



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:27 AM GMT

PDB ID : 3AV0  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

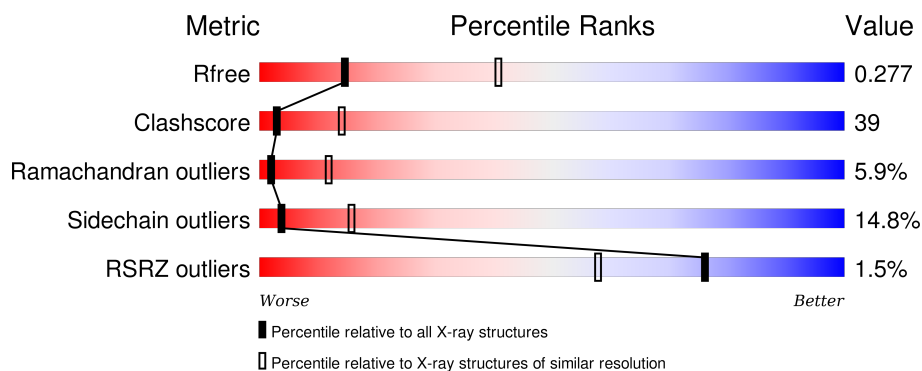
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>39%</div> <div>44%</div> <div>11%</div> <div>..</div> </div>
2	B	371	<div> <div>%</div> <div>34%</div> <div>53%</div> <div>11%</div> <div>..</div> </div>

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.

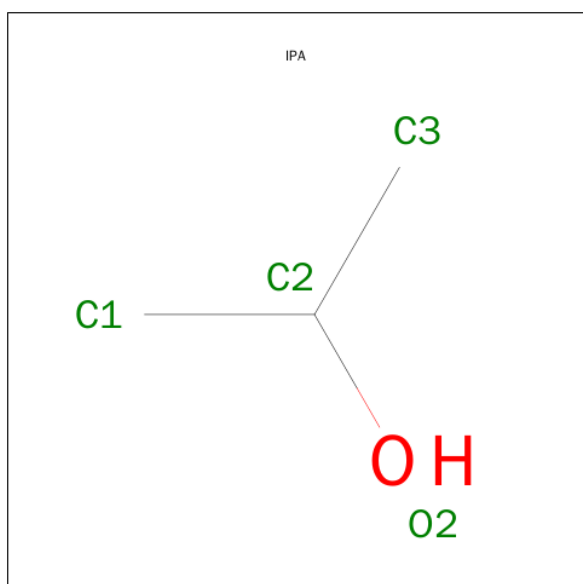
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	365	Total	C	N	O	S	0	0	0
			2937	1883	501	544	9			

- Molecule 3 is GLYCEROL (three-letter code: 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 (three-letter code: IPA) (formula:  $C_3H_8O$ ).



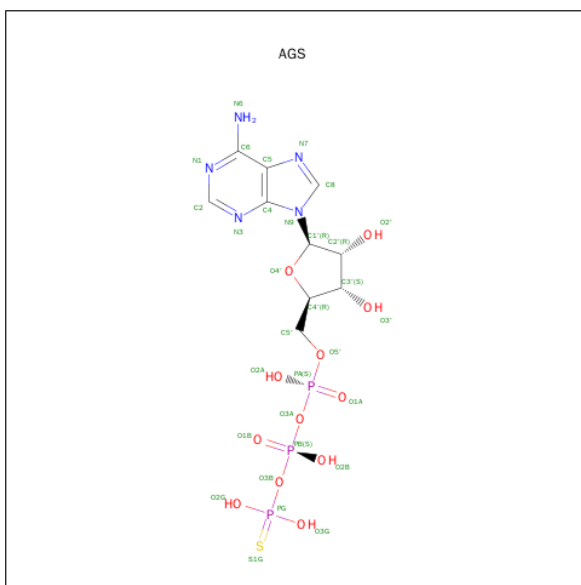
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



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 (three-letter code: MG) (formula: Mg).

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

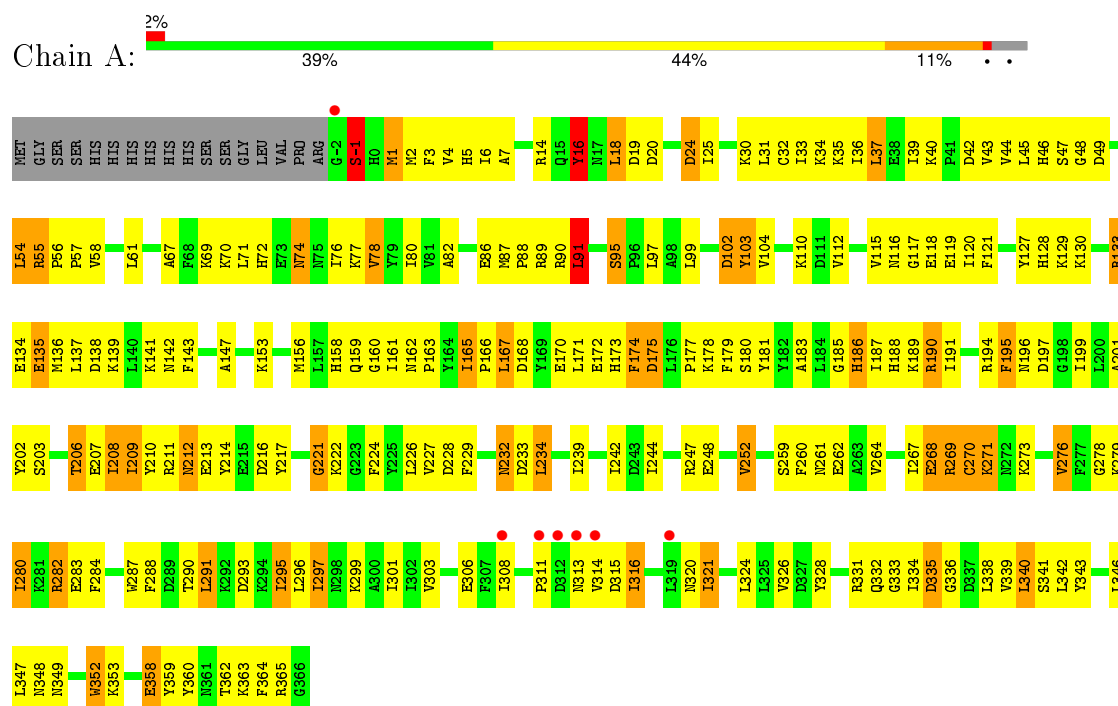
- Molecule 8 is water.

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

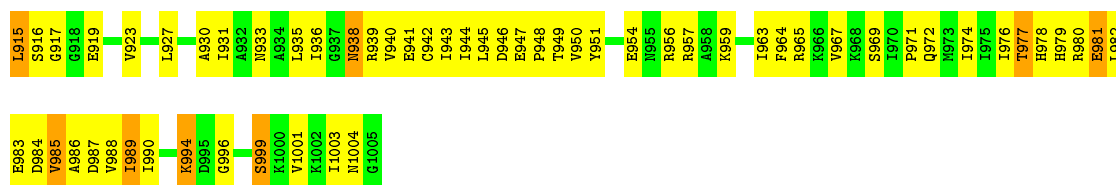
### 3 Residue-property plots

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 double-strand break repair protein mre11







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.96Å 147.13Å 175.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 3.10 46.16 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.32-3.10) 96.1 (46.16-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, $R_{free}$	0.214 , 0.276 0.202 , 0.277	Depositor DCC
$R_{free}$ test set	1960 reflections (9.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.3	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.7	EDS
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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20869 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, IPA, AGS, SO4

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	0.50	0/3128	0.65	0/4203
2	B	0.51	0/2981	0.64	0/3994
All	All	0.51	0/6109	0.64	0/8197

There are no bond length outliers.

There are no bond angle outliers.

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	239	0
2	B	2937	0	3025	263	0
3	A	6	0	8	1	0
3	B	18	0	24	11	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	479	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 39.

All (479) 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:HD2	2:B:67:LYS:H	1.29	0.96
1:A:207:GLU:HG3	1:A:208:ILE:N	1.79	0.95
1:A:133:ARG:HH21	1:A:133:ARG:HG2	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
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: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: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:886:PHE:CD1	2:B:956:ARG:HG3	2.20	0.77
2:B:880:ASN:HD21	2:B:893:VAL:H	1.32	0.77
2:B:911:THR:H	2:B:914:ASN:HD22	1.32	0.76
2:B:12:ASN:C	2:B:63:THR:HG22	2.05	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:892:PHE:HE2	2:B:904:HIS:ND1	1.87	0.73
1:A:288:PHE:O	1:A:291:LEU:HD12	1.89	0.73
2:B:105:ALA:HB1	2:B:110:ALA:HB1	1.70	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
2:B:880:ASN:HD21	2:B:893:VAL:N	1.90	0.69
1:A:46:HIS:HB3	1:A:80:ILE:HG13	1.75	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
2:B:80:ASN:CB	2:B:82:TYR:HE2	2.07	0.67
1:A:121:PHE:CE2	1:A:147:ALA:HB2	2.29	0.67
2:B:861:ASN:H	2:B:861:ASN:HD22	1.42	0.67
2:B:30:ILE:N	2:B:30:ILE:HD12	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
2:B:86:ARG:HG2	2:B:95:ALA:HB2	1.77	0.66
1:A:227:VAL:HG13	1:A:239:ILE:HG12	1.77	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:232:ASN:N	1:A:232:ASN:HD22	1.92	0.66
1:A:4:VAL:HG11	1:A:36:ILE:CD1	2.26	0.66
1:A:133:ARG:CG	1:A:133:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:10:MET:HE2	2:B:16:HIS:CB	2.27	0.65
2:B:121:VAL:HB	2:B:125:MET:HB3	1.79	0.65
2:B:186:LEU:HD12	2:B:837:LEU:HG	1.79	0.64
2:B:74:ASP:OD2	2:B:83:LYS:HE3	1.98	0.64
1:A:308:ILE:O	1:A:308:ILE:HG13	1.97	0.64
2:B:27:ILE:CG2	2:B:986:ALA:HA	2.27	0.64
1:A:347:LEU:C	1:A:349:ASN:H	2.00	0.64
1:A:234:LEU:H	1:A:234:LEU:HD12	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:CD1	2:B:30:ILE:H	2.09	0.63
1:A:112:VAL:CG1	1:A:119:GLU:HG2	2.29	0.62
1:A:4:VAL:HG11	1:A:36:ILE:HD13	1.81	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
2:B:12:ASN:CA	2:B:63:THR:CG2	2.77	0.62
2:B:985:VAL:HG23	2:B:985:VAL:O	1.97	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
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
2:B:89:ASP:O	2:B:90:SER:C	2.38	0.61
2:B:64:LYS:HZ2	3:B:1202:GOL:C1	2.13	0.61
1:A:55:ARG:NH2	2:B:980:ARG:HH11	1.98	0.61
2:B:14:LYS:HB3	6:B:1006:AGS:C5	2.31	0.61
1:A:352:TRP:CE3	2:B:171:ILE:HG12	2.36	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:315:ASP:HB3	2:B:877:LYS:HZ1	1.65	0.61
1:A:172:GLU:O	1:A:175:ASP:HB2	2.01	0.61
2:B:938:ASN:HD22	2:B:938:ASN:N	1.97	0.61
2:B:182:ILE:HD12	2:B:844:LEU:HD12	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:C	1:A:270:CYS:H	2.05	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:39:ILE:O	1:A:39:ILE:HG22	2.01	0.60
1:A:112:VAL:HG13	1:A:120:ILE:O	2.00	0.60
1:A:54:LEU:HD21	1:A:88:PRO:HA	1.83	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:116:ASN:C	1:A:118:GLU:H	2.06	0.59
2:B:877:LYS:O	2:B:881:GLU:HB2	2.01	0.59
1:A:234:LEU:HD12	1:A:234:LEU:N	2.18	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
2:B:941:GLU:O	2:B:971:PRO:HD2	2.02	0.59
2:B:99:LYS:HB3	2:B:102:LYS:O	2.02	0.59
2:B:67:LYS:CD	2:B:68:SER:H	2.16	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
2:B:977:THR:HB	2:B:979:HIS:H	1.69	0.58
2:B:47:PHE:O	2:B:48:ALA:C	2.41	0.58
1:A:166:PRO:HG2	1:A:167:LEU:HD23	1.84	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
1:A:160:GLY:CA	1:A:165:ILE:HD11	2.31	0.57
1:A:31:LEU:HB3	1:A:244:ILE:CD1	2.32	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
2:B:27:ILE:HB	2:B:987:ASP:OD1	2.04	0.57
1:A:74:ASN:N	1:A:74:ASN:HD22	2.01	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:120:ILE:HG22	1:A:121:PHE:N	2.19	0.56
1:A:3:PHE:CE2	1:A:227:VAL:HB	2.40	0.56
2:B:979:HIS:CD2	3:B:1201:GOL:H31	2.41	0.56
1:A:32:CYS:O	1:A:36:ILE:HG13	2.05	0.56
1:A:86:GLU:O	1:A:95:SER:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:162:GLU:HB2	2:B:864:GLN:HE22	1.71	0.56
1:A:283:GLU:HG3	1:A:284:PHE:CD2	2.41	0.56
2:B:978:HIS:HE1	3:B:1201:GOL:O2	1.88	0.56
2:B:30:ILE:CD1	2:B:974:ILE:HG22	2.36	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:340:LEU:O	1:A:343:TYR:HB3	2.06	0.55
1:A:260:PHE:O	1:A:264:VAL:HG23	2.06	0.55
1:A:159:GLN:HB3	1:A:170:GLU:HG2	1.88	0.55
1:A:87:MET:HE3	1:A:88:PRO:HD2	1.88	0.55
1:A:56:PRO:HG2	1:A:61:LEU:HD21	1.88	0.55
2:B:114:ALA:O	2:B:118:ILE:HG13	2.07	0.55
1:A:37:LEU:CD2	1:A:71:LEU:HD23	2.37	0.55
2:B:979:HIS:HA	8:B:1406:HOH:O	2.07	0.55
2:B:897:LYS:HD2	2:B:897:LYS:H	1.71	0.55
1:A:248:GLU:OE1	1:A:271:LYS:HB2	2.06	0.55
2:B:938:ASN:HD22	2:B:938:ASN:H	1.55	0.55
2:B:933:ASN:HD22	2:B:969:SER:CB	2.20	0.55
2:B:974:ILE:H	2:B:974:ILE:HD12	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:87:MET:CE	1:A:88:PRO:HD2	2.37	0.54
1:A:82:ALA:HB2	1:A:97:LEU:HD12	1.89	0.54
1:A:282:ARG:C	1:A:282:ARG:HD3	2.27	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
2:B:14:LYS:O	2:B:63:THR:HB	2.06	0.54
2:B:834:MET:HE2	2:B:838:GLU:HB3	1.90	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:938:ASN:ND2	2:B:938:ASN:N	2.56	0.53
2:B:67:LYS:HD3	2:B:68:SER:OG	2.08	0.53
2:B:30:ILE:HD11	2:B:974:ILE:CG2	2.39	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:900:GLU:HA	2:B:900:GLU:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:HIS:HB3	1:A:80:ILE:CG1	2.38	0.53
2:B:81:ASN:HD22	2:B:81:ASN:C	2.13	0.53
1:A:43:VAL:HG22	1:A:77:LYS:HB3	1.91	0.53
2:B:131:TYR:C	2:B:131:TYR:CD1	2.81	0.52
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
2:B:22:LYS:H	2:B:1003:ILE:HD11	1.74	0.52
1:A:162:ASN:ND2	1:A:172:GLU:OE1	2.43	0.52
1:A:69:LYS:HG3	1:A:103:TYR:CE2	2.39	0.52
2:B:9:ARG:HG2	2:B:20:ARG:HD3	1.92	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: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
2:B:141:LEU:HD13	2:B:912:ILE:HG21	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
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
1:A:2:MET:HE1	1:A:226:LEU:HG	1.93	0.51
2:B:169:GLY:O	2:B:173:LYS:HG3	2.11	0.51
1:A:260:PHE:O	1:A:260:PHE:CD2	2.64	0.51
1:A:364:PHE:HE2	2:B:847:PHE:HA	1.76	0.51
1:A:321:ILE:HD12	1:A:321:ILE:N	2.26	0.51
1:A:165:ILE:HG12	1:A:187:ILE:CD1	2.26	0.51
2:B:189:LYS:HZ1	2:B:832:LYS:HE2	1.74	0.51
2:B:36:SER:O	2:B:999:SER:HB2	2.11	0.50
2:B:897:LYS:HB2	2:B:898:ASP:OD1	2.11	0.50
1:A:55:ARG:NH2	2:B:980:ARG:NH1	2.58	0.50
1:A:147:ALA:HB1	1:A:153:LYS:HE2	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLY:O	1:A:186:HIS:CB	2.59	0.50
2:B:104:TYR:O	2:B:104:TYR:CD1	2.64	0.50
1:A:191:ILE:HB	1:A:202:TYR:HB2	1.92	0.50
2:B:28:VAL:HG12	2:B:974:ILE:HG23	1.95	0.49
2:B:6:LYS:N	2:B:74:ASP:O	2.41	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
2:B:912:ILE:HD12	2:B:913:ASP:N	2.27	0.48
2:B:897:LYS:HD2	2:B:897:LYS:N	2.28	0.48
1:A:199:ILE:HG21	1:A:239:ILE:CD1	2.43	0.48
1:A:260:PHE:C	1:A:260:PHE:CD2	2.86	0.48
1:A:347:LEU:C	1:A:349:ASN:N	2.66	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
2:B:174:GLU:C	2:B:176:GLU:H	2.17	0.48
2:B:156:LEU:HD13	2:B:871:TYR:CD1	2.48	0.48
2:B:124:ASN:N	2:B:124:ASN:ND2	2.61	0.48
2:B:8:ILE:HG13	2:B:73:LEU:HB2	1.95	0.48
2:B:95:ALA:O	2:B:111:VAL:HG21	2.14	0.48
2:B:1:MET:HG2	2:B:1:MET:O	2.13	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:ND2	1:A:232:ASN:N	2.59	0.48
2:B:10:MET:HE2	2:B:16:HIS:HB2	1.96	0.48
1:A:363:LYS:HA	1:A:365:ARG:HH12	1.79	0.48
2:B:9:ARG:HD2	2:B:72:GLU:OE1	2.14	0.47
1:A:161:ILE:HG13	1:A:171:LEU:HB2	1.96	0.47
2:B:942:CYS:CB	2:B:972:GLN:HB3	2.37	0.47
1:A:288:PHE:C	1:A:290:THR:N	2.67	0.47
2:B:111:VAL:O	2:B:115:VAL:HG23	2.13	0.47
1:A:364:PHE:CD2	2:B:847:PHE:HD2	2.33	0.47
1:A:90:ARG:O	1:A:91:LEU:C	2.52	0.47
2:B:174:GLU:HA	2:B:177:LYS:CE	2.34	0.47
1:A:326:VAL:HG21	1:A:340:LEU:HD12	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HE2	3:A:500:GOL:O2	2.14	0.47
1:A:162:ASN:HB3	1:A:163:PRO:HD3	1.96	0.47
1:A:134:GLU:C	1:A:136:MET:N	2.68	0.47
2:B:64:LYS:HA	3:B:1202:GOL:H12	1.97	0.47
1:A:70:LYS:O	1:A:71:LEU:C	2.52	0.47
1:A:259:SER:O	1:A:261:ASN:N	2.47	0.47
2:B:896:THR:HG23	2:B:900:GLU:O	2.14	0.47
1:A:158:HIS:O	1:A:158:HIS:CD2	2.67	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
2:B:107:THR:O	2:B:108:ILE:C	2.53	0.47
2:B:161:PHE:CE2	2:B:863:PHE:CE2	3.02	0.46
2:B:189:LYS:HD2	2:B:189:LYS:HA	1.62	0.46
2:B:872:VAL:O	2:B:873:PRO:C	2.52	0.46
2:B:38:LYS:HB3	2:B:976:ILE:CG2	2.45	0.46
2:B:66:LYS:O	3:B:1202:GOL:H31	2.16	0.46
2:B:8:ILE:HG13	2:B:73:LEU:CB	2.45	0.46
1:A:326:VAL:HG23	1:A:340:LEU:HD12	1.98	0.46
1:A:6:ILE:HG13	1:A:224:PHE:HB3	1.96	0.46
2:B:876:GLN:O	2:B:877:LYS:C	2.54	0.46
1:A:267:ILE:O	1:A:270:CYS:HB2	2.15	0.46
1:A:77:LYS:NZ	8:A:711:HOH:O	2.48	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
2:B:947:GLU:N	2:B:948:PRO:HD3	2.31	0.46
1:A:232:ASN:H	1:A:232:ASN:HD22	1.62	0.46
1:A:35:LYS:O	1:A:39:ILE:HG13	2.15	0.46
2:B:60:THR:O	6:B:1006:AGS:N6	2.48	0.46
2:B:28:VAL:CB	2:B:974:ILE:HG23	2.45	0.46
2:B:64:LYS:NZ	3:B:1202:GOL:H12	2.31	0.46
1:A:352:TRP:O	1:A:353:LYS:C	2.53	0.46
2:B:175:TYR:CD1	2:B:847:PHE:HE1	2.34	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:158:HIS:CG	1:A:158:HIS:O	2.69	0.45
1:A:48:GLY:O	1:A:49:ASP:HB2	2.16	0.45
2:B:116:ASN:N	2:B:116:ASN:HD22	2.14	0.45
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.71	0.45
1:A:338:LEU:O	1:A:341:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:LEU:O	2:B:179:LEU:HD22	2.16	0.45
1:A:282:ARG:NH2	2:B:907:ASN:OD1	2.49	0.45
1:A:129:LYS:HE3	2:B:986:ALA:O	2.17	0.45
1:A:162:ASN:HD22	1:A:172:GLU:CD	2.20	0.45
1:A:1:MET:HA	1:A:42:ASP:OD2	2.16	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
1:A:212:ASN:H	1:A:212:ASN:ND2	2.15	0.45
2:B:916:SER:O	2:B:917:GLY:C	2.54	0.45
2:B:852:ASP:C	2:B:854:VAL:H	2.20	0.45
2:B:118:ILE:HG22	2:B:118:ILE:O	2.16	0.45
1:A:39:ILE:O	1:A:39:ILE:CG2	2.65	0.45
2:B:47:PHE:CD1	2:B:51:GLY:HA2	2.52	0.45
1:A:308:ILE:O	1:A:308:ILE:CG1	2.61	0.45
2:B:81:ASN:ND2	2:B:81:ASN:C	2.71	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:268:GLU:C	1:A:270:CYS:N	2.70	0.45
1:A:163:PRO:HG3	1:A:173:HIS:ND1	2.32	0.44
2:B:28:VAL:HB	2:B:974:ILE:CA	2.41	0.44
1:A:252:VAL:HG13	1:A:276:VAL:HG23	1.98	0.44
1:A:57:PRO:O	1:A:58:VAL:C	2.55	0.44
1:A:316:ILE:HG22	1:A:316:ILE:O	2.17	0.44
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.51	0.44
1:A:195:PHE:CD1	1:A:196:ASN:HB2	2.52	0.44
2:B:82:TYR:N	2:B:82:TYR:CD2	2.86	0.44
1:A:259:SER:C	1:A:261:ASN:N	2.69	0.44
1:A:14:ARG:NH2	1:A:19:ASP:OD2	2.40	0.44
1:A:343:TYR:CE1	1:A:347:LEU:HD11	2.53	0.44
1:A:333:GLY:C	1:A:334:ILE:HD12	2.38	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
2:B:857:ILE:O	2:B:857:ILE:HG22	2.18	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
1:A:130:LYS:HD3	1:A:170:GLU:HA	1.99	0.44
1:A:46:HIS:O	1:A:80:ILE:HG13	2.18	0.44
1:A:190:ARG:NE	1:A:221:GLY:O	2.50	0.44
1:A:128:HIS:HB2	1:A:136:MET:HE2	1.98	0.44
1:A:352:TRP:CZ3	2:B:171:ILE:HG12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:SER:HA	2:B:940:VAL:O	2.18	0.44
2:B:64:LYS:HZ2	3:B:1202:GOL:H11	1.81	0.44
2:B:24:GLU:O	2:B:28:VAL:HG22	2.18	0.44
1:A:232:ASN:H	1:A:232:ASN:ND2	2.15	0.43
2:B:852:ASP:O	2:B:855:ARG:N	2.51	0.43
1:A:89:ARG:HH11	1:A:129:LYS:HE2	1.82	0.43
2:B:108:ILE:HG13	2:B:108:ILE:H	1.45	0.43
2:B:971:PRO:HG2	2:B:972:GLN:H	1.83	0.43
1:A:336:GLY:HA2	1:A:339:VAL:HG12	1.99	0.43
1:A:259:SER:O	1:A:260:PHE:C	2.56	0.43
1:A:191:ILE:O	1:A:201:ALA:HA	2.17	0.43
2:B:872:VAL:HB	2:B:873:PRO:HD3	2.00	0.43
2:B:179:LEU:HD13	2:B:179:LEU:C	2.39	0.43
1:A:332:GLN:OE1	2:B:856:ARG:NH2	2.51	0.43
2:B:12:ASN:O	2:B:63:THR:HG22	2.19	0.43
2:B:27:ILE:HB	2:B:987:ASP:H	1.82	0.43
1:A:139:LYS:HZ1	4:A:600:IPA:H11	1.82	0.43
2:B:50:PHE:O	2:B:51:GLY:C	2.56	0.43
2:B:82:TYR:N	2:B:82:TYR:HD2	2.16	0.43
2:B:20:ARG:C	2:B:21:ILE:HG13	2.38	0.43
2:B:965:ARG:HD3	2:B:965:ARG:HA	1.85	0.43
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.75	0.43
1:A:24:ASP:OD2	1:A:247:ARG:HB2	2.18	0.43
2:B:118:ILE:O	2:B:119:LEU:HD23	2.18	0.43
2:B:6:LYS:HD2	2:B:76:GLU:CG	2.48	0.43
2:B:36:SER:HA	2:B:994:LYS:HB2	2.01	0.43
1:A:247:ARG:HA	1:A:247:ARG:HD3	1.80	0.43
1:A:340:LEU:CD2	1:A:340:LEU:C	2.87	0.43
2:B:170:GLU:HA	2:B:173:LYS:HD2	2.01	0.43
1:A:54:LEU:HD11	1:A:87:MET:O	2.19	0.43
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: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
1:A:276:VAL:CG1	1:A:295:ILE:HG13	2.49	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
1:A:46:HIS:O	1:A:80:ILE:HA	2.18	0.42
1:A:7:ALA:HB2	1:A:47:SER:HB2	2.01	0.42
1:A:134:GLU:C	1:A:136:MET:H	2.23	0.42
2:B:63:THR:HG23	2:B:66:LYS:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:LEU:HD21	1:A:297:ILE:HG13	2.01	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
2:B:892:PHE:HE2	2:B:904:HIS:CE1	2.38	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: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
1:A:358:GLU:O	1:A:359:TYR:C	2.56	0.42
1:A:178:LYS:HG2	1:A:196:ASN:HB3	2.01	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
2:B:139:LYS:O	2:B:140:PHE:C	2.58	0.42
1:A:133:ARG:CG	1:A:133:ARG:NH2	2.70	0.41
1:A:347:LEU:O	1:A:349:ASN:N	2.53	0.41
1:A:167:LEU:H	1:A:167:LEU:HD23	1.85	0.41
1:A:208:ILE:HG12	1:A:208:ILE:H	1.48	0.41
1:A:134:GLU:O	1:A:136:MET:N	2.53	0.41
2:B:912:ILE:HA	2:B:915:LEU:HD12	2.02	0.41
2:B:181:ARG:HD2	2:B:181:ARG:HA	1.86	0.41
2:B:34:ASN:HD22	2:B:34:ASN:HA	1.66	0.41
1:A:206:THR:O	1:A:206:THR:CG2	2.68	0.41
2:B:62:ILE:HG12	2:B:69:VAL:CG1	2.49	0.41
1:A:301:ILE:HG23	2:B:891:SER:HA	2.03	0.41
2:B:945:LEU:HB3	2:B:948:PRO:HG3	2.02	0.41
1:A:166:PRO:HD2	1:A:167:LEU:CD2	2.48	0.41
2:B:954:GLU:H	2:B:954:GLU:CD	2.23	0.41
1:A:282:ARG:NH2	2:B:907:ASN:CB	2.73	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:29:ALA:O	2:B:31:ILE:CD1	2.68	0.41
2:B:896:THR:CG2	2:B:900:GLU:HB2	2.49	0.41
1:A:320:ASN:O	1:A:321:ILE:C	2.58	0.41
1:A:141:LYS:O	1:A:142:ASN:C	2.58	0.41
1:A:115:VAL:CG1	1:A:116:ASN:HD22	2.33	0.41
1:A:1:MET:HB3	1:A:115:VAL:HG12	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:O	1:A:180:SER:HB2	2.20	0.41
2:B:39:SER:HB3	8:B:1401:HOH:O	2.19	0.41
1:A:20:ASP:O	1:A:24:ASP:OD1	2.39	0.41
2:B:174:GLU:CA	2:B:177:LYS:HE2	2.36	0.41
2:B:51:GLY:O	2:B:52:ALA:C	2.59	0.41
2:B:97:LEU:O	2:B:103:PRO:HA	2.21	0.41
1:A:340:LEU:HD23	1:A:340:LEU:C	2.41	0.41
1:A:55:ARG:NH2	2:B:980:ARG:HD2	2.35	0.41
1:A:14:ARG:O	1:A:14:ARG:HG2	2.21	0.41
1:A:137:LEU:HD21	1:A:175:ASP:OD2	2.20	0.41
1:A:142:ASN:O	1:A:143:PHE:C	2.58	0.41
2:B:67:LYS:CD	2:B:68:SER:N	2.81	0.41
1:A:2:MET:O	1:A:42:ASP:N	2.45	0.41
1:A:2:MET:HE2	1:A:228:ASP:CA	2.51	0.41
2:B:911:THR:C	2:B:913:ASP:N	2.74	0.41
1:A:5:HIS:CD2	1:A:183:ALA:HB1	2.56	0.41
1:A:133:ARG:O	1:A:136:MET:HB3	2.21	0.41
1:A:39:ILE:O	1:A:40:LYS:C	2.58	0.41
2:B:168:MET:O	2:B:172:VAL:HG23	2.21	0.40
2:B:105:ALA:O	2:B:111:VAL:HG22	2.21	0.40
2:B:167:LYS:HA	2:B:167:LYS:HD2	1.92	0.40
1:A:163:PRO:HG2	1:A:173:HIS:HB3	2.02	0.40
2:B:144:LYS:HA	2:B:145:PRO:HD3	1.90	0.40
2:B:125:MET:HE3	2:B:154:LYS:HD2	2.04	0.40
1:A:363:LYS:HA	1:A:365:ARG:NH1	2.36	0.40
2:B:946:ASP:CG	8:B:1401:HOH:O	2.60	0.40
1:A:278:GLY:O	1:A:301:ILE:HD12	2.20	0.40
1:A:116:ASN:C	1:A:118:GLU:N	2.70	0.40
2:B:186:LEU:HD12	2:B:837:LEU:CG	2.49	0.40
1:A:102:ASP:C	1:A:103:TYR:CD1	2.95	0.40
2:B:69:VAL:O	2:B:87:GLU:HA	2.21	0.40
1:A:45:LEU:HD22	1:A:156:MET:SD	2.62	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%)	2	14
2	B	361/371 (97%)	279 (77%)	59 (16%)	23 (6%)	2	10
All	All	728/757 (96%)	569 (78%)	116 (16%)	43 (6%)	2	12

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
2	B	54	SER
2	B	122	ASP
2	B	853	LYS
2	B	984	ASP
1	A	195	PHE
1	A	271	LYS

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Mol	Chain	Res	Type
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%)	286 (85%)	51 (15%)	3	15
2	B	319/324 (98%)	273 (86%)	46 (14%)	4	17
All	All	656/676 (97%)	559 (85%)	97 (15%)	4	16

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	1	MET
1	A	16	TYR
1	A	18	LEU
1	A	24	ASP
1	A	25	ILE
1	A	37	LEU
1	A	54	LEU
1	A	55	ARG
1	A	72	HIS
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	78	VAL
1	A	91	LEU
1	A	95	SER
1	A	102	ASP
1	A	110	LYS
1	A	133	ARG
1	A	135	GLU
1	A	138	ASP
1	A	165	ILE
1	A	167	LEU
1	A	174	PHE
1	A	175	ASP
1	A	189	LYS
1	A	190	ARG
1	A	197	ASP
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	229	PHE
1	A	232	ASN
1	A	234	LEU
1	A	252	VAL
1	A	262	GLU
1	A	268	GLU
1	A	270	CYS
1	A	276	VAL
1	A	282	ARG
1	A	291	LEU
1	A	295	ILE
1	A	297	ILE
1	A	303	VAL
1	A	306	GLU
1	A	313	ASN
1	A	314	VAL
1	A	321	ILE
1	A	340	LEU
1	A	352	TRP
2	B	3	MET
2	B	11	ASN

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Mol	Chain	Res	Type
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	67	LYS
2	B	68	SER
2	B	69	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	131	TYR
2	B	150	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
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	914	ASN
2	B	923	VAL
2	B	935	LEU
2	B	936	ILE
2	B	938	ASN
2	B	943	ILE
2	B	944	ILE
2	B	977	THR
2	B	985	VAL

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Mol	Chain	Res	Type
2	B	994	LYS
2	B	999	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	74	ASN
1	A	162	ASN
1	A	173	HIS
1	A	212	ASN
1	A	232	ASN
1	A	253	ASN
1	A	361	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
2	B	1004	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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
5	SO4	A	400	-	4,4,4	0.26	0	6,6,6	0.18	0
3	GOL	A	500	-	5,5,5	0.29	0	5,5,5	0.52	0
4	IPA	A	600	-	3,3,3	0.59	0	3,3,3	0.23	0
6	AGS	B	1006	7	24,33,33	4.53	15 (62%)	28,52,52	2.90	9 (32%)
3	GOL	B	1200	-	5,5,5	0.29	0	5,5,5	0.65	0
3	GOL	B	1201	-	5,5,5	0.30	0	5,5,5	0.48	0
3	GOL	B	1202	-	5,5,5	0.26	0	5,5,5	0.51	0
4	IPA	B	1300	-	3,3,3	0.65	0	3,3,3	0.39	0
4	IPA	B	601	-	3,3,3	0.58	0	3,3,3	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	400	-	-	0/0/0/0	0/0/0/0
3	GOL	A	500	-	-	0/4/4/4	0/0/0/0
4	IPA	A	600	-	-	0/0/0/0	0/0/0/0
6	AGS	B	1006	7	-	0/15/38/38	0/3/3/3
3	GOL	B	1200	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1201	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1202	-	-	0/4/4/4	0/0/0/0
4	IPA	B	1300	-	-	0/0/0/0	0/0/0/0
4	IPA	B	601	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1006	AGS	PG-O3G	-2.45	1.46	1.55
6	B	1006	AGS	C2'-C3'	-2.27	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1006	AGS	PB-O2B	-2.24	1.45	1.54
6	B	1006	AGS	C5-N7	2.17	1.46	1.39
6	B	1006	AGS	PG-O2G	3.15	1.66	1.55
6	B	1006	AGS	C5-C4	3.37	1.48	1.40
6	B	1006	AGS	C6-N6	3.50	1.45	1.34
6	B	1006	AGS	PB-O1B	3.51	1.64	1.51
6	B	1006	AGS	PA-O1A	3.63	1.64	1.51
6	B	1006	AGS	O4'-C1'	3.82	1.46	1.41
6	B	1006	AGS	C8-N7	5.87	1.45	1.34
6	B	1006	AGS	C4-N3	7.56	1.46	1.35
6	B	1006	AGS	C2-N1	9.05	1.51	1.33
6	B	1006	AGS	C2-N3	9.27	1.48	1.32
6	B	1006	AGS	PG-S1G	11.29	2.12	1.90

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1006	AGS	N3-C2-N1	-10.16	121.11	128.89
6	B	1006	AGS	C2'-C1'-N9	-7.96	102.13	114.29
6	B	1006	AGS	C4'-O4'-C1'	-3.54	105.83	109.72
6	B	1006	AGS	PB-O3B-PG	-2.90	122.95	132.67
6	B	1006	AGS	C5'-C4'-C3'	-2.45	105.50	115.21
6	B	1006	AGS	PA-O3A-PB	-2.26	126.39	132.73
6	B	1006	AGS	O2'-C2'-C3'	-2.06	105.13	111.83
6	B	1006	AGS	O4'-C4'-C3'	2.13	109.44	105.15
6	B	1006	AGS	O2B-PB-O3B	2.80	117.81	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

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

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	369/386 (95%)	-0.02	7 (1%) 70 48	57, 96, 147, 191	0
2	B	365/371 (98%)	0.05	4 (1%) 82 66	54, 104, 141, 165	0
All	All	734/757 (96%)	0.02	11 (1%) 76 58	54, 100, 144, 191	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	ASP	4.4
1	A	314	VAL	3.3
2	B	98	TYR	3.3
1	A	-2	GLY	2.9
1	A	308	ILE	2.8
1	A	313	ASN	2.8
1	A	311	PRO	2.4
2	B	899	PHE	2.4
2	B	189	LYS	2.2
1	A	319	LEU	2.1
2	B	831	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	B	1007	1/1	0.95	0.28	1.92	70,70,70,70	0
3	GOL	B	1200	6/6	0.83	0.32	1.68	71,91,94,98	0
4	IPA	B	1300	4/4	0.90	0.26	0.91	68,73,75,82	0
3	GOL	B	1202	6/6	0.90	0.17	0.08	85,86,94,100	0
6	AGS	B	1006	31/31	0.98	0.20	-0.25	49,69,76,88	0
5	SO4	A	400	5/5	0.98	0.21	-1.16	84,85,94,94	0
3	GOL	B	1201	6/6	0.95	0.23	-2.29	82,84,86,89	0
4	IPA	A	600	4/4	0.93	0.35	-	98,102,104,105	0
3	GOL	A	500	6/6	0.95	0.18	-	74,85,89,95	0
4	IPA	B	601	4/4	0.88	0.26	-	93,100,102,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.