Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 05:53 PM EDT

PDB ID	:	3CMU / pdb_00003cmu
Title	:	Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors	:	Pavletich, N.P.
Deposited on	:	2008-03-24
Resolution	:	4.20 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 (i) 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 (i)) were used in the production of this report:

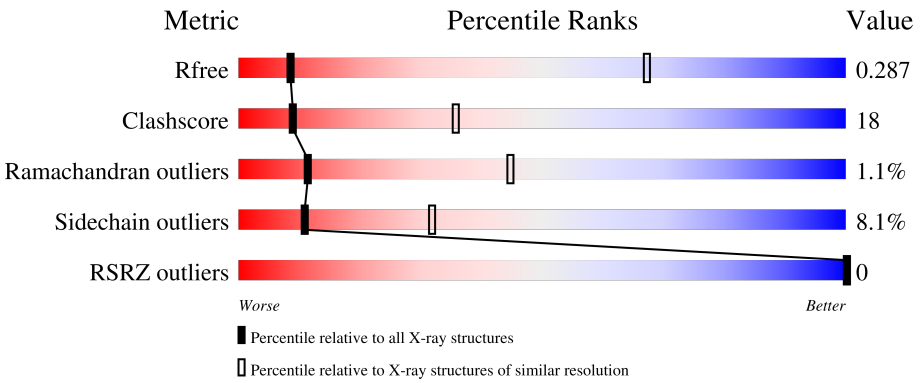
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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

Mol	Chain	Length	Quality of chain
1	B	18	50% 33% 17%
2	A	2050	60% 31% • 6%

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
4	ALF	A	1501	-	-	X	-
4	ALF	A	501	-	-	X	-
4	ALF	A	5501	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15093 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 DNA chain called DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	15	297	150	30	103	14	0	0	0

- Molecule 2 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	1937	14598	9178	2528	2824	68	0	0	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	HIS	-	linker	UNP P0A7G6
A	29	MET	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6
A	989	THR	-	linker	UNP P0A7G6
A	990	GLY	-	linker	UNP P0A7G6
A	991	SER	-	linker	UNP P0A7G6
A	992	GLY	-	linker	UNP P0A7G6
A	993	THR	-	linker	UNP P0A7G6
A	994	THR	-	linker	UNP P0A7G6
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6
A	997	THR	-	linker	UNP P0A7G6
A	998	GLY	-	linker	UNP P0A7G6
A	999	SER	-	linker	UNP P0A7G6
A	1000	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1986	THR	-	linker	UNP P0A7G6
A	1987	GLY	-	linker	UNP P0A7G6
A	1988	SER	-	linker	UNP P0A7G6
A	1989	THR	-	linker	UNP P0A7G6
A	1990	GLY	-	linker	UNP P0A7G6
A	1991	SER	-	linker	UNP P0A7G6
A	1992	MET	-	linker	UNP P0A7G6
A	1993	GLY	-	linker	UNP P0A7G6
A	1994	HIS	-	linker	UNP P0A7G6
A	1995	THR	-	linker	UNP P0A7G6
A	1996	THR	-	linker	UNP P0A7G6
A	1997	GLY	-	linker	UNP P0A7G6
A	1998	ALA	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2986	THR	-	linker	UNP P0A7G6
A	2987	GLY	-	linker	UNP P0A7G6
A	2988	SER	-	linker	UNP P0A7G6
A	2989	THR	-	linker	UNP P0A7G6
A	2990	GLY	-	linker	UNP P0A7G6
A	2991	SER	-	linker	UNP P0A7G6
A	2992	MET	-	linker	UNP P0A7G6
A	2993	ALA	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	THR	-	linker	UNP P0A7G6
A	2996	GLY	-	linker	UNP P0A7G6
A	2997	SER	-	linker	UNP P0A7G6
A	2998	THR	-	linker	UNP P0A7G6
A	2999	GLY	-	linker	UNP P0A7G6
A	3000	SER	-	linker	UNP P0A7G6
A	3989	THR	-	linker	UNP P0A7G6
A	3990	GLY	-	linker	UNP P0A7G6
A	3991	ALA	-	linker	UNP P0A7G6
A	3992	THR	-	linker	UNP P0A7G6
A	3993	GLY	-	linker	UNP P0A7G6
A	3994	ALA	-	linker	UNP P0A7G6
A	3995	MET	-	linker	UNP P0A7G6
A	3996	SER	-	linker	UNP P0A7G6
A	3997	GLY	-	linker	UNP P0A7G6
A	3998	ARG	-	linker	UNP P0A7G6
A	3999	MET	-	linker	UNP P0A7G6
A	4000	SER	-	linker	UNP P0A7G6

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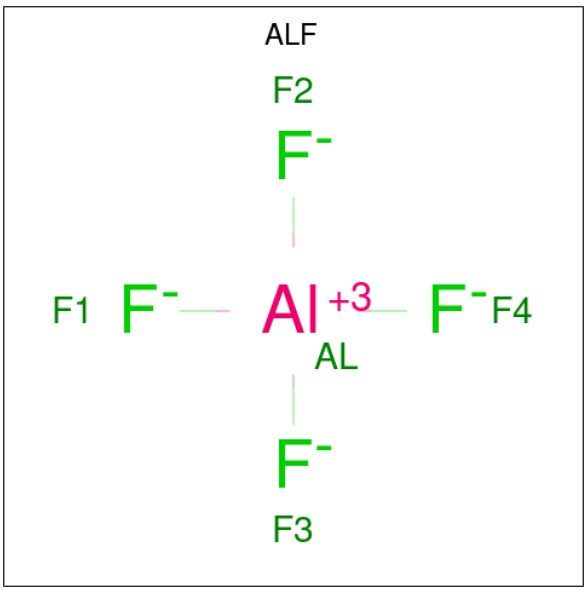
Chain	Residue	Modelled	Actual	Comment	Reference
A	4987	THR	-	linker	UNP P0A7G6
A	4988	GLY	-	linker	UNP P0A7G6
A	4989	SER	-	linker	UNP P0A7G6
A	4990	THR	-	linker	UNP P0A7G6
A	4991	GLY	-	linker	UNP P0A7G6
A	4992	SER	-	linker	UNP P0A7G6
A	4993	GLY	-	linker	UNP P0A7G6
A	4994	SER	-	linker	UNP P0A7G6
A	4995	SER	-	linker	UNP P0A7G6
A	4996	THR	-	linker	UNP P0A7G6
A	4997	GLY	-	linker	UNP P0A7G6
A	4998	SER	-	linker	UNP P0A7G6
A	4999	MET	-	linker	UNP P0A7G6
A	5000	SER	-	linker	UNP P0A7G6

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	6	6	6	0	0

- Molecule 4 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
4	A	1	5	1	4	0	0

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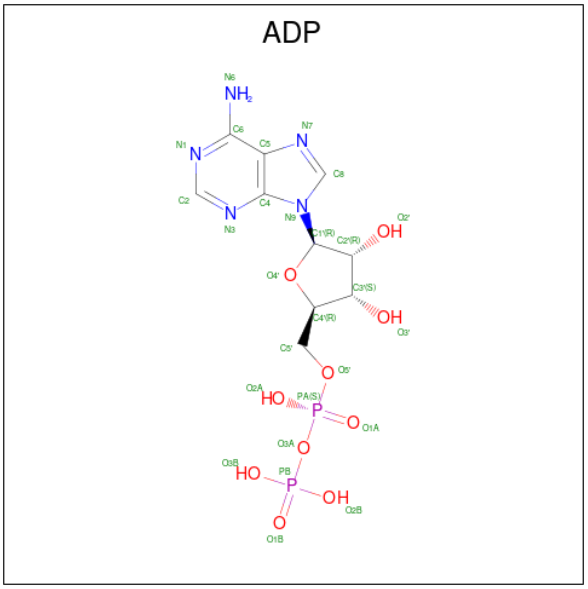
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Al	F			
4	A	1	5	1	4		0	0
			Total	Al	F			
4	A	1	5	1	4		0	0
			Total	Al	F			
4	A	1	5	1	4		0	0
			Total	Al	F			
4	A	1	5	1	4		0	0
			Total	Al	F			
4	A	1	5	1	4		0	0

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



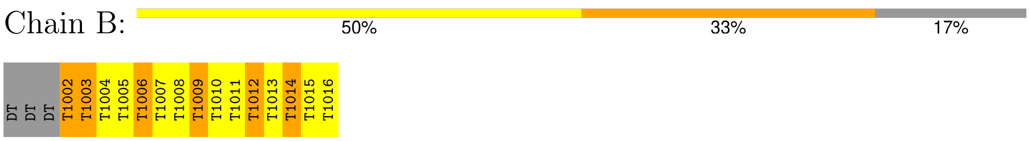
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0

3 Residue-property plots ⓘ

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

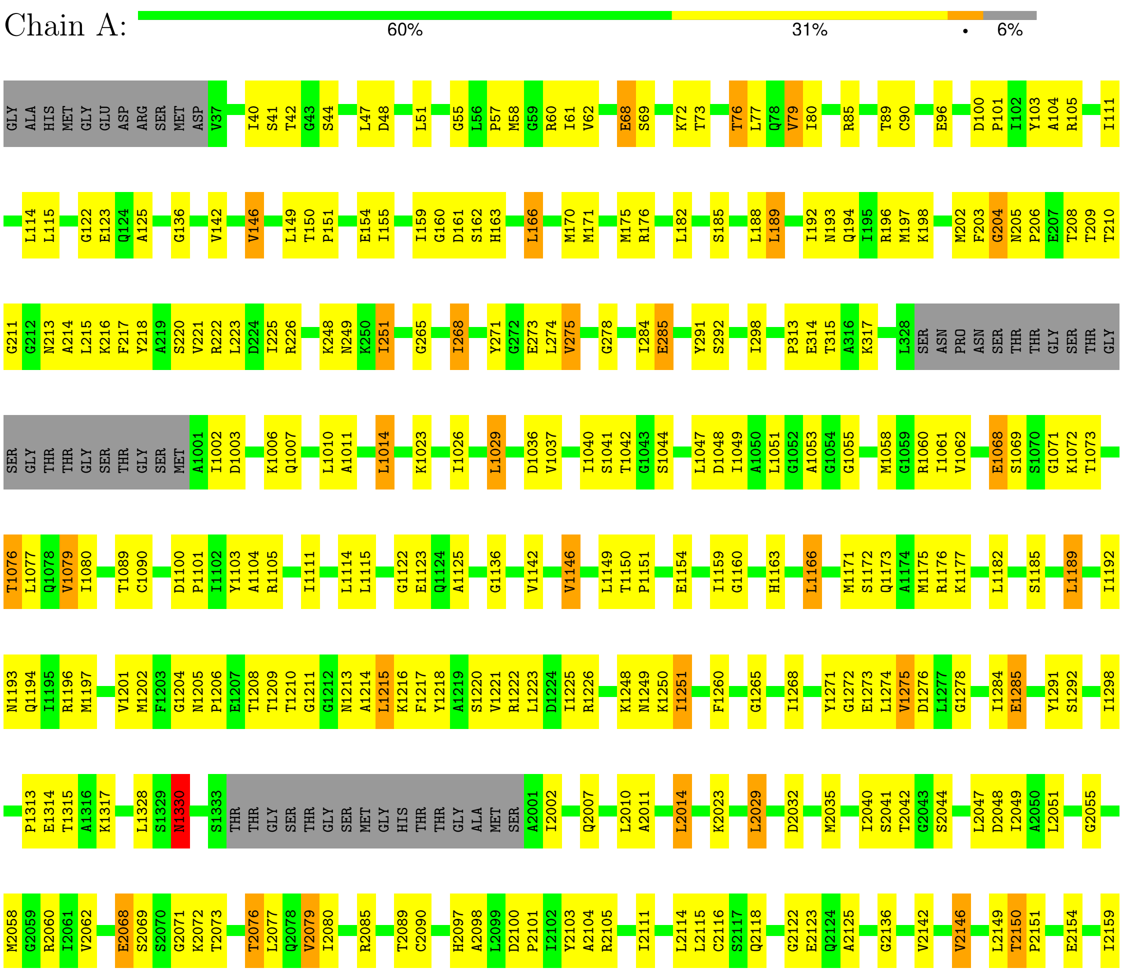
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain B:



- Molecule 2: Protein recA

Chain A:



PHE
GLY
N5205
P5206
E5207
T5208
T5209
T5210
G5211
G5212
N5213
A5214
L5215
K5216
F5217
S5220
V5221
R5222
L5223
D5224
I5225
R5226
E5235
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N5249
K5250
I5251
I5260
G5265
I5268
Y5271
G5272
E5273
L5274
V5275
G5278
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E5285
Y5291
S5292
I5298
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E5314
T5315
A5316
K5317
L5328
SER
ASN
PRO
ASN
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L5115
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E5123
Q5124
A5125
G5136
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V5146
L5149
T5150
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I5155
E5156
GLY
GLU
ILE
GLY
ASP
SER
HIS
M5164
G5165
L5166
M5170
M5171
S5172
Q5173
A5174
M5175
R5176
K5177
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R5196
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ILE
GLY
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M5058
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I5061
V5062
E5068
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T5076
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SER
THR
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E4207
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Y4218
A4219
S4220
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L4223
D4224
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R4226
K4248
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K4250
I4251
V4062
E4068
S4069
S4070
G4071
K4072
T4073
T4076
L4077
Q4078
V4079
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ALA
THR
GLY
ALA
MET
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ARG
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K4006
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L4010
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L4014
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S4044
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V3146
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S2172
Q2173
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F2217
Y2218
A2219
S2220
V2221
R2222
L2223
D2224
I2225
R2226
K2248
N2249
K2250

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	156.00Å 156.00Å 211.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 4.20 12.00 – 4.20	Depositor EDS
% Data completeness (in resolution range)	80.7 (12.00-4.20) 76.9 (12.00-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.275 , 0.298 0.271 , 0.287	Depositor DCC
R_{free} test set	1095 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	173.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 71.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15093	wwPDB-VP
Average B, all atoms (Å^2)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	B	0.90	0/326	1.70	8/502 (1.6%)
2	A	0.74	3/14765 (0.0%)	0.99	10/19866 (0.1%)
All	All	0.74	3/15091 (0.0%)	1.02	18/20368 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	268	ILE	C-N	7.34	1.43	1.33
2	A	5155	ILE	CA-CB	6.16	1.61	1.54
2	A	1036	ASP	CA-C	5.19	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5166	LEU	N-CA-C	-7.57	103.04	111.82
2	A	3166	LEU	N-CA-C	-7.35	103.34	111.36
2	A	4166	LEU	N-CA-C	-7.00	103.73	111.36
2	A	2166	LEU	N-CA-C	-6.96	103.78	111.36
1	B	1002	DT	N1-C1'-C2'	6.87	123.80	113.50
1	B	1006	DT	O3'-P-O5'	-6.83	93.76	104.00
2	A	166	LEU	N-CA-C	-6.69	104.06	111.82
2	A	1166	LEU	N-CA-C	-6.62	104.14	111.36
1	B	1012	DT	P-O3'-C3'	-6.59	110.32	120.20
1	B	1003	DT	P-O3'-C3'	5.73	128.80	120.20
2	A	5043	GLY	N-CA-C	-5.40	107.87	115.32
2	A	5178	LEU	N-CA-C	5.37	116.94	111.14
1	B	1014	DT	P-O3'-C3'	5.26	128.09	120.20
1	B	1012	DT	O3'-P-O5'	-5.25	96.12	104.00
2	A	4178	LEU	N-CA-C	5.24	116.80	111.14
1	B	1009	DT	O3'-P-O5'	-5.09	96.36	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1002	DT	C2-N1-C1'	5.06	126.94	119.35
2	A	4043	GLY	N-CA-C	-5.02	108.39	115.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	297	0	182	26	0
2	A	14598	0	14995	545	1
3	A	6	0	0	0	0
4	A	30	0	0	9	0
5	A	162	0	72	25	0
All	All	15093	0	15249	560	1

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 18.

All (560) 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:A:4194:GLN:HE21	2:A:4196:ARG:HH12	1.10	1.00
2:A:2194:GLN:HE21	2:A:2196:ARG:HH12	1.09	0.98
2:A:194:GLN:HE21	2:A:196:ARG:HH12	1.08	0.98
2:A:5194:GLN:HE21	2:A:5196:ARG:HH12	1.11	0.95
2:A:3194:GLN:HE21	2:A:3196:ARG:HH12	1.10	0.95
2:A:2068:GLU:HG2	2:A:3216:LYS:HB3	1.49	0.94
2:A:1194:GLN:HE21	2:A:1196:ARG:HH12	1.10	0.92
2:A:4160:GLY:H	2:A:5173:GLN:HE22	1.10	0.91
2:A:1160:GLY:H	2:A:2173:GLN:HE22	1.19	0.88
2:A:3194:GLN:NE2	2:A:3196:ARG:HH12	1.72	0.87
2:A:194:GLN:NE2	2:A:196:ARG:HH12	1.71	0.87
2:A:4194:GLN:NE2	2:A:4196:ARG:HH12	1.73	0.87
2:A:2194:GLN:NE2	2:A:2196:ARG:HH12	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2159:ILE:HA	2:A:3173:GLN:NE2	1.89	0.86
2:A:3068:GLU:HG2	2:A:4216:LYS:HB3	1.58	0.85
2:A:5194:GLN:NE2	2:A:5196:ARG:HH12	1.74	0.85
2:A:5146:VAL:HA	2:A:5149:LEU:HD13	1.59	0.85
2:A:1194:GLN:NE2	2:A:1196:ARG:HH12	1.73	0.85
2:A:1146:VAL:HA	2:A:1149:LEU:HD13	1.59	0.84
2:A:3159:ILE:HA	2:A:4173:GLN:NE2	1.94	0.83
2:A:4146:VAL:HA	2:A:4149:LEU:HD13	1.61	0.82
2:A:146:VAL:HA	2:A:149:LEU:HD13	1.60	0.82
2:A:2069:SER:OG	2:A:3248:LYS:HG3	1.80	0.81
2:A:2146:VAL:HA	2:A:2149:LEU:HD13	1.62	0.81
2:A:154:GLU:O	2:A:1177:LYS:HE2	1.81	0.81
2:A:4115:LEU:HD22	2:A:5026:ILE:HG12	1.62	0.80
2:A:5068:GLU:HA	4:A:5501:ALF:F1	1.71	0.80
2:A:2111:ILE:HG22	2:A:3030:GLY:HA2	1.64	0.80
2:A:3146:VAL:HA	2:A:3149:LEU:HD13	1.61	0.80
2:A:3160:GLY:H	2:A:4173:GLN:HE22	1.30	0.80
2:A:2111:ILE:HG22	2:A:3030:GLY:CA	2.13	0.79
2:A:2160:GLY:H	2:A:3173:GLN:HE22	1.28	0.79
2:A:3069:SER:OG	2:A:4248:LYS:HG3	1.85	0.77
2:A:1069:SER:OG	2:A:2248:LYS:HG3	1.86	0.76
2:A:1068:GLU:HG2	2:A:2216:LYS:HB3	1.68	0.75
2:A:3068:GLU:HG2	2:A:4216:LYS:CB	2.17	0.75
2:A:2068:GLU:HG2	2:A:3216:LYS:CB	2.16	0.74
2:A:4160:GLY:N	2:A:5173:GLN:HE22	1.84	0.74
2:A:4111:ILE:HG22	2:A:5030:GLY:CA	2.18	0.74
2:A:2071:GLY:HA2	5:A:2502:ADP:H5'1	1.72	0.72
2:A:4154:GLU:O	2:A:5177:LYS:HE2	1.89	0.72
2:A:3254:PRO:HG3	5:A:2502:ADP:O2'	1.90	0.71
2:A:42:THR:HG21	2:A:47:LEU:HD22	1.73	0.71
2:A:1042:THR:HG21	2:A:1047:LEU:HD22	1.74	0.70
2:A:4112:ASP:O	2:A:5028:ARG:HG2	1.91	0.70
2:A:96:GLU:OE2	4:A:501:ALF:F4	1.99	0.69
2:A:4159:ILE:HA	2:A:5173:GLN:NE2	2.08	0.69
2:A:4042:THR:HG21	2:A:4047:LEU:HD22	1.74	0.68
2:A:1068:GLU:HG2	2:A:2216:LYS:CB	2.23	0.68
2:A:1159:ILE:HG12	2:A:2177:LYS:HD3	1.74	0.68
2:A:2071:GLY:HA2	5:A:2502:ADP:C5'	2.24	0.68
2:A:4111:ILE:HG22	2:A:5030:GLY:N	2.09	0.68
2:A:3042:THR:HG21	2:A:3047:LEU:HD22	1.75	0.68
2:A:3171:MET:HA	2:A:3171:MET:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5042:THR:HG21	2:A:5047:LEU:HD22	1.76	0.68
2:A:160:GLY:H	2:A:1173:GLN:HE22	1.42	0.67
2:A:5072:LYS:N	5:A:5502:ADP:O2B	2.27	0.67
2:A:2049:ILE:HA	2:A:2328:LEU:CD2	2.24	0.67
2:A:4072:LYS:N	5:A:4502:ADP:O2B	2.25	0.67
2:A:2159:ILE:HA	2:A:3173:GLN:HE22	1.57	0.67
2:A:3159:ILE:HG12	2:A:4177:LYS:HD3	1.77	0.67
2:A:1159:ILE:HA	2:A:2173:GLN:NE2	2.10	0.66
2:A:4171:MET:HE2	2:A:4171:MET:HA	1.77	0.66
2:A:4159:ILE:HG12	2:A:5177:LYS:HD3	1.78	0.66
2:A:4291:TYR:O	2:A:4298:ILE:HG12	1.95	0.66
2:A:3291:TYR:O	2:A:3298:ILE:HG12	1.96	0.65
2:A:2042:THR:HG21	2:A:2047:LEU:HD22	1.76	0.65
2:A:1171:MET:HA	2:A:1171:MET:HE2	1.77	0.65
2:A:3159:ILE:HA	2:A:4173:GLN:HE22	1.60	0.65
2:A:171:MET:HE2	2:A:171:MET:HA	1.78	0.65
2:A:2171:MET:HE2	2:A:2171:MET:HA	1.77	0.65
2:A:4193:ASN:HD22	2:A:4194:GLN:H	1.45	0.65
2:A:111:ILE:HG23	2:A:1029:LEU:HD13	1.79	0.65
2:A:5171:MET:HE2	2:A:5171:MET:HA	1.78	0.64
2:A:1291:TYR:O	2:A:1298:ILE:HG12	1.97	0.64
2:A:1072:LYS:N	5:A:1502:ADP:O2B	2.31	0.64
2:A:3101:PRO:HD3	2:A:4035:MET:HG3	1.79	0.63
2:A:3248:LYS:NZ	4:A:2501:ALF:F1	2.21	0.63
2:A:2291:TYR:O	2:A:2298:ILE:HG12	1.99	0.63
2:A:3159:ILE:HG23	2:A:4173:GLN:HE21	1.64	0.63
2:A:291:TYR:O	2:A:298:ILE:HG12	1.98	0.63
2:A:1160:GLY:N	2:A:2173:GLN:HE22	1.92	0.63
2:A:2160:GLY:N	2:A:3173:GLN:HE22	1.96	0.63
2:A:5193:ASN:HD22	2:A:5194:GLN:H	1.47	0.62
2:A:5291:TYR:O	2:A:5298:ILE:HG12	1.98	0.62
2:A:2072:LYS:HB3	2:A:2192:ILE:HG23	1.80	0.62
2:A:4278:GLY:HA3	2:A:4284:ILE:HD12	1.82	0.62
2:A:193:ASN:HD22	2:A:194:GLN:H	1.47	0.62
2:A:5278:GLY:HA3	2:A:5284:ILE:HD12	1.82	0.61
2:A:3072:LYS:HB3	2:A:3192:ILE:HG23	1.83	0.61
2:A:3072:LYS:N	5:A:3502:ADP:O2B	2.31	0.61
2:A:1278:GLY:HA3	2:A:1284:ILE:HD12	1.82	0.61
2:A:4197:MET:HA	2:A:4206:PRO:O	2.01	0.61
2:A:5208:THR:HG22	2:A:5209:THR:H	1.65	0.61
2:A:2150:THR:OG1	2:A:3176:ARG:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:DT:N3	2:A:198:LYS:HB3	2.15	0.61
2:A:1193:ASN:HD22	2:A:1194:GLN:H	1.49	0.61
2:A:72:LYS:HB3	2:A:192:ILE:HG23	1.82	0.60
2:A:5072:LYS:HB3	2:A:5192:ILE:HG23	1.82	0.60
2:A:4208:THR:HG22	2:A:4209:THR:H	1.65	0.60
2:A:2159:ILE:HG12	2:A:3177:LYS:HD3	1.82	0.60
2:A:3193:ASN:HD22	2:A:3194:GLN:H	1.48	0.60
2:A:4254:PRO:HG3	5:A:3502:ADP:O2'	2.01	0.60
1:B:1003:DT:H3	2:A:198:LYS:HB3	1.66	0.60
2:A:5164:MET:O	2:A:5166:LEU:N	2.35	0.60
2:A:1072:LYS:HB3	2:A:1192:ILE:HG23	1.82	0.60
2:A:1154:GLU:O	2:A:2177:LYS:HE2	2.02	0.60
2:A:4068:GLU:HB3	2:A:5217:PHE:HA	1.83	0.60
1:B:1004:DT:C6	1:B:1005:DT:H72	2.37	0.59
2:A:1248:LYS:NZ	4:A:501:ALF:F1	2.17	0.59
2:A:2193:ASN:HD22	2:A:2194:GLN:H	1.49	0.59
2:A:3160:GLY:N	2:A:4173:GLN:HE22	1.97	0.59
2:A:1273:GLU:O	2:A:1274:LEU:C	2.45	0.59
2:A:3071:GLY:HA2	5:A:3502:ADP:O1A	2.02	0.59
2:A:4072:LYS:HB3	2:A:4192:ILE:HG23	1.83	0.59
2:A:3208:THR:HG22	2:A:3209:THR:H	1.68	0.59
2:A:208:THR:HG22	2:A:209:THR:H	1.68	0.59
2:A:4068:GLU:HG2	2:A:5216:LYS:HB3	1.84	0.59
2:A:68:GLU:HG2	2:A:1216:LYS:HB3	1.85	0.58
2:A:73:THR:O	2:A:76:THR:HB	2.04	0.58
2:A:2111:ILE:HG22	2:A:3030:GLY:N	2.18	0.58
2:A:2154:GLU:O	2:A:3177:LYS:HE2	2.04	0.58
2:A:2254:PRO:HG3	5:A:1502:ADP:O2'	2.04	0.58
2:A:3250:LYS:HA	5:A:2502:ADP:N7	2.18	0.58
2:A:3115:LEU:HD22	2:A:4026:ILE:HG12	1.85	0.58
2:A:2208:THR:HG22	2:A:2209:THR:H	1.69	0.58
2:A:3273:GLU:O	2:A:3274:LEU:C	2.46	0.58
2:A:1197:MET:HA	2:A:1206:PRO:O	2.05	0.57
2:A:2049:ILE:HA	2:A:2328:LEU:HD21	1.84	0.57
1:B:1010:DT:C6	1:B:1011:DT:H72	2.40	0.57
2:A:4069:SER:OG	2:A:5248:LYS:HG3	2.04	0.57
2:A:4273:GLU:O	2:A:4274:LEU:C	2.48	0.57
2:A:1250:LYS:HE3	4:A:501:ALF:F3	1.95	0.57
2:A:3111:ILE:HG23	2:A:4029:LEU:HD13	1.86	0.57
2:A:3053:ALA:HA	2:A:3330:ASN:O	2.05	0.56
2:A:4154:GLU:HG3	2:A:4163:HIS:HD2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5250:LYS:HE3	4:A:4501:ALF:F3	1.94	0.56
2:A:4111:ILE:HG22	2:A:5030:GLY:HA2	1.85	0.56
2:A:5073:THR:O	2:A:5076:THR:HB	2.05	0.56
1:B:1007:DT:C6	1:B:1008:DT:H72	2.40	0.56
2:A:2048:ASP:HA	2:A:2051:LEU:HD12	1.87	0.56
2:A:273:GLU:O	2:A:274:LEU:C	2.48	0.56
2:A:5076:THR:HG22	2:A:5077:LEU:N	2.21	0.56
2:A:4048:ASP:HA	2:A:4051:LEU:HD12	1.87	0.56
1:B:1013:DT:C6	1:B:1014:DT:H72	2.40	0.56
2:A:210:THR:HG22	2:A:211:GLY:H	1.71	0.56
2:A:1208:THR:HG22	2:A:1209:THR:H	1.71	0.56
2:A:1210:THR:HG22	2:A:1211:GLY:H	1.71	0.56
2:A:2210:THR:HG22	2:A:2211:GLY:H	1.70	0.56
2:A:3197:MET:HA	2:A:3206:PRO:O	2.05	0.56
2:A:3278:GLY:HA3	2:A:3284:ILE:HD12	1.87	0.56
2:A:5048:ASP:HA	2:A:5051:LEU:HD12	1.88	0.56
2:A:3048:ASP:HA	2:A:3051:LEU:HD12	1.88	0.55
2:A:4193:ASN:ND2	2:A:4194:GLN:H	2.04	0.55
2:A:2278:GLY:HA3	2:A:2284:ILE:HD12	1.88	0.55
2:A:2073:THR:O	2:A:2076:THR:HB	2.06	0.55
2:A:2273:GLU:O	2:A:2274:LEU:C	2.47	0.55
2:A:2285:GLU:HB3	2:A:2292:SER:HB2	1.89	0.55
2:A:5271:TYR:O	2:A:5275:VAL:HG23	2.06	0.55
2:A:40:ILE:HG22	2:A:41:SER:O	2.06	0.55
2:A:1271:TYR:O	2:A:1275:VAL:HG23	2.06	0.55
2:A:2136:GLY:HA2	2:A:2185:SER:HB3	1.89	0.55
2:A:4136:GLY:HA2	2:A:4185:SER:HB3	1.89	0.55
2:A:3111:ILE:HG22	2:A:4030:GLY:N	2.22	0.55
2:A:5103:TYR:O	2:A:5104:ALA:C	2.50	0.55
2:A:4073:THR:O	2:A:4076:THR:HB	2.07	0.55
2:A:5136:GLY:HA2	2:A:5185:SER:HB3	1.89	0.55
2:A:3073:THR:O	2:A:3076:THR:HB	2.07	0.54
2:A:5040:ILE:HG22	2:A:5041:SER:O	2.07	0.54
2:A:5273:GLU:O	2:A:5274:LEU:C	2.48	0.54
1:B:1003:DT:H3'	2:A:196:ARG:HB3	1.89	0.54
2:A:278:GLY:HA3	2:A:284:ILE:HD12	1.88	0.54
2:A:4210:THR:HG22	2:A:4211:GLY:H	1.72	0.54
2:A:3136:GLY:HA2	2:A:3185:SER:HB3	1.90	0.54
2:A:3210:THR:HG22	2:A:3211:GLY:H	1.72	0.54
2:A:1048:ASP:HA	2:A:1051:LEU:HD12	1.89	0.54
2:A:5210:THR:HG22	2:A:5211:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1073:THR:O	2:A:1076:THR:HB	2.08	0.54
2:A:1103:TYR:O	2:A:1104:ALA:C	2.51	0.54
2:A:3111:ILE:HG22	2:A:4030:GLY:CA	2.37	0.54
2:A:3150:THR:OG1	2:A:4176:ARG:HG2	2.08	0.54
1:B:1015:DT:O5'	1:B:1015:DT:H6	1.91	0.54
2:A:4040:ILE:HG22	2:A:4041:SER:O	2.08	0.54
2:A:4076:THR:HG22	2:A:4077:LEU:N	2.22	0.54
2:A:1111:ILE:HG23	2:A:2029:LEU:HD13	1.90	0.54
2:A:2123:GLU:OE1	2:A:2151:PRO:HA	2.08	0.53
2:A:2154:GLU:OE2	2:A:3176:ARG:HD2	2.07	0.53
2:A:3076:THR:HG22	2:A:3077:LEU:N	2.23	0.53
2:A:4007:GLN:HA	2:A:4010:LEU:HB3	1.91	0.53
2:A:5193:ASN:ND2	2:A:5194:GLN:H	2.06	0.53
2:A:40:ILE:HG12	2:A:58:MET:SD	2.48	0.53
2:A:3040:ILE:HG12	2:A:3058:MET:SD	2.48	0.53
2:A:2103:TYR:O	2:A:2104:ALA:C	2.51	0.53
2:A:4271:TYR:O	2:A:4275:VAL:HG23	2.09	0.53
2:A:5040:ILE:HG12	2:A:5058:MET:SD	2.49	0.53
1:B:1006:DT:H6	1:B:1006:DT:O5'	1.92	0.53
2:A:48:ASP:HA	2:A:51:LEU:HD12	1.90	0.53
2:A:4103:TYR:O	2:A:4104:ALA:C	2.50	0.53
2:A:76:THR:HG22	2:A:77:LEU:N	2.23	0.53
2:A:210:THR:HG22	2:A:211:GLY:N	2.24	0.53
2:A:2264:TYR:CD2	2:A:3254:PRO:HD2	2.43	0.53
2:A:4053:ALA:HA	2:A:4330:ASN:O	2.09	0.53
2:A:136:GLY:HA2	2:A:185:SER:HB3	1.90	0.53
2:A:1136:GLY:HA2	2:A:1185:SER:HB3	1.89	0.53
2:A:2076:THR:HG22	2:A:2077:LEU:N	2.24	0.53
2:A:2040:ILE:HG22	2:A:2041:SER:O	2.10	0.52
2:A:2111:ILE:CG2	2:A:3030:GLY:HA2	2.38	0.52
2:A:103:TYR:O	2:A:104:ALA:C	2.51	0.52
2:A:2007:GLN:HA	2:A:2010:LEU:HB3	1.91	0.52
2:A:3040:ILE:HG22	2:A:3041:SER:O	2.08	0.52
2:A:285:GLU:HB3	2:A:292:SER:HB2	1.90	0.52
2:A:1210:THR:HG22	2:A:1211:GLY:N	2.24	0.52
2:A:3103:TYR:O	2:A:3104:ALA:C	2.50	0.52
2:A:4115:LEU:HD13	2:A:5026:ILE:HD11	1.91	0.52
2:A:2271:TYR:O	2:A:2275:VAL:HG23	2.10	0.52
2:A:3123:GLU:OE1	2:A:3151:PRO:HA	2.09	0.52
2:A:2210:THR:HG22	2:A:2211:GLY:N	2.25	0.52
2:A:1249:ASN:OD1	2:A:1251:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4040:ILE:HG12	2:A:4058:MET:SD	2.50	0.52
2:A:5076:THR:O	2:A:5079:VAL:HG22	2.09	0.52
2:A:4210:THR:HG22	2:A:4211:GLY:N	2.25	0.52
2:A:5249:ASN:OD1	2:A:5251:ILE:HG22	2.10	0.52
2:A:76:THR:O	2:A:79:VAL:HG22	2.10	0.51
2:A:193:ASN:ND2	2:A:194:GLN:H	2.08	0.51
2:A:1076:THR:HG22	2:A:1077:LEU:N	2.23	0.51
2:A:1076:THR:O	2:A:1079:VAL:HG22	2.10	0.51
2:A:5123:GLU:OE1	2:A:5151:PRO:HA	2.09	0.51
2:A:2040:ILE:HG12	2:A:2058:MET:SD	2.50	0.51
2:A:3193:ASN:ND2	2:A:3194:GLN:H	2.07	0.51
1:B:1009:DT:O5'	1:B:1009:DT:H6	1.93	0.51
2:A:4060:ARG:HB3	2:A:4220:SER:OG	2.10	0.51
2:A:4071:GLY:HA2	5:A:4502:ADP:H5'1	1.91	0.51
2:A:2076:THR:O	2:A:2079:VAL:HG22	2.11	0.51
2:A:2197:MET:HA	2:A:2206:PRO:O	2.11	0.51
2:A:1040:ILE:HG22	2:A:1041:SER:O	2.09	0.51
2:A:3007:GLN:HA	2:A:3010:LEU:HB3	1.93	0.51
1:B:1012:DT:H6	1:B:1012:DT:O5'	1.93	0.51
2:A:159:ILE:HG12	2:A:1177:LYS:HD3	1.92	0.51
2:A:1007:GLN:HA	2:A:1010:LEU:HB3	1.92	0.51
2:A:4154:GLU:HG3	2:A:4163:HIS:CD2	2.46	0.51
2:A:5210:THR:HG22	2:A:5211:GLY:N	2.25	0.51
2:A:123:GLU:OE1	2:A:151:PRO:HA	2.10	0.51
2:A:1193:ASN:ND2	2:A:1194:GLN:H	2.09	0.51
2:A:4076:THR:O	2:A:4079:VAL:HG22	2.11	0.51
2:A:4123:GLU:OE1	2:A:4151:PRO:HA	2.11	0.51
2:A:5285:GLU:HB3	2:A:5292:SER:HB2	1.93	0.50
2:A:2193:ASN:ND2	2:A:2194:GLN:H	2.08	0.50
2:A:2069:SER:OG	2:A:3248:LYS:CG	2.56	0.50
2:A:3252:ALA:C	5:A:2502:ADP:C2	2.89	0.50
1:B:1011:DT:H2"	2:A:4169:ARG:HH11	1.76	0.50
2:A:1053:ALA:HA	2:A:1330:ASN:O	2.12	0.50
2:A:1193:ASN:HD21	2:A:1210:THR:HB	1.76	0.50
2:A:2249:ASN:OD1	2:A:2251:ILE:HG22	2.10	0.50
2:A:3249:ASN:OD1	2:A:3251:ILE:HG22	2.11	0.50
1:B:1016:DT:H72	2:A:4197:MET:HG2	1.94	0.50
2:A:2101:PRO:HD3	2:A:3035:MET:HG3	1.94	0.50
2:A:4249:ASN:OD1	2:A:4251:ILE:HG22	2.12	0.50
2:A:249:ASN:OD1	2:A:251:ILE:HG22	2.12	0.49
2:A:3111:ILE:HD12	2:A:4029:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4097:HIS:NE2	2:A:5180:GLY:HA2	2.27	0.49
2:A:3210:THR:HG22	2:A:3211:GLY:N	2.26	0.49
2:A:1123:GLU:OE1	2:A:1151:PRO:HA	2.11	0.49
2:A:1077:LEU:O	2:A:1080:ILE:HB	2.13	0.49
2:A:1285:GLU:HB3	2:A:1292:SER:HB2	1.93	0.49
2:A:1060:ARG:HB3	2:A:1220:SER:OG	2.13	0.49
2:A:1062:VAL:HG22	2:A:1221:VAL:HB	1.95	0.49
2:A:3068:GLU:HB3	2:A:4217:PHE:HA	1.93	0.49
2:A:3193:ASN:HD21	2:A:3210:THR:HB	1.78	0.49
2:A:5074:THR:OG1	5:A:5502:ADP:H5'1	2.11	0.49
1:B:1003:DT:H6	1:B:1003:DT:O5'	1.95	0.49
2:A:4049:ILE:HA	2:A:4328:LEU:CD2	2.42	0.49
2:A:69:SER:OG	2:A:1248:LYS:HG3	2.13	0.49
2:A:2011:ALA:HA	2:A:2014:LEU:HB2	1.94	0.49
2:A:2146:VAL:CA	2:A:2149:LEU:HD13	2.39	0.49
2:A:1040:ILE:HG12	2:A:1058:MET:SD	2.53	0.49
2:A:5007:GLN:HA	2:A:5010:LEU:HB3	1.94	0.49
2:A:4285:GLU:HB3	2:A:4292:SER:HB2	1.95	0.48
2:A:5060:ARG:HB3	2:A:5220:SER:OG	2.12	0.48
2:A:1011:ALA:HA	2:A:1014:LEU:HB2	1.95	0.48
2:A:3285:GLU:HB3	2:A:3292:SER:HB2	1.94	0.48
2:A:3271:TYR:O	2:A:3275:VAL:HG23	2.13	0.48
2:A:4205:ASN:HA	2:A:4206:PRO:HD3	1.64	0.48
2:A:3076:THR:O	2:A:3079:VAL:HG22	2.13	0.48
2:A:1068:GLU:HB3	2:A:2217:PHE:HA	1.96	0.48
2:A:4193:ASN:HD21	2:A:4210:THR:HB	1.78	0.48
2:A:5077:LEU:O	2:A:5080:ILE:HB	2.13	0.48
2:A:193:ASN:HD21	2:A:210:THR:HB	1.78	0.48
2:A:3011:ALA:HA	2:A:3014:LEU:HB2	1.95	0.48
2:A:4044:SER:HB2	2:A:4268:ILE:HD13	1.96	0.48
2:A:4313:PRO:O	2:A:4317:LYS:HG2	2.14	0.48
2:A:2060:ARG:HB3	2:A:2220:SER:OG	2.13	0.48
2:A:4068:GLU:HG2	2:A:5216:LYS:CB	2.43	0.48
2:A:90:CYS:HB2	2:A:114:LEU:HD23	1.96	0.48
2:A:271:TYR:O	2:A:275:VAL:HG23	2.13	0.48
2:A:1044:SER:HB2	2:A:1268:ILE:HD13	1.96	0.48
2:A:2097:HIS:CE1	2:A:3180:GLY:HA2	2.49	0.48
2:A:3154:GLU:O	2:A:4177:LYS:HE2	2.14	0.48
2:A:60:ARG:HB3	2:A:220:SER:OG	2.14	0.47
2:A:3124:GLN:HG3	2:A:4021:PHE:CD1	2.48	0.47
2:A:4071:GLY:HA2	5:A:4502:ADP:C5'	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5193:ASN:HD21	2:A:5210:THR:HB	1.79	0.47
2:A:3216:LYS:HA	2:A:3222:ARG:HD3	1.96	0.47
2:A:4077:LEU:O	2:A:4080:ILE:HB	2.14	0.47
2:A:4175:MET:O	2:A:4176:ARG:C	2.56	0.47
2:A:216:LYS:HA	2:A:222:ARG:HD3	1.96	0.47
2:A:2194:GLN:HG2	2:A:3217:PHE:CD2	2.50	0.47
2:A:4208:THR:HG22	2:A:4209:THR:N	2.29	0.47
2:A:5216:LYS:HA	2:A:5222:ARG:HD3	1.97	0.47
2:A:68:GLU:HG2	2:A:1216:LYS:CB	2.44	0.47
2:A:2193:ASN:HD21	2:A:2210:THR:HB	1.79	0.47
2:A:3032:ASP:HB3	2:A:3035:MET:HB2	1.96	0.47
2:A:5208:THR:HG22	2:A:5209:THR:N	2.29	0.47
2:A:2118:GLN:NE2	2:A:3183:LYS:HG2	2.29	0.47
2:A:3111:ILE:HG22	2:A:4030:GLY:HA2	1.95	0.47
2:A:3040:ILE:O	2:A:3055:GLY:HA3	2.15	0.47
2:A:3090:CYS:HB2	2:A:3114:LEU:HD23	1.97	0.47
2:A:205:ASN:HA	2:A:206:PRO:HD3	1.63	0.47
2:A:313:PRO:O	2:A:317:LYS:HG2	2.15	0.47
2:A:2216:LYS:HA	2:A:2222:ARG:HD3	1.95	0.47
2:A:4146:VAL:CA	2:A:4149:LEU:HD13	2.39	0.47
2:A:1105:ARG:N	2:A:1111:ILE:HD11	2.30	0.47
2:A:3077:LEU:O	2:A:3080:ILE:HB	2.15	0.47
2:A:5122:GLY:O	2:A:5125:ALA:HB3	2.14	0.47
2:A:146:VAL:CA	2:A:149:LEU:HD13	2.38	0.47
2:A:3069:SER:OG	2:A:4248:LYS:CG	2.61	0.47
2:A:4115:LEU:HD23	2:A:4115:LEU:HA	1.73	0.46
2:A:105:ARG:N	2:A:111:ILE:HD11	2.31	0.46
2:A:1313:PRO:O	2:A:1317:LYS:HG2	2.15	0.46
1:B:1016:DT:H3'	2:A:5212:GLY:HA2	1.97	0.46
2:A:2105:ARG:N	2:A:2111:ILE:HD11	2.31	0.46
2:A:3060:ARG:HB3	2:A:3220:SER:OG	2.15	0.46
2:A:1159:ILE:HG23	2:A:2173:GLN:HE21	1.81	0.46
2:A:1175:MET:O	2:A:1176:ARG:C	2.59	0.46
2:A:2159:ILE:CA	2:A:3173:GLN:HE22	2.28	0.46
2:A:4105:ARG:N	2:A:4111:ILE:HD11	2.31	0.46
2:A:2098:ALA:HA	2:A:3060:ARG:CZ	2.45	0.46
2:A:4090:CYS:HB2	2:A:4114:LEU:HD23	1.97	0.46
2:A:44:SER:HB2	2:A:268:ILE:HD13	1.96	0.46
2:A:1090:CYS:HB2	2:A:1114:LEU:HD23	1.97	0.46
2:A:2077:LEU:O	2:A:2080:ILE:HB	2.15	0.46
2:A:40:ILE:O	2:A:55:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:62:VAL:HG22	2:A:221:VAL:HB	1.98	0.46
2:A:175:MET:O	2:A:176:ARG:C	2.59	0.46
2:A:2175:MET:O	2:A:2176:ARG:C	2.59	0.46
2:A:3044:SER:HB2	2:A:3268:ILE:HD13	1.97	0.46
2:A:3159:ILE:CA	2:A:4173:GLN:HE22	2.28	0.46
2:A:77:LEU:O	2:A:80:ILE:HB	2.16	0.46
2:A:4147:ALA:O	2:A:5176:ARG:HG3	2.16	0.46
2:A:68:GLU:HB3	2:A:1217:PHE:HA	1.96	0.45
2:A:76:THR:CG2	2:A:142:VAL:HG21	2.46	0.45
2:A:4076:THR:CG2	2:A:4142:VAL:HG21	2.46	0.45
2:A:5062:VAL:HG22	2:A:5221:VAL:HB	1.98	0.45
2:A:1071:GLY:HA2	5:A:1502:ADP:C5'	2.46	0.45
2:A:2044:SER:HB2	2:A:2268:ILE:HD13	1.98	0.45
2:A:2115:LEU:HD22	2:A:3026:ILE:HG12	1.98	0.45
2:A:3213:ASN:O	2:A:3214:ALA:C	2.59	0.45
2:A:154:GLU:OE2	2:A:1176:ARG:HD2	2.16	0.45
2:A:1061:ILE:HD12	2:A:1061:ILE:N	2.32	0.45
2:A:3105:ARG:N	2:A:3111:ILE:HD11	2.31	0.45
2:A:3122:GLY:O	2:A:3125:ALA:HB3	2.16	0.45
2:A:1040:ILE:O	2:A:1055:GLY:HA3	2.16	0.45
2:A:2072:LYS:HB3	2:A:2192:ILE:CG2	2.47	0.45
2:A:4071:GLY:HA2	5:A:4502:ADP:O1A	2.16	0.45
2:A:4160:GLY:H	2:A:5173:GLN:NE2	1.94	0.45
2:A:4216:LYS:HA	2:A:4222:ARG:HD3	1.97	0.45
2:A:2208:THR:HG22	2:A:2209:THR:N	2.32	0.45
2:A:3076:THR:CG2	2:A:3142:VAL:HG21	2.46	0.45
2:A:5032:ASP:HB3	2:A:5035:MET:HB2	1.99	0.45
1:B:1007:DT:H4'	2:A:2168:ALA:CB	2.47	0.45
2:A:115:LEU:HD23	2:A:115:LEU:HA	1.73	0.45
2:A:1146:VAL:CA	2:A:1149:LEU:HD13	2.36	0.45
2:A:1216:LYS:HA	2:A:1222:ARG:HD3	1.97	0.45
2:A:2076:THR:CG2	2:A:2142:VAL:HG21	2.47	0.45
2:A:3124:GLN:HG3	2:A:4021:PHE:CG	2.52	0.45
2:A:5044:SER:HB2	2:A:5268:ILE:HD13	1.98	0.45
1:B:1006:DT:H4'	2:A:2169:ARG:HA	1.99	0.45
2:A:4040:ILE:O	2:A:4055:GLY:HA3	2.17	0.45
2:A:1213:ASN:O	2:A:1214:ALA:C	2.59	0.45
2:A:4115:LEU:HD13	2:A:5026:ILE:CD1	2.47	0.45
2:A:5090:CYS:HB2	2:A:5114:LEU:HD23	1.98	0.45
2:A:5175:MET:O	2:A:5176:ARG:C	2.60	0.45
2:A:5011:ALA:HA	2:A:5014:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3175:MET:O	2:A:3176:ARG:C	2.59	0.44
2:A:4062:VAL:HG22	2:A:4221:VAL:HB	1.98	0.44
1:B:1014:DT:C7	1:B:1015:DT:O4	2.65	0.44
2:A:208:THR:HG22	2:A:209:THR:N	2.31	0.44
2:A:2040:ILE:O	2:A:2055:GLY:HA3	2.16	0.44
2:A:2062:VAL:HG22	2:A:2221:VAL:HB	2.00	0.44
2:A:2213:ASN:O	2:A:2214:ALA:C	2.59	0.44
2:A:4193:ASN:HD22	2:A:4194:GLN:N	2.14	0.44
2:A:122:GLY:O	2:A:125:ALA:HB3	2.18	0.44
2:A:1071:GLY:HA2	5:A:1502:ADP:O1A	2.17	0.44
2:A:3071:GLY:HA2	5:A:3502:ADP:H5'1	1.99	0.44
2:A:3182:LEU:HD11	2:A:3189:LEU:HD12	1.99	0.44
2:A:4097:HIS:CD2	2:A:5180:GLY:HA2	2.53	0.44
2:A:1071:GLY:HA2	5:A:1502:ADP:H5'1	2.00	0.44
2:A:1072:LYS:HB3	2:A:1192:ILE:CG2	2.48	0.44
1:B:1002:DT:H2'	1:B:1003:DT:C5	2.53	0.44
2:A:1154:GLU:HG3	2:A:1163:HIS:HD2	1.82	0.44
2:A:2042:THR:O	2:A:2079:VAL:HG12	2.18	0.44
2:A:3154:GLU:HG3	2:A:3163:HIS:HD2	1.82	0.44
2:A:4118:GLN:NE2	2:A:5183:LYS:HG2	2.32	0.44
2:A:5213:ASN:O	2:A:5214:ALA:C	2.61	0.44
2:A:1003:ASP:HA	2:A:1006:LYS:HG3	1.99	0.44
2:A:2115:LEU:HD23	2:A:2115:LEU:HA	1.72	0.44
2:A:2122:GLY:O	2:A:2125:ALA:HB3	2.17	0.44
2:A:5040:ILE:O	2:A:5055:GLY:HA3	2.17	0.44
2:A:2170:MET:HE2	2:A:2170:MET:HB3	1.94	0.44
2:A:2182:LEU:HD11	2:A:2189:LEU:HD12	2.00	0.44
2:A:4103:TYR:HE1	2:A:4265:GLY:H	1.66	0.44
2:A:5115:LEU:HD23	2:A:5115:LEU:HA	1.73	0.44
2:A:5146:VAL:CA	2:A:5149:LEU:HD13	2.37	0.44
2:A:5225:ILE:O	2:A:5226:ARG:HG3	2.18	0.44
2:A:2090:CYS:HB2	2:A:2114:LEU:HD23	1.99	0.43
2:A:2100:ASP:OD2	2:A:3037:VAL:HG21	2.18	0.43
2:A:3146:VAL:CA	2:A:3149:LEU:HD13	2.38	0.43
2:A:5205:ASN:HA	2:A:5206:PRO:HD3	1.64	0.43
2:A:3208:THR:HG22	2:A:3209:THR:N	2.31	0.43
2:A:4116:CYS:SG	2:A:5035:MET:HE3	2.58	0.43
2:A:5061:ILE:HD12	2:A:5061:ILE:N	2.33	0.43
2:A:1042:THR:O	2:A:1079:VAL:HG12	2.18	0.43
4:A:5501:ALF:F2	5:A:5502:ADP:O1B	2.26	0.43
2:A:1103:TYR:HE1	2:A:1265:GLY:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1205:ASN:HA	2:A:1206:PRO:HD3	1.63	0.43
2:A:2097:HIS:NE2	2:A:3180:GLY:HA2	2.33	0.43
2:A:5182:LEU:HD11	2:A:5189:LEU:HD12	2.01	0.43
2:A:1122:GLY:O	2:A:1125:ALA:HB3	2.19	0.43
2:A:3071:GLY:HA2	5:A:3502:ADP:C5'	2.48	0.43
2:A:4011:ALA:HA	2:A:4014:LEU:HB2	1.99	0.43
2:A:4260:PHE:CD1	2:A:4268:ILE:HG23	2.53	0.43
2:A:5216:LYS:HG2	2:A:5222:ARG:CZ	2.49	0.43
2:A:2118:GLN:HE22	2:A:3183:LYS:HG2	1.82	0.43
2:A:2194:GLN:NE2	2:A:3217:PHE:CG	2.87	0.43
2:A:2250:LYS:HE3	4:A:1501:ALF:F3	2.08	0.43
2:A:3202:MET:HE2	2:A:3202:MET:H	1.83	0.43
2:A:3264:TYR:CD2	2:A:4254:PRO:HD2	2.54	0.43
2:A:5105:ARG:N	2:A:5111:ILE:HD11	2.33	0.43
2:A:103:TYR:HE1	2:A:265:GLY:H	1.66	0.43
2:A:197:MET:HA	2:A:206:PRO:O	2.19	0.43
2:A:1208:THR:HG22	2:A:1209:THR:N	2.33	0.43
2:A:2216:LYS:HG2	2:A:2222:ARG:CZ	2.49	0.43
2:A:4098:ALA:HA	2:A:5060:ARG:CZ	2.49	0.43
2:A:4111:ILE:CG2	2:A:5030:GLY:HA2	2.49	0.43
2:A:213:ASN:O	2:A:214:ALA:C	2.61	0.43
2:A:3103:TYR:HE1	2:A:3265:GLY:H	1.67	0.43
2:A:4122:GLY:O	2:A:4125:ALA:HB3	2.18	0.43
1:B:1004:DT:OP1	2:A:1213:ASN:N	2.51	0.43
1:B:1011:DT:C7	1:B:1012:DT:O4	2.67	0.43
2:A:3072:LYS:HB3	2:A:3192:ILE:CG2	2.49	0.43
2:A:3313:PRO:O	2:A:3317:LYS:HG2	2.19	0.43
2:A:4182:LEU:HD11	2:A:4189:LEU:HD12	2.00	0.43
2:A:4209:THR:HG22	2:A:4216:LYS:HE2	2.01	0.43
2:A:3062:VAL:HG22	2:A:3221:VAL:HB	2.00	0.42
2:A:3111:ILE:HG23	2:A:4029:LEU:HB3	2.01	0.42
2:A:4076:THR:HG23	2:A:4142:VAL:HG21	2.01	0.42
2:A:1182:LEU:HD11	2:A:1189:LEU:HD12	2.00	0.42
2:A:3175:MET:HB3	2:A:3218:TYR:CG	2.54	0.42
2:A:4097:HIS:CE1	2:A:5180:GLY:HA2	2.54	0.42
2:A:182:LEU:HD11	2:A:189:LEU:HD12	2.01	0.42
2:A:1068:GLU:HG2	2:A:2216:LYS:HB2	1.99	0.42
2:A:1159:ILE:HA	2:A:2173:GLN:HE22	1.82	0.42
2:A:2072:LYS:NZ	5:A:2502:ADP:PB	2.92	0.42
2:A:4217:PHE:O	2:A:4248:LYS:NZ	2.52	0.42
2:A:76:THR:HG23	2:A:142:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1076:THR:CG2	2:A:1142:VAL:HG21	2.49	0.42
2:A:3042:THR:O	2:A:3079:VAL:HG12	2.19	0.42
2:A:3216:LYS:HG2	2:A:3222:ARG:CZ	2.49	0.42
2:A:2032:ASP:HB3	2:A:2035:MET:HB2	2.01	0.42
2:A:2068:GLU:CG	2:A:3216:LYS:HB3	2.35	0.42
2:A:2150:THR:HG23	2:A:3176:ARG:HD2	2.01	0.42
2:A:2313:PRO:O	2:A:2317:LYS:HG2	2.19	0.42
2:A:100:ASP:HA	2:A:101:PRO:HD2	1.89	0.42
2:A:216:LYS:HG2	2:A:222:ARG:CZ	2.49	0.42
2:A:2098:ALA:HB1	2:A:3250:LYS:HD3	2.02	0.42
2:A:4042:THR:O	2:A:4079:VAL:HG12	2.19	0.42
2:A:4061:ILE:N	2:A:4061:ILE:HD12	2.35	0.42
2:A:4111:ILE:HG23	2:A:5029:LEU:HB3	2.01	0.42
2:A:3205:ASN:HA	2:A:3206:PRO:HD3	1.62	0.42
2:A:3260:PHE:CD1	2:A:3268:ILE:HG23	2.55	0.42
2:A:4213:ASN:O	2:A:4214:ALA:C	2.61	0.42
2:A:4225:ILE:O	2:A:4226:ARG:HG3	2.20	0.42
2:A:5076:THR:CG2	2:A:5142:VAL:HG21	2.50	0.42
2:A:1175:MET:HB3	2:A:1218:TYR:CG	2.55	0.42
2:A:2194:GLN:NE2	2:A:3217:PHE:HB2	2.34	0.42
2:A:2225:ILE:O	2:A:2226:ARG:HG3	2.19	0.42
2:A:3225:ILE:O	2:A:3226:ARG:HG3	2.19	0.42
2:A:3101:PRO:HB3	2:A:4029:LEU:HD22	2.00	0.42
2:A:3217:PHE:O	2:A:3248:LYS:NZ	2.52	0.42
2:A:5217:PHE:O	2:A:5248:LYS:NZ	2.53	0.42
1:B:1003:DT:H5'	2:A:1172:SER:CB	2.50	0.42
2:A:203:PHE:CG	2:A:204:GLY:N	2.88	0.42
2:A:2159:ILE:HG23	2:A:3173:GLN:HE21	1.85	0.42
2:A:5042:THR:O	2:A:5079:VAL:HG12	2.20	0.42
2:A:5103:TYR:HE1	2:A:5265:GLY:H	1.67	0.42
2:A:209:THR:HG22	2:A:216:LYS:HE2	2.00	0.41
2:A:217:PHE:O	2:A:248:LYS:NZ	2.52	0.41
2:A:42:THR:O	2:A:79:VAL:HG12	2.19	0.41
2:A:2154:GLU:OE2	2:A:3176:ARG:NH1	2.52	0.41
2:A:3159:ILE:HG12	2:A:4177:LYS:CD	2.49	0.41
2:A:4003:ASP:HA	2:A:4006:LYS:HG3	2.01	0.41
2:A:4101:PRO:HG2	2:A:4102:ILE:HD12	2.03	0.41
2:A:5170:MET:HE2	2:A:5170:MET:HB3	2.00	0.41
2:A:115:LEU:HD22	2:A:1026:ILE:HG12	2.02	0.41
2:A:3224:ASP:OD1	2:A:3226:ARG:NE	2.52	0.41
2:A:4034:SER:O	2:A:4183:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4216:LYS:HG2	2:A:4222:ARG:CZ	2.49	0.41
1:B:1007:DT:H71	2:A:1197:MET:HG2	2.03	0.41
2:A:1100:ASP:HA	2:A:1101:PRO:HD2	1.90	0.41
2:A:1225:ILE:O	2:A:1226:ARG:HG3	2.21	0.41
2:A:2103:TYR:HE1	2:A:2265:GLY:H	1.67	0.41
2:A:2209:THR:HG22	2:A:2216:LYS:HE2	2.03	0.41
2:A:3209:THR:HG22	2:A:3216:LYS:HE2	2.02	0.41
2:A:4072:LYS:HB3	2:A:4192:ILE:CG2	2.50	0.41
2:A:5101:PRO:HG2	2:A:5102:ILE:HD12	2.03	0.41
2:A:1260:PHE:CD1	2:A:1268:ILE:HG23	2.56	0.41
2:A:2217:PHE:O	2:A:2248:LYS:NZ	2.53	0.41
2:A:4175:MET:HB3	2:A:4218:TYR:CG	2.56	0.41
2:A:5100:ASP:HA	2:A:5101:PRO:HD2	1.88	0.41
2:A:1217:PHE:O	2:A:1248:LYS:NZ	2.54	0.41
2:A:4154:GLU:HA	2:A:4163:HIS:CD2	2.55	0.41
2:A:5072:LYS:HB3	2:A:5192:ILE:CG2	2.49	0.41
2:A:61:ILE:N	2:A:61:ILE:HD12	2.35	0.41
2:A:72:LYS:HB3	2:A:192:ILE:CG2	2.48	0.41
2:A:72:LYS:HE2	2:A:72:LYS:HB2	1.88	0.41
2:A:2175:MET:HB3	2:A:2218:TYR:CG	2.55	0.41
2:A:2248:LYS:NZ	4:A:1501:ALF:F1	2.32	0.41
2:A:3193:ASN:HD22	2:A:3194:GLN:N	2.16	0.41
2:A:4044:SER:OG	2:A:4273:GLU:OE2	2.22	0.41
2:A:5193:ASN:HD22	2:A:5194:GLN:N	2.15	0.41
1:B:1008:DT:C7	1:B:1009:DT:O4	2.69	0.41
1:B:1015:DT:N3	2:A:4198:LYS:HA	2.35	0.41
2:A:1154:GLU:HG3	2:A:1163:HIS:CD2	2.55	0.41
2:A:2076:THR:HG23	2:A:2142:VAL:HG21	2.02	0.41
2:A:2205:ASN:HA	2:A:2206:PRO:HD3	1.62	0.41
2:A:3076:THR:HG23	2:A:3142:VAL:HG21	2.01	0.41
2:A:3170:MET:HE2	2:A:3170:MET:HB3	1.97	0.41
2:A:3175:MET:HB3	2:A:3218:TYR:CD1	2.56	0.41
2:A:4175:MET:HB3	2:A:4218:TYR:CD1	2.56	0.41
2:A:170:MET:HE2	2:A:170:MET:HB3	1.96	0.41
2:A:1214:ALA:O	2:A:1215:LEU:C	2.64	0.41
2:A:3042:THR:HA	2:A:3079:VAL:HG12	2.03	0.41
2:A:3112:ASP:O	2:A:4028:ARG:HG2	2.21	0.41
2:A:4252:ALA:C	5:A:3502:ADP:C2	2.98	0.41
1:B:1004:DT:H2"	1:B:1005:DT:H6	1.86	0.40
2:A:4049:ILE:HD11	2:A:4323:VAL:HG12	2.03	0.40
2:A:4202:MET:H	2:A:4202:MET:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:57:PRO:O	2:A:188:LEU:HD13	2.21	0.40
2:A:175:MET:HB3	2:A:218:TYR:CG	2.57	0.40
2:A:1049:ILE:HA	2:A:1328:LEU:CD2	2.51	0.40
2:A:1068:GLU:H	2:A:1068:GLU:HG3	1.57	0.40
2:A:2116:CYS:SG	2:A:3035:MET:HE3	2.61	0.40
2:A:3254:PRO:CG	5:A:2502:ADP:O2'	2.65	0.40
2:A:4224:ASP:OD1	2:A:4226:ARG:NE	2.49	0.40
2:A:5260:PHE:CD1	2:A:5268:ILE:HG23	2.55	0.40
2:A:5313:PRO:O	2:A:5317:LYS:HG2	2.21	0.40
2:A:225:ILE:O	2:A:226:ARG:HG3	2.21	0.40
2:A:1115:LEU:HA	2:A:1115:LEU:HD23	1.75	0.40
2:A:1272:GLY:O	2:A:1275:VAL:HB	2.21	0.40
2:A:2260:PHE:CD1	2:A:2268:ILE:HG23	2.56	0.40
2:A:3251:ILE:HD12	2:A:3251:ILE:HA	1.92	0.40

All (1) 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)
2:A:1276:ASP:OD2	2:A:5235:GLU:OE2[4_556]	2.08	0.12

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
2	A	1921/2050 (94%)	1719 (90%)	180 (9%)	22 (1%)	11 45

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	5165	GLY
2	A	1204	GLY

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Mol	Chain	Res	Type
2	A	2204	GLY
2	A	3204	GLY
2	A	4204	GLY
2	A	161	ASP
2	A	1023	LYS
2	A	2023	LYS
2	A	3023	LYS
2	A	4023	LYS
2	A	5023	LYS
2	A	1037	VAL
2	A	1275	VAL
2	A	4275	VAL
2	A	275	VAL
2	A	2275	VAL
2	A	3275	VAL
2	A	5275	VAL
2	A	204	GLY
2	A	1330	ASN
2	A	3037	VAL
2	A	4330	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	1524/1606 (95%)	1401 (92%)	123 (8%)	11 32

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	68	GLU
2	A	76	THR
2	A	79	VAL
2	A	85	ARG
2	A	89	THR
2	A	146	VAL

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Mol	Chain	Res	Type
2	A	150	THR
2	A	155	ILE
2	A	162	SER
2	A	163	HIS
2	A	166	LEU
2	A	189	LEU
2	A	202	MET
2	A	215	LEU
2	A	223	LEU
2	A	251	ILE
2	A	285	GLU
2	A	314	GLU
2	A	315	THR
2	A	1002	ILE
2	A	1014	LEU
2	A	1029	LEU
2	A	1068	GLU
2	A	1076	THR
2	A	1079	VAL
2	A	1089	THR
2	A	1146	VAL
2	A	1150	THR
2	A	1166	LEU
2	A	1189	LEU
2	A	1201	VAL
2	A	1202	MET
2	A	1215	LEU
2	A	1223	LEU
2	A	1251	ILE
2	A	1285	GLU
2	A	1314	GLU
2	A	1315	THR
2	A	1330	ASN
2	A	2002	ILE
2	A	2014	LEU
2	A	2029	LEU
2	A	2068	GLU
2	A	2076	THR
2	A	2079	VAL
2	A	2085	ARG
2	A	2089	THR
2	A	2146	VAL

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Mol	Chain	Res	Type
2	A	2150	THR
2	A	2166	LEU
2	A	2189	LEU
2	A	2199	ILE
2	A	2201	VAL
2	A	2202	MET
2	A	2215	LEU
2	A	2223	LEU
2	A	2251	ILE
2	A	2285	GLU
2	A	2314	GLU
2	A	2315	THR
2	A	2330	ASN
2	A	3002	ILE
2	A	3014	LEU
2	A	3029	LEU
2	A	3068	GLU
2	A	3076	THR
2	A	3079	VAL
2	A	3089	THR
2	A	3146	VAL
2	A	3150	THR
2	A	3166	LEU
2	A	3189	LEU
2	A	3201	VAL
2	A	3202	MET
2	A	3203	PHE
2	A	3215	LEU
2	A	3223	LEU
2	A	3251	ILE
2	A	3285	GLU
2	A	3314	GLU
2	A	3315	THR
2	A	3330	ASN
2	A	4002	ILE
2	A	4014	LEU
2	A	4029	LEU
2	A	4068	GLU
2	A	4076	THR
2	A	4079	VAL
2	A	4089	THR
2	A	4146	VAL

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Mol	Chain	Res	Type
2	A	4150	THR
2	A	4155	ILE
2	A	4166	LEU
2	A	4189	LEU
2	A	4199	ILE
2	A	4201	VAL
2	A	4202	MET
2	A	4215	LEU
2	A	4223	LEU
2	A	4251	ILE
2	A	4285	GLU
2	A	4314	GLU
2	A	4315	THR
2	A	4330	ASN
2	A	5002	ILE
2	A	5014	LEU
2	A	5029	LEU
2	A	5068	GLU
2	A	5076	THR
2	A	5079	VAL
2	A	5089	THR
2	A	5146	VAL
2	A	5150	THR
2	A	5155	ILE
2	A	5164	MET
2	A	5166	LEU
2	A	5189	LEU
2	A	5215	LEU
2	A	5223	LEU
2	A	5251	ILE
2	A	5285	GLU
2	A	5314	GLU
2	A	5315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	124	GLN
2	A	181	ASN
2	A	193	ASN
2	A	194	GLN
2	A	236	ASN

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Mol	Chain	Res	Type
2	A	304	ASN
2	A	1097	HIS
2	A	1124	GLN
2	A	1163	HIS
2	A	1173	GLN
2	A	1181	ASN
2	A	1193	ASN
2	A	1194	GLN
2	A	1236	ASN
2	A	1304	ASN
2	A	2097	HIS
2	A	2118	GLN
2	A	2124	GLN
2	A	2163	HIS
2	A	2173	GLN
2	A	2181	ASN
2	A	2193	ASN
2	A	2194	GLN
2	A	2236	ASN
2	A	2300	GLN
2	A	2304	ASN
2	A	3016	GLN
2	A	3097	HIS
2	A	3118	GLN
2	A	3124	GLN
2	A	3163	HIS
2	A	3173	GLN
2	A	3181	ASN
2	A	3193	ASN
2	A	3194	GLN
2	A	3236	ASN
2	A	3300	GLN
2	A	3304	ASN
2	A	4016	GLN
2	A	4118	GLN
2	A	4124	GLN
2	A	4163	HIS
2	A	4173	GLN
2	A	4181	ASN
2	A	4193	ASN
2	A	4194	GLN
2	A	4236	ASN

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Mol	Chain	Res	Type
2	A	4300	GLN
2	A	4304	ASN
2	A	5097	HIS
2	A	5124	GLN
2	A	5173	GLN
2	A	5181	ASN
2	A	5193	ASN
2	A	5194	GLN
2	A	5236	ASN
2	A	5300	GLN
2	A	5304	ASN

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)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ALF	A	2501	5	4,4,4	1.39	0	-		
5	ADP	A	1502	3,4	28,29,29	1.53	4 (14%)	43,45,45	1.87	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	A	502	3,4	28,29,29	1.44	5 (17%)	43,45,45	1.89	12 (27%)
5	ADP	A	4502	3,4	28,29,29	1.45	5 (17%)	43,45,45	1.99	11 (25%)
5	ADP	A	5502	3,4	28,29,29	1.52	5 (17%)	43,45,45	1.83	10 (23%)
5	ADP	A	2502	3,4	28,29,29	1.44	5 (17%)	43,45,45	1.77	10 (23%)
4	ALF	A	501	5	4,4,4	1.36	0	-		
5	ADP	A	3502	3,4	28,29,29	1.46	4 (14%)	43,45,45	1.92	10 (23%)
4	ALF	A	4501	5	4,4,4	1.40	0	-		
4	ALF	A	5501	5	4,4,4	1.39	0	-		
4	ALF	A	3501	5	4,4,4	1.36	0	-		
4	ALF	A	1501	5	4,4,4	1.41	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
5	ADP	A	1502	3,4	-	0/16/32/32	0/3/3/3
5	ADP	A	502	3,4	-	1/16/32/32	0/3/3/3
5	ADP	A	4502	3,4	-	1/16/32/32	0/3/3/3
5	ADP	A	2502	3,4	-	0/16/32/32	0/3/3/3
5	ADP	A	3502	3,4	-	0/16/32/32	0/3/3/3
5	ADP	A	5502	3,4	-	0/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1502	ADP	C5-C4	5.14	1.48	1.39
5	A	3502	ADP	C5-C4	4.97	1.47	1.39
5	A	5502	ADP	C5-C4	4.95	1.47	1.39
5	A	4502	ADP	C5-C4	4.75	1.47	1.39
5	A	2502	ADP	C5-C4	4.74	1.47	1.39
5	A	502	ADP	C5-C4	4.71	1.47	1.39
5	A	5502	ADP	C5-C6	3.10	1.49	1.41
5	A	4502	ADP	C5-C6	3.09	1.49	1.41
5	A	1502	ADP	C5-C6	2.96	1.49	1.41
5	A	3502	ADP	C5-C6	2.85	1.48	1.41
5	A	2502	ADP	C5-C6	2.57	1.48	1.41
5	A	3502	ADP	C8-N7	2.50	1.36	1.31
5	A	2502	ADP	C5-N7	-2.50	1.34	1.39
5	A	5502	ADP	C4-N9	-2.50	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	ADP	C5-N7	-2.49	1.34	1.39
5	A	502	ADP	C8-N7	2.49	1.36	1.31
5	A	1502	ADP	C8-N7	2.42	1.36	1.31
5	A	4502	ADP	C8-N7	2.30	1.36	1.31
5	A	1502	ADP	C5-N7	-2.24	1.35	1.39
5	A	2502	ADP	C8-N7	2.23	1.36	1.31
5	A	5502	ADP	C5-N7	-2.20	1.35	1.39
5	A	5502	ADP	C8-N7	2.17	1.35	1.31
5	A	4502	ADP	C5-N7	-2.15	1.35	1.39
5	A	502	ADP	C5-C6	2.15	1.47	1.41
5	A	2502	ADP	C4-N9	-2.12	1.33	1.37
5	A	502	ADP	PA-O3A	2.07	1.61	1.59
5	A	4502	ADP	C4-N9	-2.03	1.33	1.37
5	A	3502	ADP	C5-N7	-2.01	1.35	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1502	ADP	C5-C4-N3	-5.82	118.70	126.72
5	A	4502	ADP	C5-C4-N3	-5.67	118.91	126.72
5	A	3502	ADP	C5-C4-N3	-5.61	118.99	126.72
5	A	502	ADP	C5-C4-N3	-5.31	119.41	126.72
5	A	5502	ADP	C5-C4-N3	-5.19	119.57	126.72
5	A	2502	ADP	C5-C4-N3	-5.19	119.57	126.72
5	A	502	ADP	N3-C4-N9	5.00	135.67	127.17
5	A	1502	ADP	N3-C4-N9	4.85	135.42	127.17
5	A	4502	ADP	N3-C4-N9	4.78	135.30	127.17
5	A	3502	ADP	N3-C4-N9	4.77	135.28	127.17
5	A	2502	ADP	N3-C4-N9	4.33	134.53	127.17
5	A	5502	ADP	N3-C4-N9	4.21	134.33	127.17
5	A	1502	ADP	C2-N3-C4	4.00	121.61	111.83
5	A	502	ADP	N3-C2-N1	-3.98	122.56	128.58
5	A	4502	ADP	C2-N3-C4	3.96	121.51	111.83
5	A	1502	ADP	N3-C2-N1	-3.93	122.64	128.58
5	A	3502	ADP	C2-N3-C4	3.87	121.29	111.83
5	A	4502	ADP	N3-C2-N1	-3.84	122.77	128.58
5	A	4502	ADP	C4-N9-C8	3.81	109.74	105.74
5	A	3502	ADP	N3-C2-N1	-3.80	122.83	128.58
5	A	5502	ADP	C4-C5-N7	-3.78	106.26	110.58
5	A	4502	ADP	C4-C5-N7	-3.75	106.29	110.58
5	A	502	ADP	C2-N3-C4	3.66	120.77	111.83
5	A	2502	ADP	C2-N3-C4	3.46	120.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2502	ADP	N3-C2-N1	-3.45	123.36	128.58
5	A	502	ADP	C4-N9-C8	3.43	109.34	105.74
5	A	5502	ADP	C2-N3-C4	3.43	120.21	111.83
5	A	5502	ADP	C4-N9-C8	3.43	109.33	105.74
5	A	3502	ADP	C4-N9-C8	3.32	109.22	105.74
5	A	3502	ADP	C4-C5-N7	-3.26	106.86	110.58
5	A	1502	ADP	C4-C5-N7	-3.25	106.87	110.58
5	A	2502	ADP	C4-C5-N7	-3.19	106.93	110.58
5	A	5502	ADP	N3-C2-N1	-3.14	123.83	128.58
5	A	2502	ADP	C4-N9-C8	3.04	108.93	105.74
5	A	4502	ADP	C5-N7-C8	2.96	108.11	103.45
5	A	1502	ADP	C4-N9-C8	2.75	108.63	105.74
5	A	4502	ADP	N9-C8-N7	-2.73	110.07	113.94
5	A	5502	ADP	C5-N7-C8	2.66	107.63	103.45
5	A	3502	ADP	C5-N7-C8	2.59	107.52	103.45
5	A	2502	ADP	C5-N7-C8	2.52	107.41	103.45
5	A	5502	ADP	C2'-C1'-N9	-2.52	107.05	113.30
5	A	502	ADP	O3B-PB-O2B	2.51	117.22	107.80
5	A	1502	ADP	C5-N7-C8	2.46	107.31	103.45
5	A	4502	ADP	C6-C5-N7	2.45	136.81	132.09
5	A	502	ADP	N6-C6-N1	2.38	123.69	118.38
5	A	502	ADP	C5-N7-C8	2.34	107.13	103.45
5	A	5502	ADP	C6-C5-N7	2.33	136.59	132.09
5	A	502	ADP	C4-C5-N7	-2.32	107.93	110.58
5	A	5502	ADP	N9-C8-N7	-2.30	110.67	113.94
5	A	3502	ADP	N9-C8-N7	-2.30	110.67	113.94
5	A	502	ADP	N9-C8-N7	-2.30	110.67	113.94
5	A	3502	ADP	C2-N1-C6	2.27	122.45	118.73
5	A	502	ADP	C2-N1-C6	2.25	122.42	118.73
5	A	4502	ADP	O3A-PA-O1A	-2.20	104.08	110.70
5	A	2502	ADP	N9-C8-N7	-2.19	110.83	113.94
5	A	2502	ADP	C6-C5-N7	2.11	136.17	132.09
5	A	3502	ADP	C6-C5-N7	2.11	136.15	132.09
5	A	502	ADP	C5-C6-N6	-2.10	118.09	123.29
5	A	1502	ADP	C6-C5-N7	2.06	136.06	132.09
5	A	4502	ADP	C2-N1-C6	2.05	122.09	118.73
5	A	2502	ADP	C2-N1-C6	2.04	122.08	118.73
5	A	1502	ADP	C2-N1-C6	2.04	122.08	118.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	ADP	PA-O3A-PB-O3B
5	A	4502	ADP	PA-O3A-PB-O3B

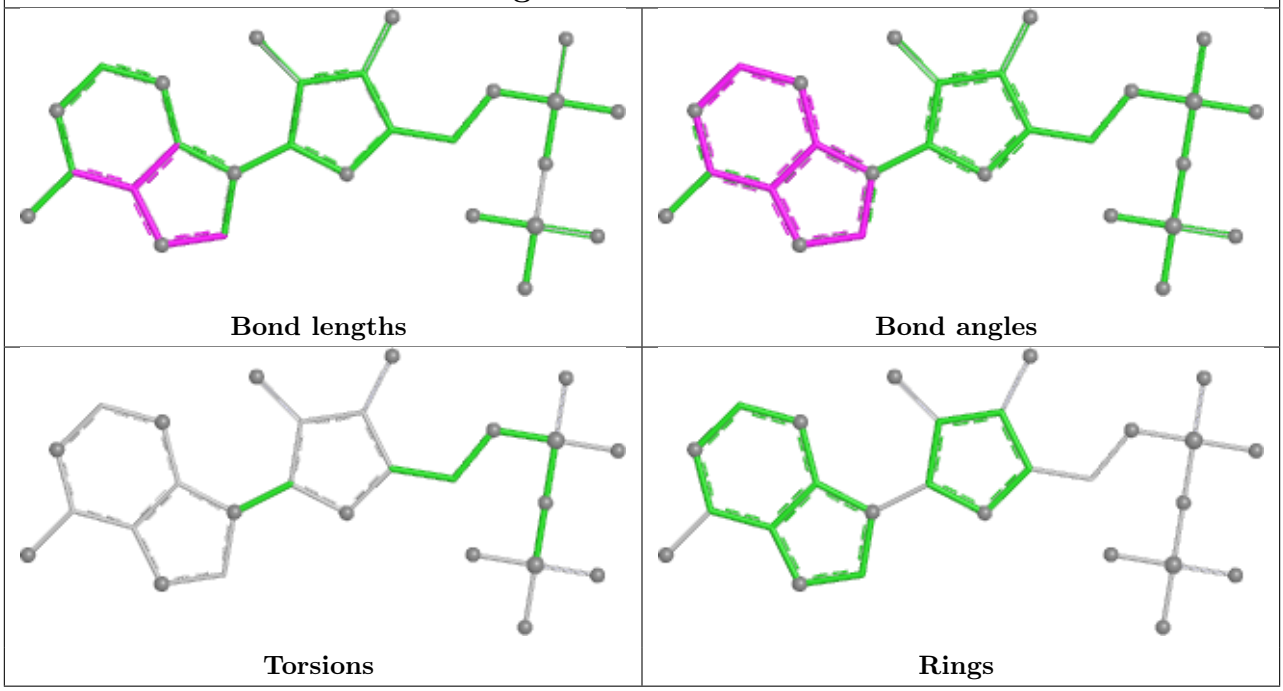
There are no ring outliers.

10 monomers are involved in 33 short contacts:

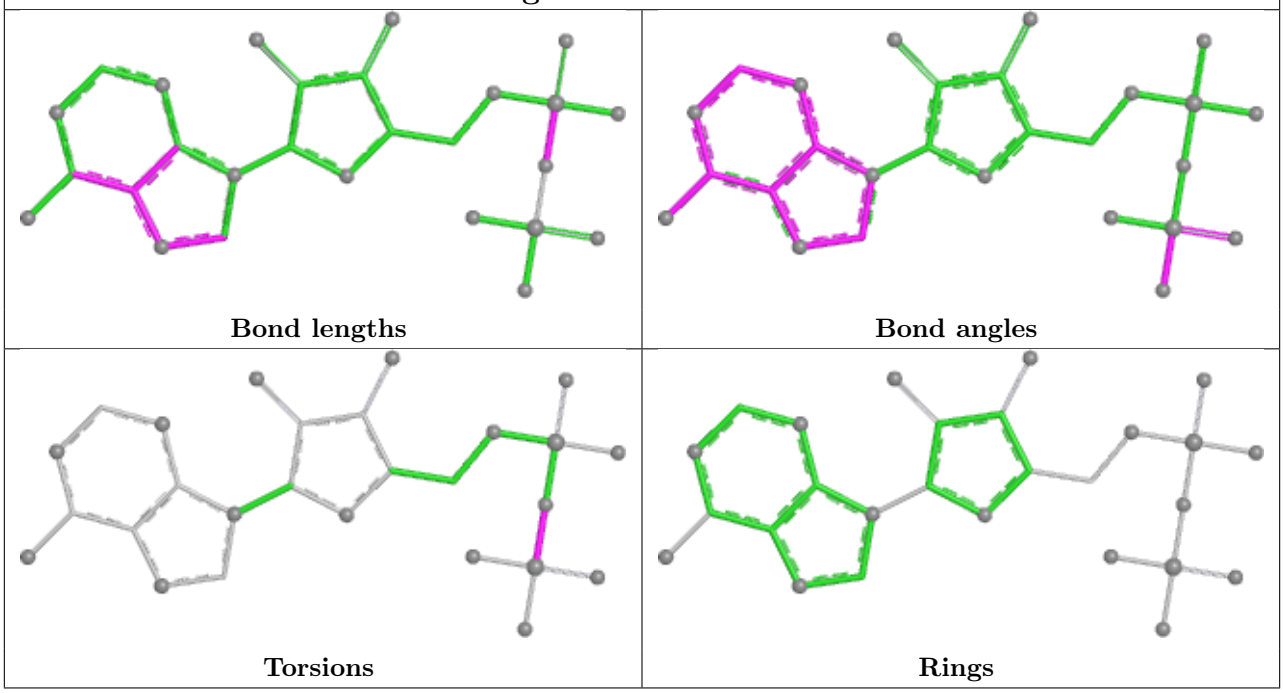
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2501	ALF	1	0
5	A	1502	ADP	5	0
5	A	4502	ADP	4	0
5	A	5502	ADP	3	0
5	A	2502	ADP	7	0
4	A	501	ALF	3	0
5	A	3502	ADP	6	0
4	A	4501	ALF	1	0
4	A	5501	ALF	2	0
4	A	1501	ALF	2	0

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

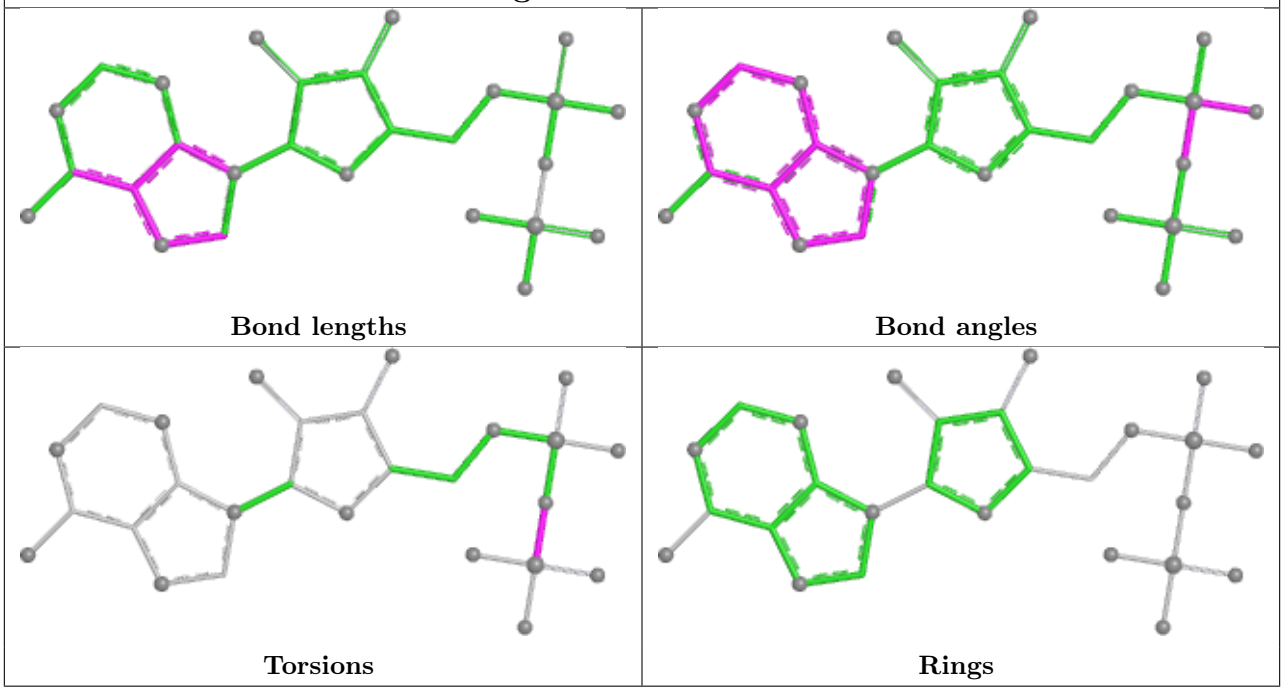
Ligand ADP A 1502



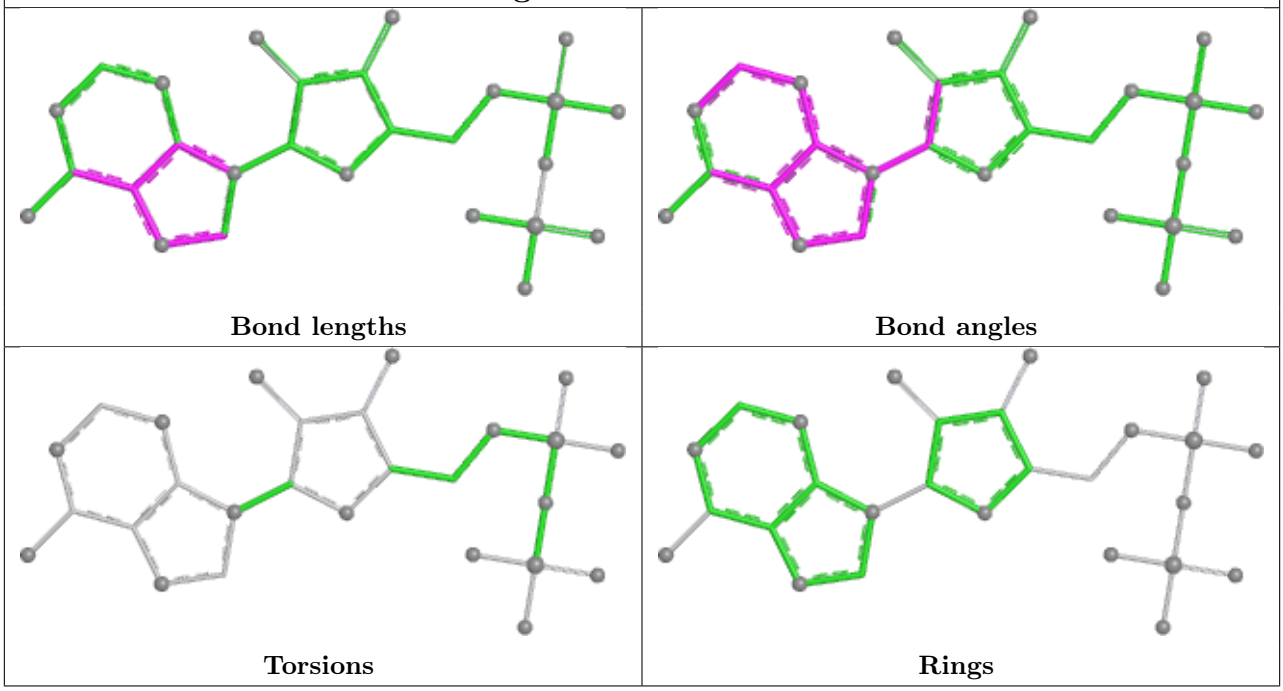
Ligand ADP A 502



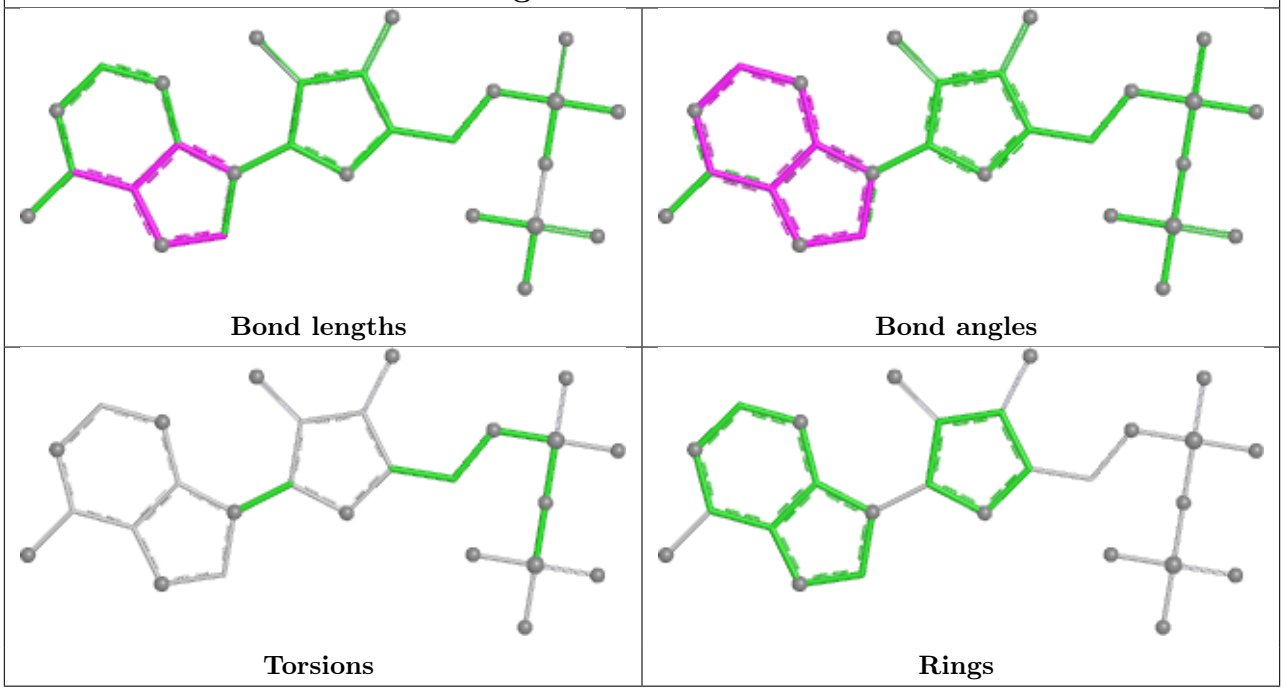
Ligand ADP A 4502



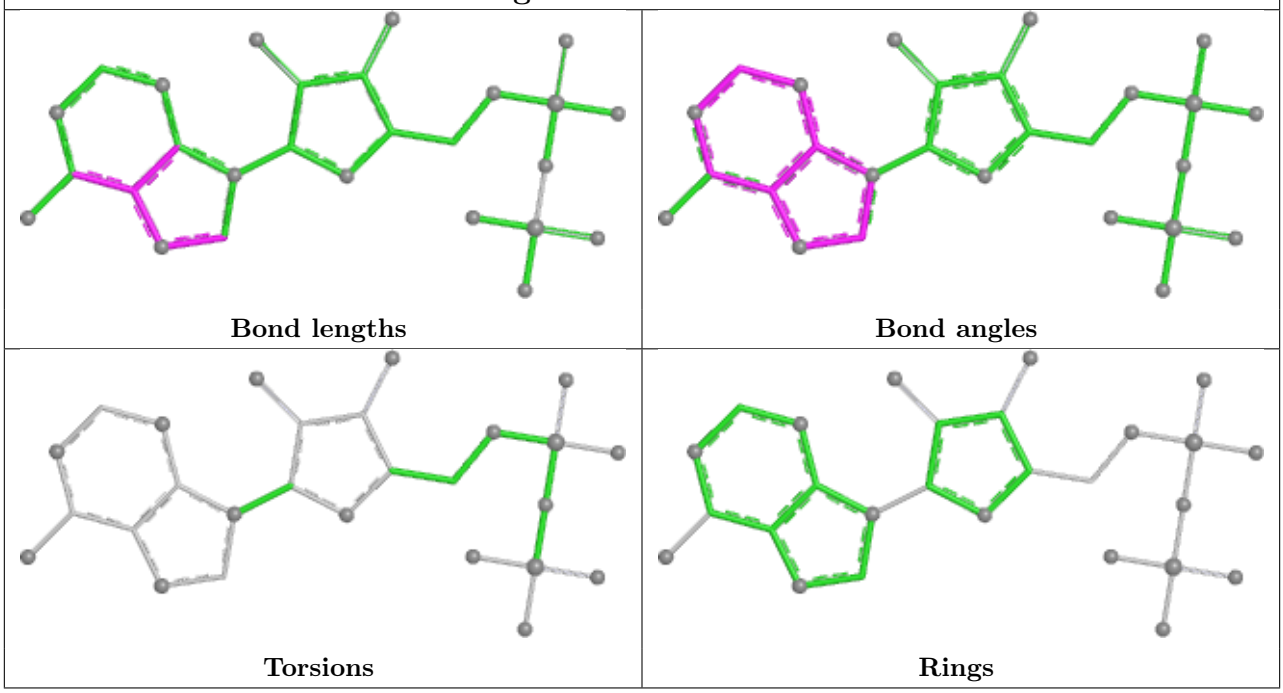
Ligand ADP A 5502



Ligand ADP A 2502



Ligand ADP A 3502



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	B	15/18 (83%)	-0.35	0	100	100	118, 147, 162, 174	0
2	A	1937/2050 (94%)	-0.74	0	100	100	147, 196, 220, 220	0
All	All	1952/2068 (94%)	-0.74	0	100	100	118, 195, 220, 220	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	4500	1/1	0.78	0.10	162,162,162,162	0
4	ALF	A	5501	5/5	0.78	0.12	167,172,172,172	0
3	MG	A	500	1/1	0.92	0.10	162,162,162,162	0
3	MG	A	3500	1/1	0.92	0.11	180,180,180,180	0
5	ADP	A	4502	27/27	0.93	0.06	157,178,183,183	0
5	ADP	A	3502	27/27	0.95	0.05	182,190,197,197	0
3	MG	A	2500	1/1	0.95	0.07	177,177,177,177	0

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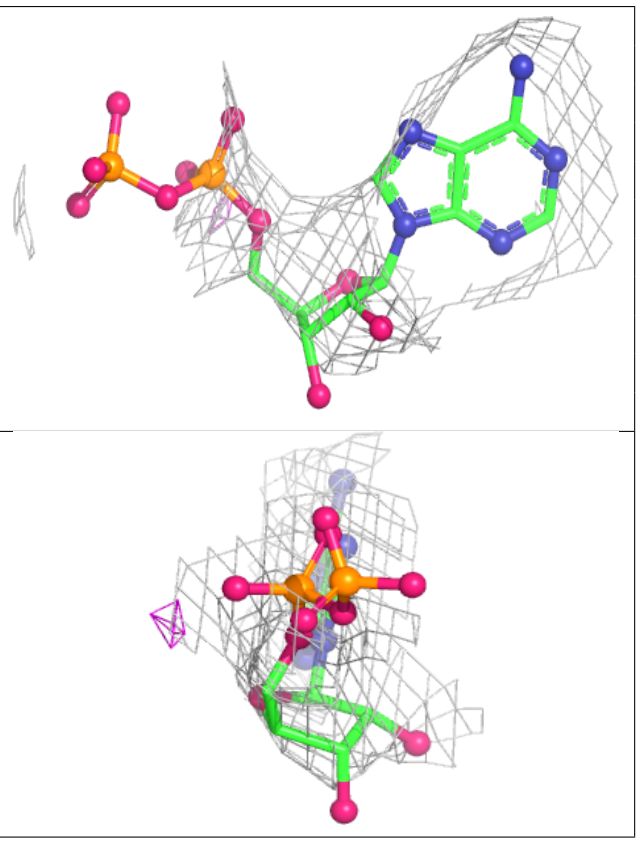
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ADP	A	5502	27/27	0.95	0.05	173,185,193,193	0
5	ADP	A	2502	27/27	0.96	0.04	176,188,192,193	0
3	MG	A	1500	1/1	0.96	0.05	186,186,186,186	0
5	ADP	A	502	27/27	0.96	0.05	169,190,193,193	0
5	ADP	A	1502	27/27	0.96	0.05	191,198,201,202	0
4	ALF	A	1501	5/5	0.97	0.06	190,194,195,196	0
4	ALF	A	3501	5/5	0.97	0.06	181,181,182,183	0
4	ALF	A	4501	5/5	0.97	0.07	159,160,161,162	0
3	MG	A	5500	1/1	0.97	0.03	53,53,53,53	0
4	ALF	A	501	5/5	0.97	0.05	165,168,169,169	0
4	ALF	A	2501	5/5	0.98	0.03	177,177,179,180	0

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

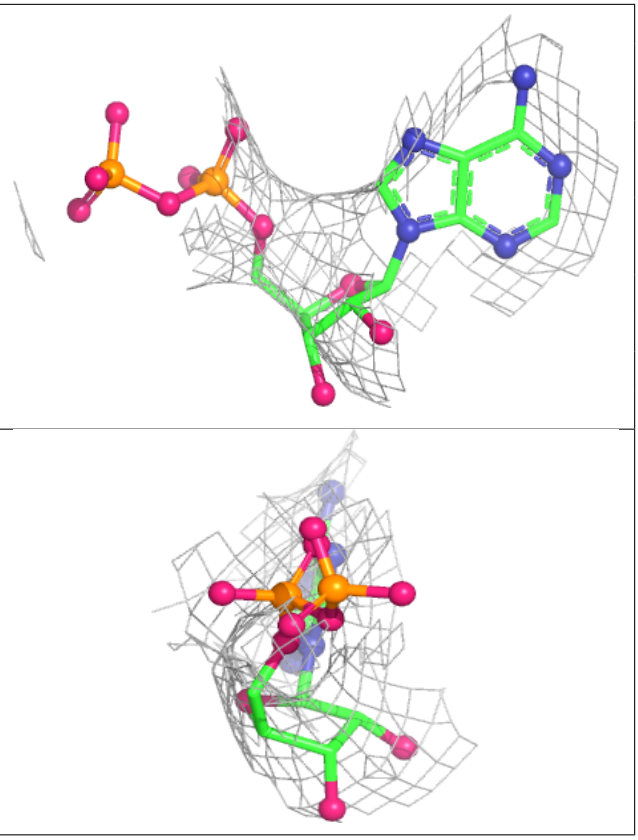
Electron density around ADP A 4502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



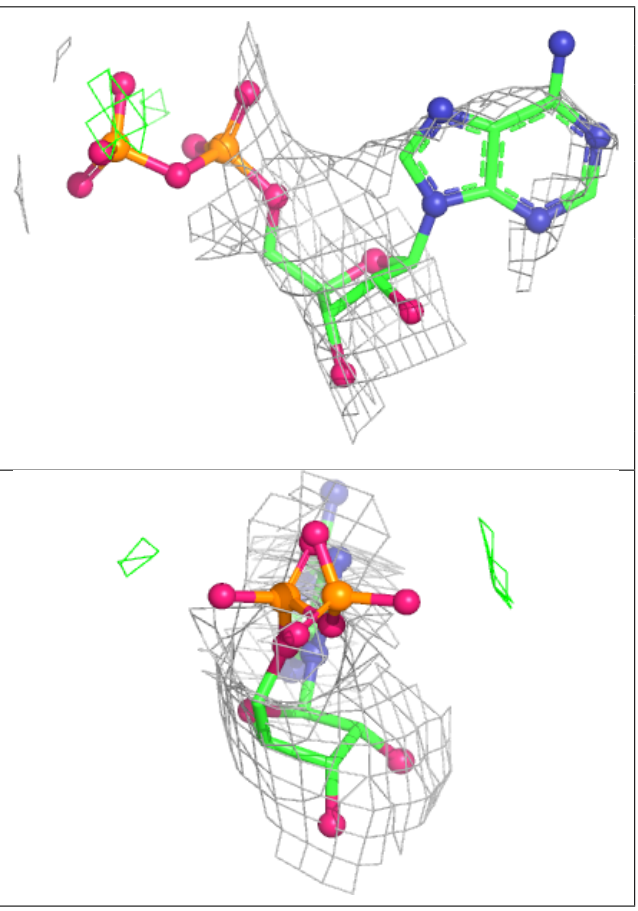
Electron density around ADP A 3502:

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



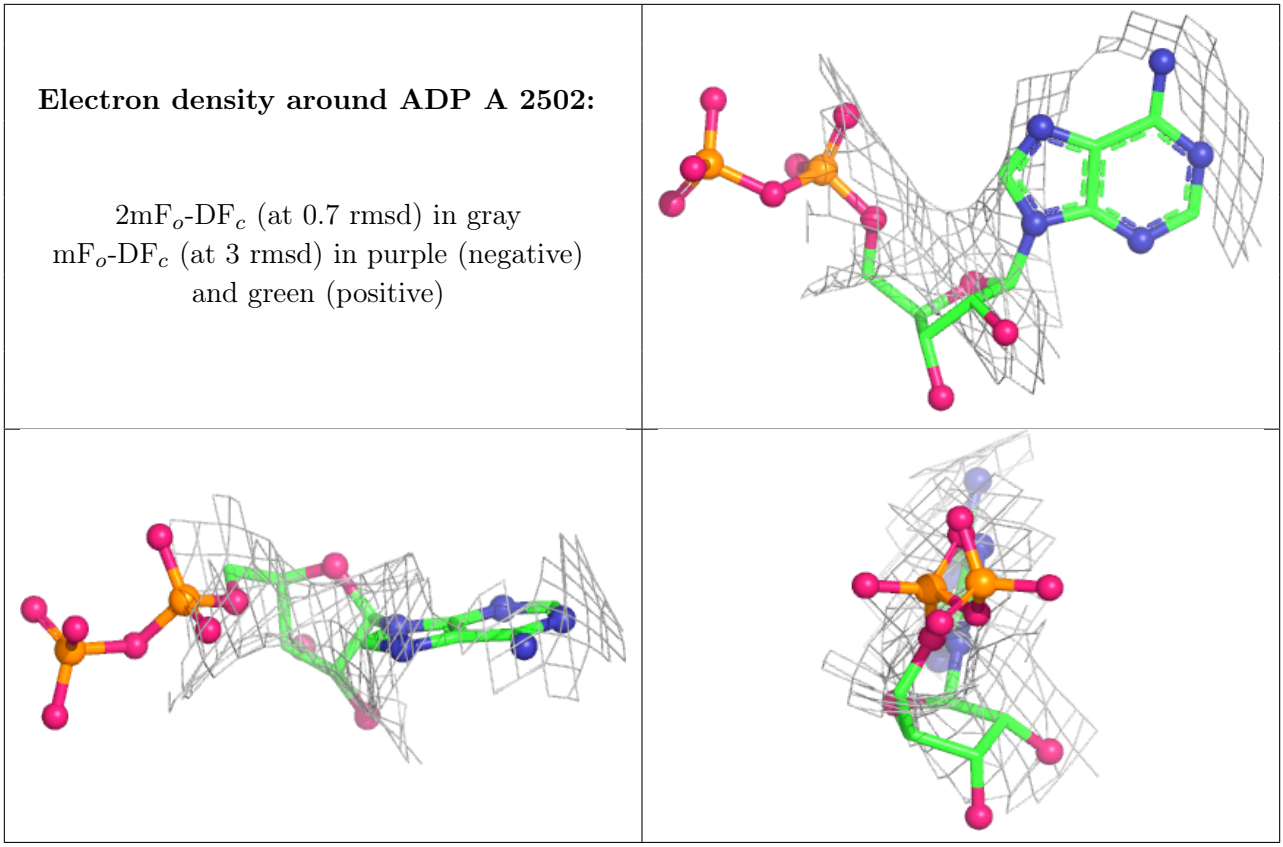
Electron density around ADP A 5502:

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



Electron density around ADP A 2502:

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



Electron density around ADP A 502:

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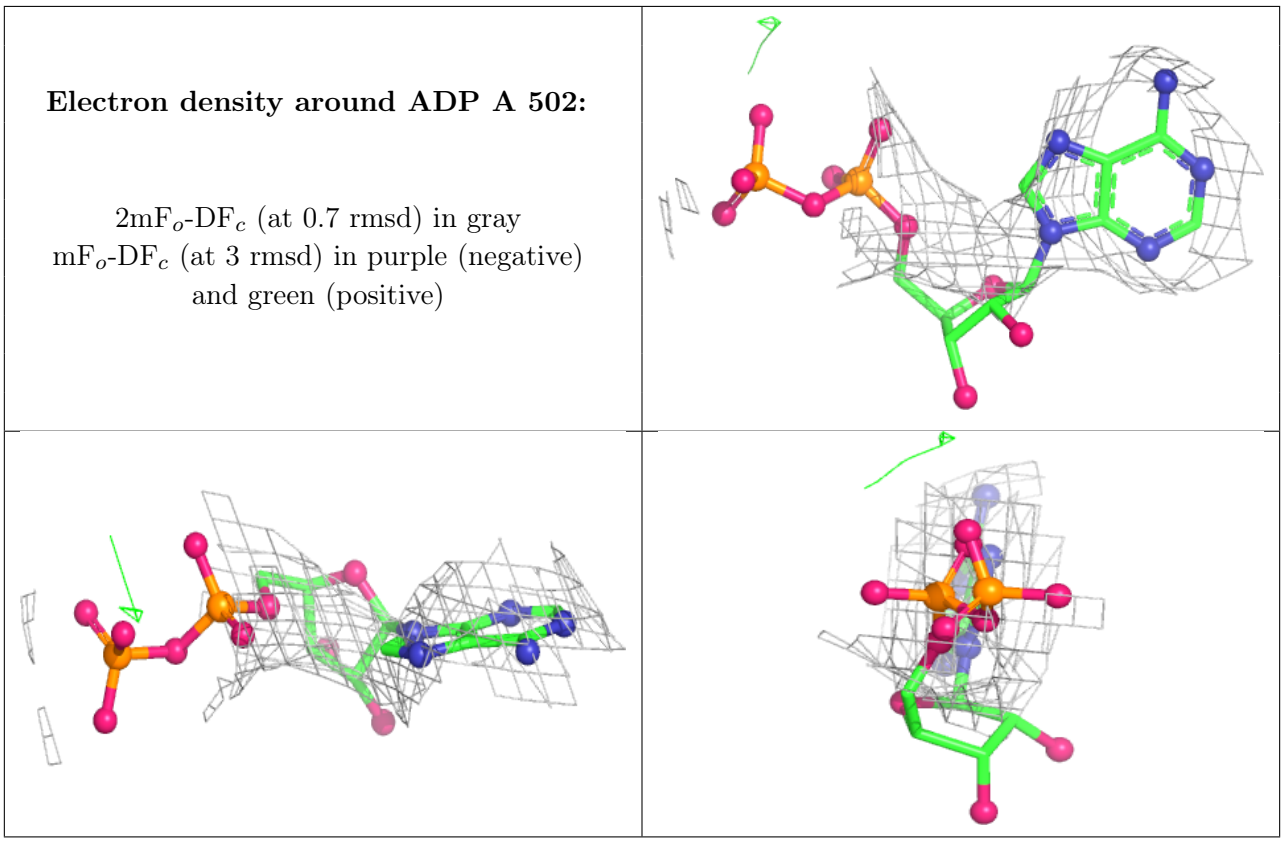
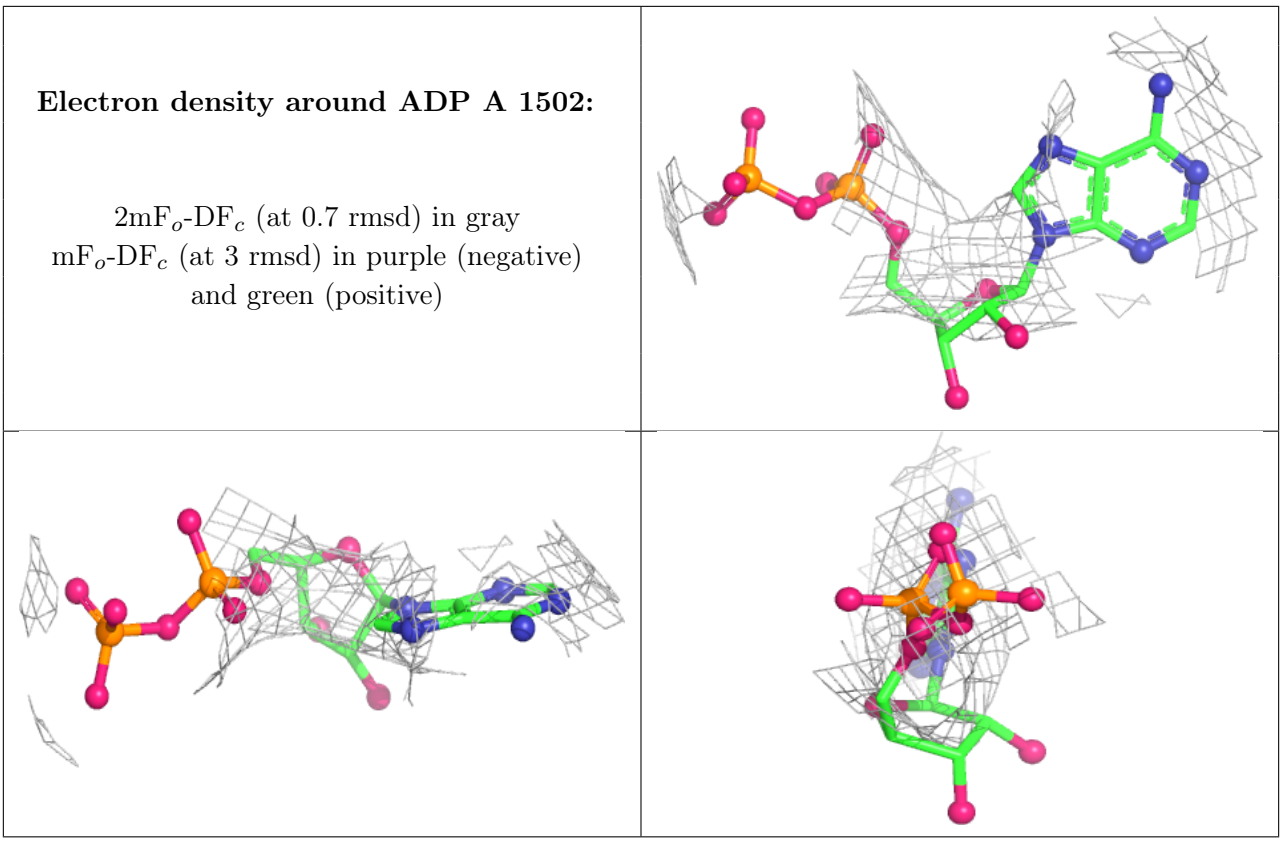
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 1502:

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



6.5 Other polymers (i)

There are no such residues in this entry.