



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:49 PM UTC

PDB ID : 8RTF / pdb_00008rtf
Title : Crystal structure of Trypanosoma congolense pyruvate kinase in complex with a single-domain antibody (TcoPYK-sdAb42)
Authors : Sterckx, Y.G.-J.
Deposited on : 2024-01-26
Resolution : 2.80 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
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

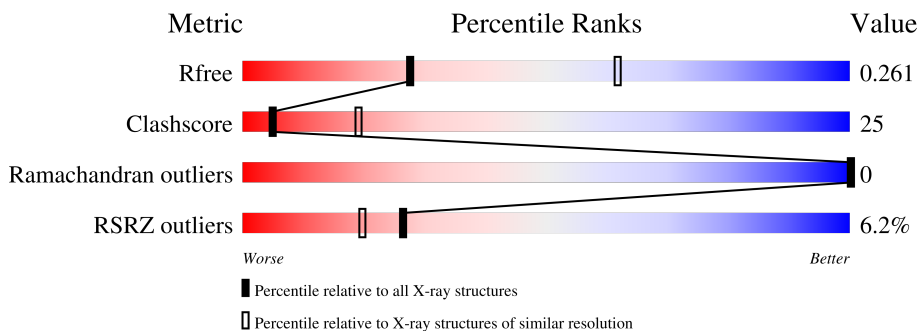
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.







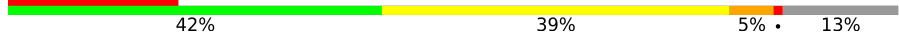
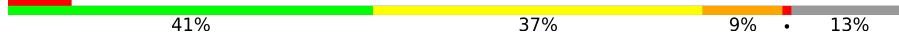
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	514	
1	B	514	
1	C	514	
1	D	514	
1	E	514	
1	F	514	

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Mol	Chain	Length	Quality of chain
2	G	149	
2	H	149	
2	I	149	
2	J	149	
2	K	149	
2	L	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	601	-	X	-	-
3	GOL	B	701	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25898 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	3687	2298	650	713	26	0	0	0
1	B	404	2996	1859	537	577	23	0	0	0
1	C	499	3672	2287	654	705	26	0	1	0
1	D	499	3691	2300	654	711	26	0	1	0
1	E	395	2920	1807	525	565	23	0	0	0
1	F	399	2901	1802	515	562	22	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	GLU	-	expression tag	UNP G0UYF4
A	501	ASN	-	expression tag	UNP G0UYF4
A	502	LEU	-	expression tag	UNP G0UYF4
A	503	TYR	-	expression tag	UNP G0UYF4
A	504	PHE	-	expression tag	UNP G0UYF4
A	505	GLN	-	expression tag	UNP G0UYF4
A	506	SER	-	expression tag	UNP G0UYF4
A	507	GLY	-	expression tag	UNP G0UYF4
A	508	GLY	-	expression tag	UNP G0UYF4
A	509	HIS	-	expression tag	UNP G0UYF4
A	510	HIS	-	expression tag	UNP G0UYF4
A	511	HIS	-	expression tag	UNP G0UYF4
A	512	HIS	-	expression tag	UNP G0UYF4
A	513	HIS	-	expression tag	UNP G0UYF4
A	514	HIS	-	expression tag	UNP G0UYF4
B	500	GLU	-	expression tag	UNP G0UYF4
B	501	ASN	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	502	LEU	-	expression tag	UNP G0UYF4
B	503	TYR	-	expression tag	UNP G0UYF4
B	504	PHE	-	expression tag	UNP G0UYF4
B	505	GLN	-	expression tag	UNP G0UYF4
B	506	SER	-	expression tag	UNP G0UYF4
B	507	GLY	-	expression tag	UNP G0UYF4
B	508	GLY	-	expression tag	UNP G0UYF4
B	509	HIS	-	expression tag	UNP G0UYF4
B	510	HIS	-	expression tag	UNP G0UYF4
B	511	HIS	-	expression tag	UNP G0UYF4
B	512	HIS	-	expression tag	UNP G0UYF4
B	513	HIS	-	expression tag	UNP G0UYF4
B	514	HIS	-	expression tag	UNP G0UYF4
C	515	GLU	-	expression tag	UNP G0UYF4
C	516	ASN	-	expression tag	UNP G0UYF4
C	517	LEU	-	expression tag	UNP G0UYF4
C	518	TYR	-	expression tag	UNP G0UYF4
C	519	PHE	-	expression tag	UNP G0UYF4
C	520	GLN	-	expression tag	UNP G0UYF4
C	521	SER	-	expression tag	UNP G0UYF4
C	522	GLY	-	expression tag	UNP G0UYF4
C	523	GLY	-	expression tag	UNP G0UYF4
C	524	HIS	-	expression tag	UNP G0UYF4
C	525	HIS	-	expression tag	UNP G0UYF4
C	526	HIS	-	expression tag	UNP G0UYF4
C	527	HIS	-	expression tag	UNP G0UYF4
C	528	HIS	-	expression tag	UNP G0UYF4
C	529	HIS	-	expression tag	UNP G0UYF4
D	515	GLU	-	expression tag	UNP G0UYF4
D	516	ASN	-	expression tag	UNP G0UYF4
D	517	LEU	-	expression tag	UNP G0UYF4
D	518	TYR	-	expression tag	UNP G0UYF4
D	519	PHE	-	expression tag	UNP G0UYF4
D	520	GLN	-	expression tag	UNP G0UYF4
D	521	SER	-	expression tag	UNP G0UYF4
D	522	GLY	-	expression tag	UNP G0UYF4
D	523	GLY	-	expression tag	UNP G0UYF4
D	524	HIS	-	expression tag	UNP G0UYF4
D	525	HIS	-	expression tag	UNP G0UYF4
D	526	HIS	-	expression tag	UNP G0UYF4
D	527	HIS	-	expression tag	UNP G0UYF4
D	528	HIS	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	529	HIS	-	expression tag	UNP G0UYF4
E	500	GLU	-	expression tag	UNP G0UYF4
E	501	ASN	-	expression tag	UNP G0UYF4
E	502	LEU	-	expression tag	UNP G0UYF4
E	503	TYR	-	expression tag	UNP G0UYF4
E	504	PHE	-	expression tag	UNP G0UYF4
E	505	GLN	-	expression tag	UNP G0UYF4
E	506	SER	-	expression tag	UNP G0UYF4
E	507	GLY	-	expression tag	UNP G0UYF4
E	508	GLY	-	expression tag	UNP G0UYF4
E	509	HIS	-	expression tag	UNP G0UYF4
E	510	HIS	-	expression tag	UNP G0UYF4
E	511	HIS	-	expression tag	UNP G0UYF4
E	512	HIS	-	expression tag	UNP G0UYF4
E	513	HIS	-	expression tag	UNP G0UYF4
E	514	HIS	-	expression tag	UNP G0UYF4
F	500	GLU	-	expression tag	UNP G0UYF4
F	501	ASN	-	expression tag	UNP G0UYF4
F	502	LEU	-	expression tag	UNP G0UYF4
F	503	TYR	-	expression tag	UNP G0UYF4
F	504	PHE	-	expression tag	UNP G0UYF4
F	505	GLN	-	expression tag	UNP G0UYF4
F	506	SER	-	expression tag	UNP G0UYF4
F	507	GLY	-	expression tag	UNP G0UYF4
F	508	GLY	-	expression tag	UNP G0UYF4
F	509	HIS	-	expression tag	UNP G0UYF4
F	510	HIS	-	expression tag	UNP G0UYF4
F	511	HIS	-	expression tag	UNP G0UYF4
F	512	HIS	-	expression tag	UNP G0UYF4
F	513	HIS	-	expression tag	UNP G0UYF4
F	514	HIS	-	expression tag	UNP G0UYF4

- Molecule 2 is a protein called Camelid single-domain antibody 42 (sdAb42).

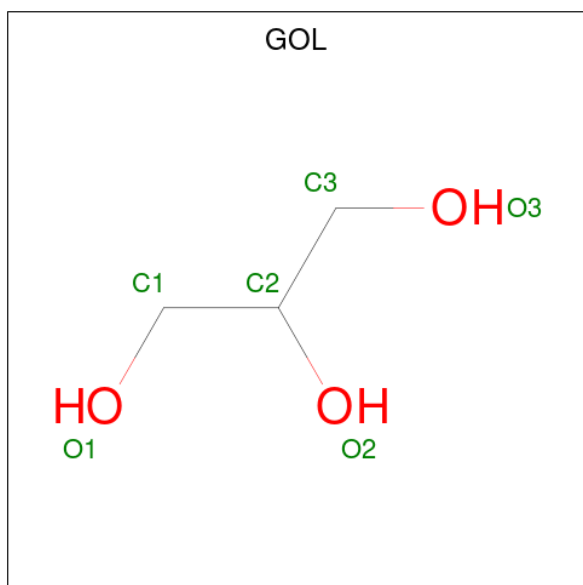
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	130	Total	C	N	O	S	0	0	0
			995	622	173	197	3			
2	H	130	Total	C	N	O	S	0	0	0
			998	623	173	199	3			
2	I	130	Total	C	N	O	S	0	0	0
			976	610	167	196	3			
2	J	131	Total	C	N	O	S	0	0	0
			1007	628	175	201	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	K	130	Total 967	C 603	N 165	O 196	S 3	0	0	0
2	L	130	Total 942	C 585	N 160	O 194	S 3	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0

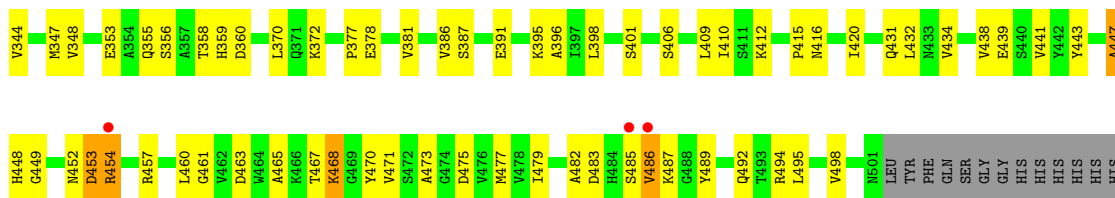
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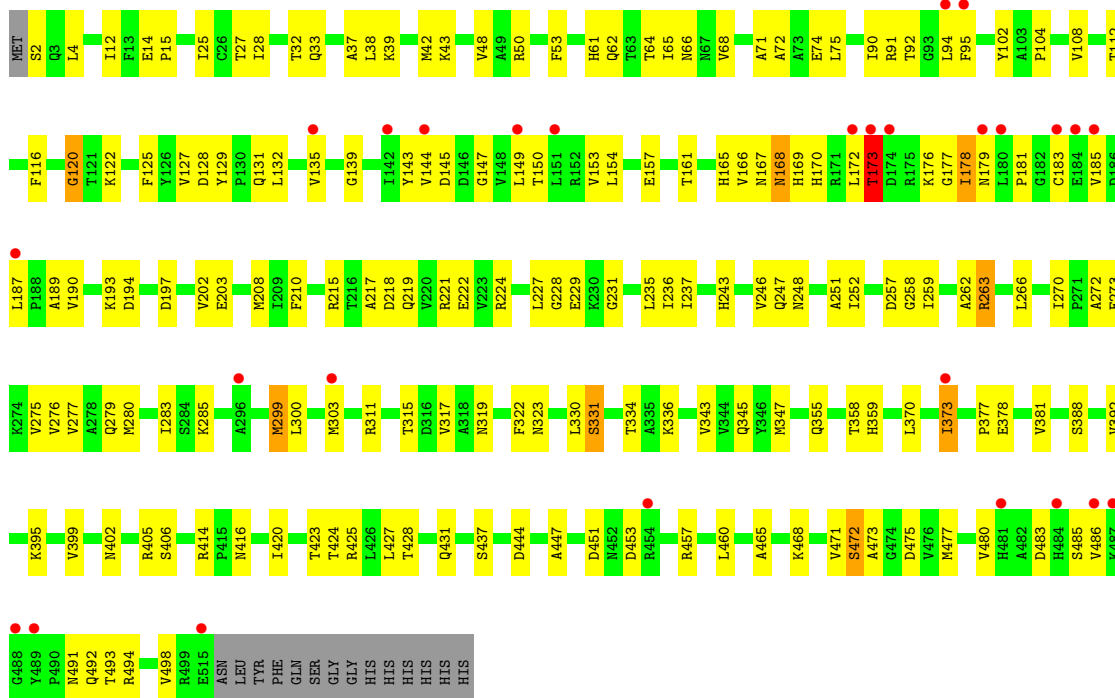
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

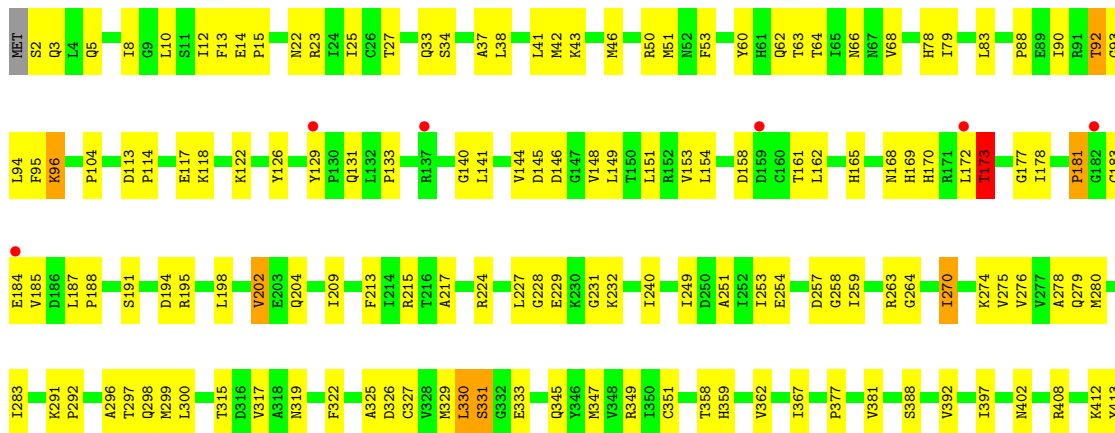
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	7	Total	O	0	0
			7	7		
4	C	25	Total	O	0	0
			25	25		
4	D	13	Total	O	0	0
			13	13		
4	E	5	Total	O	0	0
			5	5		
4	F	5	Total	O	0	0
			5	5		
4	G	2	Total	O	0	0
			2	2		
4	H	5	Total	O	0	0
			5	5		
4	I	1	Total	O	0	0
			1	1		
4	J	4	Total	O	0	0
			4	4		
4	L	1	Total	O	0	0
			1	1		

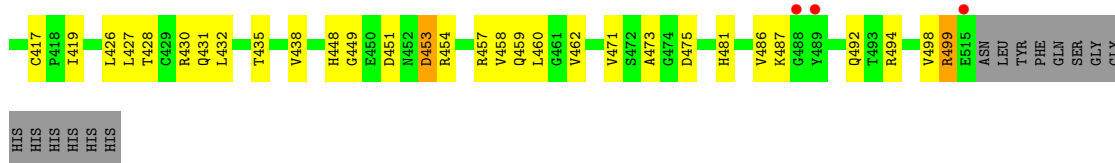


● Molecule 1: Pyruvate kinase

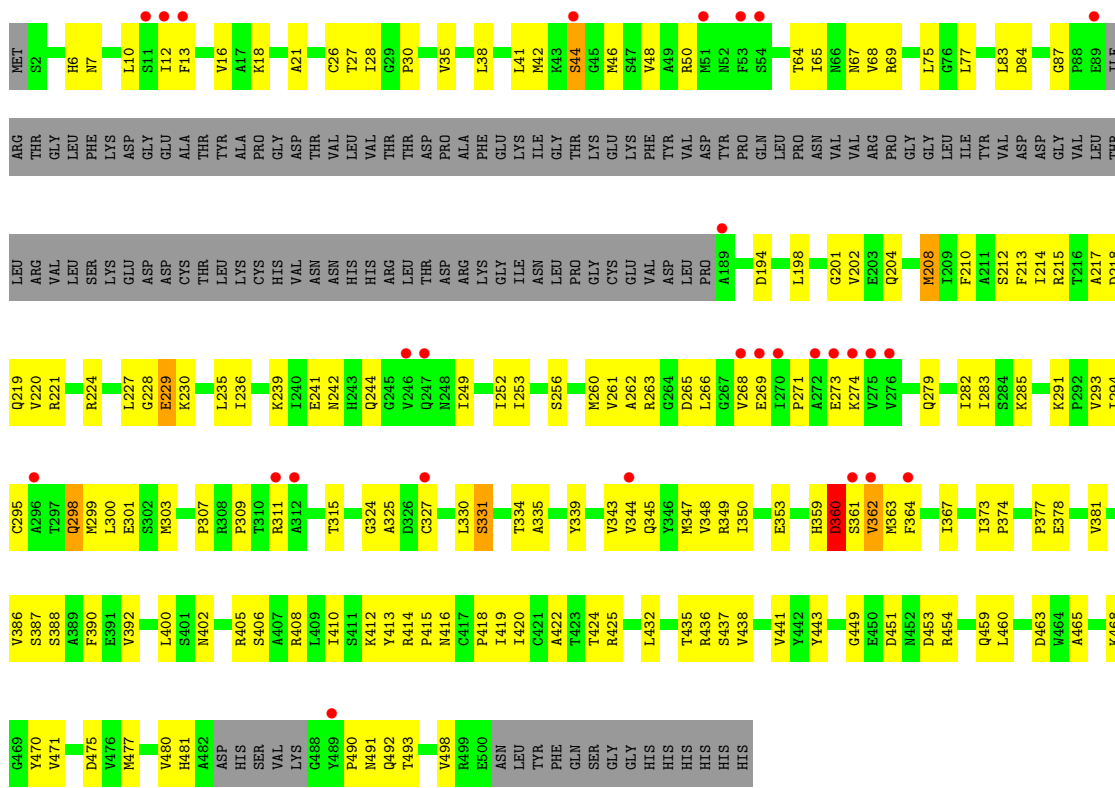


● Molecule 1: Pyruvate kinase

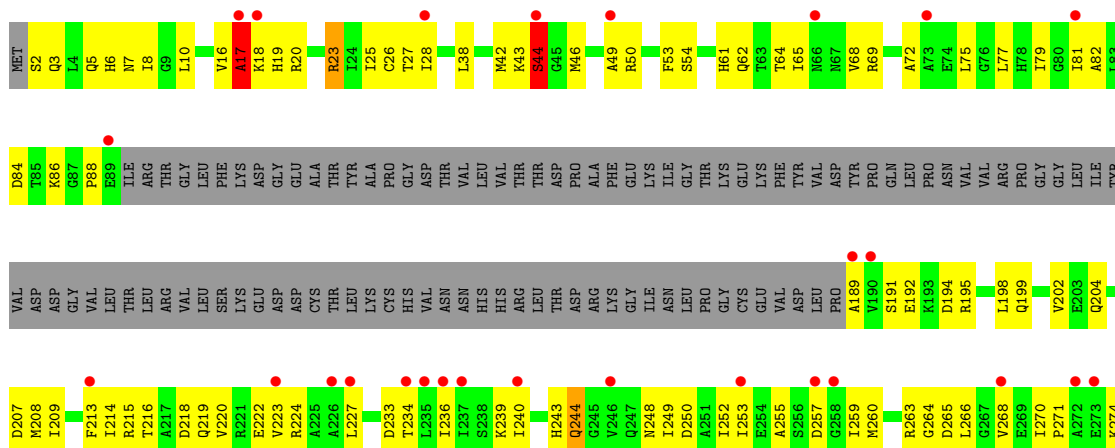


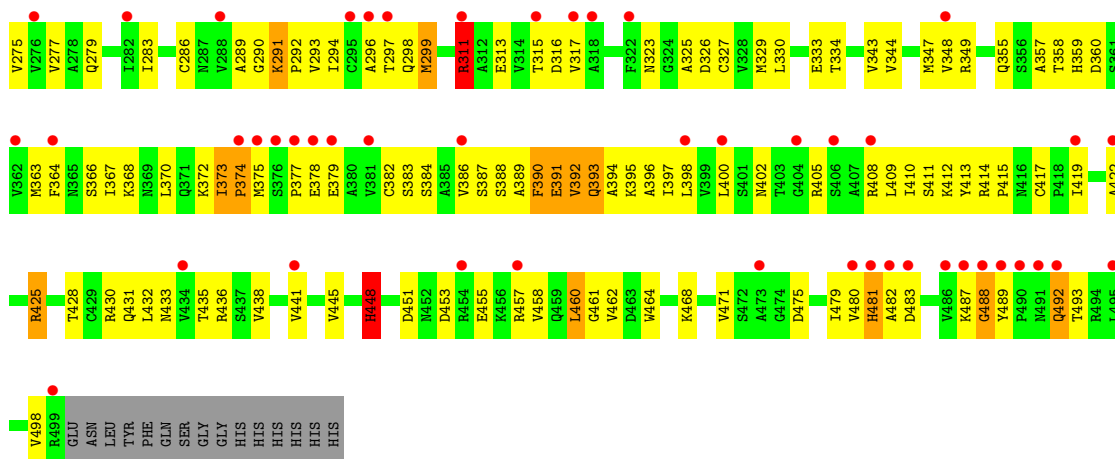


• Molecule 1: Pyruvate kinase



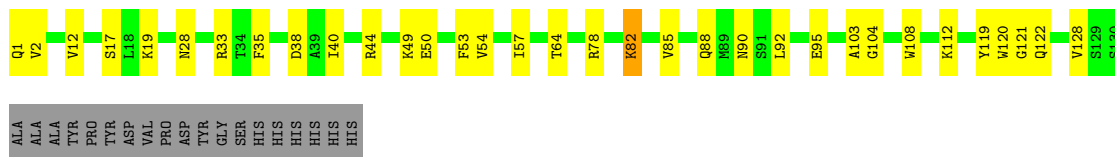
• Molecule 1: Pyruvate kinase





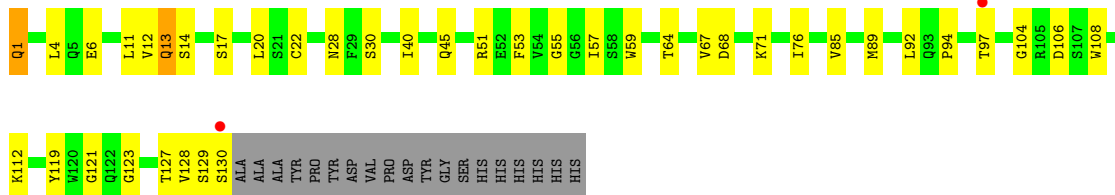
- Molecule 2: Camelid single-domain antibody 42 (sdAb42)

Chain G: 65% 21% 13%



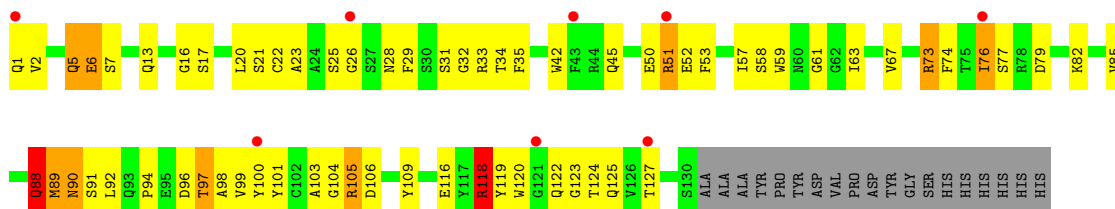
- Molecule 2: Camelid single-domain antibody 42 (sdAb42)

Chain H: 60% 26% 13%



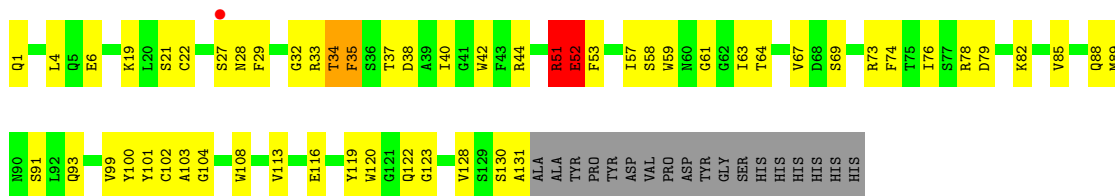
- Molecule 2: Camelid single-domain antibody 42 (sdAb42)

Chain I: 5% 43% 37% 6% 13%

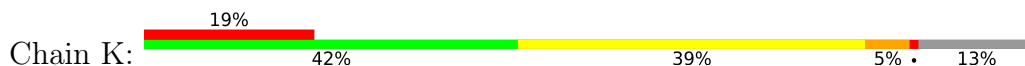


- Molecule 2: Camelid single-domain antibody 42 (sdAb42)

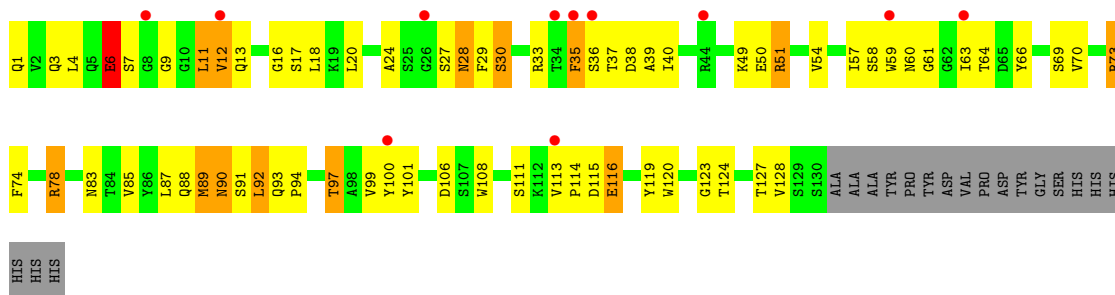
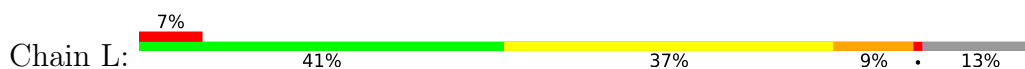
Chain J: 50% 35% 12%



• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.52Å 170.81Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.80 48.35 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.35-2.80) 99.8 (48.35-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.228 , 0.272 (Not available) , 0.261	Depositor DCC
R_{free} test set	6274 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25898	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
GOL

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	0.71	0/3744	1.03	8/5098 (0.2%)
1	B	0.69	0/3037	1.03	11/4124 (0.3%)
1	C	0.72	0/3733	1.14	22/5084 (0.4%)
1	D	0.63	0/3751	1.09	23/5107 (0.5%)
1	E	0.67	1/2958 (0.0%)	1.31	18/4015 (0.4%)
1	F	0.85	6/2940 (0.2%)	1.47	45/4002 (1.1%)
2	G	0.75	1/1018 (0.1%)	1.17	9/1377 (0.7%)
2	H	0.65	0/1021	1.02	2/1381 (0.1%)
2	I	0.80	2/999 (0.2%)	1.53	28/1356 (2.1%)
2	J	0.65	0/1030	1.21	9/1393 (0.6%)
2	K	0.78	1/989 (0.1%)	1.74	20/1343 (1.5%)
2	L	0.72	2/964 (0.2%)	1.54	29/1314 (2.2%)
All	All	0.72	13/26184 (0.0%)	1.23	224/35594 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	4
1	D	0	3
1	E	0	1
1	F	0	8
2	G	0	1
2	I	0	5
2	J	0	2
2	K	0	5
2	L	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	35

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	391	GLU	C-O	12.90	1.39	1.24
1	F	374	PRO	N-CD	10.84	1.62	1.47
2	K	91	SER	CB-OG	-9.10	1.24	1.42
2	I	88	GLN	CG-CD	-7.76	1.32	1.52
1	F	481	HIS	CA-CB	7.03	1.63	1.53
2	G	82	LYS	CE-NZ	6.20	1.68	1.49
1	F	391	GLU	CA-CB	6.07	1.63	1.53
2	L	51	ARG	CG-CD	6.00	1.70	1.52
1	F	392	VAL	C-O	-5.78	1.17	1.24
1	E	298	GLN	CD-NE2	-5.66	1.21	1.33
2	I	97	THR	CB-CG2	5.39	1.70	1.52
2	L	51	ARG	CB-CG	5.33	1.68	1.52
1	F	481	HIS	CA-C	5.30	1.59	1.52

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	361	SER	N-CA-C	35.33	152.99	112.72
2	K	90	ASN	N-CA-C	23.87	150.06	109.96
2	J	34	THR	N-CA-C	-19.58	79.67	109.24
1	F	374	PRO	N-CA-C	-19.32	72.67	112.47
2	K	50	GLU	CA-C-N	17.71	147.64	123.20
2	K	50	GLU	C-N-CA	17.71	147.64	123.20
1	D	453	ASP	N-CA-C	-16.38	86.04	110.28
1	F	17	ALA	N-CA-C	15.58	132.90	111.39
1	E	361	SER	CB-CA-C	-15.22	85.82	110.94
1	A	44	SER	CB-CA-C	-15.12	87.62	111.06
1	C	120	GLY	N-CA-C	14.96	148.64	113.18
2	L	51	ARG	CG-CD-NE	14.82	144.61	112.00
1	F	375	MET	N-CA-CB	-14.76	88.58	110.87
1	F	227	LEU	N-CA-C	-14.54	88.44	110.10
1	F	448	HIS	CA-C-N	14.50	134.12	120.34
1	F	448	HIS	C-N-CA	14.50	134.12	120.34
2	K	50	GLU	CB-CA-C	-14.15	79.74	111.30
2	J	35	PHE	N-CA-CB	-14.00	88.02	110.14
1	F	19	HIS	N-CA-C	13.98	127.26	110.91
2	G	50	GLU	CA-CB-CG	13.97	142.04	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	SER	CB-CA-C	-13.96	89.42	111.06
1	C	373	ILE	CA-C-N	13.87	137.18	119.84
1	C	373	ILE	C-N-CA	13.87	137.18	119.84
1	E	44	SER	CB-CA-C	-13.86	89.58	111.06
1	C	173	THR	N-CA-C	-13.57	90.15	109.69
1	F	391	GLU	CA-CB-CG	13.42	140.94	114.10
1	F	360	ASP	CB-CA-C	-13.40	84.53	110.65
2	I	25	SER	N-CA-C	13.32	131.94	111.56
1	E	361	SER	N-CA-CB	-13.15	91.11	110.70
1	F	44	SER	CB-CA-C	-12.90	91.06	111.06
1	C	178	ILE	CA-CB-CG1	12.82	132.20	110.40
1	D	453	ASP	CB-CA-C	12.81	131.56	109.65
1	D	92	THR	CB-CA-C	-12.77	88.91	110.24
1	C	373	ILE	N-CA-C	-12.56	95.71	108.15
1	B	485	SER	N-CA-C	12.45	133.69	107.67
1	B	485	SER	CB-CA-C	-12.39	94.37	112.09
2	K	91	SER	N-CA-CB	12.26	131.10	111.74
2	G	121	GLY	CA-C-N	-12.14	102.51	122.54
2	G	121	GLY	C-N-CA	-12.14	102.51	122.54
2	K	90	ASN	CB-CA-C	-12.05	89.65	109.53
1	D	92	THR	N-CA-C	11.87	128.47	112.68
2	L	11	LEU	CB-CA-C	-11.86	91.65	110.74
1	F	372	LYS	CB-CA-C	-11.69	86.20	109.35
1	E	360	ASP	N-CA-C	11.43	135.14	110.80
1	F	481	HIS	N-CA-C	-10.91	94.71	108.45
1	D	173	THR	N-CA-C	-10.86	93.75	109.18
1	F	227	LEU	CB-CA-C	10.73	126.64	109.90
1	F	391	GLU	CB-CG-CD	10.56	130.56	112.60
1	F	488	GLY	N-CA-C	10.46	128.81	115.21
1	E	360	ASP	CA-C-N	10.45	139.56	122.73
1	E	360	ASP	C-N-CA	10.45	139.56	122.73
1	F	448	HIS	N-CA-C	-10.43	94.68	108.34
1	F	460	LEU	CB-CG-CD2	-9.87	81.09	110.70
2	K	89	MET	CB-CA-C	-9.86	90.81	110.42
1	F	391	GLU	OE1-CD-OE2	-9.75	99.51	122.90
1	F	391	GLU	CG-CD-OE2	9.61	140.49	118.40
1	C	373	ILE	CB-CA-C	9.58	120.18	111.08
1	B	468	LYS	CB-CA-C	9.54	129.41	110.42
2	L	11	LEU	N-CA-C	9.41	124.48	108.02
1	A	298	GLN	N-CA-C	9.39	123.96	111.28
1	F	311	ARG	CB-CG-CD	-9.32	89.86	111.30
2	K	77	SER	CB-CA-C	-9.31	92.47	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	91	SER	CB-CA-C	-9.21	98.66	112.11
1	D	181	PRO	CB-CA-C	-9.20	97.91	110.88
1	D	173	THR	CB-CA-C	-9.10	92.01	111.11
1	E	362	VAL	CB-CA-C	-9.07	99.90	112.14
1	C	331	SER	N-CA-C	9.03	130.04	110.80
1	E	18	LYS	N-CA-C	-9.01	92.64	108.13
1	E	362	VAL	N-CA-C	8.94	119.74	110.62
2	I	105	ARG	CA-C-N	8.91	134.97	120.63
2	I	105	ARG	C-N-CA	8.91	134.97	120.63
2	L	13	GLN	CA-CB-CG	-8.85	96.40	114.10
1	E	468	LYS	CB-CA-C	8.80	127.53	110.46
2	I	13	GLN	N-CA-C	8.72	122.21	110.35
1	D	202	VAL	CG1-CB-CG2	-8.68	91.70	110.80
2	I	105	ARG	CB-CA-C	8.67	128.35	110.40
1	D	331	SER	N-CA-C	8.67	122.78	108.48
1	A	484	HIS	CB-CA-C	8.64	126.61	110.63
2	G	50	GLU	N-CA-CB	8.59	122.23	110.38
2	I	90	ASN	CA-C-N	8.51	134.88	122.63
2	I	90	ASN	C-N-CA	8.51	134.88	122.63
1	F	299	MET	N-CA-C	8.44	124.48	111.56
2	L	50	GLU	N-CA-CB	-8.43	96.24	110.49
2	K	50	GLU	CA-CB-CG	8.32	130.75	114.10
1	B	486	VAL	N-CA-C	-8.21	98.52	108.53
2	H	1	GLN	CB-CA-C	8.14	125.56	110.10
2	I	51	ARG	N-CA-C	-8.02	98.77	110.64
2	L	13	GLN	N-CA-CB	-7.90	97.54	110.41
1	C	173	THR	CB-CA-C	-7.88	95.31	111.22
1	E	18	LYS	CB-CA-C	7.88	121.74	110.24
1	C	183	CYS	CB-CA-C	-7.83	96.52	111.48
1	D	173	THR	CA-C-N	7.69	132.41	121.42
1	D	173	THR	C-N-CA	7.69	132.41	121.42
2	I	89	MET	CA-C-N	-7.53	107.20	121.66
2	I	89	MET	C-N-CA	-7.53	107.20	121.66
2	L	30	SER	N-CA-C	-7.51	104.08	113.55
1	A	472	SER	CB-CA-C	7.47	127.32	110.67
2	L	49	LYS	CA-C-N	7.45	135.76	121.54
2	L	49	LYS	C-N-CA	7.45	135.76	121.54
1	C	183	CYS	N-CA-C	-7.43	99.25	109.95
2	K	84	THR	CA-C-N	7.42	132.67	123.10
2	K	84	THR	C-N-CA	7.42	132.67	123.10
2	J	34	THR	CB-CA-C	7.27	126.06	110.07
2	I	25	SER	CB-CA-C	-7.24	97.49	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	360	ASP	N-CA-C	7.22	124.69	113.72
2	L	116	GLU	N-CA-CB	-7.19	98.33	110.41
2	G	82	LYS	CA-CB-CG	-7.18	99.73	114.10
2	I	51	ARG	CB-CA-C	7.18	118.63	109.80
1	D	270	ILE	CG1-CB-CG2	-7.16	89.21	110.70
2	L	50	GLU	CB-CG-CD	-7.12	100.50	112.60
2	I	91	SER	N-CA-C	-7.11	101.68	111.28
2	J	52	GLU	N-CA-C	7.10	121.15	110.64
2	L	115	ASP	CA-C-N	7.09	135.40	121.58
2	L	115	ASP	C-N-CA	7.09	135.40	121.58
2	L	35	PHE	N-CA-C	-7.06	103.52	111.07
1	C	120	GLY	CA-C-N	7.05	136.53	121.45
1	C	120	GLY	C-N-CA	7.05	136.53	121.45
2	J	52	GLU	CG-CD-OE2	-6.91	102.50	118.40
2	G	50	GLU	CB-CA-C	-6.89	96.35	111.71
1	F	375	MET	CB-CA-C	-6.88	97.31	111.22
1	F	448	HIS	CB-CA-C	-6.83	97.00	113.19
1	D	96	LYS	CB-CA-C	6.83	119.55	110.06
1	F	298	GLN	N-CA-C	6.82	120.57	111.30
2	I	91	SER	CA-C-N	6.80	131.15	121.42
2	I	91	SER	C-N-CA	6.80	131.15	121.42
1	F	213	PHE	CB-CA-C	-6.75	102.82	111.86
1	F	17	ALA	CB-CA-C	-6.72	102.34	111.89
2	K	50	GLU	N-CA-CB	6.72	119.38	110.25
2	K	91	SER	N-CA-C	6.69	120.31	111.28
2	L	12	VAL	CA-C-N	6.63	133.41	122.07
2	L	12	VAL	C-N-CA	6.63	133.41	122.07
1	F	213	PHE	N-CA-C	6.63	120.80	111.52
1	C	183	CYS	CA-C-N	6.62	132.09	122.36
1	C	183	CYS	C-N-CA	6.62	132.09	122.36
1	E	229	GLU	CA-CB-CG	-6.61	100.88	114.10
1	D	330	LEU	CB-CA-C	6.58	120.77	109.51
1	E	21	ALA	N-CA-CB	-6.57	102.31	110.98
1	C	299	MET	N-CA-C	6.56	123.29	110.56
2	I	91	SER	CA-CB-OG	6.42	123.94	111.10
1	B	454	ARG	N-CA-C	6.41	120.68	112.86
1	F	311	ARG	CD-NE-CZ	-6.40	115.43	124.40
1	D	95	PHE	CB-CA-C	6.40	120.90	109.38
1	F	408	ARG	CB-CG-CD	6.36	125.93	111.30
1	B	486	VAL	CB-CA-C	-6.34	101.65	110.91
2	I	88	GLN	CA-C-N	-6.31	111.88	122.92
2	I	88	GLN	C-N-CA	-6.31	111.88	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	331	SER	N-CA-C	6.30	124.21	110.80
1	C	453	ASP	CB-CA-C	6.28	123.58	110.32
2	G	122	GLN	N-CA-C	-6.27	105.27	113.17
1	F	244	GLN	CB-CG-CD	6.26	123.25	112.60
2	K	77	SER	N-CA-CB	6.26	120.74	110.97
2	L	91	SER	CA-C-N	6.26	130.02	120.82
2	L	91	SER	C-N-CA	6.26	130.02	120.82
1	A	489	TYR	CB-CA-C	6.19	122.36	110.17
2	L	92	LEU	CB-CG-CD2	-6.18	92.16	110.70
1	F	291	LYS	CG-CD-CE	-6.13	97.19	111.30
2	L	51	ARG	CD-NE-CZ	6.12	132.97	124.40
1	B	453	ASP	CB-CA-C	6.11	123.22	110.32
2	L	6	GLU	N-CA-C	-6.10	101.75	110.59
2	I	76	ILE	CA-CB-CG1	6.08	120.73	110.40
1	D	331	SER	CB-CA-C	-6.07	103.54	114.52
2	I	97	THR	OG1-CB-CG2	-6.06	97.18	109.30
2	J	51	ARG	CA-C-N	6.04	132.42	121.97
2	J	51	ARG	C-N-CA	6.04	132.42	121.97
1	D	95	PHE	N-CA-C	-5.91	100.08	109.59
2	J	52	GLU	CA-CB-CG	5.87	125.83	114.10
1	F	468	LYS	CB-CA-C	5.86	121.83	110.46
2	K	88	GLN	CA-CB-CG	5.86	125.82	114.10
1	F	390	PHE	CB-CA-C	-5.83	101.98	110.96
2	G	50	GLU	N-CA-C	5.82	118.38	110.35
1	F	393	GLN	CB-CA-C	-5.79	103.50	111.73
1	F	20	ARG	CB-CA-C	-5.78	102.03	110.06
2	I	6	GLU	N-CA-C	-5.77	100.73	109.85
2	H	13	GLN	CA-CB-CG	-5.76	102.57	114.10
1	D	96	LYS	N-CA-C	-5.73	101.70	110.30
1	C	472	SER	CB-CA-C	5.73	121.53	109.79
2	L	89	MET	N-CA-CB	-5.72	101.25	110.69
2	L	28	ASN	CB-CA-C	5.70	120.45	111.39
1	F	44	SER	CA-C-N	5.69	131.62	122.40
1	F	44	SER	C-N-CA	5.69	131.62	122.40
1	A	89	GLU	N-CA-C	-5.66	98.75	110.80
1	F	377	PRO	N-CA-C	5.65	119.50	110.40
2	L	91	SER	N-CA-C	5.60	118.97	111.24
1	E	208	MET	CB-CG-SD	-5.60	95.90	112.70
2	K	101	TYR	N-CA-CB	5.60	119.81	110.85
2	K	90	ASN	N-CA-CB	-5.57	101.21	110.23
2	K	49	LYS	CA-C-N	5.56	130.96	121.29
2	K	49	LYS	C-N-CA	5.56	130.96	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	296	ALA	CA-C-N	-5.55	113.07	122.67
1	D	296	ALA	C-N-CA	-5.55	113.07	122.67
1	F	244	GLN	N-CA-CB	5.50	118.80	110.28
2	L	51	ARG	CB-CG-CD	-5.50	98.66	111.30
2	I	6	GLU	CA-CB-CG	-5.44	103.21	114.10
2	I	97	THR	CA-CB-CG2	-5.40	101.33	110.50
1	C	263	ARG	CA-CB-CG	-5.38	103.33	114.10
1	F	19	HIS	CB-CA-C	-5.38	102.85	112.27
1	A	183	CYS	N-CA-C	-5.38	101.61	109.63
1	F	460	LEU	CD1-CG-CD2	-5.38	98.96	110.80
1	F	487	LYS	CB-CA-C	-5.38	99.14	111.95
2	I	118	ARG	CG-CD-NE	-5.38	100.17	112.00
1	A	66	ASN	N-CA-C	5.36	120.21	111.37
1	D	95	PHE	CA-C-N	5.35	129.77	121.26
1	D	95	PHE	C-N-CA	5.35	129.77	121.26
2	J	52	GLU	CG-CD-OE1	5.34	130.69	118.40
1	B	447	ALA	CA-C-N	-5.34	114.29	122.62
1	B	447	ALA	C-N-CA	-5.34	114.29	122.62
1	C	437	SER	CB-CA-C	-5.29	100.24	110.35
2	G	82	LYS	CB-CG-CD	5.29	123.46	111.30
1	C	203	GLU	CA-CB-CG	5.28	124.66	114.10
2	I	88	GLN	CB-CA-C	-5.28	100.62	109.53
2	L	97	THR	OG1-CB-CG2	-5.25	98.80	109.30
1	F	375	MET	N-CA-C	-5.24	102.14	109.69
2	I	76	ILE	CG1-CB-CG2	-5.15	95.24	110.70
1	E	18	LYS	CA-C-N	5.14	128.40	121.05
1	E	18	LYS	C-N-CA	5.14	128.40	121.05
1	F	23	ARG	CB-CG-CD	-5.14	99.48	111.30
2	L	50	GLU	CB-CA-C	-5.13	100.21	110.42
2	I	88	GLN	CA-CB-CG	-5.11	103.88	114.10
1	D	122	LYS	CB-CA-C	5.08	121.57	110.18
2	L	90	ASN	CA-C-N	5.03	130.07	122.68
2	L	90	ASN	C-N-CA	5.03	130.07	122.68
1	C	468	LYS	CB-CA-C	5.02	120.92	110.32
2	I	96	ASP	CB-CA-C	-5.02	105.04	111.22
1	B	299	MET	CB-CA-C	-5.02	100.43	110.42

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	372	LYS	Peptide
1	C	120	GLY	Peptide
1	C	168	ASN	Peptide
1	C	173	THR	Peptide
1	C	373	ILE	Peptide
1	D	173	THR	Peptide
1	D	195	ARG	Sidechain
1	D	499	ARG	Sidechain
1	E	360	ASP	Peptide
1	F	17	ALA	Peptide
1	F	233	ASP	Peptide
1	F	311	ARG	Sidechain
1	F	373	ILE	Peptide
1	F	425	ARG	Sidechain
1	F	44	SER	Peptide
1	F	448	HIS	Peptide
1	F	492	GLN	Peptide
2	G	49	LYS	Peptide
2	I	106	ASP	Peptide
2	I	118	ARG	Sidechain
2	I	5	GLN	Peptide
2	I	73	ARG	Sidechain
2	I	88	GLN	Sidechain
2	J	51	ARG	Peptide
2	J	52	GLU	Sidechain
2	K	101	TYR	Sidechain
2	K	50	GLU	Peptide,Mainchain
2	K	76	ILE	Peptide
2	K	90	ASN	Peptide
2	L	51	ARG	Sidechain
2	L	6	GLU	Peptide
2	L	73	ARG	Sidechain
2	L	78	ARG	Sidechain

5.2 Too-close contacts

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	3687	0	3598	169	0
1	B	2996	0	2955	139	0
1	C	3672	0	3562	196	0
1	D	3691	0	3610	179	0
1	E	2920	0	2857	152	1
1	F	2901	0	2817	184	7
2	G	995	0	932	30	1
2	H	998	0	934	35	0
2	I	976	0	891	75	0
2	J	1007	0	945	46	1
2	K	967	0	879	68	6
2	L	942	0	818	73	0
3	A	6	0	8	0	0
3	B	18	0	24	0	0
3	C	12	0	15	0	0
3	D	12	0	16	1	0
3	E	6	0	8	2	0
3	F	6	0	8	0	0
4	A	18	0	0	1	0
4	B	7	0	0	0	0
4	C	25	0	0	0	0
4	D	13	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	2	0	0	1	0
4	H	5	0	0	0	0
4	I	1	0	0	0	0
4	J	4	0	0	0	0
4	L	1	0	0	0	0
All	All	25898	0	24877	1273	8

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 25.

All (1273) 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)
2:G:82:LYS:NZ	2:G:82:LYS:CE	1.68	1.56
1:D:185:VAL:HG12	1:D:187:LEU:CD2	1.53	1.35
1:F:441:VAL:CG1	1:F:460:LEU:HD21	1.54	1.35
1:F:441:VAL:HG11	1:F:460:LEU:CD2	1.60	1.31
1:A:143:TYR:CD1	1:A:150:THR:HG22	1.66	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:O	1:B:344:VAL:HG12	1.35	1.25
2:I:16:GLY:O	2:I:92:LEU:HD12	1.27	1.25
1:A:472:SER:O	1:A:498:VAL:HG21	1.33	1.23
1:D:172:LEU:HD23	1:D:173:THR:O	1.34	1.21
1:C:27:THR:HG22	1:C:50:ARG:HD3	1.19	1.19
1:C:149:LEU:HD21	1:C:170:HIS:HB3	1.24	1.19
1:A:472:SER:O	1:A:498:VAL:CG2	1.92	1.17
1:D:185:VAL:CG1	1:D:187:LEU:CD2	2.26	1.14
2:L:11:LEU:HD23	2:L:127:THR:OG1	1.48	1.12
1:C:149:LEU:HD21	1:C:170:HIS:CB	1.80	1.11
1:C:27:THR:CG2	1:C:50:ARG:HD3	1.79	1.11
1:D:185:VAL:CG1	1:D:187:LEU:HD21	1.78	1.11
1:C:185:VAL:HG12	1:C:187:LEU:HD13	1.18	1.09
1:C:276:VAL:CG2	1:D:315:THR:HG22	1.81	1.09
2:G:1:GLN:HG2	2:G:2:VAL:H	1.02	1.09
1:A:54:SER:HA	1:A:86:LYS:HG2	1.17	1.08
1:C:149:LEU:HD21	1:C:170:HIS:CG	1.88	1.08
1:D:172:LEU:CD2	1:D:173:THR:O	2.02	1.07
2:L:18:LEU:O	2:L:89:MET:HB2	1.53	1.07
1:B:44:SER:O	1:B:344:VAL:CG1	2.02	1.07
1:D:92:THR:O	1:D:126:TYR:O	1.70	1.07
1:C:27:THR:HG21	1:C:50:ARG:HH11	0.90	1.06
2:I:16:GLY:O	2:I:92:LEU:CD1	2.04	1.05
2:G:1:GLN:HG3	2:G:28:ASN:HB2	1.38	1.04
1:C:149:LEU:CD2	1:C:170:HIS:HB3	1.87	1.04
2:H:97:THR:HG22	2:H:128:VAL:H	1.18	1.04
1:C:276:VAL:HG22	1:D:315:THR:CG2	1.89	1.03
1:C:27:THR:HG21	1:C:50:ARG:NH1	1.73	1.03
1:D:292:PRO:HA	1:D:326:ASP:OD2	1.59	1.02
1:A:143:TYR:CE1	1:A:150:THR:HG22	1.95	1.02
1:A:44:SER:O	1:A:344:VAL:CG1	2.08	1.01
1:C:27:THR:CG2	1:C:50:ARG:HH11	1.74	1.01
2:I:1:GLN:HG2	2:I:2:VAL:H	1.24	1.01
1:A:44:SER:O	1:A:344:VAL:HG12	1.57	1.01
1:C:185:VAL:CG1	1:C:187:LEU:HD13	1.90	1.01
1:F:207:ASP:OD2	1:F:430:ARG:HB3	1.61	1.00
1:C:276:VAL:HG22	1:D:315:THR:HG22	1.01	1.00
1:A:143:TYR:CE1	1:A:150:THR:CG2	2.44	1.00
1:F:441:VAL:HG12	1:F:460:LEU:HD21	1.35	1.00
1:C:149:LEU:HD11	1:C:170:HIS:ND1	1.77	1.00
1:C:179:ASN:OD1	1:C:179:ASN:O	1.79	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:441:VAL:CG1	1:F:460:LEU:CD2	2.28	0.99
2:H:13:GLN:HG3	2:H:14:SER:N	1.76	0.98
2:K:70:VAL:HB	2:K:74:PHE:CD2	1.99	0.98
1:C:303:MET:SD	1:C:343:VAL:HB	2.02	0.98
2:G:33:ARG:NH1	2:G:38:ASP:OD1	1.97	0.98
2:K:1:GLN:OE1	2:K:28:ASN:CG	2.08	0.97
1:D:451:ASP:O	1:D:457:ARG:NH2	1.96	0.96
1:F:18:LYS:O	1:F:355:GLN:NE2	1.97	0.96
1:E:27:THR:HG21	1:E:50:ARG:HH11	1.23	0.96
1:D:185:VAL:HG12	1:D:187:LEU:HD23	1.48	0.95
2:I:94:PRO:O	2:I:97:THR:OG1	1.84	0.95
1:A:90:ILE:HG23	1:A:129:TYR:HB2	1.48	0.95
1:C:185:VAL:CG1	1:C:187:LEU:CD1	2.44	0.95
2:J:79:ASP:OD2	2:J:82:LYS:NZ	1.99	0.94
1:F:289:ALA:HB1	1:F:291:LYS:HE3	1.46	0.94
2:K:70:VAL:HB	2:K:74:PHE:HD2	1.26	0.94
1:D:249:ILE:O	1:D:253:ILE:HD12	1.68	0.93
1:A:143:TYR:HD1	1:A:150:THR:HG22	1.14	0.92
1:C:185:VAL:HG11	1:C:187:LEU:HD11	1.49	0.92
2:I:1:GLN:HG2	2:I:2:VAL:N	1.82	0.92
1:A:102:TYR:CE1	1:A:172:LEU:HD12	2.05	0.92
1:C:27:THR:HG22	1:C:50:ARG:CD	2.00	0.91
1:F:270:ILE:HD11	1:F:274:LYS:HB2	1.51	0.90
2:G:1:GLN:HG2	2:G:2:VAL:N	1.74	0.90
1:F:386:VAL:HG13	1:F:415:PRO:HB3	1.54	0.90
1:C:185:VAL:HG12	1:C:187:LEU:CD1	2.01	0.89
1:A:215:ARG:HH21	1:A:219:GLN:HE22	1.17	0.89
1:A:492:GLN:HG2	1:C:494:ARG:HB3	1.54	0.89
1:E:44:SER:O	1:E:344:VAL:HG12	1.72	0.89
1:B:270:ILE:HG22	2:G:108:TRP:CH2	2.08	0.89
2:L:94:PRO:O	2:L:97:THR:OG1	1.91	0.88
1:B:239:LYS:NZ	1:B:260:MET:SD	2.45	0.88
1:D:185:VAL:HG11	1:D:187:LEU:HD21	1.53	0.88
1:C:149:LEU:HD21	1:C:170:HIS:ND1	1.88	0.88
1:D:27:THR:HG22	1:D:50:ARG:HD3	1.53	0.88
2:K:89:MET:HB3	2:K:92:LEU:HD21	1.54	0.88
2:K:82:LYS:O	2:K:84:THR:HG23	1.74	0.87
1:E:339:TYR:O	1:E:343:VAL:HG12	1.75	0.87
2:K:101:TYR:CD1	2:K:123:GLY:HA3	2.10	0.87
2:G:1:GLN:CG	2:G:2:VAL:H	1.88	0.86
1:B:270:ILE:HG22	2:G:108:TRP:CZ3	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:MET:HE2	1:F:317:VAL:HG22	1.57	0.86
1:C:243:HIS:CE1	2:I:63:ILE:HD11	2.09	0.86
1:F:349:ARG:NH1	2:L:37:THR:HG21	1.90	0.86
1:A:143:TYR:HE1	1:A:150:THR:HG21	1.40	0.86
2:I:125:GLN:OE1	2:I:127:THR:HG23	1.75	0.86
1:C:480:VAL:HG22	1:C:493:THR:HG22	1.59	0.85
1:A:41:LEU:HB3	1:A:46:MET:HE2	1.57	0.85
1:A:143:TYR:HE1	1:A:150:THR:CG2	1.88	0.84
2:K:69:SER:O	2:K:73:ARG:NH2	2.10	0.84
2:K:101:TYR:HD1	2:K:123:GLY:HA3	1.43	0.84
1:B:54:SER:HA	1:B:86:LYS:HG3	1.59	0.84
2:L:111:SER:OG	2:L:116:GLU:OE1	1.94	0.84
1:B:401:SER:HB2	1:B:406:SER:OG	1.79	0.83
1:C:247:GLN:HG3	1:D:13:PHE:CE2	2.13	0.83
1:D:41:LEU:HB3	1:D:46:MET:HE2	1.61	0.83
2:I:58:SER:HB3	2:I:63:ILE:CG2	2.08	0.83
2:I:17:SER:CB	2:I:90:ASN:HB3	2.08	0.83
2:J:51:ARG:HG2	2:J:51:ARG:HH11	1.43	0.82
2:H:11:LEU:HD12	2:H:127:THR:HB	1.60	0.82
2:G:57:ILE:HG13	2:G:64:THR:HG22	1.61	0.82
2:L:57:ILE:HD11	2:L:61:GLY:HA2	1.60	0.82
2:K:84:THR:HG1	2:K:86:TYR:HH	1.02	0.82
1:F:387:SER:O	1:F:391:GLU:HG2	1.79	0.82
1:A:5:GLN:CG	1:B:370:LEU:HD11	2.09	0.82
1:A:93:GLY:HA3	1:A:175:ARG:H	1.44	0.82
1:C:299:MET:O	1:C:300:LEU:HD23	1.79	0.81
1:C:168:ASN:HD22	1:C:170:HIS:H	1.29	0.81
2:I:58:SER:OG	2:I:63:ILE:HG22	1.80	0.81
2:I:28:ASN:HD22	2:I:33:ARG:H	1.27	0.81
1:A:143:TYR:CE1	1:A:150:THR:HG21	2.15	0.81
1:C:247:GLN:HG3	1:D:13:PHE:HE2	1.43	0.81
2:K:89:MET:O	2:K:92:LEU:HG	1.80	0.80
1:C:185:VAL:HG11	1:C:187:LEU:CD1	2.08	0.80
1:A:170:HIS:CD2	1:A:172:LEU:HD23	2.16	0.80
1:C:423:THR:HG22	1:C:425:ARG:H	1.46	0.80
1:C:172:LEU:HG	1:C:173:THR:O	1.80	0.80
1:C:303:MET:SD	1:C:343:VAL:CB	2.69	0.80
1:F:441:VAL:HG22	1:F:464:TRP:CE3	2.17	0.80
2:L:6:GLU:O	2:L:7:SER:OG	1.99	0.80
2:L:59:TRP:CD1	2:L:60:ASN:HD22	2.00	0.80
1:E:378:GLU:OE2	1:E:405:ARG:NH1	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HG12	1:D:187:LEU:HD22	1.60	0.80
1:A:51:MET:HE3	1:A:53:PHE:HE1	1.46	0.79
2:K:35:PHE:HE2	2:K:85:VAL:HG23	1.46	0.79
1:B:260:MET:HG3	1:B:294:ILE:HB	1.65	0.79
1:E:300:LEU:HG	1:E:347:MET:HE2	1.62	0.79
1:F:441:VAL:HG11	1:F:460:LEU:CG	2.12	0.79
1:E:414:ARG:HG3	1:E:436:ARG:HH21	1.48	0.79
1:A:227:LEU:HD13	1:A:234:THR:CG2	2.13	0.78
1:F:411:SER:OG	1:F:436:ARG:O	2.01	0.78
2:K:57:ILE:HD12	2:K:77:SER:HA	1.63	0.78
1:D:27:THR:HG23	1:D:330:LEU:O	1.84	0.78
1:F:62:GLN:HE22	1:F:204:GLN:HG3	1.48	0.77
2:I:1:GLN:CG	2:I:2:VAL:H	1.96	0.77
1:B:486:VAL:HG22	1:B:487:LYS:H	1.49	0.77
2:L:58:SER:O	2:L:78:ARG:NH1	2.16	0.77
1:B:355:GLN:O	1:B:358:THR:HG22	1.84	0.77
1:D:249:ILE:HG13	1:D:253:ILE:HD11	1.65	0.77
1:A:5:GLN:HG2	1:B:370:LEU:HD11	1.65	0.77
1:E:27:THR:HG22	1:E:50:ARG:HB3	1.64	0.77
2:K:84:THR:OG1	2:K:86:TYR:OH	1.85	0.76
1:F:363:MET:O	1:F:367:ILE:HG13	1.85	0.76
1:A:143:TYR:CD1	1:A:150:THR:CG2	2.56	0.75
1:D:473:ALA:HA	1:D:498:VAL:HG23	1.68	0.75
1:F:395:LYS:HG3	1:F:475:ASP:HB3	1.66	0.75
1:E:480:VAL:HG22	1:E:493:THR:HG22	1.68	0.75
1:C:92:THR:HG22	1:C:178:ILE:HD12	1.66	0.75
1:E:7:ASN:HA	1:E:10:LEU:HG	1.68	0.75
1:C:280:MET:HE1	1:D:322:PHE:CE2	2.22	0.75
1:D:377:PRO:O	1:D:381:VAL:HG23	1.87	0.75
1:F:383:SER:O	1:F:387:SER:OG	2.03	0.75
2:J:42:TRP:HD1	2:J:76:ILE:HD13	1.49	0.75
2:I:5:GLN:O	2:I:23:ALA:N	2.16	0.75
1:A:54:SER:CA	1:A:86:LYS:HG2	2.09	0.74
1:D:149:LEU:HD23	1:D:170:HIS:HB3	1.68	0.74
1:A:195:ARG:O	1:A:199:GLN:OE1	2.05	0.74
1:D:299:MET:O	1:D:300:LEU:HD23	1.88	0.74
1:F:3:GLN:O	1:F:7:ASN:ND2	2.20	0.74
1:F:397:ILE:HD12	1:F:417:CYS:SG	2.28	0.74
1:C:62:GLN:HG3	1:C:66:ASN:HD21	1.53	0.73
2:L:11:LEU:CD2	2:L:127:THR:OG1	2.31	0.73
2:L:27:SER:HB2	2:L:33:ARG:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:69:SER:O	2:L:73:ARG:NH2	2.21	0.73
1:C:104:PRO:HD3	1:C:169:HIS:CE1	2.23	0.73
2:H:97:THR:CG2	2:H:128:VAL:H	1.97	0.73
1:C:315:THR:HG22	1:D:276:VAL:HG22	1.70	0.73
1:A:227:LEU:HD13	1:A:234:THR:HG23	1.70	0.73
1:E:454:ARG:HD2	1:E:481:HIS:CD2	2.24	0.73
1:E:298:GLN:HA	1:E:301:GLU:HG3	1.70	0.72
1:A:170:HIS:CD2	1:A:172:LEU:CD2	2.72	0.72
1:F:279:GLN:OE1	1:F:323:ASN:ND2	2.22	0.72
1:C:243:HIS:CE1	2:I:63:ILE:CD1	2.71	0.72
1:D:299:MET:HE3	1:D:317:VAL:HG22	1.70	0.72
1:D:38:LEU:O	1:D:42:MET:HG3	1.89	0.72
1:F:283:ILE:HA	1:F:293:VAL:HG21	1.71	0.72
1:F:441:VAL:HG11	1:F:460:LEU:HD23	1.67	0.72
1:B:401:SER:HB2	1:B:406:SER:HG	1.54	0.72
1:D:228:GLY:O	1:D:232:LYS:HG2	1.90	0.72
1:E:44:SER:O	1:E:344:VAL:CG1	2.38	0.72
1:B:38:LEU:O	1:B:42:MET:HG3	1.91	0.71
1:F:214:ILE:HG22	1:F:252:ILE:HD13	1.72	0.71
2:L:114:PRO:HB3	2:L:120:TRP:HH2	1.55	0.71
1:A:2:SER:N	1:A:359:HIS:NE2	2.39	0.71
1:B:198:LEU:HD12	1:B:227:LEU:HD21	1.71	0.71
1:B:431:GLN:O	1:B:434:VAL:HG12	1.89	0.71
1:F:432:LEU:HD13	1:F:438:VAL:HG11	1.72	0.71
1:C:144:VAL:HG13	1:C:178:ILE:HG13	1.71	0.71
1:C:311:ARG:HH11	1:C:315:THR:HG21	1.54	0.71
1:E:27:THR:HG21	1:E:50:ARG:NH1	2.03	0.71
1:B:270:ILE:CG2	2:G:108:TRP:CH2	2.74	0.71
1:A:472:SER:C	1:A:498:VAL:HG21	2.13	0.71
1:C:473:ALA:HA	1:C:498:VAL:HG12	1.71	0.71
2:I:28:ASN:HD21	2:I:31:SER:H	1.36	0.71
1:B:386:VAL:HG13	1:B:415:PRO:HB3	1.70	0.71
2:I:104:GLY:HA3	2:I:119:TYR:CE1	2.26	0.71
1:B:192:GLU:HA	1:B:195:ARG:HG3	1.73	0.71
1:C:149:LEU:CD1	1:C:170:HIS:ND1	2.53	0.70
1:C:471:VAL:HG21	1:C:477:MET:HE2	1.71	0.70
1:B:452:ASN:OD1	1:B:453:ASP:N	2.24	0.70
1:C:154:LEU:HD11	1:C:165:HIS:HB2	1.72	0.70
1:E:349:ARG:HD2	2:K:32:GLY:O	1.90	0.70
1:A:44:SER:O	1:A:344:VAL:HG11	1.91	0.70
1:B:242:ASN:ND2	1:B:244:GLN:OE1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:SER:OG	1:E:490:PRO:CG	2.39	0.70
2:I:58:SER:CB	2:I:63:ILE:HG22	2.20	0.70
1:B:65:ILE:CG2	1:B:69:ARG:HH11	2.04	0.70
1:C:451:ASP:HB3	1:C:457:ARG:HH11	1.57	0.70
1:A:47:SER:HB3	1:A:433:ASN:HB3	1.73	0.70
1:F:387:SER:C	1:F:391:GLU:HG2	2.17	0.70
1:A:270:ILE:HG22	2:H:108:TRP:CH2	2.27	0.69
1:A:406:SER:OG	1:A:490:PRO:CG	2.40	0.69
1:A:480:VAL:HG22	1:A:493:THR:HG22	1.73	0.69
1:F:270:ILE:HG23	1:F:275:VAL:HG22	1.73	0.69
1:A:492:GLN:OE1	1:C:492:GLN:NE2	2.25	0.69
2:L:1:GLN:HG3	2:L:28:ASN:HD21	1.57	0.69
1:F:363:MET:CE	1:F:367:ILE:HD11	2.22	0.69
1:F:471:VAL:HG11	1:F:498:VAL:HG11	1.74	0.69
1:A:53:PHE:O	1:A:86:LYS:CE	2.41	0.69
1:A:170:HIS:HD2	1:A:172:LEU:CD2	2.04	0.69
1:F:53:PHE:HB2	1:F:84:ASP:O	1.92	0.69
2:L:33:ARG:HH12	2:L:106:ASP:HA	1.57	0.69
1:B:294:ILE:HG23	1:B:327:CYS:HB2	1.75	0.69
1:F:38:LEU:O	1:F:42:MET:HG3	1.93	0.69
1:F:395:LYS:HE3	1:F:475:ASP:CG	2.17	0.69
2:I:17:SER:HB3	2:I:90:ASN:HB3	1.73	0.69
1:E:454:ARG:HD2	1:E:481:HIS:HD2	1.55	0.68
1:F:224:ARG:HG2	1:F:236:ILE:HD11	1.75	0.68
2:H:97:THR:HG22	2:H:128:VAL:N	2.01	0.68
2:K:1:GLN:OE1	2:K:28:ASN:OD1	2.10	0.68
1:D:451:ASP:O	1:D:453:ASP:O	2.11	0.68
1:E:408:ARG:HG2	1:E:435:THR:HG21	1.75	0.68
1:F:290:GLY:HA2	1:F:412:LYS:HB2	1.76	0.68
1:C:247:GLN:CG	1:D:13:PHE:HE2	2.06	0.68
1:E:35:VAL:HG23	1:E:67:ASN:OD1	1.92	0.68
1:B:192:GLU:H	1:B:192:GLU:CD	2.00	0.68
1:F:234:THR:HA	1:F:431:GLN:NE2	2.09	0.68
1:A:93:GLY:CA	1:A:175:ARG:H	2.06	0.68
1:A:94:LEU:HB3	1:A:118:LYS:HA	1.75	0.68
1:B:42:MET:HE2	1:B:79:ILE:HG13	1.76	0.68
1:A:276:VAL:HG22	1:B:315:THR:HG22	1.76	0.68
1:C:42:MET:HE1	1:C:71:ALA:C	2.20	0.67
1:F:44:SER:O	1:F:344:VAL:HG22	1.94	0.67
2:J:6:GLU:H	2:J:122:GLN:NE2	1.92	0.67
1:F:386:VAL:HG21	1:F:413:TYR:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:11:LEU:HD23	2:L:127:THR:HG1	1.59	0.67
1:A:102:TYR:CE2	1:A:108:VAL:HG21	2.29	0.67
1:A:39:LYS:HG3	1:A:71:ALA:HB1	1.76	0.67
1:E:27:THR:HG23	1:E:330:LEU:O	1.95	0.67
1:C:102:TYR:O	1:C:168:ASN:ND2	2.24	0.66
1:E:271:PRO:HB2	1:E:273:GLU:HG3	1.76	0.66
1:E:87:GLY:N	1:E:194:ASP:OD1	2.23	0.66
2:L:113:VAL:HB	2:L:116:GLU:HG3	1.78	0.66
1:E:283:ILE:HD13	1:E:325:ALA:HB2	1.77	0.66
2:K:59:TRP:CD1	2:K:108:TRP:HB2	2.31	0.66
2:J:6:GLU:OE2	2:J:101:TYR:HA	1.96	0.66
1:A:278:ALA:HB2	1:B:12:ILE:HD12	1.77	0.66
1:B:190:VAL:HG22	1:B:195:ARG:HG2	1.76	0.66
1:D:240:ILE:HD13	1:D:259:ILE:HG23	1.78	0.66
1:A:471:VAL:HG21	1:A:477:MET:HE2	1.78	0.66
2:L:88:GLN:NE2	2:L:90:ASN:OD1	2.28	0.66
1:D:213:PHE:CE2	1:D:215:ARG:HD3	2.30	0.66
2:I:122:GLN:NE2	2:I:124:THR:OG1	2.26	0.66
2:K:13:GLN:NE2	2:K:130:SER:O	2.28	0.66
1:B:38:LEU:HD13	1:B:68:VAL:HG12	1.78	0.65
2:G:82:LYS:NZ	2:G:82:LYS:CD	2.58	0.65
2:K:105:ARG:NH1	2:K:116:GLU:OE1	2.30	0.65
1:A:315:THR:HG22	1:B:276:VAL:HG22	1.76	0.65
1:B:377:PRO:O	1:B:381:VAL:HG23	1.96	0.65
1:D:51:MET:HE3	1:D:53:PHE:HE1	1.61	0.65
2:K:1:GLN:OE1	2:K:28:ASN:ND2	2.30	0.65
1:B:463:ASP:O	1:B:467:THR:HG23	1.97	0.65
2:I:58:SER:CB	2:I:63:ILE:CG2	2.75	0.65
1:E:26:CYS:SG	1:E:46:MET:HG3	2.36	0.65
1:D:402:ASN:O	1:D:428:THR:HG21	1.97	0.64
2:I:42:TRP:HD1	2:I:76:ILE:HD12	1.62	0.64
1:B:398:LEU:HB3	1:B:479:ILE:HD13	1.78	0.64
1:F:2:SER:OG	1:F:359:HIS:NE2	2.23	0.64
2:K:6:GLU:CD	2:K:123:GLY:HA2	2.22	0.64
1:A:170:HIS:HD2	1:A:172:LEU:HD21	1.63	0.64
1:C:27:THR:O	1:C:334:THR:HG23	1.97	0.64
2:J:51:ARG:HG2	2:J:51:ARG:NH1	2.09	0.64
2:L:1:GLN:HG2	2:L:119:TYR:CD2	2.33	0.64
1:A:102:TYR:O	1:A:169:HIS:HA	1.98	0.64
1:F:445:VAL:O	1:F:448:HIS:O	2.16	0.64
1:F:441:VAL:CG1	1:F:460:LEU:CG	2.73	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:VAL:HG11	1:E:498:VAL:HG11	1.80	0.64
2:J:40:ILE:HG21	2:J:85:VAL:HG11	1.80	0.64
1:C:243:HIS:O	1:C:246:VAL:HG22	1.98	0.63
1:C:299:MET:HE3	1:C:317:VAL:HG22	1.80	0.63
1:C:2:SER:N	1:C:359:HIS:NE2	2.45	0.63
1:C:143:TYR:O	1:C:178:ILE:HG23	1.98	0.63
2:H:40:ILE:HG21	2:H:85:VAL:HG11	1.79	0.63
2:J:42:TRP:CD1	2:J:76:ILE:HD13	2.31	0.63
2:K:42:TRP:CG	2:K:87:LEU:HD12	2.33	0.63
1:E:324:GLY:O	1:E:414:ARG:NH2	2.32	0.63
1:F:441:VAL:HG22	1:F:464:TRP:HE3	1.62	0.63
1:D:249:ILE:HG13	1:D:253:ILE:CD1	2.28	0.63
1:E:27:THR:CG2	1:E:50:ARG:HH11	2.04	0.63
1:A:94:LEU:HB3	1:A:118:LYS:HG3	1.79	0.63
1:E:249:ILE:HG12	1:E:282:ILE:CD1	2.27	0.63
2:K:73:ARG:NH1	2:K:96:ASP:OD2	2.32	0.63
1:E:198:LEU:HD13	1:E:227:LEU:HD21	1.81	0.63
2:I:45:GLN:HB3	2:I:99:VAL:HG13	1.80	0.63
2:L:39:ALA:HA	2:L:78:ARG:HH12	1.64	0.63
2:L:113:VAL:O	2:L:116:GLU:HB2	1.97	0.63
1:E:214:ILE:HG22	1:E:252:ILE:HD13	1.80	0.63
1:E:345:GLN:HG3	2:K:32:GLY:HA2	1.80	0.62
1:F:330:LEU:HD21	1:F:343:VAL:HG22	1.80	0.62
1:B:378:GLU:HG3	1:B:489:TYR:HD2	1.64	0.62
1:C:477:MET:HE3	1:C:498:VAL:CG2	2.29	0.62
1:F:198:LEU:O	1:F:202:VAL:HG22	1.99	0.62
2:H:13:GLN:HE22	2:H:130:SER:C	2.05	0.62
2:I:6:GLU:O	2:I:6:GLU:HG2	1.81	0.62
1:A:400:LEU:HD22	1:A:422:ALA:HB3	1.80	0.62
1:E:274:LYS:O	1:E:274:LYS:HG2	1.99	0.62
1:D:217:ALA:HB2	1:D:251:ALA:HB1	1.81	0.62
1:F:363:MET:HE3	1:F:367:ILE:HD11	1.81	0.62
1:A:263:ARG:NH2	1:A:316:ASP:OD1	2.33	0.62
1:C:144:VAL:HG12	1:C:145:ASP:H	1.65	0.62
2:L:28:ASN:O	2:L:29:PHE:CD2	2.53	0.62
2:K:74:PHE:CD1	2:K:89:MET:HA	2.34	0.62
2:H:13:GLN:HE22	2:H:130:SER:HA	1.65	0.62
1:A:94:LEU:O	1:A:118:LYS:O	2.18	0.62
1:B:52:ASN:OD1	1:B:54:SER:OG	2.18	0.62
1:D:88:PRO:O	1:D:187:LEU:HD12	2.00	0.62
1:E:241:GLU:HB2	1:E:265:ASP:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:HIS:ND1	1:F:359:HIS:HA	2.15	0.62
2:L:57:ILE:HD13	2:L:64:THR:HG22	1.82	0.62
1:A:39:LYS:O	1:A:43:LYS:HG3	1.99	0.62
1:A:93:GLY:HA3	1:A:175:ARG:N	2.12	0.62
1:C:317:VAL:HG21	1:C:347:MET:HE1	1.81	0.61
1:D:94:LEU:HB2	1:D:118:LYS:HA	1.82	0.61
1:F:189:ALA:HB2	1:F:219:GLN:HE21	1.64	0.61
2:L:28:ASN:O	2:L:29:PHE:HD2	1.83	0.61
1:A:299:MET:HE3	1:A:317:VAL:HG22	1.82	0.61
1:C:300:LEU:HG	1:C:347:MET:HE3	1.82	0.61
1:D:471:VAL:HG23	1:D:475:ASP:HB2	1.82	0.61
1:F:384:SER:O	1:F:388:SER:OG	2.15	0.61
2:L:59:TRP:NE1	2:L:60:ASN:HD22	1.98	0.61
1:A:270:ILE:HG13	1:A:275:VAL:HG22	1.81	0.61
1:E:406:SER:OG	1:E:490:PRO:HG3	2.00	0.61
1:F:398:LEU:HD12	1:F:461:GLY:HA3	1.83	0.61
1:C:62:GLN:O	1:C:66:ASN:ND2	2.33	0.61
1:F:69:ARG:NH2	1:F:204:GLN:O	2.34	0.61
1:C:149:LEU:CD2	1:C:170:HIS:ND1	2.63	0.61
1:C:224:ARG:HE	1:C:236:ILE:HD12	1.65	0.61
1:B:441:VAL:HG11	1:B:460:LEU:HG	1.82	0.61
1:F:3:GLN:NE2	1:F:357:ALA:O	2.33	0.61
1:A:215:ARG:HH21	1:A:219:GLN:NE2	1.94	0.61
1:B:494:ARG:HG2	1:D:492:GLN:HB2	1.80	0.61
1:F:218:ASP:O	1:F:222:GLU:HG3	2.00	0.61
1:D:427:LEU:O	1:D:431:GLN:HG3	2.01	0.60
1:B:492:GLN:HE21	1:D:492:GLN:HE21	1.49	0.60
1:C:299:MET:CE	1:C:317:VAL:HG22	2.31	0.60
1:D:27:THR:CG2	1:D:50:ARG:HD3	2.29	0.60
2:K:38:ASP:HB2	2:K:105:ARG:O	2.01	0.60
1:A:90:ILE:HB	1:A:178:ILE:HB	1.82	0.60
1:B:265:ASP:O	1:B:268:VAL:HG22	2.01	0.60
1:D:202:VAL:HG11	1:D:231:GLY:HA3	1.82	0.60
2:G:1:GLN:HB2	2:G:28:ASN:HA	1.83	0.60
2:L:92:LEU:HB3	2:L:128:VAL:HG21	1.84	0.60
1:B:328:VAL:HG21	1:B:347:MET:HE3	1.83	0.60
1:B:447:ALA:C	1:B:448:HIS:HD1	2.10	0.60
1:E:402:ASN:HB3	1:E:425:ARG:HE	1.67	0.60
1:F:43:LYS:O	2:L:29:PHE:HB3	2.00	0.60
2:J:34:THR:O	2:J:37:THR:OG1	2.20	0.60
2:L:39:ALA:HB2	2:L:108:TRP:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:OG1	1:A:160:CYS:HB2	2.01	0.60
1:C:486:VAL:HG11	1:C:491:ASN:HD21	1.67	0.60
1:E:28:ILE:HG21	1:E:64:THR:HG23	1.84	0.60
1:F:7:ASN:HA	1:F:10:LEU:HG	1.83	0.60
2:L:73:ARG:NH1	2:L:93:GLN:HG3	2.17	0.60
1:C:27:THR:HG22	1:C:50:ARG:HB3	1.83	0.60
1:C:276:VAL:CG2	1:D:315:THR:CG2	2.66	0.60
1:C:28:ILE:HD12	1:C:38:LEU:HD21	1.83	0.60
1:D:83:LEU:HB3	1:D:209:ILE:HD13	1.83	0.60
1:D:279:GLN:O	1:D:283:ILE:HG13	2.02	0.60
1:F:25:ILE:HB	1:F:329:MET:HG3	1.84	0.60
1:B:492:GLN:NE2	1:D:492:GLN:HE21	2.00	0.59
1:F:373:ILE:HG22	1:F:373:ILE:O	2.02	0.59
1:A:2:SER:N	1:A:359:HIS:HE2	2.00	0.59
1:A:41:LEU:HB3	1:A:46:MET:CE	2.30	0.59
1:F:349:ARG:HH12	2:L:37:THR:HG21	1.66	0.59
2:G:19:LYS:HD3	2:G:88:GLN:NE2	2.17	0.59
1:B:387:SER:O	1:B:391:GLU:HG3	2.02	0.59
1:D:114:PRO:O	1:D:117:GLU:HB2	2.03	0.59
1:E:363:MET:HE2	1:E:367:ILE:HD11	1.84	0.59
2:J:44:ARG:NH2	2:J:52:GLU:OE2	2.34	0.59
1:C:388:SER:O	1:C:392:VAL:HG22	2.02	0.59
2:I:17:SER:HB2	2:I:90:ASN:HB3	1.82	0.59
2:K:42:TRP:HD1	2:K:76:ILE:HD13	1.66	0.59
1:A:87:GLY:O	1:A:89:GLU:HG2	2.03	0.59
1:A:311:ARG:HD2	1:B:275:VAL:HG11	1.83	0.59
2:J:1:GLN:HE21	2:J:28:ASN:HB2	1.67	0.59
1:A:311:ARG:HH22	1:B:316:ASP:CG	2.10	0.59
1:A:340:PRO:O	1:A:343:VAL:HG12	2.02	0.59
1:B:33:GLN:HG3	1:B:64:THR:HG22	1.84	0.59
1:E:405:ARG:HG2	1:E:405:ARG:HH11	1.68	0.59
1:A:463:ASP:O	1:A:467:THR:HG23	2.02	0.59
1:F:458:VAL:O	1:F:462:VAL:HG23	2.03	0.59
2:L:92:LEU:HD22	2:L:128:VAL:HG21	1.83	0.59
1:F:65:ILE:O	1:F:69:ARG:HG3	2.03	0.59
2:K:27:SER:HB3	2:K:29:PHE:CE2	2.38	0.59
1:C:143:TYR:HB3	1:C:147:GLY:HA2	1.84	0.59
2:L:33:ARG:HB3	2:L:38:ASP:OD1	2.03	0.59
2:L:1:GLN:HG3	2:L:28:ASN:ND2	2.17	0.58
1:B:34:SER:OG	1:B:37:ALA:CB	2.50	0.58
1:A:12:ILE:HG13	1:B:274:LYS:HD3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:VAL:HG21	1:F:413:TYR:CB	2.33	0.58
1:C:42:MET:HE3	1:C:75:LEU:HD12	1.86	0.58
1:F:207:ASP:OD2	1:F:430:ARG:CB	2.45	0.58
2:I:28:ASN:ND2	2:I:33:ARG:H	1.99	0.58
1:A:270:ILE:HG22	2:H:108:TRP:CZ3	2.37	0.58
1:E:218:ASP:HA	1:E:221:ARG:HG2	1.84	0.58
1:E:454:ARG:CD	1:E:481:HIS:HD2	2.16	0.58
1:F:270:ILE:CD1	1:F:274:LYS:HB2	2.29	0.58
1:F:330:LEU:HD22	1:F:334:THR:HG23	1.84	0.58
1:F:194:ASP:O	1:F:198:LEU:HD12	2.03	0.58
2:I:20:LEU:HD21	2:I:100:TYR:HD2	1.67	0.58
2:K:91:SER:O	2:K:91:SER:OG	1.97	0.58
1:A:311:ARG:O	1:A:315:THR:HG23	2.04	0.58
1:E:84:ASP:HA	1:E:210:PHE:HB2	1.85	0.58
1:C:285:LYS:NZ	1:D:8:ILE:O	2.37	0.58
1:D:27:THR:HG21	1:D:50:ARG:HH11	1.69	0.58
1:E:213:PHE:HD1	1:E:241:GLU:HG3	1.67	0.58
1:E:239:LYS:HD2	1:E:260:MET:HE2	1.83	0.58
1:E:415:PRO:HG2	1:E:419:ILE:HD11	1.84	0.58
1:F:388:SER:HA	1:F:391:GLU:HG3	1.86	0.58
1:A:299:MET:HE2	1:A:347:MET:HE1	1.85	0.58
1:D:146:ASP:H	1:D:148:VAL:HG23	1.68	0.58
1:F:248:ASN:O	1:F:252:ILE:HG13	2.04	0.58
1:F:482:ALA:HB2	1:F:489:TYR:O	2.03	0.58
1:F:62:GLN:NE2	1:F:62:GLN:HA	2.19	0.58
2:I:116:GLU:C	2:I:118:ARG:HH12	2.12	0.58
1:A:210:PHE:CD2	1:A:260:MET:HE1	2.39	0.57
1:F:441:VAL:HG11	1:F:460:LEU:HD21	1.22	0.57
2:H:13:GLN:HE22	2:H:130:SER:CA	2.17	0.57
1:A:378:GLU:HG3	1:A:489:TYR:CD1	2.39	0.57
1:A:260:MET:SD	1:A:329:MET:HE1	2.44	0.57
1:A:353:GLU:OE2	1:B:274:LYS:NZ	2.28	0.57
1:F:219:GLN:O	1:F:223:VAL:HG23	2.04	0.57
2:I:73:ARG:C	2:I:74:PHE:HD1	2.12	0.57
1:A:486:VAL:HG11	1:A:489:TYR:O	2.03	0.57
1:E:241:GLU:HB3	1:E:262:ALA:HB3	1.87	0.57
1:F:236:ILE:N	1:F:257:ASP:OD2	2.32	0.57
1:F:294:ILE:HG12	1:F:327:CYS:HB2	1.85	0.57
2:J:58:SER:HB3	2:J:63:ILE:HB	1.87	0.57
1:B:2:SER:N	1:B:359:HIS:HE2	2.02	0.57
1:C:218:ASP:O	1:C:222:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ILE:HB	1:D:329:MET:HG3	1.87	0.57
1:E:41:LEU:HB3	1:E:46:MET:HE2	1.86	0.57
2:I:50:GLU:O	2:I:51:ARG:C	2.47	0.57
1:B:64:THR:O	1:B:68:VAL:HG13	2.05	0.57
1:C:62:GLN:HG3	1:C:66:ASN:ND2	2.19	0.57
1:F:3:GLN:OE1	1:F:7:ASN:ND2	2.37	0.57
2:H:53:PHE:O	2:H:67:VAL:HG21	2.04	0.57
2:K:3:GLN:O	2:K:24:ALA:HA	2.05	0.57
1:C:14:GLU:HG3	1:C:15:PRO:HD2	1.87	0.57
1:F:400:LEU:HD12	1:F:422:ALA:HB3	1.86	0.57
1:D:458:VAL:O	1:D:462:VAL:HG23	2.05	0.56
1:D:359:HIS:HB3	1:D:362:VAL:HG23	1.86	0.56
1:A:93:GLY:O	1:A:94:LEU:HB2	2.05	0.56
1:A:102:TYR:HE2	1:A:108:VAL:HG21	1.67	0.56
1:C:2:SER:N	1:C:359:HIS:HE2	2.02	0.56
1:E:6:HIS:CD2	1:E:10:LEU:HD21	2.40	0.56
1:F:61:HIS:HA	1:F:64:THR:HG22	1.88	0.56
1:A:53:PHE:O	1:A:86:LYS:HE2	2.05	0.56
1:A:273:GLU:HG2	1:A:274:LYS:N	2.19	0.56
1:C:42:MET:CE	1:C:75:LEU:HD12	2.36	0.56
1:C:477:MET:HE3	1:C:498:VAL:HG21	1.87	0.56
1:F:289:ALA:HB1	1:F:291:LYS:CE	2.29	0.56
1:F:289:ALA:CB	1:F:291:LYS:HE3	2.28	0.56
1:B:34:SER:OG	1:B:37:ALA:HB3	2.05	0.56
1:E:256:SER:O	1:E:291:LYS:NZ	2.30	0.56
1:A:53:PHE:O	1:A:86:LYS:CG	2.53	0.56
1:A:148:VAL:O	1:A:168:ASN:ND2	2.34	0.56
1:F:388:SER:O	1:F:392:VAL:HG12	2.06	0.56
2:G:33:ARG:NH2	4:G:201:HOH:O	2.39	0.56
2:I:6:GLU:HG3	2:I:124:THR:OG1	2.05	0.56
1:C:280:MET:HE1	1:D:322:PHE:HE2	1.71	0.56
2:J:100:TYR:O	2:J:123:GLY:HA2	2.06	0.56
2:I:28:ASN:ND2	2:I:31:SER:H	2.04	0.56
1:D:188:PRO:O	1:D:215:ARG:NH2	2.37	0.55
1:E:69:ARG:NH2	1:E:204:GLN:O	2.38	0.55
1:E:416:ASN:CG	1:E:416:ASN:O	2.48	0.55
2:H:13:GLN:HG3	2:H:14:SER:H	1.63	0.55
2:L:106:ASP:OD1	2:L:106:ASP:N	2.37	0.55
1:A:451:ASP:OD1	1:A:454:ARG:CA	2.54	0.55
1:C:303:MET:SD	1:C:343:VAL:HA	2.46	0.55
1:C:336:LYS:O	1:C:336:LYS:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ILE:O	1:D:430:ARG:HG2	2.05	0.55
1:D:144:VAL:HG12	1:D:145:ASP:H	1.71	0.55
2:G:95:GLU:N	2:G:95:GLU:OE1	2.40	0.55
1:A:274:LYS:HD3	1:B:353:GLU:OE1	2.05	0.55
1:E:261:VAL:HG22	1:E:295:CYS:HA	1.89	0.55
2:L:89:MET:CE	2:L:92:LEU:HD21	2.36	0.55
1:A:378:GLU:CD	1:A:378:GLU:H	2.14	0.55
1:C:64:THR:O	1:C:68:VAL:HG13	2.05	0.55
1:C:150:THR:HG23	1:C:167:ASN:HB2	1.89	0.55
1:D:158:ASP:HB2	1:D:161:THR:HG22	1.89	0.55
1:A:332:GLY:HA2	1:A:335:ALA:HB3	1.89	0.55
1:D:300:LEU:HG	1:D:347:MET:HE1	1.87	0.55
1:B:44:SER:O	1:B:344:VAL:HG11	2.00	0.55
1:B:214:ILE:HG22	1:B:252:ILE:HD13	1.89	0.55
1:C:451:ASP:OD2	1:C:457:ARG:HD3	2.07	0.55
2:I:7:SER:OG	2:I:21:SER:HB3	2.07	0.55
1:A:377:PRO:O	1:A:381:VAL:HG23	2.07	0.55
1:E:38:LEU:HD13	1:E:68:VAL:HG12	1.88	0.55
1:C:322:PHE:CE2	1:D:280:MET:HE1	2.42	0.55
1:A:366:SER:O	1:A:370:LEU:HD22	2.05	0.55
1:D:34:SER:OG	1:D:37:ALA:CB	2.55	0.55
2:K:51:ARG:HE	2:K:114:PRO:HB2	1.72	0.55
1:C:270:ILE:HD12	1:D:12:ILE:HD12	1.88	0.54
1:C:451:ASP:O	1:C:457:ARG:NH1	2.41	0.54
1:E:198:LEU:O	1:E:202:VAL:HG13	2.07	0.54
2:L:36:SER:C	2:L:38:ASP:H	2.15	0.54
1:B:190:VAL:HG11	1:B:195:ARG:HH11	1.72	0.54
1:B:443:TYR:OH	1:B:449:GLY:O	2.24	0.54
2:I:74:PHE:HD1	2:I:74:PHE:N	2.05	0.54
2:K:1:GLN:HG2	2:K:28:ASN:HA	1.89	0.54
1:D:158:ASP:HB2	1:D:161:THR:CG2	2.36	0.54
1:D:388:SER:O	1:D:392:VAL:HG22	2.07	0.54
2:H:6:GLU:CD	2:H:123:GLY:H	2.15	0.54
2:K:77:SER:O	2:K:86:TYR:HD1	1.90	0.54
1:A:5:GLN:HG3	1:B:370:LEU:HD11	1.86	0.54
1:B:54:SER:HA	1:B:86:LYS:CG	2.33	0.54
1:C:92:THR:HG23	1:C:176:LYS:O	2.07	0.54
1:E:303:MET:HE3	1:E:307:PRO:O	2.08	0.54
1:C:27:THR:HG22	1:C:50:ARG:CG	2.38	0.54
1:C:444:ASP:HB3	1:C:447:ALA:HB3	1.90	0.54
2:H:104:GLY:HA3	2:H:119:TYR:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:O	1:A:232:LYS:HG2	2.08	0.54
1:B:342:GLU:OE1	1:B:342:GLU:N	2.36	0.54
1:C:420:ILE:CD1	1:C:465:ALA:HB2	2.38	0.54
1:E:454:ARG:CG	1:E:481:HIS:HD2	2.20	0.54
2:I:28:ASN:HD21	2:I:31:SER:N	2.02	0.54
1:B:199:GLN:O	1:B:203:GLU:HG3	2.07	0.54
1:C:423:THR:HG21	1:C:428:THR:HB	1.89	0.54
1:E:364:PHE:HZ	1:E:387:SER:OG	1.90	0.54
2:L:35:PHE:CD2	2:L:83:ASN:HA	2.42	0.54
1:B:471:VAL:HG12	1:B:498:VAL:HG21	1.90	0.54
1:C:311:ARG:NH1	1:C:315:THR:HG21	2.23	0.54
2:J:6:GLU:N	2:J:122:GLN:NE2	2.56	0.54
1:D:148:VAL:HB	1:D:170:HIS:CD2	2.43	0.54
1:E:364:PHE:HZ	1:E:387:SER:HG	1.52	0.54
1:A:26:CYS:HB2	1:A:46:MET:HG3	1.90	0.54
1:A:451:ASP:OD2	1:A:457:ARG:HB2	2.07	0.54
1:A:473:ALA:HA	1:A:498:VAL:HG23	1.90	0.54
1:B:39:LYS:O	1:B:43:LYS:HG3	2.08	0.54
1:F:26:CYS:HB2	1:F:46:MET:HE3	1.89	0.54
1:F:460:LEU:HD23	1:F:460:LEU:C	2.33	0.54
2:K:18:LEU:O	2:K:89:MET:HG3	2.08	0.53
2:L:113:VAL:HB	2:L:116:GLU:CG	2.37	0.53
1:E:402:ASN:HB2	1:E:425:ARG:HH21	1.72	0.53
2:J:4:LEU:HD13	2:J:22:CYS:SG	2.48	0.53
1:A:316:ASP:CG	1:B:311:ARG:HH22	2.15	0.53
1:A:363:MET:HE3	1:A:414:ARG:HG3	1.89	0.53
1:B:213:PHE:HD1	1:B:241:GLU:HG3	1.73	0.53
1:B:406:SER:O	1:B:410:ILE:HG12	2.08	0.53
1:C:303:MET:SD	1:C:343:VAL:CA	2.96	0.53
1:E:48:VAL:HG11	1:E:208:MET:HE3	1.88	0.53
1:A:246:VAL:HG11	1:B:12:ILE:HG21	1.91	0.53
1:E:217:ALA:O	1:E:220:VAL:HG12	2.08	0.53
1:E:416:ASN:O	1:E:416:ASN:ND2	2.41	0.53
2:K:35:PHE:CE1	2:K:83:ASN:HA	2.44	0.53
2:L:70:VAL:HB	2:L:74:PHE:CD2	2.44	0.53
2:G:1:GLN:CG	2:G:28:ASN:HB2	2.27	0.53
1:A:266:LEU:O	1:A:270:ILE:HG12	2.09	0.53
1:C:228:GLY:O	1:C:231:GLY:N	2.36	0.53
1:C:423:THR:CG2	1:C:425:ARG:H	2.20	0.53
1:E:271:PRO:C	1:E:273:GLU:N	2.66	0.53
1:F:405:ARG:O	1:F:409:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:111:SER:O	2:K:117:TYR:OH	2.13	0.53
1:A:13:PHE:CZ	1:B:247:GLN:HG3	2.43	0.53
1:C:92:THR:HG22	1:C:178:ILE:CD1	2.38	0.53
1:D:454:ARG:HA	1:D:457:ARG:HH21	1.73	0.53
1:C:168:ASN:HD22	1:C:170:HIS:N	2.03	0.53
2:H:94:PRO:O	2:H:97:THR:HG23	2.09	0.53
1:B:48:VAL:HG11	1:B:208:MET:CE	2.39	0.53
1:B:208:MET:HB3	1:B:235:LEU:HB2	1.90	0.53
1:C:377:PRO:O	1:C:381:VAL:HG23	2.09	0.53
1:D:145:ASP:HB3	1:D:148:VAL:HG23	1.91	0.53
1:D:229:GLU:OE2	1:D:232:LYS:HB2	2.09	0.53
1:E:65:ILE:O	1:E:69:ARG:HG3	2.09	0.53
1:F:16:VAL:HG23	1:F:17:ALA:H	1.74	0.53
1:F:23:ARG:HG3	1:F:433:ASN:O	2.09	0.53
2:G:103:ALA:HB2	2:G:120:TRP:CE3	2.44	0.53
2:I:63:ILE:HD13	2:I:109:TYR:HE1	1.73	0.53
1:C:127:VAL:HG21	1:C:132:LEU:HD22	1.91	0.53
1:F:82:ALA:HB2	1:F:208:MET:HE3	1.90	0.53
2:H:57:ILE:HG13	2:H:64:THR:HG22	1.91	0.53
2:J:44:ARG:NE	2:J:52:GLU:OE2	2.41	0.53
2:K:9:GLY:H	2:K:124:THR:HG21	1.73	0.53
1:C:53:PHE:HD2	1:C:197:ASP:OD2	1.92	0.52
1:A:8:ILE:O	1:B:285:LYS:NZ	2.42	0.52
1:D:283:ILE:HD13	1:D:325:ALA:HB2	1.91	0.52
2:I:74:PHE:N	2:I:74:PHE:CD1	2.75	0.52
1:F:27:THR:C	1:F:28:ILE:HD13	2.35	0.52
2:J:6:GLU:N	2:J:122:GLN:HE22	2.06	0.52
2:I:89:MET:HE1	2:I:100:TYR:CE2	2.44	0.52
2:I:101:TYR:HB3	2:I:120:TRP:CZ3	2.45	0.52
1:B:192:GLU:CD	1:B:192:GLU:N	2.67	0.52
1:E:345:GLN:HG3	2:K:32:GLY:CA	2.39	0.52
1:A:102:TYR:HE1	1:A:172:LEU:HD12	1.70	0.52
1:A:311:ARG:HH21	1:A:315:THR:HG21	1.75	0.52
1:A:458:VAL:O	1:A:462:VAL:HG23	2.10	0.52
1:B:194:ASP:O	1:B:198:LEU:HD23	2.09	0.52
1:D:27:THR:CG2	1:D:50:ARG:HH11	2.22	0.52
1:D:34:SER:OG	1:D:37:ALA:HB2	2.10	0.52
1:D:94:LEU:HD12	1:D:118:LYS:HG3	1.92	0.52
1:D:471:VAL:HG21	1:D:498:VAL:HG11	1.92	0.52
1:F:483:ASP:N	1:F:483:ASP:OD1	2.42	0.52
2:K:57:ILE:HD11	2:K:61:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG11	1:B:208:MET:HE3	1.92	0.52
1:D:131:GLN:O	1:D:131:GLN:HG2	2.10	0.52
2:K:92:LEU:HB3	2:K:128:VAL:HG21	1.92	0.52
1:A:264:GLY:N	1:A:297:THR:OG1	2.41	0.52
1:C:311:ARG:O	1:C:315:THR:HG23	2.10	0.52
1:D:451:ASP:C	1:D:453:ASP:O	2.53	0.52
1:F:3:GLN:HG2	1:F:359:HIS:HB2	1.91	0.52
2:L:1:GLN:HG2	2:L:119:TYR:HD2	1.75	0.52
1:C:143:TYR:HD1	1:C:181:PRO:HD3	1.73	0.52
1:D:41:LEU:HB3	1:D:46:MET:CE	2.37	0.52
1:D:185:VAL:CG1	1:D:187:LEU:HD23	2.18	0.52
1:E:27:THR:HG22	1:E:50:ARG:HD3	1.90	0.52
1:F:264:GLY:N	1:F:297:THR:OG1	2.40	0.52
2:L:101:TYR:CD1	2:L:123:GLY:HA3	2.45	0.52
1:B:68:VAL:CG2	1:B:81:ILE:HD11	2.40	0.51
1:C:149:LEU:CD2	1:C:170:HIS:CB	2.61	0.51
2:I:42:TRP:CD1	2:I:76:ILE:HD12	2.45	0.51
1:A:94:LEU:CB	1:A:118:LYS:HA	2.39	0.51
1:A:406:SER:OG	1:A:490:PRO:HG2	2.09	0.51
1:C:399:VAL:HG21	1:C:406:SER:OG	2.10	0.51
1:D:62:GLN:HE22	1:D:204:GLN:HG3	1.75	0.51
1:E:16:VAL:HG21	1:E:353:GLU:OE2	2.10	0.51
1:F:3:GLN:HE21	1:F:358:THR:HA	1.74	0.51
2:L:54:VAL:HG13	2:L:70:VAL:HG11	1.91	0.51
1:D:432:LEU:HD13	1:D:438:VAL:HG11	1.92	0.51
1:F:6:HIS:HE1	1:F:358:THR:O	1.92	0.51
2:H:14:SER:HA	2:H:92:LEU:O	2.09	0.51
2:K:74:PHE:CE1	2:K:89:MET:HA	2.44	0.51
1:E:213:PHE:CD2	1:E:215:ARG:HD2	2.46	0.51
1:A:459:GLN:HG3	1:A:463:ASP:OD1	2.11	0.51
1:C:208:MET:HE2	1:C:210:PHE:CE1	2.46	0.51
1:D:240:ILE:HD11	1:D:259:ILE:HD12	1.93	0.51
2:G:1:GLN:HB2	2:G:28:ASN:CA	2.40	0.51
2:G:1:GLN:NE2	2:G:119:TYR:CD1	2.78	0.51
2:G:17:SER:HB3	2:G:90:ASN:HA	1.93	0.51
2:K:5:GLN:OE1	2:K:122:GLN:HG3	2.10	0.51
1:A:270:ILE:HG13	1:A:275:VAL:CG2	2.40	0.51
1:C:279:GLN:O	1:C:283:ILE:HG13	2.11	0.51
1:A:381:VAL:HG21	1:A:491:ASN:HA	1.93	0.51
1:B:61:HIS:O	1:B:65:ILE:HD12	2.11	0.51
1:D:38:LEU:HD13	1:D:68:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:GLN:OE1	2:H:28:ASN:CG	2.54	0.51
1:A:16:VAL:HG21	1:A:352:ILE:HG22	1.93	0.51
1:D:263:ARG:HH11	1:D:279:GLN:HE22	1.59	0.51
1:F:62:GLN:HA	1:F:62:GLN:HE21	1.76	0.51
2:I:103:ALA:HB2	2:I:120:TRP:CE3	2.45	0.51
1:B:398:LEU:HD11	1:B:461:GLY:HA3	1.93	0.51
1:E:239:LYS:HD2	1:E:260:MET:CE	2.41	0.51
1:F:214:ILE:CG2	1:F:252:ILE:HD13	2.39	0.51
1:F:398:LEU:CD1	1:F:461:GLY:HA3	2.40	0.51
2:J:74:PHE:CZ	2:J:89:MET:HG2	2.45	0.51
1:B:328:VAL:CG2	1:B:347:MET:HE3	2.41	0.51
1:C:95:PHE:HZ	1:C:125:PHE:CD2	2.29	0.50
1:D:202:VAL:CG1	1:D:231:GLY:HA3	2.40	0.50
1:E:408:ARG:CG	1:E:435:THR:HG21	2.41	0.50
1:F:239:LYS:HG2	1:F:260:MET:HE2	1.93	0.50
1:F:293:VAL:O	1:F:326:ASP:HB2	2.11	0.50
1:B:473:ALA:HA	1:B:498:VAL:HG23	1.92	0.50
1:E:459:GLN:NE2	1:E:463:ASP:OD1	2.44	0.50
1:F:313:GLU:O	1:F:316:ASP:HB3	2.11	0.50
2:K:101:TYR:CE1	2:K:123:GLY:HA3	2.47	0.50
2:L:92:LEU:HD22	2:L:128:VAL:CG2	2.41	0.50
1:C:4:LEU:CD2	1:D:367:ILE:HD12	2.42	0.50
1:C:61:HIS:O	1:C:65:ILE:HG13	2.10	0.50
1:C:94:LEU:HD13	1:C:95:PHE:N	2.27	0.50
1:E:265:ASP:O	1:E:268:VAL:HG12	2.11	0.50
1:E:441:VAL:CG1	1:E:460:LEU:HG	2.41	0.50
1:D:499:ARG:HH11	1:D:499:ARG:H	1.58	0.50
1:E:349:ARG:HG3	2:K:31:SER:O	2.12	0.50
1:A:53:PHE:O	1:A:86:LYS:HE3	2.10	0.50
1:E:13:PHE:O	2:K:105:ARG:NH2	2.45	0.50
1:B:432:LEU:HD13	1:B:438:VAL:HG11	1.91	0.50
1:C:235:LEU:HD11	1:C:431:GLN:HB3	1.94	0.50
1:C:355:GLN:O	1:C:358:THR:HG22	2.11	0.50
1:D:270:ILE:C	1:D:270:ILE:HD12	2.37	0.50
1:A:494:ARG:HD2	1:A:496:VAL:HG12	1.93	0.50
1:B:311:ARG:HH21	1:B:315:THR:HG21	1.76	0.50
1:E:491:ASN:CG	1:E:491:ASN:O	2.54	0.50
2:J:93:GLN:C	2:J:128:VAL:HG11	2.36	0.50
1:E:441:VAL:HG11	1:E:460:LEU:HG	1.93	0.50
1:F:373:ILE:HA	1:F:374:PRO:C	2.37	0.50
1:F:400:LEU:HD21	1:F:457:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2:VAL:HG22	2:I:26:GLY:O	2.12	0.50
2:K:113:VAL:HB	2:K:116:GLU:HG3	1.94	0.50
1:E:294:ILE:HG23	1:E:327:CYS:HB2	1.94	0.50
1:F:259:ILE:HB	1:F:286:CYS:SG	2.51	0.50
2:G:40:ILE:HG21	2:G:85:VAL:HG21	1.94	0.50
2:J:27:SER:HB2	2:J:34:THR:HG22	1.94	0.50
1:C:258:GLY:O	1:C:259:ILE:HD13	2.12	0.49
1:D:154:LEU:HD11	1:D:165:HIS:HB2	1.94	0.49
1:A:406:SER:OG	1:A:490:PRO:CD	2.60	0.49
1:B:241:GLU:HB2	1:B:265:ASP:HB3	1.93	0.49
1:C:91:ARG:H	1:C:128:ASP:CB	2.24	0.49
1:C:91:ARG:H	1:C:128:ASP:HB2	1.77	0.49
1:E:261:VAL:O	1:E:263:ARG:HG2	2.12	0.49
2:G:53:PHE:CD1	2:G:112:LYS:HA	2.47	0.49
1:C:42:MET:HE1	1:C:72:ALA:N	2.27	0.49
1:E:299:MET:O	1:E:300:LEU:HD23	2.12	0.49
1:F:453:ASP:O	1:F:455:GLU:N	2.46	0.49
2:K:35:PHE:HE1	2:K:80:ASN:HA	1.78	0.49
1:A:199:GLN:O	1:A:203:GLU:HB2	2.13	0.49
1:F:263:ARG:HA	1:F:266:LEU:HB3	1.93	0.49
1:D:14:GLU:OE2	1:D:15:PRO:HD2	2.12	0.49
1:D:270:ILE:HD13	1:D:274:LYS:HB2	1.95	0.49
1:F:378:GLU:O	1:F:379:GLU:C	2.56	0.49
1:F:451:ASP:OD2	1:F:457:ARG:HD2	2.13	0.49
2:K:103:ALA:HB2	2:K:120:TRP:CD1	2.48	0.49
1:A:104:PRO:HB3	1:A:167:ASN:O	2.13	0.49
1:B:311:ARG:O	1:B:315:THR:HG23	2.13	0.49
1:B:439:GLU:OE1	1:B:470:TYR:OH	2.27	0.49
1:C:102:TYR:C	1:C:168:ASN:HD21	2.15	0.49
1:D:113:ASP:OD1	1:D:113:ASP:C	2.56	0.49
1:F:192:GLU:HA	1:F:195:ARG:HD3	1.95	0.49
1:F:239:LYS:HZ3	1:F:260:MET:HE1	1.78	0.49
2:I:45:GLN:HB3	2:I:99:VAL:CG1	2.42	0.49
2:L:89:MET:HE2	2:L:92:LEU:HD21	1.93	0.49
1:B:486:VAL:HG22	1:B:487:LYS:N	2.24	0.49
1:C:247:GLN:HG3	1:D:13:PHE:CZ	2.46	0.49
1:D:2:SER:N	1:D:359:HIS:CE1	2.81	0.49
1:E:38:LEU:HD23	1:E:38:LEU:HA	1.49	0.49
1:E:242:ASN:HB2	1:E:269:GLU:OE1	2.13	0.49
2:I:6:GLU:OE2	2:I:122:GLN:NE2	2.46	0.49
1:A:294:ILE:HG12	1:A:327:CYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HZ3	1:A:475:ASP:CG	2.21	0.49
1:B:198:LEU:HD12	1:B:227:LEU:CD2	2.38	0.49
1:B:271:PRO:HG2	1:B:274:LYS:HG3	1.94	0.49
1:C:330:LEU:HD11	1:C:347:MET:HG3	1.95	0.49
1:C:483:ASP:OD2	1:C:485:SER:HB2	2.13	0.49
1:D:270:ILE:HD11	1:D:275:VAL:CG2	2.43	0.49
1:E:28:ILE:HG21	1:E:64:THR:CG2	2.42	0.49
1:F:395:LYS:HE3	1:F:475:ASP:CB	2.42	0.49
1:F:488:GLY:O	1:F:489:TYR:HB3	2.12	0.49
2:G:57:ILE:HG13	2:G:64:THR:CG2	2.39	0.49
1:B:61:HIS:C	1:B:65:ILE:HD12	2.38	0.49
1:F:64:THR:O	1:F:68:VAL:HG12	2.13	0.49
1:A:149:LEU:HB2	1:A:170:HIS:CD2	2.48	0.49
1:C:471:VAL:HG13	1:C:475:ASP:HB2	1.94	0.49
1:F:396:ALA:HA	1:F:417:CYS:HB2	1.94	0.49
1:F:398:LEU:CD2	1:F:479:ILE:HG23	2.43	0.49
2:G:1:GLN:NE2	2:G:119:TYR:HD1	2.11	0.49
2:H:45:GLN:HG3	2:H:51:ARG:HA	1.94	0.49
1:C:247:GLN:CG	1:D:13:PHE:CE2	2.89	0.48
1:E:475:ASP:O	1:E:498:VAL:HG22	2.12	0.48
1:F:240:ILE:HD11	1:F:252:ILE:HG21	1.95	0.48
1:F:414:ARG:CZ	1:F:436:ARG:HD2	2.42	0.48
2:H:59:TRP:H	2:H:59:TRP:CD1	2.30	0.48
1:A:316:ASP:OD1	1:B:311:ARG:NH2	2.45	0.48
1:E:215:ARG:NE	1:E:219:GLN:HE22	2.12	0.48
1:E:453:ASP:OD1	1:E:453:ASP:O	2.31	0.48
1:F:42:MET:HE2	1:F:79:ILE:HG13	1.94	0.48
2:I:5:GLN:O	2:I:22:CYS:HA	2.12	0.48
2:J:113:VAL:HB	2:J:116:GLU:HG3	1.95	0.48
2:K:1:GLN:HB3	2:K:2:VAL:H	1.42	0.48
1:C:279:GLN:HE21	1:C:323:ASN:HD22	1.61	0.48
1:D:96:LYS:HD2	1:D:96:LYS:HA	1.75	0.48
1:D:117:GLU:HB3	1:D:118:LYS:NZ	2.27	0.48
1:D:133:PRO:HA	1:D:162:LEU:HD11	1.95	0.48
1:E:405:ARG:HH11	1:E:405:ARG:CG	2.26	0.48
2:K:6:GLU:HB3	2:K:22:CYS:HB2	1.96	0.48
1:A:257:ASP:O	1:A:292:PRO:HD2	2.14	0.48
1:B:84:ASP:HA	1:B:210:PHE:HB2	1.95	0.48
1:B:483:ASP:CB	1:D:494:ARG:NH1	2.77	0.48
1:C:104:PRO:HG3	1:C:168:ASN:O	2.13	0.48
1:E:418:PRO:HG2	1:E:470:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASP:OD1	1:A:454:ARG:HA	2.13	0.48
1:C:345:GLN:NE2	2:J:32:GLY:HA2	2.28	0.48
1:E:283:ILE:HA	1:E:293:VAL:HG11	1.96	0.48
1:A:153:VAL:HA	1:A:164:CYS:SG	2.54	0.48
1:C:420:ILE:HD11	1:C:465:ALA:HB2	1.95	0.48
1:E:279:GLN:O	1:E:283:ILE:HG13	2.14	0.48
1:F:54:SER:HA	1:F:86:LYS:HG3	1.95	0.48
1:F:367:ILE:HA	1:F:370:LEU:HB2	1.96	0.48
2:J:130:SER:O	2:J:131:ALA:HB3	2.13	0.48
1:C:263:ARG:HD2	1:C:279:GLN:OE1	2.14	0.48
1:E:27:THR:O	1:E:334:THR:OG1	2.31	0.48
1:E:249:ILE:HG12	1:E:282:ILE:HD13	1.96	0.48
1:E:419:ILE:O	1:E:438:VAL:HA	2.14	0.48
1:F:330:LEU:HB3	1:F:333:GLU:HB2	1.96	0.48
1:F:374:PRO:CD	1:F:374:PRO:O	2.51	0.48
2:H:53:PHE:CD2	2:H:112:LYS:HA	2.49	0.48
2:I:53:PHE:O	2:I:67:VAL:HG21	2.12	0.48
1:F:366:SER:O	1:F:370:LEU:HD13	2.13	0.48
1:F:216:THR:N	1:F:219:GLN:OE1	2.39	0.48
1:E:271:PRO:O	1:E:273:GLU:N	2.47	0.47
1:F:479:ILE:O	1:F:493:THR:HA	2.13	0.47
1:E:386:VAL:HG21	1:E:413:TYR:HB2	1.96	0.47
1:F:6:HIS:CD2	1:F:10:LEU:HD21	2.49	0.47
1:F:250:ASP:O	1:F:253:ILE:HG22	2.14	0.47
1:D:213:PHE:O	1:D:215:ARG:HG3	2.14	0.47
1:A:12:ILE:HG22	1:A:13:PHE:CE2	2.49	0.47
1:A:227:LEU:CD1	1:A:234:THR:HG23	2.42	0.47
1:B:250:ASP:OD1	1:B:285:LYS:HE3	2.14	0.47
1:C:112:THR:HG22	1:C:127:VAL:HG23	1.96	0.47
1:D:412:LYS:HD3	1:D:413:TYR:CE2	2.50	0.47
1:E:27:THR:OG1	1:E:331:SER:O	2.31	0.47
1:E:208:MET:HB3	1:E:235:LEU:HB2	1.95	0.47
2:L:101:TYR:HD1	2:L:123:GLY:HA3	1.80	0.47
1:A:94:LEU:HB3	1:A:118:LYS:CA	2.44	0.47
1:A:161:THR:C	1:A:162:LEU:HD12	2.39	0.47
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.79	0.47
1:D:198:LEU:O	1:D:202:VAL:HG22	2.14	0.47
1:F:42:MET:HE2	1:F:79:ILE:CG1	2.45	0.47
1:C:311:ARG:HH21	1:D:298:GLN:HB2	1.80	0.47
2:G:1:GLN:CG	2:G:2:VAL:N	2.53	0.47
2:J:22:CYS:HB3	2:J:85:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:104:GLY:HA3	2:J:119:TYR:CZ	2.49	0.47
1:B:482:ALA:HB1	1:B:486:VAL:HG11	1.97	0.47
1:D:258:GLY:O	1:D:259:ILE:HD13	2.13	0.47
1:D:264:GLY:H	1:D:297:THR:CB	2.28	0.47
1:E:75:LEU:CB	1:E:77:LEU:HD22	2.44	0.47
1:C:427:LEU:O	1:C:431:GLN:HG3	2.14	0.47
1:D:104:PRO:HD3	1:D:169:HIS:HB2	1.97	0.47
1:D:397:ILE:HD12	1:D:417:CYS:SG	2.54	0.47
1:E:83:LEU:HD13	1:E:201:GLY:HA3	1.97	0.47
1:E:300:LEU:HG	1:E:347:MET:CE	2.40	0.47
1:E:432:LEU:HD13	1:E:438:VAL:HG11	1.96	0.47
1:E:492:GLN:C	1:E:493:THR:HG23	2.40	0.47
1:F:46:MET:HE2	1:F:49:ALA:HA	1.96	0.47
2:K:89:MET:O	2:K:92:LEU:CG	2.59	0.47
1:C:90:ILE:HD12	1:C:129:TYR:HB2	1.96	0.47
1:D:345:GLN:HG2	2:I:32:GLY:HA2	1.97	0.47
1:E:27:THR:HG22	1:E:50:ARG:CB	2.39	0.47
1:E:406:SER:O	1:E:410:ILE:HG12	2.15	0.47
2:G:44:ARG:HG2	2:G:54:VAL:CG2	2.45	0.47
1:D:270:ILE:CD1	1:D:275:VAL:HG23	2.45	0.47
1:B:495:LEU:HD22	1:D:381:VAL:HG22	1.97	0.46
1:C:43:LYS:O	2:J:29:PHE:HB3	2.15	0.46
1:C:202:VAL:CG2	1:C:227:LEU:HD23	2.44	0.46
1:C:272:ALA:O	1:C:273:GLU:C	2.57	0.46
1:E:239:LYS:NZ	3:E:601:GOL:H11	2.30	0.46
1:E:271:PRO:O	1:E:274:LYS:N	2.49	0.46
1:F:88:PRO:HD3	1:F:189:ALA:O	2.15	0.46
2:H:6:GLU:OE2	2:H:121:GLY:HA3	2.14	0.46
2:I:88:GLN:HG3	2:I:89:MET:N	2.31	0.46
2:J:103:ALA:HB2	2:J:120:TRP:CE3	2.50	0.46
2:L:20:LEU:HD12	2:L:87:LEU:HD23	1.97	0.46
1:F:364:PHE:CD2	1:F:390:PHE:HE2	2.33	0.46
1:F:402:ASN:OD1	1:F:457:ARG:NH2	2.48	0.46
1:C:4:LEU:HD21	1:D:367:ILE:HD12	1.98	0.46
1:C:402:ASN:HA	1:C:423:THR:HG23	1.96	0.46
1:E:364:PHE:CZ	1:E:387:SER:OG	2.66	0.46
1:E:477:MET:CE	1:E:498:VAL:CG1	2.93	0.46
2:L:100:TYR:O	2:L:123:GLY:HA2	2.15	0.46
1:C:27:THR:HG22	1:C:50:ARG:CB	2.46	0.46
1:C:131:GLN:O	1:C:135:VAL:HG12	2.16	0.46
1:F:6:HIS:CE1	1:F:358:THR:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ALA:O	1:B:282:ILE:HG13	2.16	0.46
1:B:467:THR:O	1:B:468:LYS:C	2.59	0.46
1:C:311:ARG:HH11	1:C:315:THR:CG2	2.27	0.46
1:D:27:THR:HG21	1:D:50:ARG:NH1	2.31	0.46
1:E:239:LYS:HZ1	3:E:601:GOL:H11	1.79	0.46
1:E:274:LYS:O	1:E:274:LYS:CG	2.62	0.46
2:I:22:CYS:HB3	2:I:85:VAL:HG13	1.97	0.46
2:L:36:SER:C	2:L:38:ASP:N	2.73	0.46
1:A:54:SER:O	1:A:55:HIS:ND1	2.42	0.46
1:C:32:THR:HA	1:C:37:ALA:HB1	1.97	0.46
1:C:215:ARG:HB2	1:C:219:GLN:OE1	2.16	0.46
2:L:40:ILE:HG21	2:L:85:VAL:HG11	1.97	0.46
1:A:281:CYS:SG	1:A:285:LYS:HE2	2.56	0.46
1:B:38:LEU:CD1	1:B:68:VAL:HG12	2.43	0.46
2:L:1:GLN:HE21	2:L:28:ASN:HD21	1.64	0.46
1:B:249:ILE:O	1:B:253:ILE:HG13	2.15	0.46
1:B:260:MET:HE3	1:B:294:ILE:HD12	1.96	0.46
1:B:420:ILE:CD1	1:B:465:ALA:HB2	2.46	0.46
1:C:486:VAL:CG1	1:C:491:ASN:HD21	2.27	0.46
1:D:172:LEU:HD23	1:D:173:THR:N	2.31	0.46
2:I:77:SER:O	2:I:85:VAL:HG23	2.16	0.46
2:L:16:GLY:C	2:L:92:LEU:HD12	2.41	0.46
2:L:36:SER:C	2:L:37:THR:HG23	2.41	0.46
2:L:58:SER:HB3	2:L:63:ILE:HG23	1.97	0.46
1:D:5:GLN:O	1:D:8:ILE:HG13	2.15	0.46
1:F:5:GLN:O	1:F:8:ILE:HG13	2.16	0.46
1:F:61:HIS:O	1:F:65:ILE:HD12	2.16	0.46
1:F:333:GLU:OE1	1:F:333:GLU:N	2.40	0.46
1:F:410:ILE:HD11	1:F:480:VAL:HG11	1.98	0.46
2:J:6:GLU:HA	2:J:21:SER:O	2.16	0.46
2:K:6:GLU:CG	2:K:123:GLY:HA2	2.46	0.46
1:A:213:PHE:N	1:A:241:GLU:OE2	2.49	0.46
1:D:141:LEU:O	1:D:181:PRO:HD2	2.15	0.46
1:D:144:VAL:HG13	1:D:178:ILE:CD1	2.46	0.46
1:D:151:LEU:N	1:D:151:LEU:HD22	2.31	0.46
1:E:224:ARG:CZ	1:E:236:ILE:HG13	2.46	0.46
1:F:389:ALA:HB2	1:F:397:ILE:HD11	1.98	0.46
1:A:53:PHE:O	1:A:86:LYS:HG2	2.16	0.45
1:C:471:VAL:HG11	1:C:498:VAL:HG21	1.97	0.45
1:E:388:SER:O	1:E:392:VAL:HG22	2.16	0.45
1:E:436:ARG:O	1:E:437:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:GLY:CA	1:F:412:LYS:HB2	2.44	0.45
2:K:44:ARG:CB	2:K:100:TYR:HA	2.46	0.45
1:A:95:PHE:O	1:A:98:GLY:N	2.41	0.45
1:A:472:SER:O	1:A:498:VAL:HG23	2.05	0.45
1:B:65:ILE:HG21	1:B:69:ARG:HH11	1.78	0.45
1:B:224:ARG:HE	1:B:236:ILE:HG13	1.82	0.45
1:F:292:PRO:HG3	1:F:435:THR:HG22	1.99	0.45
2:H:1:GLN:OE1	2:H:28:ASN:CB	2.65	0.45
2:H:55:GLY:HA3	2:H:76:ILE:HD11	1.99	0.45
2:J:53:PHE:HD2	2:J:67:VAL:HG13	1.81	0.45
1:A:102:TYR:CD2	1:A:108:VAL:HG21	2.50	0.45
1:C:319:ASN:OD1	1:D:319:ASN:ND2	2.44	0.45
1:D:78:HIS:N	1:D:78:HIS:CD2	2.85	0.45
2:G:1:GLN:OE1	2:G:1:GLN:N	2.45	0.45
1:C:116:PHE:CD1	1:C:116:PHE:N	2.85	0.45
1:C:235:LEU:HA	1:C:257:ASP:OD2	2.16	0.45
1:D:22:ASN:HB2	1:D:351:CYS:SG	2.56	0.45
1:D:270:ILE:HG22	2:J:108:TRP:CH2	2.51	0.45
1:D:331:SER:N	1:D:333:GLU:OE1	2.49	0.45
1:E:261:VAL:O	1:E:261:VAL:HG23	2.17	0.45
1:F:270:ILE:HD11	1:F:274:LYS:CB	2.34	0.45
2:I:7:SER:N	2:I:21:SER:O	2.50	0.45
2:K:1:GLN:CD	2:K:28:ASN:CG	2.82	0.45
1:D:140:GLY:O	1:D:153:VAL:HG22	2.16	0.45
1:D:253:ILE:O	1:D:291:LYS:NZ	2.49	0.45
1:E:420:ILE:HD12	1:E:465:ALA:HB2	1.98	0.45
1:F:26:CYS:SG	1:F:46:MET:HG3	2.56	0.45
1:F:75:LEU:HB2	1:F:77:LEU:HD12	1.99	0.45
1:F:191:SER:O	1:F:195:ARG:HD2	2.16	0.45
1:F:234:THR:HA	1:F:431:GLN:HE22	1.81	0.45
1:F:330:LEU:HG	1:F:347:MET:HE2	1.97	0.45
2:H:20:LEU:HG	2:H:89:MET:HE3	1.99	0.45
2:L:4:LEU:HD12	2:L:120:TRP:HA	1.98	0.45
1:A:281:CYS:O	1:A:285:LYS:HG3	2.16	0.45
1:B:26:CYS:HB2	1:B:46:MET:SD	2.57	0.45
1:B:53:PHE:HD2	1:B:197:ASP:OD2	1.99	0.45
1:C:149:LEU:HD11	1:C:170:HIS:CE1	2.48	0.45
1:D:270:ILE:HD11	1:D:275:VAL:HG23	1.98	0.45
1:D:426:LEU:HA	1:D:426:LEU:HD23	1.63	0.45
1:E:345:GLN:O	1:E:349:ARG:HD3	2.17	0.45
1:A:140:GLY:O	1:A:153:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HD2	1:B:279:GLN:OE1	2.17	0.45
1:C:273:GLU:H	1:C:273:GLU:HG3	1.41	0.45
2:H:106:ASP:OD1	2:H:106:ASP:N	2.46	0.45
1:C:280:MET:HE1	1:D:322:PHE:CZ	2.52	0.45
1:D:50:ARG:HD2	1:D:329:MET:SD	2.56	0.45
1:F:62:GLN:NE2	1:F:204:GLN:HG3	2.23	0.45
1:F:234:THR:HA	1:F:431:GLN:HE21	1.82	0.45
1:F:311:ARG:O	1:F:315:THR:HG23	2.17	0.45
2:H:28:ASN:OD1	2:H:30:SER:OG	2.34	0.45
2:J:19:LYS:HD3	2:J:88:GLN:HE22	1.82	0.45
2:K:35:PHE:CE1	2:K:80:ASN:HA	2.50	0.45
2:L:3:GLN:O	2:L:24:ALA:HA	2.17	0.45
1:C:157:GLU:HB3	1:C:161:THR:O	2.16	0.45
1:D:133:PRO:CA	1:D:162:LEU:HD11	2.46	0.45
1:F:68:VAL:CG1	1:F:81:ILE:HD11	2.46	0.45
1:F:249:ILE:O	1:F:253:ILE:HB	2.17	0.45
1:F:293:VAL:HG13	1:F:325:ALA:HA	1.98	0.45
1:C:102:TYR:HE1	1:C:122:LYS:O	2.00	0.45
1:D:92:THR:OG1	1:D:93:GLY:N	2.47	0.45
2:J:59:TRP:CD1	2:J:108:TRP:HB2	2.52	0.45
2:L:99:VAL:HG22	2:L:101:TYR:CE1	2.52	0.45
1:A:483:ASP:CB	1:A:491:ASN:HD21	2.30	0.44
1:B:409:LEU:HD23	1:B:412:LYS:HD3	1.99	0.44
1:C:215:ARG:HH11	1:C:215:ARG:HG2	1.81	0.44
1:D:83:LEU:HB3	1:D:209:ILE:CD1	2.46	0.44
1:D:292:PRO:HG3	1:D:435:THR:HG22	1.99	0.44
2:H:13:GLN:NE2	2:H:129:SER:O	2.50	0.44
2:I:50:GLU:O	2:I:52:GLU:HG2	2.17	0.44
1:A:136:VAL:HG12	1:A:153:VAL:HG21	1.98	0.44
1:A:141:LEU:HA	1:A:151:LEU:O	2.17	0.44
1:D:129:TYR:CZ	1:D:131:GLN:HB3	2.52	0.44
1:F:364:PHE:CZ	1:F:368:LYS:HD2	2.51	0.44
2:I:45:GLN:O	2:I:99:VAL:HG12	2.17	0.44
2:L:73:ARG:HH11	2:L:93:GLN:HG3	1.81	0.44
1:B:330:LEU:HD21	1:B:347:MET:HE2	1.99	0.44
1:D:300:LEU:HG	1:D:347:MET:CE	2.46	0.44
1:E:400:LEU:HD12	1:E:422:ALA:HB3	1.99	0.44
1:F:270:ILE:HG23	1:F:275:VAL:CG2	2.44	0.44
2:I:101:TYR:HB3	2:I:120:TRP:CE3	2.52	0.44
1:A:144:VAL:HG22	1:A:178:ILE:HD12	2.00	0.44
1:B:310:THR:HG23	1:B:313:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:LEU:HD12	1:E:266:LEU:HA	1.67	0.44
1:F:18:LYS:CB	1:F:355:GLN:HE21	2.30	0.44
1:F:243:HIS:ND1	1:F:243:HIS:C	2.76	0.44
2:J:59:TRP:CD1	2:J:59:TRP:H	2.35	0.44
2:K:43:PHE:HZ	2:K:117:TYR:CE1	2.35	0.44
2:L:9:GLY:H	2:L:124:THR:HG21	1.82	0.44
2:L:37:THR:H	2:L:59:TRP:HE3	1.65	0.44
1:B:46:MET:HE3	1:B:49:ALA:HA	1.98	0.44
1:C:416:ASN:OD1	1:C:416:ASN:C	2.59	0.44
1:D:104:PRO:HG3	1:D:168:ASN:C	2.42	0.44
1:D:161:THR:C	1:D:162:LEU:HD12	2.42	0.44
1:D:454:ARG:HG3	1:D:457:ARG:NH2	2.32	0.44
1:F:382:CYS:HB2	1:F:413:TYR:HE2	1.83	0.44
1:A:218:ASP:OD1	1:A:221:ARG:NH1	2.51	0.44
1:B:51:MET:HE3	1:B:53:PHE:CE1	2.53	0.44
1:B:195:ARG:HE	1:B:195:ARG:HB3	1.68	0.44
1:C:217:ALA:HB2	1:C:251:ALA:HB1	1.99	0.44
1:D:3:GLN:NE2	1:D:358:THR:HA	2.32	0.44
1:E:363:MET:HE2	1:E:363:MET:HB3	1.73	0.44
1:F:215:ARG:HD3	1:F:219:GLN:HE22	1.83	0.44
1:F:392:VAL:O	1:F:393:GLN:HB2	2.18	0.44
2:H:17:SER:HA	2:H:89:MET:O	2.17	0.44
2:K:122:GLN:OE1	2:K:123:GLY:N	2.51	0.44
2:K:9:GLY:HA3	2:K:124:THR:HG22	1.99	0.44
2:L:59:TRP:CD1	2:L:60:ASN:ND2	2.78	0.44
1:A:270:ILE:HD12	1:B:12:ILE:HD11	1.99	0.44
1:E:7:ASN:HA	1:E:10:LEU:CG	2.44	0.44
1:F:265:ASP:O	1:F:268:VAL:HG12	2.18	0.44
2:H:12:VAL:HG22	2:H:13:GLN:H	1.83	0.44
1:A:51:MET:HE3	1:A:53:PHE:CE1	2.37	0.44
1:A:216:THR:OG1	1:A:219:GLN:HG3	2.18	0.44
1:C:149:LEU:CD2	1:C:170:HIS:CG	2.78	0.44
1:E:228:GLY:O	1:E:229:GLU:C	2.59	0.44
2:J:101:TYR:CE1	2:J:123:GLY:HA3	2.53	0.44
1:E:253:ILE:HD12	1:E:285:LYS:HG2	1.98	0.43
1:F:271:PRO:HB2	1:F:274:LYS:HG3	2.00	0.43
2:I:101:TYR:CB	2:I:120:TRP:CZ3	3.01	0.43
1:B:227:LEU:HD13	1:B:234:THR:OG1	2.18	0.43
1:F:239:LYS:NZ	1:F:260:MET:HE1	2.33	0.43
2:I:17:SER:HB3	2:I:90:ASN:CB	2.46	0.43
2:I:34:THR:O	2:I:35:PHE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:53:PHE:HD1	2:I:67:VAL:HG22	1.83	0.43
1:C:90:ILE:HB	1:C:178:ILE:O	2.19	0.43
1:C:414:ARG:HG3	1:C:414:ARG:HH11	1.83	0.43
1:F:344:VAL:O	1:F:348:VAL:HG23	2.18	0.43
2:H:12:VAL:O	2:H:128:VAL:HA	2.18	0.43
2:I:88:GLN:CG	2:I:89:MET:N	2.77	0.43
1:A:378:GLU:HG3	1:A:489:TYR:CG	2.54	0.43
1:B:20:ARG:CD	1:B:348:VAL:HG22	2.48	0.43
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.58	0.43
1:B:46:MET:HE3	1:B:48:VAL:O	2.17	0.43
1:F:27:THR:HA	1:F:50:ARG:HB3	2.01	0.43
1:A:64:THR:O	1:A:68:VAL:HG13	2.18	0.43
1:A:280:MET:HE1	1:B:322:PHE:CE2	2.53	0.43
1:A:445:VAL:HG23	1:A:450:GLU:HA	2.00	0.43
1:C:94:LEU:HD13	1:C:95:PHE:H	1.83	0.43
1:C:104:PRO:HA	1:C:166:VAL:O	2.19	0.43
1:C:395:LYS:HG3	1:C:475:ASP:HB3	2.01	0.43
1:E:311:ARG:NH2	1:E:315:THR:HG21	2.33	0.43
1:E:348:VAL:HG12	2:K:31:SER:O	2.19	0.43
1:F:481:HIS:H	1:F:492:GLN:HB3	1.83	0.43
2:I:28:ASN:O	2:I:29:PHE:HB2	2.17	0.43
2:L:28:ASN:C	2:L:30:SER:H	2.27	0.43
1:A:26:CYS:SG	1:A:46:MET:HG3	2.58	0.43
1:A:274:LYS:HD2	1:A:274:LYS:HA	1.74	0.43
1:A:386:VAL:HG21	1:A:413:TYR:HB2	1.99	0.43
1:F:311:ARG:HE	1:F:311:ARG:HB3	1.31	0.43
1:F:419:ILE:O	1:F:438:VAL:HA	2.18	0.43
1:B:83:LEU:HD23	1:B:83:LEU:C	2.44	0.43
1:C:102:TYR:CD1	1:C:108:VAL:HG21	2.54	0.43
1:C:127:VAL:HG21	1:C:132:LEU:CD2	2.49	0.43
1:E:48:VAL:HG21	1:E:208:MET:HE1	2.00	0.43
1:E:359:HIS:HB3	1:E:362:VAL:HG23	2.01	0.43
1:F:236:ILE:HG21	1:F:236:ILE:HD13	1.77	0.43
2:J:35:PHE:C	2:J:37:THR:H	2.27	0.43
2:K:103:ALA:HB1	2:K:117:TYR:HB3	2.01	0.43
1:B:35:VAL:HG13	1:B:71:ALA:HB2	2.00	0.43
1:C:149:LEU:CG	1:C:170:HIS:ND1	2.81	0.43
1:C:262:ALA:O	1:C:266:LEU:HB2	2.18	0.43
1:C:378:GLU:OE1	1:C:405:ARG:HD3	2.19	0.43
1:D:33:GLN:HG3	1:D:64:THR:HG22	2.01	0.43
1:D:459:GLN:O	1:D:460:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ASN:CA	1:E:10:LEU:HG	2.44	0.43
1:E:373:ILE:HG22	1:E:374:PRO:HD3	2.00	0.43
1:F:243:HIS:CD2	1:F:244:GLN:OE1	2.72	0.43
2:I:5:GLN:N	2:I:23:ALA:O	2.50	0.43
2:L:33:ARG:HH12	2:L:106:ASP:CA	2.27	0.43
1:A:264:GLY:CA	1:A:298:GLN:HE21	2.32	0.43
1:A:399:VAL:O	1:A:421:CYS:HA	2.18	0.43
1:D:23:ARG:HB2	1:D:327:CYS:SG	2.58	0.43
1:D:62:GLN:O	1:D:66:ASN:ND2	2.50	0.43
2:I:57:ILE:HD11	2:I:61:GLY:HA2	2.00	0.43
2:L:12:VAL:O	2:L:128:VAL:HA	2.18	0.43
1:E:27:THR:CG2	1:E:50:ARG:HD3	2.49	0.43
1:E:367:ILE:HD13	1:E:412:LYS:O	2.19	0.43
2:J:99:VAL:HG12	2:J:101:TYR:CE2	2.53	0.43
1:C:208:MET:HE2	1:C:210:PHE:CZ	2.54	0.42
1:C:277:VAL:HG12	1:D:12:ILE:HG22	2.00	0.42
1:E:13:PHE:CD1	1:E:13:PHE:N	2.87	0.42
1:E:420:ILE:CD1	1:E:465:ALA:HB2	2.48	0.42
1:F:274:LYS:HA	1:F:277:VAL:HG12	2.00	0.42
2:H:4:LEU:HB3	2:H:22:CYS:SG	2.58	0.42
2:K:4:LEU:HD21	2:K:119:TYR:CE1	2.54	0.42
1:A:168:ASN:OD1	1:A:168:ASN:N	2.52	0.42
1:A:482:ALA:HA	1:A:490:PRO:HA	2.01	0.42
1:B:65:ILE:CG2	1:B:69:ARG:NH1	2.78	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.66	0.42
1:D:198:LEU:HD22	1:D:227:LEU:HD21	2.00	0.42
1:F:283:ILE:HD13	1:F:325:ALA:HB2	2.00	0.42
2:J:33:ARG:NH1	2:J:38:ASP:OD1	2.51	0.42
2:L:78:ARG:HB2	2:L:85:VAL:HG23	2.01	0.42
1:C:471:VAL:HG12	1:C:472:SER:N	2.35	0.42
1:B:2:SER:N	1:B:359:HIS:NE2	2.66	0.42
1:C:266:LEU:O	1:C:270:ILE:HG23	2.19	0.42
1:D:62:GLN:HG3	1:D:66:ASN:HD21	1.83	0.42
1:D:177:GLY:C	1:D:178:ILE:HD13	2.44	0.42
1:E:212:SER:HA	1:E:239:LYS:CE	2.49	0.42
1:F:389:ALA:HA	1:F:394:ALA:CB	2.49	0.42
2:I:1:GLN:HB2	2:I:28:ASN:HA	2.00	0.42
2:L:38:ASP:O	2:L:78:ARG:NH2	2.52	0.42
1:A:378:GLU:HG3	1:A:489:TYR:CE1	2.55	0.42
1:D:254:GLU:O	3:D:602:GOL:O2	2.29	0.42
1:E:330:LEU:N	1:E:330:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:460:LEU:HD23	1:F:461:GLY:N	2.34	0.42
2:I:105:ARG:HG3	2:I:116:GLU:O	2.20	0.42
2:L:33:ARG:HG3	2:L:33:ARG:HH11	1.85	0.42
1:A:13:PHE:CE2	1:B:247:GLN:HG3	2.55	0.42
1:D:181:PRO:O	2:J:64:THR:OG1	2.31	0.42
1:F:283:ILE:HD12	1:F:323:ASN:HB2	2.01	0.42
1:C:27:THR:HA	1:C:50:ARG:HB3	2.01	0.42
1:C:27:THR:OG1	1:C:331:SER:O	2.38	0.42
1:C:190:VAL:HG13	1:C:194:ASP:HB3	2.02	0.42
1:C:228:GLY:O	1:C:229:GLU:C	2.62	0.42
1:D:224:ARG:NH2	1:D:257:ASP:OD2	2.53	0.42
1:D:408:ARG:HG2	1:D:435:THR:HG21	2.01	0.42
1:D:419:ILE:O	1:D:438:VAL:HA	2.20	0.42
1:F:389:ALA:HA	1:F:394:ALA:HB3	2.00	0.42
2:H:104:GLY:HA3	2:H:119:TYR:CZ	2.55	0.42
2:K:75:THR:HB	2:K:88:GLN:HB3	2.00	0.42
2:L:88:GLN:HA	2:L:88:GLN:OE1	2.20	0.42
1:A:136:VAL:CG1	1:A:153:VAL:HG21	2.49	0.42
1:B:16:VAL:HG21	1:B:356:SER:CB	2.50	0.42
1:E:350:ILE:HD13	1:E:350:ILE:HG21	1.85	0.42
1:F:208:MET:C	1:F:209:ILE:HD13	2.45	0.42
1:D:114:PRO:O	1:D:117:GLU:CB	2.68	0.42
1:F:388:SER:HA	1:F:391:GLU:CG	2.48	0.42
2:I:63:ILE:CD1	2:I:109:TYR:HE1	2.33	0.42
2:L:99:VAL:HG13	2:L:101:TYR:OH	2.19	0.42
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.94	0.42
1:C:90:ILE:O	1:C:177:GLY:HA2	2.20	0.42
1:C:460:LEU:HD12	1:C:460:LEU:HA	1.84	0.42
1:D:471:VAL:HG23	1:D:475:ASP:CB	2.49	0.42
1:E:12:ILE:HA	1:E:12:ILE:HD13	1.78	0.42
2:I:97:THR:O	2:I:98:ALA:HB2	2.20	0.42
2:K:41:GLY:HA3	2:K:117:TYR:CE2	2.55	0.42
1:A:84:ASP:HA	1:A:210:PHE:HB2	2.01	0.41
1:A:494:ARG:HD2	1:A:496:VAL:CG1	2.50	0.41
1:B:276:VAL:O	1:B:280:MET:HG3	2.20	0.41
1:F:199:GLN:HA	1:F:199:GLN:OE1	2.20	0.41
2:J:38:ASP:O	2:J:78:ARG:NH2	2.40	0.41
2:J:51:ARG:NH1	2:J:101:TYR:CD2	2.84	0.41
1:B:441:VAL:CG1	1:B:460:LEU:HG	2.50	0.41
1:B:454:ARG:HA	1:B:457:ARG:HH21	1.86	0.41
1:D:42:MET:HE2	1:D:79:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:HD12	1:D:162:LEU:N	2.36	0.41
1:E:402:ASN:CB	1:E:425:ARG:HH21	2.33	0.41
2:G:35:PHE:O	2:G:78:ARG:NH2	2.53	0.41
2:J:6:GLU:HG3	2:J:102:CYS:SG	2.61	0.41
2:L:17:SER:HA	2:L:89:MET:O	2.20	0.41
1:C:39:LYS:HD2	1:C:74:GLU:OE1	2.21	0.41
1:C:208:MET:HE3	1:C:237:ILE:CD1	2.50	0.41
1:E:212:SER:OG	1:E:239:LYS:HE2	2.20	0.41
1:E:377:PRO:O	1:E:381:VAL:HG23	2.21	0.41
2:K:4:LEU:HD21	2:K:119:TYR:HE1	1.85	0.41
1:A:264:GLY:HA2	1:A:298:GLN:HE21	1.86	0.41
1:B:90:ILE:HD13	1:B:90:ILE:HG21	1.84	0.41
1:B:492:GLN:NE2	1:D:492:GLN:NE2	2.66	0.41
1:D:42:MET:O	1:D:43:LYS:C	2.60	0.41
1:D:60:TYR:O	1:D:63:THR:HB	2.19	0.41
1:F:398:LEU:HD21	1:F:400:LEU:HD13	2.02	0.41
2:I:58:SER:HB3	2:I:63:ILE:HG23	1.97	0.41
2:I:100:TYR:O	2:I:123:GLY:HA2	2.20	0.41
2:L:120:TRP:N	2:L:120:TRP:CD1	2.88	0.41
1:A:240:ILE:HD11	1:A:252:ILE:HG21	2.01	0.41
1:B:396:ALA:HB3	1:B:477:MET:HG2	2.03	0.41
1:D:90:ILE:HD13	1:D:129:TYR:HB2	2.01	0.41
1:D:349:ARG:HD3	2:I:32:GLY:O	2.20	0.41
1:E:360:ASP:O	1:E:390:PHE:HZ	2.03	0.41
1:F:220:VAL:HG21	1:F:255:ALA:CB	2.50	0.41
1:F:398:LEU:HD22	1:F:479:ILE:HG23	2.02	0.41
1:F:409:LEU:HD13	1:F:409:LEU:HA	1.90	0.41
1:F:432:LEU:HD23	1:F:432:LEU:HA	1.64	0.41
2:G:104:GLY:HA3	2:G:119:TYR:CE2	2.56	0.41
2:L:66:TYR:HB3	2:L:70:VAL:HG23	2.02	0.41
1:A:237:ILE:HG23	1:A:237:ILE:HD12	1.80	0.41
1:A:311:ARG:HD2	1:B:275:VAL:CG1	2.47	0.41
1:C:143:TYR:HE1	1:C:181:PRO:HG3	1.86	0.41
1:C:423:THR:HG22	1:C:424:THR:N	2.36	0.41
1:D:486:VAL:HG12	1:D:487:LYS:N	2.35	0.41
1:E:449:GLY:C	1:E:451:ASP:N	2.77	0.41
1:F:88:PRO:HG3	1:F:189:ALA:HA	2.02	0.41
1:F:389:ALA:CB	1:F:397:ILE:HD11	2.51	0.41
2:I:59:TRP:H	2:I:59:TRP:CD1	2.38	0.41
2:I:103:ALA:HB2	2:I:120:TRP:CD2	2.56	0.41
1:C:303:MET:O	1:C:303:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:GLN:HE22	1:D:204:GLN:CG	2.33	0.41
1:D:183:CYS:HB3	1:D:184:GLU:H	1.79	0.41
1:E:214:ILE:HD13	1:E:214:ILE:HA	1.91	0.41
1:E:424:THR:HG22	1:E:443:TYR:HB3	2.02	0.41
1:E:477:MET:HE2	1:E:477:MET:HB2	1.78	0.41
2:I:79:ASP:CG	2:I:82:LYS:HG3	2.45	0.41
1:A:406:SER:O	1:A:410:ILE:HG13	2.21	0.41
1:B:263:ARG:H	1:B:263:ARG:HG3	1.59	0.41
1:E:75:LEU:HB2	1:E:77:LEU:HD22	2.02	0.41
2:J:44:ARG:HB3	2:J:100:TYR:CE2	2.56	0.41
2:K:51:ARG:HE	2:K:114:PRO:CB	2.33	0.41
1:A:89:GLU:HB3	4:A:706:HOH:O	2.21	0.41
1:B:214:ILE:HD13	1:B:214:ILE:HA	1.89	0.41
1:B:229:GLU:OE1	1:B:229:GLU:HA	2.20	0.41
1:C:12:ILE:HG12	1:D:278:ALA:HB2	2.02	0.41
1:C:139:GLY:N	1:C:153:VAL:O	2.33	0.41
1:C:272:ALA:O	1:C:275:VAL:N	2.54	0.41
1:D:62:GLN:HE22	1:D:204:GLN:CD	2.29	0.41
1:D:451:ASP:OD2	1:D:457:ARG:HG3	2.21	0.41
1:E:236:ILE:HD13	1:E:236:ILE:HG21	1.64	0.41
1:E:242:ASN:OD1	1:E:244:GLN:NE2	2.50	0.41
1:E:260:MET:HG3	1:E:294:ILE:HB	2.01	0.41
1:E:363:MET:C	1:E:367:ILE:HD12	2.45	0.41
2:I:16:GLY:C	2:I:92:LEU:CD1	2.88	0.41
2:J:57:ILE:HD11	2:J:61:GLY:HA2	2.02	0.41
2:K:77:SER:HB2	2:K:78:ARG:H	1.38	0.41
1:A:231:GLY:O	1:A:234:THR:HG22	2.21	0.41
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.91	0.41
1:D:454:ARG:HD3	1:D:481:HIS:ND1	2.36	0.41
1:E:42:MET:HE2	1:E:42:MET:HB2	1.73	0.41
1:F:425:ARG:O	1:F:428:THR:HB	2.21	0.41
2:J:33:ARG:HA	2:J:37:THR:OG1	2.21	0.41
2:L:9:GLY:HA3	2:L:124:THR:CG2	2.51	0.41
1:A:109:LEU:HD22	1:A:161:THR:HG21	2.03	0.40
1:B:12:ILE:HG21	1:B:12:ILE:HD13	1.84	0.40
1:C:39:LYS:HG3	1:C:71:ALA:HB1	2.03	0.40
1:C:277:VAL:HG13	1:D:10:LEU:HD13	2.03	0.40
1:D:209:ILE:HD13	1:D:209:ILE:HA	1.94	0.40
1:D:213:PHE:CD2	1:D:215:ARG:NH1	2.88	0.40
1:D:240:ILE:CD1	1:D:259:ILE:HD12	2.51	0.40
1:E:30:PRO:HD2	1:E:335:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:MET:HE3	1:F:296:ALA:CB	2.52	0.40
2:G:12:VAL:HG21	2:G:92:LEU:HD13	2.03	0.40
2:I:1:GLN:HE21	2:I:119:TYR:HB3	1.86	0.40
1:A:96:LYS:O	1:A:97:ASP:HB2	2.21	0.40
1:A:263:ARG:HH22	1:A:316:ASP:CG	2.30	0.40
1:B:83:LEU:HD23	1:B:83:LEU:O	2.21	0.40
1:C:25:ILE:HG23	1:C:48:VAL:HB	2.04	0.40
1:D:191:SER:O	1:D:194:ASP:HB2	2.21	0.40
1:E:27:THR:HA	1:E:50:ARG:HB3	2.03	0.40
2:I:118:ARG:HA	2:I:118:ARG:HD3	1.50	0.40
2:J:69:SER:O	2:J:73:ARG:NH1	2.49	0.40
1:B:395:LYS:HD2	1:B:475:ASP:CG	2.46	0.40
1:C:193:LYS:O	1:C:197:ASP:OD1	2.38	0.40
1:C:218:ASP:OD1	1:C:221:ARG:NH1	2.54	0.40
1:C:300:LEU:HG	1:C:347:MET:CE	2.49	0.40
1:D:129:TYR:OH	1:D:131:GLN:HB3	2.21	0.40
1:D:448:HIS:HB3	1:D:449:GLY:H	1.74	0.40
1:E:228:GLY:C	1:E:230:LYS:N	2.77	0.40
1:E:303:MET:SD	1:E:309:PRO:HD3	2.61	0.40
1:F:42:MET:HE1	1:F:72:ALA:HB2	2.04	0.40
1:F:68:VAL:HG13	1:F:81:ILE:HD11	2.03	0.40
2:H:68:ASP:HA	2:H:71:LYS:HB2	2.03	0.40
2:I:1:GLN:OE1	2:I:1:GLN:N	2.43	0.40
1:B:82:ALA:HB2	1:B:208:MET:HE3	2.03	0.40
1:B:360:ASP:CG	1:B:416:ASN:OD1	2.64	0.40
1:C:33:GLN:HG3	1:C:64:THR:HG22	2.03	0.40
1:C:224:ARG:HE	1:C:236:ILE:CD1	2.30	0.40
2:J:22:CYS:HB3	2:J:85:VAL:CG1	2.50	0.40
2:K:28:ASN:O	2:K:29:PHE:HB2	2.20	0.40
2:L:28:ASN:C	2:L:29:PHE:CD2	2.99	0.40
1:C:189:ALA:HB3	1:C:222:GLU:OE1	2.22	0.40
1:C:248:ASN:O	1:C:252:ILE:HG13	2.22	0.40
1:C:266:LEU:HD12	1:C:266:LEU:HA	1.76	0.40
1:C:480:VAL:HG22	1:C:493:THR:CG2	2.40	0.40
1:D:249:ILE:C	1:D:253:ILE:HD12	2.42	0.40
1:D:276:VAL:O	1:D:280:MET:HG3	2.22	0.40
2:K:42:TRP:CD2	2:K:87:LEU:HD12	2.57	0.40
2:K:66:TYR:HE1	2:K:76:ILE:HG13	1.86	0.40

All (8) 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:F:274:LYS:NZ	2:K:108:TRP:CD1[3_455]	1.04	1.16
1:F:274:LYS:NZ	2:K:108:TRP:NE1[3_455]	1.49	0.71
1:F:274:LYS:NZ	2:K:108:TRP:CG[3_455]	1.59	0.61
1:E:311:ARG:NH2	1:F:316:ASP:OD1[3_445]	1.77	0.43
2:G:128:VAL:O	2:J:91:SER:OG[4_454]	2.10	0.10
1:F:274:LYS:NZ	2:K:108:TRP:CE2[3_455]	2.12	0.08
1:F:274:LYS:NZ	2:K:108:TRP:CD2[3_455]	2.18	0.02
1:F:274:LYS:CE	2:K:108:TRP:CD1[3_455]	2.19	0.01

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	497/514 (97%)	461 (93%)	36 (7%)	0	100	100
1	B	400/514 (78%)	386 (96%)	14 (4%)	0	100	100
1	C	171/514 (33%)	163 (95%)	8 (5%)	0	100	100
1	D	245/514 (48%)	233 (95%)	12 (5%)	0	100	100
1	E	66/514 (13%)	66 (100%)	0	0	100	100
1	F	309/514 (60%)	289 (94%)	20 (6%)	0	100	100
2	G	128/149 (86%)	126 (98%)	2 (2%)	0	100	100
2	H	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
2	I	128/149 (86%)	121 (94%)	7 (6%)	0	100	100
2	J	129/149 (87%)	123 (95%)	6 (5%)	0	100	100
2	K	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
2	L	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
All	All	2457/3978 (62%)	2334 (95%)	123 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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	GOL	D	601	-	5,5,5	1.34	1 (20%)	5,5,5	1.03	0
3	GOL	B	703	-	5,5,5	0.93	0	5,5,5	0.94	0
3	GOL	B	701	-	5,5,5	1.56	2 (40%)	5,5,5	1.06	0
3	GOL	C	601	-	5,5,5	1.69	1 (20%)	5,5,5	1.55	1 (20%)
3	GOL	F	601	-	5,5,5	1.34	1 (20%)	5,5,5	0.77	0
3	GOL	B	702	-	5,5,5	0.95	0	5,5,5	1.23	1 (20%)
3	GOL	E	601	-	5,5,5	0.88	0	5,5,5	1.01	0
3	GOL	C	602	-	5,5,5	1.54	2 (40%)	5,5,5	1.44	0
3	GOL	A	601	-	5,5,5	2.58	2 (40%)	5,5,5	1.00	0
3	GOL	D	602	-	5,5,5	0.96	0	5,5,5	1.00	0

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	GOL	D	601	-	-	0/4/4/4	-
3	GOL	B	703	-	-	0/4/4/4	-
3	GOL	B	701	-	-	4/4/4/4	-
3	GOL	C	601	-	-	1/4/4/4	-
3	GOL	F	601	-	-	2/4/4/4	-
3	GOL	B	702	-	-	4/4/4/4	-
3	GOL	E	601	-	-	4/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	A	601	-	-	4/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	GOL	C3-C2	4.74	1.69	1.51
3	C	601	GOL	C1-C2	3.26	1.64	1.51
3	C	602	GOL	C1-C2	2.44	1.61	1.51
3	B	701	GOL	C3-C2	2.40	1.60	1.51
3	D	601	GOL	C3-C2	2.36	1.60	1.51
3	A	601	GOL	C1-C2	2.35	1.60	1.51
3	C	602	GOL	C3-C2	2.23	1.60	1.51
3	F	601	GOL	C1-C2	2.19	1.60	1.51
3	B	701	GOL	C1-C2	2.18	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	GOL	O3-C3-C2	-2.57	98.82	110.38
3	B	702	GOL	C3-C2-C1	-2.19	103.77	111.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	C1-C2-C3-O3
3	B	701	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	701	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2
3	B	702	GOL	O1-C1-C2-C3
3	C	602	GOL	C1-C2-C3-O3
3	A	601	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-C3
3	B	702	GOL	C1-C2-C3-O3
3	D	602	GOL	O1-C1-C2-C3
3	E	601	GOL	O1-C1-C2-C3
3	E	601	GOL	C1-C2-C3-O3
3	F	601	GOL	C1-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2
3	B	701	GOL	O1-C1-C2-O2
3	B	701	GOL	O2-C2-C3-O3
3	B	702	GOL	O2-C2-C3-O3
3	F	601	GOL	O2-C2-C3-O3
3	C	602	GOL	O2-C2-C3-O3
3	E	601	GOL	O2-C2-C3-O3
3	E	601	GOL	O1-C1-C2-O2
3	C	601	GOL	C1-C2-C3-O3
3	D	602	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	GOL	2	0
3	D	602	GOL	1	0

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	499/514 (97%)	0.09	21 (4%) 40 32	57, 71, 179, 197	0
1	B	404/514 (78%)	-0.01	5 (1%) 76 68	61, 83, 120, 173	0
1	C	499/514 (97%)	0.20	27 (5%) 31 24	51, 78, 173, 191	1 (0%)
1	D	499/514 (97%)	0.18	9 (1%) 67 58	64, 92, 140, 182	1 (0%)
1	E	395/514 (76%)	0.63	28 (7%) 22 16	73, 108, 130, 164	0
1	F	399/514 (77%)	1.25	74 (18%) 3 2	100, 124, 182, 219	0
2	G	130/149 (87%)	-0.03	0 100 100	64, 78, 100, 130	0
2	H	130/149 (87%)	0.06	2 (1%) 72 63	75, 92, 127, 152	0
2	I	130/149 (87%)	0.74	8 (6%) 26 20	90, 131, 188, 206	0
2	J	131/149 (87%)	0.15	1 (0%) 82 75	69, 88, 112, 136	0
2	K	130/149 (87%)	1.46	29 (22%) 2 1	100, 170, 223, 236	0
2	L	130/149 (87%)	0.99	11 (8%) 16 12	115, 163, 211, 218	0
All	All	3476/3978 (87%)	0.41	215 (6%) 26 20	51, 96, 179, 236	2 (0%)

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	61	GLY	5.3
1	E	272	ALA	4.8
2	K	100	TYR	4.8
1	F	237	ILE	4.7
1	A	179	ASN	4.5
1	F	318	ALA	4.5
1	F	236	ILE	4.4
1	C	174	ASP	4.3
1	F	273	GLU	4.2
2	K	109	TYR	4.1
1	C	172	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	K	20	LEU	3.9
1	A	141	LEU	3.8
1	F	481	HIS	3.8
1	B	90	ILE	3.7
1	C	173	THR	3.7
1	F	376	SER	3.7
2	K	84	THR	3.7
1	F	257	ASP	3.7
1	E	189	ALA	3.6
1	E	270	ILE	3.6
1	F	406	SER	3.6
1	F	44	SER	3.5
1	F	272	ALA	3.5
1	F	66	ASN	3.4
1	F	422	ALA	3.4
1	C	515	GLU	3.4
1	E	247	GLN	3.3
1	D	515	GLU	3.3
1	F	315	THR	3.3
2	L	35	PHE	3.2
1	A	92	THR	3.2
1	E	89	GLU	3.2
1	F	375	MET	3.2
2	K	22	CYS	3.1
1	F	234	THR	3.1
1	F	486	VAL	3.1
1	B	485	SER	3.1
1	A	94	LEU	3.1
1	F	296	ALA	3.0
1	D	489	TYR	3.0
1	E	53	PHE	3.0
1	E	364	PHE	3.0
1	E	362	VAL	3.0
1	F	288	VAL	3.0
2	K	110	PHE	2.9
2	K	62	GLY	2.9
2	K	77	SER	2.9
2	K	75	THR	2.9
2	I	51	ARG	2.9
2	L	44	ARG	2.9
1	F	364	PHE	2.9
2	K	40	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	483	ASP	2.8
2	K	63	ILE	2.8
1	F	398	LEU	2.8
2	K	60	ASN	2.8
1	A	488	GLY	2.8
1	C	187	LEU	2.8
1	F	487	LYS	2.8
1	C	303	MET	2.7
1	E	11	SER	2.7
2	K	24	ALA	2.7
1	F	419	ILE	2.7
1	C	484	HIS	2.7
1	F	499	ARG	2.7
2	K	118	ARG	2.7
1	F	362	VAL	2.7
1	F	213	PHE	2.7
2	K	23	ALA	2.7
1	F	258	GLY	2.7
2	K	74	PHE	2.6
2	L	100	TYR	2.6
1	C	184	GLU	2.6
1	E	246	VAL	2.6
1	E	273	GLU	2.6
1	F	223	VAL	2.6
1	F	246	VAL	2.6
1	E	13	PHE	2.6
1	E	296	ALA	2.6
1	A	185	VAL	2.6
1	F	317	VAL	2.6
1	C	183	CYS	2.6
1	E	327	CYS	2.6
2	L	113	VAL	2.6
1	F	378	GLU	2.6
1	C	179	ASN	2.6
1	F	408	ARG	2.5
2	K	130	SER	2.5
1	A	86	LYS	2.5
1	C	488	GLY	2.5
1	C	185	VAL	2.5
1	E	489	TYR	2.5
1	F	492	GLN	2.5
1	F	189	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	454	ARG	2.5
1	D	137	ARG	2.5
2	K	12	VAL	2.5
1	F	297	THR	2.5
1	D	182	GLY	2.5
1	F	81	ILE	2.5
1	F	348	VAL	2.5
1	F	89	GLU	2.5
1	E	276	VAL	2.4
1	F	381	VAL	2.4
1	A	500	GLU	2.4
1	E	312	ALA	2.4
1	E	12	ILE	2.4
1	C	144	VAL	2.4
1	D	488	GLY	2.4
1	F	276	VAL	2.4
2	I	121	GLY	2.4
1	A	489	TYR	2.4
1	D	129	TYR	2.4
1	A	484	HIS	2.4
1	F	495	LEU	2.4
1	A	174	ASP	2.4
2	K	33	ARG	2.4
2	K	89	MET	2.4
1	C	151	LEU	2.4
1	F	374	PRO	2.4
1	F	490	PRO	2.4
1	E	275	VAL	2.3
2	I	26	GLY	2.3
1	F	73	ALA	2.3
1	C	489	TYR	2.3
1	F	489	TYR	2.3
2	K	86	TYR	2.3
1	F	454	ARG	2.3
2	K	70	VAL	2.3
1	D	184	GLU	2.3
1	F	379	GLU	2.3
2	J	27	SER	2.3
1	F	282	ILE	2.3
1	B	190	VAL	2.3
1	F	480	VAL	2.3
1	F	49	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	159	ASP	2.3
1	D	172	LEU	2.3
2	L	63	ILE	2.3
2	L	34	THR	2.3
2	I	1	GLN	2.3
1	F	457	ARG	2.3
1	F	377	PRO	2.3
1	F	235	LEU	2.2
2	K	92	LEU	2.2
1	C	142	ILE	2.2
2	K	108	TRP	2.2
1	A	31	SER	2.2
1	C	486	VAL	2.2
2	L	8	GLY	2.2
1	C	95	PHE	2.2
1	C	296	ALA	2.2
1	E	269	GLU	2.2
1	F	482	ALA	2.2
1	F	227	LEU	2.2
1	C	135	VAL	2.2
1	E	54	SER	2.2
1	E	361	SER	2.2
1	C	149	LEU	2.2
1	F	473	ALA	2.2
1	F	491	ASN	2.2
1	F	311	ARG	2.2
2	H	130	SER	2.2
2	K	2	VAL	2.2
2	L	12	VAL	2.2
1	A	173	THR	2.2
1	A	297	THR	2.2
1	F	488	GLY	2.2
1	C	94	LEU	2.2
1	A	119	ILE	2.1
1	E	268	VAL	2.1
1	E	344	VAL	2.1
1	E	51	MET	2.1
1	E	274	LYS	2.1
2	I	127	THR	2.1
1	F	322	PHE	2.1
1	F	295	CYS	2.1
2	L	36	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	253	ILE	2.1
1	F	386	VAL	2.1
1	F	434	VAL	2.1
1	A	176	LYS	2.1
2	L	26	GLY	2.1
1	C	454	ARG	2.1
1	F	17	ALA	2.1
2	I	100	TYR	2.1
1	A	134	ASN	2.1
1	B	486	VAL	2.1
1	F	18	LYS	2.1
2	K	47	PRO	2.1
1	C	180	LEU	2.1
1	F	400	LEU	2.1
1	F	404	GLY	2.1
1	F	28	ILE	2.1
1	C	481	HIS	2.1
2	I	76	ILE	2.1
1	A	44	SER	2.0
1	C	487	LYS	2.0
1	F	190	VAL	2.0
1	F	268	VAL	2.0
1	A	93	GLY	2.0
1	A	140	GLY	2.0
1	E	311	ARG	2.0
2	I	43	PHE	2.0
1	C	373	ILE	2.0
2	H	97	THR	2.0
1	E	44	SER	2.0
2	K	36	SER	2.0
1	A	270	ILE	2.0
1	F	240	ILE	2.0
2	K	76	ILE	2.0
1	F	226	ALA	2.0
2	L	59	TRP	2.0
1	F	441	VAL	2.0

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

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
3	GOL	C	602	6/6	0.58	0.22	89,93,95,98	0
3	GOL	C	601	6/6	0.65	0.16	84,87,94,108	0
3	GOL	A	601	6/6	0.66	0.21	78,85,85,86	0
3	GOL	F	601	6/6	0.74	0.14	104,110,112,112	0
3	GOL	B	702	6/6	0.79	0.12	92,94,95,101	0
3	GOL	E	601	6/6	0.81	0.10	112,115,116,118	0
3	GOL	D	602	6/6	0.82	0.13	90,92,94,94	0
3	GOL	B	703	6/6	0.87	0.11	95,100,100,103	0
3	GOL	B	701	6/6	0.87	0.17	82,84,85,87	0
3	GOL	D	601	6/6	0.90	0.12	85,89,92,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.