Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:16 AM UTC

PDB ID	:	5OPX / pdb_00005opx
Title	:	Crystal structure of the GroEL mutant A109C in complex with GroES and ADP BeF2
Authors	:	Yan, X.; Shi, Q.; Bracher, A.; Milicic, G.; Singh, A.K.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on	:	2017-08-10
Resolution	:	3.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

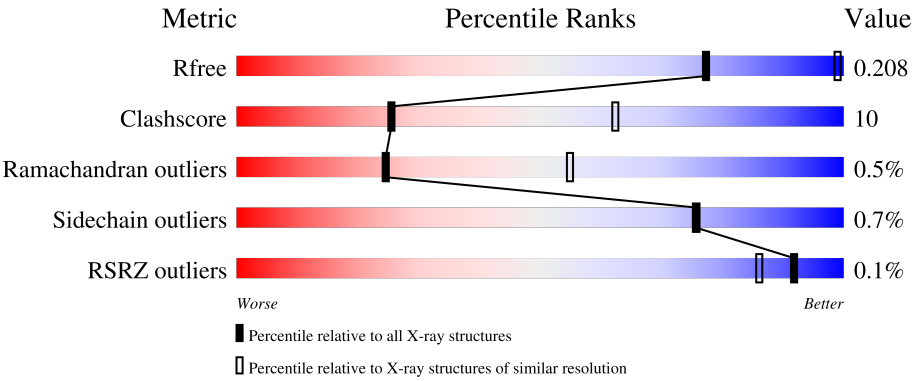
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	77% 18% 5%
1	B	548	76% 19% 5%
1	C	548	76% 19% 5%
1	D	548	79% 16% 5%

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Mol	Chain	Length	Quality of chain
1	E	548	77% 17% 5%
1	F	548	77% 18% 5%
1	G	548	76% 18% 5%
1	H	548	78% 17% 5%
1	I	548	77% 18% 5%
1	J	548	76% 19% 5%
1	K	548	78% 17% 5%
1	L	548	76% 18% 5%
1	M	548	76% 19% 5%
1	N	548	78% 17% 5%
2	1	97	71% 23% 5%
2	2	97	69% 26% 5%
2	O	97	68% 28%
2	P	97	73% 23%
2	Q	97	66% 26% 7%
2	R	97	75% 20% 5%
2	S	97	69% 25% 5%
2	T	97	71% 22% 5%
2	U	97	65% 28% 5%
2	V	97	70% 23%
2	W	97	73% 21%
2	X	97	68% 25% 5%
2	Y	97	70% 24% 5%
2	Z	97	68% 27% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 63865 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	B	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	C	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	D	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	E	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	F	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	G	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	H	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	I	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	J	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	K	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	L	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	M	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0
1	N	520	Total 3835	C 2386	N 661	O 767	S 21	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	CYS	ALA	engineered mutation	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	109	CYS	ALA	engineered mutation	UNP P0A6F5
C	109	CYS	ALA	engineered mutation	UNP P0A6F5
D	109	CYS	ALA	engineered mutation	UNP P0A6F5
E	109	CYS	ALA	engineered mutation	UNP P0A6F5
F	109	CYS	ALA	engineered mutation	UNP P0A6F5
G	109	CYS	ALA	engineered mutation	UNP P0A6F5
H	109	CYS	ALA	engineered mutation	UNP P0A6F5
I	109	CYS	ALA	engineered mutation	UNP P0A6F5
J	109	CYS	ALA	engineered mutation	UNP P0A6F5
K	109	CYS	ALA	engineered mutation	UNP P0A6F5
L	109	CYS	ALA	engineered mutation	UNP P0A6F5
M	109	CYS	ALA	engineered mutation	UNP P0A6F5
N	109	CYS	ALA	engineered mutation	UNP P0A6F5

- Molecule 2 is a protein called 10 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	2	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	O	93	Total	C	N	O	S	0	0	0
			701	437	122	140	2			
2	P	94	Total	C	N	O	S	0	0	0
			707	440	123	142	2			
2	Q	90	Total	C	N	O	S	0	0	0
			675	421	118	135	1			
2	R	92	Total	C	N	O	S	0	0	0
			691	431	120	139	1			
2	S	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	T	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	U	92	Total	C	N	O	S	0	0	0
			690	430	121	138	1			
2	V	93	Total	C	N	O	S	0	0	0
			699	435	122	141	1			
2	W	93	Total	C	N	O	S	0	0	0
			699	435	122	141	1			
2	X	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	Y	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			

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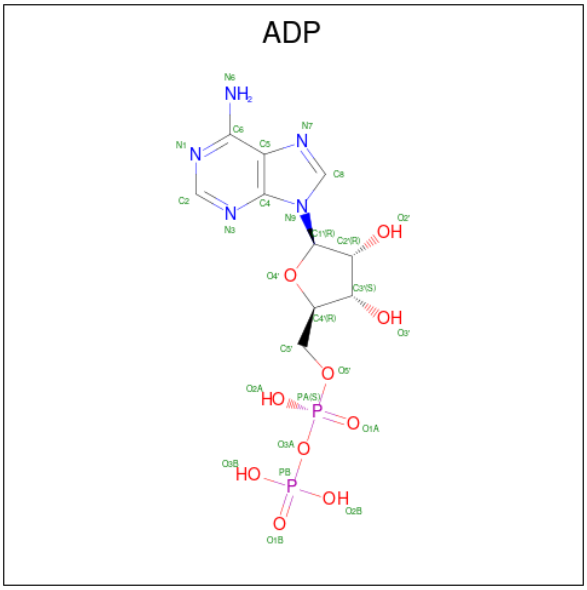
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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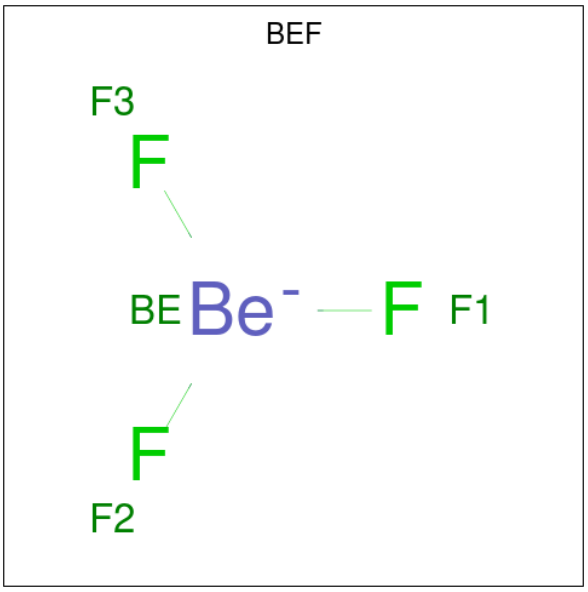
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
5	A	1	4	1	3	0	0
5	B	1	4	1	3	0	0
5	C	1	4	1	3	0	0
5	D	1	4	1	3	0	0
5	E	1	4	1	3	0	0
5	F	1	4	1	3	0	0
5	G	1	4	1	3	0	0
5	H	1	4	1	3	0	0
5	I	1	4	1	3	0	0
5	J	1	4	1	3	0	0
5	K	1	4	1	3	0	0
5	L	1	4	1	3	0	0
5	M	1	4	1	3	0	0
5	N	1	4	1	3	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	E	1	Total K 1 1	0	0
6	F	1	Total K 1 1	0	0
6	G	1	Total K 1 1	0	0
6	H	1	Total K 1 1	0	0
6	I	1	Total K 1 1	0	0
6	J	1	Total K 1 1	0	0
6	K	1	Total K 1 1	0	0
6	L	1	Total K 1 1	0	0
6	M	1	Total K 1 1	0	0
6	N	1	Total K 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 60 kDa chaperonin

Chain A:

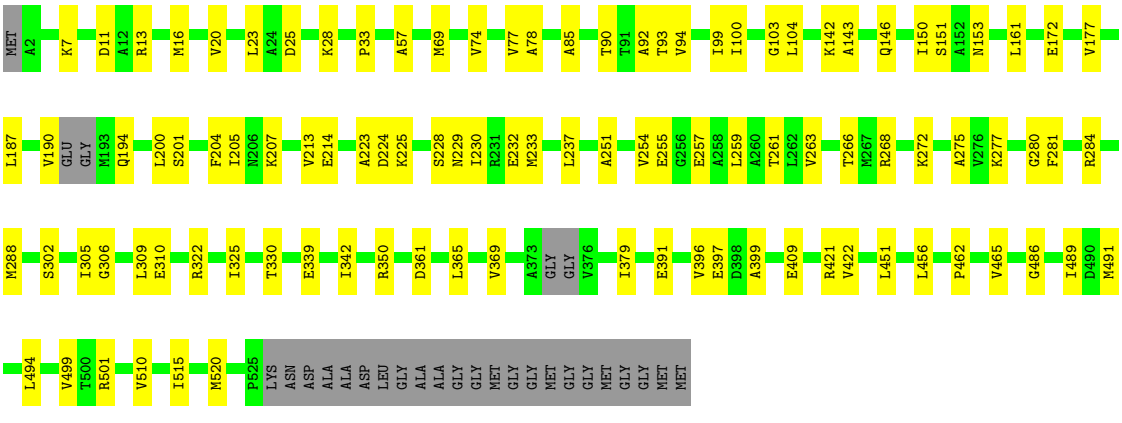




- Molecule 1: 60 kDa chaperonin

Chain B:

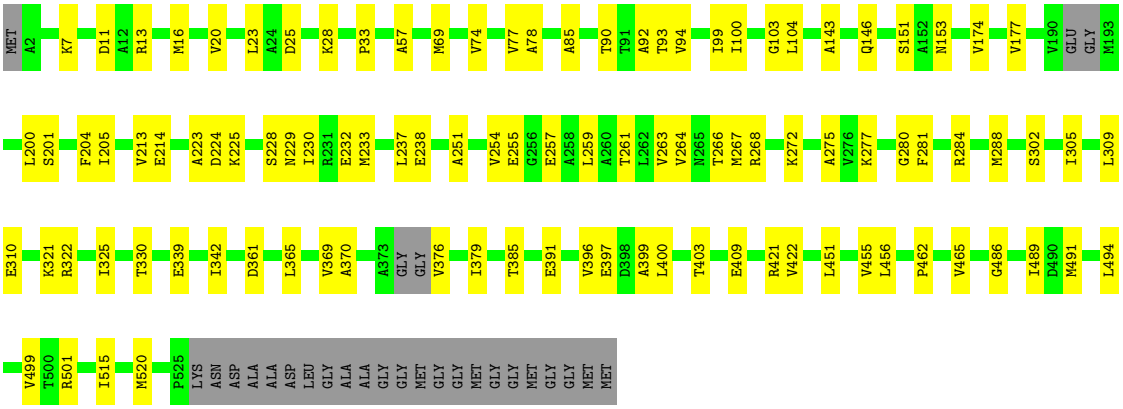




- Molecule 1: 60 kDa chaperonin

Chain C:

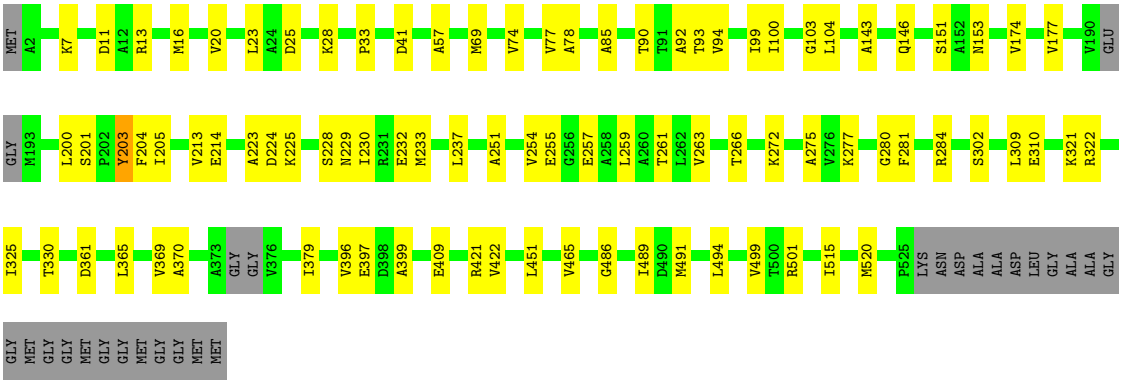




• Molecule 1: 60 kDa chaperonin

Chain D:

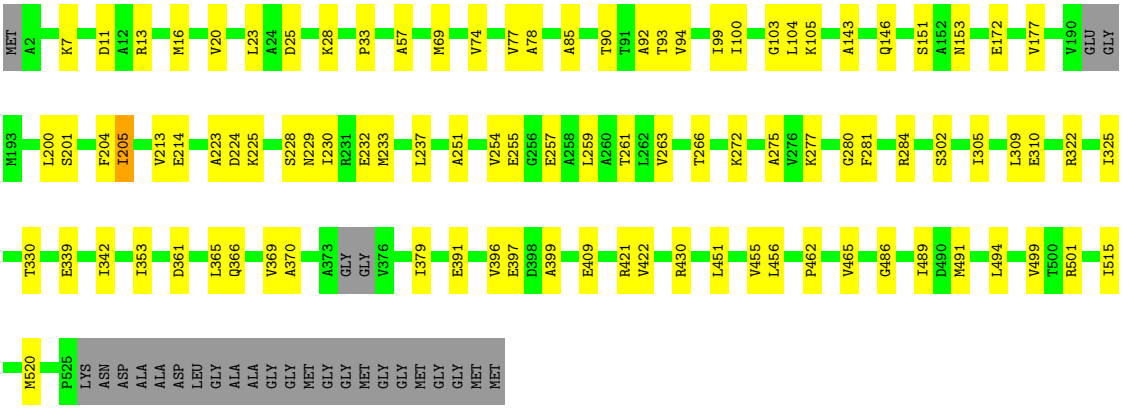




• Molecule 1: 60 kDa chaperonin

Chain E:

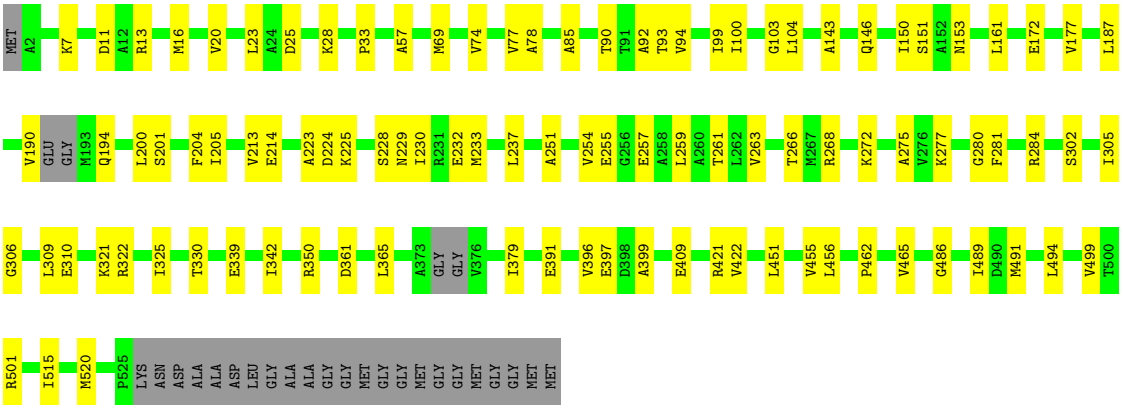




• Molecule 1: 60 kDa chaperonin

Chain F:

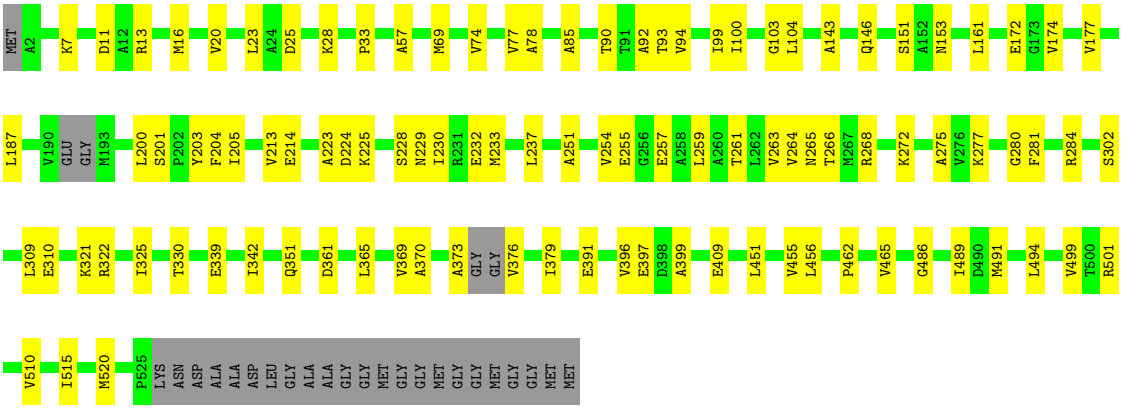




• Molecule 1: 60 kDa chaperonin

Chain G:

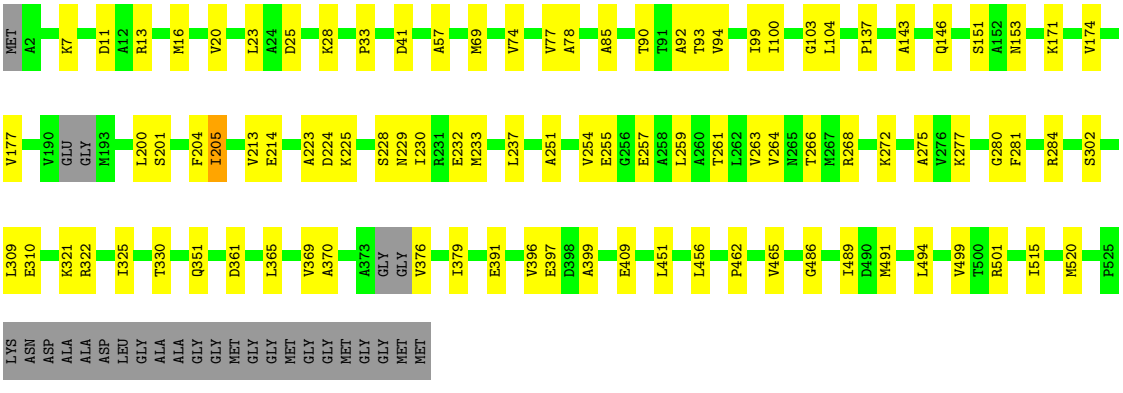




• Molecule 1: 60 kDa chaperonin

Chain H:

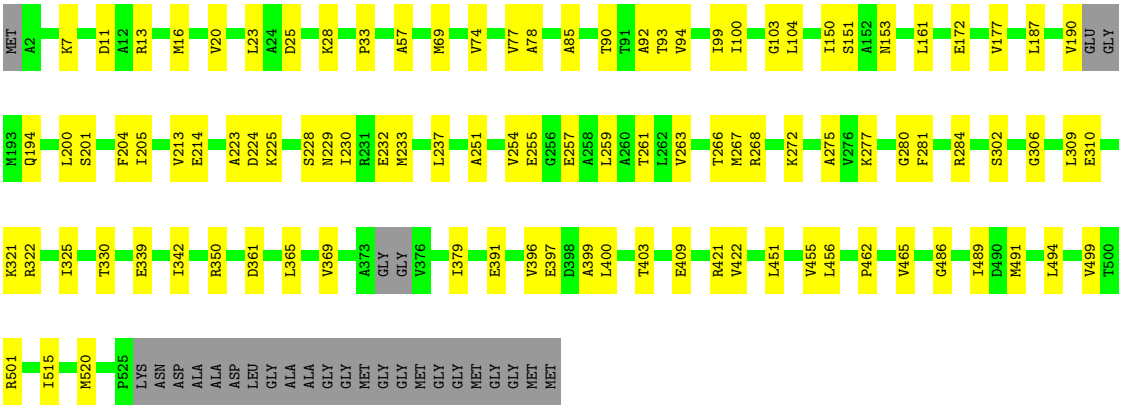




• Molecule 1: 60 kDa chaperonin

Chain I:

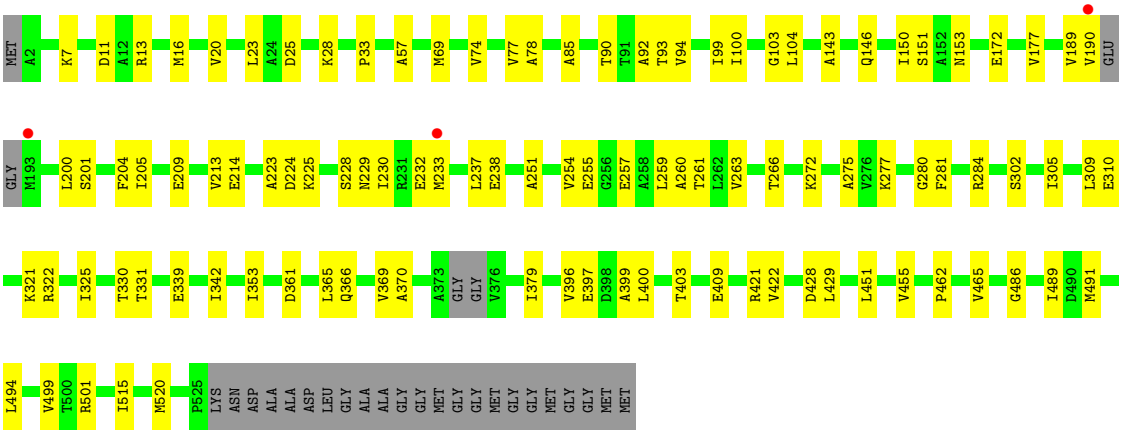




• Molecule 1: 60 kDa chaperonin

Chain J:

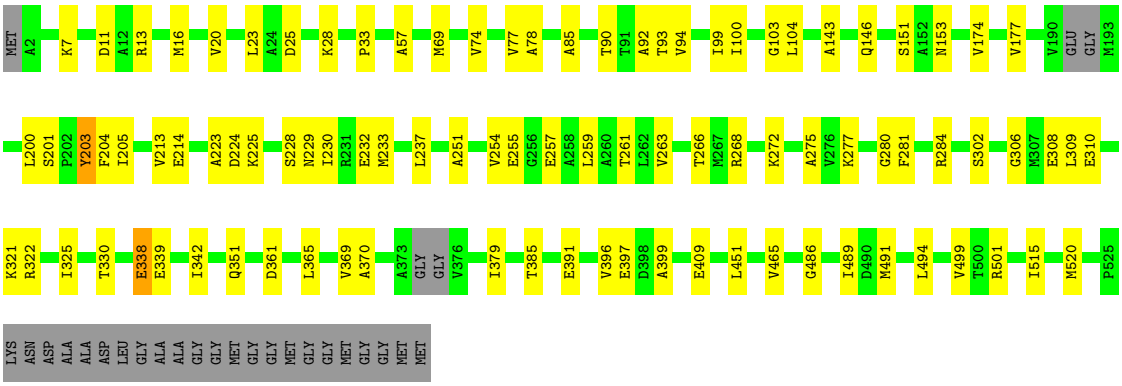




• Molecule 1: 60 kDa chaperonin

Chain K:

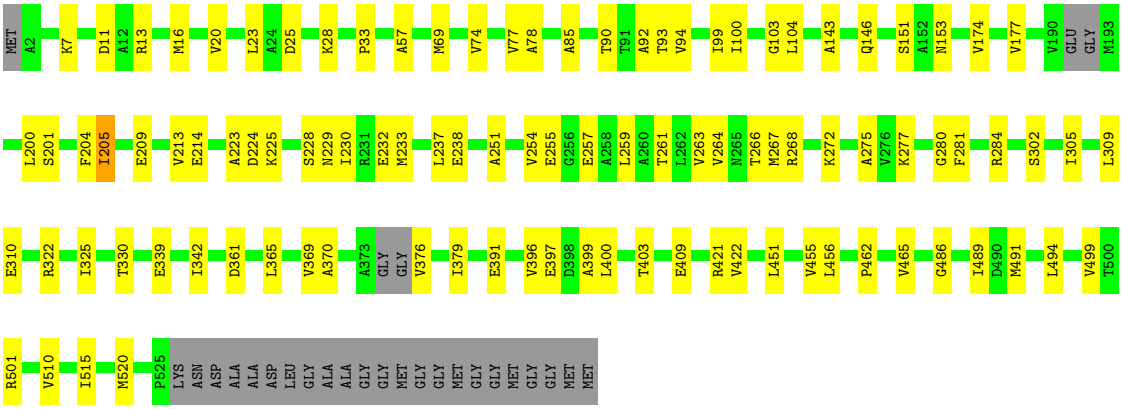




• Molecule 1: 60 kDa chaperonin

Chain L:

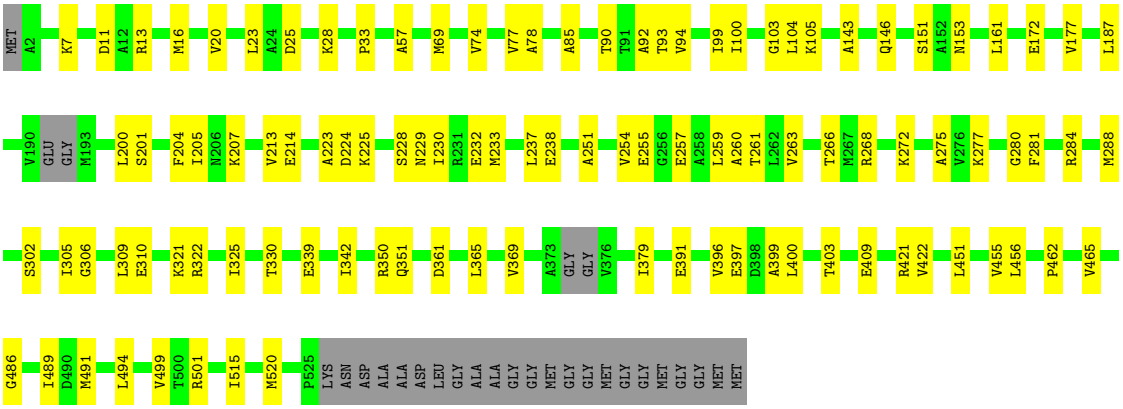




• Molecule 1: 60 kDa chaperonin

Chain M:

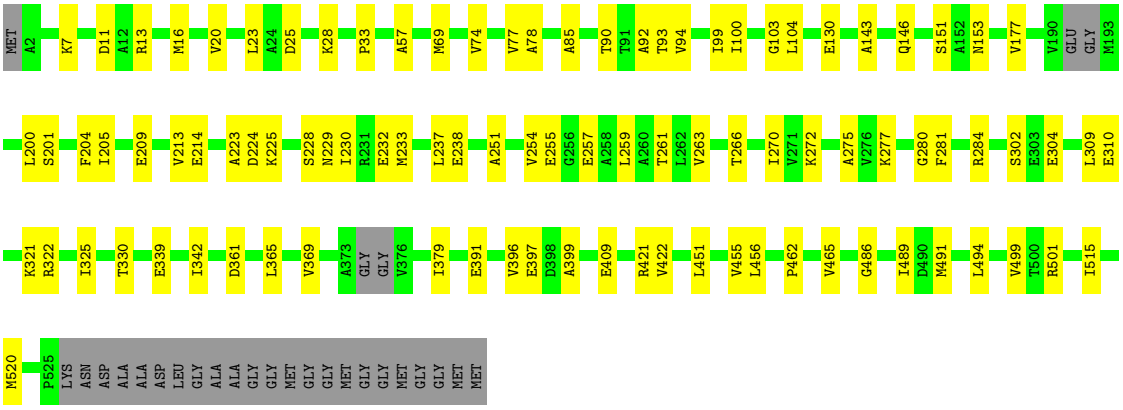




• Molecule 1: 60 kDa chaperonin

Chain N:

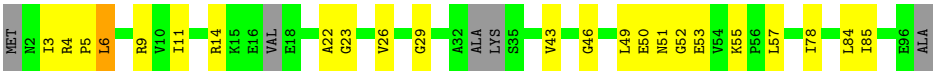




• Molecule 2: 10 kDa chaperonin

Chain 1:

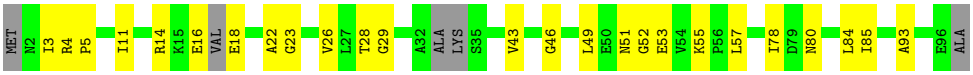




• Molecule 2: 10 kDa chaperonin

Chain 2:

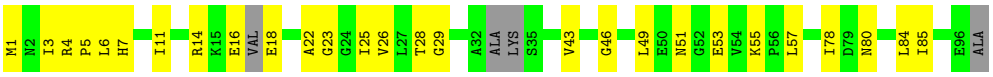




• Molecule 2: 10 kDa chaperonin

Chain O:

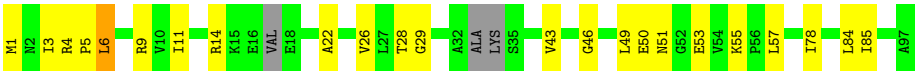




• Molecule 2: 10 kDa chaperonin

Chain P:

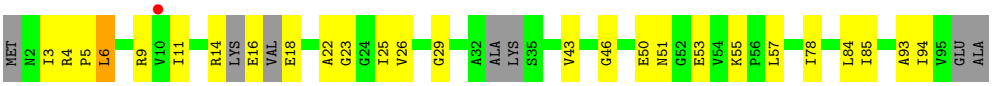




• Molecule 2: 10 kDa chaperonin

Chain Q:

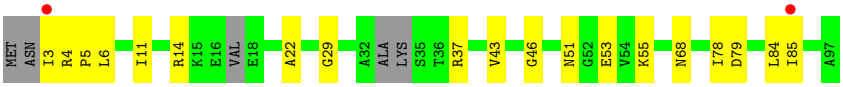




• Molecule 2: 10 kDa chaperonin

Chain R:





• Molecule 2: 10 kDa chaperonin

Chain S:

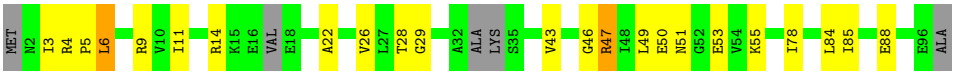




• Molecule 2: 10 kDa chaperonin

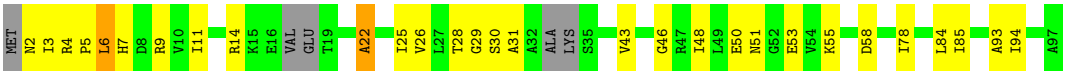
Chain T:





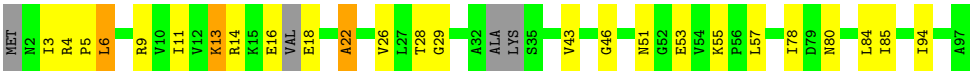
• Molecule 2: 10 kDa chaperonin

Chain U:



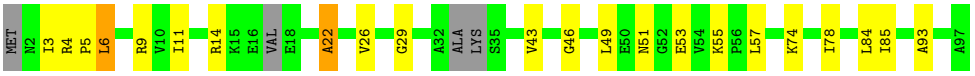
• Molecule 2: 10 kDa chaperonin

Chain V:



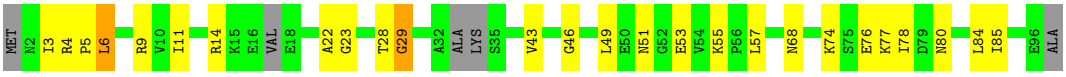
• Molecule 2: 10 kDa chaperonin

Chain W:



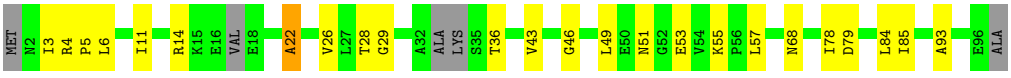
• Molecule 2: 10 kDa chaperonin

Chain X:



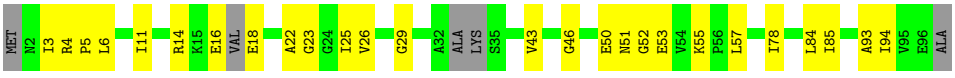
• Molecule 2: 10 kDa chaperonin

Chain Y:



• Molecule 2: 10 kDa chaperonin

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	217.57Å 230.50Å 235.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.64 50.01 – 3.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.01-3.64) 99.7 (50.01-3.64)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.231 , 0.256 (Not available) , 0.208	Depositor DCC
R_{free} test set	6583 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	101.3	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 113.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	63865	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1222e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, BEF, MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.79	0/3861	1.01	1/5211 (0.0%)
1	B	0.79	0/3861	1.01	1/5211 (0.0%)
1	C	0.78	0/3861	1.01	1/5211 (0.0%)
1	D	0.79	0/3861	1.01	0/5211
1	E	0.80	0/3861	1.01	1/5211 (0.0%)
1	F	0.79	0/3861	1.01	1/5211 (0.0%)
1	G	0.79	0/3861	1.01	1/5211 (0.0%)
1	H	0.80	0/3861	1.01	1/5211 (0.0%)
1	I	0.79	0/3861	1.01	1/5211 (0.0%)
1	J	0.79	1/3861 (0.0%)	1.01	0/5211
1	K	0.80	0/3861	1.02	2/5211 (0.0%)
1	L	0.79	0/3861	1.01	1/5211 (0.0%)
1	M	0.79	0/3861	1.01	1/5211 (0.0%)
1	N	0.80	0/3861	1.01	1/5211 (0.0%)
2	1	0.80	0/695	0.90	0/932
2	2	0.77	0/695	0.92	0/932
2	O	0.87	0/703	0.93	0/942
2	P	0.79	0/709	0.90	0/949
2	Q	0.76	0/676	0.89	0/906
2	R	0.83	0/693	0.89	0/928
2	S	0.76	0/695	0.88	0/932
2	T	0.80	0/695	0.90	0/932
2	U	0.90	0/692	0.96	1/927 (0.1%)
2	V	0.80	0/701	0.94	1/939 (0.1%)
2	W	0.79	0/701	0.92	0/939
2	X	0.78	0/695	0.90	0/932
2	Y	0.87	0/695	0.92	0/932
2	Z	0.83	0/695	0.92	0/932
All	All	0.79	1/63794 (0.0%)	1.00	15/86008 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	189	VAL	C-O	-5.02	1.19	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	13	LYS	CG-CD-CE	6.87	127.10	111.30
1	K	338	GLU	CA-CB-CG	6.66	127.42	114.10
1	C	391	GLU	N-CA-CB	5.48	118.27	110.16
1	M	391	GLU	N-CA-CB	5.38	118.13	110.16
2	U	2	ASN	CB-CA-C	5.37	120.30	110.10
1	H	391	GLU	N-CA-CB	5.34	118.07	110.16
1	G	391	GLU	N-CA-CB	5.24	117.92	110.16
1	N	391	GLU	N-CA-CB	5.22	117.89	110.16
1	L	391	GLU	N-CA-CB	5.20	117.76	110.12
1	B	391	GLU	N-CA-CB	5.19	117.75	110.12
1	A	391	GLU	N-CA-CB	5.17	117.81	110.16
1	K	391	GLU	N-CA-CB	5.11	117.72	110.16
1	E	391	GLU	N-CA-CB	5.10	117.70	110.16
1	I	391	GLU	N-CA-CB	5.09	117.61	110.12
1	F	391	GLU	N-CA-CB	5.08	117.68	110.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3835	0	3956	78	0
1	B	3835	0	3958	77	2
1	C	3835	0	3956	84	0
1	D	3835	0	3958	71	0
1	E	3835	0	3958	70	7
1	F	3835	0	3957	77	0
1	G	3835	0	3958	82	0
1	H	3835	0	3958	73	0
1	I	3835	0	3958	75	0
1	J	3835	0	3958	78	5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3835	0	3957	76	0
1	L	3835	0	3958	85	0
1	M	3835	0	3957	77	1
1	N	3835	0	3958	75	1
2	1	693	0	716	20	0
2	2	693	0	716	25	0
2	O	701	0	728	29	0
2	P	707	0	733	14	0
2	Q	675	0	696	17	0
2	R	691	0	715	12	5
2	S	693	0	716	17	0
2	T	693	0	716	18	0
2	U	690	0	715	29	0
2	V	699	0	721	23	0
2	W	699	0	721	19	0
2	X	693	0	716	22	0
2	Y	693	0	716	23	7
2	Z	693	0	716	20	0
3	A	27	0	12	1	0
3	B	27	0	12	3	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
3	G	27	0	12	1	0
3	H	27	0	12	1	0
3	I	27	0	12	2	0
3	J	27	0	12	2	0
3	K	27	0	12	1	0
3	L	27	0	12	1	0
3	M	27	0	12	1	0
3	N	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
5	D	4	0	0	1	0
5	E	4	0	0	1	0
5	F	4	0	0	1	0
5	G	4	0	0	1	0
5	H	4	0	0	1	0
5	I	4	0	0	1	0
5	J	4	0	0	1	0
5	K	4	0	0	1	0
5	L	4	0	0	1	0
5	M	4	0	0	1	0
5	N	4	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
All	All	63865	0	65614	1247	14

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:VAL:HG21	1:D:370:ALA:HB2	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:80:ASN:OD1	2:U:22:ALA:HA	1.54	1.08
2:V:80:ASN:ND2	2:W:22:ALA:HB2	1.71	1.05
1:K:203:TYR:CD2	1:L:305:ILE:HD13	1.91	1.03
1:G:229:ASN:HA	1:G:257:GLU:OE1	1.68	0.94
1:N:229:ASN:HA	1:N:257:GLU:OE1	1.68	0.94
1:H:229:ASN:HA	1:H:257:GLU:OE1	1.68	0.94
1:F:229:ASN:HA	1:F:257:GLU:OE1	1.68	0.93
1:C:229:ASN:HA	1:C:257:GLU:OE1	1.68	0.93
1:L:229:ASN:HA	1:L:257:GLU:OE1	1.68	0.93
1:A:229:ASN:HA	1:A:257:GLU:OE1	1.68	0.93
1:J:229:ASN:HA	1:J:257:GLU:OE1	1.68	0.93
1:I:229:ASN:HA	1:I:257:GLU:OE1	1.68	0.93
1:M:229:ASN:HA	1:M:257:GLU:OE1	1.68	0.93
1:E:229:ASN:HA	1:E:257:GLU:OE1	1.68	0.92
1:B:229:ASN:HA	1:B:257:GLU:OE1	1.68	0.92
1:D:229:ASN:HA	1:D:257:GLU:OE1	1.68	0.92
1:K:229:ASN:HA	1:K:257:GLU:OE1	1.68	0.91
1:G:174:VAL:HG21	1:G:370:ALA:HB2	1.51	0.90
2:V:80:ASN:HD22	2:W:22:ALA:HB2	1.37	0.85
1:D:174:VAL:HG21	1:D:370:ALA:CB	2.08	0.84
1:H:264:VAL:HG21	1:I:306:GLY:HA3	1.61	0.81
1:H:351:GLN:OE1	1:N:209:GLU:O	1.97	0.81
1:B:306:GLY:HA3	1:C:264:VAL:HG21	1.64	0.80
1:L:264:VAL:HG21	1:M:306:GLY:HA3	1.64	0.79
1:K:204:PHE:HE1	1:K:263:VAL:HA	1.48	0.78
1:E:204:PHE:HE1	1:E:263:VAL:HA	1.48	0.78
1:H:174:VAL:CG2	1:H:370:ALA:HB2	2.14	0.78
1:J:204:PHE:HE1	1:J:263:VAL:HA	1.48	0.78
1:A:238:GLU:OE2	2:O:23:GLY:HA3	1.83	0.78
1:L:174:VAL:CG2	1:L:370:ALA:HB2	2.14	0.78
1:C:204:PHE:HE1	1:C:263:VAL:HA	1.49	0.78
1:A:204:PHE:HE1	1:A:263:VAL:HA	1.47	0.78
1:D:204:PHE:HE1	1:D:263:VAL:HA	1.48	0.78
1:I:204:PHE:HE1	1:I:263:VAL:HA	1.48	0.78
1:L:204:PHE:HE1	1:L:263:VAL:HA	1.49	0.78
1:N:204:PHE:HE1	1:N:263:VAL:HA	1.48	0.77
1:F:204:PHE:HE1	1:F:263:VAL:HA	1.48	0.77
1:C:174:VAL:CG2	1:C:370:ALA:HB2	2.14	0.77
1:G:204:PHE:HE1	1:G:263:VAL:HA	1.48	0.77
1:C:174:VAL:HG23	1:C:370:ALA:HB2	1.66	0.77
1:K:203:TYR:CE2	1:L:305:ILE:HD13	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:PHE:HE1	1:H:263:VAL:HA	1.48	0.76
1:M:204:PHE:HE1	1:M:263:VAL:HA	1.48	0.76
1:B:204:PHE:HE1	1:B:263:VAL:HA	1.48	0.76
1:L:267:MET:HE3	1:M:305:ILE:HD12	1.66	0.76
1:G:257:GLU:HG2	2:U:30:SER:HB2	1.67	0.76
2:Y:4:ARG:O	2:Z:93:ALA:HB1	1.86	0.75
2:P:3:ILE:HD11	2:P:78:ILE:HG13	1.68	0.75
1:K:174:VAL:HG21	1:K:370:ALA:CB	2.17	0.74
2:O:80:ASN:OD1	2:U:22:ALA:CA	2.35	0.74
1:E:232:GLU:HG3	1:E:310:GLU:OE2	1.88	0.74
1:F:232:GLU:HG3	1:F:310:GLU:OE2	1.88	0.74
1:I:232:GLU:HG3	1:I:310:GLU:OE2	1.88	0.74
1:M:232:GLU:HG3	1:M:310:GLU:OE2	1.88	0.74
1:D:232:GLU:HG3	1:D:310:GLU:OE2	1.88	0.73
1:B:232:GLU:HG3	1:B:310:GLU:OE2	1.88	0.73
1:C:305:ILE:HD13	1:D:203:TYR:CD2	2.24	0.73
1:A:232:GLU:HG3	1:A:310:GLU:OE2	1.88	0.73
1:E:228:SER:OG	1:E:255:GLU:HG3	1.89	0.73
1:G:232:GLU:HG3	1:G:310:GLU:OE2	1.88	0.73
2:W:3:ILE:HD11	2:W:78:ILE:HG13	1.70	0.73
1:H:232:GLU:HG3	1:H:310:GLU:OE2	1.89	0.73
2:V:80:ASN:ND2	2:W:22:ALA:CB	2.50	0.73
1:E:213:VAL:HB	1:E:325:ILE:CG1	2.19	0.73
1:G:213:VAL:HB	1:G:325:ILE:CG1	2.19	0.73
1:H:228:SER:OG	1:H:255:GLU:HG3	1.89	0.73
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.19	0.73
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.19	0.73
1:C:232:GLU:HG3	1:C:310:GLU:OE2	1.88	0.73
1:F:223:ALA:HB3	1:F:251:ALA:HB2	1.71	0.73
1:N:228:SER:OG	1:N:255:GLU:HG3	1.89	0.73
1:A:213:VAL:HB	1:A:325:ILE:CG1	2.19	0.73
1:B:213:VAL:HB	1:B:325:ILE:CG1	2.19	0.73
1:C:213:VAL:HB	1:C:325:ILE:CG1	2.19	0.73
1:I:223:ALA:HB3	1:I:251:ALA:HB2	1.71	0.73
1:K:232:GLU:HG3	1:K:310:GLU:OE2	1.88	0.73
1:N:213:VAL:HB	1:N:325:ILE:CG1	2.19	0.73
1:A:228:SER:OG	1:A:255:GLU:HG3	1.89	0.72
1:B:228:SER:OG	1:B:255:GLU:HG3	1.89	0.72
1:M:228:SER:OG	1:M:255:GLU:HG3	1.89	0.72
2:2:3:ILE:HD11	2:2:78:ILE:HG13	1.71	0.72
1:D:213:VAL:HB	1:D:325:ILE:CG1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:232:GLU:HG3	1:L:310:GLU:OE2	1.88	0.72
1:L:213:VAL:HB	1:L:325:ILE:CG1	2.19	0.72
1:C:228:SER:OG	1:C:255:GLU:HG3	1.89	0.72
1:I:213:VAL:HB	1:I:325:ILE:CG1	2.19	0.72
1:J:228:SER:OG	1:J:255:GLU:HG3	1.89	0.72
2:Z:3:ILE:HD11	2:Z:78:ILE:HG13	1.70	0.72
1:A:223:ALA:HB3	1:A:251:ALA:HB2	1.71	0.72
1:F:213:VAL:HB	1:F:325:ILE:CG1	2.19	0.72
1:G:228:SER:OG	1:G:255:GLU:HG3	1.89	0.72
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.19	0.72
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.72	0.72
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.71	0.72
1:L:228:SER:OG	1:L:255:GLU:HG3	1.89	0.72
1:J:232:GLU:HG3	1:J:310:GLU:OE2	1.88	0.72
1:H:223:ALA:HB3	1:H:251:ALA:HB2	1.71	0.72
1:I:228:SER:OG	1:I:255:GLU:HG3	1.89	0.72
2:Q:3:ILE:HD11	2:Q:78:ILE:HG13	1.70	0.72
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.72	0.72
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.71	0.72
1:N:232:GLU:HG3	1:N:310:GLU:OE2	1.88	0.72
1:C:23:LEU:HD23	1:C:74:VAL:HG13	1.72	0.72
1:C:223:ALA:HB3	1:C:251:ALA:HB2	1.71	0.72
1:L:23:LEU:HD23	1:L:74:VAL:HG13	1.72	0.72
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.72	0.71
1:N:238:GLU:OE2	2:2:23:GLY:HA3	1.90	0.71
1:B:223:ALA:HB3	1:B:251:ALA:HB2	1.71	0.71
1:N:223:ALA:HB3	1:N:251:ALA:HB2	1.71	0.71
1:D:223:ALA:HB3	1:D:251:ALA:HB2	1.71	0.71
1:E:223:ALA:HB3	1:E:251:ALA:HB2	1.72	0.71
1:G:223:ALA:HB3	1:G:251:ALA:HB2	1.71	0.71
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.72	0.71
1:C:228:SER:HA	1:C:255:GLU:HB2	1.72	0.71
1:K:213:VAL:HB	1:K:325:ILE:CG1	2.19	0.71
1:K:228:SER:OG	1:K:255:GLU:HG3	1.89	0.71
1:F:228:SER:OG	1:F:255:GLU:HG3	1.89	0.71
1:L:174:VAL:HG23	1:L:370:ALA:HB2	1.73	0.71
1:L:228:SER:HA	1:L:255:GLU:HB2	1.72	0.71
2:V:3:ILE:HD11	2:V:78:ILE:HG13	1.72	0.71
1:D:23:LEU:HD23	1:D:74:VAL:HG13	1.72	0.71
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.71	0.71
1:D:228:SER:OG	1:D:255:GLU:HG3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:SER:HA	1:G:255:GLU:HB2	1.72	0.71
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.72	0.71
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.72	0.71
2:X:3:ILE:HD11	2:X:78:ILE:HG13	1.71	0.71
1:A:228:SER:HA	1:A:255:GLU:HB2	1.73	0.71
1:K:223:ALA:HB3	1:K:251:ALA:HB2	1.72	0.71
2:S:3:ILE:HD11	2:S:78:ILE:HG13	1.71	0.71
1:J:23:LEU:HD23	1:J:74:VAL:HG13	1.73	0.71
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.72	0.71
1:F:23:LEU:HD23	1:F:74:VAL:HG13	1.72	0.70
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.72	0.70
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.72	0.70
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.72	0.70
1:L:232:GLU:HA	1:L:310:GLU:HG3	1.73	0.70
1:D:232:GLU:HA	1:D:310:GLU:HG3	1.73	0.70
1:E:23:LEU:HD23	1:E:74:VAL:HG13	1.73	0.70
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.73	0.70
1:I:23:LEU:HD23	1:I:74:VAL:HG13	1.72	0.70
1:K:228:SER:HA	1:K:255:GLU:HB2	1.72	0.70
1:N:228:SER:HA	1:N:255:GLU:HB2	1.72	0.70
1:N:232:GLU:HA	1:N:310:GLU:HG3	1.73	0.70
1:A:232:GLU:HA	1:A:310:GLU:HG3	1.73	0.70
1:F:228:SER:HA	1:F:255:GLU:HB2	1.72	0.70
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.72	0.70
1:H:232:GLU:HA	1:H:310:GLU:HG3	1.73	0.70
1:C:232:GLU:HA	1:C:310:GLU:HG3	1.73	0.70
1:E:228:SER:HA	1:E:255:GLU:HB2	1.72	0.70
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.72	0.70
1:K:23:LEU:HD23	1:K:74:VAL:HG13	1.73	0.70
1:K:203:TYR:CD2	1:L:305:ILE:CD1	2.74	0.70
2:T:3:ILE:HD11	2:T:78:ILE:HG13	1.73	0.70
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.72	0.70
2:1:52:GLY:HA2	2:2:55:LYS:HE3	1.73	0.70
1:H:228:SER:HA	1:H:255:GLU:HB2	1.72	0.70
2:O:4:ARG:O	2:U:93:ALA:HB1	1.91	0.70
1:A:23:LEU:HD23	1:A:74:VAL:HG13	1.73	0.69
1:H:23:LEU:HD23	1:H:74:VAL:HG13	1.73	0.69
1:I:228:SER:HA	1:I:255:GLU:HB2	1.72	0.69
1:J:228:SER:HA	1:J:255:GLU:HB2	1.72	0.69
1:G:265:ASN:OD1	2:U:25:ILE:HG23	1.92	0.69
1:M:228:SER:HA	1:M:255:GLU:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:23:LEU:HD23	1:N:74:VAL:HG13	1.73	0.69
2:R:3:ILE:HD11	2:R:78:ILE:HG13	1.74	0.69
1:I:232:GLU:HA	1:I:310:GLU:HG3	1.73	0.69
1:B:228:SER:HA	1:B:255:GLU:HB2	1.72	0.69
1:D:228:SER:HA	1:D:255:GLU:HB2	1.72	0.69
1:E:232:GLU:HA	1:E:310:GLU:HG3	1.73	0.69
1:E:325:ILE:HG22	1:E:330:THR:HG23	1.74	0.69
1:H:325:ILE:HG22	1:H:330:THR:HG23	1.75	0.69
1:H:174:VAL:HG23	1:H:370:ALA:HB2	1.75	0.69
1:G:23:LEU:HD23	1:G:74:VAL:HG13	1.73	0.69
1:G:232:GLU:HA	1:G:310:GLU:HG3	1.73	0.69
1:B:232:GLU:HA	1:B:310:GLU:HG3	1.73	0.69
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.75	0.69
3:G:600:ADP:O3B	5:G:602:BEF:F3	2.01	0.69
1:K:232:GLU:HA	1:K:310:GLU:HG3	1.73	0.69
1:M:23:LEU:HD23	1:M:74:VAL:HG13	1.73	0.69
2:O:3:ILE:HD11	2:O:78:ILE:HG13	1.75	0.69
1:J:232:GLU:HA	1:J:310:GLU:HG3	1.73	0.69
1:I:325:ILE:HG22	1:I:330:THR:HG23	1.75	0.69
2:1:3:ILE:HD11	2:1:78:ILE:HG13	1.73	0.69
1:F:325:ILE:HG22	1:F:330:THR:HG23	1.75	0.68
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.75	0.68
1:M:232:GLU:HA	1:M:310:GLU:HG3	1.73	0.68
1:B:23:LEU:HD23	1:B:74:VAL:HG13	1.73	0.68
1:J:325:ILE:HG22	1:J:330:THR:HG23	1.75	0.68
1:L:238:GLU:OE2	2:Z:23:GLY:HA3	1.94	0.68
1:K:325:ILE:HG22	1:K:330:THR:HG23	1.75	0.68
3:J:600:ADP:O3B	5:J:602:BEF:F3	2.01	0.68
1:A:325:ILE:HG22	1:A:330:THR:HG23	1.75	0.68
1:F:232:GLU:HA	1:F:310:GLU:HG3	1.73	0.68
1:F:306:GLY:HA3	1:G:264:VAL:HG21	1.75	0.68
3:M:600:ADP:O3B	5:M:602:BEF:F3	2.02	0.68
1:C:325:ILE:HG22	1:C:330:THR:HG23	1.75	0.68
1:N:325:ILE:HG22	1:N:330:THR:HG23	1.75	0.68
1:B:325:ILE:HG22	1:B:330:THR:HG23	1.75	0.67
3:H:600:ADP:O3B	5:H:602:BEF:F3	2.03	0.67
2:Y:3:ILE:HD11	2:Y:78:ILE:HG13	1.77	0.67
2:O:80:ASN:CG	2:U:22:ALA:HA	2.18	0.67
1:D:325:ILE:HG22	1:D:330:THR:HG23	1.75	0.67
1:M:325:ILE:HG22	1:M:330:THR:HG23	1.75	0.67
1:G:265:ASN:CG	2:U:25:ILE:HG23	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:600:ADP:O1B	5:C:602:BEF:F3	2.04	0.66
1:A:237:LEU:HB3	2:O:25:ILE:HD13	1.78	0.66
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.78	0.65
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.78	0.65
1:C:238:GLU:OE2	2:Q:23:GLY:HA3	1.97	0.65
1:K:174:VAL:HG21	1:K:370:ALA:HB2	1.78	0.65
1:D:174:VAL:CG2	1:D:370:ALA:HB2	2.20	0.65
1:G:268:ARG:NH1	2:U:26:VAL:HG21	2.11	0.65
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.79	0.65
1:E:172:GLU:O	1:E:370:ALA:HA	1.96	0.65
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.78	0.64
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.78	0.64
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.79	0.64
3:F:600:ADP:O3B	5:F:602:BEF:F3	2.06	0.64
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.78	0.64
3:B:600:ADP:O1B	5:B:602:BEF:F3	2.06	0.64
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.78	0.64
1:F:268:ARG:NH1	2:T:26:VAL:HG21	2.12	0.64
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.78	0.64
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.79	0.64
3:N:600:ADP:O3B	5:N:602:BEF:F3	2.05	0.64
1:L:267:MET:CE	1:M:305:ILE:HD12	2.29	0.64
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.78	0.63
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.79	0.63
3:I:600:ADP:O3B	5:I:602:BEF:F3	2.06	0.63
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.79	0.63
2:2:52:GLY:HA2	2:V:55:LYS:HE3	1.79	0.63
1:A:261:THR:HG23	2:O:28:THR:OG1	1.98	0.63
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.78	0.63
1:J:228:SER:O	1:J:257:GLU:OE1	2.17	0.63
1:D:228:SER:O	1:D:257:GLU:OE1	2.17	0.62
1:B:228:SER:O	1:B:257:GLU:OE1	2.17	0.62
1:F:228:SER:O	1:F:257:GLU:OE1	2.17	0.62
1:M:228:SER:O	1:M:257:GLU:OE1	2.18	0.62
1:A:228:SER:O	1:A:257:GLU:OE1	2.17	0.62
1:B:305:ILE:HD12	1:C:267:MET:HE3	1.81	0.62
1:K:228:SER:O	1:K:257:GLU:OE1	2.17	0.62
1:K:203:TYR:CE2	1:L:305:ILE:CD1	2.83	0.62
2:T:49:LEU:HD11	2:T:55:LYS:HE3	1.82	0.62
1:A:261:THR:CG2	2:O:28:THR:OG1	2.47	0.62
1:E:228:SER:O	1:E:257:GLU:OE1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:228:SER:O	1:I:257:GLU:OE1	2.17	0.61
1:G:228:SER:O	1:G:257:GLU:OE1	2.17	0.61
2:V:80:ASN:HD22	2:W:22:ALA:CB	2.09	0.61
2:Y:4:ARG:O	2:Z:93:ALA:CB	2.48	0.61
3:A:600:ADP:O3B	5:A:602:BEF:F3	2.08	0.61
1:A:172:GLU:O	1:A:370:ALA:HA	2.01	0.61
3:K:600:ADP:O3B	5:K:602:BEF:F3	2.07	0.61
2:O:4:ARG:HB3	2:U:94:ILE:O	1.99	0.61
1:H:228:SER:O	1:H:257:GLU:OE1	2.17	0.61
1:L:228:SER:O	1:L:257:GLU:OE1	2.17	0.61
1:J:261:THR:HG23	2:X:28:THR:OG1	2.00	0.61
1:N:228:SER:O	1:N:257:GLU:OE1	2.17	0.61
1:A:204:PHE:CE1	1:A:263:VAL:HA	2.34	0.61
1:B:305:ILE:HD12	1:C:267:MET:CE	2.30	0.61
1:C:228:SER:O	1:C:257:GLU:OE1	2.17	0.61
3:L:600:ADP:O3B	5:L:602:BEF:F3	2.09	0.61
2:V:80:ASN:CG	2:W:22:ALA:HB2	2.26	0.61
1:A:238:GLU:OE2	2:O:23:GLY:CA	2.49	0.61
2:Y:4:ARG:HB3	2:Z:94:ILE:O	2.00	0.61
1:D:204:PHE:CE1	1:D:263:VAL:HA	2.35	0.60
1:E:280:GLY:O	1:E:281:PHE:CD1	2.54	0.60
1:H:281:PHE:O	1:H:284:ARG:HG2	2.01	0.60
1:K:281:PHE:O	1:K:284:ARG:HG2	2.01	0.60
1:N:280:GLY:O	1:N:281:PHE:CD1	2.54	0.60
1:B:281:PHE:O	1:B:284:ARG:HG2	2.01	0.60
1:J:238:GLU:OE2	2:X:23:GLY:HA3	2.01	0.60
1:J:280:GLY:O	1:J:281:PHE:CD1	2.54	0.60
1:K:204:PHE:CE1	1:K:263:VAL:HA	2.35	0.60
1:B:280:GLY:O	1:B:281:PHE:CD1	2.54	0.60
1:C:280:GLY:O	1:C:281:PHE:CD1	2.54	0.60
1:D:281:PHE:O	1:D:284:ARG:HG2	2.01	0.60
1:G:281:PHE:O	1:G:284:ARG:HG2	2.01	0.60
1:I:69:MET:HE2	1:I:520:MET:HE2	1.84	0.60
1:J:281:PHE:O	1:J:284:ARG:HG2	2.01	0.60
1:M:281:PHE:O	1:M:284:ARG:HG2	2.02	0.60
1:D:280:GLY:O	1:D:281:PHE:CD1	2.54	0.60
1:M:280:GLY:O	1:M:281:PHE:CD1	2.55	0.60
1:N:204:PHE:CE1	1:N:263:VAL:HA	2.34	0.60
2:O:80:ASN:ND2	2:U:22:ALA:O	2.35	0.60
1:A:280:GLY:O	1:A:281:PHE:CD1	2.54	0.60
1:E:281:PHE:O	1:E:284:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:PHE:O	1:F:284:ARG:HG2	2.02	0.60
1:I:204:PHE:CE1	1:I:263:VAL:HA	2.35	0.60
1:F:280:GLY:O	1:F:281:PHE:CD1	2.54	0.60
1:K:280:GLY:O	1:K:281:PHE:CD1	2.54	0.60
1:H:280:GLY:O	1:H:281:PHE:CD1	2.54	0.60
1:I:281:PHE:O	1:I:284:ARG:HG2	2.02	0.60
1:G:280:GLY:O	1:G:281:PHE:CD1	2.54	0.60
1:L:280:GLY:O	1:L:281:PHE:CD1	2.54	0.60
1:N:281:PHE:O	1:N:284:ARG:HG2	2.02	0.60
1:A:209:GLU:O	1:G:351:GLN:OE1	2.20	0.59
1:I:280:GLY:O	1:I:281:PHE:CD1	2.54	0.59
1:C:69:MET:HE2	1:C:520:MET:HE2	1.83	0.59
1:A:281:PHE:O	1:A:284:ARG:HG2	2.01	0.59
3:D:600:ADP:O3B	5:D:602:BEF:F3	2.10	0.59
1:F:204:PHE:CE1	1:F:263:VAL:HA	2.35	0.59
1:G:204:PHE:CE1	1:G:263:VAL:HA	2.35	0.59
2:P:49:LEU:HD11	2:P:55:LYS:HE3	1.83	0.59
1:C:281:PHE:O	1:C:284:ARG:HG2	2.01	0.59
3:E:600:ADP:O3B	5:E:602:BEF:F3	2.10	0.59
1:H:204:PHE:CE1	1:H:263:VAL:HA	2.35	0.59
1:L:281:PHE:O	1:L:284:ARG:HG2	2.01	0.59
2:1:4:ARG:O	2:2:93:ALA:HB1	2.03	0.58
1:H:370:ALA:HB1	1:H:376:VAL:HG22	1.85	0.58
1:D:174:VAL:CG2	1:D:370:ALA:CB	2.79	0.58
1:N:261:THR:CG2	2:2:28:THR:OG1	2.51	0.58
1:J:204:PHE:CE1	1:J:263:VAL:HA	2.35	0.58
1:C:268:ARG:NH1	2:Q:26:VAL:HG21	2.19	0.58
1:H:261:THR:HG23	2:V:28:THR:OG1	2.04	0.57
1:C:281:PHE:N	1:C:284:ARG:HE	2.03	0.57
1:H:281:PHE:N	1:H:284:ARG:HE	2.03	0.57
1:I:281:PHE:N	1:I:284:ARG:HE	2.03	0.57
1:A:281:PHE:N	1:A:284:ARG:HE	2.03	0.57
1:G:281:PHE:N	1:G:284:ARG:HE	2.03	0.57
1:A:69:MET:HE2	1:A:520:MET:HE2	1.85	0.57
1:C:370:ALA:HB1	1:C:376:VAL:HG22	1.87	0.57
1:D:281:PHE:N	1:D:284:ARG:HE	2.03	0.57
1:C:177:VAL:HG12	1:C:379:ILE:HB	1.87	0.57
1:G:174:VAL:CG2	1:G:370:ALA:HB2	2.29	0.57
1:M:281:PHE:N	1:M:284:ARG:HE	2.03	0.57
1:B:281:PHE:N	1:B:284:ARG:HE	2.03	0.57
1:K:13:ARG:HD2	1:K:104:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:PHE:N	1:F:284:ARG:HE	2.03	0.57
1:K:281:PHE:N	1:K:284:ARG:HE	2.03	0.57
1:A:177:VAL:HG12	1:A:379:ILE:HB	1.87	0.57
1:J:281:PHE:N	1:J:284:ARG:HE	2.03	0.57
1:L:177:VAL:HG12	1:L:379:ILE:HB	1.87	0.57
2:X:49:LEU:HD11	2:X:55:LYS:HE3	1.85	0.57
1:E:281:PHE:N	1:E:284:ARG:HE	2.02	0.56
1:L:281:PHE:N	1:L:284:ARG:HE	2.03	0.56
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.87	0.56
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.88	0.56
1:E:177:VAL:HG12	1:E:379:ILE:HB	1.88	0.56
1:E:204:PHE:CE1	1:E:263:VAL:HA	2.35	0.56
1:L:13:ARG:HD2	1:L:104:LEU:HD22	1.86	0.56
1:N:177:VAL:HG12	1:N:379:ILE:HB	1.87	0.56
1:J:13:ARG:HD2	1:J:104:LEU:HD22	1.87	0.56
1:J:177:VAL:HG12	1:J:379:ILE:HB	1.87	0.56
2:X:80:ASN:OD1	2:Y:22:ALA:HA	2.05	0.56
1:N:281:PHE:N	1:N:284:ARG:HE	2.03	0.56
1:B:204:PHE:CE1	1:B:263:VAL:HA	2.35	0.56
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.88	0.56
1:E:177:VAL:HG11	1:E:396:VAL:HG12	1.88	0.56
1:I:177:VAL:HG12	1:I:379:ILE:HB	1.87	0.56
1:G:229:ASN:HA	1:G:257:GLU:CD	2.31	0.56
1:H:229:ASN:HA	1:H:257:GLU:CD	2.31	0.56
1:K:177:VAL:HG12	1:K:379:ILE:HB	1.88	0.56
1:B:177:VAL:HG12	1:B:379:ILE:HB	1.87	0.56
1:L:370:ALA:HB1	1:L:376:VAL:HG22	1.87	0.56
1:M:204:PHE:CE1	1:M:263:VAL:HA	2.35	0.56
1:E:229:ASN:HA	1:E:257:GLU:CD	2.31	0.56
1:F:229:ASN:HA	1:F:257:GLU:CD	2.31	0.56
1:N:13:ARG:HD2	1:N:104:LEU:HD22	1.88	0.56
2:1:55:LYS:HE3	2:Z:52:GLY:HA2	1.88	0.55
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.88	0.55
1:C:201:SER:HB3	1:C:204:PHE:CE2	2.42	0.55
1:H:69:MET:HE2	1:H:520:MET:HE2	1.89	0.55
1:H:177:VAL:HG12	1:H:379:ILE:HB	1.87	0.55
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.88	0.55
1:A:177:VAL:HG11	1:A:396:VAL:HG12	1.88	0.55
1:I:229:ASN:HA	1:I:257:GLU:CD	2.31	0.55
1:C:204:PHE:CE1	1:C:263:VAL:HA	2.36	0.55
1:D:177:VAL:HG12	1:D:379:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:VAL:HG12	1:F:379:ILE:HB	1.87	0.55
1:M:13:ARG:HD2	1:M:104:LEU:HD22	1.87	0.55
1:M:177:VAL:HG12	1:M:379:ILE:HB	1.87	0.55
2:X:4:ARG:O	2:Y:93:ALA:HB1	2.06	0.55
1:J:261:THR:CG2	2:X:28:THR:OG1	2.54	0.55
1:L:204:PHE:CE1	1:L:263:VAL:HA	2.36	0.55
2:O:4:ARG:O	2:U:93:ALA:CB	2.55	0.55
1:D:69:MET:HE2	1:D:520:MET:HE2	1.88	0.55
1:N:177:VAL:HG11	1:N:396:VAL:HG12	1.89	0.55
1:A:229:ASN:HA	1:A:257:GLU:CD	2.31	0.55
1:D:201:SER:HB3	1:D:204:PHE:CE2	2.42	0.55
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.88	0.55
1:F:190:VAL:HG11	1:F:194:GLN:HB3	1.88	0.55
1:J:229:ASN:HA	1:J:257:GLU:CD	2.31	0.55
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.87	0.55
1:D:177:VAL:HG11	1:D:396:VAL:HG12	1.88	0.55
1:G:177:VAL:HG12	1:G:379:ILE:HB	1.88	0.55
1:H:13:ARG:HD2	1:H:104:LEU:HD22	1.87	0.55
1:J:172:GLU:O	1:J:370:ALA:HA	2.07	0.55
1:J:177:VAL:HG11	1:J:396:VAL:HG12	1.89	0.55
1:K:229:ASN:HA	1:K:257:GLU:CD	2.31	0.55
2:2:16:GLU:HB3	2:2:18:GLU:N	2.21	0.55
1:L:201:SER:HB3	1:L:204:PHE:CE2	2.42	0.54
2:2:51:ASN:HD21	2:2:53:GLU:CD	2.15	0.54
2:R:51:ASN:HD21	2:R:53:GLU:CD	2.15	0.54
2:T:51:ASN:HD21	2:T:53:GLU:CD	2.15	0.54
2:V:51:ASN:HD21	2:V:53:GLU:CD	2.15	0.54
2:W:49:LEU:HD11	2:W:55:LYS:HE3	1.89	0.54
2:W:51:ASN:HD21	2:W:53:GLU:CD	2.15	0.54
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.88	0.54
1:E:201:SER:HB3	1:E:204:PHE:CE2	2.43	0.54
1:K:69:MET:HE2	1:K:520:MET:HE2	1.88	0.54
1:K:201:SER:HB3	1:K:204:PHE:CE2	2.42	0.54
1:L:229:ASN:HA	1:L:257:GLU:CD	2.31	0.54
1:B:201:SER:HB3	1:B:204:PHE:CE2	2.43	0.54
1:J:201:SER:HB3	1:J:204:PHE:CE2	2.43	0.54
1:M:201:SER:HB3	1:M:204:PHE:CE2	2.43	0.54
1:C:229:ASN:HA	1:C:257:GLU:CD	2.31	0.54
1:D:229:ASN:HA	1:D:257:GLU:CD	2.31	0.54
1:E:223:ALA:HB3	1:E:251:ALA:CB	2.37	0.54
1:H:201:SER:HB3	1:H:204:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:51:ASN:HD21	2:O:53:GLU:CD	2.16	0.54
2:X:51:ASN:HD21	2:X:53:GLU:CD	2.15	0.54
2:Y:51:ASN:HD21	2:Y:53:GLU:CD	2.16	0.54
1:A:201:SER:HB3	1:A:204:PHE:CE2	2.43	0.54
1:G:177:VAL:HG11	1:G:396:VAL:HG12	1.90	0.54
1:J:223:ALA:HB3	1:J:251:ALA:CB	2.38	0.54
1:N:201:SER:HB3	1:N:204:PHE:CE2	2.42	0.54
2:S:49:LEU:HD11	2:S:55:LYS:HE3	1.88	0.54
2:Z:51:ASN:HD21	2:Z:53:GLU:CD	2.15	0.54
1:F:177:VAL:HG11	1:F:396:VAL:HG12	1.90	0.54
1:F:201:SER:HB3	1:F:204:PHE:CE2	2.43	0.54
1:M:223:ALA:HB3	1:M:251:ALA:CB	2.37	0.54
2:P:51:ASN:HD21	2:P:53:GLU:CD	2.16	0.54
1:C:177:VAL:HG11	1:C:396:VAL:HG12	1.90	0.54
1:G:69:MET:HE2	1:G:520:MET:HE2	1.90	0.54
1:H:177:VAL:HG11	1:H:396:VAL:HG12	1.90	0.54
1:L:177:VAL:HG11	1:L:396:VAL:HG12	1.90	0.54
1:M:229:ASN:HA	1:M:257:GLU:CD	2.31	0.54
1:N:229:ASN:HA	1:N:257:GLU:CD	2.31	0.54
2:S:51:ASN:HD21	2:S:53:GLU:CD	2.15	0.54
1:B:223:ALA:HB3	1:B:251:ALA:CB	2.38	0.54
1:B:229:ASN:HA	1:B:257:GLU:CD	2.31	0.54
1:G:201:SER:HB3	1:G:204:PHE:CE2	2.43	0.54
2:1:51:ASN:HD21	2:1:53:GLU:CD	2.15	0.54
1:A:223:ALA:HB3	1:A:251:ALA:CB	2.38	0.54
2:U:51:ASN:HD21	2:U:53:GLU:CD	2.16	0.54
2:O:16:GLU:HB3	2:O:18:GLU:HA	1.90	0.53
1:B:214:GLU:CD	1:B:322:ARG:HH21	2.17	0.53
1:G:223:ALA:HB3	1:G:251:ALA:CB	2.37	0.53
1:I:201:SER:HB3	1:I:204:PHE:CE2	2.42	0.53
2:O:4:ARG:CB	2:U:94:ILE:O	2.57	0.53
2:Q:51:ASN:HD21	2:Q:53:GLU:CD	2.15	0.53
1:A:214:GLU:CD	1:A:322:ARG:HH21	2.17	0.53
1:D:223:ALA:HB3	1:D:251:ALA:CB	2.37	0.53
1:E:214:GLU:CD	1:E:322:ARG:HH21	2.17	0.53
1:F:214:GLU:CD	1:F:322:ARG:HH21	2.17	0.53
1:I:177:VAL:HG11	1:I:396:VAL:HG12	1.90	0.53
1:K:177:VAL:HG11	1:K:396:VAL:HG12	1.88	0.53
1:K:223:ALA:HB3	1:K:251:ALA:CB	2.38	0.53
1:N:214:GLU:CD	1:N:322:ARG:HH21	2.17	0.53
1:J:214:GLU:CD	1:J:322:ARG:HH21	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:214:GLU:CD	1:L:322:ARG:HH21	2.17	0.53
1:L:268:ARG:NH1	2:Z:26:VAL:HG21	2.23	0.53
1:N:223:ALA:HB3	1:N:251:ALA:CB	2.37	0.53
1:I:214:GLU:CD	1:I:322:ARG:HH21	2.17	0.53
1:K:177:VAL:HG21	1:K:397:GLU:HG3	1.91	0.53
1:C:223:ALA:HB3	1:C:251:ALA:CB	2.37	0.53
1:N:261:THR:HG23	2:2:28:THR:OG1	2.08	0.53
1:G:214:GLU:CD	1:G:322:ARG:HH21	2.17	0.53
1:L:223:ALA:HB3	1:L:251:ALA:CB	2.37	0.53
1:C:214:GLU:CD	1:C:322:ARG:HH21	2.17	0.52
1:I:190:VAL:HG11	1:I:194:GLN:HB3	1.91	0.52
1:H:223:ALA:HB3	1:H:251:ALA:CB	2.38	0.52
1:N:225:LYS:HE2	1:N:309:LEU:HB2	1.91	0.52
1:M:214:GLU:CD	1:M:322:ARG:HH21	2.17	0.52
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.92	0.52
1:K:214:GLU:CD	1:K:322:ARG:HH21	2.17	0.52
1:N:69:MET:HE2	1:N:520:MET:HE2	1.91	0.52
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.91	0.52
1:H:214:GLU:CD	1:H:322:ARG:HH21	2.17	0.52
1:D:214:GLU:CD	1:D:322:ARG:HH21	2.17	0.52
1:M:177:VAL:HG11	1:M:396:VAL:HG12	1.91	0.52
1:J:177:VAL:HG21	1:J:397:GLU:HG3	1.92	0.52
1:N:201:SER:HB3	1:N:204:PHE:CD2	2.45	0.52
1:F:229:ASN:CA	1:F:257:GLU:OE1	2.52	0.52
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.92	0.52
1:L:177:VAL:HG21	1:L:397:GLU:HG3	1.92	0.52
1:B:177:VAL:HG11	1:B:396:VAL:HG12	1.91	0.51
1:D:225:LYS:HE2	1:D:309:LEU:HB2	1.93	0.51
1:H:201:SER:HB3	1:H:204:PHE:CD2	2.45	0.51
1:N:232:GLU:HG3	1:N:310:GLU:CD	2.35	0.51
1:B:232:GLU:HG3	1:B:310:GLU:CD	2.36	0.51
1:E:69:MET:HE2	1:E:520:MET:HE2	1.92	0.51
1:G:201:SER:HB3	1:G:204:PHE:CD2	2.46	0.51
1:F:69:MET:HE2	1:F:520:MET:HE2	1.93	0.51
1:J:201:SER:HB3	1:J:204:PHE:CD2	2.46	0.51
1:N:270:ILE:HD13	2:2:26:VAL:HG23	1.91	0.51
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.92	0.51
1:E:201:SER:HB3	1:E:204:PHE:CD2	2.45	0.51
1:F:225:LYS:HE2	1:F:309:LEU:HB2	1.93	0.51
1:I:223:ALA:HB3	1:I:251:ALA:CB	2.37	0.51
1:K:201:SER:HB3	1:K:204:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:232:GLU:HG3	1:L:310:GLU:CD	2.35	0.51
1:I:229:ASN:CA	1:I:257:GLU:OE1	2.52	0.51
1:A:225:LYS:HE2	1:A:309:LEU:HB2	1.93	0.51
1:F:232:GLU:HG3	1:F:310:GLU:CD	2.36	0.51
1:H:232:GLU:HG3	1:H:310:GLU:CD	2.35	0.51
1:M:232:GLU:HG3	1:M:310:GLU:CD	2.36	0.51
1:C:201:SER:HB3	1:C:204:PHE:CD2	2.45	0.51
1:I:177:VAL:HG21	1:I:397:GLU:HG3	1.92	0.51
1:I:225:LYS:HE2	1:I:309:LEU:HB2	1.93	0.51
2:Q:94:ILE:O	2:R:4:ARG:HB3	2.11	0.51
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.92	0.51
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.92	0.51
1:G:225:LYS:HE2	1:G:309:LEU:HB2	1.92	0.51
1:H:177:VAL:HG21	1:H:397:GLU:HG3	1.93	0.51
1:I:232:GLU:HG3	1:I:310:GLU:CD	2.36	0.51
1:L:201:SER:HB3	1:L:204:PHE:CD2	2.45	0.51
1:B:201:SER:HB3	1:B:204:PHE:CD2	2.46	0.51
1:C:232:GLU:HG3	1:C:310:GLU:CD	2.35	0.51
1:D:201:SER:HB3	1:D:204:PHE:CD2	2.45	0.51
1:G:232:GLU:HG3	1:G:310:GLU:CD	2.36	0.51
1:H:225:LYS:HE2	1:H:309:LEU:HB2	1.93	0.51
1:J:260:ALA:HB1	1:K:306:GLY:N	2.25	0.51
1:M:260:ALA:CB	1:N:304:GLU:O	2.59	0.51
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.92	0.51
1:J:190:VAL:HG13	1:J:331:THR:HG21	1.92	0.51
1:M:201:SER:HB3	1:M:204:PHE:CD2	2.45	0.51
1:K:232:GLU:HG3	1:K:310:GLU:CD	2.35	0.50
1:N:177:VAL:HG21	1:N:397:GLU:HG3	1.92	0.50
1:E:225:LYS:HE2	1:E:309:LEU:HB2	1.93	0.50
1:F:223:ALA:HB3	1:F:251:ALA:CB	2.37	0.50
1:K:268:ARG:NH1	2:Y:26:VAL:HG21	2.25	0.50
2:R:37:ARG:NE	2:S:76:GLU:OE1	2.44	0.50
1:D:232:GLU:HG3	1:D:310:GLU:CD	2.35	0.50
1:M:229:ASN:CA	1:M:257:GLU:OE1	2.52	0.50
1:M:268:ARG:NH1	2:1:26:VAL:HG21	2.26	0.50
1:A:232:GLU:HG3	1:A:310:GLU:CD	2.35	0.50
1:C:225:LYS:HE2	1:C:309:LEU:HB2	1.92	0.50
1:C:305:ILE:HD13	1:D:203:TYR:CE2	2.47	0.50
1:J:232:GLU:HG3	1:J:310:GLU:CD	2.36	0.50
1:A:201:SER:HB3	1:A:204:PHE:CD2	2.45	0.50
1:F:201:SER:HB3	1:F:204:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:SER:HB3	1:I:204:PHE:CD2	2.46	0.50
1:K:225:LYS:HE2	1:K:309:LEU:HB2	1.94	0.50
1:M:177:VAL:HG21	1:M:397:GLU:HG3	1.93	0.50
2:1:49:LEU:HD11	2:1:55:LYS:HE3	1.93	0.50
1:B:225:LYS:HE2	1:B:309:LEU:HB2	1.93	0.50
1:J:209:GLU:O	1:K:351:GLN:OE1	2.30	0.50
1:L:225:LYS:HE2	1:L:309:LEU:HB2	1.93	0.50
2:Y:49:LEU:HD11	2:Y:55:LYS:HE3	1.93	0.50
1:M:238:GLU:OE2	2:1:23:GLY:HA3	2.12	0.50
1:B:99:ILE:O	1:B:100:ILE:C	2.56	0.49
1:M:99:ILE:O	1:M:100:ILE:C	2.55	0.49
2:S:93:ALA:HB1	2:T:4:ARG:O	2.12	0.49
1:B:489:ILE:HG23	1:B:494:LEU:HD21	1.94	0.49
1:I:99:ILE:O	1:I:100:ILE:C	2.55	0.49
1:J:225:LYS:HE2	1:J:309:LEU:HB2	1.93	0.49
1:F:99:ILE:O	1:F:100:ILE:C	2.56	0.49
1:M:225:LYS:HE2	1:M:309:LEU:HB2	1.94	0.49
1:M:489:ILE:HG23	1:M:494:LEU:HD21	1.94	0.49
2:Z:16:GLU:HB3	2:Z:18:GLU:HA	1.95	0.49
1:E:232:GLU:HG3	1:E:310:GLU:CD	2.36	0.49
1:I:489:ILE:HG23	1:I:494:LEU:HD21	1.94	0.49
1:L:99:ILE:O	1:L:100:ILE:C	2.55	0.49
1:B:229:ASN:CA	1:B:257:GLU:OE1	2.52	0.49
1:E:99:ILE:O	1:E:100:ILE:C	2.55	0.49
1:J:229:ASN:CA	1:J:257:GLU:OE1	2.52	0.49
1:L:229:ASN:CA	1:L:257:GLU:OE1	2.52	0.49
1:F:489:ILE:HG23	1:F:494:LEU:HD21	1.94	0.49
1:K:99:ILE:O	1:K:100:ILE:C	2.55	0.49
1:G:99:ILE:O	1:G:100:ILE:C	2.55	0.49
1:G:489:ILE:HG23	1:G:494:LEU:HD21	1.95	0.49
1:H:489:ILE:HG23	1:H:494:LEU:HD21	1.95	0.49
1:I:267:MET:CE	1:J:305:ILE:HB	2.43	0.49
1:J:99:ILE:O	1:J:100:ILE:C	2.55	0.49
2:1:50:GLU:HG2	2:Z:50:GLU:OE1	2.11	0.49
1:A:99:ILE:O	1:A:100:ILE:C	2.56	0.48
1:C:238:GLU:OE2	2:Q:23:GLY:CA	2.61	0.48
1:C:266:THR:HG23	1:C:272:LYS:HG2	1.94	0.48
1:K:229:ASN:CA	1:K:257:GLU:OE1	2.52	0.48
1:N:261:THR:HG22	2:2:28:THR:OG1	2.13	0.48
1:B:268:ARG:NH1	2:P:26:VAL:HG21	2.28	0.48
1:D:489:ILE:HG23	1:D:494:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:ILE:HG23	1:E:494:LEU:HD21	1.95	0.48
1:C:99:ILE:O	1:C:100:ILE:C	2.56	0.48
1:K:489:ILE:HG23	1:K:494:LEU:HD21	1.95	0.48
1:N:99:ILE:O	1:N:100:ILE:C	2.56	0.48
1:A:325:ILE:CG2	1:A:330:THR:HG23	2.43	0.48
1:I:268:ARG:NH1	2:W:26:VAL:HG21	2.29	0.48
1:N:229:ASN:CA	1:N:257:GLU:OE1	2.52	0.48
2:P:50:GLU:HG2	2:Q:50:GLU:OE1	2.13	0.48
2:Y:4:ARG:CB	2:Z:94:ILE:O	2.61	0.48
1:C:229:ASN:CA	1:C:257:GLU:OE1	2.52	0.48
1:D:99:ILE:O	1:D:100:ILE:C	2.56	0.48
1:F:325:ILE:CG2	1:F:330:THR:HG23	2.43	0.48
1:L:69:MET:HE2	1:L:520:MET:HE2	1.95	0.48
1:L:489:ILE:HG23	1:L:494:LEU:HD21	1.95	0.48
2:1:4:ARG:O	2:2:93:ALA:CB	2.61	0.48
1:A:489:ILE:HG23	1:A:494:LEU:HD21	1.95	0.48
1:H:99:ILE:O	1:H:100:ILE:C	2.56	0.48
1:L:238:GLU:OE2	2:Z:23:GLY:CA	2.61	0.48
1:G:229:ASN:CA	1:G:257:GLU:OE1	2.52	0.48
1:J:489:ILE:HG23	1:J:494:LEU:HD21	1.95	0.48
2:P:5:PRO:HG2	2:P:43:VAL:C	2.39	0.48
2:Y:5:PRO:HG2	2:Y:43:VAL:C	2.39	0.48
1:I:7:LYS:HD3	1:I:11:ASP:HB3	1.94	0.48
1:K:7:LYS:HD3	1:K:11:ASP:HB3	1.95	0.48
1:N:325:ILE:CG2	1:N:330:THR:HG23	2.43	0.48
2:U:5:PRO:HG2	2:U:43:VAL:C	2.39	0.48
1:B:103:GLY:HA3	1:B:515:ILE:HD13	1.96	0.47
1:C:489:ILE:HG23	1:C:494:LEU:HD21	1.94	0.47
2:S:5:PRO:HG2	2:S:43:VAL:C	2.39	0.47
1:I:263:VAL:HG11	1:J:305:ILE:HG22	1.95	0.47
2:1:5:PRO:HG2	2:1:43:VAL:C	2.39	0.47
2:X:5:PRO:HG2	2:X:43:VAL:C	2.39	0.47
1:A:229:ASN:CA	1:A:257:GLU:OE1	2.52	0.47
1:D:229:ASN:CA	1:D:257:GLU:OE1	2.52	0.47
1:G:325:ILE:CG2	1:G:330:THR:HG23	2.43	0.47
1:I:325:ILE:CG2	1:I:330:THR:HG23	2.43	0.47
2:1:52:GLY:HA2	2:2:55:LYS:CE	2.43	0.47
2:O:5:PRO:HG2	2:O:43:VAL:C	2.39	0.47
2:R:5:PRO:HG2	2:R:43:VAL:C	2.39	0.47
2:V:5:PRO:HG2	2:V:43:VAL:C	2.39	0.47
1:B:90:THR:O	1:B:94:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:93:ALA:HB1	2:R:4:ARG:O	2.14	0.47
1:B:172:GLU:CD	1:B:350:ARG:HH21	2.22	0.47
1:J:260:ALA:HB1	1:K:306:GLY:CA	2.44	0.47
1:M:90:THR:O	1:M:94:VAL:HG23	2.15	0.47
2:1:52:GLY:CA	2:2:55:LYS:HE3	2.44	0.47
2:X:74:LYS:HD2	2:Y:68:ASN:ND2	2.29	0.47
1:D:7:LYS:HD3	1:D:11:ASP:HB3	1.96	0.47
1:H:90:THR:O	1:H:94:VAL:HG23	2.15	0.47
1:M:103:GLY:HA3	1:M:515:ILE:HD13	1.97	0.47
1:B:325:ILE:CG2	1:B:330:THR:HG23	2.43	0.47
1:E:7:LYS:HD3	1:E:11:ASP:HB3	1.96	0.47
1:E:259:LEU:O	1:E:263:VAL:HG23	2.15	0.47
1:G:103:GLY:HA3	1:G:515:ILE:HD13	1.97	0.47
1:H:7:LYS:HD3	1:H:11:ASP:HB3	1.97	0.47
1:H:325:ILE:CG2	1:H:330:THR:HG23	2.43	0.47
1:J:7:LYS:HD3	1:J:11:ASP:HB3	1.97	0.47
1:J:259:LEU:O	1:J:263:VAL:HG23	2.15	0.47
1:K:259:LEU:O	1:K:263:VAL:HG23	2.15	0.47
1:M:325:ILE:CG2	1:M:330:THR:HG23	2.43	0.47
1:N:90:THR:O	1:N:94:VAL:HG23	2.15	0.47
2:W:5:PRO:HG2	2:W:43:VAL:C	2.39	0.47
1:D:90:THR:O	1:D:94:VAL:HG23	2.15	0.47
1:H:103:GLY:HA3	1:H:515:ILE:HD13	1.97	0.47
1:I:90:THR:O	1:I:94:VAL:HG23	2.15	0.47
1:L:237:LEU:HB3	2:Z:25:ILE:HD13	1.96	0.47
1:N:489:ILE:HG23	1:N:494:LEU:HD21	1.95	0.47
2:2:11:ILE:HG12	2:2:85:ILE:HG12	1.96	0.47
1:E:325:ILE:CG2	1:E:330:THR:HG23	2.43	0.47
1:F:261:THR:HG23	2:T:28:THR:OG1	2.15	0.47
1:J:103:GLY:HA3	1:J:515:ILE:HD13	1.96	0.47
1:K:90:THR:O	1:K:94:VAL:HG23	2.15	0.47
1:L:7:LYS:HD3	1:L:11:ASP:HB3	1.97	0.47
1:A:259:LEU:O	1:A:263:VAL:HG23	2.15	0.47
1:C:7:LYS:HD3	1:C:11:ASP:HB3	1.97	0.47
1:D:259:LEU:O	1:D:263:VAL:HG23	2.15	0.47
1:F:103:GLY:HA3	1:F:515:ILE:HD13	1.97	0.47
1:F:172:GLU:CD	1:F:350:ARG:HH21	2.23	0.47
1:J:90:THR:O	1:J:94:VAL:HG23	2.15	0.47
2:2:5:PRO:HG2	2:2:43:VAL:C	2.39	0.47
1:A:232:GLU:HA	1:A:310:GLU:CG	2.45	0.46
1:C:103:GLY:HA3	1:C:515:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:THR:O	1:G:94:VAL:HG23	2.15	0.46
1:H:268:ARG:NH1	2:V:26:VAL:HG21	2.30	0.46
1:I:172:GLU:CD	1:I:350:ARG:HH21	2.23	0.46
1:I:266:THR:HG23	1:I:272:LYS:HG2	1.97	0.46
1:L:90:THR:O	1:L:94:VAL:HG23	2.15	0.46
1:L:103:GLY:HA3	1:L:515:ILE:HD13	1.96	0.46
2:Z:5:PRO:HG2	2:Z:43:VAL:C	2.39	0.46
1:B:361:ASP:O	1:B:365:LEU:HG	2.15	0.46
1:D:361:ASP:O	1:D:365:LEU:HG	2.16	0.46
1:F:90:THR:O	1:F:94:VAL:HG23	2.15	0.46
1:F:361:ASP:O	1:F:365:LEU:HG	2.16	0.46
1:L:228:SER:O	1:L:257:GLU:HB3	2.16	0.46
1:L:325:ILE:CG2	1:L:330:THR:HG23	2.43	0.46
2:T:5:PRO:HG2	2:T:43:VAL:C	2.39	0.46
2:W:74:LYS:HE3	2:X:68:ASN:ND2	2.30	0.46
1:A:254:VAL:HG21	1:A:275:ALA:HB1	1.98	0.46
1:C:228:SER:O	1:C:257:GLU:HB3	2.16	0.46
1:M:361:ASP:O	1:M:365:LEU:HG	2.16	0.46
1:N:103:GLY:HA3	1:N:515:ILE:HD13	1.97	0.46
1:N:259:LEU:O	1:N:263:VAL:HG23	2.15	0.46
2:O:49:LEU:HD11	2:O:55:LYS:HE3	1.97	0.46
1:A:385:THR:HG21	1:G:510:VAL:HG23	1.97	0.46
1:B:259:LEU:O	1:B:263:VAL:HG23	2.15	0.46
1:F:259:LEU:O	1:F:263:VAL:HG23	2.15	0.46
1:J:232:GLU:HA	1:J:310:GLU:CG	2.45	0.46
1:M:259:LEU:O	1:M:263:VAL:HG23	2.15	0.46
2:Q:5:PRO:HG2	2:Q:43:VAL:C	2.39	0.46
2:S:11:ILE:HG12	2:S:85:ILE:HG12	1.98	0.46
1:A:361:ASP:O	1:A:365:LEU:HG	2.16	0.46
1:E:103:GLY:HA3	1:E:515:ILE:HD13	1.97	0.46
1:F:254:VAL:HG21	1:F:275:ALA:HB1	1.97	0.46
1:G:361:ASP:O	1:G:365:LEU:HG	2.16	0.46
1:H:361:ASP:O	1:H:365:LEU:HG	2.16	0.46
1:I:103:GLY:HA3	1:I:515:ILE:HD13	1.97	0.46
1:C:90:THR:O	1:C:94:VAL:HG23	2.15	0.46
1:I:361:ASP:O	1:I:365:LEU:HG	2.16	0.46
1:M:172:GLU:CD	1:M:350:ARG:HH21	2.23	0.46
2:U:3:ILE:HD11	2:U:78:ILE:HD12	1.98	0.46
1:A:90:THR:O	1:A:94:VAL:HG23	2.15	0.46
1:G:261:THR:HG22	2:U:28:THR:H	1.81	0.46
1:H:41:ASP:HB2	1:I:69:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:46:GLY:HA3	2:T:55:LYS:O	2.16	0.46
2:U:11:ILE:HG12	2:U:85:ILE:HG12	1.97	0.46
1:C:232:GLU:HA	1:C:310:GLU:CG	2.45	0.46
1:D:232:GLU:HA	1:D:310:GLU:CG	2.45	0.46
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.98	0.46
1:I:254:VAL:HG21	1:I:275:ALA:HB1	1.98	0.46
1:K:232:GLU:HA	1:K:310:GLU:CG	2.45	0.46
2:R:11:ILE:HG12	2:R:85:ILE:HG12	1.97	0.46
2:Y:11:ILE:HG12	2:Y:85:ILE:HG12	1.97	0.46
1:A:103:GLY:HA3	1:A:515:ILE:HD13	1.98	0.46
1:C:325:ILE:CG2	1:C:330:THR:HG23	2.43	0.46
1:D:409:GLU:OE2	1:D:501:ARG:NH2	2.49	0.46
1:E:90:THR:O	1:E:94:VAL:HG23	2.15	0.46
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.49	0.46
1:G:261:THR:HG22	2:U:28:THR:N	2.31	0.46
1:H:229:ASN:CA	1:H:257:GLU:OE1	2.52	0.46
1:H:259:LEU:O	1:H:263:VAL:HG23	2.15	0.46
1:J:409:GLU:OE2	1:J:501:ARG:NH2	2.49	0.46
1:M:69:MET:HE2	1:M:520:MET:HE2	1.98	0.46
1:M:228:SER:O	1:M:257:GLU:HB3	2.15	0.46
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.98	0.46
1:E:228:SER:O	1:E:257:GLU:HB3	2.16	0.46
1:E:361:ASP:O	1:E:365:LEU:HG	2.16	0.46
1:F:232:GLU:HA	1:F:310:GLU:CG	2.45	0.46
1:G:228:SER:O	1:G:257:GLU:HB3	2.16	0.46
1:L:361:ASP:O	1:L:365:LEU:HG	2.16	0.46
2:S:93:ALA:CB	2:T:4:ARG:O	2.64	0.46
2:V:11:ILE:HG12	2:V:85:ILE:HG12	1.98	0.46
1:A:261:THR:HG22	2:O:28:THR:OG1	2.16	0.45
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.98	0.45
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.98	0.45
1:A:228:SER:O	1:A:257:GLU:HB3	2.16	0.45
1:D:228:SER:O	1:D:257:GLU:HB3	2.16	0.45
1:H:78:ALA:HB2	1:H:93:THR:OG1	2.17	0.45
1:I:259:LEU:O	1:I:263:VAL:HG23	2.15	0.45
1:L:232:GLU:HA	1:L:310:GLU:CG	2.45	0.45
1:L:232:GLU:HB3	1:L:309:LEU:HD23	1.98	0.45
1:M:409:GLU:OE2	1:M:501:ARG:NH2	2.49	0.45
2:T:50:GLU:HG2	2:U:50:GLU:OE1	2.17	0.45
1:A:270:ILE:HD13	2:O:26:VAL:HG23	1.99	0.45
1:B:254:VAL:HG21	1:B:275:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ASP:O	1:C:365:LEU:HG	2.16	0.45
1:H:254:VAL:HG21	1:H:275:ALA:HB1	1.98	0.45
1:J:228:SER:O	1:J:257:GLU:HB3	2.16	0.45
1:K:325:ILE:CG2	1:K:330:THR:HG23	2.43	0.45
1:K:361:ASP:O	1:K:365:LEU:HG	2.16	0.45
1:L:259:LEU:O	1:L:263:VAL:HG23	2.15	0.45
1:M:232:GLU:HB3	1:M:309:LEU:HD23	1.98	0.45
1:A:409:GLU:OE2	1:A:501:ARG:NH2	2.49	0.45
1:C:259:LEU:O	1:C:263:VAL:HG23	2.15	0.45
1:F:228:SER:O	1:F:257:GLU:HB3	2.16	0.45
1:G:78:ALA:HB2	1:G:93:THR:OG1	2.17	0.45
1:K:228:SER:O	1:K:257:GLU:HB3	2.16	0.45
1:K:409:GLU:OE2	1:K:501:ARG:NH2	2.49	0.45
1:N:409:GLU:OE2	1:N:501:ARG:NH2	2.49	0.45
1:B:228:SER:O	1:B:257:GLU:HB3	2.16	0.45
1:B:232:GLU:HB3	1:B:309:LEU:HD23	1.98	0.45
1:G:254:VAL:HG21	1:G:275:ALA:HB1	1.98	0.45
1:G:259:LEU:O	1:G:263:VAL:HG23	2.15	0.45
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.99	0.45
1:L:409:GLU:OE2	1:L:501:ARG:NH2	2.49	0.45
1:M:78:ALA:HB2	1:M:93:THR:OG1	2.17	0.45
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.98	0.45
2:2:80:ASN:OD1	2:V:22:ALA:HB2	2.16	0.45
2:Z:11:ILE:HG12	2:Z:85:ILE:HG12	1.98	0.45
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.98	0.45
1:D:266:THR:HG23	1:D:272:LYS:HG2	1.98	0.45
1:K:103:GLY:HA3	1:K:515:ILE:HD13	1.97	0.45
1:M:254:VAL:HG21	1:M:275:ALA:HB1	1.99	0.45
1:N:254:VAL:HG21	1:N:275:ALA:HB1	1.99	0.45
1:B:409:GLU:OE2	1:B:501:ARG:NH2	2.49	0.45
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.99	0.45
1:C:232:GLU:HB3	1:C:309:LEU:HD23	1.98	0.45
1:D:103:GLY:HA3	1:D:515:ILE:HD13	1.97	0.45
1:D:232:GLU:HB3	1:D:309:LEU:HD23	1.98	0.45
1:E:25:ASP:HA	1:E:28:LYS:HD3	1.99	0.45
1:J:25:ASP:HA	1:J:28:LYS:HD3	1.99	0.45
1:J:25:ASP:HA	1:J:28:LYS:CD	2.47	0.45
1:J:325:ILE:CG2	1:J:330:THR:HG23	2.43	0.45
1:K:78:ALA:HB2	1:K:93:THR:OG1	2.17	0.45
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.99	0.45
2:U:46:GLY:HA3	2:U:55:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:HB2	1:A:93:THR:OG1	2.17	0.45
1:C:78:ALA:HB2	1:C:93:THR:OG1	2.17	0.45
1:E:229:ASN:CA	1:E:257:GLU:OE1	2.52	0.45
1:F:230:ILE:HD12	1:F:261:THR:CB	2.47	0.45
1:G:25:ASP:HA	1:G:28:LYS:CD	2.47	0.45
1:H:25:ASP:HA	1:H:28:LYS:CD	2.47	0.45
1:I:409:GLU:OE2	1:I:501:ARG:NH2	2.49	0.45
1:N:232:GLU:HB3	1:N:309:LEU:HD23	1.97	0.45
2:O:4:ARG:N	2:U:94:ILE:O	2.50	0.45
2:W:46:GLY:HA3	2:W:55:LYS:O	2.17	0.45
1:B:78:ALA:HB2	1:B:93:THR:OG1	2.17	0.45
1:D:78:ALA:HB2	1:D:93:THR:OG1	2.17	0.45
1:E:78:ALA:HB2	1:E:93:THR:OG1	2.17	0.45
1:F:25:ASP:HA	1:F:28:LYS:CD	2.47	0.45
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.49	0.45
1:G:25:ASP:HA	1:G:28:LYS:HD3	1.99	0.45
1:H:409:GLU:OE2	1:H:501:ARG:NH2	2.50	0.45
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.99	0.45
1:I:232:GLU:HA	1:I:310:GLU:CG	2.45	0.45
1:J:78:ALA:HB2	1:J:93:THR:OG1	2.17	0.45
1:J:232:GLU:HB3	1:J:309:LEU:HD23	1.98	0.45
1:J:361:ASP:O	1:J:365:LEU:HG	2.16	0.45
1:L:78:ALA:HB2	1:L:93:THR:OG1	2.17	0.45
1:L:254:VAL:HG21	1:L:275:ALA:HB1	1.98	0.45
1:N:361:ASP:O	1:N:365:LEU:HG	2.16	0.45
1:F:7:LYS:HD3	1:F:11:ASP:HB3	1.99	0.45
2:Y:46:GLY:HA3	2:Y:55:LYS:O	2.17	0.45
1:A:25:ASP:HA	1:A:28:LYS:CD	2.48	0.44
1:A:224:ASP:HB3	1:A:302:SER:HA	1.99	0.44
1:B:7:LYS:HD3	1:B:11:ASP:HB3	1.98	0.44
1:C:254:VAL:HG21	1:C:275:ALA:HB1	1.99	0.44
1:D:224:ASP:HB3	1:D:302:SER:HA	1.99	0.44
1:F:78:ALA:HB2	1:F:93:THR:OG1	2.17	0.44
1:H:25:ASP:HA	1:H:28:LYS:HD3	1.99	0.44
1:H:228:SER:O	1:H:257:GLU:HB3	2.16	0.44
1:H:232:GLU:HB3	1:H:309:LEU:HD23	1.99	0.44
1:I:25:ASP:HA	1:I:28:LYS:CD	2.47	0.44
1:I:78:ALA:HB2	1:I:93:THR:OG1	2.17	0.44
1:K:266:THR:HG23	1:K:272:LYS:HG2	1.99	0.44
1:L:224:ASP:HB3	1:L:302:SER:HA	1.99	0.44
1:N:25:ASP:HA	1:N:28:LYS:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:78:ALA:HB2	1:N:93:THR:OG1	2.17	0.44
2:1:11:ILE:HG12	2:1:85:ILE:HG12	1.99	0.44
2:Z:4:ARG:NH1	2:Z:5:PRO:O	2.50	0.44
1:B:261:THR:HG23	2:P:28:THR:OG1	2.18	0.44
1:E:25:ASP:HA	1:E:28:LYS:CD	2.47	0.44
1:E:232:GLU:HB3	1:E:309:LEU:HD23	1.98	0.44
1:G:172:GLU:O	1:G:373:ALA:HB1	2.17	0.44
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.98	0.44
1:I:228:SER:O	1:I:257:GLU:HB3	2.16	0.44
1:J:254:VAL:HG21	1:J:275:ALA:HB1	1.99	0.44
1:K:232:GLU:HB3	1:K:309:LEU:HD23	1.98	0.44
1:M:25:ASP:HA	1:M:28:LYS:HD3	1.99	0.44
2:S:46:GLY:HA3	2:S:55:LYS:O	2.17	0.44
1:B:69:MET:HE2	1:B:520:MET:HE2	1.99	0.44
1:C:224:ASP:HB3	1:C:302:SER:HA	1.99	0.44
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.99	0.44
1:H:266:THR:HG23	1:H:272:LYS:HG2	1.99	0.44
1:I:25:ASP:HA	1:I:28:LYS:HD3	2.00	0.44
1:L:25:ASP:HA	1:L:28:LYS:CD	2.47	0.44
1:L:177:VAL:HG11	1:L:396:VAL:CG1	2.48	0.44
1:L:230:ILE:HD12	1:L:261:THR:CB	2.48	0.44
1:L:339:GLU:HA	1:L:342:ILE:HD12	2.00	0.44
2:P:11:ILE:HG12	2:P:85:ILE:HG12	1.98	0.44
2:X:4:ARG:O	2:Y:93:ALA:CB	2.64	0.44
2:X:11:ILE:HG12	2:X:85:ILE:HG12	2.00	0.44
2:Y:4:ARG:NH1	2:Y:5:PRO:O	2.50	0.44
1:B:25:ASP:HA	1:B:28:LYS:HD3	2.00	0.44
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.99	0.44
1:C:409:GLU:OE2	1:C:501:ARG:NH2	2.50	0.44
1:G:232:GLU:HA	1:G:310:GLU:CG	2.45	0.44
1:H:177:VAL:HG11	1:H:396:VAL:CG1	2.48	0.44
1:N:224:ASP:HB3	1:N:302:SER:HA	2.00	0.44
1:N:228:SER:O	1:N:257:GLU:HB3	2.16	0.44
1:N:339:GLU:HA	1:N:342:ILE:HD12	1.99	0.44
2:2:80:ASN:OD1	2:V:22:ALA:CB	2.65	0.44
2:O:4:ARG:NH1	2:O:5:PRO:O	2.51	0.44
2:P:4:ARG:NH1	2:P:5:PRO:O	2.51	0.44
2:V:46:GLY:HA3	2:V:55:LYS:O	2.17	0.44
2:X:46:GLY:HA3	2:X:55:LYS:O	2.17	0.44
1:B:224:ASP:HB3	1:B:302:SER:HA	1.99	0.44
1:F:25:ASP:HA	1:F:28:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:MET:HB3	1:G:237:LEU:CD1	2.48	0.44
1:G:409:GLU:OE2	1:G:501:ARG:NH2	2.49	0.44
1:H:232:GLU:HA	1:H:310:GLU:CG	2.45	0.44
1:I:224:ASP:HB3	1:I:302:SER:HA	1.99	0.44
2:R:46:GLY:HA3	2:R:55:LYS:O	2.18	0.44
1:E:254:VAL:HG21	1:E:275:ALA:HB1	2.00	0.44
1:H:224:ASP:HB3	1:H:302:SER:HA	1.99	0.44
1:J:69:MET:HE2	1:J:520:MET:HE2	2.00	0.44
1:M:7:LYS:HD3	1:M:11:ASP:HB3	1.98	0.44
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.99	0.44
1:B:25:ASP:HA	1:B:28:LYS:CD	2.47	0.44
1:B:266:THR:HG23	1:B:272:LYS:HG2	2.00	0.44
1:G:257:GLU:HG2	2:U:30:SER:CB	2.42	0.44
1:J:150:ILE:HG23	3:J:600:ADP:C8	2.53	0.44
1:K:25:ASP:HA	1:K:28:LYS:CD	2.47	0.44
1:A:232:GLU:HB3	1:A:309:LEU:HD23	1.99	0.44
1:B:177:VAL:HG11	1:B:396:VAL:CG1	2.48	0.44
1:C:177:VAL:HG11	1:C:396:VAL:CG1	2.48	0.44
1:D:25:ASP:HA	1:D:28:LYS:CD	2.47	0.44
1:D:25:ASP:HA	1:D:28:LYS:HD3	1.99	0.44
1:I:232:GLU:HB3	1:I:309:LEU:HD23	1.98	0.44
1:J:177:VAL:HG11	1:J:396:VAL:CG1	2.48	0.44
1:K:23:LEU:CD1	1:K:57:ALA:HA	2.48	0.44
1:K:25:ASP:HA	1:K:28:LYS:HD3	1.99	0.44
1:M:25:ASP:HA	1:M:28:LYS:CD	2.47	0.44
2:O:7:HIS:CE1	2:U:58:ASP:OD1	2.70	0.44
2:Q:46:GLY:HA3	2:Q:55:LYS:O	2.17	0.44
2:X:4:ARG:NH1	2:X:5:PRO:O	2.51	0.44
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.99	0.44
1:K:233:MET:HB3	1:K:237:LEU:CD1	2.48	0.44
1:K:385:THR:HG21	1:L:510:VAL:HG23	2.00	0.44
1:M:224:ASP:HB3	1:M:302:SER:HA	1.99	0.44
2:Q:4:ARG:NH1	2:Q:5:PRO:O	2.51	0.44
2:V:4:ARG:O	2:W:93:ALA:HB1	2.18	0.44
1:C:25:ASP:HA	1:C:28:LYS:CD	2.47	0.43
1:C:230:ILE:HD12	1:C:261:THR:CB	2.48	0.43
1:D:254:VAL:HG21	1:D:275:ALA:HB1	1.99	0.43
1:F:305:ILE:HG21	1:G:203:TYR:CD2	2.53	0.43
1:J:224:ASP:HB3	1:J:302:SER:HA	1.99	0.43
2:U:4:ARG:NH1	2:U:5:PRO:O	2.51	0.43
1:C:339:GLU:HA	1:C:342:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:LEU:CD1	1:H:57:ALA:HA	2.48	0.43
1:M:486:GLY:C	1:M:491:MET:HE2	2.43	0.43
2:P:14:ARG:NH2	2:P:84:LEU:HD21	2.34	0.43
2:V:16:GLU:HG3	2:V:18:GLU:HA	1.99	0.43
2:Y:4:ARG:HB3	2:Z:94:ILE:H	1.83	0.43
1:B:150:ILE:HG23	3:B:600:ADP:C8	2.53	0.43
1:E:23:LEU:CD1	1:E:57:ALA:HA	2.48	0.43
1:I:230:ILE:HD12	1:I:261:THR:CB	2.48	0.43
1:L:266:THR:HG23	1:L:272:LYS:HG2	1.99	0.43
1:M:233:MET:HB3	1:M:237:LEU:HG	2.00	0.43
1:M:266:THR:HG23	1:M:272:LYS:HG2	2.00	0.43
1:N:451:LEU:HD21	1:N:465:VAL:HG12	2.01	0.43
2:2:46:GLY:HA3	2:2:55:LYS:O	2.18	0.43
2:P:49:LEU:CD1	2:P:55:LYS:HE3	2.48	0.43
2:T:4:ARG:NH1	2:T:5:PRO:O	2.51	0.43
2:X:14:ARG:NH2	2:X:84:LEU:HD21	2.33	0.43
1:A:177:VAL:HG11	1:A:396:VAL:CG1	2.48	0.43
1:A:233:MET:HB3	1:A:237:LEU:CD1	2.48	0.43
1:B:233:MET:HB3	1:B:237:LEU:CD1	2.48	0.43
1:D:325:ILE:CG2	1:D:330:THR:HG23	2.43	0.43
1:F:233:MET:HB3	1:F:237:LEU:CD1	2.48	0.43
1:G:23:LEU:CD1	1:G:57:ALA:HA	2.49	0.43
1:G:230:ILE:HD12	1:G:261:THR:CB	2.48	0.43
1:K:254:VAL:HG21	1:K:275:ALA:HB1	1.99	0.43
1:L:25:ASP:HA	1:L:28:LYS:HD3	1.99	0.43
2:1:14:ARG:NH2	2:1:84:LEU:HD21	2.34	0.43
2:R:4:ARG:NH1	2:R:5:PRO:O	2.51	0.43
2:X:76:GLU:OE2	2:Y:36:THR:OG1	2.25	0.43
1:A:77:VAL:HG12	1:A:92:ALA:HB1	2.01	0.43
1:B:23:LEU:CD1	1:B:57:ALA:HA	2.49	0.43
1:C:233:MET:HB3	1:C:237:LEU:CD1	2.48	0.43
1:D:77:VAL:HG12	1:D:92:ALA:HB1	2.01	0.43
1:E:224:ASP:HB3	1:E:302:SER:HA	1.99	0.43
1:E:339:GLU:HA	1:E:342:ILE:HD12	2.01	0.43
1:F:232:GLU:HB3	1:F:309:LEU:HD23	1.98	0.43
1:G:232:GLU:HB3	1:G:309:LEU:HD23	1.99	0.43
1:H:233:MET:HB3	1:H:237:LEU:CD1	2.48	0.43
1:M:23:LEU:CD1	1:M:57:ALA:HA	2.49	0.43
1:M:233:MET:HB3	1:M:237:LEU:CD1	2.48	0.43
1:N:77:VAL:HG12	1:N:92:ALA:HB1	2.01	0.43
2:1:4:ARG:NH1	2:1:5:PRO:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:14:ARG:NH2	2:R:84:LEU:HD21	2.34	0.43
2:S:4:ARG:NH1	2:S:5:PRO:O	2.51	0.43
2:T:14:ARG:NH2	2:T:84:LEU:HD21	2.33	0.43
2:U:14:ARG:NH2	2:U:84:LEU:HD21	2.34	0.43
2:W:4:ARG:NH1	2:W:5:PRO:O	2.51	0.43
2:W:14:ARG:NH2	2:W:84:LEU:HD21	2.34	0.43
2:Z:46:GLY:HA3	2:Z:55:LYS:O	2.18	0.43
1:A:151:SER:HB3	1:A:399:ALA:HA	2.01	0.43
1:F:23:LEU:CD1	1:F:57:ALA:HA	2.48	0.43
1:I:233:MET:HB3	1:I:237:LEU:HG	2.00	0.43
1:K:230:ILE:HD12	1:K:261:THR:CB	2.48	0.43
1:M:177:VAL:HG11	1:M:396:VAL:CG1	2.48	0.43
2:2:4:ARG:NH1	2:2:5:PRO:O	2.51	0.43
2:V:4:ARG:O	2:W:93:ALA:CB	2.66	0.43
2:V:4:ARG:NH1	2:V:5:PRO:O	2.51	0.43
2:W:11:ILE:HG12	2:W:85:ILE:HG12	2.01	0.43
1:A:23:LEU:CD1	1:A:57:ALA:HA	2.49	0.43
1:A:25:ASP:HA	1:A:28:LYS:HD3	2.00	0.43
1:B:230:ILE:HD12	1:B:261:THR:CB	2.48	0.43
1:B:233:MET:HB3	1:B:237:LEU:HG	2.00	0.43
1:B:486:GLY:C	1:B:491:MET:HE2	2.44	0.43
1:D:23:LEU:CD1	1:D:57:ALA:HA	2.49	0.43
1:D:230:ILE:HD12	1:D:261:THR:CB	2.48	0.43
1:F:224:ASP:HB3	1:F:302:SER:HA	1.99	0.43
1:F:486:GLY:C	1:F:491:MET:HE2	2.43	0.43
1:H:77:VAL:HG12	1:H:92:ALA:HB1	2.01	0.43
1:I:23:LEU:CD1	1:I:57:ALA:HA	2.48	0.43
1:I:233:MET:HB3	1:I:237:LEU:CD1	2.48	0.43
1:J:233:MET:HB3	1:J:237:LEU:CD1	2.48	0.43
1:M:230:ILE:HD12	1:M:261:THR:CB	2.48	0.43
1:N:23:LEU:CD1	1:N:57:ALA:HA	2.49	0.43
1:N:177:VAL:HG11	1:N:396:VAL:CG1	2.49	0.43
1:N:233:MET:HB3	1:N:237:LEU:CD1	2.49	0.43
2:O:14:ARG:NH2	2:O:84:LEU:HD21	2.33	0.43
2:T:49:LEU:CD1	2:T:55:LYS:HE3	2.48	0.43
2:Z:14:ARG:NH2	2:Z:84:LEU:HD21	2.34	0.43
1:A:265:ASN:OD1	2:O:26:VAL:N	2.51	0.43
1:C:233:MET:HB3	1:C:237:LEU:HG	2.01	0.43
1:E:266:THR:HG23	1:E:272:LYS:HG2	2.01	0.43
1:G:7:LYS:HD3	1:G:11:ASP:HB3	2.00	0.43
1:G:177:VAL:HG11	1:G:396:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:ASP:HB3	1:G:302:SER:HA	1.99	0.43
1:K:224:ASP:HB3	1:K:302:SER:HA	2.00	0.43
1:L:451:LEU:HD21	1:L:465:VAL:HG12	2.00	0.43
2:1:46:GLY:HA3	2:1:55:LYS:O	2.18	0.43
2:P:46:GLY:HA3	2:P:55:LYS:O	2.18	0.43
2:Q:14:ARG:NH2	2:Q:84:LEU:HD21	2.34	0.43
1:E:233:MET:HB3	1:E:237:LEU:CD1	2.49	0.43
1:G:486:GLY:C	1:G:491:MET:HE2	2.44	0.43
2:O:46:GLY:HA3	2:O:55:LYS:O	2.17	0.43
1:A:7:LYS:HD3	1:A:11:ASP:HB3	2.01	0.43
1:B:451:LEU:HD21	1:B:465:VAL:HG12	2.01	0.43
1:J:266:THR:HG23	1:J:272:LYS:HG2	2.00	0.43
1:N:25:ASP:HA	1:N:28:LYS:HD3	2.00	0.43
2:T:11:ILE:HG12	2:T:85:ILE:HG12	2.01	0.43
1:C:25:ASP:HA	1:C:28:LYS:HD3	1.99	0.42
1:D:16:MET:O	1:D:20:VAL:HG23	2.19	0.42
1:D:177:VAL:HG11	1:D:396:VAL:CG1	2.48	0.42
1:F:77:VAL:HG12	1:F:92:ALA:HB1	2.01	0.42
1:G:16:MET:O	1:G:20:VAL:HG23	2.19	0.42
1:G:456:LEU:HD13	1:G:462:PRO:HG2	2.01	0.42
1:H:230:ILE:HD12	1:H:261:THR:CB	2.48	0.42
1:J:339:GLU:HA	1:J:342:ILE:HD12	2.01	0.42
1:J:486:GLY:C	1:J:491:MET:HE2	2.44	0.42
1:K:177:VAL:HG11	1:K:396:VAL:CG1	2.49	0.42
1:L:233:MET:HB3	1:L:237:LEU:HG	2.01	0.42
1:L:233:MET:HB3	1:L:237:LEU:CD1	2.49	0.42
1:N:230:ILE:HD12	1:N:261:THR:CB	2.49	0.42
1:A:233:MET:HB3	1:A:237:LEU:HG	2.00	0.42
1:A:451:LEU:HD21	1:A:465:VAL:HG12	2.02	0.42
1:D:233:MET:HB3	1:D:237:LEU:CD1	2.48	0.42
1:D:486:GLY:C	1:D:491:MET:HE2	2.44	0.42
1:F:16:MET:O	1:F:20:VAL:HG23	2.20	0.42
1:I:16:MET:O	1:I:20:VAL:HG23	2.20	0.42
1:I:77:VAL:HG12	1:I:92:ALA:HB1	2.02	0.42
1:I:486:GLY:C	1:I:491:MET:HE2	2.44	0.42
1:L:23:LEU:CD1	1:L:57:ALA:HA	2.49	0.42
2:W:43:VAL:HG13	2:W:57:LEU:HD12	2.01	0.42
1:A:230:ILE:HD12	1:A:261:THR:CB	2.49	0.42
1:E:230:ILE:HD12	1:E:261:THR:CB	2.48	0.42
1:E:451:LEU:HD21	1:E:465:VAL:HG12	2.02	0.42
1:F:233:MET:HB3	1:F:237:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:LEU:CD1	1:J:57:ALA:HA	2.49	0.42
1:K:77:VAL:HG12	1:K:92:ALA:HB1	2.01	0.42
1:K:486:GLY:C	1:K:491:MET:HE2	2.44	0.42
1:N:233:MET:HB3	1:N:237:LEU:HG	2.00	0.42
2:W:6:LEU:O	2:W:9:ARG:HG2	2.20	0.42
1:A:16:MET:O	1:A:20:VAL:HG23	2.19	0.42
1:C:486:GLY:C	1:C:491:MET:HE2	2.44	0.42
1:E:486:GLY:C	1:E:491:MET:HE2	2.44	0.42
1:F:339:GLU:HA	1:F:342:ILE:HD12	2.00	0.42
1:G:77:VAL:HG12	1:G:92:ALA:HB1	2.01	0.42
1:G:339:GLU:HA	1:G:342:ILE:HD12	2.01	0.42
1:J:151:SER:HB3	1:J:399:ALA:HA	2.01	0.42
1:K:224:ASP:CB	1:K:302:SER:HA	2.50	0.42
1:K:233:MET:HB3	1:K:237:LEU:HG	2.01	0.42
1:L:77:VAL:HG12	1:L:92:ALA:HB1	2.01	0.42
1:L:486:GLY:C	1:L:491:MET:HE2	2.44	0.42
1:N:266:THR:HG23	1:N:272:LYS:HG2	2.00	0.42
2:2:4:ARG:HB3	2:V:94:ILE:HB	2.02	0.42
2:2:14:ARG:NH2	2:2:84:LEU:HD21	2.34	0.42
2:Y:14:ARG:NH2	2:Y:84:LEU:HD21	2.34	0.42
1:B:456:LEU:HD13	1:B:462:PRO:HG2	2.01	0.42
1:F:266:THR:HG23	1:F:272:LYS:HG2	2.01	0.42
1:H:16:MET:O	1:H:20:VAL:HG23	2.19	0.42
1:J:230:ILE:HD12	1:J:261:THR:CB	2.49	0.42
1:J:233:MET:HB3	1:J:237:LEU:HG	2.01	0.42
1:N:7:LYS:HD3	1:N:11:ASP:HB3	2.02	0.42
1:N:151:SER:HB3	1:N:399:ALA:HA	2.02	0.42
1:N:486:GLY:C	1:N:491:MET:HE2	2.44	0.42
2:1:43:VAL:HG13	2:1:57:LEU:HD12	2.02	0.42
1:C:23:LEU:CD1	1:C:57:ALA:HA	2.49	0.42
1:C:305:ILE:CD1	1:D:203:TYR:CD2	3.00	0.42
1:D:151:SER:HB3	1:D:399:ALA:HA	2.01	0.42
1:J:77:VAL:HG12	1:J:92:ALA:HB1	2.01	0.42
1:M:400:LEU:O	1:M:403:THR:OG1	2.34	0.42
1:N:456:LEU:HD13	1:N:462:PRO:HG2	2.01	0.42
2:2:43:VAL:HG13	2:2:57:LEU:HD12	2.02	0.42
2:P:43:VAL:HG13	2:P:57:LEU:HD12	2.02	0.42
1:B:421:ARG:O	1:B:422:VAL:C	2.63	0.42
1:I:400:LEU:O	1:I:403:THR:OG1	2.34	0.42
1:J:421:ARG:O	1:J:422:VAL:C	2.63	0.42
1:K:451:LEU:HD21	1:K:465:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:456:LEU:HD13	1:M:462:PRO:HG2	2.02	0.42
1:N:33:PRO:HA	1:N:153:ASN:OD1	2.20	0.42
2:X:43:VAL:HG13	2:X:57:LEU:HD12	2.02	0.42
1:A:143:ALA:HA	1:A:146:GLN:HE21	1.85	0.42
1:A:339:GLU:HA	1:A:342:ILE:HD12	2.01	0.42
1:B:288:MET:HE2	1:B:288:MET:HB3	1.98	0.42
1:G:266:THR:HG23	1:G:272:LYS:HG2	2.00	0.42
1:I:451:LEU:HD21	1:I:465:VAL:HG12	2.02	0.42
1:L:151:SER:HB3	1:L:399:ALA:HA	2.02	0.42
1:M:421:ARG:O	1:M:422:VAL:C	2.63	0.42
2:V:14:ARG:NH2	2:V:84:LEU:HD21	2.34	0.42
1:A:486:GLY:C	1:A:491:MET:HE2	2.45	0.42
1:B:77:VAL:HG12	1:B:92:ALA:HB1	2.01	0.42
1:C:151:SER:HB3	1:C:399:ALA:HA	2.02	0.42
1:C:451:LEU:HD21	1:C:465:VAL:HG12	2.02	0.42
1:E:421:ARG:O	1:E:422:VAL:C	2.63	0.42
1:G:143:ALA:HA	1:G:146:GLN:HE21	1.85	0.42
1:G:230:ILE:HG22	2:U:31:ALA:HB2	2.02	0.42
1:H:456:LEU:HD13	1:H:462:PRO:HG2	2.02	0.42
1:K:143:ALA:HA	1:K:146:GLN:HE21	1.85	0.42
1:B:224:ASP:CB	1:B:302:SER:HA	2.50	0.42
1:D:451:LEU:HD21	1:D:465:VAL:HG12	2.01	0.42
1:F:281:PHE:H	1:F:284:ARG:HE	1.68	0.42
1:H:33:PRO:HA	1:H:153:ASN:OD1	2.20	0.42
1:H:224:ASP:CB	1:H:302:SER:HA	2.50	0.42
1:I:456:LEU:HD13	1:I:462:PRO:HG2	2.01	0.42
1:J:451:LEU:HD21	1:J:465:VAL:HG12	2.02	0.42
1:L:456:LEU:HD13	1:L:462:PRO:HG2	2.02	0.42
1:M:451:LEU:HD21	1:M:465:VAL:HG12	2.01	0.42
1:N:16:MET:O	1:N:20:VAL:HG23	2.19	0.42
2:R:68:ASN:ND2	2:S:74:LYS:CE	2.83	0.42
1:A:33:PRO:HA	1:A:153:ASN:OD1	2.20	0.41
1:A:224:ASP:CB	1:A:302:SER:HA	2.50	0.41
1:B:16:MET:O	1:B:20:VAL:HG23	2.19	0.41
1:C:224:ASP:CB	1:C:302:SER:HA	2.50	0.41
1:D:224:ASP:CB	1:D:302:SER:HA	2.50	0.41
1:E:16:MET:O	1:E:20:VAL:HG23	2.19	0.41
1:F:150:ILE:HG23	3:F:600:ADP:C8	2.55	0.41
1:F:451:LEU:HD21	1:F:465:VAL:HG12	2.01	0.41
1:G:224:ASP:CB	1:G:302:SER:HA	2.50	0.41
1:H:233:MET:HB3	1:H:237:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:281:PHE:H	1:I:284:ARG:HE	1.68	0.41
1:K:16:MET:O	1:K:20:VAL:HG23	2.19	0.41
1:L:33:PRO:HA	1:L:153:ASN:OD1	2.20	0.41
1:M:224:ASP:CB	1:M:302:SER:HA	2.50	0.41
1:N:213:VAL:HB	1:N:325:ILE:HG13	2.02	0.41
2:Q:16:GLU:HB3	2:Q:18:GLU:HA	2.02	0.41
2:X:6:LEU:O	2:X:9:ARG:HG2	2.20	0.41
1:A:456:LEU:HD13	1:A:462:PRO:HG2	2.02	0.41
1:C:77:VAL:HG12	1:C:92:ALA:HB1	2.02	0.41
1:D:233:MET:HB3	1:D:237:LEU:HG	2.01	0.41
1:E:224:ASP:CB	1:E:302:SER:HA	2.50	0.41
1:G:233:MET:HB3	1:G:237:LEU:HG	2.01	0.41
1:H:281:PHE:H	1:H:284:ARG:HE	1.68	0.41
1:I:224:ASP:CB	1:I:302:SER:HA	2.50	0.41
1:J:33:PRO:HA	1:J:153:ASN:OD1	2.20	0.41
1:L:209:GLU:O	1:M:351:GLN:OE1	2.37	0.41
1:N:224:ASP:CB	1:N:302:SER:HA	2.50	0.41
1:N:232:GLU:HA	1:N:310:GLU:CG	2.45	0.41
2:1:50:GLU:O	2:2:49:LEU:HD13	2.20	0.41
2:S:14:ARG:NH2	2:S:84:LEU:HD21	2.34	0.41
2:T:6:LEU:O	2:T:9:ARG:HG2	2.20	0.41
1:D:33:PRO:HA	1:D:153:ASN:OD1	2.20	0.41
1:G:33:PRO:HA	1:G:153:ASN:OD1	2.20	0.41
1:H:143:ALA:HA	1:H:146:GLN:HE21	1.85	0.41
1:H:486:GLY:C	1:H:491:MET:HE2	2.44	0.41
1:J:16:MET:O	1:J:20:VAL:HG23	2.19	0.41
1:J:143:ALA:HA	1:J:146:GLN:HE21	1.85	0.41
1:K:151:SER:HB3	1:K:399:ALA:HA	2.01	0.41
1:M:16:MET:O	1:M:20:VAL:HG23	2.19	0.41
1:N:143:ALA:HA	1:N:146:GLN:HE21	1.85	0.41
1:C:456:LEU:HD13	1:C:462:PRO:HG2	2.03	0.41
1:E:77:VAL:HG12	1:E:92:ALA:HB1	2.01	0.41
1:I:339:GLU:HA	1:I:342:ILE:HD12	2.01	0.41
1:J:353:ILE:HD13	1:J:366:GLN:HG2	2.02	0.41
1:L:224:ASP:CB	1:L:302:SER:HA	2.50	0.41
1:L:421:ARG:O	1:L:422:VAL:C	2.63	0.41
2:S:43:VAL:HG13	2:S:57:LEU:HD12	2.02	0.41
1:C:16:MET:O	1:C:20:VAL:HG23	2.19	0.41
1:C:421:ARG:O	1:C:422:VAL:C	2.63	0.41
1:D:143:ALA:HA	1:D:146:GLN:HE21	1.85	0.41
1:E:233:MET:HB3	1:E:237:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:ILE:HG22	1:F:263:VAL:HG11	2.03	0.41
1:J:224:ASP:CB	1:J:302:SER:HA	2.50	0.41
1:L:264:VAL:HG22	1:M:305:ILE:O	2.21	0.41
2:Q:11:ILE:HG12	2:Q:85:ILE:HG12	2.02	0.41
2:R:68:ASN:ND2	2:S:74:LYS:HE3	2.35	0.41
2:X:77:LYS:HE2	2:Y:22:ALA:HA	2.00	0.41
1:C:33:PRO:HA	1:C:153:ASN:OD1	2.20	0.41
1:F:33:PRO:HA	1:F:153:ASN:OD1	2.20	0.41
1:F:224:ASP:CB	1:F:302:SER:HA	2.50	0.41
1:H:451:LEU:HD21	1:H:465:VAL:HG12	2.01	0.41
1:I:150:ILE:HG23	3:I:600:ADP:C8	2.56	0.41
1:I:161:LEU:HD11	1:I:187:LEU:HB2	2.03	0.41
1:L:143:ALA:HA	1:L:146:GLN:HE21	1.85	0.41
1:M:77:VAL:HG12	1:M:92:ALA:HB1	2.01	0.41
1:M:288:MET:HE2	1:M:288:MET:HB3	1.98	0.41
2:P:6:LEU:O	2:P:9:ARG:HG2	2.21	0.41
1:B:33:PRO:HA	1:B:153:ASN:OD1	2.20	0.41
1:B:161:LEU:HD11	1:B:187:LEU:HB2	2.03	0.41
1:E:143:ALA:HA	1:E:146:GLN:HE21	1.85	0.41
1:F:177:VAL:HG11	1:F:396:VAL:CG1	2.49	0.41
1:G:161:LEU:HD11	1:G:187:LEU:HB2	2.03	0.41
1:G:451:LEU:HD21	1:G:465:VAL:HG12	2.01	0.41
1:K:308:GLU:OE2	2:X:29:GLY:HA3	2.20	0.41
1:M:339:GLU:HA	1:M:342:ILE:HD12	2.02	0.41
1:N:421:ARG:O	1:N:422:VAL:C	2.63	0.41
2:O:43:VAL:HG13	2:O:57:LEU:HD12	2.01	0.41
2:V:6:LEU:O	2:V:9:ARG:HG2	2.21	0.41
1:A:455:VAL:HG11	1:A:462:PRO:HA	2.03	0.41
1:E:151:SER:HB3	1:E:399:ALA:HA	2.02	0.41
1:E:353:ILE:HD13	1:E:366:GLN:HG2	2.03	0.41
1:F:151:SER:HB3	1:F:399:ALA:HA	2.03	0.41
1:F:161:LEU:HD11	1:F:187:LEU:HB2	2.03	0.41
1:I:151:SER:HB3	1:I:399:ALA:HA	2.02	0.41
1:K:33:PRO:HA	1:K:153:ASN:OD1	2.21	0.41
1:K:261:THR:HG23	2:Y:28:THR:OG1	2.21	0.41
1:M:33:PRO:HA	1:M:153:ASN:OD1	2.20	0.41
1:M:161:LEU:HD11	1:M:187:LEU:HB2	2.03	0.41
2:U:6:LEU:O	2:U:9:ARG:HG2	2.21	0.41
1:B:151:SER:HB3	1:B:399:ALA:HA	2.02	0.41
1:B:339:GLU:HA	1:B:342:ILE:HD12	2.02	0.41
1:C:69:MET:SD	1:D:41:ASP:HB2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:LEU:O	1:C:403:THR:OG1	2.34	0.41
1:E:33:PRO:HA	1:E:153:ASN:OD1	2.20	0.41
1:F:421:ARG:O	1:F:422:VAL:C	2.63	0.41
1:G:455:VAL:HG21	1:G:465:VAL:HG11	2.03	0.41
1:I:421:ARG:O	1:I:422:VAL:C	2.63	0.41
1:I:455:VAL:HG11	1:I:462:PRO:HA	2.03	0.41
1:J:455:VAL:HG11	1:J:462:PRO:HA	2.03	0.41
1:L:16:MET:O	1:L:20:VAL:HG23	2.19	0.41
1:M:151:SER:HB3	1:M:399:ALA:HA	2.02	0.41
2:Q:6:LEU:O	2:Q:9:ARG:HG2	2.20	0.41
2:T:47:ARG:HH22	2:U:48:ILE:HB	1.86	0.41
2:V:43:VAL:HG13	2:V:57:LEU:HD12	2.03	0.41
2:X:80:ASN:ND2	2:Y:22:ALA:O	2.54	0.41
1:B:33:PRO:HG3	3:B:600:ADP:C6	2.56	0.41
1:B:190:VAL:HG11	1:B:194:GLN:HB3	2.03	0.41
1:B:232:GLU:HA	1:B:310:GLU:CG	2.45	0.41
1:C:143:ALA:HA	1:C:146:GLN:HE21	1.86	0.41
1:H:205:ILE:HA	1:H:213:VAL:HG22	2.03	0.41
2:S:6:LEU:O	2:S:9:ARG:HG2	2.21	0.41
1:A:270:ILE:CD1	2:O:26:VAL:HG23	2.51	0.40
1:F:143:ALA:HA	1:F:146:GLN:HE21	1.86	0.40
1:F:455:VAL:HG11	1:F:462:PRO:HA	2.04	0.40
1:J:400:LEU:O	1:J:403:THR:OG1	2.34	0.40
1:L:400:LEU:O	1:L:403:THR:OG1	2.34	0.40
2:Z:43:VAL:HG13	2:Z:57:LEU:HD12	2.03	0.40
1:B:143:ALA:HA	1:B:146:GLN:HE21	1.86	0.40
1:E:455:VAL:HG11	1:E:462:PRO:HA	2.03	0.40
1:E:456:LEU:HD13	1:E:462:PRO:HG2	2.02	0.40
1:F:261:THR:HG22	2:T:28:THR:N	2.36	0.40
1:F:456:LEU:HD13	1:F:462:PRO:HG2	2.02	0.40
1:I:33:PRO:HA	1:I:153:ASN:OD1	2.20	0.40
1:N:270:ILE:CD1	2:2:26:VAL:HG23	2.50	0.40
2:1:6:LEU:O	2:1:9:ARG:HG2	2.21	0.40
2:T:88:GLU:OE1	2:U:7:HIS:CE1	2.74	0.40
1:A:421:ARG:O	1:A:422:VAL:C	2.63	0.40
1:B:510:VAL:HG23	1:C:385:THR:HG21	2.04	0.40
1:C:237:LEU:HB3	2:Q:25:ILE:HD13	2.03	0.40
1:C:288:MET:HE2	1:C:288:MET:HB3	1.98	0.40
1:E:205:ILE:HA	1:E:213:VAL:HG22	2.04	0.40
1:G:370:ALA:O	1:G:376:VAL:CG2	2.69	0.40
1:N:455:VAL:HG11	1:N:462:PRO:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:HG21	1:A:465:VAL:HG11	2.03	0.40
1:C:281:PHE:H	1:C:284:ARG:HE	1.68	0.40
1:E:177:VAL:HG11	1:E:396:VAL:CG1	2.50	0.40
1:H:151:SER:HB3	1:H:399:ALA:HA	2.02	0.40
1:K:339:GLU:HA	1:K:342:ILE:HD12	2.03	0.40
1:M:455:VAL:HG21	1:M:465:VAL:HG11	2.04	0.40
2:Q:43:VAL:HG13	2:Q:57:LEU:HD12	2.03	0.40
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.04	0.40
1:D:421:ARG:O	1:D:422:VAL:C	2.63	0.40
1:E:261:THR:CG2	2:S:28:THR:OG1	2.70	0.40
1:G:151:SER:HB3	1:G:399:ALA:HA	2.02	0.40
1:L:205:ILE:HA	1:L:213:VAL:HG22	2.03	0.40
1:L:455:VAL:HG21	1:L:465:VAL:HG11	2.04	0.40
1:M:143:ALA:HA	1:M:146:GLN:HE21	1.86	0.40
2:S:16:GLU:HB3	2:S:18:GLU:HA	2.04	0.40
2:Y:43:VAL:HG13	2:Y:57:LEU:HD12	2.03	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:ARG:C	2:Y:79:ASP:OD1[2_454]	1.25	0.95
1:E:430:ARG:CA	2:Y:79:ASP:OD1[2_454]	1.57	0.63
1:E:430:ARG:O	2:Y:79:ASP:OD1[2_454]	1.61	0.59
1:J:429:LEU:CA	2:R:79:ASP:OD1[2_465]	1.71	0.49
1:J:428:ASP:O	2:R:79:ASP:OD2[2_465]	1.84	0.36
1:E:430:ARG:CB	2:Y:79:ASP:OD1[2_454]	1.90	0.30
1:J:428:ASP:O	2:R:79:ASP:OD1[2_465]	2.04	0.16
1:E:430:ARG:C	2:Y:79:ASP:CG[2_454]	2.12	0.08
1:J:429:LEU:N	2:R:79:ASP:OD1[2_465]	2.13	0.07
1:B:207:LYS:NZ	1:M:207:LYS:NZ[3_554]	2.14	0.06
1:J:428:ASP:O	2:R:79:ASP:CG[2_465]	2.14	0.06
1:E:430:ARG:CB	2:Y:79:ASP:OD2[2_454]	2.16	0.04
1:E:430:ARG:N	2:Y:79:ASP:OD1[2_454]	2.17	0.03
1:B:142:LYS:NZ	1:N:130:GLU:OE2[3_554]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	43	71
1	B	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	43	71
1	C	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	43	71
1	D	514/548 (94%)	490 (95%)	22 (4%)	2 (0%)	30	59
1	E	514/548 (94%)	492 (96%)	21 (4%)	1 (0%)	43	71
1	F	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	43	71
1	G	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	43	71
1	H	514/548 (94%)	489 (95%)	24 (5%)	1 (0%)	43	71
1	I	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	43	71
1	J	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	43	71
1	K	514/548 (94%)	491 (96%)	21 (4%)	2 (0%)	30	59
1	L	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	43	71
1	M	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	43	71
1	N	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	43	71
2	1	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5	26
2	2	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5	26
2	O	87/97 (90%)	81 (93%)	4 (5%)	2 (2%)	5	26
2	P	88/97 (91%)	82 (93%)	4 (4%)	2 (2%)	5	26
2	Q	83/97 (86%)	77 (93%)	4 (5%)	2 (2%)	4	25
2	R	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5	26
2	S	86/97 (89%)	81 (94%)	3 (4%)	2 (2%)	5	26
2	T	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5	26
2	U	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5	26
2	V	87/97 (90%)	81 (93%)	4 (5%)	2 (2%)	5	26
2	W	87/97 (90%)	81 (93%)	4 (5%)	2 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	X	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5 26
2	Y	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5 26
2	Z	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	5 26
All	All	8402/9030 (93%)	7989 (95%)	369 (4%)	44 (0%)	24 55

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	22	ALA
2	W	29	GLY
2	Y	22	ALA
2	1	22	ALA
2	2	22	ALA
2	O	22	ALA
2	P	22	ALA
2	Q	22	ALA
2	R	22	ALA
2	S	22	ALA
2	T	22	ALA
2	V	22	ALA
2	W	22	ALA
2	X	22	ALA
2	Z	22	ALA
1	D	203	TYR
1	K	203	TYR
2	T	29	GLY
1	A	205	ILE
1	B	205	ILE
1	C	205	ILE
1	D	205	ILE
1	E	205	ILE
1	F	205	ILE
1	G	205	ILE
1	H	205	ILE
1	I	205	ILE
1	J	205	ILE
1	K	205	ILE
1	L	205	ILE
1	M	205	ILE
1	N	205	ILE
2	Z	29	GLY

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Mol	Chain	Res	Type
2	O	29	GLY
2	Q	29	GLY
2	1	29	GLY
2	2	29	GLY
2	P	29	GLY
2	R	29	GLY
2	S	29	GLY
2	U	29	GLY
2	X	29	GLY
2	Y	29	GLY
2	V	29	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/416 (97%)	401 (99%)	3 (1%)	76	75
1	B	404/416 (97%)	403 (100%)	1 (0%)	87	84
1	C	404/416 (97%)	402 (100%)	2 (0%)	81	78
1	D	404/416 (97%)	402 (100%)	2 (0%)	81	78
1	E	404/416 (97%)	402 (100%)	2 (0%)	81	78
1	F	404/416 (97%)	403 (100%)	1 (0%)	87	84
1	G	404/416 (97%)	402 (100%)	2 (0%)	81	78
1	H	404/416 (97%)	400 (99%)	4 (1%)	68	72
1	I	404/416 (97%)	402 (100%)	2 (0%)	81	78
1	J	404/416 (97%)	402 (100%)	2 (0%)	81	78
1	K	404/416 (97%)	401 (99%)	3 (1%)	76	75
1	L	404/416 (97%)	403 (100%)	1 (0%)	87	84
1	M	404/416 (97%)	401 (99%)	3 (1%)	76	75
1	N	404/416 (97%)	402 (100%)	2 (0%)	81	78
2	1	77/80 (96%)	76 (99%)	1 (1%)	61	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	77/80 (96%)	77 (100%)	0	100	100
2	O	78/80 (98%)	76 (97%)	2 (3%)	40	58
2	P	78/80 (98%)	76 (97%)	2 (3%)	40	58
2	Q	75/80 (94%)	74 (99%)	1 (1%)	61	69
2	R	76/80 (95%)	75 (99%)	1 (1%)	61	69
2	S	77/80 (96%)	76 (99%)	1 (1%)	61	69
2	T	77/80 (96%)	75 (97%)	2 (3%)	40	58
2	U	76/80 (95%)	75 (99%)	1 (1%)	61	69
2	V	77/80 (96%)	75 (97%)	2 (3%)	40	58
2	W	77/80 (96%)	76 (99%)	1 (1%)	61	69
2	X	77/80 (96%)	76 (99%)	1 (1%)	61	69
2	Y	77/80 (96%)	76 (99%)	1 (1%)	61	69
2	Z	77/80 (96%)	76 (99%)	1 (1%)	61	69
All	All	6732/6944 (97%)	6685 (99%)	47 (1%)	76	75

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	A	321	LYS
1	A	369	VAL
1	B	369	VAL
1	C	321	LYS
1	C	369	VAL
1	D	321	LYS
1	D	369	VAL
1	E	105	LYS
1	E	369	VAL
1	F	321	LYS
1	G	321	LYS
1	G	369	VAL
1	H	137	PRO
1	H	171	LYS
1	H	321	LYS
1	H	369	VAL
1	I	321	LYS
1	I	369	VAL

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Mol	Chain	Res	Type
1	J	321	LYS
1	J	369	VAL
1	K	321	LYS
1	K	338	GLU
1	K	369	VAL
1	L	369	VAL
1	M	105	LYS
1	M	321	LYS
1	M	369	VAL
1	N	321	LYS
1	N	369	VAL
2	1	6	LEU
2	O	1	MET
2	O	6	LEU
2	P	1	MET
2	P	6	LEU
2	Q	6	LEU
2	R	6	LEU
2	S	6	LEU
2	T	6	LEU
2	T	47	ARG
2	U	6	LEU
2	V	6	LEU
2	V	13	LYS
2	W	6	LEU
2	X	6	LEU
2	Y	6	LEU
2	Z	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	37	ASN
1	A	146	GLN
1	A	348	GLN
1	A	366	GLN
1	A	453	GLN
1	A	457	ASN
1	B	21	ASN
1	B	37	ASN
1	B	146	GLN

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Mol	Chain	Res	Type
1	B	348	GLN
1	B	366	GLN
1	B	457	ASN
1	C	21	ASN
1	C	37	ASN
1	C	72	GLN
1	C	146	GLN
1	C	348	GLN
1	C	366	GLN
1	C	457	ASN
1	D	21	ASN
1	D	37	ASN
1	D	146	GLN
1	D	348	GLN
1	D	366	GLN
1	D	457	ASN
1	E	21	ASN
1	E	37	ASN
1	E	146	GLN
1	E	348	GLN
1	E	366	GLN
1	E	457	ASN
1	F	21	ASN
1	F	37	ASN
1	F	72	GLN
1	F	146	GLN
1	F	194	GLN
1	F	348	GLN
1	F	366	GLN
1	F	453	GLN
1	F	457	ASN
1	G	21	ASN
1	G	37	ASN
1	G	72	GLN
1	G	146	GLN
1	G	348	GLN
1	G	366	GLN
1	G	453	GLN
1	G	457	ASN
1	H	21	ASN
1	H	37	ASN
1	H	72	GLN

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Mol	Chain	Res	Type
1	H	146	GLN
1	H	348	GLN
1	H	366	GLN
1	H	453	GLN
1	H	457	ASN
1	I	21	ASN
1	I	37	ASN
1	I	72	GLN
1	I	146	GLN
1	I	194	GLN
1	I	348	GLN
1	I	366	GLN
1	I	453	GLN
1	I	457	ASN
1	J	21	ASN
1	J	37	ASN
1	J	72	GLN
1	J	146	GLN
1	J	319	GLN
1	J	348	GLN
1	J	366	GLN
1	J	457	ASN
1	K	21	ASN
1	K	37	ASN
1	K	146	GLN
1	K	348	GLN
1	K	366	GLN
1	K	457	ASN
1	L	21	ASN
1	L	37	ASN
1	L	146	GLN
1	L	348	GLN
1	L	366	GLN
1	L	457	ASN
1	M	21	ASN
1	M	37	ASN
1	M	146	GLN
1	M	348	GLN
1	M	366	GLN
1	M	457	ASN
1	N	21	ASN
1	N	37	ASN

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Mol	Chain	Res	Type
1	N	146	GLN
1	N	348	GLN
1	N	366	GLN
1	N	453	GLN
1	N	457	ASN
2	1	45	ASN
2	2	45	ASN
2	2	68	ASN
2	O	7	HIS
2	O	45	ASN
2	O	68	ASN
2	P	7	HIS
2	P	45	ASN
2	P	68	ASN
2	Q	7	HIS
2	Q	45	ASN
2	Q	68	ASN
2	R	45	ASN
2	R	68	ASN
2	S	45	ASN
2	S	68	ASN
2	T	7	HIS
2	T	45	ASN
2	T	51	ASN
2	T	68	ASN
2	U	7	HIS
2	U	45	ASN
2	U	68	ASN
2	V	7	HIS
2	V	45	ASN
2	V	51	ASN
2	V	68	ASN
2	W	7	HIS
2	W	45	ASN
2	W	68	ASN
2	X	45	ASN
2	X	68	ASN
2	Y	45	ASN
2	Y	68	ASN
2	Z	45	ASN
2	Z	68	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	D	600	6,5,4	28,29,29	1.43	4 (14%)	43,45,45	2.02	15 (34%)
3	ADP	E	600	6,5,4	28,29,29	1.44	5 (17%)	43,45,45	2.17	17 (39%)
3	ADP	B	600	6,5,4	28,29,29	1.59	5 (17%)	43,45,45	2.01	16 (37%)
3	ADP	J	600	6,5,4	28,29,29	1.46	5 (17%)	43,45,45	1.97	18 (41%)
5	BEF	N	602	3	0,3,3	-	-	-		
3	ADP	A	600	6,5,4	28,29,29	1.27	5 (17%)	43,45,45	2.37	15 (34%)
3	ADP	N	600	6,5,4	28,29,29	1.52	4 (14%)	43,45,45	1.96	13 (30%)
5	BEF	C	602	3	0,3,3	-	-	-		
5	BEF	I	602	3	0,3,3	-	-	-		
5	BEF	F	602	3	0,3,3	-	-	-		
5	BEF	H	602	3	0,3,3	-	-	-		
5	BEF	K	602	3	0,3,3	-	-	-		
5	BEF	E	602	3	0,3,3	-	-	-		
5	BEF	B	602	3	0,3,3	-	-	-		
3	ADP	C	600	6,5,4	28,29,29	1.39	6 (21%)	43,45,45	1.90	14 (32%)
3	ADP	I	600	6,5,4	28,29,29	1.39	4 (14%)	43,45,45	2.05	16 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BEF	A	602	3	0,3,3	-	-	-		
3	ADP	L	600	6,5,4	28,29,29	1.41	4 (14%)	43,45,45	2.11	18 (41%)
5	BEF	G	602	3	0,3,3	-	-	-		
5	BEF	D	602	3	0,3,3	-	-	-		
5	BEF	J	602	3	0,3,3	-	-	-		
3	ADP	H	600	6,5,4	28,29,29	1.45	3 (10%)	43,45,45	2.00	15 (34%)
3	ADP	G	600	6,5,4	28,29,29	1.59	5 (17%)	43,45,45	2.03	17 (39%)
3	ADP	K	600	6,5,4	28,29,29	1.45	6 (21%)	43,45,45	2.15	16 (37%)
5	BEF	L	602	3	0,3,3	-	-	-		
5	BEF	M	602	3	0,3,3	-	-	-		
3	ADP	F	600	6,5,4	28,29,29	1.38	5 (17%)	43,45,45	2.03	16 (37%)
3	ADP	M	600	6,5,4	28,29,29	1.35	4 (14%)	43,45,45	2.26	20 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	H	600	6,5,4	-	6/16/32/32	0/3/3/3
3	ADP	D	600	6,5,4	-	7/16/32/32	0/3/3/3
3	ADP	E	600	6,5,4	-	7/16/32/32	0/3/3/3
3	ADP	B	600	6,5,4	-	6/16/32/32	0/3/3/3
3	ADP	J	600	6,5,4	-	5/16/32/32	0/3/3/3
3	ADP	C	600	6,5,4	-	6/16/32/32	0/3/3/3
3	ADP	I	600	6,5,4	-	6/16/32/32	0/3/3/3
3	ADP	G	600	6,5,4	-	7/16/32/32	0/3/3/3
3	ADP	F	600	6,5,4	-	7/16/32/32	0/3/3/3
3	ADP	A	600	6,5,4	-	7/16/32/32	0/3/3/3
3	ADP	K	600	6,5,4	-	6/16/32/32	0/3/3/3
3	ADP	M	600	6,5,4	-	6/16/32/32	0/3/3/3
3	ADP	L	600	6,5,4	-	7/16/32/32	0/3/3/3
3	ADP	N	600	6,5,4	-	7/16/32/32	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	600	ADP	C4-N9	-4.57	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	600	ADP	C4-N9	-4.31	1.28	1.37
3	E	600	ADP	C4-N9	-4.31	1.28	1.37
3	B	600	ADP	C5-C4	4.31	1.46	1.39
3	D	600	ADP	C5-C4	4.16	1.46	1.39
3	G	600	ADP	C4-N9	-4.14	1.29	1.37
3	G	600	ADP	C5-C4	4.14	1.46	1.39
3	H	600	ADP	C4-N9	-4.11	1.29	1.37
3	J	600	ADP	C4-N9	-4.01	1.29	1.37
3	B	600	ADP	C4-N9	-3.97	1.29	1.37
3	N	600	ADP	C5-C4	3.97	1.46	1.39
3	M	600	ADP	C4-N9	-3.93	1.29	1.37
3	F	600	ADP	C4-N9	-3.88	1.29	1.37
3	L	600	ADP	C5-C4	3.82	1.45	1.39
3	C	600	ADP	C4-N9	-3.76	1.29	1.37
3	K	600	ADP	C5-C4	3.74	1.45	1.39
3	J	600	ADP	C5-C4	3.67	1.45	1.39
3	H	600	ADP	C5-C4	3.58	1.45	1.39
3	D	600	ADP	C4-N9	-3.55	1.30	1.37
3	L	600	ADP	C4-N9	-3.52	1.30	1.37
3	F	600	ADP	C5-C4	3.50	1.45	1.39
3	C	600	ADP	C5-C4	3.34	1.45	1.39
3	A	600	ADP	C4-N9	-3.17	1.31	1.37
3	K	600	ADP	C4-N9	-3.15	1.31	1.37
3	H	600	ADP	C5-N7	-2.91	1.33	1.39
3	I	600	ADP	C5-C4	2.85	1.44	1.39
3	M	600	ADP	C5-C4	2.81	1.44	1.39
3	A	600	ADP	C5-C6	2.71	1.48	1.41
3	B	600	ADP	C5-N7	-2.67	1.34	1.39
3	F	600	ADP	C8-N7	2.65	1.36	1.31
3	E	600	ADP	C5-C4	2.65	1.43	1.39
3	G	600	ADP	C8-N7	2.61	1.36	1.31
3	J	600	ADP	C5-N7	-2.59	1.34	1.39
3	A	600	ADP	C5-C4	2.59	1.43	1.39
3	K	600	ADP	PA-O3A	2.58	1.62	1.59
3	K	600	ADP	C5-C6	2.54	1.48	1.41
3	G	600	ADP	C5-C6	2.53	1.48	1.41
3	C	600	ADP	C5-N7	-2.53	1.34	1.39
3	E	600	ADP	C5-N7	-2.52	1.34	1.39
3	D	600	ADP	C5-C6	2.49	1.47	1.41
3	A	600	ADP	C8-N7	2.47	1.36	1.31
3	E	600	ADP	C5-C6	2.46	1.47	1.41
3	L	600	ADP	C8-N7	2.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	600	ADP	C5-C6	2.38	1.47	1.41
3	A	600	ADP	C8-N9	-2.37	1.33	1.37
3	B	600	ADP	C8-N7	2.36	1.36	1.31
3	N	600	ADP	C5-C6	2.33	1.47	1.41
3	M	600	ADP	C5-C6	2.30	1.47	1.41
3	I	600	ADP	C5-N7	-2.27	1.34	1.39
3	C	600	ADP	C8-N7	2.24	1.36	1.31
3	K	600	ADP	C8-N7	2.18	1.35	1.31
3	J	600	ADP	PA-O3A	2.17	1.61	1.59
3	J	600	ADP	C8-N7	2.15	1.35	1.31
3	G	600	ADP	C5-N7	-2.13	1.35	1.39
3	E	600	ADP	C8-N9	-2.11	1.34	1.37
3	M	600	ADP	C5-N7	-2.11	1.35	1.39
3	D	600	ADP	C8-N7	2.11	1.35	1.31
3	B	600	ADP	PA-O3A	2.07	1.61	1.59
3	I	600	ADP	C5-C6	2.06	1.46	1.41
3	K	600	ADP	C5-N7	-2.06	1.35	1.39
3	F	600	ADP	C5-C6	2.06	1.46	1.41
3	C	600	ADP	C5-C6	2.06	1.46	1.41
3	C	600	ADP	C8-N9	-2.02	1.34	1.37
3	N	600	ADP	C2-N1	2.01	1.37	1.33
3	F	600	ADP	C5-N7	-2.00	1.35	1.39

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	600	ADP	C4-N9-C8	5.79	111.82	105.74
3	N	600	ADP	C4-N9-C8	5.76	111.78	105.74
3	E	600	ADP	C4-N9-C8	5.52	111.54	105.74
3	A	600	ADP	C5-C4-N3	-5.22	119.53	126.72
3	B	600	ADP	N3-C2-N1	-5.10	120.86	128.58
3	D	600	ADP	C4-N9-C8	5.07	111.06	105.74
3	A	600	ADP	C4-N9-C8	4.94	110.93	105.74
3	L	600	ADP	N3-C2-N1	-4.72	121.44	128.58
3	G	600	ADP	N3-C2-N1	-4.71	121.46	128.58
3	J	600	ADP	N3-C2-N1	-4.67	121.51	128.58
3	K	600	ADP	C4-N9-C8	4.66	110.63	105.74
3	I	600	ADP	C4-N9-C8	4.66	110.63	105.74
3	M	600	ADP	N3-C2-N1	-4.56	121.68	128.58
3	A	600	ADP	C4-C5-N7	-4.56	105.37	110.58
3	E	600	ADP	N3-C2-N1	-4.52	121.74	128.58
3	A	600	ADP	C2-N3-C4	4.41	122.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	600	ADP	N3-C2-N1	-4.37	121.96	128.58
3	I	600	ADP	N3-C2-N1	-4.34	122.02	128.58
3	L	600	ADP	C4-N9-C8	4.31	110.27	105.74
3	A	600	ADP	N3-C2-N1	-4.27	122.12	128.58
3	A	600	ADP	N9-C8-N7	-4.27	107.89	113.94
3	F	600	ADP	N3-C2-N1	-4.22	122.19	128.58
3	H	600	ADP	C4-N9-C8	4.18	110.13	105.74
3	H	600	ADP	N3-C2-N1	-4.12	122.34	128.58
3	D	600	ADP	N3-C2-N1	-4.08	122.40	128.58
3	K	600	ADP	C5-C4-N3	-4.06	121.13	126.72
3	K	600	ADP	N3-C2-N1	-3.97	122.57	128.58
3	C	600	ADP	C4-N9-C8	3.96	109.89	105.74
3	G	600	ADP	C2-N3-C4	3.95	121.48	111.83
3	A	600	ADP	C6-C5-N7	3.89	139.59	132.09
3	J	600	ADP	C4-N9-C8	3.88	109.81	105.74
3	E	600	ADP	C4-N9-C1'	-3.79	117.77	126.63
3	L	600	ADP	C2-N3-C4	3.78	121.07	111.83
3	K	600	ADP	C4-C5-N7	-3.78	106.26	110.58
3	E	600	ADP	C2-N3-C4	3.75	120.98	111.83
3	M	600	ADP	N9-C8-N7	-3.70	108.68	113.94
3	M	600	ADP	C2-N3-C4	3.69	120.84	111.83
3	G	600	ADP	C5-C4-N3	-3.68	121.65	126.72
3	A	600	ADP	N3-C4-N9	3.67	133.41	127.17
3	B	600	ADP	C4-N9-C8	3.65	109.57	105.74
3	I	600	ADP	C2-N3-C4	3.63	120.70	111.83
3	F	600	ADP	C4-N9-C8	3.62	109.54	105.74
3	E	600	ADP	N9-C8-N7	-3.60	108.83	113.94
3	C	600	ADP	C2-N3-C4	3.59	120.61	111.83
3	F	600	ADP	C4-N9-C1'	-3.54	118.36	126.63
3	K	600	ADP	C2-N3-C4	3.51	120.41	111.83
3	M	600	ADP	C4-N9-C1'	-3.50	118.45	126.63
3	F	600	ADP	C2-N3-C4	3.46	120.28	111.83
3	K	600	ADP	N9-C8-N7	-3.44	109.05	113.94
3	C	600	ADP	C5-C4-N3	-3.43	121.99	126.72
3	A	600	ADP	C5-N7-C8	3.38	108.77	103.45
3	J	600	ADP	C2-N3-C4	3.38	120.08	111.83
3	F	600	ADP	C2'-C3'-C4'	3.38	109.13	102.61
3	D	600	ADP	C4-N9-C1'	-3.36	118.76	126.63
3	B	600	ADP	N6-C6-N1	3.36	125.86	118.38
3	M	600	ADP	N3-C4-N9	3.33	132.83	127.17
3	K	600	ADP	N3-C4-N9	3.30	132.78	127.17
3	I	600	ADP	C4-N9-C1'	-3.27	118.98	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	ADP	C2-N3-C4	3.27	119.81	111.83
3	D	600	ADP	N3-C4-N9	3.26	132.71	127.17
3	L	600	ADP	C4-N9-C1'	-3.25	119.02	126.63
3	L	600	ADP	C6-C5-N7	3.25	138.36	132.09
3	G	600	ADP	C4-N9-C1'	-3.23	119.07	126.63
3	D	600	ADP	C2-N3-C4	3.21	119.67	111.83
3	M	600	ADP	C5-C4-N3	-3.21	122.30	126.72
3	F	600	ADP	C6-C5-N7	3.20	138.26	132.09
3	L	600	ADP	C5-C4-N3	-3.20	122.31	126.72
3	E	600	ADP	C6-C5-N7	3.18	138.21	132.09
3	E	600	ADP	C2'-C3'-C4'	3.17	108.73	102.61
3	N	600	ADP	C4-N9-C1'	-3.17	119.23	126.63
3	B	600	ADP	C4-N9-C1'	-3.16	119.24	126.63
3	G	600	ADP	C6-C5-N7	3.15	138.16	132.09
3	C	600	ADP	N3-C4-N9	3.14	132.50	127.17
3	N	600	ADP	N3-C4-N9	3.13	132.49	127.17
3	J	600	ADP	C4-N9-C1'	-3.13	119.32	126.63
3	B	600	ADP	C2-N1-C6	3.12	123.86	118.73
3	E	600	ADP	O5'-C5'-C4'	3.12	119.62	108.99
3	G	600	ADP	C4-N9-C8	3.11	109.00	105.74
3	H	600	ADP	N6-C6-N1	3.10	125.28	118.38
3	A	600	ADP	C4-N9-C1'	-3.10	119.38	126.63
3	G	600	ADP	O5'-C5'-C4'	3.08	119.48	108.99
3	K	600	ADP	C6-C5-N7	3.06	138.00	132.09
3	F	600	ADP	C5-C4-N3	-3.03	122.54	126.72
3	I	600	ADP	N3-C4-N9	3.01	132.29	127.17
3	I	600	ADP	C5-C4-N3	-3.00	122.59	126.72
3	N	600	ADP	N9-C8-N7	-2.99	109.69	113.94
3	L	600	ADP	N3-C4-N9	2.98	132.24	127.17
3	E	600	ADP	C5-C4-N3	-2.97	122.63	126.72
3	H	600	ADP	O3A-PA-O1A	-2.94	101.85	110.70
3	E	600	ADP	N3-C4-N9	2.93	132.16	127.17
3	H	600	ADP	C2-N3-C4	2.93	118.98	111.83
3	H	600	ADP	N3-C4-N9	2.93	132.14	127.17
3	F	600	ADP	C6-C5-C4	-2.92	113.19	117.18
3	F	600	ADP	O5'-C5'-C4'	2.91	118.91	108.99
3	B	600	ADP	C5-C6-N6	-2.88	116.15	123.29
3	K	600	ADP	C4-N9-C1'	-2.88	119.90	126.63
3	I	600	ADP	O3A-PA-O1A	-2.88	102.04	110.70
3	N	600	ADP	O3'-C3'-C2'	-2.88	102.59	111.82
3	K	600	ADP	C5-N7-C8	2.87	107.97	103.45
3	M	600	ADP	C6-C5-N7	2.87	137.62	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	600	ADP	C2'-C3'-C4'	2.87	108.15	102.61
3	J	600	ADP	N6-C6-N1	2.83	124.68	118.38
3	L	600	ADP	C6-C5-C4	-2.83	113.31	117.18
3	H	600	ADP	C2'-C3'-C4'	2.82	108.06	102.61
3	M	600	ADP	O3A-PA-O1A	-2.80	102.27	110.70
3	C	600	ADP	C4-N9-C1'	-2.79	120.10	126.63
3	L	600	ADP	O3A-PA-O1A	-2.78	102.33	110.70
3	A	600	ADP	O4'-C1'-N9	2.77	113.42	108.09
3	H	600	ADP	C4-N9-C1'	-2.77	120.16	126.63
3	B	600	ADP	O4'-C1'-N9	2.76	113.38	108.09
3	D	600	ADP	C5-C4-N3	-2.75	122.93	126.72
3	B	600	ADP	N3-C4-N9	2.75	131.85	127.17
3	N	600	ADP	C5-C4-N3	-2.74	122.94	126.72
3	G	600	ADP	N3-C4-N9	2.74	131.83	127.17
3	D	600	ADP	C6-C5-N7	2.73	137.35	132.09
3	K	600	ADP	O4'-C1'-N9	2.71	113.29	108.09
3	L	600	ADP	O5'-C5'-C4'	2.69	118.16	108.99
3	M	600	ADP	O5'-C5'-C4'	2.67	118.08	108.99
3	K	600	ADP	O5'-C5'-C4'	2.66	118.06	108.99
3	I	600	ADP	C6-C5-N7	2.65	137.20	132.09
3	J	600	ADP	O5'-C5'-C4'	2.62	117.91	108.99
3	H	600	ADP	C5-C4-N3	-2.61	123.12	126.72
3	L	600	ADP	N9-C8-N7	-2.61	110.23	113.94
3	H	600	ADP	O3A-PB-O1B	-2.61	97.32	111.04
3	C	600	ADP	C6-C5-N7	2.60	137.09	132.09
3	J	600	ADP	N3-C4-N9	2.59	131.58	127.17
3	J	600	ADP	C5-C4-N3	-2.59	123.16	126.72
3	H	600	ADP	C2-N1-C6	2.57	122.95	118.73
3	G	600	ADP	C2'-C3'-C4'	2.55	107.54	102.61
3	A	600	ADP	O5'-C5'-C4'	2.54	117.65	108.99
3	N	600	ADP	C2'-C3'-C4'	2.53	107.50	102.61
3	N	600	ADP	O3A-PB-O1B	-2.53	97.75	111.04
3	G	600	ADP	C6-C5-C4	-2.52	113.74	117.18
3	J	600	ADP	C2-N1-C6	2.52	122.87	118.73
3	I	600	ADP	O3A-PB-O1B	-2.52	97.80	111.04
3	I	600	ADP	C6-C5-C4	-2.51	113.74	117.18
3	D	600	ADP	C6-C5-C4	-2.51	113.75	117.18
3	J	600	ADP	O4'-C1'-N9	2.51	112.91	108.09
3	D	600	ADP	N9-C8-N7	-2.51	110.38	113.94
3	J	600	ADP	C5-C6-N6	-2.51	117.08	123.29
3	L	600	ADP	C5-C6-N6	-2.50	117.10	123.29
3	H	600	ADP	C5-C6-N6	-2.50	117.11	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	600	ADP	O4'-C1'-N9	2.49	112.87	108.09
3	H	600	ADP	O5'-C5'-C4'	2.48	117.44	108.99
3	G	600	ADP	C5-C6-N6	-2.48	117.15	123.29
3	E	600	ADP	C4-C5-N7	-2.47	107.76	110.58
3	D	600	ADP	O5'-C5'-C4'	2.47	117.40	108.99
3	I	600	ADP	C5-C6-N6	-2.46	117.20	123.29
3	K	600	ADP	O3A-PA-O1A	-2.46	103.31	110.70
3	I	600	ADP	O3'-C3'-C2'	-2.45	103.95	111.82
3	K	600	ADP	C3'-C2'-C1'	2.45	106.09	101.46
3	D	600	ADP	N6-C6-N1	2.45	123.83	118.38
3	J	600	ADP	C6-C5-N7	2.43	136.78	132.09
3	M	600	ADP	O2A-PA-O1A	2.43	123.76	112.44
3	F	600	ADP	N3-C4-N9	2.41	131.27	127.17
3	M	600	ADP	C4-C5-N7	-2.41	107.83	110.58
3	N	600	ADP	N6-C6-N1	2.38	123.69	118.38
3	C	600	ADP	C5-C6-N6	-2.38	117.39	123.29
3	N	600	ADP	C2'-C1'-N9	-2.38	107.39	113.30
3	J	600	ADP	C3'-C2'-C1'	2.37	105.95	101.46
3	D	600	ADP	C5-C6-N6	-2.37	117.42	123.29
3	M	600	ADP	N6-C6-N1	2.37	123.66	118.38
3	N	600	ADP	O3A-PA-O1A	-2.37	103.58	110.70
3	B	600	ADP	O5'-C5'-C4'	2.36	117.03	108.99
3	M	600	ADP	C3'-C2'-C1'	2.35	105.92	101.46
3	B	600	ADP	C5-C4-N3	-2.35	123.48	126.72
3	I	600	ADP	N9-C8-N7	-2.35	110.61	113.94
3	B	600	ADP	C6-C5-C4	-2.34	113.98	117.18
3	E	600	ADP	O4'-C1'-N9	2.34	112.59	108.09
3	L	600	ADP	C2'-C3'-C4'	2.33	107.10	102.61
3	C	600	ADP	N6-C6-N1	2.32	123.53	118.38
3	E	600	ADP	C6-C5-C4	-2.31	114.03	117.18
3	D	600	ADP	C2-N1-C6	2.30	122.50	118.73
3	A	600	ADP	C3'-C2'-C1'	2.29	105.80	101.46
3	F	600	ADP	C5-C6-N6	-2.28	117.63	123.29
3	H	600	ADP	O4'-C1'-N9	2.28	112.47	108.09
3	K	600	ADP	C2-N1-C6	2.27	122.46	118.73
3	F	600	ADP	O3'-C3'-C2'	-2.25	104.61	111.82
3	N	600	ADP	C4-C5-N7	-2.25	108.01	110.58
3	F	600	ADP	N9-C8-N7	-2.25	110.75	113.94
3	F	600	ADP	C1'-N9-C8	2.24	132.07	127.09
3	D	600	ADP	C2'-C3'-C4'	2.24	106.94	102.61
3	G	600	ADP	N6-C6-N1	2.24	123.37	118.38
3	J	600	ADP	C6-C5-C4	-2.23	114.13	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	ADP	O2A-PA-O1A	2.23	122.80	112.44
3	E	600	ADP	N6-C6-N1	2.21	123.31	118.38
3	L	600	ADP	N6-C6-N1	2.21	123.29	118.38
3	I	600	ADP	N6-C6-N1	2.20	123.27	118.38
3	J	600	ADP	O3A-PB-O1B	-2.19	99.52	111.04
3	G	600	ADP	C1'-N9-C8	2.18	131.93	127.09
3	G	600	ADP	C4-C5-N7	-2.17	108.10	110.58
3	B	600	ADP	C3'-C2'-C1'	2.17	105.57	101.46
3	A	600	ADP	O2'-C2'-C1'	-2.17	102.64	110.10
3	A	600	ADP	O2B-PB-O3A	-2.17	97.36	104.64
3	M	600	ADP	C5-C6-N6	-2.17	117.92	123.29
3	D	600	ADP	C3'-C2'-C1'	2.15	105.53	101.46
3	F	600	ADP	C4'-O4'-C1'	2.14	114.19	109.47
3	M	600	ADP	C5-N7-C8	2.13	106.80	103.45
3	L	600	ADP	C2-N1-C6	2.12	122.22	118.73
3	M	600	ADP	C2-N1-C6	2.12	122.22	118.73
3	J	600	ADP	O2A-PA-O1A	2.12	122.28	112.44
3	G	600	ADP	O2A-PA-O1A	2.11	122.28	112.44
3	M	600	ADP	C2'-C3'-C4'	2.11	106.69	102.61
3	G	600	ADP	C3'-C2'-C1'	2.11	105.46	101.46
3	L	600	ADP	O2A-PA-O1A	2.11	122.25	112.44
3	N	600	ADP	C2-N3-C4	2.10	116.96	111.83
3	H	600	ADP	C2'-C1'-N9	-2.09	108.10	113.30
3	C	600	ADP	N9-C8-N7	-2.09	110.97	113.94
3	E	600	ADP	C5-C6-N6	-2.09	118.11	123.29
3	B	600	ADP	C6-C5-N7	2.09	136.12	132.09
3	C	600	ADP	O5'-C5'-C4'	2.09	116.11	108.99
3	L	600	ADP	C3'-C2'-C1'	2.09	105.41	101.46
3	G	600	ADP	C2-N1-C6	2.09	122.16	118.73
3	C	600	ADP	C3'-C2'-C1'	2.08	105.40	101.46
3	I	600	ADP	O2A-PA-O1A	2.06	122.05	112.44
3	M	600	ADP	O2A-PA-O3A	2.06	112.85	107.27
3	K	600	ADP	N6-C6-N1	2.06	122.97	118.38
3	C	600	ADP	C6-C5-C4	-2.05	114.37	117.18
3	L	600	ADP	O4'-C1'-N9	2.05	112.02	108.09
3	E	600	ADP	C5-N7-C8	2.05	106.67	103.45
3	F	600	ADP	O4'-C1'-N9	2.04	112.01	108.09
3	J	600	ADP	N9-C8-N7	-2.02	111.06	113.94
3	C	600	ADP	O2A-PA-O1A	2.02	121.85	112.44
3	J	600	ADP	O2'-C2'-C1'	-2.02	103.15	110.10
3	B	600	ADP	O2'-C2'-C1'	-2.01	103.18	110.10
3	E	600	ADP	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	ADP	C5'-O5'-PA-O1A
3	A	600	ADP	C5'-O5'-PA-O2A
3	A	600	ADP	C5'-O5'-PA-O3A
3	B	600	ADP	PA-O3A-PB-O3B
3	B	600	ADP	C5'-O5'-PA-O1A
3	B	600	ADP	C5'-O5'-PA-O2A
3	B	600	ADP	C5'-O5'-PA-O3A
3	C	600	ADP	PA-O3A-PB-O3B
3	C	600	ADP	C5'-O5'-PA-O1A
3	C	600	ADP	C5'-O5'-PA-O2A
3	C	600	ADP	C5'-O5'-PA-O3A
3	D	600	ADP	C5'-O5'-PA-O1A
3	D	600	ADP	C5'-O5'-PA-O2A
3	D	600	ADP	C5'-O5'-PA-O3A
3	E	600	ADP	C5'-O5'-PA-O1A
3	E	600	ADP	C5'-O5'-PA-O2A
3	E	600	ADP	C5'-O5'-PA-O3A
3	F	600	ADP	C5'-O5'-PA-O1A
3	F	600	ADP	C5'-O5'-PA-O2A
3	F	600	ADP	C5'-O5'-PA-O3A
3	G	600	ADP	C5'-O5'-PA-O1A
3	G	600	ADP	C5'-O5'-PA-O2A
3	G	600	ADP	C5'-O5'-PA-O3A
3	H	600	ADP	PA-O3A-PB-O2B
3	H	600	ADP	C5'-O5'-PA-O1A
3	H	600	ADP	C5'-O5'-PA-O3A
3	I	600	ADP	PA-O3A-PB-O2B
3	I	600	ADP	C5'-O5'-PA-O1A
3	I	600	ADP	C5'-O5'-PA-O2A
3	I	600	ADP	C5'-O5'-PA-O3A
3	J	600	ADP	PA-O3A-PB-O2B
3	J	600	ADP	C5'-O5'-PA-O1A
3	J	600	ADP	C5'-O5'-PA-O2A
3	J	600	ADP	C5'-O5'-PA-O3A
3	K	600	ADP	PA-O3A-PB-O2B
3	K	600	ADP	C5'-O5'-PA-O1A
3	K	600	ADP	C5'-O5'-PA-O3A
3	L	600	ADP	PA-O3A-PB-O2B
3	L	600	ADP	C5'-O5'-PA-O1A
3	L	600	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	M	600	ADP	PA-O3A-PB-O2B
3	M	600	ADP	C5'-O5'-PA-O1A
3	M	600	ADP	C5'-O5'-PA-O2A
3	M	600	ADP	C5'-O5'-PA-O3A
3	N	600	ADP	PA-O3A-PB-O2B
3	N	600	ADP	C5'-O5'-PA-O1A
3	N	600	ADP	C5'-O5'-PA-O2A
3	N	600	ADP	C5'-O5'-PA-O3A
3	H	600	ADP	O4'-C4'-C5'-O5'
3	D	600	ADP	PA-O3A-PB-O1B
3	E	600	ADP	PA-O3A-PB-O1B
3	F	600	ADP	PA-O3A-PB-O1B
3	G	600	ADP	PA-O3A-PB-O1B
3	H	600	ADP	C5'-O5'-PA-O2A
3	K	600	ADP	C5'-O5'-PA-O2A
3	L	600	ADP	C5'-O5'-PA-O2A
3	G	600	ADP	O4'-C4'-C5'-O5'
3	A	600	ADP	PA-O3A-PB-O1B
3	D	600	ADP	O4'-C4'-C5'-O5'
3	E	600	ADP	O4'-C4'-C5'-O5'
3	A	600	ADP	O4'-C4'-C5'-O5'
3	K	600	ADP	O4'-C4'-C5'-O5'
3	C	600	ADP	O4'-C4'-C5'-O5'
3	I	600	ADP	PA-O3A-PB-O1B
3	L	600	ADP	PA-O3A-PB-O1B
3	M	600	ADP	PA-O3A-PB-O1B
3	N	600	ADP	PA-O3A-PB-O1B
3	A	600	ADP	PA-O3A-PB-O2B
3	A	600	ADP	PA-O3A-PB-O3B
3	B	600	ADP	PA-O3A-PB-O2B
3	C	600	ADP	PA-O3A-PB-O2B
3	D	600	ADP	PA-O3A-PB-O2B
3	D	600	ADP	PA-O3A-PB-O3B
3	E	600	ADP	PA-O3A-PB-O2B
3	E	600	ADP	PA-O3A-PB-O3B
3	F	600	ADP	PA-O3A-PB-O2B
3	F	600	ADP	PA-O3A-PB-O3B
3	G	600	ADP	PA-O3A-PB-O2B
3	G	600	ADP	PA-O3A-PB-O3B
3	H	600	ADP	PA-O3A-PB-O3B
3	I	600	ADP	PA-O3A-PB-O3B
3	J	600	ADP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	K	600	ADP	PA-O3A-PB-O3B
3	L	600	ADP	PA-O3A-PB-O3B
3	M	600	ADP	PA-O3A-PB-O3B
3	N	600	ADP	PA-O3A-PB-O3B
3	F	600	ADP	O4'-C4'-C5'-O5'
3	N	600	ADP	O4'-C4'-C5'-O5'
3	L	600	ADP	O4'-C4'-C5'-O5'
3	B	600	ADP	PA-O3A-PB-O1B

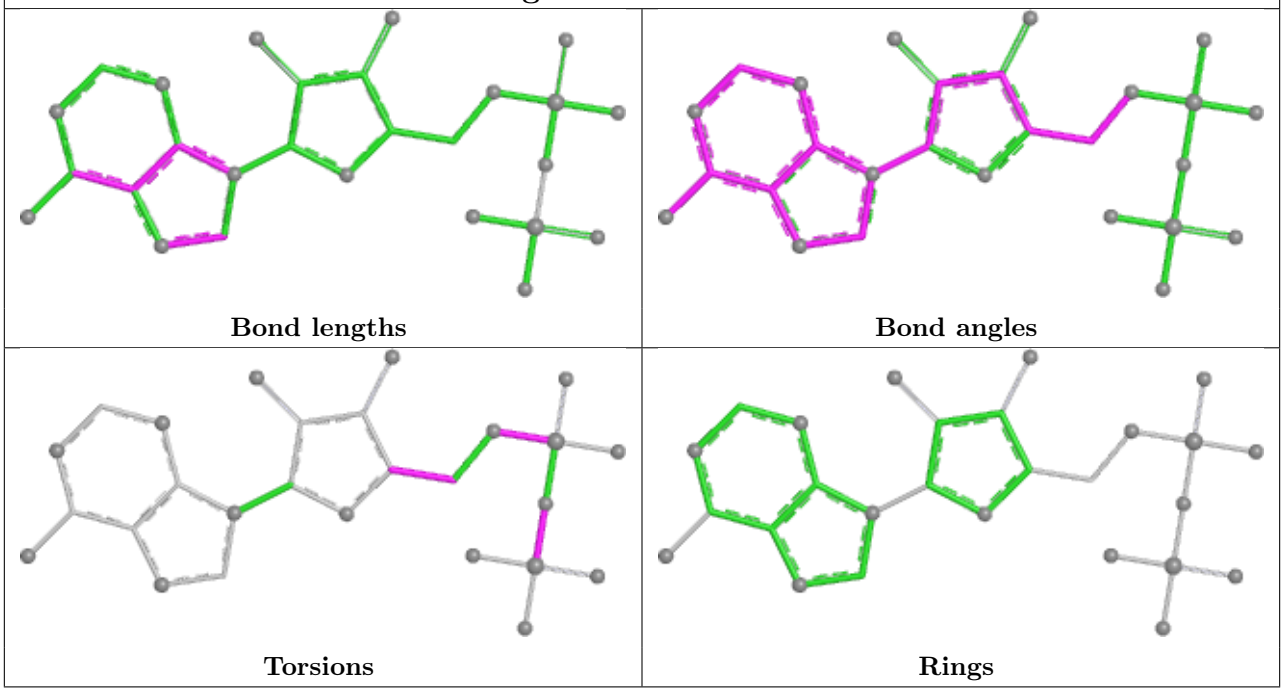
There are no ring outliers.

28 monomers are involved in 19 short contacts:

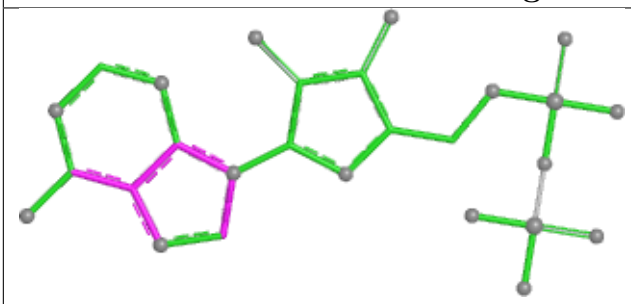
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	600	ADP	1	0
3	E	600	ADP	1	0
3	B	600	ADP	3	0
3	J	600	ADP	2	0
5	N	602	BEF	1	0
3	A	600	ADP	1	0
3	N	600	ADP	1	0
5	C	602	BEF	1	0
5	I	602	BEF	1	0
5	F	602	BEF	1	0
5	H	602	BEF	1	0
5	K	602	BEF	1	0
5	E	602	BEF	1	0
5	B	602	BEF	1	0
3	C	600	ADP	1	0
3	I	600	ADP	2	0
5	A	602	BEF	1	0
3	L	600	ADP	1	0
5	G	602	BEF	1	0
5	D	602	BEF	1	0
5	J	602	BEF	1	0
3	H	600	ADP	1	0
3	G	600	ADP	1	0
3	K	600	ADP	1	0
5	L	602	BEF	1	0
5	M	602	BEF	1	0
3	F	600	ADP	2	0
3	M	600	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

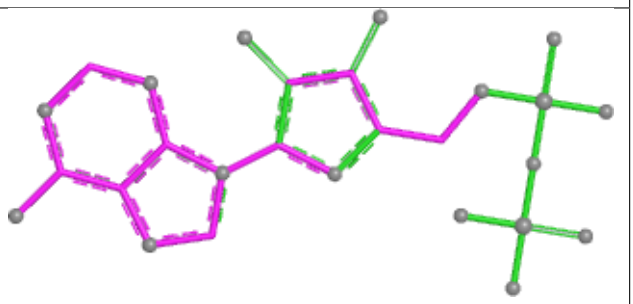
Ligand ADP D 600



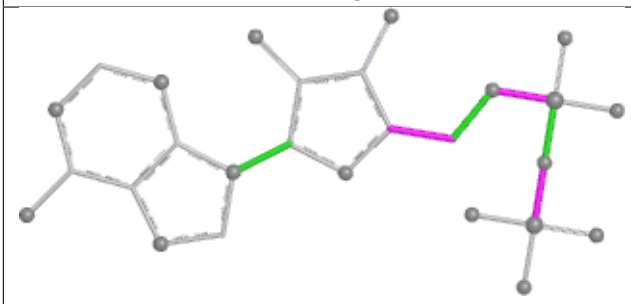
Ligand ADP E 600



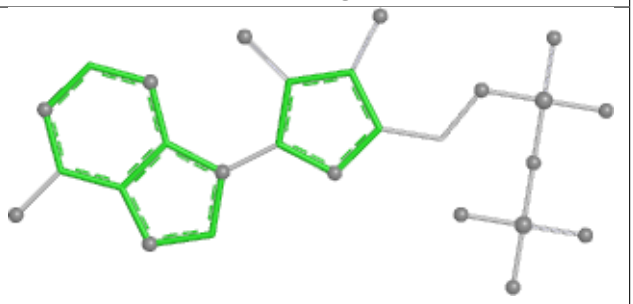
Bond lengths



Bond angles

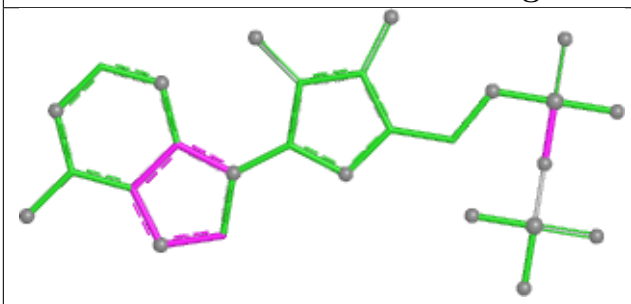


Torsions

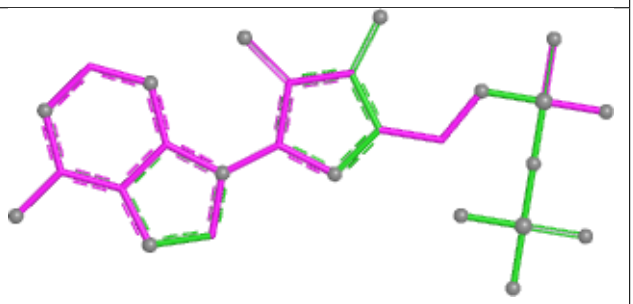


Rings

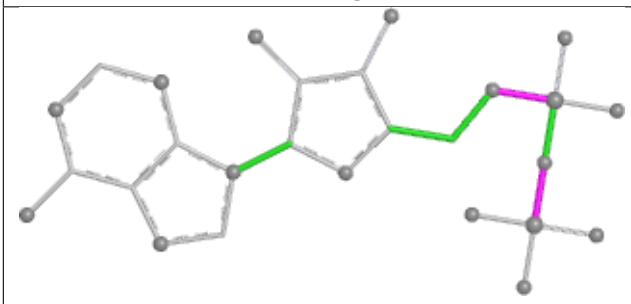
Ligand ADP B 600



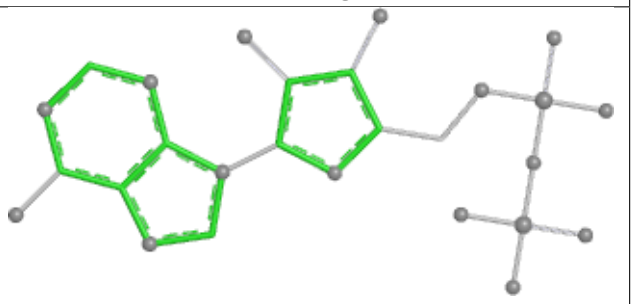
Bond lengths



Bond angles

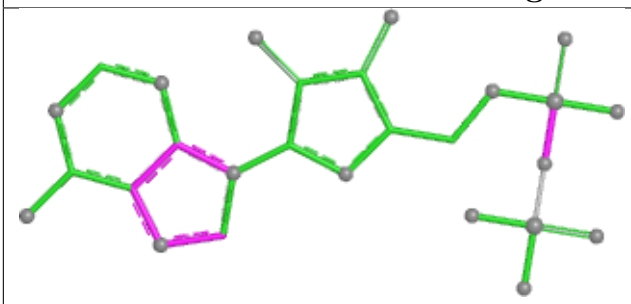


Torsions



Rings

Ligand ADP J 600



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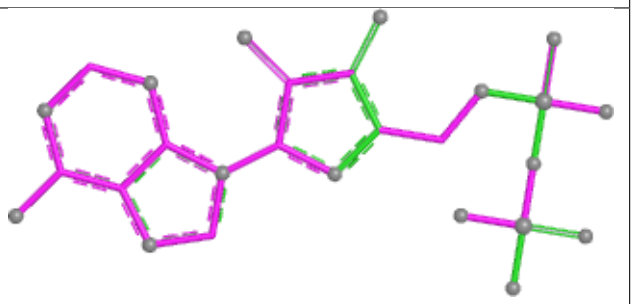

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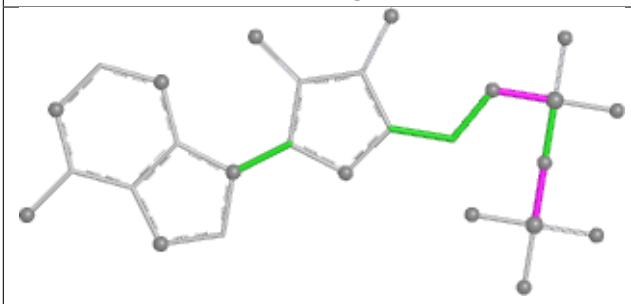
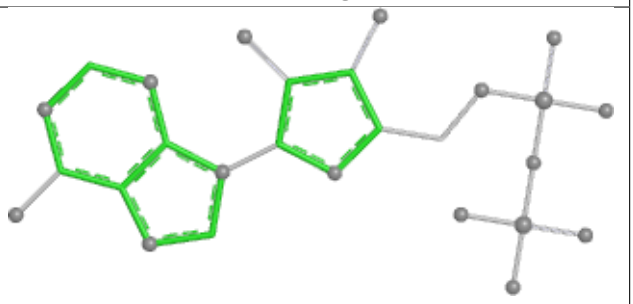
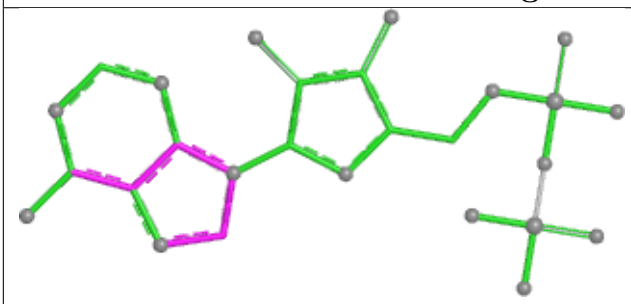


Torsions



Rings

Ligand ADP A 600



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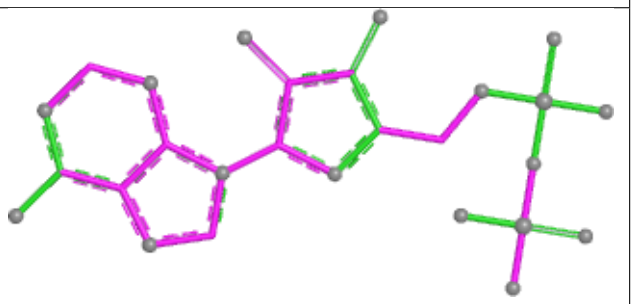
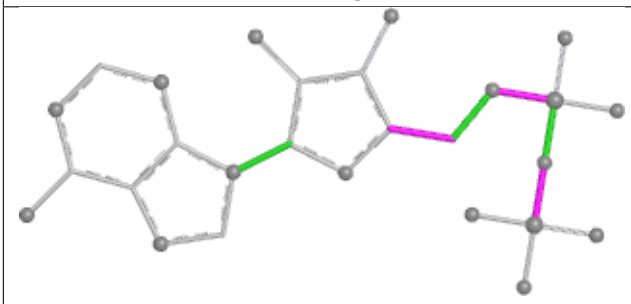


Bond angles



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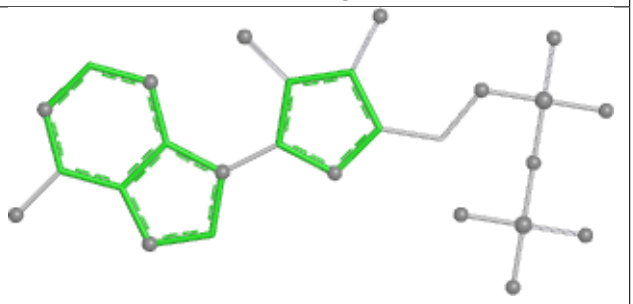
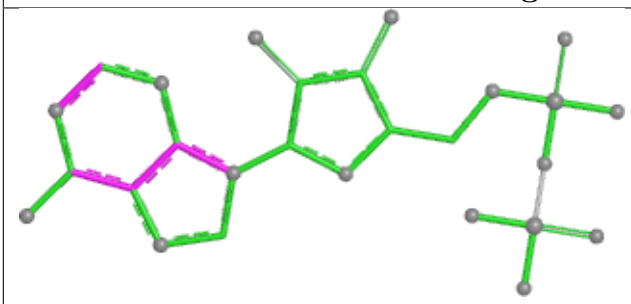


Rings

Ligand ADP N 600



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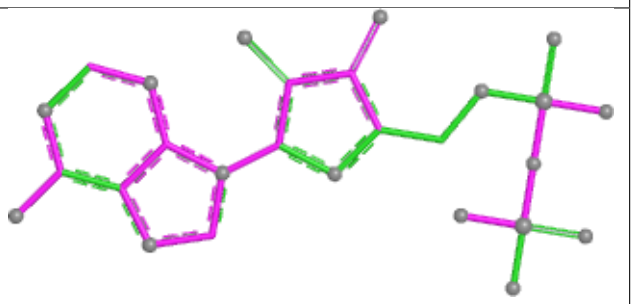
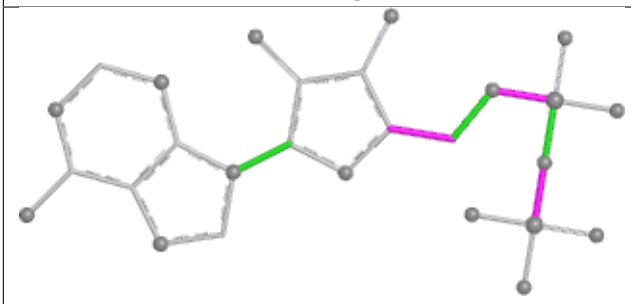
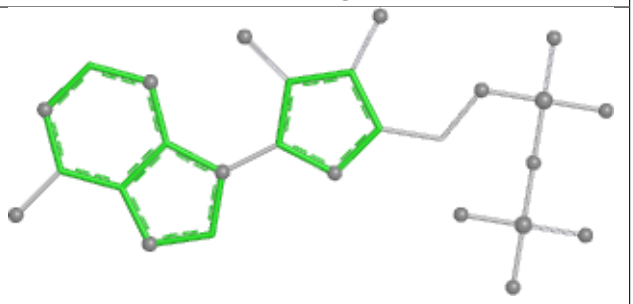


Bond angles

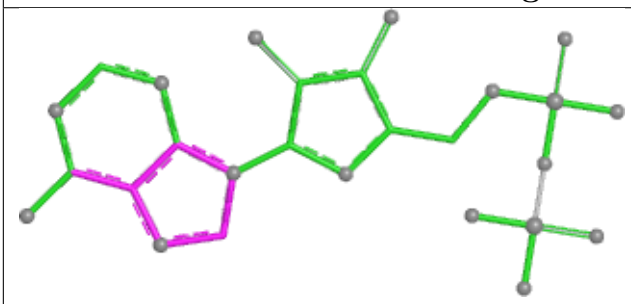


Torsions

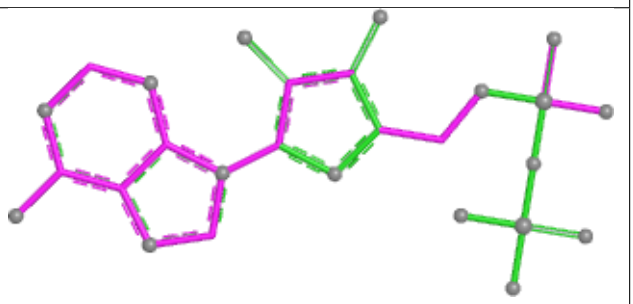


Rings

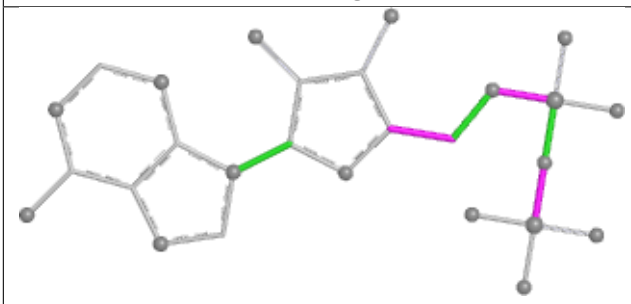
Ligand ADP C 600



Bond lengths



Bond angles



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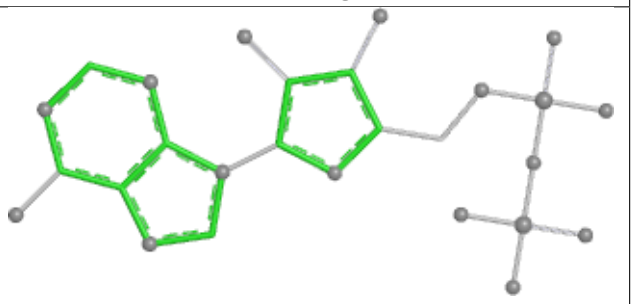
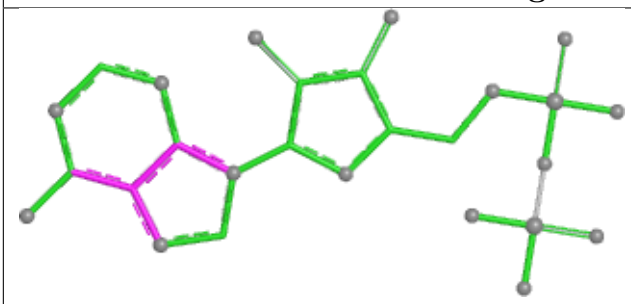


Rings

Ligand ADP I 600



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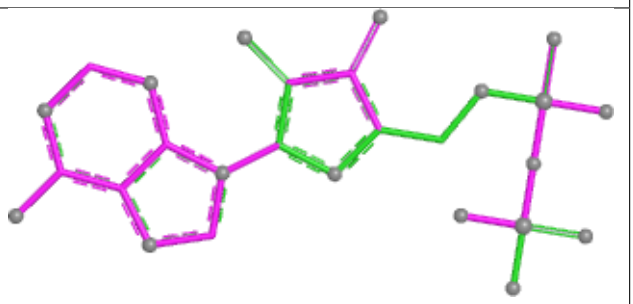

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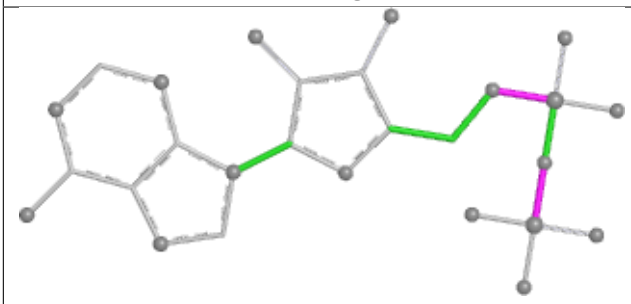

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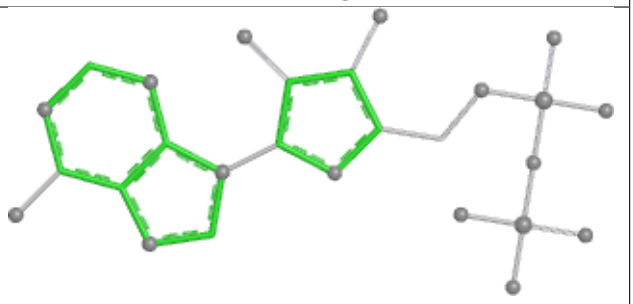
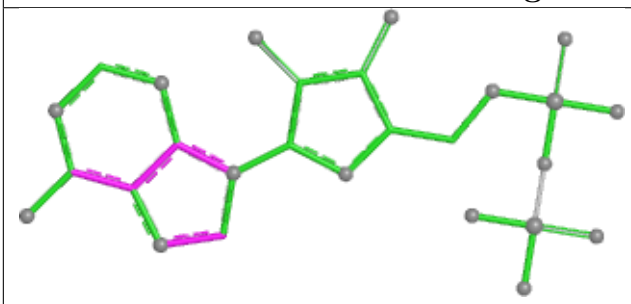
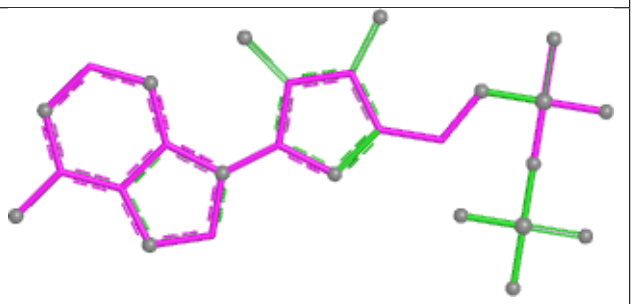


Rings

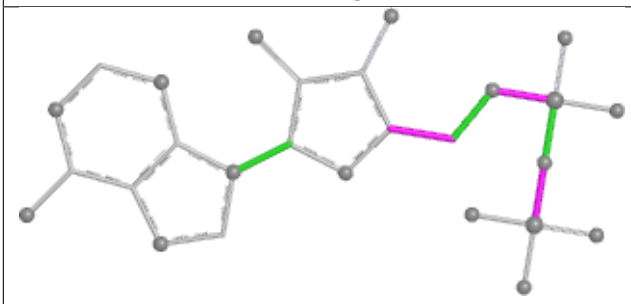
Ligand ADP L 600



Bond lengths



Bond angles



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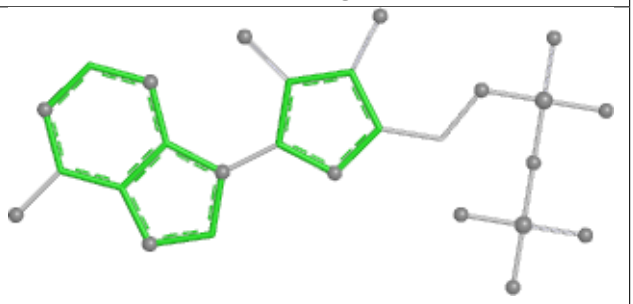
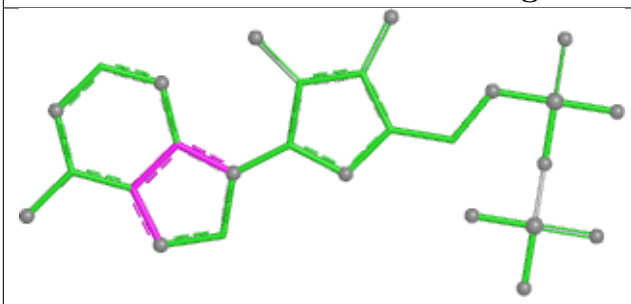


Rings

Ligand ADP H 600



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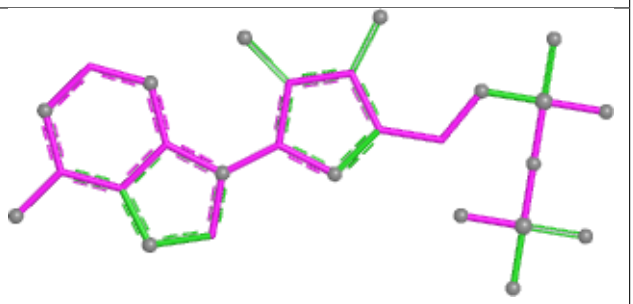
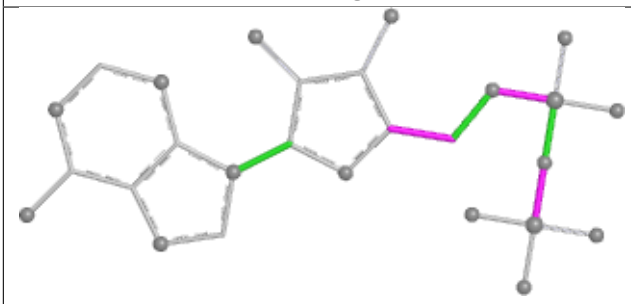


Bond angles



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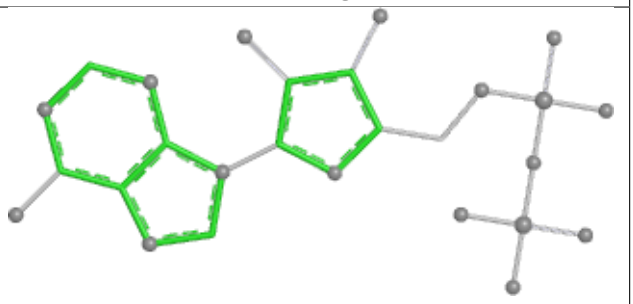
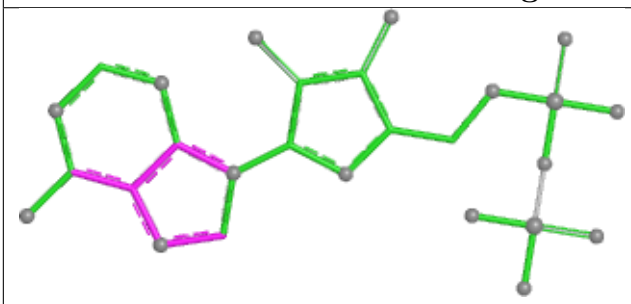
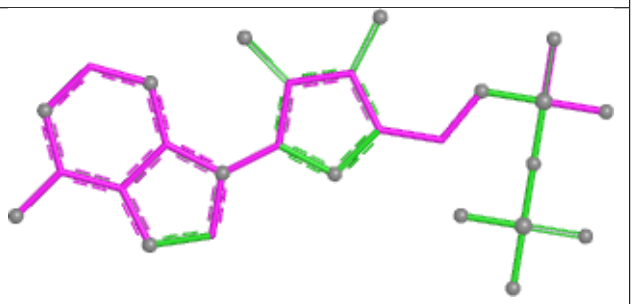


Rings

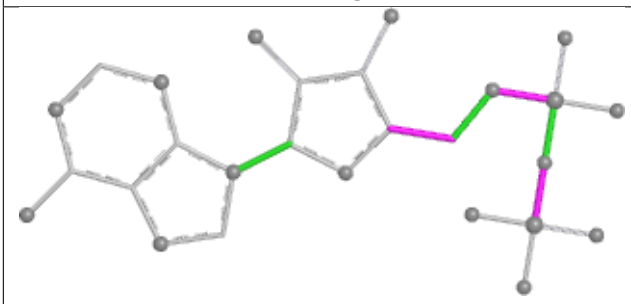
Ligand ADP G 600



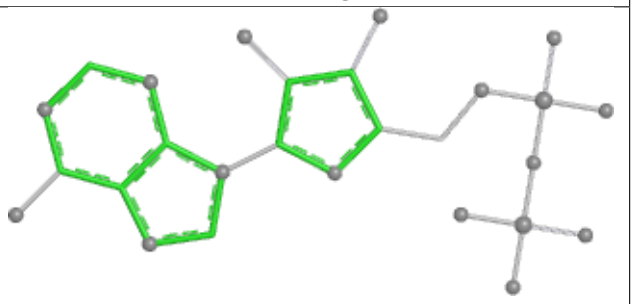
Bond lengths



Bond angles

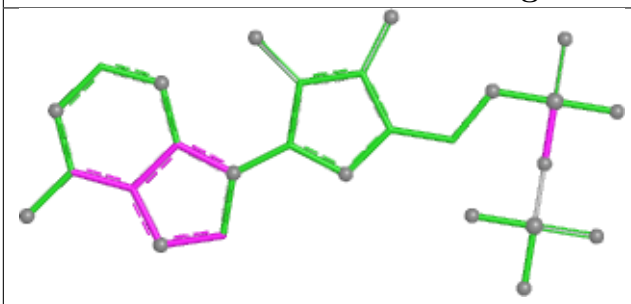


Torsions

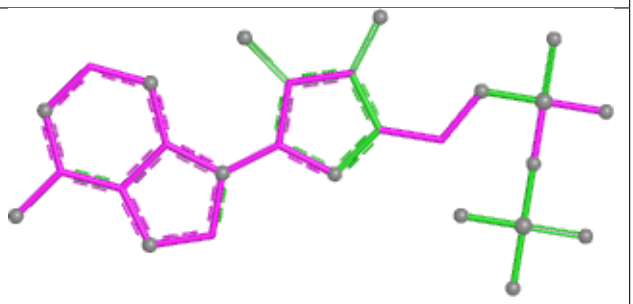


Rings

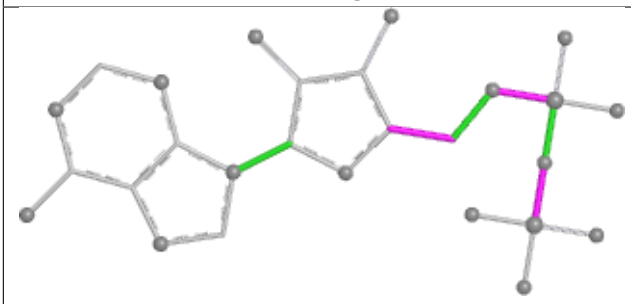
Ligand ADP K 600



Bond lengths



Bond angles



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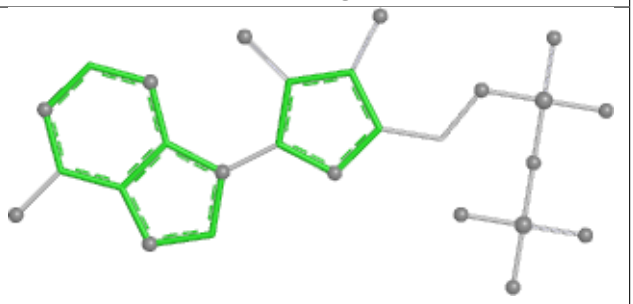
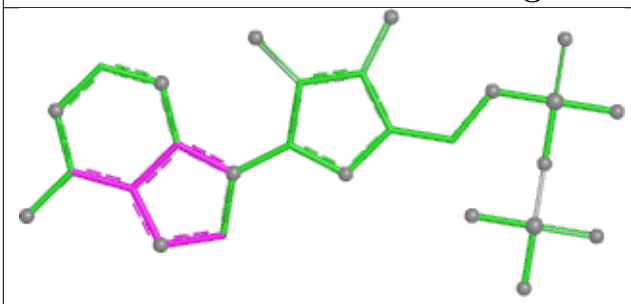
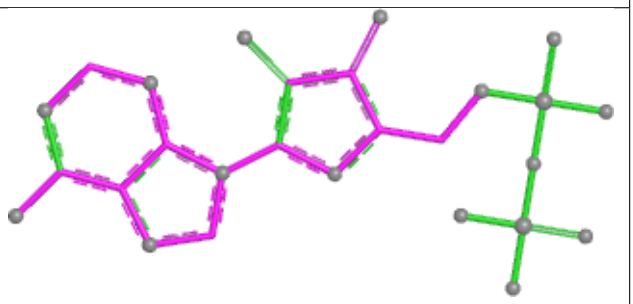


Rings

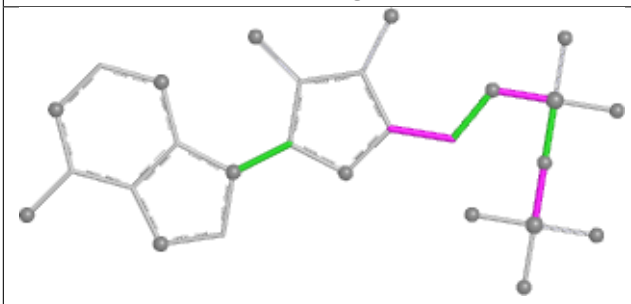
Ligand ADP F 600



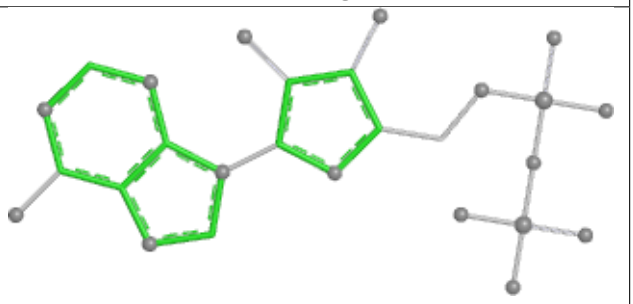
Bond lengths



Bond angles

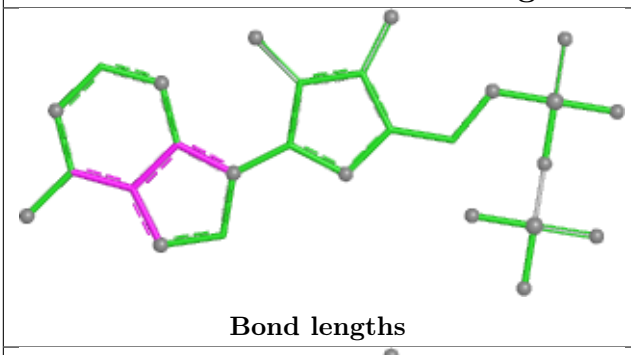


Torsions



Rings

Ligand ADP M 600



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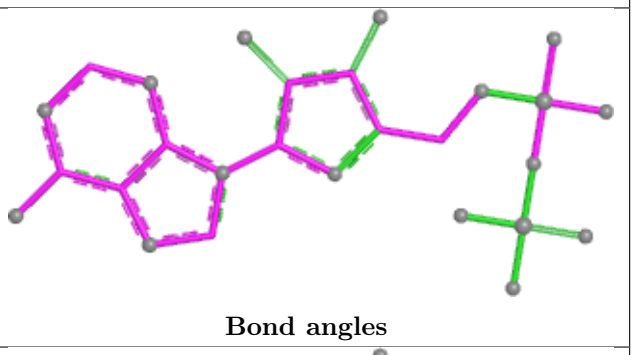
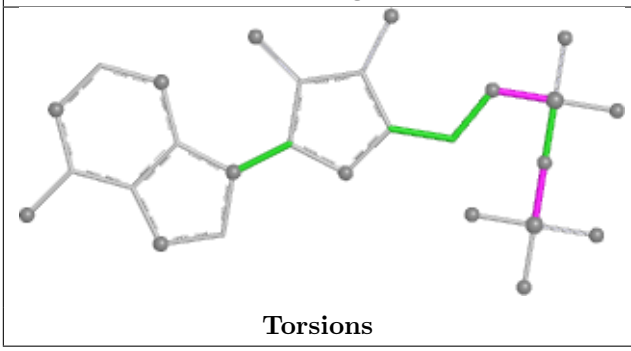
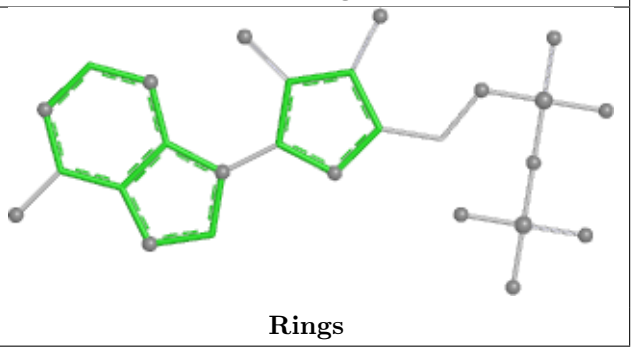


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	520/548 (94%)	-0.45	1 (0%) 91 80	59, 109, 191, 228	0
1	B	520/548 (94%)	-0.51	0 100 100	61, 107, 198, 222	0
1	C	520/548 (94%)	-0.43	0 100 100	74, 124, 231, 257	0
1	D	520/548 (94%)	-0.38	0 100 100	76, 133, 234, 259	0
1	E	520/548 (94%)	-0.48	0 100 100	60, 116, 203, 258	0
1	F	520/548 (94%)	-0.51	0 100 100	58, 109, 188, 213	0
1	G	520/548 (94%)	-0.41	0 100 100	58, 113, 206, 228	0
1	H	520/548 (94%)	-0.45	0 100 100	55, 109, 200, 241	0
1	I	520/548 (94%)	-0.53	0 100 100	60, 107, 191, 212	0
1	J	520/548 (94%)	-0.44	3 (0%) 85 65	63, 118, 192, 222	0
1	K	520/548 (94%)	-0.39	0 100 100	74, 134, 201, 239	0
1	L	520/548 (94%)	-0.45	0 100 100	73, 121, 222, 270	0
1	M	520/548 (94%)	-0.51	0 100 100	61, 108, 195, 220	0
1	N	520/548 (94%)	-0.49	0 100 100	56, 100, 182, 226	0
2	1	92/97 (94%)	-0.15	0 100 100	133, 170, 220, 238	0
2	2	92/97 (94%)	-0.15	0 100 100	132, 170, 212, 237	0
2	O	93/97 (95%)	-0.08	0 100 100	158, 178, 241, 293	0
2	P	94/97 (96%)	-0.01	0 100 100	173, 194, 233, 243	0
2	Q	90/97 (92%)	0.17	1 (1%) 78 53	162, 200, 235, 253	0
2	R	92/97 (94%)	0.16	2 (2%) 62 37	198, 220, 246, 257	0
2	S	92/97 (94%)	-0.22	0 100 100	167, 204, 227, 249	0
2	T	92/97 (94%)	-0.07	0 100 100	162, 189, 224, 234	0
2	U	92/97 (94%)	0.03	0 100 100	162, 186, 222, 232	0
2	V	93/97 (95%)	0.08	0 100 100	139, 180, 219, 239	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	W	93/97 (95%)	-0.20	0	100	100	148, 170, 206, 214	0
2	X	92/97 (94%)	-0.09	0	100	100	163, 180, 216, 235	0
2	Y	92/97 (94%)	-0.02	0	100	100	128, 160, 220, 248	0
2	Z	92/97 (94%)	-0.05	0	100	100	124, 154, 200, 231	0
All	All	8571/9030 (94%)	-0.40	7 (0%)	92	86	55, 130, 214, 293	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	190	VAL	2.2
2	Q	10	VAL	2.1
1	A	233	MET	2.1
1	J	193	MET	2.1
2	R	85	ILE	2.1
1	J	233	MET	2.1
2	R	3	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	K	L	603	1/1	0.92	0.05	80,80,80,80	0
5	BEF	J	602	4/4	0.93	0.08	81,82,83,84	0
5	BEF	E	602	4/4	0.94	0.05	96,96,97,98	0
6	K	E	603	1/1	0.94	0.04	91,91,91,91	0
5	BEF	G	602	4/4	0.94	0.06	68,69,70,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BEF	K	602	4/4	0.95	0.06	80,83,83,85	0
5	BEF	M	602	4/4	0.95	0.07	75,78,79,81	0
5	BEF	N	602	4/4	0.95	0.06	74,78,79,79	0
5	BEF	C	602	4/4	0.95	0.06	101,103,103,107	0
6	K	G	603	1/1	0.95	0.05	69,69,69,69	0
4	MG	D	601	1/1	0.95	0.06	78,78,78,78	0
5	BEF	F	602	4/4	0.96	0.07	84,88,90,91	0
6	K	A	603	1/1	0.96	0.05	94,94,94,94	0
5	BEF	B	602	4/4	0.96	0.07	85,89,90,91	0
5	BEF	L	602	4/4	0.96	0.05	91,92,92,95	0
6	K	J	603	1/1	0.96	0.04	97,97,97,97	0
5	BEF	H	602	4/4	0.96	0.05	82,85,86,87	0
5	BEF	I	602	4/4	0.97	0.05	76,80,80,83	0
4	MG	G	601	1/1	0.97	0.07	57,57,57,57	0
4	MG	M	601	1/1	0.97	0.07	52,52,52,52	0
4	MG	N	601	1/1	0.97	0.07	46,46,46,46	0
5	BEF	A	602	4/4	0.97	0.06	78,79,79,81	0
3	ADP	F	600	27/27	0.97	0.06	73,77,84,86	0
3	ADP	G	600	27/27	0.97	0.06	64,69,75,78	0
6	K	C	603	1/1	0.97	0.05	81,81,81,81	0
3	ADP	H	600	27/27	0.97	0.05	64,70,75,77	0
3	ADP	K	600	27/27	0.97	0.05	89,93,98,99	0
6	K	H	603	1/1	0.97	0.03	69,69,69,69	0
3	ADP	N	600	27/27	0.97	0.06	62,68,72,75	0
6	K	K	603	1/1	0.97	0.04	87,87,87,87	0
3	ADP	E	600	27/27	0.97	0.06	83,87,94,96	0
6	K	M	603	1/1	0.97	0.04	86,86,86,86	0
6	K	N	603	1/1	0.97	0.06	83,83,83,83	0
3	ADP	C	600	27/27	0.98	0.04	82,86,91,95	0
4	MG	E	601	1/1	0.98	0.05	62,62,62,62	0
3	ADP	D	600	27/27	0.98	0.05	88,95,103,106	0
4	MG	H	601	1/1	0.98	0.04	47,47,47,47	0
4	MG	I	601	1/1	0.98	0.05	52,52,52,52	0
4	MG	K	601	1/1	0.98	0.05	68,68,68,68	0
3	ADP	I	600	27/27	0.98	0.05	70,74,82,86	0
3	ADP	J	600	27/27	0.98	0.04	83,88,93,96	0
3	ADP	A	600	27/27	0.98	0.05	69,77,84,88	0
3	ADP	L	600	27/27	0.98	0.05	81,86,91,93	0
3	ADP	M	600	27/27	0.98	0.05	65,69,74,75	0
5	BEF	D	602	4/4	0.98	0.05	106,106,107,107	0
3	ADP	B	600	27/27	0.98	0.04	63,73,79,81	0
4	MG	A	601	1/1	0.98	0.05	59,59,59,59	0

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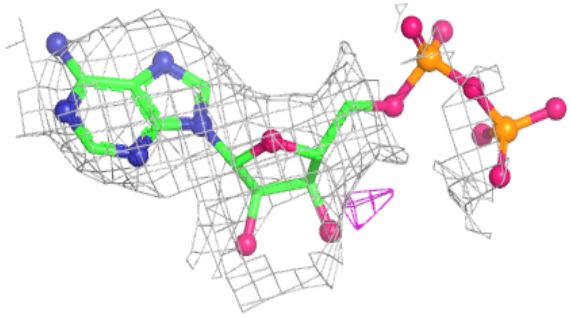
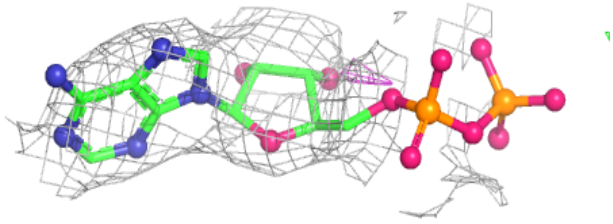
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	601	1/1	0.98	0.07	48,48,48,48	0
4	MG	C	601	1/1	0.98	0.06	57,57,57,57	0
6	K	B	603	1/1	0.99	0.03	84,84,84,84	0
4	MG	L	601	1/1	0.99	0.05	56,56,56,56	0
6	K	D	603	1/1	0.99	0.02	89,89,89,89	0
4	MG	J	601	1/1	0.99	0.06	52,52,52,52	0
6	K	F	603	1/1	0.99	0.02	80,80,80,80	0
4	MG	F	601	1/1	0.99	0.05	59,59,59,59	0
6	K	I	603	1/1	1.00	0.02	67,67,67,67	0

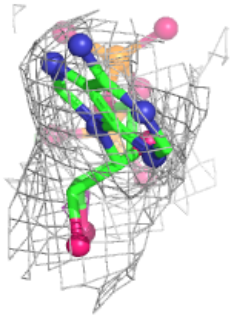
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP F 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



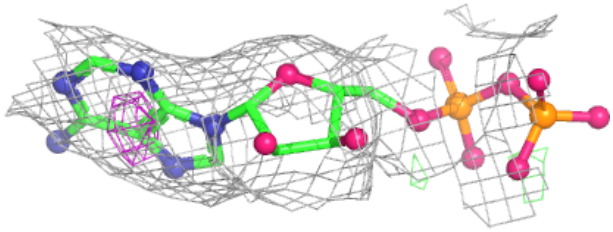


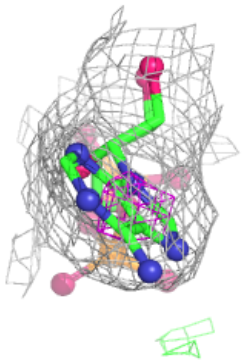


Electron density around ADP G 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

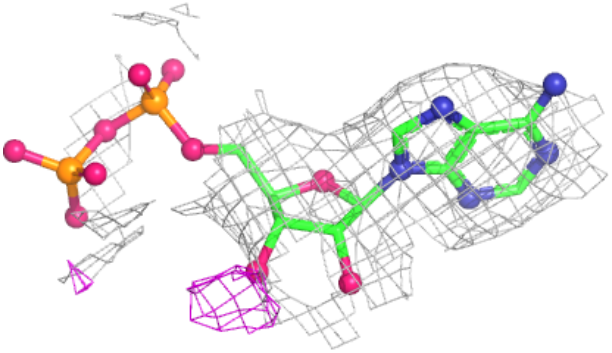


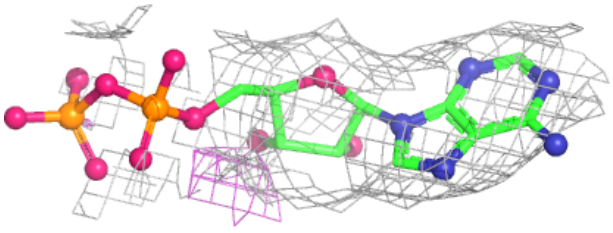


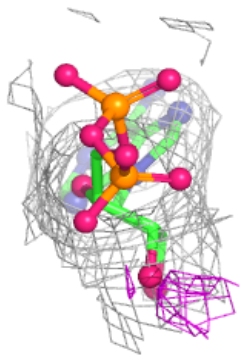


Electron density around ADP H 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

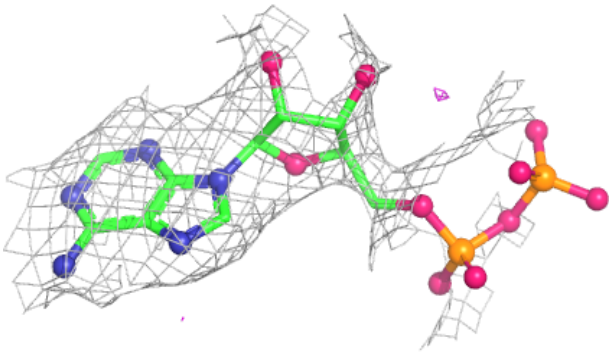


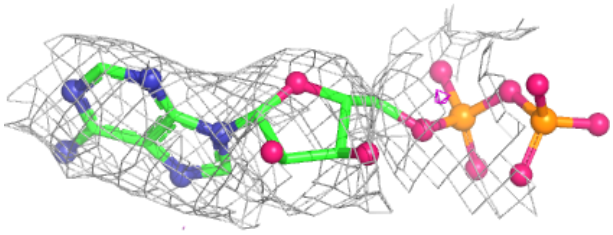


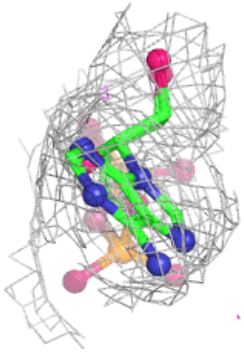


Electron density around ADP K 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

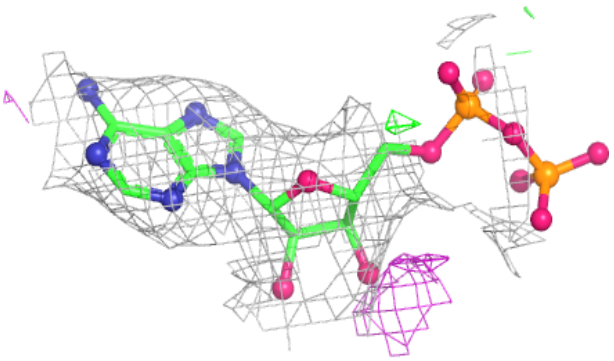


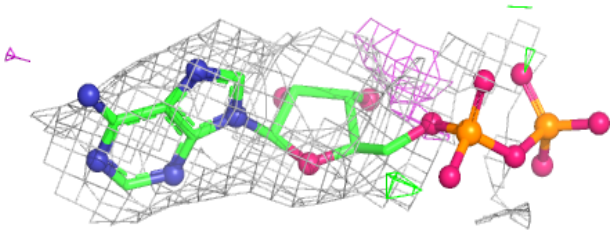


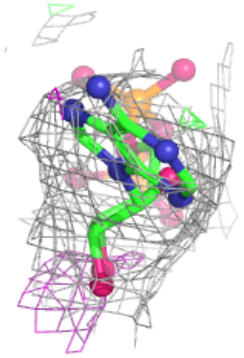


Electron density around ADP N 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

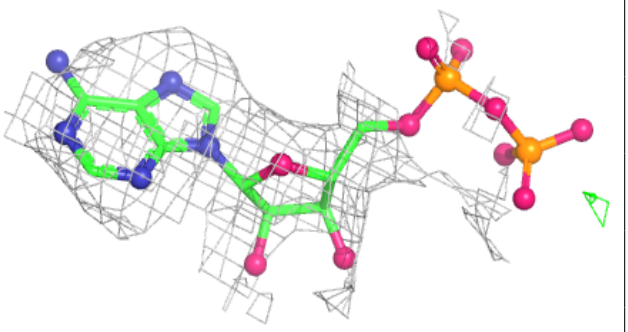


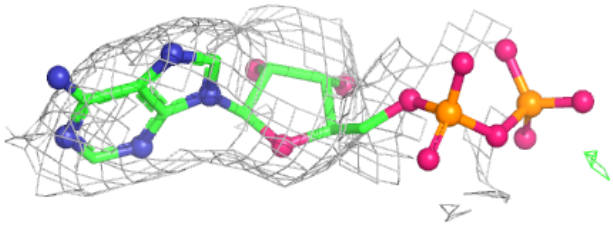


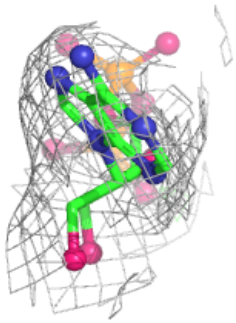


Electron density around ADP E 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

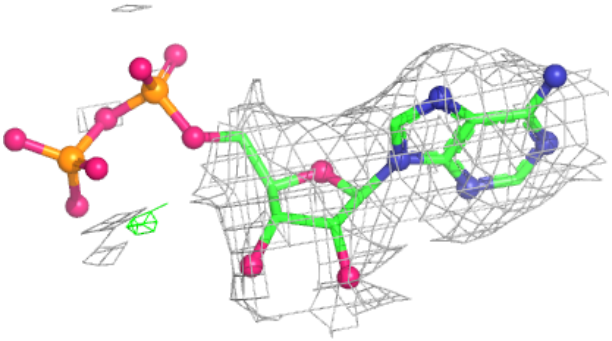


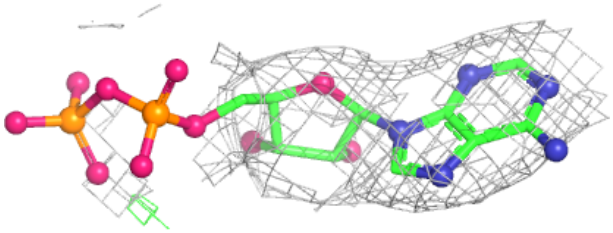


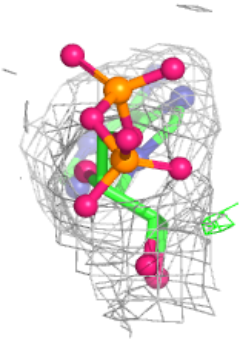


Electron density around ADP C 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

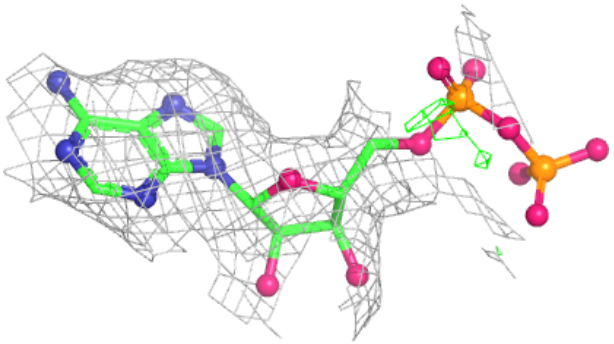


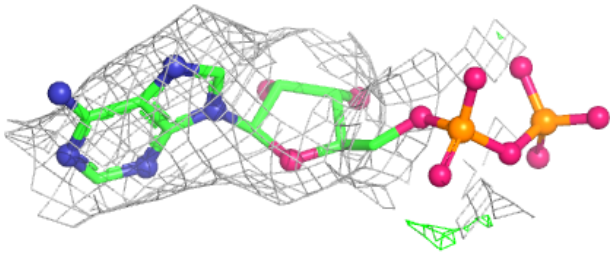


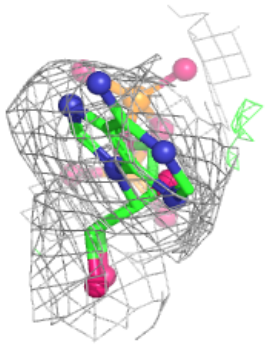


Electron density around ADP D 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

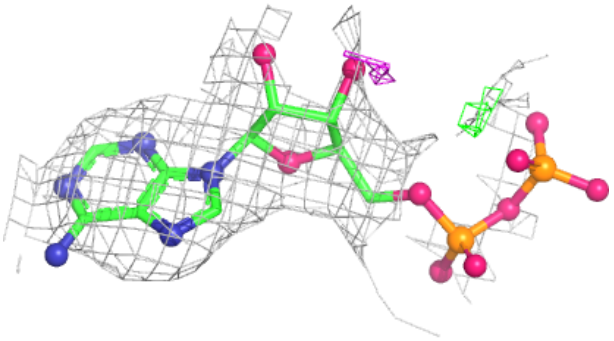


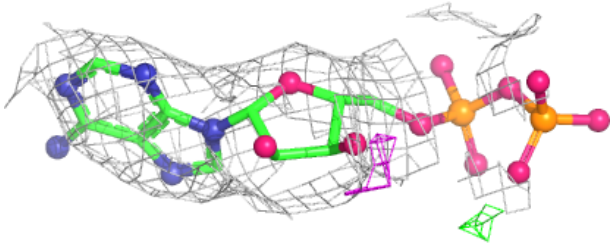


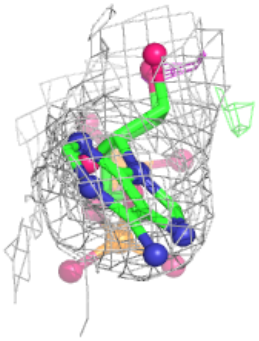


Electron density around ADP I 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

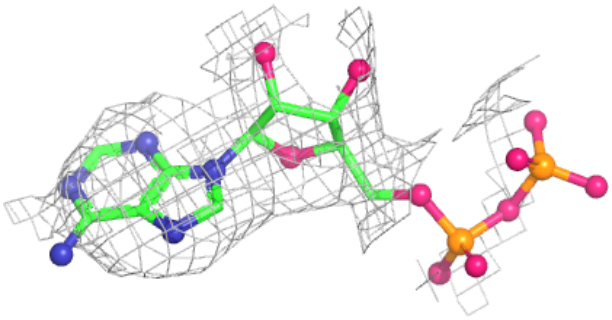


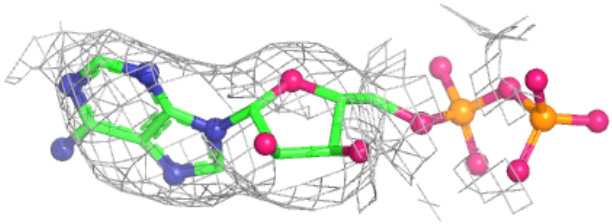


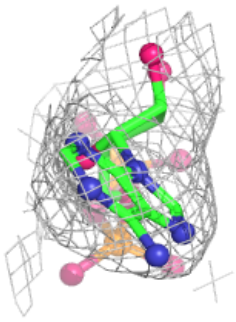


Electron density around ADP J 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

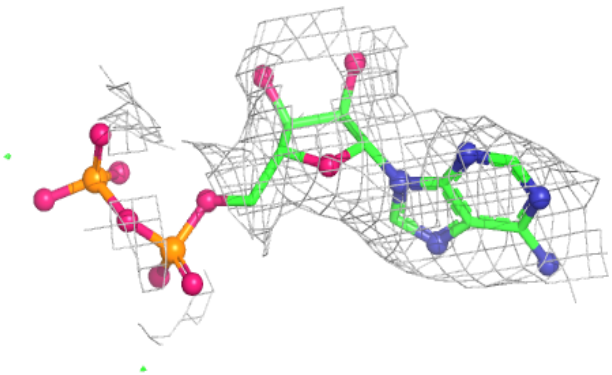


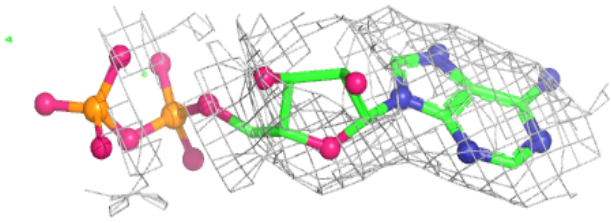


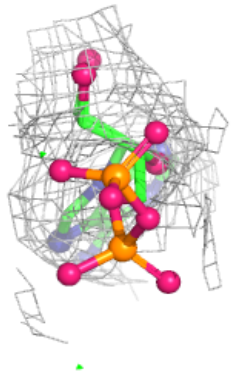


Electron density around ADP A 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

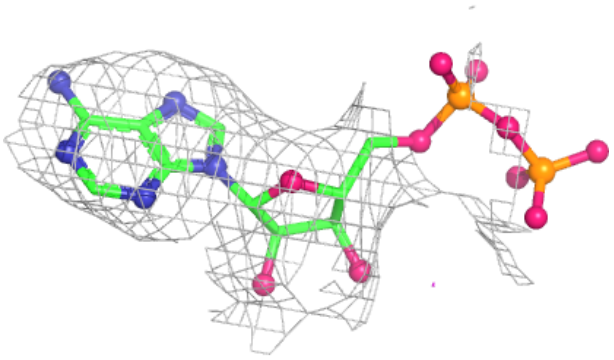


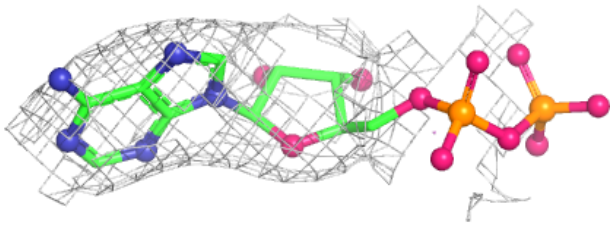


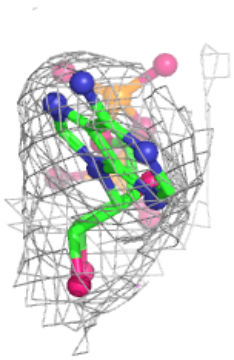


Electron density around ADP L 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

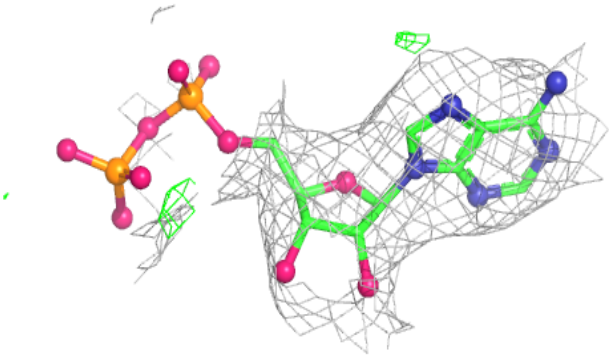


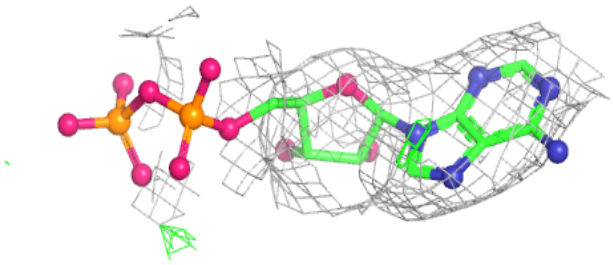


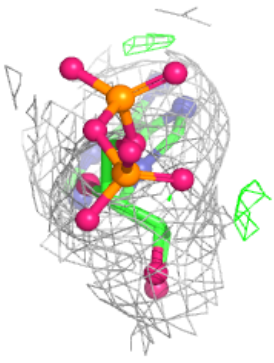


Electron density around ADP M 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

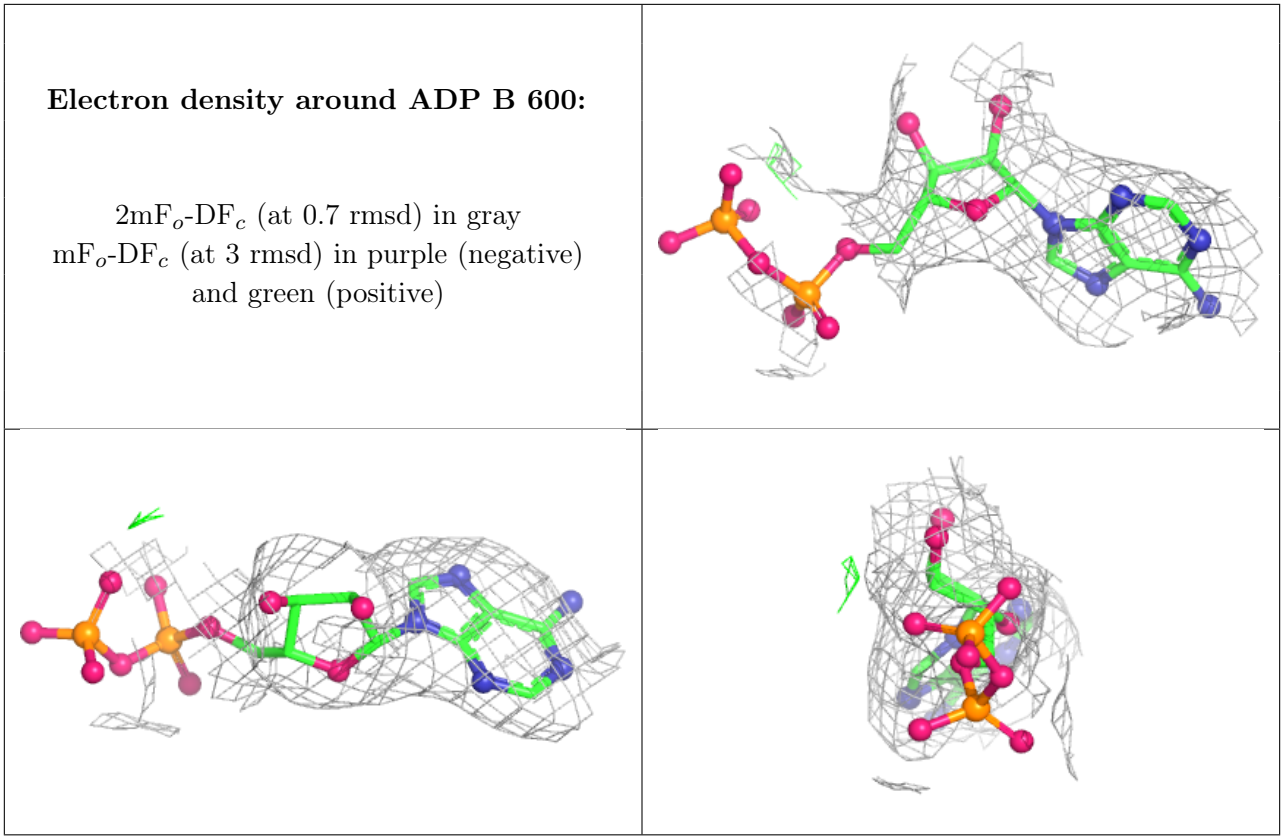






Electron density around ADP B 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.