Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:24 AM GMT

PDB ID	:	3EIS
Title	:	Crystal Structure of Arylmalonate Decarboxylase
Authors	:	Nakasako, M.; Obata, R.; Miyamoto, K.; Ohta, H.
Deposited on	:	2008-09-17
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

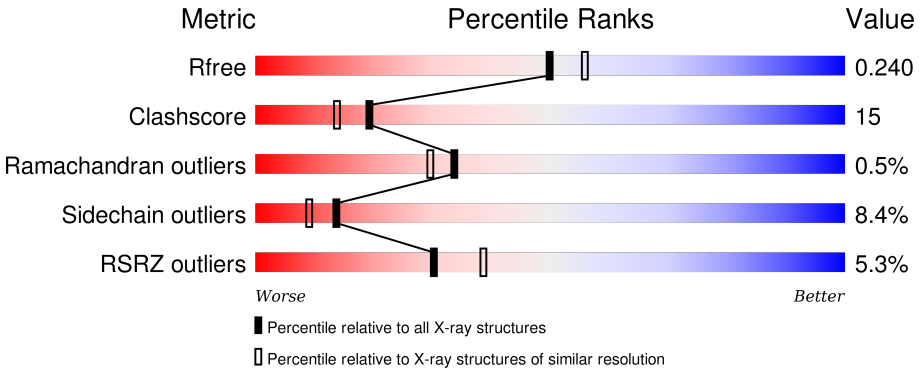
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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	5% 70% 20% 7%
1	B	240	4% 68% 25% 5%
1	C	240	5% 74% 19%
1	D	240	7% 79% 18%

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
1	CME	C	188	-	-	X	-
2	SO4	D	1004	-	-	X	X
3	GOL	A	1100	-	-	-	X
3	GOL	B	1102	-	-	-	X
3	GOL	D	1103	-	-	X	X

2 Entry composition

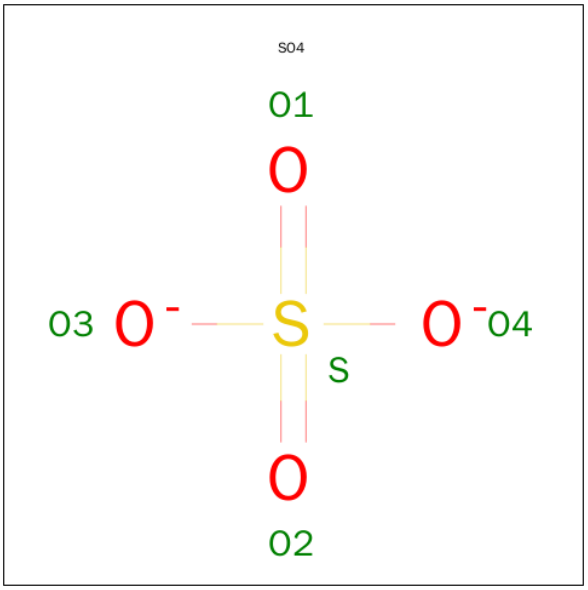
There are 4 unique types of molecules in this entry. The entry contains 7212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	224	Total	C	N	O	S	0	0	0
			1635	1030	285	309	11			
1	B	234	Total	C	N	O	S	0	0	0
			1695	1067	295	322	11			
1	C	236	Total	C	N	O	S	0	0	0
			1711	1075	297	328	11			
1	D	237	Total	C	N	O	S	0	0	0
			1716	1078	298	329	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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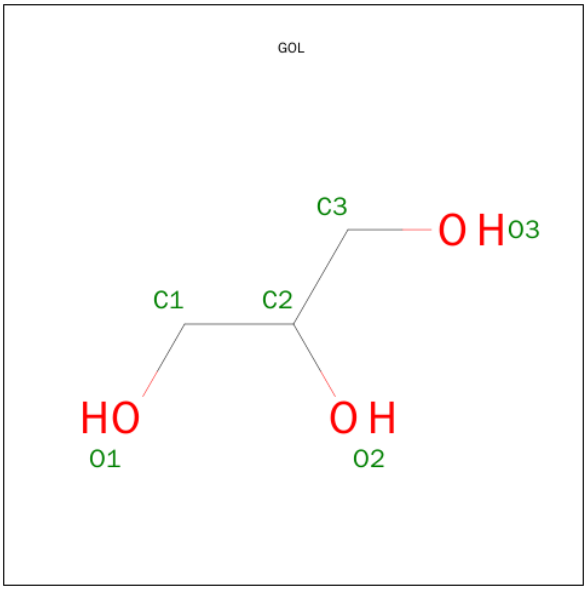
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	88	Total O 88 88	0	0
4	B	121	Total O 121 121	0	0

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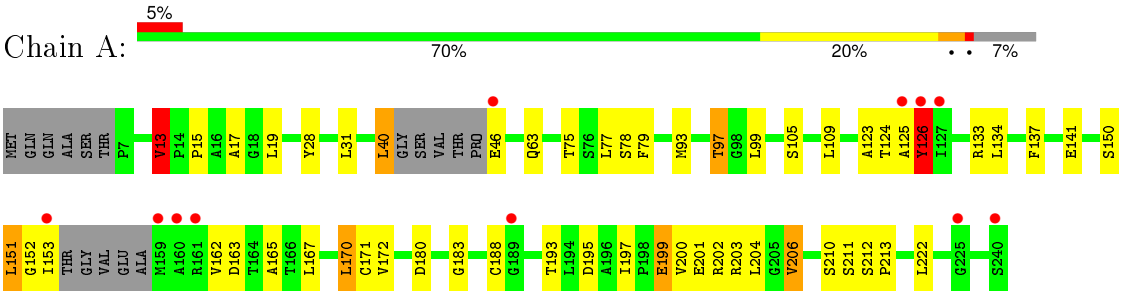
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	121	Total O 121 121	0	0
4	D	76	Total O 76 76	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

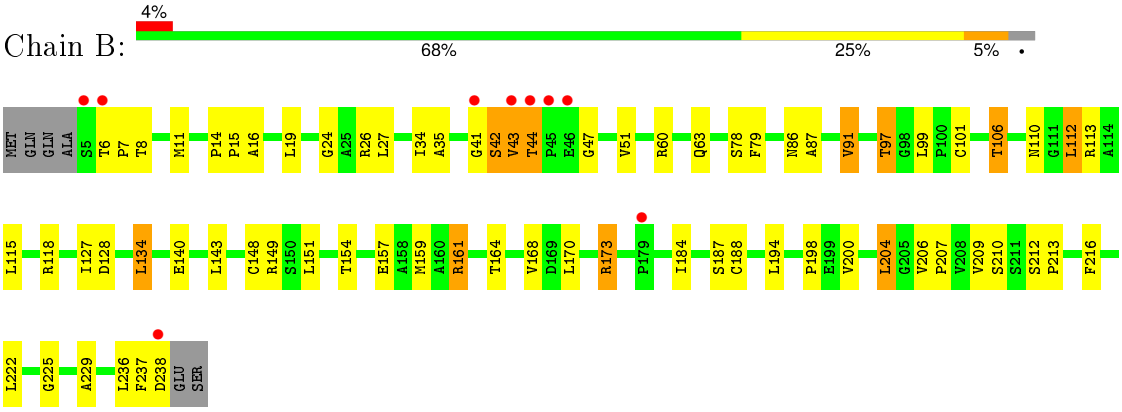
- Molecule 1: Arylmalonate decarboxylase

Chain A:



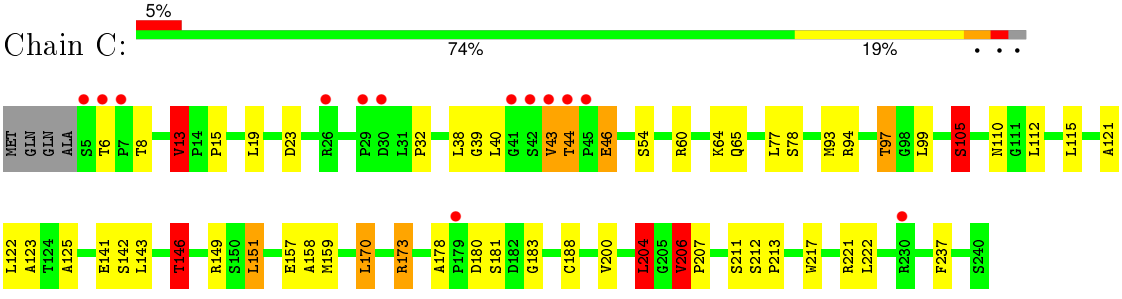
- Molecule 1: Arylmalonate decarboxylase

Chain B:



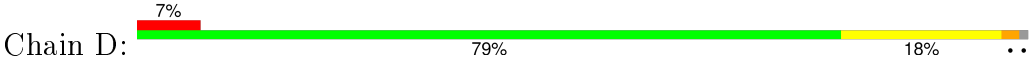
- Molecule 1: Arylmalonate decarboxylase

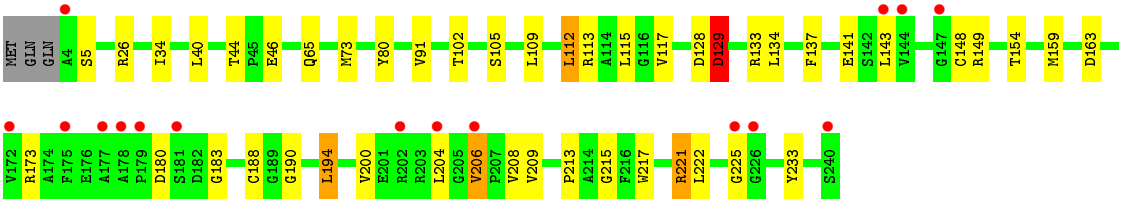
Chain C:



- Molecule 1: Arylmalonate decarboxylase

Chain D:




MET GLN GLN A4 S5 R26 I34 L40 T44 P45 E46 Q65 M73 Y80 V91 T102 S105 L109 L112 R113 A114 L115 G116 V117 D128 D129 R133 L134 F137 E141 S142 L143 V144 G147 C148 R149 T154 M159 D163
V172 R173 A174 F175 E176 A177 A178 P179 D180 S181 D182 G183 C188 G189 G190 L194 V200 E201 R202 R203 L204 G205 V206 P207 V208 V209 P213 A214 G215 F216 W217 R221 L222 G225 G226 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	83.51Å 99.39Å 139.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 49.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.10) 99.3 (49.70-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.240 0.198 , 0.240	Depositor DCC
R_{free} test set	3453 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 78730 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7212	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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, 0.375 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, CME, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.87	2/1638 (0.1%)	0.92	1/2222 (0.0%)
1	B	0.94	2/1701 (0.1%)	0.97	3/2316 (0.1%)
1	C	1.03	2/1717 (0.1%)	1.03	9/2336 (0.4%)
1	D	0.83	1/1722 (0.1%)	0.93	3/2343 (0.1%)
All	All	0.92	7/6778 (0.1%)	0.96	16/9217 (0.2%)

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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	SER	CB-OG	-7.71	1.32	1.42
1	B	78	SER	CB-OG	-7.04	1.33	1.42
1	A	171	CYS	CB-SG	-6.90	1.70	1.82
1	D	129	ASP	CB-CG	6.00	1.64	1.51
1	C	105	SER	CB-OG	-5.99	1.34	1.42
1	A	199	GLU	CG-CD	5.15	1.59	1.51
1	B	101	CYS	CB-SG	-5.09	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	26	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	D	26	ARG	NE-CZ-NH2	-10.30	115.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	163	ASP	CB-CG-OD1	-7.85	111.24	118.30
1	B	91	VAL	CG1-CB-CG2	6.49	121.28	110.90
1	C	60	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	C	211	SER	CB-CA-C	-5.83	99.03	110.10
1	C	206	VAL	CG1-CB-CG2	5.78	120.15	110.90
1	C	13	VAL	CG1-CB-CG2	5.78	120.14	110.90
1	C	146	THR	N-CA-CB	-5.68	99.52	110.30
1	C	204	LEU	CB-CG-CD1	5.60	120.51	111.00
1	B	51	VAL	CB-CA-C	-5.36	101.22	111.40
1	B	134	LEU	CB-CG-CD2	5.18	119.81	111.00
1	A	13	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	C	60	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	146	THR	OG1-CB-CG2	5.05	121.61	110.00
1	C	64	LYS	CD-CE-NZ	-5.00	100.19	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	225	GLY	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	1635	0	1659	49	0
1	B	1695	0	1722	50	0
1	C	1711	0	1733	58	0
1	D	1716	0	1738	51	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	3	0
3	A	12	0	16	2	0
3	B	6	0	8	3	0
3	D	6	0	8	4	0
4	A	88	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	121	0	0	6	3
4	C	121	0	0	3	2
4	D	76	0	0	5	0
All	All	7212	0	6884	207	3

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 15.

All (207) 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:D:154:THR:HG21	1:D:159:MET:HE2	1.21	1.18
1:C:151:LEU:HD23	1:C:188:CME:HZ2	1.18	1.13
1:A:202:ARG:HD2	4:B:1125:HOH:O	1.47	1.12
1:D:221:ARG:HB3	1:D:221:ARG:NH1	1.72	1.03
1:C:146:THR:HG21	1:C:181:SER:OG	1.57	1.02
1:D:154:THR:HG21	1:D:159:MET:CE	1.88	1.02
1:C:125:ALA:HB2	1:C:188:CME:HZ3	1.42	0.99
1:C:146:THR:HG23	1:C:178:ALA:HB1	1.48	0.96
1:A:124:THR:HG22	1:A:126:TYR:H	1.31	0.95
1:D:154:THR:CG2	1:D:159:MET:HE2	1.96	0.95
1:C:78:SER:HB3	1:C:105:SER:HB2	1.49	0.94
1:D:154:THR:CG2	1:D:159:MET:CE	2.45	0.94
1:B:97:THR:HG23	1:B:99:LEU:H	1.33	0.94
1:D:221:ARG:HG2	4:D:1127:HOH:O	1.68	0.93
1:B:140:GLU:OE2	4:B:1182:HOH:O	1.84	0.93
1:C:125:ALA:CB	1:C:188:CME:HZ3	1.98	0.92
1:D:173:ARG:HG3	2:D:1004:SO4:O4	1.71	0.90
1:C:151:LEU:HD23	1:C:188:CME:CZ	2.03	0.88
1:B:44:THR:HB	1:B:47:GLY:HA3	1.56	0.87
1:D:221:ARG:HB3	1:D:221:ARG:HH11	1.36	0.86
1:C:125:ALA:HB1	1:C:159:MET:HE1	1.59	0.84
1:A:17:ALA:HB1	1:A:19:LEU:HD21	1.62	0.81
1:C:183:GLY:HA2	1:C:206:VAL:HG13	1.62	0.80
1:B:60:ARG:HD3	4:B:1218:HOH:O	1.81	0.80
1:A:195:ASP:OD2	4:A:1148:HOH:O	1.99	0.80
1:D:5:SER:HB3	1:D:225:GLY:HA2	1.65	0.78
1:A:125:ALA:O	1:A:151:LEU:HB2	1.84	0.78
1:B:110:ASN:ND2	1:B:113:ARG:HH22	1.82	0.77
1:C:151:LEU:CD2	1:C:188:CME:HZ2	2.08	0.77
1:C:123:ALA:HB1	1:C:170:LEU:HD13	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:MET:O	1:C:97:THR:HB	1.85	0.76
1:D:46:GLU:OE1	3:D:1103:GOL:H11	1.85	0.75
1:A:75:THR:H	3:A:1101:GOL:H2	1.51	0.75
1:B:97:THR:CG2	1:B:99:LEU:H	2.00	0.74
1:C:13:VAL:HG13	1:C:15:PRO:HD2	1.69	0.73
1:B:97:THR:HG23	1:B:99:LEU:N	2.04	0.73
1:A:153:ILE:HG22	1:A:153:ILE:O	1.87	0.73
1:D:221:ARG:CB	1:D:221:ARG:HH11	2.01	0.72
1:C:125:ALA:HB2	1:C:188:CME:CZ	2.18	0.72
1:D:109:LEU:HD13	1:D:141:GLU:HG2	1.71	0.72
1:D:154:THR:CG2	1:D:159:MET:HE3	2.18	0.72
1:A:46:GLU:HA	1:A:46:GLU:OE2	1.90	0.72
1:A:97:THR:CG2	1:A:99:LEU:H	2.02	0.72
1:A:17:ALA:HB1	1:A:19:LEU:CD2	2.20	0.72
1:C:151:LEU:CD2	1:C:188:CME:HE3	2.20	0.71
1:A:13:VAL:HG13	1:A:15:PRO:HD2	1.72	0.71
1:D:173:ARG:CG	2:D:1004:SO4:O4	2.40	0.69
1:A:199:GLU:O	1:A:203:ARG:HG3	1.92	0.69
1:C:146:THR:HG23	1:C:178:ALA:CB	2.22	0.68
1:A:124:THR:HG22	1:A:126:TYR:N	2.06	0.68
1:B:6:THR:CG2	1:B:7:PRO:HD2	2.24	0.68
1:B:79:PHE:CG	1:B:134:LEU:HD22	2.29	0.67
1:C:115:LEU:HD13	1:C:207:PRO:HB2	1.76	0.67
1:A:152:GLY:O	1:A:153:ILE:HD13	1.95	0.66
1:C:200:VAL:HG13	1:C:204:LEU:HD22	1.77	0.66
1:B:115:LEU:HD13	1:B:207:PRO:HB2	1.77	0.66
1:C:23:ASP:OD1	4:C:1259:HOH:O	2.14	0.65
1:A:193:THR:HG21	1:A:210:SER:OG	1.95	0.65
1:A:151:LEU:HD13	1:A:170:LEU:HG	1.77	0.65
1:B:27:LEU:HD22	1:B:229:ALA:HB1	1.79	0.65
1:C:157:GLU:HG2	1:C:158:ALA:N	2.13	0.64
1:D:173:ARG:HD2	4:D:1166:HOH:O	1.97	0.64
1:C:97:THR:CG2	1:C:99:LEU:H	2.12	0.63
1:C:65:GLN:NE2	4:C:1309:HOH:O	2.32	0.63
1:B:210:SER:HB3	1:B:213:PRO:HG2	1.81	0.62
1:B:154:THR:O	1:B:157:GLU:HG2	1.99	0.62
1:D:113:ARG:NH2	1:D:141:GLU:HG3	2.14	0.62
1:A:93:MET:O	1:A:97:THR:HB	2.00	0.62
1:A:204:LEU:N	1:A:204:LEU:HD12	2.13	0.62
1:D:129:ASP:HB3	4:D:1177:HOH:O	1.99	0.62
1:A:19:LEU:HD22	1:A:19:LEU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:HB	3:B:1102:GOL:H32	1.82	0.61
1:B:24:GLY:HA3	1:B:216:PHE:CZ	2.36	0.61
1:B:161:ARG:H	1:B:161:ARG:NE	1.98	0.61
1:D:173:ARG:HG3	2:D:1004:SO4:S	2.40	0.60
1:D:46:GLU:HG2	4:D:1176:HOH:O	1.99	0.60
1:B:127:ILE:HA	3:B:1102:GOL:H12	1.82	0.60
1:C:110:ASN:ND2	4:C:1272:HOH:O	2.31	0.60
1:D:109:LEU:CD1	1:D:141:GLU:HG2	2.32	0.60
1:A:124:THR:HG23	1:A:188:CME:SG	2.42	0.60
1:C:40:LEU:CD2	1:C:44:THR:HG21	2.32	0.59
1:A:109:LEU:HD11	1:A:137:PHE:CE2	2.37	0.59
1:B:24:GLY:HA3	1:B:216:PHE:CE2	2.38	0.58
1:A:183:GLY:HA2	1:A:206:VAL:HG13	1.86	0.58
1:A:97:THR:HG23	1:A:99:LEU:H	1.69	0.58
1:D:217:TRP:O	1:D:221:ARG:HG3	2.04	0.57
1:A:17:ALA:CB	1:A:19:LEU:CD2	2.82	0.57
1:B:128:ASP:HB2	3:B:1102:GOL:H31	1.86	0.57
1:D:112:LEU:HD13	1:D:209:VAL:HG13	1.87	0.57
1:A:75:THR:N	3:A:1101:GOL:H2	2.18	0.57
1:A:172:VAL:HG22	1:A:204:LEU:HD11	1.87	0.57
1:A:109:LEU:HD11	1:A:137:PHE:HE2	1.70	0.57
1:A:151:LEU:CD1	1:A:170:LEU:HG	2.33	0.57
1:D:221:ARG:CB	1:D:221:ARG:NH1	2.57	0.57
1:D:44:THR:OG1	3:D:1103:GOL:H31	2.05	0.56
1:D:105:SER:HB3	1:D:137:PHE:CZ	2.40	0.56
1:B:6:THR:HG23	1:B:7:PRO:HD2	1.88	0.55
1:C:43:VAL:O	1:C:44:THR:HB	2.06	0.55
1:B:86:ASN:HD21	1:B:106:THR:CG2	2.19	0.55
1:A:200:VAL:O	1:A:204:LEU:HD13	2.07	0.55
1:A:153:ILE:CG2	1:A:153:ILE:O	2.56	0.54
1:D:154:THR:HG22	1:D:159:MET:HE3	1.88	0.54
1:A:109:LEU:HD11	1:A:141:GLU:HG3	1.90	0.54
1:D:154:THR:HG22	1:D:159:MET:CE	2.34	0.54
1:D:102:THR:HB	1:D:222:LEU:CD1	2.38	0.54
1:B:110:ASN:ND2	1:B:113:ARG:NH2	2.53	0.54
1:C:97:THR:HG23	1:C:99:LEU:H	1.73	0.54
1:D:200:VAL:HG22	1:D:208:VAL:HG21	1.91	0.53
1:C:217:TRP:HB2	1:C:237:PHE:CE1	2.43	0.53
1:A:97:THR:HG22	1:A:99:LEU:H	1.71	0.53
1:A:197:ILE:O	1:A:201:GLU:HG3	2.09	0.53
1:D:102:THR:HB	1:D:222:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:HD13	1:D:209:VAL:CG1	2.40	0.52
1:A:199:GLU:O	1:A:203:ARG:CG	2.57	0.52
1:C:151:LEU:CD2	1:C:188:CME:CE	2.87	0.52
1:D:115:LEU:HB2	1:D:117:VAL:HG23	1.91	0.52
1:C:217:TRP:CZ2	1:C:221:ARG:HD2	2.45	0.51
1:C:125:ALA:CA	1:C:188:CME:HZ3	2.40	0.51
1:A:125:ALA:HA	1:A:151:LEU:HD22	1.93	0.51
1:D:188:CME:HZ3	1:D:190:GLY:HA3	1.91	0.51
1:C:151:LEU:HD22	1:C:188:CME:HE3	1.92	0.51
1:B:200:VAL:HG13	1:B:204:LEU:HD22	1.93	0.50
1:B:184:ILE:HD11	1:B:204:LEU:HD23	1.93	0.50
1:C:40:LEU:HD11	1:C:77:LEU:HD11	1.92	0.50
1:D:129:ASP:CB	4:D:1177:HOH:O	2.59	0.50
1:C:40:LEU:HD23	1:C:44:THR:HG21	1.92	0.50
1:A:212:SER:HB3	1:A:213:PRO:HD3	1.93	0.50
1:C:149:ARG:HG3	1:C:173:ARG:HG2	1.94	0.49
1:A:79:PHE:CG	1:A:134:LEU:HD22	2.47	0.49
1:B:112:LEU:HD13	1:B:209:VAL:HG21	1.94	0.49
1:D:34:ILE:HG21	1:D:65:GLN:HE21	1.77	0.49
1:B:14:PRO:HD2	1:B:15:PRO:HD3	1.93	0.49
1:B:173:ARG:HG2	4:B:1153:HOH:O	2.11	0.49
1:C:151:LEU:CD2	1:C:188:CME:CZ	2.82	0.49
1:B:6:THR:HG22	1:B:7:PRO:HD2	1.95	0.49
1:B:87:ALA:O	1:B:91:VAL:HG13	2.13	0.49
1:B:43:VAL:HG23	1:B:43:VAL:O	2.14	0.48
1:B:118:ARG:NE	4:B:1225:HOH:O	2.47	0.48
1:C:97:THR:HG22	1:C:99:LEU:H	1.77	0.48
1:A:97:THR:HG23	1:A:99:LEU:N	2.29	0.48
1:D:194:LEU:HD13	1:D:233:TYR:CD2	2.49	0.48
1:C:40:LEU:HD22	1:C:44:THR:HG21	1.96	0.47
1:C:44:THR:O	1:C:44:THR:HG23	2.12	0.47
1:C:44:THR:O	1:C:44:THR:CG2	2.61	0.47
1:C:212:SER:HB3	1:C:213:PRO:HD3	1.96	0.47
1:C:97:THR:HG23	1:C:99:LEU:HB2	1.95	0.47
1:D:80:TYR:O	1:D:133:ARG:HD2	2.13	0.47
1:C:200:VAL:CG1	1:C:204:LEU:HD22	2.44	0.47
1:D:115:LEU:HD12	1:D:209:VAL:HG12	1.97	0.47
1:D:200:VAL:HG22	1:D:208:VAL:CG2	2.45	0.46
1:A:163:ASP:OD1	1:A:165:ALA:HB3	2.16	0.46
1:B:44:THR:O	1:B:47:GLY:N	2.46	0.46
1:C:141:GLU:O	1:C:142:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:O	1:A:150:SER:HA	2.16	0.46
1:C:39:GLY:O	1:C:43:VAL:N	2.48	0.46
1:D:5:SER:HB3	1:D:225:GLY:CA	2.43	0.46
1:B:27:LEU:HD11	1:B:237:PHE:CZ	2.51	0.45
1:C:180:ASP:N	1:C:180:ASP:OD2	2.43	0.45
1:B:24:GLY:HA3	1:B:216:PHE:CE1	2.51	0.45
1:A:124:THR:CG2	1:A:188:CME:SG	3.04	0.45
1:A:109:LEU:CD1	1:A:137:PHE:HE2	2.30	0.45
1:B:24:GLY:HA3	1:B:216:PHE:CD2	2.52	0.45
1:C:112:LEU:HD13	1:C:143:LEU:HD13	1.99	0.45
1:B:212:SER:HB3	1:B:213:PRO:HD3	1.99	0.45
1:B:79:PHE:CB	1:B:134:LEU:HD22	2.46	0.44
1:C:38:LEU:HB2	1:C:40:LEU:HG	1.99	0.44
1:B:148:CME:O	1:B:149:ARG:HD2	2.18	0.44
1:A:28:TYR:HB3	1:A:31:LEU:HG	2.00	0.44
1:B:8:THR:CG2	1:B:34:ILE:HG12	2.48	0.44
1:A:40:LEU:O	1:A:40:LEU:HD23	2.18	0.44
1:D:44:THR:OG1	3:D:1103:GOL:C3	2.66	0.43
1:C:217:TRP:HB2	1:C:237:PHE:HE1	1.83	0.43
1:B:200:VAL:CG1	1:B:204:LEU:HD22	2.49	0.43
1:B:63:GLN:HG3	1:B:99:LEU:HD11	1.99	0.43
1:C:146:THR:CG2	1:C:181:SER:OG	2.47	0.43
1:D:46:GLU:OE1	3:D:1103:GOL:C1	2.63	0.43
1:B:110:ASN:HD22	1:B:113:ARG:NH2	2.16	0.43
1:A:105:SER:HB3	1:A:137:PHE:CZ	2.53	0.43
1:C:122:LEU:N	1:C:122:LEU:HD12	2.34	0.43
1:D:149:ARG:HE	1:D:173:ARG:HE	1.66	0.43
1:B:42:SER:HB3	1:B:43:VAL:H	1.47	0.43
1:B:194:LEU:O	1:B:198:PRO:HD2	2.19	0.43
1:C:157:GLU:CG	1:C:158:ALA:N	2.82	0.43
1:A:165:ALA:HB2	4:B:1126:HOH:O	2.19	0.42
1:A:133:ARG:HD3	1:A:133:ARG:HA	1.68	0.42
1:B:164:THR:O	1:B:168:VAL:HG23	2.19	0.42
1:C:46:GLU:HG2	1:C:46:GLU:H	1.72	0.42
1:D:128:ASP:HA	1:D:148:CME:OH	2.19	0.42
1:D:115:LEU:CB	1:D:117:VAL:HG23	2.49	0.42
1:A:123:ALA:HB1	1:A:170:LEU:HD13	2.01	0.42
1:B:11:MET:O	1:B:35:ALA:HA	2.20	0.41
1:C:8:THR:HA	1:C:32:PRO:HG2	2.02	0.41
1:B:187:SER:O	1:B:188:CME:C	2.67	0.41
1:C:40:LEU:HA	1:C:40:LEU:HD23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ALA:HB3	1:C:204:LEU:HD12	2.02	0.41
1:B:86:ASN:HD21	1:B:106:THR:HG23	1.85	0.41
1:D:34:ILE:HG21	1:D:65:GLN:NE2	2.35	0.41
1:D:194:LEU:HD23	1:D:213:PRO:HG3	2.03	0.41
1:D:73:MET:HE1	1:D:215:GLY:HA3	2.02	0.41
1:B:236:LEU:O	1:B:238:ASP:N	2.47	0.41
1:C:121:ALA:HA	1:C:146:THR:HG22	2.03	0.41
1:C:97:THR:HG23	1:C:99:LEU:CB	2.51	0.41
1:D:113:ARG:HH22	1:D:141:GLU:HG3	1.85	0.41
1:D:128:ASP:OD2	1:D:148:CME:OH	2.39	0.41
1:D:183:GLY:HA2	1:D:206:VAL:HG13	2.03	0.41
1:A:204:LEU:CD1	1:A:204:LEU:N	2.83	0.40
1:C:77:LEU:HA	1:C:77:LEU:HD23	1.92	0.40

All (3) 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)
4:B:1177:HOH:O	4:C:1267:HOH:O[3_656]	1.92	0.28
4:B:1222:HOH:O	4:C:1299:HOH:O[3_656]	1.92	0.28
4:A:1183:HOH:O	4:B:1141:HOH:O[4_456]	2.17	0.03

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	216/240 (90%)	210 (97%)	5 (2%)	1 (0%)	34 30
1	B	230/240 (96%)	221 (96%)	6 (3%)	3 (1%)	15 9
1	C	232/240 (97%)	223 (96%)	8 (3%)	1 (0%)	39 37
1	D	233/240 (97%)	226 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	911/960 (95%)	880 (97%)	26 (3%)	5 (0%)	34 30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	GLY
1	A	126	TYR
1	C	44	THR
1	B	159	MET
1	B	43	VAL

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	164/176 (93%)	149 (91%)	15 (9%)	12 7
1	B	171/176 (97%)	156 (91%)	15 (9%)	12 8
1	C	173/176 (98%)	157 (91%)	16 (9%)	11 7
1	D	173/176 (98%)	162 (94%)	11 (6%)	22 18
All	All	681/704 (97%)	624 (92%)	57 (8%)	14 9

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	40	LEU
1	A	63	GLN
1	A	77	LEU
1	A	78	SER
1	A	97	THR
1	A	126	TYR
1	A	151	LEU
1	A	162	VAL
1	A	167	LEU

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Mol	Chain	Res	Type
1	A	170	LEU
1	A	180	ASP
1	A	206	VAL
1	A	211	SER
1	A	222	LEU
1	B	19	LEU
1	B	26	ARG
1	B	42	SER
1	B	44	THR
1	B	97	THR
1	B	106	THR
1	B	112	LEU
1	B	143	LEU
1	B	151	LEU
1	B	161	ARG
1	B	170	LEU
1	B	173	ARG
1	B	204	LEU
1	B	206	VAL
1	B	222	LEU
1	C	6	THR
1	C	13	VAL
1	C	19	LEU
1	C	43	VAL
1	C	46	GLU
1	C	54	SER
1	C	94	ARG
1	C	97	THR
1	C	105	SER
1	C	146	THR
1	C	151	LEU
1	C	170	LEU
1	C	173	ARG
1	C	204	LEU
1	C	206	VAL
1	C	222	LEU
1	D	40	LEU
1	D	91	VAL
1	D	112	LEU
1	D	129	ASP
1	D	134	LEU
1	D	143	LEU

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Mol	Chain	Res	Type
1	D	180	ASP
1	D	194	LEU
1	D	204	LEU
1	D	206	VAL
1	D	221	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	110	ASN
1	B	65	GLN
1	B	86	ASN
1	B	110	ASN
1	C	110	ASN
1	D	63	GLN
1	D	65	GLN
1	D	110	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 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	CME	A	148	1	8,9,10	0.63	0	6,9,11	2.12	3 (50%)
1	CME	A	188	1	8,9,10	0.65	0	6,9,11	1.61	1 (16%)
1	CME	B	148	1	8,9,10	0.58	0	6,9,11	1.30	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CME	B	188	1	8,9,10	0.54	0	6,9,11	1.51	2 (33%)
1	CME	C	148	1	8,9,10	0.69	0	6,9,11	2.46	3 (50%)
1	CME	C	188	1	8,9,10	0.62	0	6,9,11	1.45	1 (16%)
1	CME	D	148	1	8,9,10	0.68	0	6,9,11	1.62	1 (16%)
1	CME	D	188	1	8,9,10	1.57	1 (12%)	6,9,11	2.43	3 (50%)

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
1	CME	A	148	1	-	0/5/8/10	0/0/0/0
1	CME	A	188	1	-	0/5/8/10	0/0/0/0
1	CME	B	148	1	-	0/5/8/10	0/0/0/0
1	CME	B	188	1	-	0/5/8/10	0/0/0/0
1	CME	C	148	1	-	0/5/8/10	0/0/0/0
1	CME	C	188	1	-	0/5/8/10	0/0/0/0
1	CME	D	148	1	-	0/5/8/10	0/0/0/0
1	CME	D	188	1	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	188	CME	CB-CA	4.02	1.64	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	148	CME	CZ-CE-SD	-2.67	106.64	113.16
1	D	188	CME	O-C-CA	-2.58	118.77	125.49
1	B	148	CME	CB-SG-SD	-2.30	99.46	103.95
1	A	148	CME	O-C-CA	-2.27	119.58	125.49
1	C	148	CME	O-C-CA	-2.23	119.67	125.49
1	B	148	CME	O-C-CA	-2.16	119.85	125.49
1	B	188	CME	O-C-CA	-2.15	119.88	125.49
1	A	148	CME	CZ-CE-SD	-2.05	108.16	113.16
1	B	188	CME	CE-SD-SG	2.29	115.45	103.56
1	C	148	CME	CE-SD-SG	2.62	117.14	103.56
1	A	188	CME	CB-SG-SD	2.73	109.28	103.95
1	D	188	CME	CZ-CE-SD	3.05	120.62	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	188	CME	CB-SG-SD	3.06	109.91	103.95
1	D	188	CME	CB-SG-SD	3.79	111.35	103.95
1	A	148	CME	CB-SG-SD	3.98	111.71	103.95
1	C	148	CME	CB-SG-SD	4.87	113.44	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	188	CME	2	0
1	B	148	CME	1	0
1	B	188	CME	1	0
1	C	188	CME	11	0
1	D	148	CME	2	0
1	D	188	CME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
2	SO4	A	1000	-	4,4,4	0.21	0	6,6,6	0.22	0
3	GOL	A	1100	-	5,5,5	0.28	0	5,5,5	0.58	0
3	GOL	A	1101	-	5,5,5	0.33	0	5,5,5	0.42	0
2	SO4	B	1001	-	4,4,4	0.16	0	6,6,6	0.31	0
3	GOL	B	1102	-	5,5,5	0.27	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	C	1002	-	4,4,4	0.92	0	6,6,6	1.12	0
2	SO4	C	1003	-	4,4,4	0.17	0	6,6,6	0.33	0
2	SO4	D	1004	-	4,4,4	0.09	0	6,6,6	0.43	0
3	GOL	D	1103	-	5,5,5	0.36	0	5,5,5	1.09	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	SO4	A	1000	-	-	0/0/0/0	0/0/0/0
3	GOL	A	1100	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1101	-	-	0/4/4/4	0/0/0/0
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
3	GOL	B	1102	-	-	0/4/4/4	0/0/0/0
2	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1004	-	-	0/0/0/0	0/0/0/0
3	GOL	D	1103	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	GOL	2	0
3	B	1102	GOL	3	0
2	D	1004	SO4	3	0
3	D	1103	GOL	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	222/240 (92%)	0.23	11 (4%)	32	41	20, 35, 62, 97	0
1	B	232/240 (96%)	0.32	9 (3%)	43	52	20, 31, 55, 73	0
1	C	234/240 (97%)	0.17	13 (5%)	28	36	18, 29, 54, 83	0
1	D	235/240 (97%)	0.34	16 (6%)	20	28	22, 36, 61, 68	0
All	All	923/960 (96%)	0.26	49 (5%)	30	39	18, 33, 59, 97	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	VAL	10.6
1	C	6	THR	8.1
1	C	5	SER	6.7
1	C	42	SER	5.8
1	B	43	VAL	5.7
1	A	126	TYR	5.2
1	C	44	THR	5.0
1	A	189	GLY	4.7
1	A	161	ARG	4.5
1	B	44	THR	4.4
1	B	6	THR	4.2
1	D	177	ALA	3.9
1	B	5	SER	3.8
1	B	46	GLU	3.8
1	A	125	ALA	3.7
1	D	225	GLY	3.6
1	A	46	GLU	3.4
1	D	240	SER	3.4
1	D	179	PRO	3.4
1	A	160	ALA	3.2
1	B	179	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	45	PRO	3.1
1	A	240	SER	3.1
1	B	41	GLY	3.0
1	C	41	GLY	2.9
1	D	4	ALA	2.8
1	D	202	ARG	2.8
1	C	26	ARG	2.8
1	A	127	ILE	2.7
1	C	30	ASP	2.7
1	C	29	PRO	2.6
1	D	178	ALA	2.6
1	D	144	VAL	2.6
1	C	230	ARG	2.5
1	D	147	GLY	2.5
1	D	181	SER	2.4
1	A	153	ILE	2.4
1	D	204	LEU	2.4
1	C	7	PRO	2.3
1	D	206	VAL	2.3
1	C	179	PRO	2.3
1	D	172	VAL	2.3
1	D	175	PHE	2.2
1	A	159	MET	2.2
1	B	238	ASP	2.2
1	A	225	GLY	2.1
1	B	45	PRO	2.1
1	D	143	LEU	2.1
1	D	226	GLY	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. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
1	CME	C	188	10/11	0.96	0.15	-	20,26,46,51	0
1	CME	D	148	10/11	0.91	0.22	-	45,51,58,61	0
1	CME	A	188	10/11	0.89	0.15	-	49,56,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CME	B	148	10/11	0.88	0.14	-	35,39,53,54	0
1	CME	A	148	10/11	0.89	0.14	-	47,53,69,71	0
1	CME	B	188	10/11	0.96	0.12	-	25,28,37,37	0
1	CME	C	148	10/11	0.86	0.13	-	32,34,42,43	0
1	CME	D	188	10/11	0.85	0.17	-	30,33,42,49	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. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	B	1102	6/6	0.82	0.26	8.31	62,64,65,66	0
2	SO4	D	1004	5/5	0.81	0.54	6.75	94,95,95,95	0
3	GOL	D	1103	6/6	0.61	0.34	3.85	53,53,55,56	0
3	GOL	A	1100	6/6	0.74	0.24	2.85	69,71,71,71	0
2	SO4	C	1002	5/5	0.96	0.11	-0.05	36,39,39,41	0
2	SO4	C	1003	5/5	0.90	0.27	-	90,91,91,91	0
2	SO4	B	1001	5/5	0.91	0.20	-	72,73,73,74	0
2	SO4	A	1000	5/5	0.93	0.22	-	78,79,79,79	0
3	GOL	A	1101	6/6	0.68	0.20	-	62,64,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.