



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:23 AM UTC

PDB ID : 3AV0 / pdb_00003av0
Title : Crystal structure of Mre11-Rad50 bound to ATP S
Authors : Lim, H.S.; Kim, J.S.; Cho, Y.
Deposited on : 2011-02-18
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

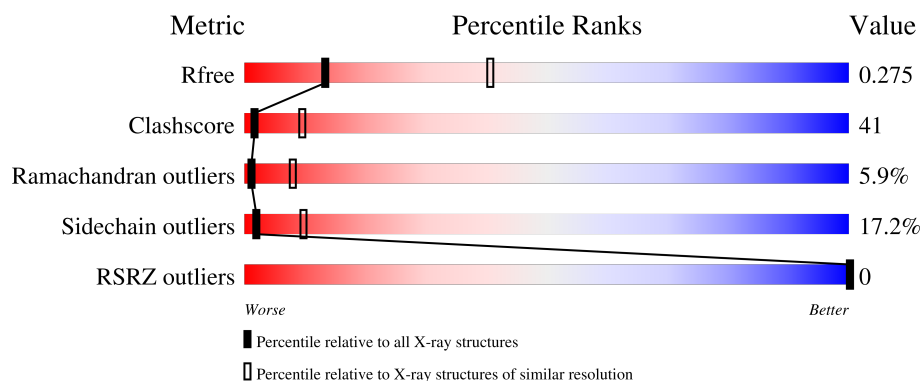
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

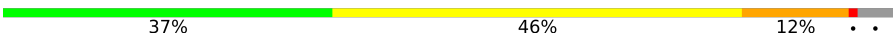
The reported resolution of this entry is 3.10 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	386	
2	B	371	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	1201	-	-	X	-
3	GOL	B	1202	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6094 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA double-strand break repair protein mre11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			3064	1973	511	569	11			

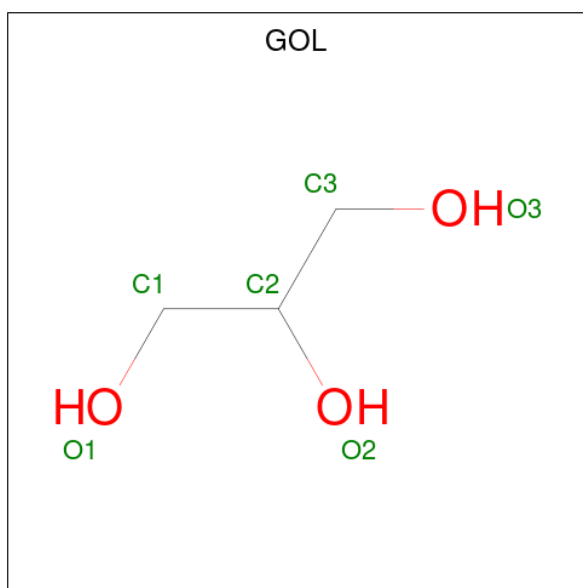
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q58719
A	-18	GLY	-	expression tag	UNP Q58719
A	-17	SER	-	expression tag	UNP Q58719
A	-16	SER	-	expression tag	UNP Q58719
A	-15	HIS	-	expression tag	UNP Q58719
A	-14	HIS	-	expression tag	UNP Q58719
A	-13	HIS	-	expression tag	UNP Q58719
A	-12	HIS	-	expression tag	UNP Q58719
A	-11	HIS	-	expression tag	UNP Q58719
A	-10	HIS	-	expression tag	UNP Q58719
A	-9	SER	-	expression tag	UNP Q58719
A	-8	SER	-	expression tag	UNP Q58719
A	-7	GLY	-	expression tag	UNP Q58719
A	-6	LEU	-	expression tag	UNP Q58719
A	-5	VAL	-	expression tag	UNP Q58719
A	-4	PRO	-	expression tag	UNP Q58719
A	-3	ARG	-	expression tag	UNP Q58719
A	-2	GLY	-	expression tag	UNP Q58719
A	-1	SER	-	expression tag	UNP Q58719
A	0	HIS	-	expression tag	UNP Q58719

- Molecule 2 is a protein called DNA double-strand break repair rad50 ATPase.

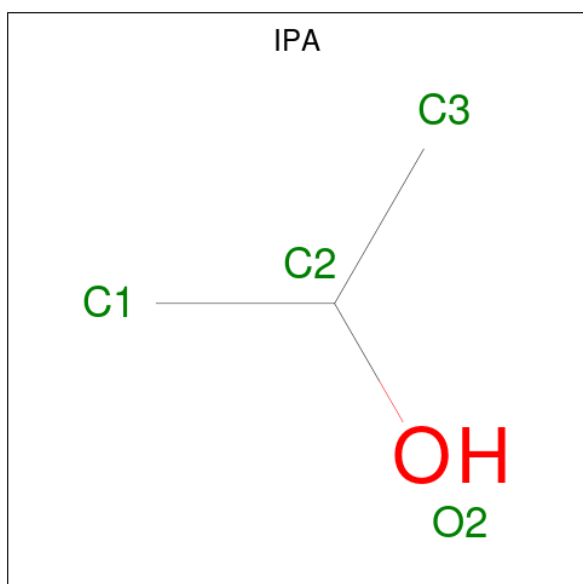
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	365	Total	C	N	O	S	0	0	0
			2937	1883	501	544	9			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



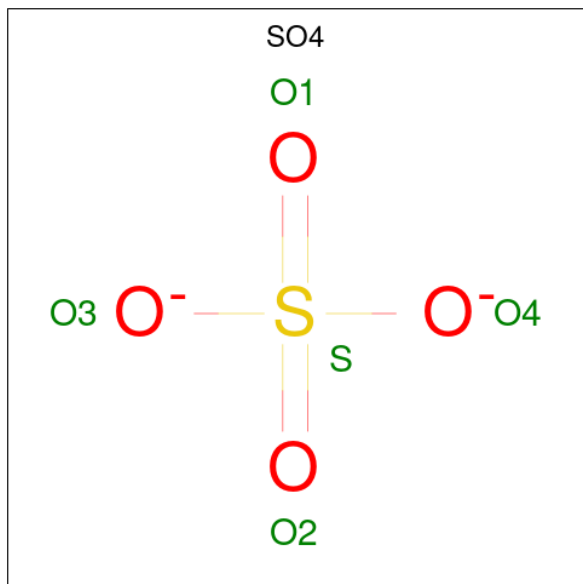
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



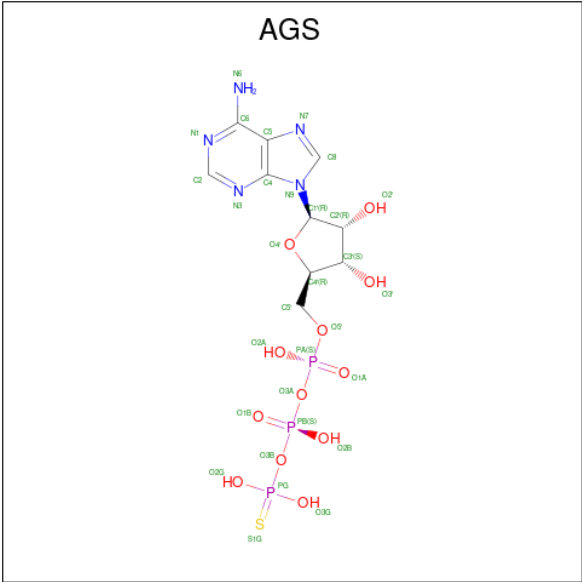
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		

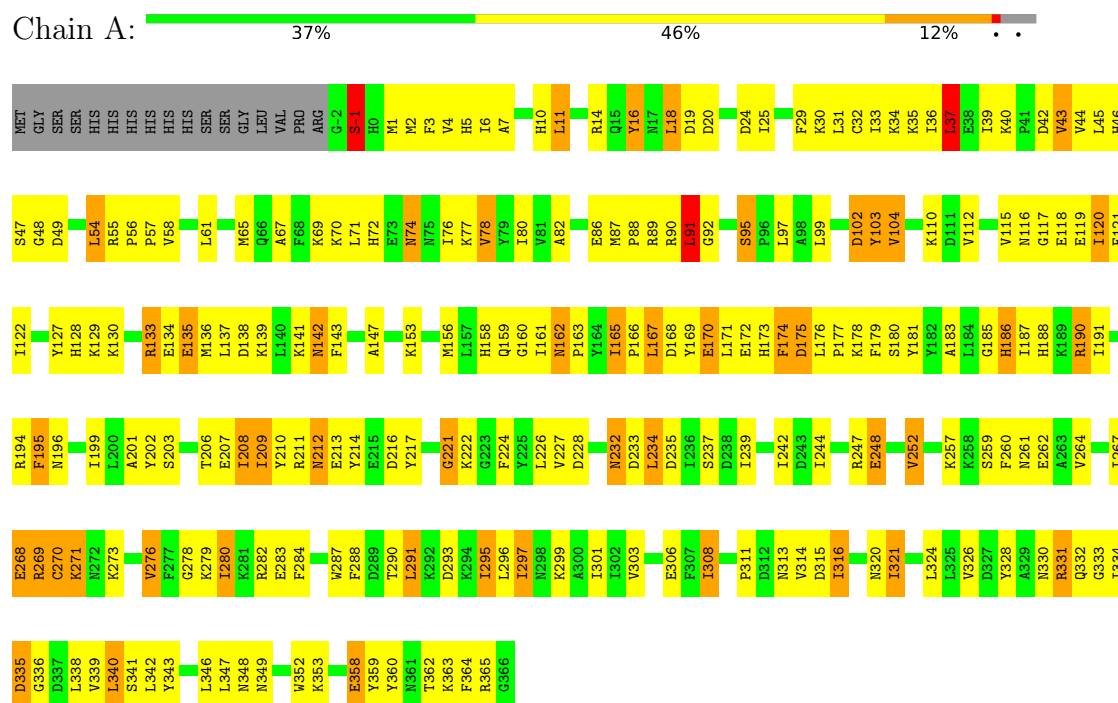
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	10	Total	O	0	0
			10	10		
8	B	10	Total	O	0	0
			10	10		

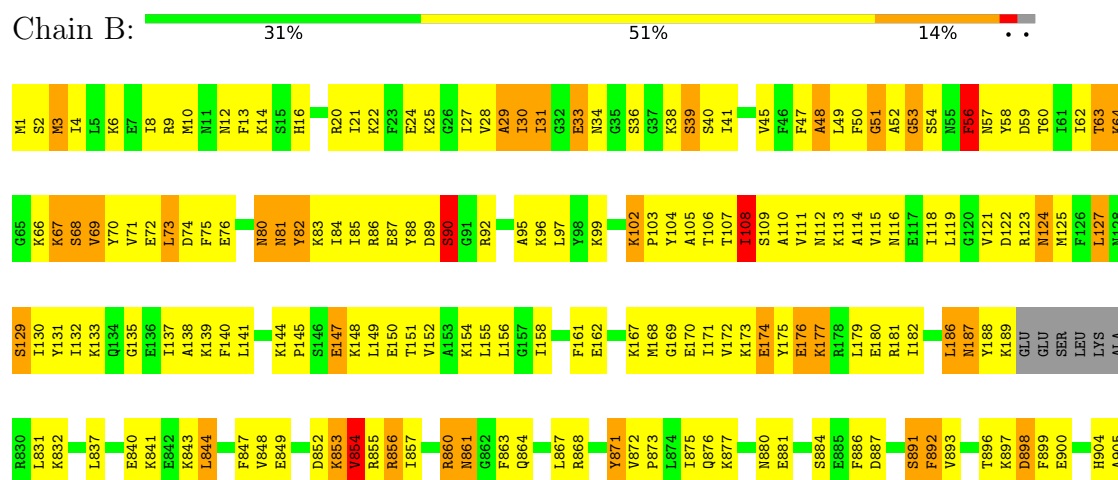
3 Residue-property plots

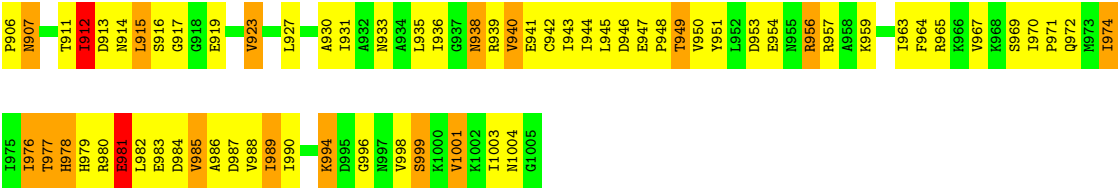
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 double-strand break repair mre11



- Molecule 2: DNA double-strand break repair rad50 ATPase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	86.96Å 147.13Å 175.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 3.10 29.32 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.32-3.10) 96.5 (29.32-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.214 , 0.276 0.204 , 0.275	Depositor DCC
R_{free} test set	2021 reflections (9.68%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.030 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6094	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, IPA, AGS, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/3128	1.00	7/4203 (0.2%)
2	B	0.62	0/2981	1.01	10/3994 (0.3%)
All	All	0.60	0/6109	1.00	17/8197 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LEU	CA-C-N	9.36	129.20	120.21
1	A	176	LEU	C-N-CA	9.36	129.20	120.21
1	A	162	ASN	CA-C-N	-7.65	111.91	119.87
1	A	162	ASN	C-N-CA	-7.65	111.91	119.87
2	B	102	LYS	CA-C-N	7.44	127.86	119.83
2	B	102	LYS	C-N-CA	7.44	127.86	119.83
2	B	135	GLY	N-CA-C	-6.99	106.16	114.48
2	B	923	VAL	CB-CA-C	-6.74	103.25	111.88
1	A	37	LEU	N-CA-C	-6.46	104.08	112.23
2	B	949	THR	CB-CA-C	-6.14	103.67	111.22
1	A	92	GLY	N-CA-C	-5.94	106.84	113.79
2	B	29	ALA	N-CA-C	5.91	117.08	107.32
2	B	1001	VAL	N-CA-C	5.76	116.09	107.51
1	A	29	PHE	N-CA-C	-5.42	105.48	112.68
2	B	854	VAL	N-CA-C	-5.25	107.71	112.96
2	B	978	HIS	N-CA-C	-5.22	105.58	112.94
2	B	176	GLU	N-CA-C	-5.18	108.72	114.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3064	0	3070	252	0
2	B	2937	0	3025	279	0
3	A	6	0	8	1	0
3	B	18	0	24	12	0
4	A	4	0	8	2	0
4	B	8	0	16	0	0
5	A	5	0	0	1	0
6	B	31	0	12	3	0
7	B	1	0	0	0	0
8	A	10	0	0	2	0
8	B	10	0	0	4	0
All	All	6094	0	6163	507	0

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 41.

All (507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:HG3	1:A:208:ILE:H	1.13	1.12
1:A:165:ILE:HG12	1:A:187:ILE:HD11	1.38	1.04
2:B:949:THR:O	3:B:1201:GOL:H32	1.57	1.02
1:A:282:ARG:HH22	2:B:907:ASN:HB3	1.26	1.01
1:A:173:HIS:CD2	1:A:174:PHE:H	1.84	0.96
1:A:173:HIS:HD2	1:A:174:PHE:H	1.05	0.96
2:B:67:LYS:H	2:B:67:LYS:HD2	1.29	0.96
1:A:207:GLU:HG3	1:A:208:ILE:N	1.79	0.95
1:A:133:ARG:HG2	1:A:133:ARG:HH21	1.31	0.95
1:A:1:MET:HB3	1:A:115:VAL:HG11	1.47	0.94
2:B:30:ILE:HD12	2:B:30:ILE:H	1.31	0.94
1:A:160:GLY:HA3	1:A:165:ILE:HD11	1.53	0.91
2:B:174:GLU:HA	2:B:177:LYS:HE2	1.52	0.90
2:B:911:THR:H	2:B:914:ASN:ND2	1.68	0.90
1:A:31:LEU:HB3	1:A:244:ILE:HD11	1.54	0.90
1:A:69:LYS:HA	1:A:103:TYR:CE2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HB	1:A:78:VAL:HG13	1.55	0.86
2:B:942:CYS:HB2	2:B:972:GLN:HB3	1.56	0.86
2:B:50:PHE:CD1	2:B:123:ARG:HG3	2.11	0.84
1:A:342:LEU:O	1:A:346:LEU:HG	1.78	0.84
2:B:947:GLU:O	2:B:950:VAL:HG23	1.78	0.83
1:A:1:MET:HB3	1:A:115:VAL:CG1	2.08	0.83
2:B:12:ASN:C	2:B:63:THR:HG22	2.05	0.82
2:B:12:ASN:HA	2:B:63:THR:CG2	2.10	0.82
1:A:33:ILE:HG13	1:A:67:ALA:HB1	1.63	0.80
2:B:979:HIS:NE2	3:B:1201:GOL:H31	1.97	0.80
2:B:10:MET:HE2	2:B:16:HIS:CG	2.17	0.79
2:B:28:VAL:HB	2:B:974:ILE:HA	1.61	0.79
2:B:80:ASN:HB2	2:B:82:TYR:HE2	1.48	0.79
1:A:69:LYS:HA	1:A:103:TYR:CD2	2.17	0.79
2:B:49:LEU:HB2	2:B:50:PHE:HD2	1.48	0.79
1:A:78:VAL:HB	1:A:104:VAL:HG22	1.66	0.78
2:B:144:LYS:HG2	2:B:145:PRO:HD2	1.66	0.78
2:B:67:LYS:HD2	2:B:67:LYS:N	1.97	0.78
1:A:282:ARG:HH22	2:B:907:ASN:CB	1.96	0.77
2:B:880:ASN:HD21	2:B:893:VAL:H	1.32	0.77
2:B:886:PHE:CD1	2:B:956:ARG:HG3	2.20	0.77
2:B:911:THR:H	2:B:914:ASN:HD22	1.32	0.76
1:A:-1:SER:HA	1:A:116:ASN:OD1	1.86	0.76
1:A:127:TYR:HA	1:A:159:GLN:HE22	1.50	0.75
1:A:1:MET:CB	1:A:115:VAL:HG11	2.18	0.74
2:B:12:ASN:CA	2:B:63:THR:HG22	2.18	0.74
1:A:69:LYS:HG3	1:A:103:TYR:HE2	1.53	0.74
2:B:49:LEU:HB2	2:B:50:PHE:CD2	2.24	0.73
1:A:65:MET:HE3	1:A:99:LEU:O	1.89	0.73
1:A:288:PHE:O	1:A:291:LEU:HD12	1.89	0.73
2:B:892:PHE:HE2	2:B:904:HIS:ND1	1.87	0.73
2:B:105:ALA:HB1	2:B:110:ALA:HB1	1.70	0.72
1:A:352:TRP:H	1:A:352:TRP:CD1	2.05	0.72
2:B:64:LYS:HZ2	3:B:1202:GOL:C1	2.03	0.72
2:B:50:PHE:O	2:B:51:GLY:O	2.08	0.71
2:B:905:ALA:HB1	2:B:906:PRO:HD2	1.70	0.71
2:B:938:ASN:O	2:B:939:ARG:HG3	1.90	0.70
1:A:326:VAL:CG2	1:A:340:LEU:HD12	2.21	0.70
2:B:860:ARG:HD3	2:B:860:ARG:H	1.56	0.70
2:B:28:VAL:CG1	2:B:974:ILE:HG23	2.22	0.69
1:A:46:HIS:HB3	1:A:80:ILE:HG13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:880:ASN:HD21	2:B:893:VAL:N	1.90	0.69
1:A:347:LEU:C	1:A:349:ASN:H	2.00	0.69
2:B:50:PHE:HD1	2:B:123:ARG:HG3	1.57	0.69
1:A:222:LYS:O	1:A:244:ILE:HG22	1.92	0.68
2:B:21:ILE:HG12	2:B:1001:VAL:HG11	1.75	0.68
2:B:985:VAL:CG2	2:B:985:VAL:O	2.41	0.68
2:B:12:ASN:HA	2:B:63:THR:HG22	1.74	0.68
1:A:121:PHE:CE2	1:A:147:ALA:HB2	2.29	0.67
2:B:80:ASN:CB	2:B:82:TYR:HE2	2.07	0.67
2:B:861:ASN:H	2:B:861:ASN:HD22	1.42	0.67
2:B:30:ILE:HD12	2:B:30:ILE:N	2.06	0.67
2:B:898:ASP:OD1	2:B:898:ASP:N	2.26	0.67
2:B:53:GLY:H	2:B:123:ARG:HH12	1.43	0.67
2:B:978:HIS:CE1	3:B:1201:GOL:O2	2.48	0.67
2:B:170:GLU:O	2:B:173:LYS:HB2	1.95	0.67
1:A:227:VAL:HG13	1:A:239:ILE:HG12	1.77	0.66
2:B:86:ARG:HG2	2:B:95:ALA:HB2	1.77	0.66
2:B:89:ASP:O	2:B:90:SER:C	2.38	0.66
2:B:53:GLY:H	2:B:123:ARG:NH1	1.94	0.66
2:B:886:PHE:HD1	2:B:956:ARG:HG3	1.59	0.66
2:B:988:VAL:HG12	2:B:989:ILE:H	1.60	0.66
1:A:4:VAL:HG11	1:A:36:ILE:CD1	2.26	0.66
1:A:232:ASN:N	1:A:232:ASN:HD22	1.92	0.66
1:A:133:ARG:HH21	1:A:133:ARG:CG	2.08	0.65
2:B:84:ILE:HG12	2:B:97:LEU:HD13	1.78	0.65
2:B:963:ILE:O	2:B:967:VAL:HG23	1.95	0.65
1:A:166:PRO:HD2	1:A:167:LEU:HD23	1.77	0.65
1:A:112:VAL:HG11	1:A:119:GLU:HG2	1.79	0.65
1:A:315:ASP:HB3	2:B:877:LYS:NZ	2.12	0.65
1:A:268:GLU:C	1:A:270:CYS:H	2.05	0.65
2:B:121:VAL:HB	2:B:125:MET:HB3	1.79	0.65
2:B:74:ASP:OD2	2:B:83:LYS:HE3	1.98	0.64
2:B:186:LEU:HD12	2:B:837:LEU:HG	1.79	0.64
1:A:308:ILE:O	1:A:308:ILE:HG13	1.97	0.64
1:A:116:ASN:C	1:A:118:GLU:H	2.06	0.64
2:B:27:ILE:CG2	2:B:986:ALA:HA	2.27	0.64
1:A:234:LEU:HD12	1:A:234:LEU:H	1.62	0.64
2:B:880:ASN:ND2	2:B:893:VAL:H	1.96	0.63
2:B:144:LYS:HG2	2:B:145:PRO:CD	2.28	0.63
2:B:30:ILE:H	2:B:30:ILE:CD1	2.09	0.63
2:B:47:PHE:O	2:B:48:ALA:C	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG11	1:A:36:ILE:HD13	1.81	0.62
1:A:112:VAL:CG1	1:A:119:GLU:HG2	2.29	0.62
1:A:116:ASN:O	1:A:118:GLU:N	2.26	0.62
1:A:133:ARG:NH1	1:A:175:ASP:OD1	2.32	0.62
1:A:165:ILE:HD12	1:A:168:ASP:O	2.00	0.62
1:A:139:LYS:NZ	4:A:600:IPA:H11	2.15	0.62
1:A:214:TYR:O	1:A:217:TYR:HB3	2.00	0.62
2:B:12:ASN:CA	2:B:63:THR:CG2	2.77	0.62
2:B:985:VAL:O	2:B:985:VAL:HG23	1.97	0.62
2:B:125:MET:HE3	2:B:154:LYS:HD2	1.80	0.62
2:B:10:MET:HE2	2:B:16:HIS:CB	2.29	0.62
1:A:173:HIS:CD2	1:A:174:PHE:N	2.63	0.61
1:A:31:LEU:CB	1:A:244:ILE:HD11	2.28	0.61
1:A:2:MET:HE3	1:A:228:ASP:HB2	1.81	0.61
1:A:55:ARG:NH2	2:B:980:ARG:HH11	1.98	0.61
1:A:352:TRP:CE3	2:B:171:ILE:HG12	2.36	0.61
2:B:14:LYS:HB3	6:B:1006:AGS:C5	2.31	0.61
2:B:950:VAL:O	2:B:951:TYR:HB2	2.01	0.61
1:A:282:ARG:O	1:A:282:ARG:HD3	2.00	0.61
1:A:172:GLU:O	1:A:175:ASP:HB2	2.01	0.61
2:B:182:ILE:HD12	2:B:844:LEU:HD12	1.83	0.61
2:B:938:ASN:N	2:B:938:ASN:HD22	1.97	0.61
1:A:287:TRP:O	1:A:290:THR:HG22	2.01	0.60
2:B:27:ILE:HG21	2:B:986:ALA:HA	1.82	0.60
1:A:69:LYS:HA	1:A:103:TYR:HE2	1.60	0.60
2:B:22:LYS:HG2	2:B:1003:ILE:HD13	1.83	0.60
2:B:27:ILE:HG22	2:B:27:ILE:O	2.01	0.60
1:A:360:TYR:CE1	2:B:843:LYS:HD3	2.36	0.60
1:A:39:ILE:HG22	1:A:39:ILE:O	2.01	0.60
2:B:860:ARG:HA	2:B:864:GLN:OE1	2.02	0.60
2:B:875:ILE:HD13	2:B:931:ILE:HG12	1.83	0.60
1:A:54:LEU:HD21	1:A:88:PRO:HA	1.83	0.60
1:A:112:VAL:HG13	1:A:120:ILE:O	2.00	0.60
2:B:80:ASN:HB2	2:B:82:TYR:CE2	2.34	0.60
2:B:29:ALA:O	2:B:31:ILE:HD12	2.02	0.60
2:B:82:TYR:CE1	2:B:118:ILE:HG21	2.37	0.59
2:B:964:PHE:HD2	2:B:982:LEU:HD21	1.67	0.59
1:A:234:LEU:HD12	1:A:234:LEU:N	2.18	0.59
2:B:877:LYS:O	2:B:881:GLU:HB2	2.01	0.59
2:B:67:LYS:HD2	2:B:68:SER:H	1.68	0.59
1:A:226:LEU:HB2	1:A:242:ILE:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LYS:HB3	2:B:102:LYS:O	2.02	0.59
2:B:941:GLU:O	2:B:971:PRO:HD2	2.02	0.59
2:B:67:LYS:CD	2:B:68:SER:H	2.16	0.59
1:A:282:ARG:HD3	1:A:282:ARG:C	2.27	0.59
1:A:177:PRO:HG2	1:A:179:PHE:HE2	1.68	0.58
2:B:988:VAL:HG12	2:B:989:ILE:N	2.18	0.58
2:B:129:SER:OG	2:B:130:ILE:HD12	2.03	0.58
1:A:166:PRO:HG2	1:A:167:LEU:HD23	1.84	0.58
2:B:977:THR:HB	2:B:979:HIS:H	1.69	0.58
2:B:189:LYS:NZ	2:B:832:LYS:HE2	2.19	0.58
2:B:12:ASN:HA	2:B:63:THR:HG21	1.84	0.58
1:A:133:ARG:HG2	1:A:133:ARG:NH2	2.10	0.58
1:A:211:ARG:HG3	5:A:400:SO4:O4	2.03	0.58
2:B:81:ASN:HD22	2:B:81:ASN:C	2.13	0.57
1:A:31:LEU:HB3	1:A:244:ILE:CD1	2.32	0.57
1:A:160:GLY:CA	1:A:165:ILE:HD11	2.31	0.57
1:A:78:VAL:HB	1:A:104:VAL:CG2	2.35	0.57
1:A:269:ARG:O	1:A:269:ARG:HG2	2.04	0.57
1:A:74:ASN:N	1:A:74:ASN:HD22	2.01	0.57
2:B:27:ILE:HB	2:B:987:ASP:OD1	2.04	0.57
1:A:279:LYS:O	1:A:280:ILE:HG13	2.04	0.57
1:A:273:LYS:HE2	1:A:293:ASP:O	2.04	0.57
1:A:3:PHE:CE2	1:A:227:VAL:HB	2.40	0.56
1:A:120:ILE:HG22	1:A:121:PHE:N	2.19	0.56
1:A:32:CYS:O	1:A:36:ILE:HG13	2.05	0.56
2:B:979:HIS:CD2	3:B:1201:GOL:H31	2.41	0.56
1:A:86:GLU:O	1:A:95:SER:HB2	2.05	0.56
1:A:315:ASP:HB3	2:B:877:LYS:HZ3	1.70	0.56
2:B:131:TYR:C	2:B:131:TYR:CD1	2.81	0.56
2:B:911:THR:N	2:B:914:ASN:HD22	2.01	0.56
2:B:957:ARG:HB3	2:B:981:GLU:HG3	1.87	0.56
1:A:283:GLU:HG3	1:A:284:PHE:CD2	2.41	0.56
2:B:162:GLU:HB2	2:B:864:GLN:HE22	1.71	0.56
2:B:30:ILE:CD1	2:B:974:ILE:HG22	2.36	0.56
2:B:978:HIS:HE1	3:B:1201:GOL:O2	1.88	0.56
1:A:335:ASP:HB3	1:A:338:LEU:HB3	1.88	0.56
1:A:71:LEU:HD22	1:A:76:ILE:HD12	1.89	0.56
1:A:260:PHE:O	1:A:264:VAL:HG23	2.06	0.55
1:A:340:LEU:O	1:A:343:TYR:HB3	2.06	0.55
1:A:159:GLN:HB3	1:A:170:GLU:HG2	1.88	0.55
1:A:56:PRO:HG2	1:A:61:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:CD2	1:A:71:LEU:HD23	2.37	0.55
2:B:114:ALA:O	2:B:118:ILE:HG13	2.07	0.55
2:B:897:LYS:H	2:B:897:LYS:HD2	1.71	0.55
2:B:979:HIS:HA	8:B:1406:HOH:O	2.07	0.55
1:A:248:GLU:OE1	1:A:271:LYS:HB2	2.06	0.55
2:B:933:ASN:HD22	2:B:969:SER:CB	2.20	0.55
2:B:938:ASN:HD22	2:B:938:ASN:H	1.55	0.55
2:B:974:ILE:HD12	2:B:974:ILE:H	1.71	0.54
1:A:340:LEU:O	1:A:340:LEU:HD23	2.07	0.54
2:B:22:LYS:HG2	2:B:1003:ILE:CD1	2.37	0.54
1:A:82:ALA:HB2	1:A:97:LEU:HD12	1.89	0.54
1:A:87:MET:CE	1:A:88:PRO:HD2	2.37	0.54
1:A:166:PRO:CD	1:A:167:LEU:HD23	2.38	0.54
2:B:6:LYS:HD2	2:B:76:GLU:HG3	1.90	0.54
1:A:347:LEU:C	1:A:349:ASN:N	2.66	0.54
2:B:14:LYS:O	2:B:63:THR:HB	2.06	0.54
2:B:4:ILE:O	2:B:75:PHE:HB2	2.08	0.54
1:A:338:LEU:HG	1:A:339:VAL:N	2.23	0.54
1:A:137:LEU:O	1:A:141:LYS:HG2	2.07	0.53
2:B:172:VAL:HG12	2:B:172:VAL:O	2.08	0.53
2:B:30:ILE:HD11	2:B:974:ILE:CG2	2.39	0.53
2:B:67:LYS:HD3	2:B:68:SER:OG	2.08	0.53
1:A:260:PHE:C	1:A:260:PHE:CD2	2.86	0.53
2:B:959:LYS:O	2:B:963:ILE:HG13	2.08	0.53
1:A:4:VAL:HG13	1:A:224:PHE:CD2	2.43	0.53
1:A:296:LEU:O	1:A:296:LEU:HD12	2.08	0.53
2:B:174:GLU:C	2:B:176:GLU:H	2.17	0.53
2:B:900:GLU:OE1	2:B:900:GLU:HA	2.07	0.53
1:A:153:LYS:HB2	1:A:179:PHE:HD1	1.74	0.53
2:B:933:ASN:HD22	2:B:969:SER:HB2	1.74	0.53
1:A:43:VAL:HG22	1:A:77:LYS:HB3	1.91	0.53
1:A:46:HIS:HB3	1:A:80:ILE:CG1	2.38	0.53
2:B:149:LEU:HA	2:B:152:VAL:HG12	1.91	0.52
1:A:16:TYR:CD1	1:A:299:LYS:HD2	2.44	0.52
1:A:186:HIS:ND1	8:A:709:HOH:O	2.34	0.52
1:A:87:MET:HE3	1:A:88:PRO:HD2	1.91	0.52
1:A:90:ARG:O	1:A:91:LEU:C	2.52	0.52
1:A:288:PHE:C	1:A:290:THR:N	2.67	0.52
2:B:22:LYS:H	2:B:1003:ILE:HD11	1.74	0.52
1:A:69:LYS:HG3	1:A:103:TYR:CE2	2.39	0.52
1:A:162:ASN:ND2	1:A:172:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ARG:HG2	2:B:20:ARG:HD3	1.92	0.52
2:B:938:ASN:N	2:B:938:ASN:ND2	2.56	0.52
2:B:886:PHE:CE1	2:B:956:ARG:HG3	2.44	0.52
1:A:342:LEU:HD21	2:B:168:MET:SD	2.49	0.52
1:A:364:PHE:CE2	2:B:847:PHE:HA	2.44	0.52
1:A:70:LYS:O	1:A:71:LEU:C	2.52	0.52
1:A:199:ILE:HG21	1:A:239:ILE:HD12	1.92	0.52
2:B:28:VAL:HB	2:B:974:ILE:HG23	1.91	0.51
2:B:989:ILE:HG23	2:B:1004:ASN:HB3	1.91	0.51
1:A:69:LYS:HA	1:A:103:TYR:HD2	1.75	0.51
1:A:334:ILE:HD12	1:A:334:ILE:N	2.24	0.51
2:B:107:THR:O	2:B:108:ILE:C	2.53	0.51
2:B:141:LEU:HD13	2:B:912:ILE:HG21	1.91	0.51
1:A:134:GLU:C	1:A:136:MET:N	2.68	0.51
1:A:209:ILE:HD11	1:A:210:TYR:CE2	2.45	0.51
2:B:70:TYR:OH	2:B:85:ILE:HD13	2.10	0.51
2:B:872:VAL:O	2:B:873:PRO:C	2.52	0.51
1:A:260:PHE:O	1:A:260:PHE:CD2	2.64	0.51
2:B:169:GLY:O	2:B:173:LYS:HG3	2.11	0.51
1:A:364:PHE:HE2	2:B:847:PHE:HA	1.76	0.51
2:B:876:GLN:O	2:B:877:LYS:C	2.54	0.51
1:A:321:ILE:N	1:A:321:ILE:HD12	2.26	0.51
1:A:165:ILE:HG12	1:A:187:ILE:CD1	2.26	0.51
2:B:64:LYS:HZ2	3:B:1202:GOL:H12	1.74	0.51
2:B:189:LYS:HZ1	2:B:832:LYS:HE2	1.74	0.51
1:A:352:TRP:O	1:A:353:LYS:C	2.53	0.50
2:B:36:SER:O	2:B:999:SER:HB2	2.11	0.50
1:A:55:ARG:NH2	2:B:980:ARG:NH1	2.58	0.50
2:B:1:MET:HE1	2:B:130:ILE:HD11	1.93	0.50
2:B:897:LYS:HB2	2:B:898:ASP:OD1	2.11	0.50
1:A:147:ALA:HB1	1:A:153:LYS:HE2	1.92	0.50
1:A:128:HIS:HB2	1:A:136:MET:HE2	1.94	0.50
2:B:22:LYS:H	2:B:1003:ILE:CD1	2.23	0.50
1:A:115:VAL:HG13	1:A:116:ASN:HD22	1.76	0.50
2:B:50:PHE:HB3	2:B:123:ARG:HG3	1.93	0.50
2:B:896:THR:HG21	2:B:900:GLU:HB2	1.93	0.50
1:A:268:GLU:C	1:A:270:CYS:N	2.70	0.50
2:B:149:LEU:HD22	2:B:868:ARG:HD2	1.93	0.50
1:A:33:ILE:HG21	1:A:67:ALA:HB1	1.94	0.50
1:A:185:GLY:O	1:A:186:HIS:CB	2.59	0.50
1:A:191:ILE:HB	1:A:202:TYR:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TYR:CD1	2:B:104:TYR:O	2.64	0.50
2:B:852:ASP:C	2:B:854:VAL:H	2.20	0.50
1:A:162:ASN:HD22	1:A:172:GLU:CD	2.20	0.49
2:B:916:SER:O	2:B:917:GLY:C	2.54	0.49
1:A:57:PRO:O	1:A:58:VAL:C	2.55	0.49
2:B:6:LYS:N	2:B:74:ASP:O	2.41	0.49
2:B:28:VAL:HG12	2:B:974:ILE:HG23	1.95	0.49
2:B:64:LYS:HZ2	3:B:1202:GOL:H11	1.77	0.49
2:B:170:GLU:HA	2:B:173:LYS:CD	2.43	0.49
2:B:950:VAL:HG22	3:B:1201:GOL:H11	1.95	0.49
2:B:980:ARG:O	2:B:983:GLU:HB2	2.13	0.49
2:B:63:THR:HG23	2:B:66:LYS:HG2	1.94	0.49
1:A:333:GLY:C	1:A:334:ILE:HD12	2.38	0.48
2:B:897:LYS:HD2	2:B:897:LYS:N	2.28	0.48
2:B:912:ILE:HD12	2:B:913:ASP:N	2.27	0.48
1:A:199:ILE:HG21	1:A:239:ILE:CD1	2.43	0.48
1:A:364:PHE:CE2	2:B:847:PHE:HD2	2.31	0.48
1:A:37:LEU:HD23	1:A:71:LEU:HD23	1.95	0.48
2:B:147:GLU:O	2:B:151:THR:HG23	2.14	0.48
2:B:58:TYR:CE2	2:B:88:TYR:CD1	3.02	0.48
1:A:259:SER:O	1:A:260:PHE:C	2.56	0.48
2:B:81:ASN:C	2:B:81:ASN:ND2	2.71	0.48
2:B:156:LEU:HD13	2:B:871:TYR:CD1	2.48	0.48
2:B:179:LEU:C	2:B:179:LEU:HD13	2.39	0.48
2:B:124:ASN:N	2:B:124:ASN:ND2	2.61	0.48
2:B:1:MET:O	2:B:1:MET:HG2	2.13	0.48
2:B:8:ILE:HG13	2:B:73:LEU:HB2	1.95	0.48
2:B:50:PHE:O	2:B:51:GLY:C	2.56	0.48
2:B:95:ALA:O	2:B:111:VAL:HG21	2.14	0.48
2:B:853:LYS:O	2:B:857:ILE:HG13	2.13	0.48
1:A:153:LYS:HB2	1:A:179:PHE:CD1	2.48	0.48
2:B:916:SER:OG	2:B:919:GLU:HB2	2.14	0.48
1:A:232:ASN:N	1:A:232:ASN:ND2	2.59	0.48
1:A:363:LYS:HA	1:A:365:ARG:HH12	1.79	0.48
2:B:20:ARG:C	2:B:21:ILE:HG13	2.38	0.48
1:A:161:ILE:HG13	1:A:171:LEU:HB2	1.96	0.47
2:B:9:ARG:HD2	2:B:72:GLU:OE1	2.14	0.47
1:A:364:PHE:CD2	2:B:847:PHE:HD2	2.33	0.47
2:B:111:VAL:O	2:B:115:VAL:HG23	2.13	0.47
2:B:942:CYS:CB	2:B:972:GLN:HB3	2.37	0.47
1:A:2:MET:HE3	1:A:228:ASP:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:HG21	1:A:340:LEU:HD12	1.94	0.47
1:A:340:LEU:C	1:A:340:LEU:CD2	2.87	0.47
2:B:174:GLU:HA	2:B:177:LYS:CE	2.34	0.47
1:A:30:LYS:HE2	3:A:500:GOL:O2	2.14	0.47
2:B:49:LEU:CD2	2:B:73:LEU:HD21	2.44	0.47
2:B:861:ASN:HD22	2:B:861:ASN:N	2.06	0.47
1:A:162:ASN:HB3	1:A:163:PRO:HD3	1.96	0.47
1:A:2:MET:HE3	1:A:228:ASP:CB	2.45	0.47
1:A:134:GLU:C	1:A:136:MET:H	2.23	0.47
1:A:158:HIS:O	1:A:158:HIS:CD2	2.67	0.47
1:A:259:SER:O	1:A:261:ASN:N	2.47	0.47
2:B:64:LYS:HA	3:B:1202:GOL:H12	1.97	0.47
2:B:896:THR:HG23	2:B:900:GLU:O	2.14	0.47
1:A:69:LYS:CG	1:A:103:TYR:HE2	2.26	0.47
1:A:166:PRO:CG	1:A:167:LEU:HD23	2.45	0.47
1:A:188:HIS:HB3	1:A:213:GLU:OE1	2.15	0.47
1:A:102:ASP:O	1:A:103:TYR:CD1	2.68	0.47
1:A:358:GLU:O	1:A:359:TYR:C	2.56	0.47
1:A:259:SER:C	1:A:261:ASN:N	2.69	0.47
2:B:161:PHE:CE2	2:B:863:PHE:CE2	3.02	0.46
2:B:139:LYS:O	2:B:140:PHE:C	2.58	0.46
2:B:189:LYS:HD2	2:B:189:LYS:HA	1.62	0.46
2:B:954:GLU:CD	2:B:954:GLU:H	2.23	0.46
2:B:38:LYS:HB3	2:B:976:ILE:CG2	2.45	0.46
1:A:6:ILE:HG13	1:A:224:PHE:HB3	1.96	0.46
1:A:77:LYS:NZ	8:A:711:HOH:O	2.48	0.46
1:A:267:ILE:O	1:A:270:CYS:HB2	2.15	0.46
1:A:326:VAL:HG23	1:A:340:LEU:HD12	1.98	0.46
2:B:8:ILE:HG13	2:B:73:LEU:CB	2.45	0.46
2:B:66:LYS:O	3:B:1202:GOL:H31	2.16	0.46
1:A:36:ILE:HG12	1:A:224:PHE:CZ	2.51	0.46
2:B:39:SER:CB	8:B:1401:HOH:O	2.63	0.46
1:A:35:LYS:O	1:A:39:ILE:HG13	2.15	0.46
1:A:232:ASN:HD22	1:A:232:ASN:H	1.62	0.46
1:A:320:ASN:O	1:A:321:ILE:C	2.58	0.46
2:B:947:GLU:N	2:B:948:PRO:HD3	2.31	0.46
2:B:28:VAL:CB	2:B:974:ILE:HG23	2.45	0.46
2:B:60:THR:O	6:B:1006:AGS:N6	2.48	0.46
2:B:175:TYR:CD1	2:B:847:PHE:HE1	2.34	0.46
1:A:141:LYS:O	1:A:142:ASN:C	2.58	0.46
1:A:340:LEU:HD23	1:A:340:LEU:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:NZ	3:B:1202:GOL:H12	2.31	0.46
2:B:132:ILE:HD12	2:B:132:ILE:N	2.31	0.46
2:B:156:LEU:HB2	2:B:158:ILE:HD13	1.98	0.45
1:A:142:ASN:O	1:A:143:PHE:C	2.58	0.45
1:A:39:ILE:O	1:A:40:LYS:C	2.58	0.45
1:A:48:GLY:O	1:A:49:ASP:HB2	2.16	0.45
1:A:158:HIS:O	1:A:158:HIS:CG	2.69	0.45
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.71	0.45
2:B:116:ASN:N	2:B:116:ASN:HD22	2.14	0.45
1:A:128:HIS:CG	1:A:136:MET:HE2	2.51	0.45
1:A:338:LEU:O	1:A:341:SER:N	2.50	0.45
2:B:179:LEU:O	2:B:179:LEU:HD22	2.16	0.45
1:A:129:LYS:HE3	2:B:986:ALA:O	2.17	0.45
1:A:282:ARG:NH2	2:B:907:ASN:OD1	2.49	0.45
1:A:1:MET:HA	1:A:42:ASP:OD2	2.16	0.45
1:A:212:ASN:H	1:A:212:ASN:ND2	2.15	0.45
2:B:105:ALA:HB1	2:B:110:ALA:CB	2.44	0.45
2:B:127:LEU:HD22	2:B:133:LYS:HD2	1.99	0.45
2:B:911:THR:C	2:B:913:ASP:N	2.74	0.45
1:A:102:ASP:C	1:A:103:TYR:CD1	2.95	0.45
1:A:39:ILE:O	1:A:39:ILE:CG2	2.65	0.45
2:B:118:ILE:O	2:B:118:ILE:HG22	2.16	0.45
1:A:308:ILE:O	1:A:308:ILE:CG1	2.61	0.45
2:B:47:PHE:CD1	2:B:51:GLY:HA2	2.52	0.45
2:B:51:GLY:O	2:B:52:ALA:C	2.59	0.45
2:B:124:ASN:HA	2:B:127:LEU:HD12	1.97	0.45
1:A:69:LYS:CA	1:A:103:TYR:CE2	2.93	0.45
1:A:288:PHE:C	1:A:290:THR:H	2.25	0.45
1:A:163:PRO:HG3	1:A:173:HIS:ND1	2.32	0.44
1:A:169:TYR:C	1:A:169:TYR:CD2	2.95	0.44
1:A:252:VAL:HG13	1:A:276:VAL:HG23	1.98	0.44
1:A:316:ILE:O	1:A:316:ILE:HG22	2.17	0.44
2:B:28:VAL:HB	2:B:974:ILE:CA	2.41	0.44
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.51	0.44
1:A:195:PHE:CD1	1:A:196:ASN:HB2	2.52	0.44
1:A:14:ARG:NH2	1:A:19:ASP:OD2	2.40	0.44
2:B:82:TYR:N	2:B:82:TYR:CD2	2.86	0.44
1:A:343:TYR:CE1	1:A:347:LEU:HD11	2.53	0.44
2:B:56:PHE:CG	2:B:57:ASN:N	2.84	0.44
1:A:89:ARG:NH1	1:A:129:LYS:HE2	2.33	0.44
1:A:55:ARG:HH21	2:B:980:ARG:NH1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:ILE:O	2:B:857:ILE:HG22	2.18	0.44
2:B:911:THR:C	2:B:913:ASP:H	2.26	0.44
2:B:946:ASP:CG	8:B:1401:HOH:O	2.60	0.44
1:A:46:HIS:O	1:A:80:ILE:HG13	2.18	0.44
1:A:116:ASN:C	1:A:118:GLU:N	2.70	0.44
1:A:130:LYS:HD3	1:A:170:GLU:HA	1.99	0.44
1:A:190:ARG:NE	1:A:221:GLY:O	2.50	0.44
1:A:194:ARG:O	1:A:195:PHE:HB2	2.17	0.44
2:B:911:THR:O	2:B:913:ASP:N	2.51	0.44
2:B:981:GLU:CD	2:B:981:GLU:H	2.25	0.44
1:A:352:TRP:CZ3	2:B:171:ILE:HG12	2.53	0.44
2:B:2:SER:HA	2:B:940:VAL:O	2.18	0.44
2:B:24:GLU:O	2:B:28:VAL:HG22	2.18	0.44
1:A:232:ASN:ND2	1:A:232:ASN:H	2.15	0.43
2:B:852:ASP:C	2:B:854:VAL:N	2.75	0.43
2:B:852:ASP:O	2:B:855:ARG:N	2.51	0.43
2:B:980:ARG:O	2:B:981:GLU:C	2.60	0.43
1:A:89:ARG:HH11	1:A:129:LYS:HE2	1.82	0.43
2:B:108:ILE:H	2:B:108:ILE:HG13	1.45	0.43
1:A:191:ILE:O	1:A:201:ALA:HA	2.17	0.43
1:A:332:GLN:OE1	2:B:856:ARG:NH2	2.51	0.43
1:A:336:GLY:HA2	1:A:339:VAL:HG12	1.99	0.43
2:B:840:GLU:O	2:B:841:LYS:C	2.60	0.43
2:B:872:VAL:HB	2:B:873:PRO:HD3	2.00	0.43
2:B:971:PRO:HG2	2:B:972:GLN:H	1.83	0.43
1:A:139:LYS:HZ1	4:A:600:IPA:H11	1.82	0.43
1:A:235:ASP:C	1:A:237:SER:H	2.26	0.43
2:B:27:ILE:HB	2:B:987:ASP:H	1.82	0.43
2:B:82:TYR:N	2:B:82:TYR:HD2	2.16	0.43
2:B:884:SER:C	2:B:886:PHE:H	2.26	0.43
2:B:965:ARG:HD3	2:B:965:ARG:HA	1.85	0.43
1:A:24:ASP:OD2	1:A:247:ARG:HB2	2.18	0.43
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.75	0.43
2:B:6:LYS:HD2	2:B:76:GLU:CG	2.48	0.43
2:B:118:ILE:O	2:B:119:LEU:HD23	2.18	0.43
1:A:45:LEU:HB3	1:A:156:MET:HE3	2.01	0.43
1:A:247:ARG:HA	1:A:247:ARG:HD3	1.80	0.43
2:B:36:SER:HA	2:B:994:LYS:HB2	2.01	0.43
2:B:983:GLU:C	2:B:985:VAL:H	2.27	0.43
1:A:54:LEU:HD11	1:A:87:MET:O	2.19	0.43
2:B:170:GLU:HA	2:B:173:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:CZ	2:B:980:ARG:HD2	2.48	0.43
1:A:212:ASN:H	1:A:212:ASN:HD22	1.66	0.43
2:B:187:ASN:C	2:B:189:LYS:H	2.25	0.43
2:B:129:SER:HB2	2:B:155:LEU:HD13	2.01	0.42
2:B:148:LYS:HE3	2:B:899:PHE:O	2.19	0.42
2:B:969:SER:C	2:B:970:ILE:HG13	2.43	0.42
1:A:276:VAL:CG1	1:A:295:ILE:HG13	2.49	0.42
1:A:7:ALA:HB2	1:A:47:SER:HB2	2.01	0.42
1:A:46:HIS:O	1:A:80:ILE:HA	2.18	0.42
2:B:66:LYS:HB3	2:B:67:LYS:HD2	2.01	0.42
2:B:102:LYS:HA	2:B:103:PRO:HD3	1.83	0.42
2:B:847:PHE:O	2:B:848:VAL:C	2.60	0.42
2:B:63:THR:HG23	2:B:66:LYS:CG	2.49	0.42
1:A:18:LEU:HD21	1:A:297:ILE:HG13	2.01	0.42
2:B:14:LYS:HA	6:B:1006:AGS:C6	2.50	0.42
2:B:97:LEU:HB2	2:B:111:VAL:HG13	2.02	0.42
1:A:181:TYR:HA	1:A:199:ILE:O	2.19	0.42
1:A:232:ASN:HD22	1:A:233:ASP:H	1.67	0.42
2:B:33:GLU:O	2:B:38:LYS:NZ	2.53	0.42
2:B:852:ASP:O	2:B:854:VAL:N	2.52	0.42
1:A:120:ILE:CG2	1:A:121:PHE:N	2.83	0.42
1:A:158:HIS:O	1:A:186:HIS:HB2	2.20	0.42
1:A:173:HIS:C	1:A:175:ASP:H	2.27	0.42
1:A:328:TYR:HE2	2:B:857:ILE:HG23	1.85	0.42
2:B:96:LYS:HD3	2:B:106:THR:HB	2.02	0.42
2:B:892:PHE:HE2	2:B:904:HIS:CE1	2.38	0.42
1:A:178:LYS:HG2	1:A:196:ASN:HB3	2.01	0.42
1:A:330:ASN:O	1:A:331:ARG:C	2.61	0.42
1:A:287:TRP:O	1:A:290:THR:CG2	2.67	0.42
2:B:162:GLU:HB2	2:B:864:GLN:NE2	2.35	0.42
2:B:927:LEU:O	2:B:930:ALA:HB3	2.20	0.42
1:A:133:ARG:CG	1:A:133:ARG:NH2	2.70	0.41
1:A:167:LEU:HD23	1:A:167:LEU:H	1.85	0.41
1:A:347:LEU:O	1:A:349:ASN:N	2.53	0.41
1:A:134:GLU:O	1:A:136:MET:N	2.53	0.41
1:A:208:ILE:H	1:A:208:ILE:HG12	1.48	0.41
2:B:34:ASN:HD22	2:B:34:ASN:HA	1.66	0.41
2:B:181:ARG:HD2	2:B:181:ARG:HA	1.86	0.41
2:B:912:ILE:HD12	2:B:912:ILE:C	2.44	0.41
2:B:912:ILE:HA	2:B:915:LEU:HD12	2.02	0.41
1:A:301:ILE:HG23	2:B:891:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ILE:HG12	2:B:69:VAL:CG1	2.49	0.41
1:A:166:PRO:HD2	1:A:167:LEU:CD2	2.48	0.41
2:B:945:LEU:HB3	2:B:948:PRO:HG3	2.02	0.41
2:B:953:ASP:OD1	2:B:953:ASP:C	2.63	0.41
1:A:235:ASP:C	1:A:237:SER:N	2.76	0.41
1:A:282:ARG:NH2	2:B:907:ASN:CB	2.73	0.41
1:A:315:ASP:HB3	2:B:877:LYS:HZ1	1.83	0.41
2:B:29:ALA:O	2:B:31:ILE:CD1	2.68	0.41
2:B:41:ILE:O	2:B:45:VAL:HG23	2.20	0.41
2:B:45:VAL:O	2:B:49:LEU:HG	2.21	0.41
2:B:896:THR:CG2	2:B:900:GLU:HB2	2.49	0.41
1:A:1:MET:HB3	1:A:115:VAL:HG12	1.98	0.41
1:A:20:ASP:O	1:A:24:ASP:OD1	2.39	0.41
1:A:115:VAL:CG1	1:A:116:ASN:HD22	2.33	0.41
1:A:153:LYS:O	1:A:180:SER:HB2	2.20	0.41
2:B:10:MET:HE3	2:B:13:PHE:HB3	2.02	0.41
2:B:39:SER:HB3	8:B:1401:HOH:O	2.19	0.41
2:B:174:GLU:CA	2:B:177:LYS:HE2	2.36	0.41
1:A:14:ARG:HG2	1:A:14:ARG:O	2.21	0.41
1:A:55:ARG:NH2	2:B:980:ARG:HD2	2.35	0.41
2:B:97:LEU:O	2:B:103:PRO:HA	2.21	0.41
1:A:2:MET:O	1:A:42:ASP:N	2.45	0.41
1:A:5:HIS:CD2	1:A:183:ALA:HB1	2.56	0.41
1:A:137:LEU:HD21	1:A:175:ASP:OD2	2.20	0.41
2:B:67:LYS:CD	2:B:68:SER:N	2.81	0.41
1:A:133:ARG:O	1:A:136:MET:HB3	2.21	0.41
1:A:291:LEU:C	1:A:293:ASP:H	2.28	0.41
2:B:105:ALA:O	2:B:111:VAL:HG22	2.21	0.40
2:B:167:LYS:HD2	2:B:167:LYS:HA	1.92	0.40
2:B:168:MET:O	2:B:172:VAL:HG23	2.21	0.40
1:A:163:PRO:HG2	1:A:173:HIS:HB3	2.02	0.40
1:A:278:GLY:O	1:A:301:ILE:HD12	2.20	0.40
1:A:363:LYS:HA	1:A:365:ARG:NH1	2.36	0.40
2:B:144:LYS:HA	2:B:145:PRO:HD3	1.90	0.40
2:B:3:MET:HE2	2:B:3:MET:HB2	1.98	0.40
2:B:138:ALA:O	2:B:139:LYS:C	2.63	0.40
2:B:186:LEU:HD12	2:B:837:LEU:CG	2.49	0.40
1:A:45:LEU:HD22	1:A:156:MET:SD	2.62	0.40
2:B:69:VAL:O	2:B:87:GLU:HA	2.21	0.40
1:A:10:HIS:O	1:A:11:LEU:C	2.65	0.40

There are no symmetry-related clashes.

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	
1	A	367/386 (95%)	290 (79%)	57 (16%)	20 (5%)	1	9
2	B	361/371 (97%)	279 (77%)	59 (16%)	23 (6%)	1	6
All	All	728/757 (96%)	569 (78%)	116 (16%)	43 (6%)	1	8

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ILE
2	B	33	GLU
2	B	51	GLY
2	B	80	ASN
2	B	187	ASN
2	B	891	SER
2	B	981	GLU
1	A	-1	SER
1	A	16	TYR
1	A	91	LEU
1	A	117	GLY
1	A	186	HIS
1	A	221	GLY
1	A	335	ASP
1	A	348	ASN
2	B	90	SER
2	B	188	TYR
2	B	915	LEU
2	B	989	ILE
2	B	990	ILE
2	B	996	GLY
1	A	269	ARG
1	A	358	GLU
2	B	48	ALA
2	B	53	GLY

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Mol	Chain	Res	Type
2	B	54	SER
2	B	122	ASP
2	B	853	LYS
2	B	984	ASP
1	A	195	PHE
1	A	271	LYS
1	A	362	THR
2	B	56	PHE
2	B	108	ILE
2	B	912	ILE
1	A	103	TYR
1	A	331	ARG
2	B	112	ASN
1	A	34	LYS
1	A	135	GLU
2	B	129	SER
1	A	280	ILE
1	A	311	PRO

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	
1	A	337/352 (96%)	285 (85%)	52 (15%)	2	12
2	B	319/324 (98%)	258 (81%)	61 (19%)	1	7
All	All	656/676 (97%)	543 (83%)	113 (17%)	2	10

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	11	LEU
1	A	18	LEU
1	A	25	ILE
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	43	VAL
1	A	54	LEU
1	A	72	HIS
1	A	74	ASN
1	A	78	VAL
1	A	91	LEU
1	A	95	SER
1	A	102	ASP
1	A	104	VAL
1	A	110	LYS
1	A	120	ILE
1	A	122	ILE
1	A	133	ARG
1	A	135	GLU
1	A	138	ASP
1	A	142	ASN
1	A	165	ILE
1	A	167	LEU
1	A	170	GLU
1	A	174	PHE
1	A	175	ASP
1	A	190	ARG
1	A	203	SER
1	A	206	THR
1	A	208	ILE
1	A	209	ILE
1	A	212	ASN
1	A	216	ASP
1	A	232	ASN
1	A	234	LEU
1	A	248	GLU
1	A	252	VAL
1	A	257	LYS
1	A	262	GLU
1	A	268	GLU
1	A	270	CYS
1	A	276	VAL
1	A	291	LEU
1	A	295	ILE
1	A	297	ILE
1	A	303	VAL
1	A	306	GLU

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Mol	Chain	Res	Type
1	A	308	ILE
1	A	313	ASN
1	A	314	VAL
1	A	321	ILE
1	A	340	LEU
2	B	3	MET
2	B	25	LYS
2	B	30	ILE
2	B	31	ILE
2	B	39	SER
2	B	40	SER
2	B	56	PHE
2	B	59	ASP
2	B	63	THR
2	B	64	LYS
2	B	67	LYS
2	B	68	SER
2	B	69	VAL
2	B	71	VAL
2	B	73	LEU
2	B	81	ASN
2	B	82	TYR
2	B	90	SER
2	B	92	ARG
2	B	108	ILE
2	B	109	SER
2	B	113	LYS
2	B	124	ASN
2	B	127	LEU
2	B	137	ILE
2	B	147	GLU
2	B	150	GLU
2	B	174	GLU
2	B	177	LYS
2	B	180	GLU
2	B	186	LEU
2	B	831	LEU
2	B	844	LEU
2	B	849	GLU
2	B	854	VAL
2	B	856	ARG
2	B	860	ARG

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Mol	Chain	Res	Type
2	B	861	ASN
2	B	867	LEU
2	B	871	TYR
2	B	887	ASP
2	B	892	PHE
2	B	898	ASP
2	B	907	ASN
2	B	912	ILE
2	B	923	VAL
2	B	935	LEU
2	B	936	ILE
2	B	938	ASN
2	B	940	VAL
2	B	943	ILE
2	B	944	ILE
2	B	956	ARG
2	B	974	ILE
2	B	976	ILE
2	B	977	THR
2	B	981	GLU
2	B	985	VAL
2	B	994	LYS
2	B	998	VAL
2	B	999	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	72	HIS
1	A	74	ASN
1	A	84	ASN
1	A	85	HIS
1	A	142	ASN
1	A	162	ASN
1	A	173	HIS
1	A	212	ASN
1	A	232	ASN
1	A	253	ASN
1	A	313	ASN
1	A	330	ASN
1	A	361	ASN

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Mol	Chain	Res	Type
2	B	11	ASN
2	B	12	ASN
2	B	34	ASN
2	B	80	ASN
2	B	116	ASN
2	B	124	ASN
2	B	166	GLN
2	B	836	ASN
2	B	861	ASN
2	B	880	ASN
2	B	914	ASN
2	B	933	ASN
2	B	938	ASN
2	B	978	HIS

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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	IPA	B	1300	-	3,3,3	0.64	0	3,3,3	0.43	0
6	AGS	B	1006	7	32,33,33	4.51	21 (65%)	45,52,52	2.13	17 (37%)
4	IPA	A	600	-	3,3,3	0.57	0	3,3,3	0.23	0
3	GOL	A	500	-	5,5,5	0.32	0	5,5,5	0.57	0
4	IPA	B	601	-	3,3,3	0.57	0	3,3,3	0.19	0
5	SO4	A	400	-	4,4,4	0.21	0	6,6,6	0.20	0
3	GOL	B	1200	-	5,5,5	0.37	0	5,5,5	0.63	0
3	GOL	B	1201	-	5,5,5	0.33	0	5,5,5	0.55	0
3	GOL	B	1202	-	5,5,5	0.28	0	5,5,5	0.58	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
6	AGS	B	1006	7	-	3/21/38/38	0/3/3/3
3	GOL	A	500	-	-	2/4/4/4	-
3	GOL	B	1200	-	-	3/4/4/4	-
3	GOL	B	1201	-	-	3/4/4/4	-
3	GOL	B	1202	-	-	0/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1006	AGS	PG-S1G	10.07	2.12	1.90
6	B	1006	AGS	C2-N1	9.67	1.51	1.33
6	B	1006	AGS	C2-N3	8.24	1.48	1.33
6	B	1006	AGS	C8-N7	7.39	1.45	1.31
6	B	1006	AGS	C4-N3	6.64	1.46	1.34
6	B	1006	AGS	C8-N9	6.60	1.48	1.37
6	B	1006	AGS	PB-O3A	5.40	1.65	1.59
6	B	1006	AGS	PB-O3B	5.11	1.65	1.59
6	B	1006	AGS	C5-C4	5.06	1.48	1.39
6	B	1006	AGS	PA-O3A	4.75	1.64	1.59
6	B	1006	AGS	C6-N6	4.52	1.45	1.34
6	B	1006	AGS	C5-N7	4.22	1.46	1.39
6	B	1006	AGS	PA-O1A	3.93	1.64	1.50
6	B	1006	AGS	PB-O1B	3.80	1.64	1.50
6	B	1006	AGS	C5-C6	3.57	1.50	1.41
6	B	1006	AGS	PG-O2G	3.53	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1006	AGS	C6-N1	3.38	1.45	1.35
6	B	1006	AGS	C4-N9	2.86	1.43	1.37
6	B	1006	AGS	PG-O3G	-2.49	1.46	1.54
6	B	1006	AGS	C2'-C3'	-2.27	1.47	1.53
6	B	1006	AGS	PB-O2B	-2.15	1.45	1.55

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1006	AGS	N3-C2-N1	-4.93	121.11	128.58
6	B	1006	AGS	N9-C8-N7	-4.81	107.11	113.94
6	B	1006	AGS	C2'-C1'-N9	-4.50	102.13	113.30
6	B	1006	AGS	O2B-PB-O3B	3.90	117.81	107.27
6	B	1006	AGS	C5-C4-N3	-3.74	121.57	126.72
6	B	1006	AGS	C4-N9-C8	3.15	109.04	105.74
6	B	1006	AGS	C5-N7-C8	3.01	108.18	103.45
6	B	1006	AGS	PB-O3B-PG	-2.79	122.95	133.17
6	B	1006	AGS	C5'-C4'-C3'	-2.70	105.50	115.21
6	B	1006	AGS	O3A-PA-O1A	2.53	118.30	110.70
6	B	1006	AGS	C2-N3-C4	2.49	117.92	111.83
6	B	1006	AGS	C6-C5-C4	2.35	120.39	117.18
6	B	1006	AGS	C4-C5-N7	-2.24	108.02	110.58
6	B	1006	AGS	PA-O5'-C5'	-2.23	108.56	121.35
6	B	1006	AGS	O4'-C4'-C3'	2.16	109.44	105.15
6	B	1006	AGS	N3-C4-N9	2.14	130.80	127.17
6	B	1006	AGS	O2'-C2'-C3'	-2.09	105.13	111.82

There are no chirality outliers.

All (11) torsion outliers are listed below:

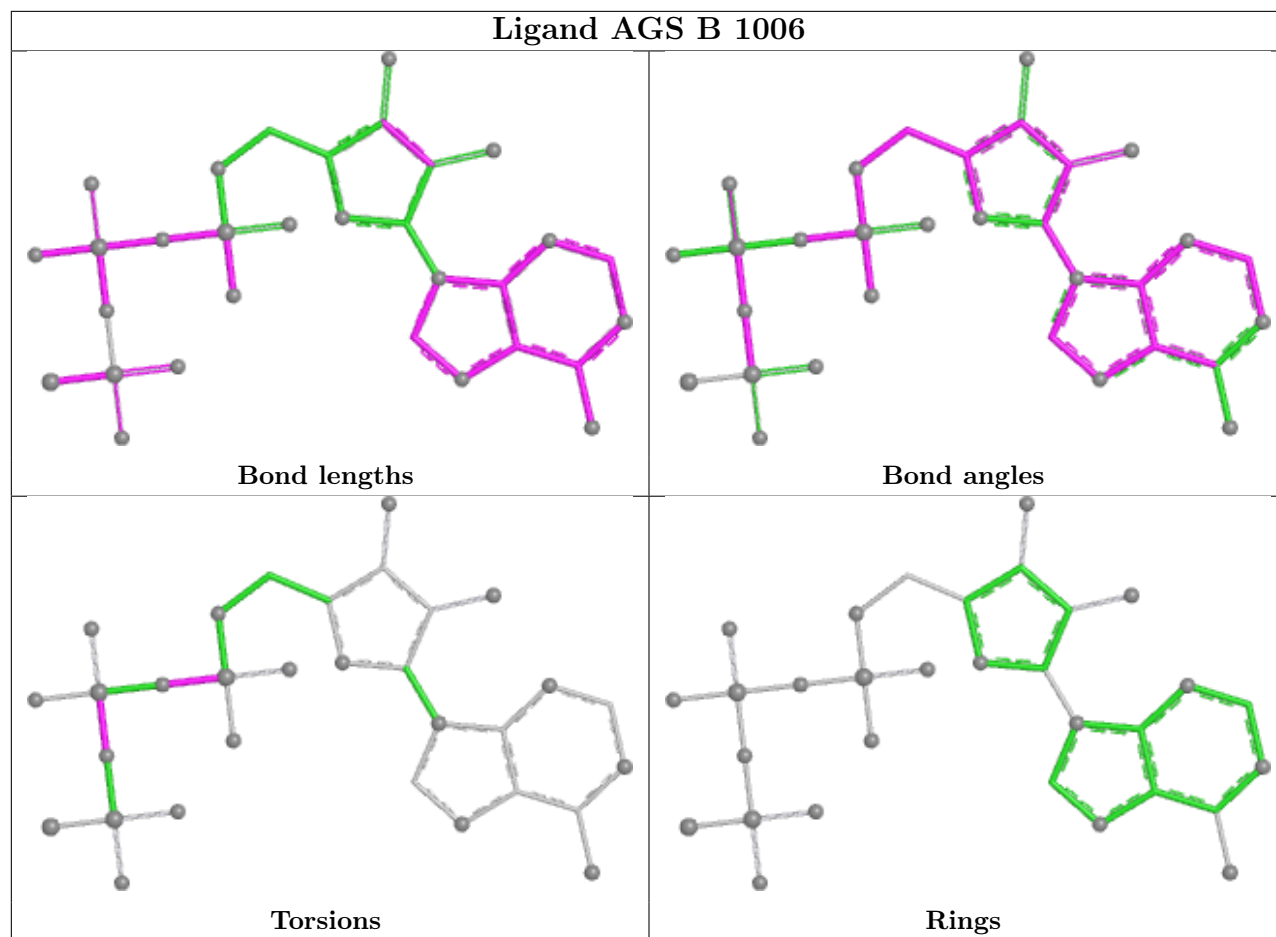
Mol	Chain	Res	Type	Atoms
3	A	500	GOL	O1-C1-C2-C3
3	B	1200	GOL	O1-C1-C2-C3
3	B	1201	GOL	O1-C1-C2-C3
3	B	1201	GOL	C1-C2-C3-O3
3	B	1200	GOL	O1-C1-C2-O2
3	A	500	GOL	O1-C1-C2-O2
3	B	1201	GOL	O1-C1-C2-O2
3	B	1200	GOL	O2-C2-C3-O3
6	B	1006	AGS	PG-O3B-PB-O1B
6	B	1006	AGS	PB-O3A-PA-O1A
6	B	1006	AGS	PB-O3A-PA-O2A

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1006	AGS	3	0
4	A	600	IPA	2	0
3	A	500	GOL	1	0
5	A	400	SO4	1	0
3	B	1201	GOL	6	0
3	B	1202	GOL	6	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 than 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.



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	A	369/386 (95%)	-0.51	0 100 100	57, 96, 147, 191	0
2	B	365/371 (98%)	-0.42	0 100 100	54, 104, 141, 165	0
All	All	734/757 (96%)	-0.47	0 100 100	54, 100, 144, 191	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.

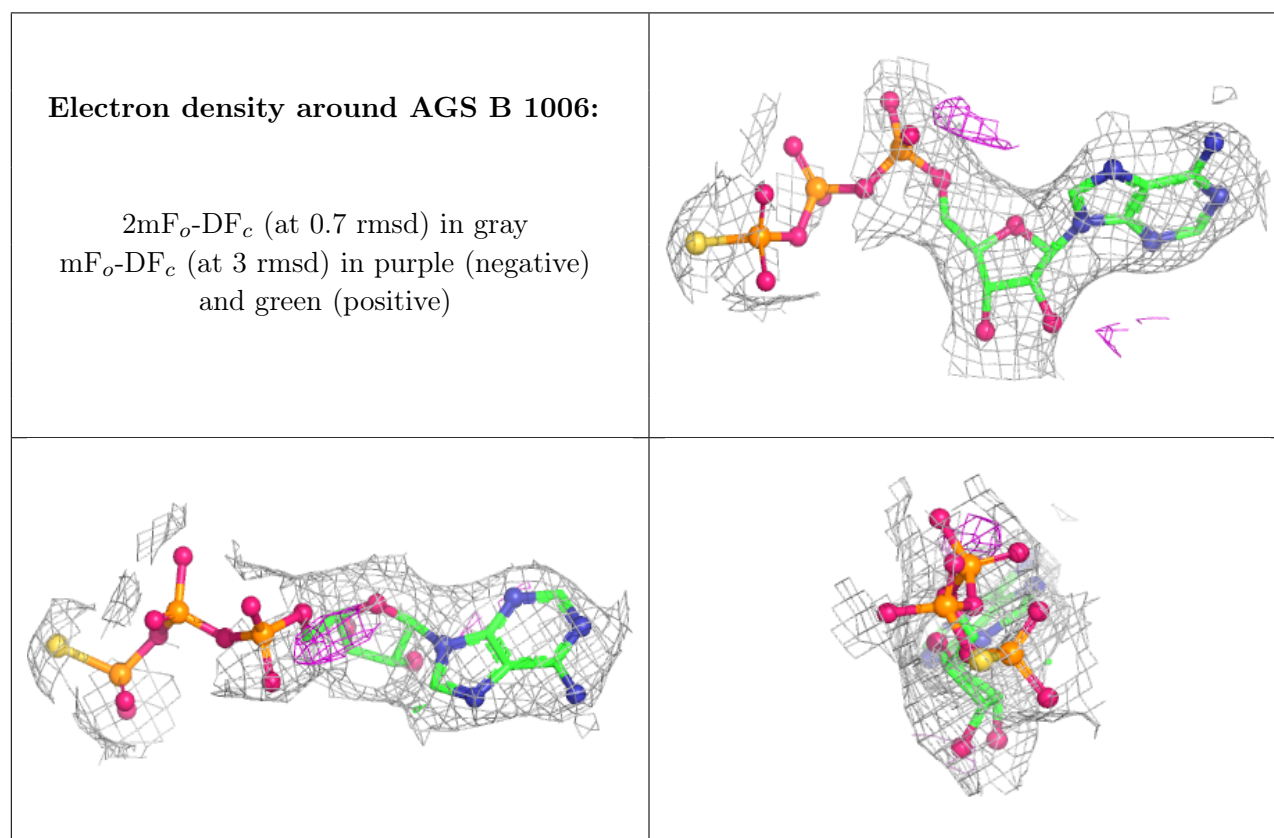
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IPA	B	601	4/4	0.81	0.30	93,100,102,103	0
3	GOL	B	1202	6/6	0.86	0.09	85,86,94,100	0
3	GOL	B	1200	6/6	0.88	0.13	71,91,94,98	0
3	GOL	A	500	6/6	0.90	0.08	74,85,89,95	0
4	IPA	B	1300	4/4	0.90	0.18	68,73,75,82	0
4	IPA	A	600	4/4	0.91	0.14	98,102,104,105	0
3	GOL	B	1201	6/6	0.95	0.09	82,84,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	AGS	B	1006	31/31	0.97	0.06	49,69,76,88	0
7	MG	B	1007	1/1	0.97	0.09	70,70,70,70	0
5	SO4	A	400	5/5	0.98	0.04	84,85,94,94	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.