



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:46 AM GMT

PDB ID : 3CMU
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

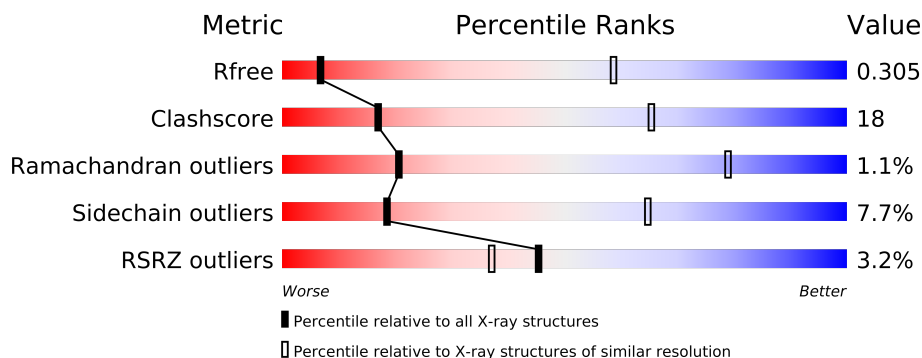
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



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}	66092	1001 (4.84-3.50)
Clashscore	79885	1259 (4.84-3.50)
Ramachandran outliers	78287	1192 (4.84-3.50)
Sidechain outliers	78261	1175 (4.84-3.50)
RSRZ outliers	66119	1001 (4.84-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	18	
2	A	2050	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	1500	-	X
3	MG	A	3500	-	X
3	MG	A	500	-	X
4	ALF	A	3501	-	X
4	ALF	A	501	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15093 atoms, of which 0 are hydrogen and 0 are deuterium.

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*DT)-3').

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

- Molecule 2 is a protein called Protein recA.

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

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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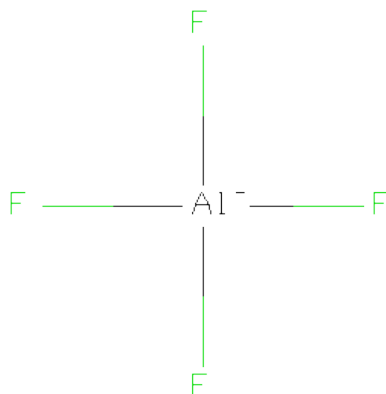
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Chain	Residue	Modelled	Actual	Comment	Reference
A	4987	THR	-	LINKER	UNP P0A7G6
A	4988	GLY	-	LINKER	UNP P0A7G6
A	4989	SER	-	LINKER	UNP P0A7G6
A	4990	THR	-	LINKER	UNP P0A7G6
A	4991	GLY	-	LINKER	UNP P0A7G6
A	4992	SER	-	LINKER	UNP P0A7G6
A	4993	GLY	-	LINKER	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 (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4^-).



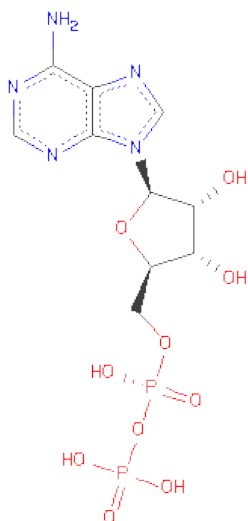
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Al F 5 1 4	0	0

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

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



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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

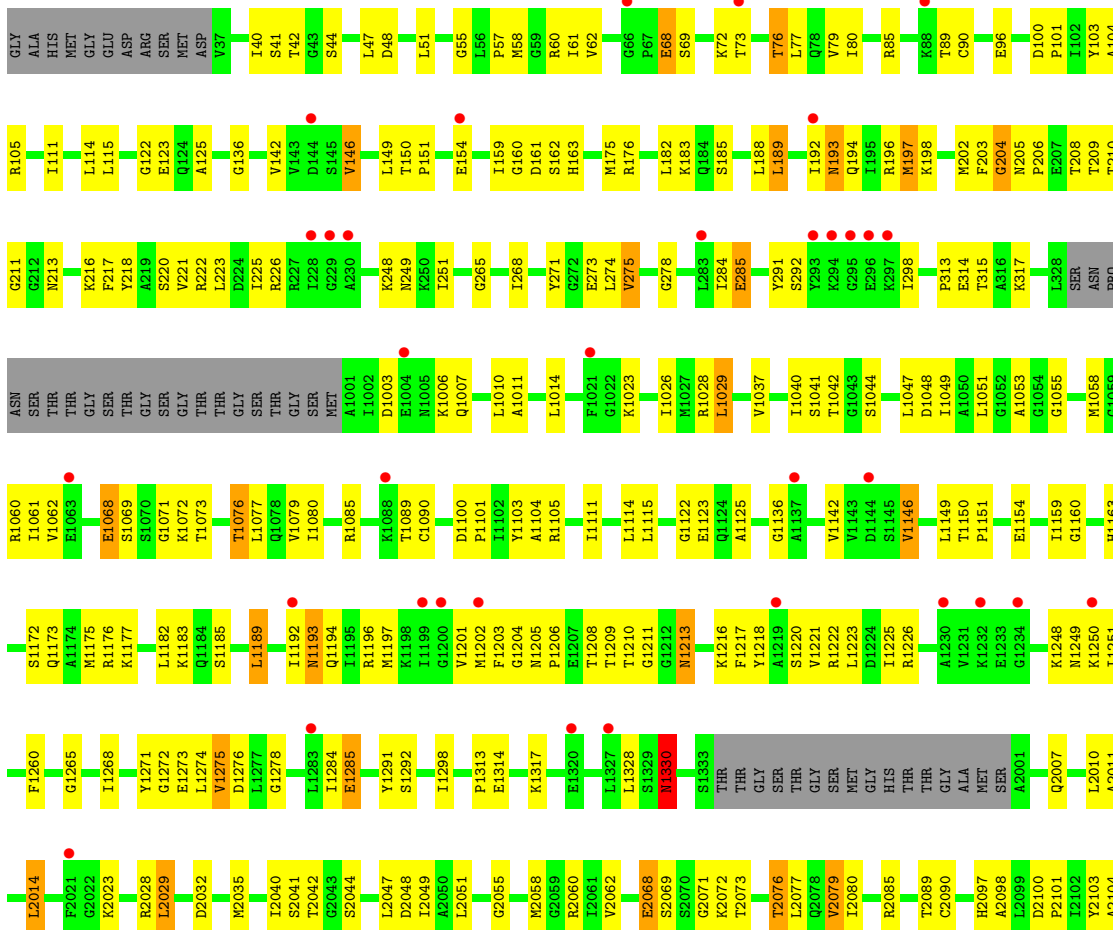
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain B: 



- Molecule 2: Protein recA

Chain A: 





4 Data and refinement statistics

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 38.35 – 4.20	Depositor EDS
% Data completeness (in resolution range)	80.7 (12.00-4.20) 81.1 (38.35-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.275 , 0.298 0.284 , 0.305	Depositor DCC
R_{free} test set	937 reflections (5.51%)	DCC
Wilson B-factor (Å ²)	173.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 77.2	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21286 reflections	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	2.06	5/326 (1.5%)	2.67	39/502 (7.8%)
2	A	0.59	0/14765	0.67	0/19866
All	All	0.66	5/15091 (0.0%)	0.79	39/20368 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1002	DT	N3-C4	6.64	1.44	1.38
1	B	1002	DT	C1'-N1	6.34	1.57	1.49
1	B	1012	DT	O3'-P	-6.04	1.53	1.61
1	B	1002	DT	N1-C6	5.66	1.42	1.38
1	B	1002	DT	N1-C2	5.58	1.42	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1014	DT	O4'-C1'-N1	11.00	115.70	108.00
1	B	1011	DT	O4'-C1'-N1	10.59	115.41	108.00
1	B	1005	DT	O4'-C1'-N1	9.55	114.69	108.00
1	B	1008	DT	O4'-C1'-N1	9.30	114.51	108.00
1	B	1002	DT	N3-C4-O4	9.05	125.33	119.90
1	B	1012	DT	C5-C4-O4	-8.23	119.14	124.90
1	B	1015	DT	C5-C4-O4	-7.85	119.40	124.90
1	B	1012	DT	P-O3'-C3'	-7.82	110.32	119.70
1	B	1009	DT	C5-C4-O4	-7.78	119.45	124.90
1	B	1003	DT	P-O3'-C3'	7.58	128.80	119.70
1	B	1006	DT	C5-C4-O4	-7.58	119.59	124.90
1	B	1003	DT	N3-C4-O4	7.38	124.33	119.90
1	B	1014	DT	P-O3'-C3'	6.99	128.09	119.70
1	B	1002	DT	C5-C4-O4	-6.94	120.04	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1012	DT	N3-C4-O4	6.91	124.04	119.90
1	B	1003	DT	C5-C4-O4	-6.87	120.09	124.90
1	B	1008	DT	P-O3'-C3'	6.65	127.68	119.70
1	B	1015	DT	N3-C4-O4	6.61	123.87	119.90
1	B	1009	DT	N3-C4-O4	6.59	123.85	119.90
1	B	1005	DT	P-O3'-C3'	6.42	127.40	119.70
1	B	1006	DT	N3-C4-O4	6.35	123.71	119.90
1	B	1002	DT	C5-C6-N1	6.23	127.44	123.70
1	B	1008	DT	C4'-C3'-C2'	-6.23	97.49	103.10
1	B	1011	DT	C4'-C3'-C2'	-6.20	97.52	103.10
1	B	1011	DT	P-O3'-C3'	6.14	127.07	119.70
1	B	1005	DT	C4'-C3'-C2'	-5.92	97.78	103.10
1	B	1002	DT	N1-C1'-C2'	5.89	123.80	112.60
1	B	1014	DT	C4'-C3'-C2'	-5.79	97.89	103.10
1	B	1003	DT	O4'-C1'-N1	5.67	111.97	108.00
1	B	1012	DT	O4'-C1'-N1	5.63	111.94	108.00
1	B	1002	DT	C2-N1-C1'	5.46	126.94	118.20
1	B	1006	DT	O3'-P-O5'	-5.39	93.76	104.00
1	B	1007	DT	N3-C4-O4	5.24	123.04	119.90
1	B	1009	DT	O4'-C1'-N1	5.20	111.64	108.00
1	B	1012	DT	OP2-P-O3'	5.14	116.50	105.20
1	B	1010	DT	N3-C4-O4	5.11	122.97	119.90
1	B	1015	DT	O4'-C1'-N1	5.11	111.57	108.00
1	B	1008	DT	C1'-O4'-C4'	-5.05	105.05	110.10
1	B	1006	DT	O4'-C1'-N1	5.01	111.51	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	297	0	182	25	0
2	A	14598	0	14995	523	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	0	0	0
4	A	30	0	0	8	0
5	A	162	0	72	24	0
All	All	15093	0	15249	538	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (538) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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:2160:GLY:H	2:A:3173:GLN:HE22	1.28	0.79
2:A:2111:ILE:HG22	2:A:3030:GLY:CA	2.13	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:4159:ILE:HA	2:A:5173:GLN:NE2	2.08	0.69
2:A:96:GLU:OE2	4:A:501:ALF:F4	1.99	0.69
2:A:4042:THR:HG21	2:A:4047:LEU:HD22	1.74	0.68
2:A:1159:ILE:HG12	2:A:2177:LYS:HD3	1.74	0.68
2:A:1068:GLU:HG2	2:A:2216:LYS:CB	2.23	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: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: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:3159:ILE:HA	2:A:4173:GLN:HE22	1.60	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: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:3159:ILE:HG23	2:A:4173:GLN:HE21	1.64	0.63
2:A:2291:TYR:O	2:A:2298:ILE:HG12	1.99	0.63
2:A:1160:GLY:N	2:A:2173:GLN:HE22	1.92	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:291:TYR:O	2:A:298:ILE:HG12	1.98	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:5208:THR:HG22	2:A:5209:THR:H	1.65	0.61
2:A:4197:MET:HA	2:A:4206:PRO:O	2.01	0.61
2:A:2150:THR:OG1	2:A:3176:ARG:HG2	2.01	0.61
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:5072:LYS:HB3	2:A:5192:ILE:HG23	1.82	0.60
2:A:72:LYS:HB3	2:A:192:ILE:HG23	1.82	0.60
2:A:4208:THR:HG22	2:A:4209:THR:H	1.65	0.60
2:A:3193:ASN:HD22	2:A:3194:GLN:H	1.48	0.60
2:A:2159:ILE:HG12	2:A:3177:LYS:HD3	1.82	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:1154:GLU:O	2:A:2177:LYS:HE2	2.02	0.60
2:A:1072:LYS:HB3	2:A:1192:ILE:HG23	1.82	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: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:4072:LYS:HB3	2:A:4192:ILE:HG23	1.83	0.59
2:A:3071:GLY:HA2	5:A:3502:ADP:O1A	2.02	0.59
2:A:3208:THR:HG22	2:A:3209:THR:H	1.68	0.59
2:A:4068:GLU:HG2	2:A:5216:LYS:HB3	1.84	0.59
2:A:208:THR:HG22	2:A:209:THR:H	1.68	0.59
2:A:73:THR:O	2:A:76:THR:HB	2.04	0.58
2:A:68:GLU:HG2	2:A:1216:LYS:HB3	1.85	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:3250:LYS:HA	5:A:2502:ADP:N7	2.18	0.58
2:A:2254:PRO:HG3	5:A:1502:ADP:O2'	2.04	0.58
2:A:3115:LEU:HD22	2:A:4026:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:2208:THR:HG22	2:A:2209:THR:H	1.69	0.58
2:A:2049:ILE:HA	2:A:2328:LEU:HD21	1.84	0.57
2:A:1197:MET:HA	2:A:1206:PRO:O	2.05	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: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:4154:GLU:HG3	2:A:4163:HIS:HD2	1.69	0.56
2:A:3053:ALA:HA	2:A:3330:ASN:O	2.05	0.56
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: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
2:A:2210:THR:HG22	2:A:2211:GLY:H	1.70	0.56
2:A:210:THR:HG22	2:A:211:GLY:H	1.71	0.56
2:A:1210:THR:HG22	2:A:1211:GLY:H	1.71	0.56
1:B:1013:DT:C6	1:B:1014:DT:H72	2.40	0.56
2:A:1208:THR:HG22	2:A:1209:THR:H	1.71	0.56
2:A:5048:ASP:HA	2:A:5051:LEU:HD12	1.88	0.56
2:A:3278:GLY:HA3	2:A:3284:ILE:HD12	1.87	0.56
2:A:3197:MET:HA	2:A:3206:PRO:O	2.05	0.56
2:A:4193:ASN:ND2	2:A:4194:GLN:H	2.04	0.55
2:A:3048:ASP:HA	2:A:3051:LEU:HD12	1.88	0.55
2:A:2278:GLY:HA3	2:A:2284:ILE:HD12	1.88	0.55
2:A:3248:LYS:NZ	4:A:2501:ALF:F1	2.21	0.55
2:A:2073:THR:O	2:A:2076:THR:HB	2.06	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: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
1:B:1003:DT:H3'	2:A:196:ARG:HB3	1.89	0.54
2:A:1273:GLU:O	2:A:1274:LEU:C	2.45	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:4210:THR:HG22	2:A:4211:GLY:H	1.72	0.54
2:A:278:GLY:HA3	2:A:284:ILE:HD12	1.88	0.54
2:A:3210:THR:HG22	2:A:3211:GLY:H	1.72	0.54
2:A:3136:GLY:HA2	2:A:3185:SER:HB3	1.90	0.54
2:A:5210:THR:HG22	2:A:5211:GLY:H	1.72	0.54
2:A:1048:ASP:HA	2:A:1051:LEU:HD12	1.89	0.54
2:A:1073:THR:O	2:A:1076:THR:HB	2.08	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
2:A:4076:THR:HG22	2:A:4077:LEU:N	2.22	0.54
1:B:1015:DT:H6	1:B:1015:DT:O5'	1.91	0.54
2:A:4040:ILE:HG22	2:A:4041:SER:O	2.08	0.54
2:A:1111:ILE:HG23	2:A:2029:LEU:HD13	1.90	0.54
2:A:2154:GLU:OE2	2:A:3176:ARG:HD2	2.07	0.53
2:A:2123:GLU:OE1	2:A:2151:PRO:HA	2.08	0.53
2:A:3076:THR:HG22	2:A:3077:LEU:N	2.23	0.53
2:A:5193:ASN:ND2	2:A:5194:GLN:H	2.06	0.53
2:A:4007:GLN:HA	2:A:4010:LEU:HB3	1.91	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:3273:GLU:O	2:A:3274:LEU:C	2.46	0.53
2:A:5040:ILE:HG12	2:A:5058:MET:SD	2.49	0.53
2:A:4271:TYR:O	2:A:4275:VAL:HG23	2.09	0.53
2:A:48:ASP:HA	2:A:51:LEU:HD12	1.90	0.53
1:B:1006:DT:O5'	1:B:1006:DT:H6	1.92	0.53
2:A:210:THR:HG22	2:A:211:GLY:N	2.24	0.53
2:A:76:THR:HG22	2:A:77:LEU:N	2.23	0.53
2:A:2264:TYR:CD2	2:A:3254:PRO:HD2	2.43	0.53
2:A:1248:LYS:NZ	4:A:501:ALF:F1	2.17	0.53
2:A:4053:ALA:HA	2:A:4330:ASN:O	2.09	0.53
2:A:2076:THR:HG22	2:A:2077:LEU:N	2.24	0.53
2:A:1136:GLY:HA2	2:A:1185:SER:HB3	1.89	0.53
2:A:136:GLY:HA2	2:A:185:SER:HB3	1.90	0.53
2:A:2111:ILE:CG2	2:A:3030:GLY:HA2	2.38	0.52
2:A:2040:ILE:HG22	2:A:2041:SER:O	2.10	0.52
2:A:3040:ILE:HG22	2:A:3041:SER:O	2.08	0.52
2:A:2007:GLN:HA	2:A:2010:LEU:HB3	1.91	0.52
2:A:1210:THR:HG22	2:A:1211:GLY:N	2.24	0.52
2:A:4115:LEU:HD13	2:A:5026:ILE:HD11	1.91	0.52
2:A:285:GLU:HB3	2:A:292:SER:HB2	1.90	0.52
2:A:4273:GLU:O	2:A:4274:LEU:C	2.48	0.52
2:A:2271:TYR:O	2:A:2275:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:5076:THR:O	2:A:5079:VAL:HG22	2.09	0.52
2:A:4040:ILE:HG12	2:A:4058:MET:SD	2.50	0.52
2:A:1249:ASN:OD1	2:A:1251:ILE:HG22	2.10	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:193:ASN:ND2	2:A:194:GLN:H	2.08	0.51
2:A:76:THR:O	2:A:79:VAL:HG22	2.10	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:273:GLU:O	2:A:274:LEU:C	2.48	0.51
2:A:3193:ASN:ND2	2:A:3194:GLN:H	2.07	0.51
2:A:2040:ILE:HG12	2:A:2058:MET:SD	2.50	0.51
2:A:4071:GLY:HA2	5:A:4502:ADP:H5'1	1.91	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: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
2:A:5210:THR:HG22	2:A:5211:GLY:N	2.25	0.51
2:A:4154:GLU:HG3	2:A:4163:HIS:CD2	2.46	0.51
2:A:159:ILE:HG12	2:A:1177:LYS:HD3	1.92	0.51
1:B:1012:DT:O5'	1:B:1012:DT:H6	1.93	0.51
2:A:1007:GLN:HA	2:A:1010:LEU:HB3	1.92	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:123:GLU:OE1	2:A:151:PRO:HA	2.10	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:2273:GLU:O	2:A:2274:LEU:C	2.47	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:1193:ASN:HD21	2:A:1210:THR:HB	1.76	0.50
1:B:1011:DT:H2''	2:A:4169:ARG:HH11	1.76	0.50
2:A:5103:TYR:O	2:A:5104:ALA:C	2.50	0.50
2:A:1053:ALA:HA	2:A:1330:ASN:O	2.12	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
2:A:5273:GLU:O	2:A:5274:LEU:C	2.48	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:4249:ASN:OD1	2:A:4251:ILE:HG22	2.12	0.50
2:A:2101:PRO:HD3	2:A:3035:MET:HG3	1.94	0.50
2:A:3111:ILE:HD12	2:A:4029:LEU:HD13	1.94	0.49
2:A:249:ASN:OD1	2:A:251:ILE:HG22	2.12	0.49
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:3193:ASN:HD21	2:A:3210:THR:HB	1.78	0.49
2:A:3068:GLU:HB3	2:A:4217:PHE:HA	1.93	0.49
2:A:5074:THR:OG1	5:A:5502:ADP:H5'1	2.11	0.49
2:A:1062:VAL:HG22	2:A:1221:VAL:HB	1.95	0.49
2:A:1060:ARG:HB3	2:A:1220:SER:OG	2.13	0.49
2:A:1103:TYR:O	2:A:1104:ALA:C	2.51	0.49
1:B:1003:DT:O5'	1:B:1003:DT:H6	1.95	0.49
2:A:4049:ILE:HA	2:A:4328:LEU:CD2	2.42	0.49
2:A:2146:VAL:CA	2:A:2149:LEU:HD13	2.39	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: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:4205:ASN:HA	2:A:4206:PRO:HD3	1.64	0.48
2:A:2103:TYR:O	2:A:2104:ALA:C	2.51	0.48
2:A:3271:TYR:O	2:A:3275:VAL:HG23	2.13	0.48
2:A:3076:THR:O	2:A:3079:VAL:HG22	2.13	0.48
2:A:4193:ASN:HD21	2:A:4210:THR:HB	1.78	0.48
2:A:1068:GLU:HB3	2:A:2217:PHE:HA	1.96	0.48
2:A:5077:LEU:O	2:A:5080:ILE:HB	2.13	0.48
2:A:4103:TYR:O	2:A:4104:ALA:C	2.50	0.48
2:A:193:ASN:HD21	2:A:210:THR:HB	1.78	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:3011:ALA:HA	2:A:3014:LEU:HB2	1.95	0.48
2:A:4068:GLU:HG2	2:A:5216:LYS:CB	2.43	0.48
2:A:2060:ARG:HB3	2:A:2220:SER:OG	2.13	0.48
2:A:3154:GLU:O	2:A:4177:LYS:HE2	2.14	0.48
2:A:1044:SER:HB2	2:A:1268:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:103:TYR:O	2:A:104:ALA:C	2.51	0.48
2:A:271:TYR:O	2:A:275:VAL:HG23	2.13	0.48
2:A:90:CYS:HB2	2:A:114:LEU:HD23	1.96	0.48
2:A:2097:HIS:CE1	2:A:3180:GLY:HA2	2.49	0.48
2:A:4071:GLY:HA2	5:A:4502:ADP:C5'	2.43	0.47
2:A:3124:GLN:HG3	2:A:4021:PHE:CD1	2.48	0.47
2:A:60:ARG:HB3	2:A:220:SER:OG	2.14	0.47
2:A:3103:TYR:O	2:A:3104:ALA:C	2.50	0.47
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: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:216:LYS:HA	2:A:222:ARG:HD3	1.96	0.47
2:A:2193:ASN:HD21	2:A:2210:THR:HB	1.79	0.47
2:A:68:GLU:HG2	2:A:1216:LYS:CB	2.44	0.47
2:A:5208:THR:HG22	2:A:5209:THR:N	2.29	0.47
2:A:3032:ASP:HB3	2:A:3035:MET:HB2	1.96	0.47
2:A:3111:ILE:HG22	2:A:4030:GLY:HA2	1.95	0.47
2:A:2118:GLN:NE2	2:A:3183:LYS:HG2	2.29	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:4146:VAL:CA	2:A:4149:LEU:HD13	2.39	0.47
2:A:2216:LYS:HA	2:A:2222:ARG:HD3	1.95	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:3077:LEU:O	2:A:3080:ILE:HB	2.15	0.47
2:A:1105:ARG:N	2:A:1111:ILE:HD11	2.30	0.47
2:A:5122:GLY:O	2:A:5125:ALA:HB3	2.14	0.47
2:A:3069:SER:OG	2:A:4248:LYS:CG	2.61	0.47
2:A:146:VAL:CA	2:A:149:LEU:HD13	2.38	0.47
2:A:4115:LEU:HA	2:A:4115:LEU:HD23	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
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
1:B:1016:DT:H3'	2:A:5212:GLY:HA2	1.97	0.46
2:A:1159:ILE:HG23	2:A:2173:GLN:HE21	1.81	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:4090:CYS:HB2	2:A:4114:LEU:HD23	1.97	0.46
2:A:2077:LEU:O	2:A:2080:ILE:HB	2.15	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:3159:ILE:CA	2:A:4173:GLN:HE22	2.28	0.46
2:A:40:ILE:O	2:A:55:GLY:HA3	2.16	0.46
2:A:3044:SER:HB2	2:A:3268:ILE:HD13	1.97	0.46
2:A:62:VAL:HG22	2:A:221:VAL:HB	1.98	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:3252:ALA:C	5:A:2502:ADP:C2	2.89	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:154:GLU:OE2	2:A:1176:ARG:HD2	2.16	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:1061:ILE:HD12	2:A:1061:ILE:N	2.32	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: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:1040:ILE:O	2:A:1055:GLY:HA3	2.16	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
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
1:B:1007:DT:H4'	2:A:2168:ALA:CB	2.47	0.45
2:A:5044:SER:HB2	2:A:5268:ILE:HD13	1.98	0.45
2:A:3124:GLN:HG3	2:A:4021:PHE:CG	2.52	0.45
2:A:115:LEU:HD23	2:A:115:LEU:HA	1.73	0.45
2:A:4040:ILE:O	2:A:4055:GLY:HA3	2.17	0.45
1:B:1006:DT:H4'	2:A:2169:ARG:HA	1.99	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:5011:ALA:HA	2:A:5014:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:4062:VAL:HG22	2:A:4221:VAL:HB	1.98	0.44
2:A:4193:ASN:HD22	2:A:4194:GLN:N	2.14	0.44
2:A:208:THR:HG22	2:A:209:THR:N	2.31	0.44
1:B:1014:DT:C7	1:B:1015:DT:O4	2.65	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: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:4097:HIS:CD2	2:A:5180:GLY:HA2	2.53	0.44
2:A:3182:LEU:HD11	2:A:3189:LEU:HD12	1.99	0.44
2:A:122:GLY:O	2:A:125:ALA:HB3	2.18	0.44
2:A:1072:LYS:HB3	2:A:1192:ILE:CG2	2.48	0.44
2:A:1071:GLY:HA2	5:A:1502:ADP:H5'1	2.00	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:3154:GLU:HG3	2:A:3163:HIS:HD2	1.82	0.44
2:A:2042:THR:O	2:A:2079:VAL:HG12	2.18	0.44
2:A:4118:GLN:NE2	2:A:5183:LYS:HG2	2.32	0.44
2:A:1003:ASP:HA	2:A:1006:LYS:HG3	1.99	0.44
2:A:5040:ILE:O	2:A:5055:GLY:HA3	2.17	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:5146:VAL:CA	2:A:5149:LEU:HD13	2.37	0.44
2:A:4103:TYR:HE1	2:A:4265:GLY:H	1.66	0.44
2:A:5225:ILE:O	2:A:5226:ARG:HG3	2.18	0.44
2:A:5115:LEU:HD23	2:A:5115:LEU:HA	1.73	0.44
2:A:2182:LEU:HD11	2:A:2189:LEU:HD12	2.00	0.44
2:A:3146:VAL:CA	2:A:3149:LEU:HD13	2.38	0.43
2:A:2100:ASP:OD2	2:A:3037:VAL:HG21	2.18	0.43
2:A:2090:CYS:HB2	2:A:2114:LEU:HD23	1.99	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:5061:ILE:N	2:A:5061:ILE:HD12	2.33	0.43
4:A:5501:ALF:F2	5:A:5502:ADP:O1B	2.26	0.43
2:A:1042:THR:O	2:A:1079:VAL:HG12	2.18	0.43
2:A:1205:ASN:HA	2:A:1206:PRO:HD3	1.63	0.43
2:A:1103:TYR:HE1	2:A:1265:GLY:H	1.67	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:5216:LYS:HG2	2:A:5222:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:4260:PHE:CD1	2:A:4268:ILE:HG23	2.53	0.43
2:A:4011:ALA:HA	2:A:4014:LEU:HB2	1.99	0.43
2:A:2194:GLN:NE2	2:A:3217:PHE:CG	2.87	0.43
2:A:3264:TYR:CD2	2:A:4254:PRO:HD2	2.54	0.43
2:A:2118:GLN:HE22	2:A:3183:LYS:HG2	1.82	0.43
2:A:5105:ARG:N	2:A:5111:ILE:HD11	2.33	0.43
2:A:2250:LYS:HE3	4:A:1501:ALF:F3	2.08	0.43
2:A:2216:LYS:HG2	2:A:2222:ARG:CZ	2.49	0.43
2:A:4111:ILE:CG2	2:A:5030:GLY:HA2	2.49	0.43
2:A:1208:THR:HG22	2:A:1209:THR:N	2.33	0.43
2:A:4098:ALA:HA	2:A:5060:ARG:CZ	2.49	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: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
2:A:4209:THR:HG22	2:A:4216:LYS:HE2	2.01	0.43
2:A:3072:LYS:HB3	2:A:3192:ILE:CG2	2.49	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:4175:MET:O	2:A:4176:ARG:C	2.56	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:4076:THR:HG23	2:A:4142:VAL:HG21	2.01	0.42
2:A:3111:ILE:HG23	2:A:4029:LEU:HB3	2.01	0.42
2:A:3062:VAL:HG22	2:A:3221:VAL:HB	2.00	0.42
2:A:4097:HIS:CE1	2:A:5180:GLY:HA2	2.54	0.42
2:A:3175:MET:HB3	2:A:3218:TYR:CG	2.54	0.42
2:A:1182:LEU:HD11	2:A:1189:LEU:HD12	2.00	0.42
2:A:1159:ILE:HA	2:A:2173:GLN:HE22	1.82	0.42
2:A:4217:PHE:O	2:A:4248:LYS:NZ	2.52	0.42
2:A:1068:GLU:HG2	2:A:2216:LYS:HB2	1.99	0.42
2:A:2072:LYS:NZ	5:A:2502:ADP:PB	2.92	0.42
2:A:182:LEU:HD11	2:A:189:LEU:HD12	2.01	0.42
2:A:3216:LYS:HG2	2:A:3222:ARG:CZ	2.49	0.42
2:A:76:THR:HG23	2:A:142:VAL:HG21	2.01	0.42
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: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:2032:ASP:HB3	2:A:2035:MET:HB2	2.01	0.42
2:A:2313:PRO:O	2:A:2317:LYS:HG2	2.19	0.42
2:A:4111:ILE:HG23	2:A:5029:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:216:LYS:HG2	2:A:222:ARG:CZ	2.49	0.42
2:A:100:ASP:HA	2:A:101:PRO:HD2	1.89	0.42
2:A:4061:ILE:HD12	2:A:4061:ILE:N	2.35	0.42
2:A:5076:THR:CG2	2:A:5142:VAL:HG21	2.50	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:4225:ILE:O	2:A:4226:ARG:HG3	2.20	0.42
2:A:2194:GLN:NE2	2:A:3217:PHE:HB2	2.34	0.42
2:A:1175:MET:HB3	2:A:1218:TYR:CG	2.55	0.42
2:A:3225:ILE:O	2:A:3226:ARG:HG3	2.19	0.42
2:A:2225:ILE:O	2:A:2226:ARG:HG3	2.19	0.42
2:A:3202:MET:H	2:A:3202:MET:HE2	1.84	0.42
2:A:3217:PHE:O	2:A:3248:LYS:NZ	2.52	0.42
2:A:3101:PRO:HB3	2:A:4029:LEU:HD22	2.00	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: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:203:PHE:CG	2:A:204:GLY:N	2.88	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:2154:GLU:OE2	2:A:3176:ARG:NH1	2.52	0.41
2:A:1175:MET:O	2:A:1176:ARG:C	2.59	0.41
2:A:42:THR:O	2:A:79:VAL:HG12	2.19	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:4216:LYS:HG2	2:A:4222:ARG:CZ	2.49	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
2:A:3209:THR:HG22	2:A:3216:LYS:HE2	2.02	0.41
2:A:2209:THR:HG22	2:A:2216:LYS:HE2	2.03	0.41
2:A:4072:LYS:HB3	2:A:4192:ILE:CG2	2.50	0.41
1:B:1007:DT:H71	2:A:1197:MET:HG2	2.03	0.41
2:A:2103:TYR:HE1	2:A:2265:GLY:H	1.67	0.41
2:A:5101:PRO:HG2	2:A:5102:ILE:HD12	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:1260:PHE:CD1	2:A:1268:ILE:HG23	2.56	0.41
2:A:5100:ASP:HA	2:A:5101:PRO:HD2	1.88	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:1217:PHE:O	2:A:1248:LYS:NZ	2.54	0.41
2:A:2213:ASN:O	2:A:2214:ALA:C	2.59	0.41
2:A:175:MET:O	2:A:176:ARG:C	2.59	0.41
2:A:2175:MET:O	2:A:2176:ARG:C	2.59	0.41
2:A:5193:ASN:HD22	2:A:5194:GLN:N	2.15	0.41
2:A:3193:ASN:HD22	2:A:3194:GLN:N	2.16	0.41
2:A:72:LYS:HB2	2:A:72:LYS:HE2	1.88	0.41
2:A:72:LYS:HB3	2:A:192:ILE:CG2	2.48	0.41
2:A:2175:MET:HB3	2:A:2218:TYR:CG	2.55	0.41
2:A:61:ILE:N	2:A:61:ILE:HD12	2.35	0.41
2:A:1154:GLU:HG3	2:A:1163:HIS:CD2	2.55	0.41
2:A:3076:THR:HG23	2:A:3142:VAL:HG21	2.01	0.41
2:A:2076:THR:HG23	2:A:2142:VAL:HG21	2.02	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:4175:MET:HB3	2:A:4218:TYR:CD1	2.56	0.41
2:A:2205:ASN:HA	2:A:2206:PRO:HD3	1.62	0.41
2:A:3175:MET:HB3	2:A:3218:TYR:CD1	2.56	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
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:3213:ASN:O	2:A:3214:ALA:C	2.59	0.40
2:A:4202:MET:H	2:A:4202:MET:HE2	1.86	0.40
2:A:1068:GLU:HG3	2:A:1068:GLU:H	1.57	0.40
2:A:3254:PRO:CG	5:A:2502:ADP:O2'	2.65	0.40
2:A:5044:SER:OG	2:A:5273:GLU:OE2	2.27	0.40
2:A:4224:ASP:OD1	2:A:4226:ARG:NE	2.49	0.40
2:A:175:MET:HB3	2:A:218:TYR:CG	2.57	0.40
2:A:57:PRO:O	2:A:188:LEU:HD13	2.21	0.40
2:A:1049:ILE:HA	2:A:1328:LEU:CD2	2.51	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:1272:GLY:O	2:A:1275:VAL:HB	2.21	0.40
2:A:3251:ILE:HD12	2:A:3251:ILE:HA	1.92	0.40
2:A:2260:PHE:CD1	2:A:2268:ILE:HG23	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1115:LEU:HA	2:A:1115:LEU:HD23	1.75	0.40
2:A:225:ILE:O	2:A:226:ARG:HG3	2.21	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	Distance(Å)	Clash(Å)
2:A:1276:ASP:OD2	2:A:5235:GLU:OE2[4_556]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	21 79

All (22) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	1406 (92%)	118 (8%)	18 65

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	68	GLU
2	A	76	THR
2	A	85	ARG
2	A	89	THR
2	A	146	VAL
2	A	150	THR
2	A	162	SER
2	A	163	HIS
2	A	183	LYS
2	A	189	LEU
2	A	193	ASN
2	A	197	MET
2	A	202	MET
2	A	213	ASN
2	A	223	LEU
2	A	285	GLU
2	A	314	GLU
2	A	315	THR
2	A	1028	ARG
2	A	1029	LEU
2	A	1068	GLU
2	A	1076	THR
2	A	1085	ARG

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Mol	Chain	Res	Type
2	A	1089	THR
2	A	1146	VAL
2	A	1150	THR
2	A	1183	LYS
2	A	1189	LEU
2	A	1193	ASN
2	A	1201	VAL
2	A	1202	MET
2	A	1203	PHE
2	A	1213	ASN
2	A	1223	LEU
2	A	1285	GLU
2	A	1314	GLU
2	A	1330	ASN
2	A	2014	LEU
2	A	2028	ARG
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
2	A	2150	THR
2	A	2183	LYS
2	A	2189	LEU
2	A	2193	ASN
2	A	2201	VAL
2	A	2202	MET
2	A	2203	PHE
2	A	2213	ASN
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	3027	MET
2	A	3028	ARG
2	A	3029	LEU
2	A	3068	GLU
2	A	3076	THR

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Mol	Chain	Res	Type
2	A	3085	ARG
2	A	3089	THR
2	A	3146	VAL
2	A	3150	THR
2	A	3183	LYS
2	A	3189	LEU
2	A	3193	ASN
2	A	3201	VAL
2	A	3202	MET
2	A	3203	PHE
2	A	3213	ASN
2	A	3223	LEU
2	A	3285	GLU
2	A	3314	GLU
2	A	3330	ASN
2	A	4028	ARG
2	A	4029	LEU
2	A	4068	GLU
2	A	4076	THR
2	A	4079	VAL
2	A	4085	ARG
2	A	4089	THR
2	A	4146	VAL
2	A	4183	LYS
2	A	4189	LEU
2	A	4193	ASN
2	A	4201	VAL
2	A	4202	MET
2	A	4203	PHE
2	A	4213	ASN
2	A	4223	LEU
2	A	4251	ILE
2	A	4285	GLU
2	A	4314	GLU
2	A	4330	ASN
2	A	5014	LEU
2	A	5027	MET
2	A	5028	ARG
2	A	5029	LEU
2	A	5068	GLU
2	A	5076	THR
2	A	5085	ARG

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Mol	Chain	Res	Type
2	A	5089	THR
2	A	5146	VAL
2	A	5155	ILE
2	A	5164	MET
2	A	5183	LYS
2	A	5189	LEU
2	A	5193	ASN
2	A	5213	ASN
2	A	5223	LEU
2	A	5285	GLU
2	A	5314	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	181	ASN
2	A	193	ASN
2	A	194	GLN
2	A	236	ASN
2	A	304	ASN
2	A	1118	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	2118	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	2304	ASN
2	A	3097	HIS
2	A	3118	GLN
2	A	3163	HIS
2	A	3173	GLN
2	A	3181	ASN
2	A	3193	ASN

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Mol	Chain	Res	Type
2	A	3194	GLN
2	A	3236	ASN
2	A	3304	ASN
2	A	4118	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
2	A	4304	ASN
2	A	5097	HIS
2	A	5173	GLN
2	A	5181	ASN
2	A	5193	ASN
2	A	5194	GLN
2	A	5236	ASN
2	A	5304	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1501	-	4,4,4	1.92	0	0,6,6	0.00	-
5	ADP	A	1502	3	29,29,29	1.14	2 (6%)	45,45,45	1.90	8 (17%)
4	ALF	A	2501	-	4,4,4	1.90	0	0,6,6	0.00	-
5	ADP	A	2502	3	29,29,29	1.13	2 (6%)	45,45,45	1.78	8 (17%)
4	ALF	A	3501	-	4,4,4	1.87	0	0,6,6	0.00	-
5	ADP	A	3502	3	29,29,29	1.08	2 (6%)	45,45,45	1.92	8 (17%)
4	ALF	A	4501	-	4,4,4	1.91	1 (25%)	0,6,6	0.00	-
5	ADP	A	4502	3	29,29,29	1.11	2 (6%)	45,45,45	1.98	8 (17%)
4	ALF	A	501	-	4,4,4	1.87	0	0,6,6	0.00	-
5	ADP	A	502	3	29,29,29	1.03	2 (6%)	45,45,45	1.94	9 (20%)
4	ALF	A	5501	-	4,4,4	1.89	1 (25%)	0,6,6	0.00	-
5	ADP	A	5502	3	29,29,29	1.24	2 (6%)	45,45,45	1.83	8 (17%)

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
4	ALF	A	1501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	1502	3	-	0/16/32/32	0/1/3/3
4	ALF	A	2501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	2502	3	-	0/16/32/32	0/1/3/3
4	ALF	A	3501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	3502	3	-	0/16/32/32	0/1/3/3
4	ALF	A	4501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	4502	3	-	0/16/32/32	0/1/3/3
4	ALF	A	501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	502	3	-	0/16/32/32	0/1/3/3
4	ALF	A	5501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	5502	3	-	0/16/32/32	0/1/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5502	ADP	C4-N9	-3.60	1.32	1.37
5	A	1502	ADP	C5-C4	3.44	1.48	1.40
5	A	3502	ADP	C5-C4	3.30	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5502	ADP	C5-C4	3.29	1.47	1.40
5	A	4502	ADP	C5-C4	3.13	1.47	1.40
5	A	2502	ADP	C5-C4	3.12	1.47	1.40
5	A	502	ADP	C5-C4	3.10	1.47	1.40
5	A	2502	ADP	C4-N9	-3.06	1.33	1.37
5	A	4502	ADP	C4-N9	-2.93	1.33	1.37
5	A	3502	ADP	C4-N9	-2.47	1.34	1.37
5	A	1502	ADP	C4-N9	-2.37	1.34	1.37
5	A	502	ADP	C4-N9	-2.09	1.34	1.37
4	A	4501	ALF	F1-AL	2.03	1.80	1.58
4	A	5501	ALF	F2-AL	2.02	1.80	1.58

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	ADP	N3-C2-N1	-7.36	122.56	128.71
5	A	1502	ADP	N3-C2-N1	-7.26	122.64	128.71
5	A	4502	ADP	N3-C2-N1	-7.10	122.77	128.71
5	A	3502	ADP	N3-C2-N1	-7.03	122.83	128.71
5	A	2502	ADP	N3-C2-N1	-6.40	123.36	128.71
5	A	5502	ADP	N3-C2-N1	-5.84	123.83	128.71
5	A	502	ADP	N3-C4-N9	5.67	135.67	125.43
5	A	1502	ADP	N3-C4-N9	5.53	135.42	125.43
5	A	4502	ADP	N3-C4-N9	5.47	135.30	125.43
5	A	3502	ADP	N3-C4-N9	5.45	135.28	125.43
5	A	2502	ADP	N3-C4-N9	5.04	134.53	125.43
5	A	5502	ADP	N3-C4-N9	4.93	134.33	125.43
5	A	5502	ADP	PA-O3A-PB	-3.98	120.00	131.68
5	A	5502	ADP	C4-C5-N7	-3.81	106.26	109.52
5	A	4502	ADP	C4-C5-N7	-3.77	106.29	109.52
5	A	4502	ADP	C8-N9-C4	3.72	109.74	106.90
5	A	502	ADP	PA-O3A-PB	-3.67	120.91	131.68
5	A	4502	ADP	PA-O3A-PB	-3.61	121.11	131.68
5	A	3502	ADP	PA-O3A-PB	-3.48	121.48	131.68
5	A	1502	ADP	PA-O3A-PB	-3.45	121.57	131.68
5	A	2502	ADP	PA-O3A-PB	-3.35	121.86	131.68
5	A	1502	ADP	C5-C4-N3	-3.22	118.70	125.70
5	A	502	ADP	C8-N9-C4	3.20	109.34	106.90
5	A	5502	ADP	C8-N9-C4	3.19	109.33	106.90
5	A	4502	ADP	C5-C4-N3	-3.12	118.91	125.70
5	A	3502	ADP	C4-C5-N7	-3.11	106.86	109.52
5	A	1502	ADP	C4-C5-N7	-3.10	106.87	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3502	ADP	C5-C4-N3	-3.08	118.99	125.70
5	A	3502	ADP	C8-N9-C4	3.04	109.22	106.90
5	A	2502	ADP	C4-C5-N7	-3.02	106.93	109.52
5	A	502	ADP	C5-C4-N3	-2.89	119.41	125.70
5	A	5502	ADP	C5-C4-N3	-2.82	119.57	125.70
5	A	2502	ADP	C5-C4-N3	-2.81	119.57	125.70
5	A	1502	ADP	C2-N3-C4	2.67	121.61	114.01
5	A	2502	ADP	C8-N9-C4	2.66	108.93	106.90
5	A	4502	ADP	C2-N3-C4	2.64	121.51	114.01
5	A	3502	ADP	C2-N3-C4	2.56	121.29	114.01
5	A	502	ADP	O3B-PB-O2B	2.47	117.22	107.61
5	A	4502	ADP	O2B-PB-O1B	2.44	118.42	110.44
5	A	5502	ADP	C2'-C1'-N9	-2.42	107.05	113.27
5	A	502	ADP	C2-N3-C4	2.38	120.77	114.01
5	A	1502	ADP	C8-N9-C4	2.27	108.63	106.90
5	A	1502	ADP	O4'-C1'-N9	2.21	110.50	108.44
5	A	2502	ADP	C2-N3-C4	2.21	120.29	114.01
5	A	502	ADP	N6-C6-N1	2.20	123.69	119.36
5	A	5502	ADP	C2-N3-C4	2.18	120.21	114.01
5	A	2502	ADP	O4'-C1'-N9	2.07	110.37	108.44
5	A	3502	ADP	C2-N1-C6	2.04	122.45	118.77
5	A	502	ADP	C2-N1-C6	2.02	122.42	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	B	15/18 (83%)	0.16	1 (6%) 17 19	118, 147, 162, 174	0
2	A	1937/2050 (94%)	0.20	59 (3%) 48 38	147, 196, 220, 220	0
All	All	1952/2068 (94%)	0.20	60 (3%) 45 38	118, 195, 220, 220	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	3283	LEU	4.2
2	A	294	LYS	3.9
2	A	1219	ALA	3.8
2	A	4001	ALA	3.7
2	A	1234	GLY	3.6
2	A	1200	GLY	3.5
2	A	1202	MET	3.5
2	A	3001	ALA	3.5
2	A	2144	ASP	3.3
2	A	1327	LEU	3.3
2	A	1063	GLU	3.3
2	A	1199	ILE	3.2
2	A	144	ASP	3.2
2	A	4234	GLY	3.1
2	A	4297	LYS	3.0
2	A	3002	ILE	3.0
2	A	296	GLU	2.9
2	A	2294	LYS	2.9
2	A	295	GLY	2.8
2	A	1232	LYS	2.8
2	A	3038	GLU	2.8
2	A	192	ILE	2.8
2	A	1192	ILE	2.8
2	A	3192	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	4257	GLN	2.7
2	A	5205	ASN	2.7
2	A	3144	ASP	2.7
2	A	5230	ALA	2.6
2	A	229	GLY	2.6
2	A	4002	ILE	2.6
2	A	73	THR	2.5
2	A	230	ALA	2.5
2	A	228	ILE	2.4
2	A	3193	ASN	2.4
2	A	1004	GLU	2.4
2	A	1144	ASP	2.4
2	A	297	LYS	2.3
2	A	283	LEU	2.3
2	A	293	TYR	2.3
2	A	2192	ILE	2.3
2	A	4063	GLU	2.3
2	A	1283	LEU	2.3
2	A	66	GLY	2.2
2	A	4200	GLY	2.2
1	B	1016	DT	2.2
2	A	1230	ALA	2.2
2	A	2021	PHE	2.1
2	A	88	LYS	2.1
2	A	4296	GLU	2.1
2	A	2284	ILE	2.1
2	A	154	GLU	2.1
2	A	1021	PHE	2.1
2	A	2293	TYR	2.1
2	A	1250	LYS	2.1
2	A	5235	GLU	2.1
2	A	4202	MET	2.0
2	A	1320	GLU	2.0
2	A	1088	LYS	2.0
2	A	4195	ILE	2.0
2	A	1137	ALA	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

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	4500	1/1	0.48	0.88	162,162,162,162	0
3	MG	A	1500	1/1	0.53	0.85	186,186,186,186	0
4	ALF	A	1501	5/5	0.46	0.79	190,194,195,196	0
4	ALF	A	3501	5/5	0.52	0.70	181,181,182,183	0
4	ALF	A	5501	5/5	0.23	0.63	167,172,172,172	0
4	ALF	A	4501	5/5	0.38	0.58	159,160,161,162	0
3	MG	A	500	1/1	0.67	0.38	162,162,162,162	0
3	MG	A	3500	1/1	0.59	0.37	180,180,180,180	0
5	ADP	A	502	27/27	0.42	0.22	169,190,193,193	0
5	ADP	A	1502	27/27	0.31	0.13	191,198,201,202	0
5	ADP	A	3502	27/27	0.33	0.11	182,190,197,197	0
5	ADP	A	2502	27/27	0.26	-0.05	176,188,192,193	0
4	ALF	A	2501	5/5	0.33	-0.13	177,177,179,180	0
4	ALF	A	501	5/5	0.54	-0.22	165,168,169,169	0
3	MG	A	2500	1/1	0.39	-0.24	177,177,177,177	0
5	ADP	A	5502	27/27	0.17	-0.32	173,185,193,193	0
5	ADP	A	4502	27/27	0.22	-0.51	157,178,183,183	0
3	MG	A	5500	1/1	0.16	-1.13	53,53,53,53	0

6.5 Other polymers

There are no such residues in this entry.