Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:01 pm BST

PDB ID	:	3DTV
Title	:	Crystal structure of arylmalonate decarboxylase
Authors	:	Nakasako, M.; Obata, R.; Miyamaoto, K.; Ohta, H.
Deposited on	:	2008-07-16
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

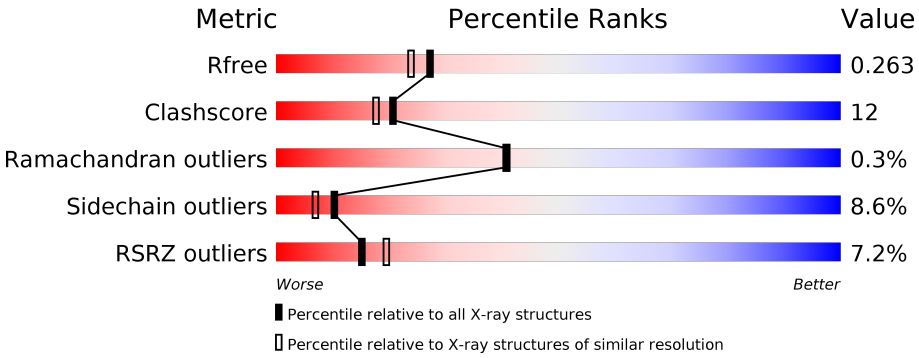
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	240	3% 69% 20% • 10%
2	B	240	9% 70% 23% • •
2	C	240	5% 72% 18% 6% 5%
3	D	240	10% 76% 20% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	1102	-	-	X	-
5	GOL	C	1103	-	-	-	X
5	GOL	D	1104	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7069 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 Arylmalonate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1576	993	275	300	8			

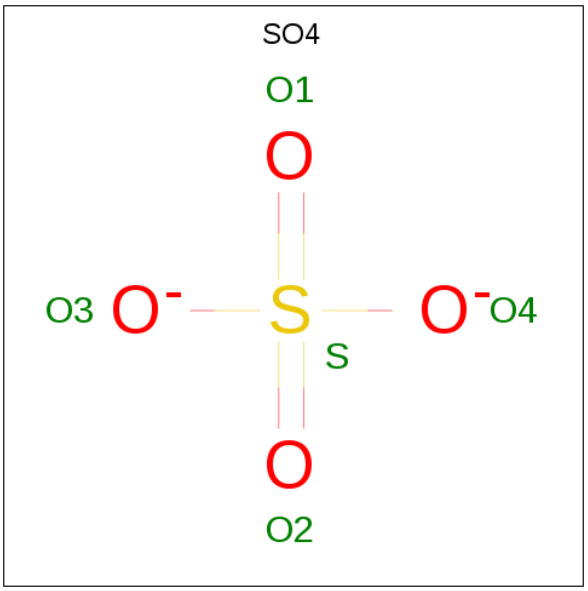
- Molecule 2 is a protein called Arylmalonate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1691	1065	295	321	10			
2	C	228	Total	C	N	O	S	0	0	0
			1654	1042	289	313	10			

- Molecule 3 is a protein called Arylmalonate decarboxylase.

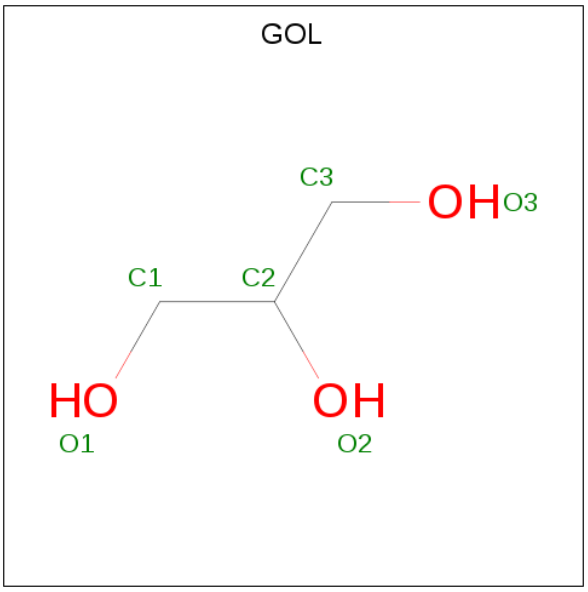
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	236	Total	C	N	O	S	0	0	0
			1707	1073	297	327	10			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



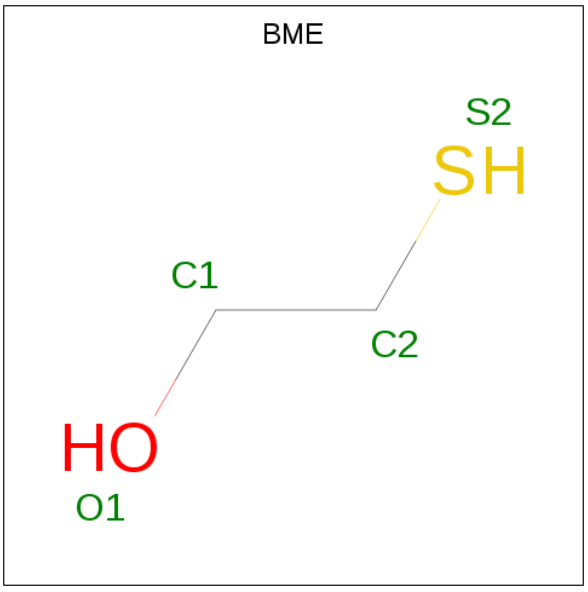
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 7 is water.

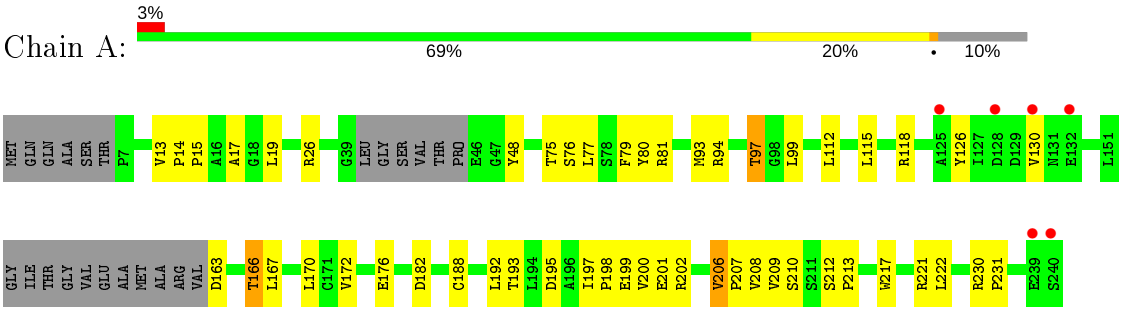
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	82	Total O 82 82	0	0
7	B	98	Total O 98 98	0	0
7	C	103	Total O 103 103	0	0
7	D	80	Total O 80 80	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

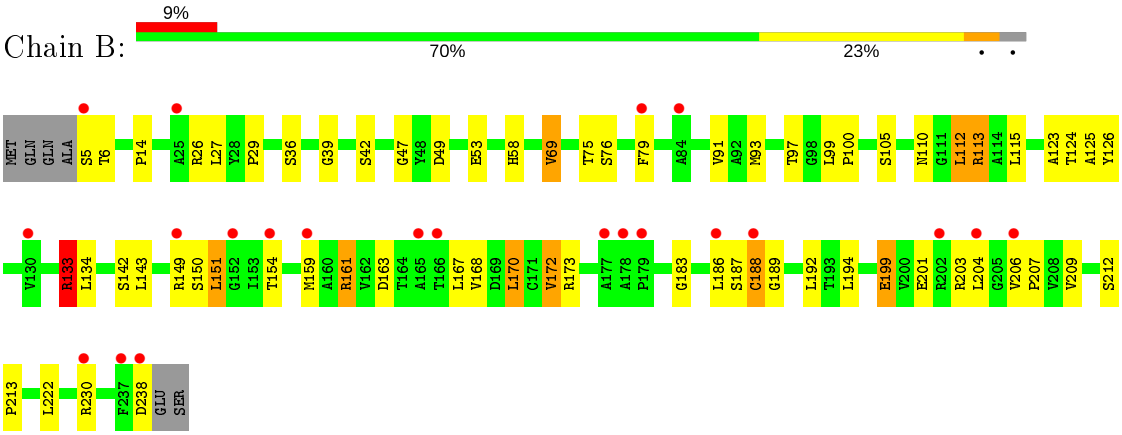
- Molecule 1: Arylmalonate decarboxylase

Chain A:



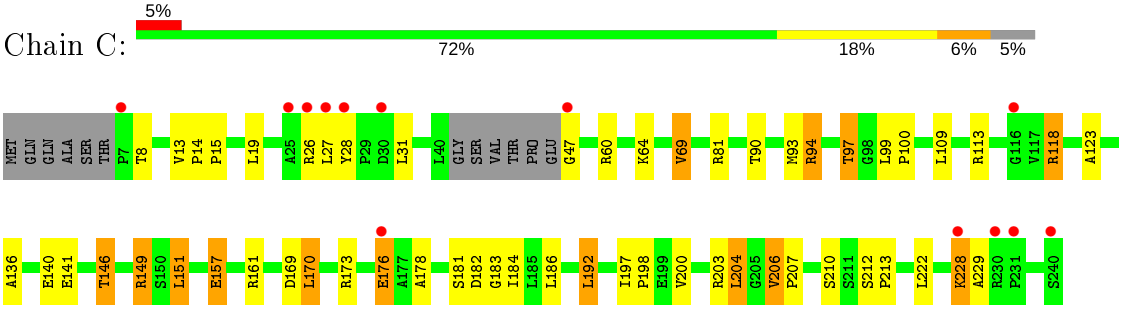
- Molecule 2: Arylmalonate decarboxylase

Chain B:



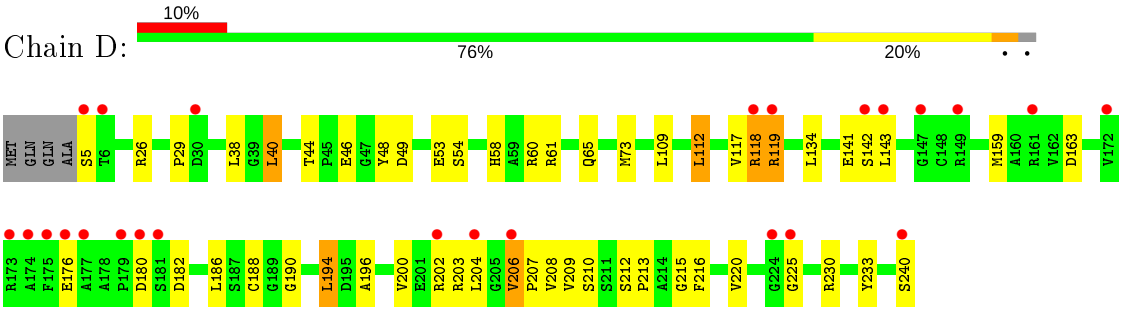
- Molecule 2: Arylmalonate decarboxylase

Chain C:



- Molecule 3: Arylmalonate decarboxylase

Chain D:


10%
76%
20%
MET GLN GLN ALA S5 T6 R26 P29 D30 L38 G39 L40 T44 P45 E46 G47 Y48 D49 E53 S54 H58 A59 R60 R61 Q65 M73 L109 L112 V117 R118 R119 L134 E141 S142 L143 G147 C148 R149 M159 A160 R161 V162 D163 V172
R173 A174 F175 E176 A177 A178 P179 D180 S181 D182 L186 S187 C188 G189 G190 L194 D195 A196 V200 E201 R202 R203 L204 G205 V206 P207 V208 V209 S210 S211 S212 P213 A214 G215 F216 V220 G224 G225 R230 Y233 S240

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.63Å 99.32Å 140.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 42.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.10) 98.6 (42.56-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.241 0.229 , 0.263	Depositor DCC
R_{free} test set	3386 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7069	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CME, SO4, BME

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	0.85	0/1601	0.76	2/2176 (0.1%)
2	B	0.99	7/1708 (0.4%)	0.90	4/2327 (0.2%)
2	C	1.00	3/1669 (0.2%)	0.88	3/2268 (0.1%)
3	D	0.87	3/1724 (0.2%)	0.75	1/2347 (0.0%)
All	All	0.93	13/6702 (0.2%)	0.83	10/9118 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	GLU	CD-OE1	8.85	1.35	1.25
2	B	142	SER	CB-OG	8.78	1.53	1.42
3	D	176	GLU	CD-OE1	7.80	1.34	1.25
2	B	142	SER	CA-CB	7.01	1.63	1.52
2	B	199	GLU	CD-OE2	6.85	1.33	1.25
3	D	203	ARG	CZ-NH1	6.72	1.41	1.33
2	B	203	ARG	CZ-NH1	5.99	1.40	1.33
3	D	176	GLU	CD-OE2	5.61	1.31	1.25
2	C	176	GLU	CG-CD	5.36	1.59	1.51
2	B	201	GLU	CD-OE2	5.25	1.31	1.25
2	B	203	ARG	CZ-NH2	5.24	1.39	1.33
2	C	157	GLU	CG-CD	5.13	1.59	1.51
2	C	47	GLY	N-CA	5.07	1.53	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	203	ARG	NE-CZ-NH2	-11.78	114.41	120.30
2	C	81	ARG	NE-CZ-NH1	9.72	125.16	120.30
2	B	203	ARG	NE-CZ-NH1	7.41	124.01	120.30
2	B	133	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	C	81	ARG	NE-CZ-NH2	-7.15	116.73	120.30
2	B	133	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	C	149	ARG	NE-CZ-NH2	-6.34	117.13	120.30
3	D	60	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	230	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	94	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	LEU	Peptide

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	1576	0	1592	36	1
2	B	1691	0	1719	50	0
2	C	1654	0	1681	44	0
3	D	1707	0	1730	43	1
4	A	20	0	0	0	0
4	B	15	0	0	1	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	9	0
5	C	6	0	8	0	0
5	D	6	0	8	4	0
6	B	4	0	6	2	0
7	A	82	0	0	1	0
7	B	98	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	103	0	0	1	0
7	D	80	0	0	0	0
All	All	7069	0	6760	166	1

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 (166) 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)
2:B:75:THR:H	5:B:1102:GOL:H12	1.10	1.10
2:C:118:ARG:HH21	2:C:118:ARG:CG	1.69	1.05
1:A:13:VAL:HG13	1:A:15:PRO:HD2	1.41	1.03
2:B:97:THR:HG23	2:B:99:LEU:H	1.22	1.02
2:B:14:PRO:HG2	5:B:1102:GOL:H2	1.44	0.99
1:A:199:GLU:OE2	2:B:161:ARG:HD3	1.63	0.99
2:C:146:THR:HG23	2:C:178:ALA:HB1	1.43	0.97
2:B:49:ASP:O	2:B:53:GLU:HG2	1.65	0.94
2:C:146:THR:HG21	2:C:181:SER:OG	1.71	0.91
2:C:97:THR:HG23	2:C:99:LEU:H	1.37	0.88
2:C:228:LYS:HD2	2:C:229:ALA:O	1.75	0.87
1:A:193:THR:HG21	1:A:210:SER:OG	1.74	0.86
2:C:118:ARG:HH21	2:C:118:ARG:HG3	1.39	0.86
2:C:13:VAL:CG1	2:C:15:PRO:HD2	2.06	0.85
1:A:163:ASP:OD1	1:A:166:THR:HG23	1.80	0.82
3:D:26:ARG:HD2	3:D:194:LEU:HD12	1.61	0.81
3:D:200:VAL:CG2	3:D:208:VAL:HG21	2.11	0.80
3:D:112:LEU:HD13	3:D:209:VAL:HG11	1.63	0.79
3:D:196:ALA:O	3:D:200:VAL:HG13	1.83	0.79
3:D:200:VAL:HG21	3:D:208:VAL:HG21	1.63	0.78
4:B:1004:SO4:O2	6:B:1101:BME:O1	2.00	0.78
3:D:112:LEU:HD13	3:D:209:VAL:CG1	2.13	0.78
2:C:146:THR:HG23	2:C:178:ALA:CB	2.12	0.78
2:C:183:GLY:HA2	2:C:206:VAL:HG13	1.64	0.78
2:C:13:VAL:HG12	2:C:15:PRO:HD2	1.65	0.77
3:D:5:SER:CB	3:D:225:GLY:HA2	2.16	0.76
2:B:75:THR:H	5:B:1102:GOL:C1	1.96	0.75
2:C:118:ARG:HH21	2:C:118:ARG:HG2	1.50	0.74
3:D:46:GLU:HG2	5:D:1104:GOL:H2	1.67	0.74
2:B:75:THR:N	5:B:1102:GOL:H12	1.95	0.74
1:A:202:ARG:HD2	2:B:161:ARG:NH1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:THR:HG23	2:B:99:LEU:N	2.02	0.70
1:A:202:ARG:HD2	2:B:161:ARG:HH12	1.56	0.70
1:A:206:VAL:HG22	1:A:207:PRO:HD2	1.74	0.70
2:B:76:SER:H	5:B:1102:GOL:H31	1.57	0.69
2:C:146:THR:CG2	2:C:178:ALA:HB1	2.21	0.68
1:A:13:VAL:CG1	1:A:15:PRO:HD2	2.23	0.67
1:A:97:THR:CG2	1:A:99:LEU:H	2.08	0.66
2:C:169:ASP:OD2	2:C:173:ARG:NH1	2.28	0.66
2:C:97:THR:HG23	2:C:99:LEU:N	2.11	0.66
2:C:97:THR:CG2	2:C:99:LEU:H	2.06	0.66
1:A:198:PRO:HB2	1:A:202:ARG:HH21	1.62	0.64
2:B:29:PRO:HG3	2:B:230:ARG:HD2	1.78	0.64
1:A:212:SER:HB3	1:A:213:PRO:HD3	1.80	0.64
2:B:47:GLY:HA2	6:B:1101:BME:H12	1.80	0.63
1:A:199:GLU:CD	2:B:161:ARG:HD3	2.19	0.63
2:C:118:ARG:NH2	2:C:118:ARG:HG2	2.12	0.62
2:B:69:VAL:HG22	2:B:100:PRO:HB2	1.81	0.62
3:D:44:THR:OG1	5:D:1104:GOL:H12	1.99	0.62
2:C:182:ASP:O	2:C:207:PRO:HD2	1.99	0.62
3:D:5:SER:HB3	3:D:225:GLY:HA2	1.81	0.62
2:B:26:ARG:O	2:B:230:ARG:HD3	1.99	0.62
2:B:14:PRO:CG	5:B:1102:GOL:H2	2.26	0.61
2:B:76:SER:H	5:B:1102:GOL:C3	2.13	0.61
3:D:61:ARG:O	3:D:65:GLN:HG3	2.01	0.61
2:B:79:PHE:CG	2:B:134:LEU:HD22	2.36	0.60
2:C:118:ARG:CG	2:C:118:ARG:NH2	2.43	0.60
2:C:13:VAL:HG13	2:C:15:PRO:HD2	1.85	0.59
1:A:231:PRO:HG2	2:B:230:ARG:HH12	1.68	0.59
3:D:159:MET:HE3	3:D:188:CME:OH	2.02	0.58
1:A:97:THR:HG23	1:A:99:LEU:H	1.68	0.58
2:B:183:GLY:HA2	2:B:206:VAL:HG13	1.86	0.57
2:C:109:LEU:HD11	2:C:141:GLU:HG3	1.86	0.57
2:B:124:THR:C	2:B:170:LEU:HD11	2.25	0.57
2:C:14:PRO:HB2	2:C:15:PRO:HD3	1.87	0.57
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.86	0.56
2:C:157:GLU:O	2:C:161:ARG:HG2	2.05	0.56
3:D:216:PHE:O	3:D:220:VAL:HG23	2.05	0.56
3:D:54:SER:O	3:D:58:HIS:HD2	1.88	0.56
1:A:172:VAL:O	1:A:176:GLU:HG3	2.06	0.56
1:A:217:TRP:CE2	1:A:221:ARG:HD2	2.41	0.56
2:C:200:VAL:HG13	2:C:204:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:212:SER:HB2	3:D:213:PRO:HD3	1.87	0.56
1:A:112:LEU:HG	1:A:209:VAL:HG21	1.88	0.55
1:A:26:ARG:NH2	1:A:195:ASP:OD1	2.36	0.55
3:D:112:LEU:HD13	3:D:209:VAL:HG13	1.89	0.55
2:B:36:SER:OG	2:B:58:HIS:HD2	1.89	0.54
2:C:184:ILE:HD11	2:C:204:LEU:HD23	1.89	0.54
1:A:118:ARG:HH11	1:A:118:ARG:HG3	1.73	0.53
1:A:197:ILE:O	1:A:201:GLU:HG3	2.08	0.53
3:D:200:VAL:CG2	3:D:208:VAL:CG2	2.84	0.53
1:A:199:GLU:OE2	2:B:161:ARG:CD	2.46	0.53
3:D:186:LEU:O	3:D:210:SER:HA	2.09	0.53
3:D:212:SER:HB2	3:D:213:PRO:CD	2.37	0.53
2:C:28:TYR:HB3	2:C:31:LEU:HG	1.90	0.53
2:B:115:LEU:HD13	2:B:207:PRO:HB2	1.89	0.53
2:C:60:ARG:O	2:C:64:LYS:HG3	2.10	0.52
2:C:151:LEU:HD13	2:C:170:LEU:HG	1.91	0.52
1:A:93:MET:O	1:A:97:THR:HB	2.09	0.52
1:A:126:TYR:HB3	1:A:130:VAL:HB	1.93	0.51
1:A:14:PRO:HB2	1:A:15:PRO:HD3	1.92	0.51
3:D:159:MET:HE3	3:D:190:GLY:HA3	1.93	0.51
3:D:46:GLU:CG	5:D:1104:GOL:H2	2.37	0.51
3:D:49:ASP:O	3:D:53:GLU:HG2	2.11	0.51
2:C:149:ARG:CD	2:C:173:ARG:HB3	2.41	0.51
2:B:212:SER:HB3	2:B:213:PRO:HD3	1.93	0.50
3:D:112:LEU:CD1	3:D:209:VAL:CG1	2.88	0.50
2:B:124:THR:O	2:B:170:LEU:HD11	2.12	0.50
2:C:69:VAL:HG22	2:C:100:PRO:HB2	1.94	0.49
3:D:194:LEU:HD13	3:D:233:TYR:CD2	2.47	0.49
1:A:97:THR:HG22	1:A:99:LEU:H	1.78	0.49
1:A:193:THR:HB	7:A:1165:HOH:O	2.13	0.48
1:A:97:THR:HG23	1:A:99:LEU:N	2.28	0.48
2:C:146:THR:CG2	2:C:178:ALA:CB	2.88	0.48
3:D:194:LEU:HD13	3:D:233:TYR:CG	2.49	0.48
2:C:184:ILE:CD1	2:C:204:LEU:HD23	2.44	0.47
3:D:112:LEU:CD1	3:D:209:VAL:HG13	2.44	0.47
3:D:119:ARG:NH1	3:D:180:ASP:OD1	2.47	0.47
3:D:182:ASP:O	3:D:206:VAL:HG22	2.14	0.47
2:C:212:SER:HB3	2:C:213:PRO:HD3	1.97	0.47
3:D:44:THR:OG1	5:D:1104:GOL:C1	2.62	0.47
2:B:29:PRO:CG	2:B:230:ARG:HD2	2.44	0.47
1:A:79:PHE:C	1:A:79:PHE:CD1	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASP:O	1:A:206:VAL:HG22	2.15	0.46
2:C:197:ILE:N	2:C:198:PRO:HD2	2.30	0.46
3:D:159:MET:HE3	3:D:188:CME:CZ	2.45	0.46
2:B:112:LEU:HD13	2:B:209:VAL:HG21	1.97	0.46
2:C:149:ARG:NE	2:C:173:ARG:HB3	2.31	0.46
2:C:192:LEU:HA	2:C:192:LEU:HD23	1.82	0.46
2:B:39:GLY:HA2	2:C:203:ARG:O	2.16	0.46
3:D:118:ARG:HG2	3:D:118:ARG:HH11	1.81	0.46
2:C:136:ALA:O	2:C:140:GLU:HG3	2.16	0.45
3:D:5:SER:CB	3:D:225:GLY:CA	2.92	0.45
1:A:217:TRP:CZ2	1:A:221:ARG:HD2	2.52	0.45
2:C:90:THR:HA	2:C:93:MET:CE	2.46	0.45
2:B:75:THR:OG1	5:B:1102:GOL:H11	2.17	0.45
2:B:133:ARG:HD3	2:B:133:ARG:HA	1.45	0.45
2:B:199:GLU:OE2	2:B:199:GLU:HA	2.17	0.45
3:D:109:LEU:HD11	3:D:141:GLU:HG3	1.99	0.44
2:B:93:MET:O	2:B:97:THR:HG22	2.17	0.44
3:D:141:GLU:O	3:D:142:SER:HB2	2.18	0.44
1:A:17:ALA:HB1	1:A:19:LEU:CD2	2.48	0.44
2:B:110:ASN:ND2	2:B:113:ARG:HH12	2.15	0.44
2:B:126:TYR:CE2	2:B:154:THR:HA	2.53	0.44
1:A:231:PRO:HG2	2:B:230:ARG:NH1	2.33	0.44
2:B:110:ASN:HD22	2:B:113:ARG:HH12	1.64	0.43
2:C:94:ARG:HA	2:C:97:THR:HG22	2.01	0.43
2:B:97:THR:CG2	2:B:99:LEU:H	2.11	0.43
3:D:73:MET:HE1	3:D:215:GLY:HA3	2.00	0.43
3:D:26:ARG:CD	3:D:194:LEU:HD12	2.40	0.43
2:B:124:THR:O	2:B:150:SER:HA	2.19	0.43
2:B:167:LEU:O	2:B:170:LEU:HB2	2.18	0.43
3:D:29:PRO:HG2	3:D:230:ARG:CZ	2.49	0.42
2:C:109:LEU:CD1	2:C:141:GLU:HG3	2.49	0.42
2:B:125:ALA:HA	2:B:151:LEU:HB2	2.02	0.42
3:D:230:ARG:HA	3:D:230:ARG:HD2	1.77	0.42
2:B:125:ALA:HB3	2:B:189:GLY:HA2	2.02	0.42
3:D:38:LEU:C	3:D:40:LEU:H	2.23	0.42
2:B:123:ALA:O	2:B:186:LEU:HA	2.19	0.42
2:C:186:LEU:O	2:C:210:SER:HA	2.20	0.41
2:B:168:VAL:O	2:B:172:VAL:HG23	2.20	0.41
1:A:200:VAL:HG11	1:A:208:VAL:HG21	2.03	0.41
2:B:187:SER:O	2:B:188:CYS:C	2.58	0.41
3:D:159:MET:HE1	3:D:188:CME:HZ2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:206:VAL:HG22	3:D:207:PRO:HD2	2.03	0.41
1:A:115:LEU:HD13	1:A:207:PRO:HB2	2.03	0.41
2:B:29:PRO:CD	2:B:230:ARG:HD2	2.51	0.41
2:B:79:PHE:CZ	2:B:105:SER:HA	2.56	0.41
3:D:117:VAL:HG13	3:D:182:ASP:HB2	2.03	0.41
1:A:76:SER:O	1:A:80:TYR:HB2	2.21	0.41
2:C:27:LEU:HD22	2:C:229:ALA:HB1	2.02	0.41
3:D:5:SER:HB2	3:D:225:GLY:CA	2.50	0.40
2:B:27:LEU:HD11	2:B:194:LEU:HD21	2.03	0.40
2:C:123:ALA:O	2:C:186:LEU:HD12	2.21	0.40
2:C:113:ARG:HD2	7:C:1106:HOH:O	2.22	0.40
2:B:75:THR:CB	5:B:1102:GOL:H11	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:OH	3:D:141:GLU:OE1[2_554]	2.13	0.07

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	211/240 (88%)	204 (97%)	6 (3%)	1 (0%)	29	26
2	B	231/240 (96%)	223 (96%)	7 (3%)	1 (0%)	34	32
2	C	223/240 (93%)	219 (98%)	3 (1%)	1 (0%)	34	32
3	D	233/240 (97%)	228 (98%)	5 (2%)	0	100	100
All	All	898/960 (94%)	874 (97%)	21 (2%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	188	CYS
1	A	188	CYS
2	C	8	THR

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	161/178 (90%)	152 (94%)	9 (6%)	21 18
2	B	172/177 (97%)	151 (88%)	21 (12%)	5 2
2	C	167/177 (94%)	152 (91%)	15 (9%)	9 6
3	D	174/177 (98%)	161 (92%)	13 (8%)	13 10
All	All	674/709 (95%)	616 (91%)	58 (9%)	10 7

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	77	LEU
1	A	81	ARG
1	A	97	THR
1	A	166	THR
1	A	167	LEU
1	A	170	LEU
1	A	206	VAL
1	A	222	LEU
2	B	5	SER
2	B	6	THR
2	B	42	SER
2	B	69	VAL
2	B	91	VAL
2	B	112	LEU
2	B	113	ARG
2	B	133	ARG
2	B	143	LEU
2	B	149	ARG

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Mol	Chain	Res	Type
2	B	151	LEU
2	B	159	MET
2	B	161	ARG
2	B	163	ASP
2	B	170	LEU
2	B	172	VAL
2	B	173	ARG
2	B	192	LEU
2	B	204	LEU
2	B	222	LEU
2	B	238	ASP
2	C	19	LEU
2	C	26	ARG
2	C	69	VAL
2	C	94	ARG
2	C	97	THR
2	C	118	ARG
2	C	146	THR
2	C	151	LEU
2	C	170	LEU
2	C	176	GLU
2	C	192	LEU
2	C	204	LEU
2	C	206	VAL
2	C	222	LEU
2	C	228	LYS
3	D	40	LEU
3	D	48	TYR
3	D	112	LEU
3	D	118	ARG
3	D	119	ARG
3	D	134	LEU
3	D	143	LEU
3	D	163	ASP
3	D	194	LEU
3	D	202	ARG
3	D	204	LEU
3	D	206	VAL
3	D	240	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	110	ASN
2	B	58	HIS
2	B	65	GLN
2	B	110	ASN
2	C	63	GLN
2	C	65	GLN
2	C	110	ASN
3	D	63	GLN
3	D	65	GLN
3	D	110	ASN
3	D	131	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
2	CME	B	148	2	8,9,10	0.63	0	5,9,11	1.76	2 (40%)
3	CME	D	188	3	8,9,10	0.49	0	5,9,11	1.12	0
2	CME	C	148	2	8,9,10	0.68	0	5,9,11	1.43	1 (20%)

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	CME	B	148	2	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CME	D	188	3	-	0/5/8/10	-
2	CME	C	148	2	-	1/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	148	CME	CB-SG-SD	3.08	111.81	103.82
2	B	148	CME	CB-SG-SD	2.73	110.89	103.82
2	B	148	CME	CZ-CE-SD	-2.32	105.31	113.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	148	CME	SD-CE-CZ-OH
2	B	148	CME	CZ-CE-SD-SG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	188	CME	3	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\|>2$
4	SO4	B	1004	-	4,4,4	0.19	0	6,6,6	0.29	0
5	GOL	D	1104	-	5,5,5	0.32	0	5,5,5	0.95	0
4	SO4	A	1000	-	4,4,4	0.07	0	6,6,6	0.28	0
4	SO4	C	1007	-	4,4,4	0.47	0	6,6,6	0.55	0
5	GOL	B	1102	-	5,5,5	0.55	0	5,5,5	0.95	0
6	BME	B	1101	-	3,3,3	0.18	0	1,2,2	1.38	0
4	SO4	A	1003	-	4,4,4	0.15	0	6,6,6	0.46	0
4	SO4	B	1006	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	A	1002	-	4,4,4	0.65	0	6,6,6	0.77	0
4	SO4	D	1009	-	4,4,4	0.23	0	6,6,6	0.39	0
4	SO4	B	1005	-	4,4,4	0.25	0	6,6,6	0.40	0
4	SO4	C	1008	-	4,4,4	0.16	0	6,6,6	0.30	0
5	GOL	C	1103	-	5,5,5	0.39	0	5,5,5	0.70	0
4	SO4	A	1001	-	4,4,4	0.32	0	6,6,6	0.43	0
5	GOL	A	1100	-	5,5,5	0.44	0	5,5,5	0.63	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	GOL	D	1104	-	-	0/4/4/4	-
6	BME	B	1101	-	-	0/1/1/1	-
5	GOL	B	1102	-	-	0/4/4/4	-
5	GOL	A	1100	-	-	3/4/4/4	-
5	GOL	C	1103	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1103	GOL	O1-C1-C2-C3
5	A	1100	GOL	O1-C1-C2-C3
5	C	1103	GOL	O1-C1-C2-O2
5	A	1100	GOL	O1-C1-C2-O2
5	C	1103	GOL	O2-C2-C3-O3
5	C	1103	GOL	C1-C2-C3-O3
5	A	1100	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1004	SO4	1	0
5	D	1104	GOL	4	0
5	B	1102	GOL	9	0
6	B	1101	BME	2	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	217/240 (90%)	0.26	6 (2%) 53 59	26, 46, 71, 99	0
2	B	233/240 (97%)	0.80	22 (9%) 8 11	26, 52, 84, 101	0
2	C	227/240 (94%)	0.39	13 (5%) 23 29	24, 38, 68, 81	0
3	D	235/240 (97%)	0.70	25 (10%) 6 7	27, 45, 74, 91	0
All	All	912/960 (95%)	0.54	66 (7%) 15 19	24, 45, 77, 101	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	240	SER	6.0
3	D	225	GLY	5.1
3	D	206	VAL	5.0
3	D	179	PRO	4.8
3	D	175	PHE	4.8
2	B	179	PRO	4.5
2	B	25	ALA	4.3
1	A	240	SER	4.1
3	D	143	LEU	4.0
2	B	238	ASP	3.9
2	C	27	LEU	3.8
3	D	172	VAL	3.5
3	D	142	SER	3.5
3	D	174	ALA	3.5
3	D	177	ALA	3.4
2	C	231	PRO	3.3
2	B	178	ALA	3.1
3	D	202	ARG	3.1
2	C	230	ARG	3.1
2	C	116	GLY	3.0
3	D	5	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	177	ALA	3.0
2	B	206	VAL	2.9
2	C	28	TYR	2.9
2	C	25	ALA	2.8
2	B	152	GLY	2.8
2	C	30	ASP	2.7
3	D	6	THR	2.7
2	B	5	SER	2.6
1	A	239	GLU	2.6
3	D	147	GLY	2.5
3	D	204	LEU	2.5
2	B	202	ARG	2.5
3	D	224	GLY	2.4
3	D	118	ARG	2.4
2	B	237	PHE	2.4
2	B	130	VAL	2.4
1	A	128	ASP	2.4
2	C	7	PRO	2.3
2	B	188	CYS	2.3
2	C	228	LYS	2.3
1	A	125	ALA	2.3
3	D	161	ARG	2.3
3	D	30	ASP	2.3
2	C	240	SER	2.3
2	B	149	ARG	2.3
1	A	130	VAL	2.2
2	B	230	ARG	2.2
3	D	181	SER	2.2
3	D	176	GLU	2.2
2	C	47	GLY	2.2
3	D	173	ARG	2.2
2	B	154	THR	2.2
2	B	159	MET	2.2
2	B	204	LEU	2.1
2	B	84	ALA	2.1
2	B	165	ALA	2.1
2	C	26	ARG	2.1
2	C	176	GLU	2.1
2	B	79	PHE	2.1
1	A	132	GLU	2.1
3	D	149	ARG	2.1
3	D	119	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	166	THR	2.0
2	B	186	LEU	2.0
3	D	180	ASP	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CME	B	148	10/11	0.77	0.17	62,65,72,74	0
2	CME	C	148	10/11	0.86	0.13	39,42,51,53	0
3	CME	D	188	10/11	0.95	0.14	39,44,47,47	0

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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	C	1103	6/6	0.76	0.46	61,67,68,70	0
4	SO4	B	1006	5/5	0.78	0.29	133,133,133,133	0
5	GOL	B	1102	6/6	0.80	0.27	53,55,57,57	0
4	SO4	B	1005	5/5	0.81	0.46	98,98,98,99	0
5	GOL	D	1104	6/6	0.83	0.27	61,61,61,62	0
5	GOL	A	1100	6/6	0.85	0.17	56,59,59,60	0
6	BME	B	1101	4/4	0.90	0.21	71,72,72,75	0
4	SO4	B	1004	5/5	0.91	0.14	86,86,87,87	0
4	SO4	C	1008	5/5	0.93	0.20	92,93,93,93	0
4	SO4	D	1009	5/5	0.93	0.19	75,77,78,78	0
4	SO4	A	1003	5/5	0.93	0.20	77,78,79,80	0
4	SO4	A	1002	5/5	0.94	0.14	53,54,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1000	5/5	0.96	0.16	83,83,84,84	0
4	SO4	A	1001	5/5	0.97	0.08	46,48,49,49	0
4	SO4	C	1007	5/5	0.99	0.07	35,35,36,37	0

6.5 Other polymers (i)

There are no such residues in this entry.