



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 07:38 AM EDT

PDB ID : 3PDB  
Title : Crystal structure of mouse mitochondrial aspartate aminotransferase in complex with oxaloacetic acid  
Authors : Han, Q.; Robinson, H.; Cai, T.; Tagle, D.A.; Li, J.  
Deposited on : 2010-10-22  
Resolution : 2.40 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

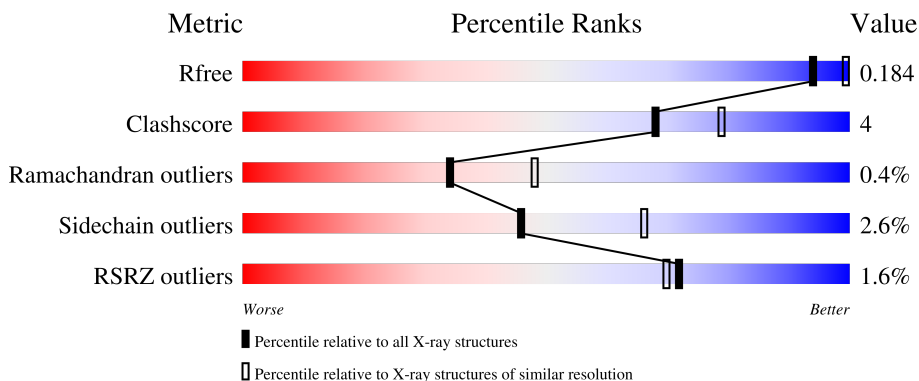
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	401	 90% 9%
1	C	401	 90% 9%
2	B	401	 87% 12%
2	D	401	 92% 7%

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
5	OAA	B	1	-	X	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13409 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.

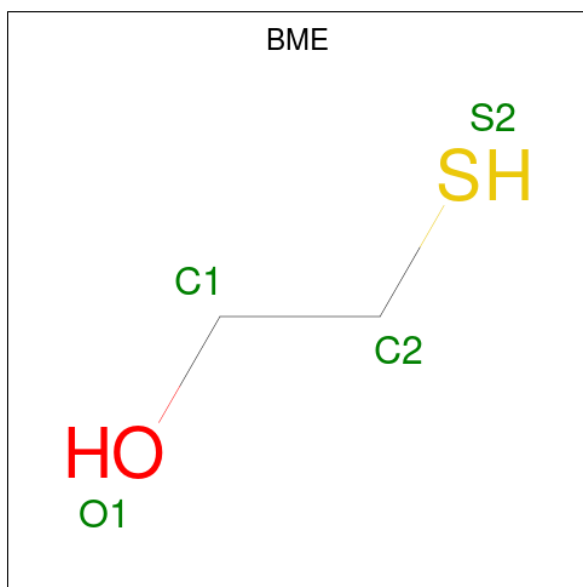
- Molecule 1 is a protein called Aspartate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	401	Total 3155	C 2005	N 551	O 582	P 1	S 16	0	0	0
1	C	401	Total 3162	C 2010	N 553	O 582	P 1	S 16	0	1	0

- Molecule 2 is a protein called Aspartate aminotransferase, mitochondrial.

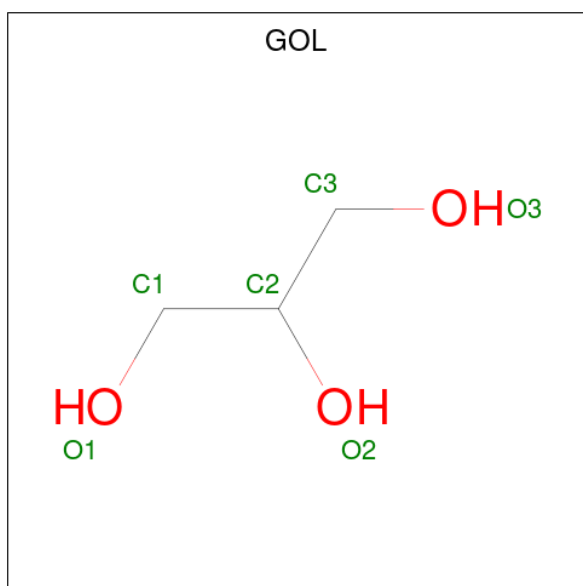
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	401	Total 3140	C 1997	N 550	O 577	S 16	0	0	0
2	D	401	Total 3147	C 2002	N 552	O 577	S 16	0	1	0

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



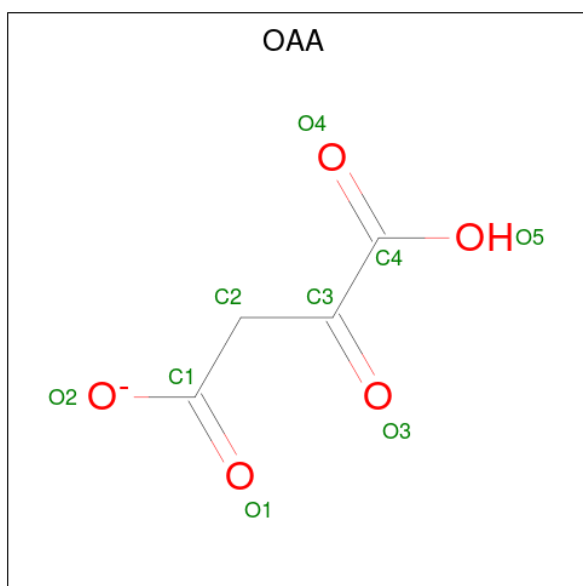
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



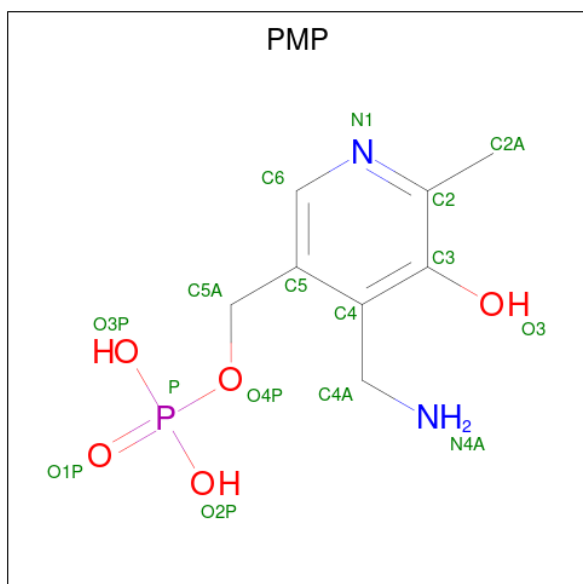
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula:  $C_4H_3O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

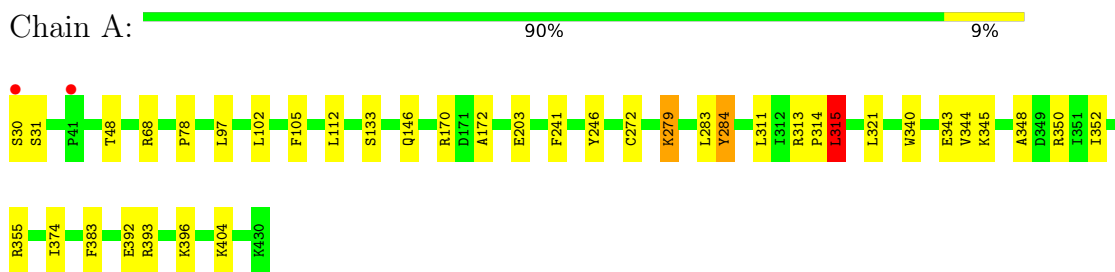
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	191	Total	O	0	0
			191	191		
7	B	137	Total	O	0	0
			137	137		
7	C	184	Total	O	0	0
			184	184		
7	D	194	Total	O	0	0
			194	194		

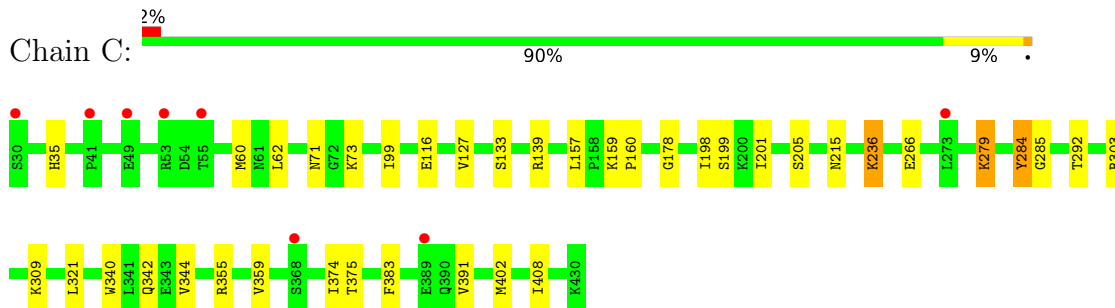
### 3 Residue-property plots [i](#)

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.

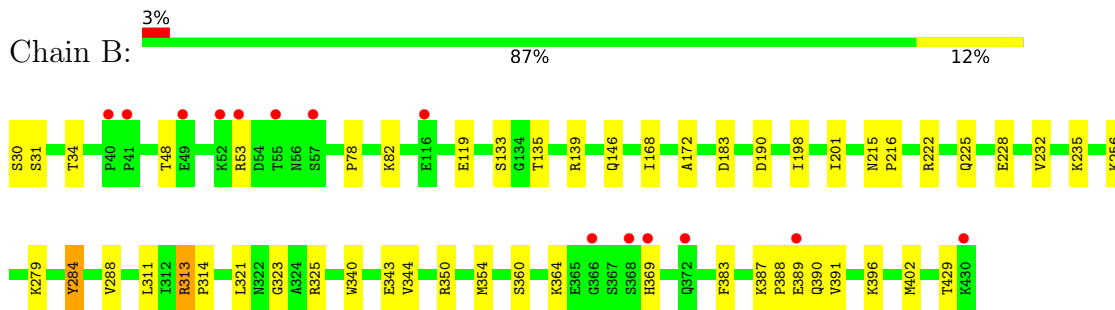
- Molecule 1: Aspartate aminotransferase, mitochondrial



- Molecule 1: Aspartate aminotransferase, mitochondrial



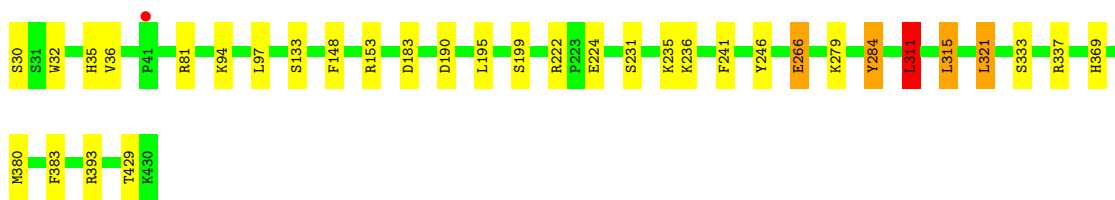
- Molecule 2: Aspartate aminotransferase, mitochondrial



- Molecule 2: Aspartate aminotransferase, mitochondrial







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	282.42Å 77.89Å 87.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.40) 92.8 (30.01-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.177 , 0.190 0.173 , 0.184	Depositor DCC
$R_{free}$ test set	3554 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtrriage
Anisotropy	0.155	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13409	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PMP, OAA, BME, GOL, LLP

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	0.81	0/3203	0.78	1/4326 (0.0%)
1	C	0.75	0/3214	0.74	1/4341 (0.0%)
2	B	0.69	0/3213	0.72	0/4340
2	D	0.80	0/3224	0.79	2/4355 (0.0%)
All	All	0.76	0/12854	0.76	4/17362 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	LEU	CA-CB-CG	6.21	129.58	115.30
2	D	311	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	315	LEU	CB-CG-CD1	5.78	120.82	111.00
2	D	321	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3155	0	3128	20	0
1	C	3162	0	3135	23	0
2	B	3140	0	3125	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3147	0	3132	29	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	8	0	12	2	0
3	D	8	0	12	1	0
4	A	12	0	16	1	0
4	C	6	0	8	0	0
4	D	12	0	16	0	0
5	B	9	0	2	3	0
6	B	16	0	11	2	0
6	D	16	0	11	4	0
7	A	191	0	0	4	0
7	B	137	0	0	5	0
7	C	184	0	0	1	0
7	D	194	0	0	6	0
All	All	13409	0	12626	97	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 4.

All (97) 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:C:198:ILE:HA	1:C:201:ILE:HD12	1.52	0.91
2:B:279:LYS:HE3	7:B:711:HOH:O	1.73	0.87
2:B:183:ASP:HB2	2:B:190:ASP:HB2	1.58	0.84
2:D:279:LYS:HG2	7:D:712:HOH:O	1.79	0.82
2:B:198:ILE:HA	2:B:201:ILE:HD12	1.65	0.77
1:A:203:GLU:HB3	7:A:539:HOH:O	1.85	0.75
2:D:369:HIS:HE1	2:D:429:THR:O	1.69	0.75
1:C:340:TRP:O	1:C:344:VAL:HG23	1.92	0.69
2:D:279:LYS:HD2	2:D:380:MET:CE	2.23	0.69
2:D:279:LYS:HE2	6:D:432:PMP:HNA2	1.60	0.67
2:D:279:LYS:CE	6:D:432:PMP:HNA2	2.08	0.66
1:A:311:LEU:O	1:A:315:LEU:HD22	1.96	0.66
1:A:355:ARG:HD3	1:A:374:ILE:O	1.95	0.66
2:D:279:LYS:HD2	2:D:380:MET:HE2	1.78	0.64
1:A:393:ARG:HD3	7:A:482:HOH:O	1.98	0.63
2:B:31:SER:HB3	2:B:34:THR:HG22	1.81	0.61
6:B:432:PMP:H4A1	7:B:711:HOH:O	1.99	0.60
2:B:31:SER:HB3	2:B:34:THR:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ASN:HD21	3:C:1:BME:H22	1.67	0.58
2:B:387:LYS:HB3	2:B:388:PRO:HD2	1.86	0.58
2:B:390:GLN:NE2	2:B:429:THR:HG22	2.20	0.57
1:C:359:VAL:HG21	1:C:375:THR:HG23	1.87	0.56
6:B:432:PMP:C4A	7:B:711:HOH:O	2.52	0.56
2:D:222:ARG:NH1	2:D:224:GLU:OE1	2.37	0.55
1:C:355:ARG:O	1:C:359:VAL:HG23	2.06	0.55
2:B:313:ARG:HH12	5:B:1:OAA:C2	2.20	0.54
1:C:73:LYS:NZ	7:C:561:HOH:O	2.37	0.54
1:A:78:PRO:HD2	1:A:343:GLU:OE1	2.08	0.54
2:B:288:VAL:HG22	2:B:323:GLY:HA3	1.92	0.52
2:B:215:ASN:OD1	2:B:216:PRO:HA	2.10	0.52
2:B:340:TRP:O	2:B:344:VAL:HG23	2.09	0.52
2:B:222:ARG:HB2	2:B:225:GLN:HG3	1.92	0.52
2:B:313:ARG:HH12	5:B:1:OAA:H22	1.73	0.52
1:C:60:MET:HE2	1:C:62:LEU:HD21	1.92	0.52
1:C:303:ARG:HD2	2:D:36:VAL:O	2.10	0.52
2:B:288:VAL:CG2	2:B:323:GLY:HA3	2.40	0.51
2:D:279:LYS:HD3	2:D:284:TYR:HE1	1.76	0.51
1:A:246:TYR:HE1	1:A:279:LLP:HD3	1.76	0.51
2:D:279:LYS:HD3	2:D:284:TYR:CE1	2.47	0.49
1:A:97:LEU:HG	1:A:321:LEU:HD13	1.94	0.49
1:C:35[A]:HIS:CE1	2:D:148:PHE:O	2.64	0.49
2:B:311:LEU:O	2:B:314:PRO:HD2	2.12	0.49
3:D:1:BME:H11	6:D:432:PMP:H4A1	1.95	0.49
2:D:337:ARG:NE	7:D:467:HOH:O	2.44	0.48
2:B:279:LYS:HD3	2:B:284:TYR:CE1	2.49	0.47
1:C:279:LLP:H4'1	3:C:1:BME:H12	1.95	0.47
2:D:393:ARG:HD3	7:D:462:HOH:O	2.14	0.47
1:A:102:LEU:HB3	1:A:105:PHE:HB3	1.97	0.47
2:D:199:SER:O	2:D:236:LYS:HD2	2.15	0.47
2:D:246:TYR:CE1	2:D:279:LYS:HG3	2.50	0.47
5:B:1:OAA:O1	7:B:482:HOH:O	2.20	0.47
2:B:350:ARG:O	2:B:354:MET:HG2	2.14	0.47
1:A:404:LYS:HE2	7:A:547:HOH:O	2.14	0.46
2:D:97:LEU:HG	2:D:321:LEU:HD13	1.96	0.46
2:D:183:ASP:HB2	2:D:190:ASP:HB2	1.98	0.46
2:B:321:LEU:HD22	2:B:325:ARG:CZ	2.45	0.46
2:B:146:GLN:HG3	2:B:172:ALA:O	2.16	0.46
2:B:390:GLN:HE22	2:B:429:THR:HG22	1.80	0.46
1:A:146:GLN:HG3	1:A:172:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:LYS:HD3	2:D:235:LYS:HA	1.58	0.45
1:A:241:PHE:CD1	1:A:272:CYS:SG	3.09	0.45
2:D:153:ARG:HA	2:D:153:ARG:HE	1.82	0.45
1:A:283:LEU:O	1:A:284:TYR:C	2.55	0.44
1:C:99:ILE:HB	1:C:309:LYS:HG2	1.99	0.44
1:C:159:LYS:HA	1:C:160:PRO:HA	1.74	0.44
1:A:340:TRP:O	1:A:344:VAL:HG23	2.18	0.44
2:D:279:LYS:CE	6:D:432:PMP:N4A	2.79	0.43
1:A:315:LEU:HD13	2:B:139:ARG:NH1	2.33	0.43
1:C:285:GLY:HA3	2:D:321:LEU:HD22	1.99	0.43
1:A:313:ARG:HB2	1:A:314:PRO:HD3	1.99	0.43
1:C:139:ARG:NH1	2:D:315:LEU:HD13	2.34	0.43
2:D:311:LEU:HD22	7:D:489:HOH:O	2.18	0.43
1:A:68:ARG:O	1:A:350:ARG:NH1	2.52	0.42
1:A:30:SER:HB2	1:A:31:SER:H	1.65	0.42
2:B:82:LYS:HD2	7:B:461:HOH:O	2.18	0.42
2:B:135:THR:HG23	2:B:168:ILE:HD11	2.01	0.42
1:A:348:ALA:O	1:A:352:ILE:HG13	2.19	0.42
1:C:284:TYR:HB2	2:D:94:LYS:O	2.19	0.42
2:D:337:ARG:HD3	7:D:467:HOH:O	2.21	0.41
1:A:112:LEU:HD12	4:A:432:GOL:H31	2.01	0.41
1:C:199:SER:O	1:C:236:LYS:HD2	2.20	0.41
1:C:355:ARG:HD3	1:C:374:ILE:O	2.20	0.41
1:A:203:GLU:CD	7:A:539:HOH:O	2.58	0.41
2:D:32:TRP:O	2:D:35[B]:HIS:HE1	2.03	0.41
2:D:266:GLU:O	2:D:266:GLU:HG2	2.19	0.41
2:B:53:ARG:HB2	2:B:53:ARG:CZ	2.51	0.41
2:B:228:GLU:O	2:B:232:VAL:HG23	2.20	0.41
2:D:393:ARG:NH2	7:D:477:HOH:O	2.53	0.41
1:C:201:ILE:CG2	1:C:205:SER:HB2	2.51	0.40
1:C:402:MET:HE2	1:C:408:ILE:HG22	2.02	0.40
2:B:391:VAL:HG13	2:B:402:MET:HG2	2.03	0.40
1:C:157:LEU:O	1:C:178:GLY:HA2	2.21	0.40
2:D:81:ARG:HD3	2:D:81:ARG:HA	1.79	0.40
2:B:78:PRO:HD2	2:B:343:GLU:CD	2.41	0.40
1:C:127:VAL:O	1:C:292:THR:HA	2.20	0.40
1:C:342:GLN:HE21	1:C:342:GLN:HB2	1.65	0.40
1:C:391:VAL:HG13	1:C:402:MET:HG3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/401 (99%)	388 (98%)	9 (2%)	1 (0%)	41	55
1	C	399/401 (100%)	386 (97%)	12 (3%)	1 (0%)	41	55
2	B	399/401 (100%)	380 (95%)	16 (4%)	3 (1%)	19	29
2	D	400/401 (100%)	386 (96%)	13 (3%)	1 (0%)	41	55
All	All	1596/1604 (100%)	1540 (96%)	50 (3%)	6 (0%)	34	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	TYR
2	B	284	TYR
1	C	284	TYR
2	D	284	TYR
2	B	364	LYS
2	B	119	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/333 (100%)	325 (98%)	8 (2%)	49	68
1	C	334/333 (100%)	328 (98%)	6 (2%)	59	76
2	B	334/334 (100%)	323 (97%)	11 (3%)	38	57
2	D	335/334 (100%)	325 (97%)	10 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1336/1334 (100%)	1301 (97%)	35 (3%)	46 66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	133	SER
1	A	170	ARG
1	A	315	LEU
1	A	345	LYS
1	A	383	PHE
1	A	392	GLU
1	A	396	LYS
2	B	30	SER
2	B	48	THR
2	B	133	SER
2	B	235	LYS
2	B	256	LYS
2	B	313	ARG
2	B	360	SER
2	B	369	HIS
2	B	383	PHE
2	B	389	GLU
2	B	396	LYS
1	C	71	ASN
1	C	116	GLU
1	C	133	SER
1	C	236	LYS
1	C	266	GLU
1	C	383	PHE
2	D	30	SER
2	D	133	SER
2	D	195	LEU
2	D	231	SER
2	D	241	PHE
2	D	266	GLU
2	D	311	LEU
2	D	315	LEU
2	D	333	SER
2	D	383	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)



such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	342	GLN
1	A	361	ASN
1	A	369	HIS
1	A	372	GLN
2	B	86	GLN
2	B	322	ASN
2	B	361	ASN
1	C	86	GLN
1	C	342	GLN
1	C	361	ASN
1	C	369	HIS
1	C	372	GLN
2	D	86	GLN
2	D	204	GLN
2	D	322	ASN
2	D	361	ASN
2	D	369	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	LLP	C	279	1	23,24,25	1.93	5 (21%)	25,32,34	1.58	4 (16%)
1	LLP	A	279	1	23,24,25	2.78	8 (34%)	25,32,34	2.14	8 (32%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	279	1	-	8/16/17/19	0/1/1/1
1	LLP	A	279	1	-	9/16/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	LLP	CE-NZ	7.63	1.63	1.46
1	A	279	LLP	O3-C3	-6.50	1.21	1.37
1	C	279	LLP	O3-C3	-5.40	1.24	1.37
1	C	279	LLP	CE-NZ	4.77	1.57	1.46
1	A	279	LLP	C4-C4'	4.67	1.55	1.46
1	A	279	LLP	C4'-NZ	3.41	1.38	1.27
1	C	279	LLP	C4-C4'	3.02	1.52	1.46
1	A	279	LLP	CD-CE	3.00	1.61	1.51
1	A	279	LLP	CB-CA	2.60	1.57	1.53
1	C	279	LLP	C4'-NZ	2.54	1.35	1.27
1	C	279	LLP	C2-N1	2.30	1.38	1.33
1	A	279	LLP	C2-N1	2.28	1.38	1.33
1	A	279	LLP	CG-CB	2.13	1.61	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	LLP	CD-CE-NZ	5.31	123.95	110.93
1	A	279	LLP	OP2-P-OP4	-4.27	95.37	106.73
1	A	279	LLP	OP4-C5'-C5	4.06	117.08	109.35
1	C	279	LLP	OP4-C5'-C5	3.97	116.92	109.35
1	C	279	LLP	OP2-P-OP4	-3.86	96.45	106.73
1	A	279	LLP	C4-C3-C2	3.13	122.13	120.19
1	A	279	LLP	CE-NZ-C4'	-2.73	110.53	118.90
1	A	279	LLP	C5-C6-N1	-2.38	119.86	123.82
1	A	279	LLP	C3-C4-C5	-2.28	116.51	118.26
1	C	279	LLP	C4-C4'-NZ	-2.17	114.36	124.31
1	C	279	LLP	CE-NZ-C4'	-2.06	112.57	118.90
1	A	279	LLP	C6-C5-C4	2.00	121.84	118.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	279	LLP	C4-C5-C5'-OP4
1	A	279	LLP	N-CA-CB-CG
1	C	279	LLP	C5'-OP4-P-OP1
1	C	279	LLP	C5'-OP4-P-OP2
1	C	279	LLP	C4-C4'-NZ-CE
1	A	279	LLP	C3-C4-C4'-NZ
1	C	279	LLP	C3-C4-C4'-NZ
1	C	279	LLP	CA-CB-CG-CD
1	A	279	LLP	CA-CB-CG-CD
1	A	279	LLP	C5-C4-C4'-NZ
1	C	279	LLP	C5-C4-C4'-NZ
1	A	279	LLP	C6-C5-C5'-OP4
1	C	279	LLP	C5'-OP4-P-OP3
1	A	279	LLP	C5'-OP4-P-OP1
1	C	279	LLP	CD-CE-NZ-C4'
1	A	279	LLP	C-CA-CB-CG
1	A	279	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	279	LLP	1	0
1	A	279	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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
3	BME	A	1	-	3,3,3	0.74	0	1,2,2	2.04	1 (100%)
4	GOL	D	433	-	5,5,5	0.25	0	5,5,5	0.64	0
4	GOL	A	432	-	5,5,5	0.35	0	5,5,5	0.94	0
6	PMP	B	432	-	16,16,16	0.93	1 (6%)	21,23,23	1.02	2 (9%)
6	PMP	D	432	-	16,16,16	0.93	1 (6%)	21,23,23	1.00	2 (9%)
3	BME	B	431	-	3,3,3	0.32	0	1,2,2	0.33	0
3	BME	C	1	-	3,3,3	0.31	0	1,2,2	0.29	0
3	BME	D	1	-	3,3,3	0.63	0	1,2,2	0.08	0
4	GOL	A	431	-	5,5,5	0.43	0	5,5,5	0.41	0
4	GOL	C	432	-	5,5,5	0.29	0	5,5,5	0.52	0
4	GOL	D	434	-	5,5,5	0.33	0	5,5,5	0.39	0
5	OAA	B	1	-	8,8,8	2.46	3 (37%)	9,10,10	2.69	4 (44%)
3	BME	C	431	-	3,3,3	0.30	0	1,2,2	2.03	1 (100%)
3	BME	D	431	-	3,3,3	0.32	0	1,2,2	0.34	0
3	BME	B	433	-	3,3,3	0.24	0	1,2,2	0.01	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
3	BME	A	1	-	-	1/1/1/1	-
4	GOL	D	433	-	-	3/4/4/4	-
4	GOL	A	432	-	-	1/4/4/4	-
6	PMP	B	432	-	-	3/8/8/8	0/1/1/1
6	PMP	D	432	-	-	3/8/8/8	0/1/1/1
3	BME	B	431	-	-	1/1/1/1	-
3	BME	C	1	-	-	1/1/1/1	-
3	BME	D	1	-	-	1/1/1/1	-
4	GOL	A	431	-	-	2/4/4/4	-
4	GOL	C	432	-	-	4/4/4/4	-
4	GOL	D	434	-	-	2/4/4/4	-
5	OAA	B	1	-	-	5/8/8/8	-
3	BME	C	431	-	-	0/1/1/1	-
3	BME	D	431	-	-	0/1/1/1	-
3	BME	B	433	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	OAA	O3-C3	4.38	1.31	1.23
5	B	1	OAA	C2-C1	3.69	1.56	1.51
5	B	1	OAA	O1-C1	2.99	1.32	1.22
6	D	432	PMP	C2-N1	2.46	1.38	1.33
6	B	432	PMP	C2-N1	2.41	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	OAA	O5-C4-O4	-4.98	112.22	123.61
5	B	1	OAA	O5-C4-C3	3.58	123.76	113.97
5	B	1	OAA	O2-C1-O1	-3.28	115.12	123.30
6	B	432	PMP	C6-C5-C4	2.45	119.85	118.12
6	D	432	PMP	C6-C5-C4	2.36	119.79	118.12
6	B	432	PMP	C5-C6-N1	-2.26	120.05	123.82
6	D	432	PMP	C5-C6-N1	-2.23	120.10	123.82
5	B	1	OAA	O2-C1-C2	2.19	121.52	114.54
3	A	1	BME	O1-C1-C2	-2.04	102.79	110.83
3	C	431	BME	O1-C1-C2	2.03	118.85	110.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	BME	O1-C1-C2-S2
3	B	431	BME	O1-C1-C2-S2
3	B	433	BME	O1-C1-C2-S2
3	C	1	BME	O1-C1-C2-S2
3	D	1	BME	O1-C1-C2-S2
4	A	431	GOL	C1-C2-C3-O3
4	C	432	GOL	O1-C1-C2-C3
4	D	433	GOL	C1-C2-C3-O3
4	D	434	GOL	O1-C1-C2-C3
5	B	1	OAA	O3-C3-C4-O4
5	B	1	OAA	O3-C3-C4-O5
5	B	1	OAA	C2-C3-C4-O4
5	B	1	OAA	C2-C3-C4-O5
6	B	432	PMP	C5A-O4P-P-O3P
6	D	432	PMP	C5A-O4P-P-O2P
6	D	432	PMP	C5A-O4P-P-O3P
4	C	432	GOL	C1-C2-C3-O3
4	A	431	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	433	GOL	O2-C2-C3-O3
4	C	432	GOL	O1-C1-C2-O2
4	C	432	GOL	O2-C2-C3-O3
4	D	434	GOL	O1-C1-C2-O2
6	B	432	PMP	C5A-O4P-P-O1P
6	D	432	PMP	C5A-O4P-P-O1P
6	B	432	PMP	C5A-O4P-P-O2P
5	B	1	OAA	O2-C1-C2-C3
4	D	433	GOL	O1-C1-C2-O2
4	A	432	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	432	GOL	1	0
6	B	432	PMP	2	0
6	D	432	PMP	4	0
3	C	1	BME	2	0
3	D	1	BME	1	0
5	B	1	OAA	3	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 [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	400/401 (99%)	-0.47	2 (0%) 91 89	9, 21, 34, 44	0
1	C	400/401 (99%)	-0.26	8 (2%) 65 63	14, 27, 46, 56	0
2	B	401/401 (100%)	-0.06	14 (3%) 44 43	15, 35, 63, 74	0
2	D	401/401 (100%)	-0.42	1 (0%) 95 94	12, 22, 36, 44	0
All	All	1602/1604 (99%)	-0.30	25 (1%) 72 70	9, 25, 49, 74	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	SER	3.5
2	B	53	ARG	3.2
1	C	368	SER	3.1
1	C	41	PRO	3.1
2	D	41	PRO	3.1
1	A	30	SER	3.0
1	A	41	PRO	2.8
1	C	53	ARG	2.7
2	B	369	HIS	2.7
1	C	55	THR	2.6
2	B	116	GLU	2.6
2	B	57	SER	2.5
2	B	52	LYS	2.5
2	B	49	GLU	2.5
2	B	372	GLN	2.4
2	B	430	LYS	2.4
2	B	55	THR	2.3
2	B	41	PRO	2.2
2	B	389	GLU	2.2
1	C	49	GLU	2.1
2	B	366	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	273	LEU	2.1
2	B	368	SER	2.1
1	C	389	GLU	2.1
2	B	40	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	A	279	24/25	0.96	0.19	16,23,29,32	0
1	LLP	C	279	24/25	0.98	0.20	19,27,33,33	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	D	433	6/6	0.74	0.23	53,55,56,56	0
5	OAA	B	1	9/9	0.78	0.28	42,49,51,51	0
3	BME	C	431	4/4	0.80	0.26	50,53,55,55	0
4	GOL	A	432	6/6	0.82	0.22	44,47,49,49	0
3	BME	B	433	4/4	0.83	0.29	65,66,66,66	0
4	GOL	A	431	6/6	0.85	0.23	55,57,57,57	0
4	GOL	C	432	6/6	0.87	0.26	47,49,50,50	0
3	BME	A	1	4/4	0.88	0.14	46,48,49,53	0
4	GOL	D	434	6/6	0.94	0.15	48,50,51,52	0
3	BME	C	1	4/4	0.94	0.31	58,60,60,63	0
3	BME	B	431	4/4	0.95	0.23	52,54,55,59	0
3	BME	D	1	4/4	0.95	0.33	52,54,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BME	D	431	4/4	0.96	0.10	43,44,45,48	0
6	PMP	B	432	16/16	0.96	0.18	28,35,41,42	0
6	PMP	D	432	16/16	0.96	0.20	20,24,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.