



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 PM GMT

PDB ID : 4IA5  
Title : Hydratase from Lactobacillus acidophilus - SeMet derivative (apo LAH)  
Authors : Khoshnevis, S.; Neumann, P.; Ficner, R.  
Deposited on : 2012-12-06  
Resolution : 2.22 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

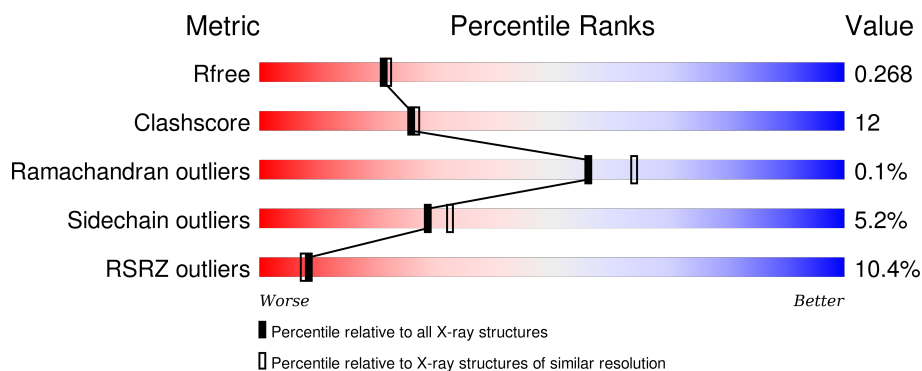
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	591	
1	B	591	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	A	604	-	-	-	X
4	MPD	A	605	-	-	-	X
4	MPD	A	606	-	-	-	X
4	MPD	B	604	-	-	-	X
4	MPD	B	605	-	-	-	X
5	NA	B	601	-	-	-	X
7	GOL	B	606	-	-	-	X
7	GOL	B	607	-	-	-	X
7	GOL	B	608	-	-	X	-

## 2 Entry composition [i](#)

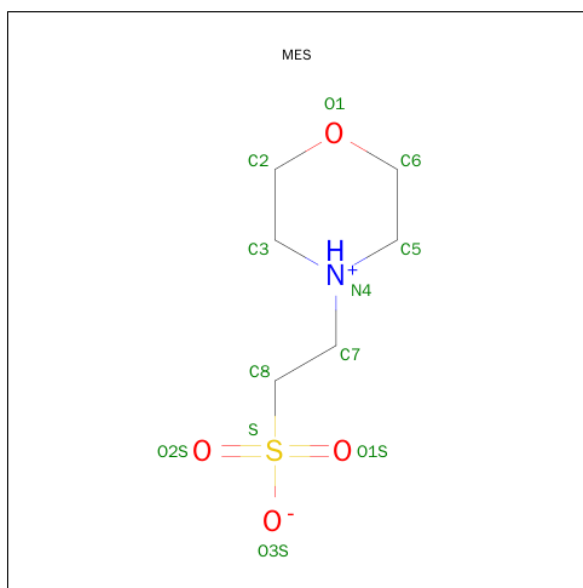
There are 8 unique types of molecules in this entry. The entry contains 9939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myosin-crossreactive antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	Se	0	0	0
			4679	2992	771	892	6	18			
1	B	579	Total	C	N	O	S	Se	0	1	0
			4696	3002	774	895	6	19			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

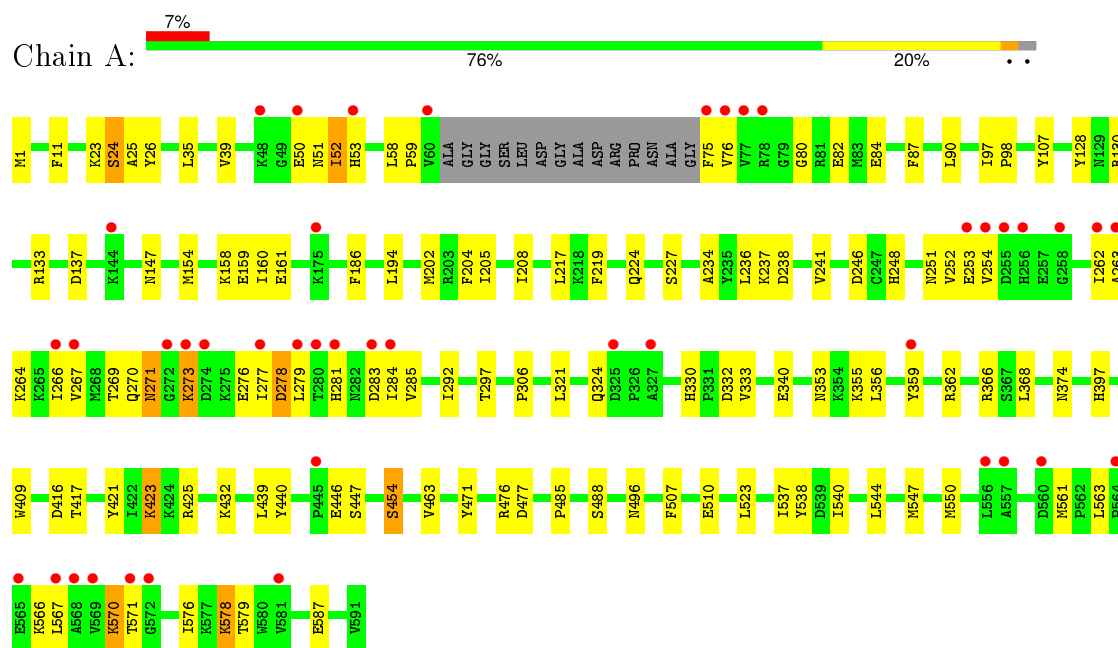
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	209	Total 209	O 209	0	0
8	B	264	Total 265	O 265	0	1

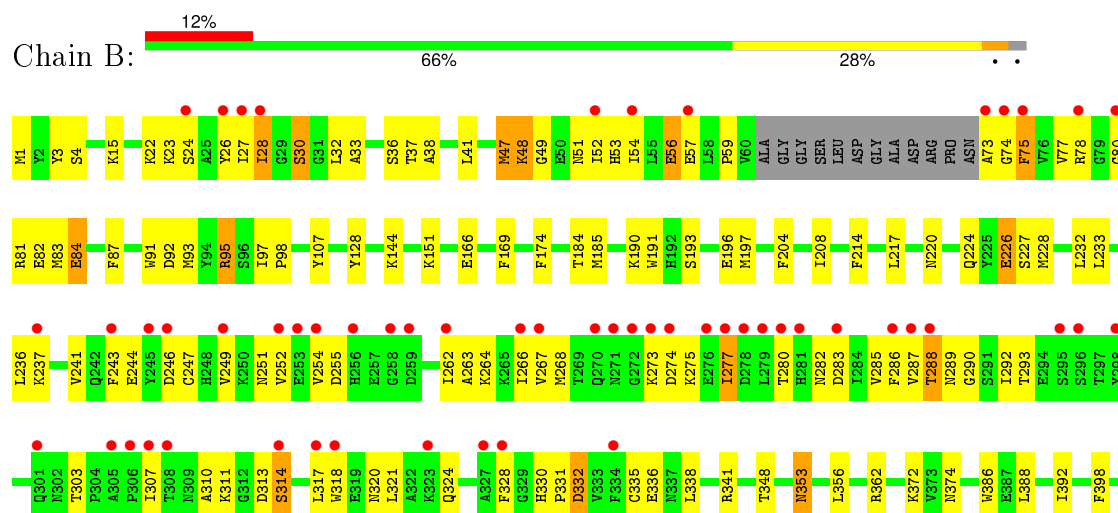
### 3 Residue-property plots

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.

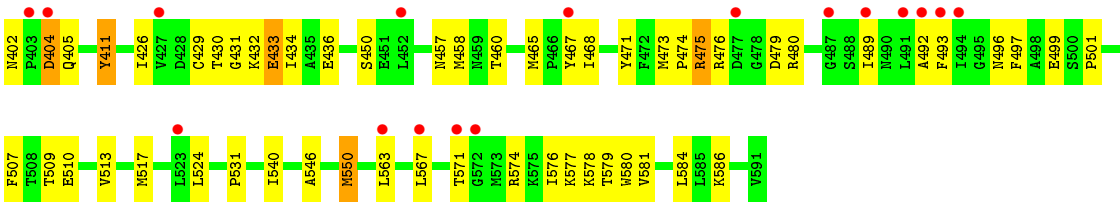
#### • Molecule 1: Myosin-crossreactive antigen



#### • Molecule 1: Myosin-crossreactive antigen







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.75Å 78.97Å 108.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.79 – 2.22 45.82 – 2.22	Depositor EDS
% Data completeness (in resolution range)	88.4 (44.79-2.22) 92.9 (45.82-2.22)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 2.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.214 , 0.259 0.233 , 0.268	Depositor DCC
$R_{free}$ test set	3370 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 57.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 67437 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, MPD, NA, PO4, MES, K

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	0.36	0/4781	0.54	0/6448
1	B	0.40	0/4798	0.61	0/6470
All	All	0.38	0/9579	0.57	0/12918

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	4679	0	4543	88	0
1	B	4696	0	4558	145	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	2	0	0	0	0
4	A	24	0	42	5	0
4	B	16	0	28	6	0
5	B	1	0	0	0	0
6	B	5	0	0	0	0
7	B	18	0	24	5	0
8	A	209	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	265	0	0	10	0
All	All	9939	0	9219	232	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 12.

All (232) 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:52:ILE:HB	1:A:241:VAL:HG23	1.57	0.87
1:B:47[A]:MSE:HE3	1:B:524:LEU:HD11	1.63	0.81
1:A:186:PHE:HE1	4:A:604:MPD:H31	1.46	0.81
1:B:28:ILE:HD11	1:B:287:VAL:HG22	1.63	0.80
1:B:266:ILE:HB	1:B:277:ILE:HG13	1.65	0.78
1:B:429:CYS:HB3	1:B:433:GLU:HB2	1.64	0.77
1:B:36:SER:HB3	1:B:93:MSE:HE1	1.69	0.75
1:A:23:LYS:O	1:A:51:ASN:ND2	2.20	0.73
1:A:158:LYS:NZ	1:A:477:ASP:OD2	2.19	0.72
1:B:92:ASP:O	1:B:95:ARG:HG3	1.90	0.71
1:B:196:GLU:OE1	1:B:475:ARG:NH2	2.24	0.71
1:A:236:LEU:HB3	1:A:241:VAL:HG11	1.73	0.71
1:B:49:GLY:HA2	1:B:52:ILE:HD12	1.73	0.71
1:B:249:VAL:HA	1:B:268:MSE:HB2	1.70	0.71
1:B:41:LEU:HB3	1:B:47[B]:MSE:HE2	1.73	0.70
1:B:290:GLY:H	1:B:314:SER:HB3	1.56	0.70
1:B:338:LEU:HG	1:B:473:MSE:HE3	1.74	0.70
1:B:47[B]:MSE:HE3	1:B:52:ILE:HG12	1.73	0.69
1:B:252:VAL:HG22	1:B:266:ILE:HG12	1.73	0.69
1:B:411:TYR:HB2	4:B:604:MPD:H11	1.73	0.69
1:B:266:ILE:HD11	1:B:285:VAL:HG21	1.75	0.68
1:B:236:LEU:HD23	1:B:241:VAL:HG21	1.75	0.68
1:B:479:ASP:O	8:B:961:HOH:O	2.14	0.65
1:A:26:TYR:HB2	1:A:285:VAL:HG22	1.79	0.64
1:A:359:TYR:O	1:A:362:ARG:HG2	1.97	0.64
1:B:208:ILE:HG21	1:B:546:ALA:HA	1.80	0.64
1:B:251:ASN:OD1	1:B:252:VAL:N	2.31	0.63
1:B:307:ILE:O	7:B:608:GOL:H31	1.99	0.62
1:A:538:TYR:HD1	1:B:540:ILE:HD11	1.63	0.61
1:B:540:ILE:HD13	1:B:584:LEU:HD13	1.82	0.61
1:B:228:MSE:HE1	1:B:509:THR:HG21	1.82	0.61
1:B:26:TYR:HB2	1:B:285:VAL:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASP:O	1:B:317:LEU:HG	2.01	0.61
1:B:52:ILE:HB	1:B:241:VAL:HG13	1.82	0.61
1:A:254:VAL:H	1:A:324:GLN:HE22	1.49	0.61
1:A:82:GLU:OE2	4:A:604:MPD:O2	2.18	0.60
1:A:82:GLU:HG3	1:A:217:LEU:HD22	1.82	0.60
1:B:41:LEU:HD13	1:B:47[B]:MSE:HE1	1.83	0.60
1:A:366:ARG:NH1	1:A:374:ASN:O	2.31	0.60
1:B:303:THR:N	1:B:430:THR:OG1	2.35	0.59
1:A:154:MSE:HE3	1:B:579:THR:HG21	1.84	0.59
1:A:566:LYS:O	1:A:570:LYS:HG2	2.03	0.59
1:A:340:GLU:OE2	1:A:425:ARG:NH1	2.36	0.59
1:A:561:MSE:HE3	1:A:566:LYS:HD3	1.85	0.58
1:B:36:SER:CB	1:B:93:MSE:HE1	2.32	0.58
1:A:252:VAL:HG13	1:A:321:LEU:HD21	1.86	0.58
1:B:185:MSE:HE3	1:B:214:PHE:HE1	1.68	0.58
1:B:73:ALA:HB1	1:B:398:PHE:CD2	2.39	0.57
1:A:297:THR:HB	1:A:306:PRO:HD2	1.86	0.57
1:B:54:ILE:HD11	1:B:243:PHE:CD2	2.40	0.57
1:A:262:ILE:HD13	1:A:281:HIS:CE1	2.40	0.57
1:A:567:LEU:HD12	1:A:570:LYS:HZ2	1.69	0.57
1:B:32:LEU:N	8:B:834:HOH:O	2.37	0.56
1:A:186:PHE:CE1	4:A:604:MPD:H31	2.35	0.56
1:B:576:ILE:HD13	1:B:581:VAL:HG12	1.87	0.56
1:A:254:VAL:HG22	1:A:263:ALA:HA	1.88	0.56
1:B:332:ASP:OD1	1:B:332:ASP:N	2.37	0.55
1:B:289:ASN:ND2	8:B:896:HOH:O	2.36	0.55
1:A:205:ILE:O	1:A:208:ILE:HG12	2.06	0.55
1:B:26:TYR:CE2	1:B:283:ASP:HB3	2.41	0.55
1:A:80:GLY:HA3	1:A:224:GLN:HB2	1.88	0.55
1:A:11:PHE:CG	1:B:95:ARG:HG2	2.42	0.54
1:B:430:THR:H	1:B:433:GLU:HG3	1.71	0.54
1:B:432:LYS:HE3	1:B:436:GLU:OE2	2.07	0.54
1:B:286:PHE:CD1	1:B:492:ALA:HB3	2.42	0.54
1:B:208:ILE:HD11	1:B:550:MSE:HG3	1.88	0.54
1:B:232:LEU:O	1:B:236:LEU:HD12	2.08	0.54
1:B:318:TRP:CD2	1:B:331:PRO:HB3	2.43	0.53
1:A:330:HIS:O	1:A:333:VAL:HG12	2.09	0.53
1:B:82:GLU:HG3	1:B:217:LEU:HD22	1.91	0.53
1:A:87:PHE:CG	1:A:510:GLU:HB2	2.42	0.53
1:A:292:ILE:HD13	1:A:471:TYR:CE2	2.43	0.53
1:A:416:ASP:HA	1:A:425:ARG:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG12	1:A:276:GLU:HG2	1.91	0.53
1:B:74:GLY:HA2	1:B:348:THR:HG21	1.90	0.53
1:B:402:ASN:ND2	1:B:404:ASP:OD1	2.42	0.52
1:B:57:GLU:HA	1:B:247:CYS:O	2.09	0.52
1:B:252:VAL:O	1:B:324:GLN:NE2	2.42	0.52
1:B:87:PHE:CG	1:B:510:GLU:HB2	2.45	0.52
1:B:166:GLU:HB2	1:B:190:LYS:O	2.10	0.52
1:B:22:LYS:O	1:B:282:ASN:HB3	2.10	0.52
1:A:246:ASP:OD1	1:A:248:HIS:NE2	2.34	0.52
1:B:374:ASN:HD22	1:B:392:ILE:HG22	1.73	0.52
1:B:80:GLY:HA3	1:B:224:GLN:HB2	1.90	0.52
1:A:264:LYS:O	1:A:279:LEU:N	2.40	0.52
1:B:27:ILE:HB	1:B:54:ILE:HG22	1.91	0.52
1:A:87:PHE:CD2	1:A:510:GLU:HB2	2.45	0.52
1:B:311:LYS:NZ	1:B:336:GLU:OE1	2.21	0.51
1:B:262:ILE:HG12	1:B:489:ILE:HD12	1.92	0.51
1:B:204:PHE:CZ	4:B:605:MPD:HM2	2.46	0.51
1:B:579:THR:HG22	1:B:580:TRP:N	2.26	0.51
1:B:93:MSE:HE3	1:B:513:VAL:HG13	1.93	0.51
1:B:184:THR:O	4:B:604:MPD:O4	2.28	0.51
1:B:307:ILE:HB	7:B:608:GOL:H31	1.93	0.50
1:B:274:ASP:OD1	1:B:275:LYS:N	2.44	0.50
1:A:544:LEU:HA	1:A:547:MSE:HE2	1.94	0.50
1:A:76:VAL:HA	1:A:409:TRP:CH2	2.47	0.50
1:A:266:ILE:HD12	1:A:277:ILE:HD11	1.94	0.50
1:A:50:GLU:HG2	8:A:897:HOH:O	2.10	0.50
1:A:133:ARG:HE	1:A:137:ASP:HB3	1.77	0.50
1:B:30:SER:OG	1:B:56:GLU:HG2	2.12	0.50
1:B:310:ALA:O	1:B:467:TYR:OH	2.16	0.49
1:B:37:THR:HG21	1:B:286:PHE:CD2	2.47	0.49
1:B:81:ARG:NH2	8:B:804:HOH:O	2.30	0.49
1:B:465:MSE:SE	1:B:468:ILE:HD13	2.62	0.49
1:B:38:ALA:HA	1:B:41:LEU:HD12	1.95	0.49
1:B:321:LEU:HB3	1:B:328:PHE:CD2	2.47	0.49
1:B:307:ILE:HB	7:B:608:GOL:C3	2.43	0.48
1:A:270:GLN:O	1:A:273:LYS:HG3	2.12	0.48
1:A:161:GLU:HG2	1:A:476:ARG:HG2	1.94	0.48
1:B:480:ARG:NE	1:B:499:GLU:OE1	2.43	0.48
1:A:471:TYR:CZ	1:A:496:ASN:HB2	2.48	0.48
1:B:292:ILE:HD11	7:B:606:GOL:H12	1.95	0.48
1:A:26:TYR:CD1	1:A:53:HIS:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:ND2	8:A:829:HOH:O	2.47	0.48
1:B:23:LYS:HA	1:B:282:ASN:HB3	1.94	0.48
1:B:251:ASN:HB3	1:B:267:VAL:CG2	2.44	0.48
1:B:426:ILE:HG13	1:B:434:ILE:HD11	1.95	0.47
1:A:234:ALA:O	1:A:238:ASP:HB2	2.13	0.47
1:B:26:TYR:HE1	1:B:53:HIS:HD1	1.62	0.47
1:A:368:LEU:HA	1:A:374:ASN:HD21	1.80	0.47
1:B:3:TYR:OH	1:B:501:PRO:HG2	2.14	0.47
1:A:423:LYS:HD3	1:A:423:LYS:HA	1.68	0.47
1:B:193:SER:HB2	1:B:474:PRO:HA	1.96	0.47
1:B:320:ASN:O	1:B:324:GLN:HG3	2.15	0.47
1:A:51:ASN:HA	8:A:898:HOH:O	2.13	0.47
1:A:421:TYR:CE1	1:A:446:GLU:HG2	2.49	0.47
1:B:28:ILE:HG13	1:B:287:VAL:HA	1.96	0.47
1:B:432:LYS:HD2	8:B:924:HOH:O	2.14	0.47
1:A:24:SER:HB3	1:A:51:ASN:OD1	2.14	0.47
1:B:75:PHE:HB3	1:B:78:ARG:HG3	1.97	0.47
1:B:280:THR:HG22	1:B:282:ASN:H	1.80	0.46
1:B:476:ARG:O	1:B:479:ASP:HB2	2.15	0.46
1:A:421:TYR:HE1	1:A:446:GLU:HG2	1.80	0.46
1:B:330:HIS:HB2	1:B:479:ASP:OD1	2.16	0.46
1:B:292:ILE:HD13	1:B:471:TYR:CE2	2.51	0.46
1:B:23:LYS:HG2	1:B:282:ASN:HA	1.97	0.46
1:B:307:ILE:H	7:B:608:GOL:H12	1.80	0.46
1:B:546:ALA:O	1:B:550:MSE:HB2	2.15	0.46
1:B:386:TRP:HE3	1:B:388:LEU:HD13	1.81	0.46
1:B:233:LEU:HD22	1:B:243:PHE:CE2	2.51	0.46
1:B:431:GLY:HA3	1:B:460:THR:O	2.15	0.46
1:B:174:PHE:CD1	1:B:190:LYS:HE2	2.51	0.46
1:B:356:LEU:HD13	1:B:458:MSE:SE	2.66	0.46
1:A:130:ARG:HD3	1:A:440:TYR:CZ	2.51	0.45
1:B:430:THR:HG22	1:B:433:GLU:CG	2.46	0.45
1:A:35:LEU:O	1:A:39:VAL:HG23	2.16	0.45
1:A:24:SER:OG	1:A:283:ASP:OD1	2.34	0.45
1:B:318:TRP:CG	1:B:331:PRO:HB3	2.51	0.45
1:B:318:TRP:HZ2	8:B:961:HOH:O	1.99	0.45
1:B:335:CYS:HB2	1:B:467:TYR:CE2	2.51	0.45
1:B:567:LEU:O	1:B:571:THR:HG23	2.16	0.45
1:A:82:GLU:CD	1:A:82:GLU:H	2.20	0.45
1:B:430:THR:HG22	1:B:433:GLU:HG3	1.99	0.45
1:B:33:ALA:HB3	1:B:288:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:THR:O	1:A:425:ARG:HA	2.16	0.45
1:A:353:ASN:OD1	1:A:355:LYS:HG3	2.16	0.45
1:B:47[B]:MSE:HE2	1:B:47[B]:MSE:HB3	1.82	0.45
1:B:290:GLY:N	1:B:314:SER:HB3	2.26	0.45
1:A:485:PRO:HG2	1:A:488:SER:HB2	1.99	0.45
1:A:24:SER:HA	1:A:51:ASN:ND2	2.31	0.45
1:A:204:PHE:CZ	4:A:604:MPD:HM2	2.52	0.45
1:A:251:ASN:OD1	1:A:252:VAL:N	2.49	0.45
1:B:59:PRO:HB3	1:B:246:ASP:HB2	1.99	0.45
1:A:82:GLU:HB3	1:A:219:PHE:CE2	2.52	0.44
1:B:91:TRP:CE3	1:B:91:TRP:HA	2.51	0.44
1:B:226:GLU:HG3	8:B:956:HOH:O	2.18	0.44
1:B:471:TYR:CZ	1:B:496:ASN:HB2	2.53	0.44
1:B:430:THR:N	1:B:433:GLU:HG3	2.32	0.44
1:A:279:LEU:HD22	1:A:283:ASP:CG	2.38	0.44
1:A:567:LEU:HD12	1:A:570:LYS:NZ	2.32	0.44
1:B:47[B]:MSE:HE3	1:B:52:ILE:CG1	2.43	0.44
1:B:144:LYS:HG2	8:B:864:HOH:O	2.17	0.44
1:A:578:LYS:HD2	1:A:578:LYS:HA	1.73	0.44
1:B:220:ASN:HD21	1:B:228:MSE:SE	2.51	0.43
1:A:26:TYR:HD1	1:A:53:HIS:HB2	1.83	0.43
1:A:278:ASP:O	1:A:279:LEU:HD23	2.18	0.43
1:B:286:PHE:CE1	1:B:492:ALA:HB3	2.54	0.43
1:B:15:LYS:HB2	1:B:15:LYS:HE3	1.86	0.43
1:B:28:ILE:CD1	1:B:287:VAL:HG22	2.41	0.43
1:B:237:LYS:HD3	1:B:243:PHE:CE1	2.53	0.43
1:B:450:SER:HA	8:B:957:HOH:O	2.19	0.43
1:B:23:LYS:HB3	1:B:47[A]:MSE:HE2	1.99	0.43
1:B:54:ILE:HD11	1:B:243:PHE:CE2	2.54	0.43
1:B:254:VAL:HG22	1:B:263:ALA:HA	2.00	0.43
1:A:236:LEU:HB3	1:A:241:VAL:CG1	2.46	0.42
1:B:24:SER:N	1:B:282:ASN:O	2.38	0.42
1:B:318:TRP:CH2	1:B:497:PHE:HB3	2.53	0.42
1:A:76:VAL:HB	1:A:463:VAL:HG21	2.00	0.42
1:A:236:LEU:O	1:A:241:VAL:HG12	2.19	0.42
1:A:340:GLU:HG3	1:A:416:ASP:HB3	2.00	0.42
1:A:368:LEU:HA	1:A:374:ASN:ND2	2.33	0.42
1:B:97:ILE:HA	1:B:98:PRO:HD3	1.94	0.42
1:B:517:MSE:SE	1:B:531:PRO:HD2	2.70	0.42
1:B:321:LEU:HD13	1:B:493:PHE:CZ	2.54	0.42
1:B:255:ASP:OD2	1:B:264:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HB	1:A:194:LEU:HD23	2.02	0.42
1:B:244:GLU:HB3	1:B:247:CYS:SG	2.60	0.42
1:B:563:LEU:H	1:B:563:LEU:HD12	1.84	0.42
1:A:270:GLN:HG2	1:A:271:ASN:OD1	2.20	0.42
1:A:237:LYS:HE3	1:A:237:LYS:HB2	1.89	0.42
1:A:432:LYS:HE3	1:A:454:SER:HA	2.02	0.42
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.90	0.41
1:A:356:LEU:HD22	1:A:439:LEU:HD22	2.02	0.41
1:A:540:ILE:O	1:A:544:LEU:HG	2.21	0.41
1:B:75:PHE:HD1	1:B:77:VAL:HG12	1.85	0.41
1:B:169:PHE:CZ	1:B:197:MSE:HE2	2.55	0.41
1:A:576:ILE:O	1:A:579:THR:OG1	2.27	0.41
1:A:202:MSE:HE3	1:A:537:ILE:HG12	2.01	0.41
1:B:402:ASN:H	1:B:405:GLN:NE2	2.18	0.41
1:A:97:ILE:HA	1:A:98:PRO:HD3	1.87	0.41
1:A:253:GLU:HA	1:A:324:GLN:HE22	1.85	0.41
1:A:397:HIS:HD2	8:A:742:HOH:O	2.02	0.41
1:A:107:TYR:OH	1:A:227:SER:HB3	2.20	0.41
1:A:87:PHE:HB3	1:A:90:LEU:HB3	2.02	0.41
1:A:471:TYR:CE1	1:A:496:ASN:HB2	2.56	0.41
4:B:605:MPD:H4	4:B:605:MPD:HM1	1.90	0.41
1:B:321:LEU:HD13	1:B:493:PHE:HZ	1.85	0.41
1:B:353:ASN:OD1	1:B:457:ASN:HA	2.20	0.41
1:A:25:ALA:HA	1:A:284:ILE:O	2.20	0.41
1:B:191:TRP:CZ3	1:B:341:ARG:HG2	2.56	0.41
1:B:277:ILE:HG12	8:B:962:HOH:O	2.19	0.41
1:B:411:TYR:HB2	4:B:604:MPD:C1	2.46	0.41
1:B:84:GLU:HG2	4:B:605:MPD:H32	2.03	0.41
1:B:4:SER:O	1:B:531:PRO:HA	2.21	0.40
1:B:107:TYR:OH	1:B:227:SER:HB3	2.21	0.40
1:A:58:LEU:HA	1:A:59:PRO:HD3	1.92	0.40
4:A:606:MPD:HM1	4:A:606:MPD:H4	1.78	0.40
1:B:24:SER:OG	1:B:51:ASN:O	2.32	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	573/591 (97%)	563 (98%)	9 (2%)	1 (0%)	52	59
1	B	576/591 (98%)	565 (98%)	11 (2%)	0	100	100
All	All	1149/1182 (97%)	1128 (98%)	20 (2%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LYS

### 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	511/500 (102%)	490 (96%)	21 (4%)	37	45
1	B	512/500 (102%)	479 (94%)	33 (6%)	22	23
All	All	1023/1000 (102%)	969 (95%)	54 (5%)	29	31

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	24	SER
1	A	52	ILE
1	A	75	PHE
1	A	84	GLU

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Mol	Chain	Res	Type
1	A	128	TYR
1	A	159	GLU
1	A	269	THR
1	A	271	ASN
1	A	273	LYS
1	A	278	ASP
1	A	332	ASP
1	A	447	SER
1	A	454	SER
1	A	507	PHE
1	A	550	MSE
1	A	563	LEU
1	A	570	LYS
1	A	571	THR
1	A	578	LYS
1	A	587	GLU
1	B	1	MSE
1	B	28	ILE
1	B	30	SER
1	B	47[A]	MSE
1	B	47[B]	MSE
1	B	48	LYS
1	B	56	GLU
1	B	75	PHE
1	B	83	MSE
1	B	84	GLU
1	B	95	ARG
1	B	128	TYR
1	B	151	LYS
1	B	226	GLU
1	B	273	LYS
1	B	277	ILE
1	B	288	THR
1	B	293	THR
1	B	314	SER
1	B	332	ASP
1	B	353	ASN
1	B	362	ARG
1	B	372	LYS
1	B	404	ASP
1	B	411	TYR
1	B	433	GLU

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Mol	Chain	Res	Type
1	B	475	ARG
1	B	507	PHE
1	B	550	MSE
1	B	574	ARG
1	B	577	LYS
1	B	578	LYS
1	B	586	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	A	324	GLN
1	A	374	ASN
1	B	385	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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
2	MES	A	601	-	11,12,12	0.68	0	14,16,16	2.43	6 (42%)
4	MPD	A	604	-	6,7,7	0.24	0	7,10,10	0.50	0
4	MPD	A	605	-	6,7,7	0.30	0	7,10,10	0.19	0
4	MPD	A	606	-	6,7,7	0.26	0	7,10,10	0.33	0
2	MES	B	602	-	11,12,12	0.65	0	14,16,16	3.09	7 (50%)
6	PO4	B	603	-	4,4,4	0.51	0	6,6,6	0.28	0
4	MPD	B	604	-	6,7,7	0.21	0	7,10,10	0.40	0
4	MPD	B	605	-	6,7,7	0.22	0	7,10,10	0.49	0
7	GOL	B	606	-	5,5,5	0.27	0	5,5,5	0.32	0
7	GOL	B	607	-	5,5,5	0.32	0	5,5,5	0.26	0
7	GOL	B	608	-	5,5,5	0.34	0	5,5,5	0.47	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
2	MES	A	601	-	-	0/6/14/14	0/1/1/1
4	MPD	A	604	-	-	0/5/5/5	0/0/0/0
4	MPD	A	605	-	-	0/5/5/5	0/0/0/0
4	MPD	A	606	-	-	0/5/5/5	0/0/0/0
2	MES	B	602	-	-	0/6/14/14	0/1/1/1
6	PO4	B	603	-	-	0/0/0/0	0/0/0/0
4	MPD	B	604	-	-	0/5/5/5	0/0/0/0
4	MPD	B	605	-	-	0/5/5/5	0/0/0/0
7	GOL	B	606	-	-	0/4/4/4	0/0/0/0
7	GOL	B	607	-	-	0/4/4/4	0/0/0/0
7	GOL	B	608	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MES	C6-C5-N4	-2.44	106.43	110.12
2	B	602	MES	C6-C5-N4	-2.33	106.59	110.12
2	B	602	MES	C2-C3-N4	-2.15	106.87	110.12
2	A	601	MES	C7-N4-C3	2.22	116.96	111.27
2	A	601	MES	C7-N4-C5	2.50	117.67	111.27
2	B	602	MES	C7-N4-C5	3.08	119.16	111.27
2	B	602	MES	C7-N4-C3	3.47	120.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MES	O1S-S-C8	3.81	110.16	106.91
2	B	602	MES	O2S-S-C8	3.86	110.20	106.91
2	A	601	MES	C5-N4-C3	4.18	117.95	108.90
2	A	601	MES	O2S-S-C8	5.35	111.47	106.91
2	B	602	MES	C5-N4-C3	5.37	120.53	108.90
2	B	602	MES	O1S-S-C8	6.86	112.76	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	MPD	4	0
4	A	606	MPD	1	0
4	B	604	MPD	3	0
4	B	605	MPD	3	0
7	B	606	GOL	1	0
7	B	608	GOL	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	559/591 (94%)	0.43	43 (7%) 16 16	29, 61, 99, 127	0
1	B	561/591 (94%)	0.73	73 (13%) 5 4	25, 67, 109, 127	4 (0%)
All	All	1120/1182 (94%)	0.58	116 (10%) 8 7	25, 63, 105, 127	4 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	HIS	7.2
1	B	266	ILE	7.1
1	B	267	VAL	6.1
1	A	564	PRO	5.6
1	B	254	VAL	5.5
1	B	279	LEU	5.3
1	A	77	VAL	4.9
1	B	73	ALA	4.7
1	A	568	ALA	4.7
1	B	327	ALA	4.5
1	B	563	LEU	4.4
1	A	75	PHE	4.4
1	B	75	PHE	4.3
1	A	272	GLY	4.2
1	B	491	LEU	4.2
1	B	567	LEU	4.2
1	A	254	VAL	4.2
1	B	278	ASP	4.2
1	A	266	ILE	4.2
1	B	54	ILE	4.0
1	B	252	VAL	4.0
1	B	328	PHE	3.9
1	A	78	ARG	3.9
1	A	569	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	286	PHE	3.8
1	B	258	GLY	3.8
1	A	556	LEU	3.7
1	A	76	VAL	3.7
1	A	267	VAL	3.7
1	B	272	GLY	3.7
1	A	60	VAL	3.6
1	A	256	HIS	3.6
1	B	78	ARG	3.5
1	B	280	THR	3.5
1	A	263	ALA	3.4
1	B	243	PHE	3.4
1	A	50	GLU	3.4
1	A	262	ILE	3.4
1	B	27	ILE	3.3
1	B	277	ILE	3.3
1	B	493	PHE	3.3
1	A	567	LEU	3.3
1	B	281	HIS	3.3
1	B	296	SER	3.2
1	B	571	THR	3.2
1	A	144	LYS	3.2
1	B	256	HIS	3.2
1	B	283	ASP	3.1
1	B	270	GLN	3.1
1	B	271	ASN	3.1
1	B	489	ILE	3.0
1	B	403	PRO	3.0
1	A	327	ALA	3.0
1	B	307	ILE	3.0
1	B	28	ILE	3.0
1	A	258	GLY	3.0
1	B	494	ILE	2.9
1	B	287	VAL	2.9
1	A	277	ILE	2.9
1	A	279	LEU	2.8
1	A	572	GLY	2.7
1	A	280	THR	2.7
1	B	314	SER	2.7
1	B	305	ALA	2.7
1	B	477	ASP	2.7
1	B	26	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	467	TYR	2.7
1	B	74	GLY	2.7
1	B	306	PRO	2.6
1	B	273	LYS	2.6
1	B	317	LEU	2.6
1	A	274	ASP	2.5
1	A	565	GLU	2.5
1	B	259	ASP	2.5
1	A	581	VAL	2.5
1	B	262	ILE	2.5
1	A	175	LYS	2.5
1	B	404	ASP	2.5
1	A	253	GLU	2.5
1	B	253	GLU	2.5
1	B	301	GLN	2.4
1	B	249	VAL	2.4
1	A	283	ASP	2.3
1	B	572	GLY	2.3
1	B	80	GLY	2.3
1	B	276	GLU	2.3
1	B	52	ILE	2.3
1	B	298	TYR	2.3
1	B	308	THR	2.3
1	A	48	LYS	2.2
1	B	237	LYS	2.2
1	B	288	THR	2.2
1	B	274	ASP	2.2
1	A	571	THR	2.2
1	A	557	ALA	2.2
1	B	492	ALA	2.2
1	B	245	TYR	2.1
1	A	53	HIS	2.1
1	B	487	GLY	2.1
1	A	359	TYR	2.1
1	B	57	GLU	2.1
1	B	452	LEU	2.1
1	A	273	LYS	2.1
1	B	318	TRP	2.1
1	B	523	LEU	2.1
1	A	445	PRO	2.1
1	A	560	ASP	2.1
1	B	334	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	246	ASP	2.1
1	B	323	LYS	2.1
1	A	325	ASP	2.0
1	B	295	SER	2.0
1	A	284	ILE	2.0
1	A	255	ASP	2.0
1	B	427	VAL	2.0
1	B	24	SER	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	GOL	B	607	6/6	0.90	0.22	12.12	87,91,92,96	0
4	MPD	A	606	8/8	0.54	0.40	9.86	75,84,87,87	0
5	NA	B	601	1/1	0.80	0.33	7.74	58,58,58,58	0
4	MPD	A	604	8/8	0.85	0.34	6.59	57,68,74,74	0
4	MPD	A	605	8/8	0.86	0.26	4.38	47,60,66,69	0
4	MPD	B	605	8/8	0.94	0.27	3.19	61,64,66,69	0
4	MPD	B	604	8/8	0.76	0.29	3.09	39,45,54,60	0
7	GOL	B	606	6/6	0.73	0.24	2.83	48,59,61,65	0
2	MES	B	602	12/12	0.89	0.15	-0.00	49,67,81,84	0
2	MES	A	601	12/12	0.96	0.14	-0.35	45,70,84,84	0
6	PO4	B	603	5/5	0.95	0.12	-0.51	50,67,70,83	0
3	K	A	603	1/1	0.96	0.09	-1.61	54,54,54,54	0
3	K	A	602	1/1	0.96	0.12	-1.93	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	608	6/6	0.63	0.42	-	73,84,90,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.