Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:48 PM GMT

PDB ID	:	1M4T
Title	:	Biosynthetic thiolase, Cys89 butyrylated
Authors	:	Kursula, P.; Ojala, J.; Lambeir, A.-M.; Wierenga, R.K.
Deposited on	:	2002-07-03
Resolution	:	1.77 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:

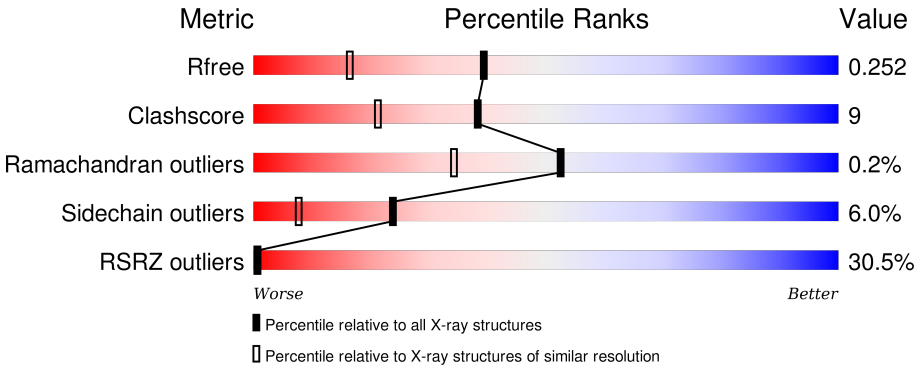
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.77 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	392	2% 85% 12%
1	B	392	2% 87% 11%
1	C	392	55% 76% 20%
1	D	392	62% 76% 22%

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
3	GOL	B	6394	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12421 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.

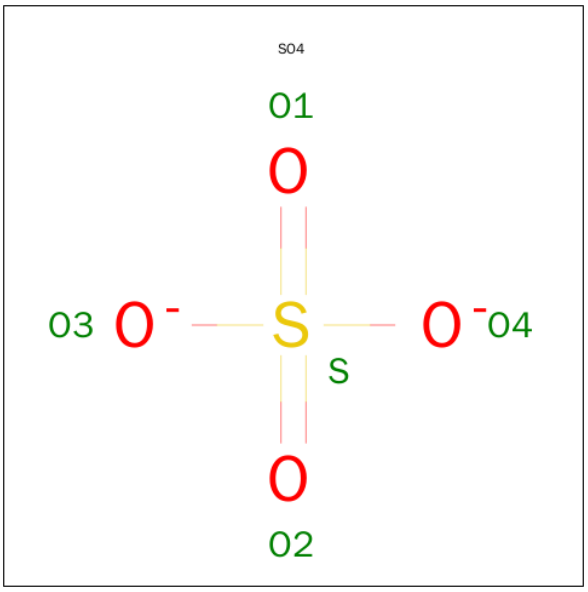
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	1	0
			2827	1756	510	540	21			
1	B	390	Total	C	N	O	S	0	1	0
			2827	1756	510	540	21			
1	C	390	Total	C	N	O	S	0	1	0
			2822	1752	510	539	21			
1	D	390	Total	C	N	O	S	0	1	0
			2822	1752	510	539	21			

There are 12 discrepancies between the modelled and reference sequences:

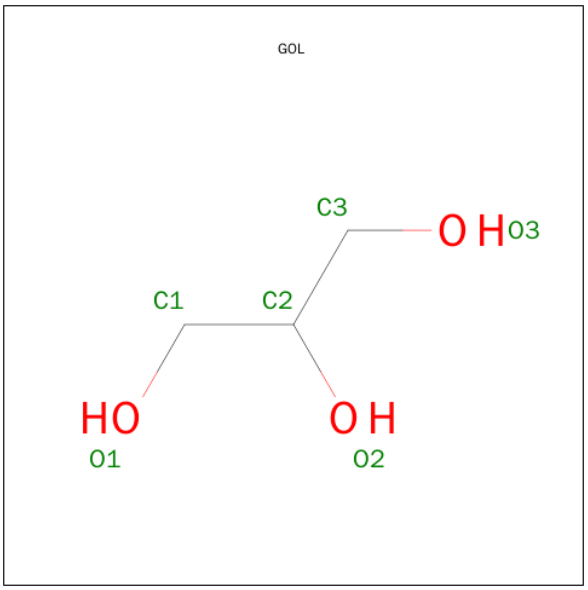
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	CY4	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	CY4	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	CY4	CYS	MODIFIED RESIDUE	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	10	ALA	-	INSERTION	UNP P07097
D	89	CY4	CYS	MODIFIED RESIDUE	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	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	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

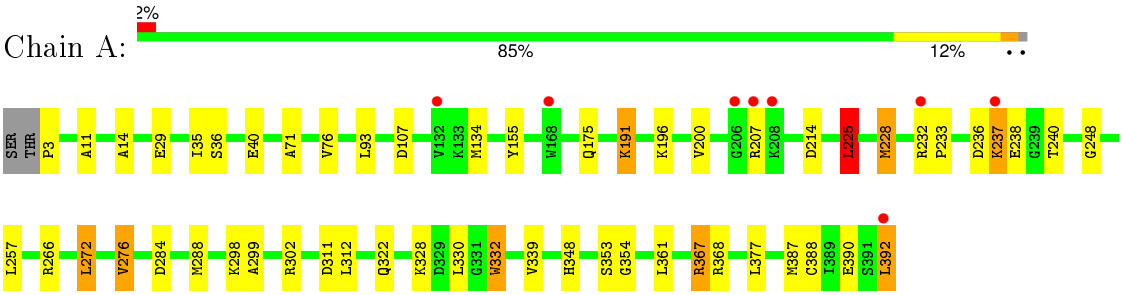
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	403	Total O 403 403	0	0
4	B	406	Total O 406 406	0	0
4	C	144	Total O 144 144	0	0
4	D	138	Total O 138 138	0	0

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 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.

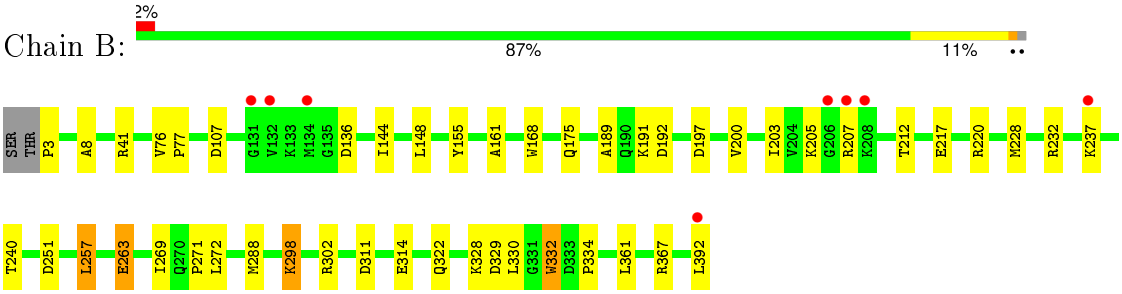
- Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



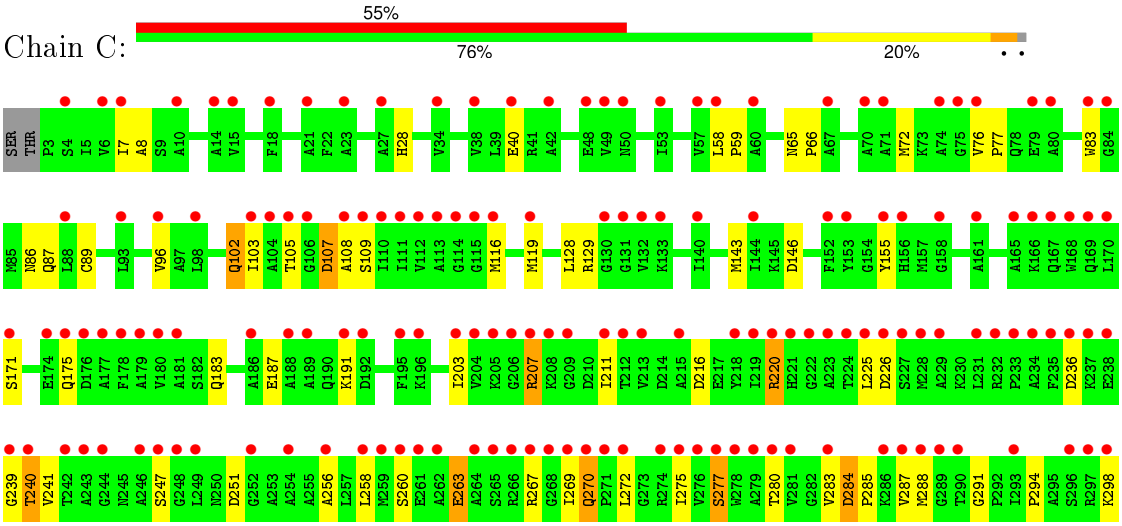
- Molecule 1: Acetyl-CoA acetyltransferase

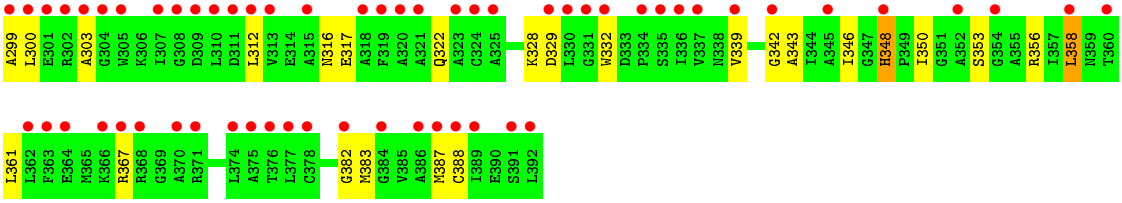
Chain B:



- Molecule 1: Acetyl-CoA acetyltransferase

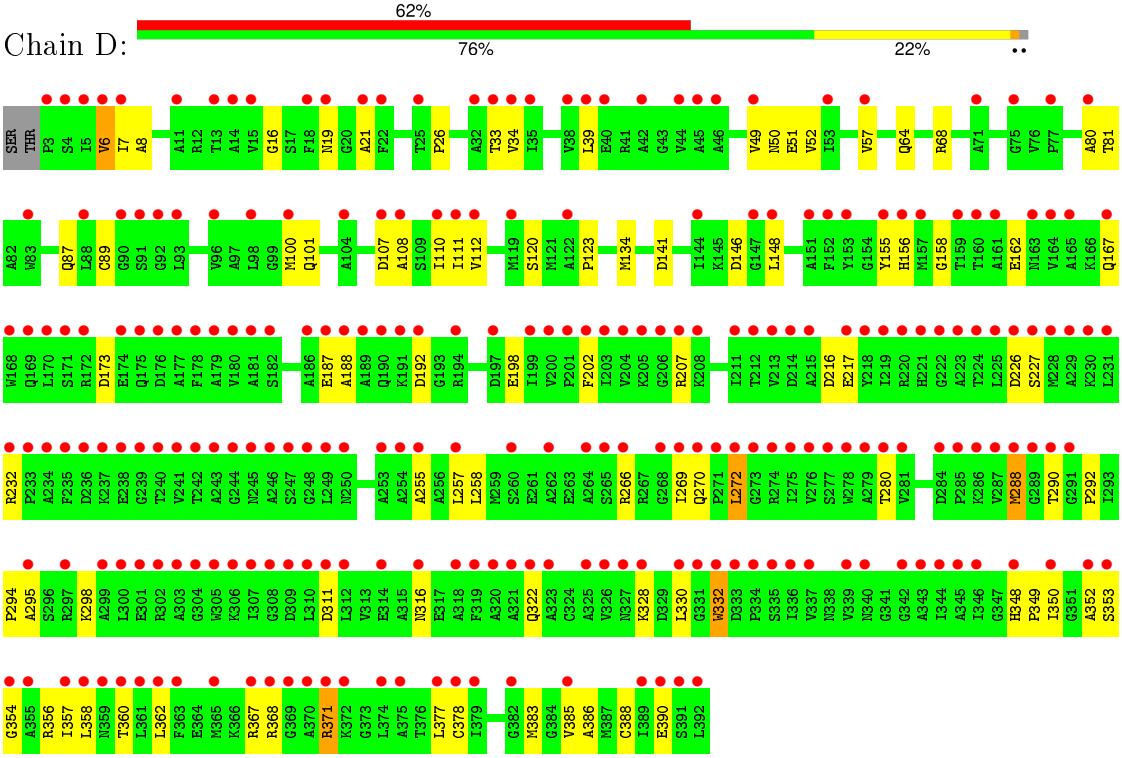
Chain C:





- Molecule 1: Acetyl-CoA acetyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.35Å 79.31Å 147.32Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	20.00 – 1.77 37.17 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-1.77) 80.8 (37.17-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.206 , 0.242 0.220 , 0.252	Depositor DCC
R_{free} test set	8647 reflections (4.85%)	DCC
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 187197 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12421	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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, SO4, CY4

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	1.02	1/2861 (0.0%)	1.02	13/3861 (0.3%)
1	B	1.00	3/2861 (0.1%)	0.99	9/3861 (0.2%)
1	C	0.57	3/2861 (0.1%)	0.77	7/3861 (0.2%)
1	D	0.52	2/2861 (0.1%)	0.77	7/3861 (0.2%)
All	All	0.81	9/11444 (0.1%)	0.90	36/15444 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	277	SER	CB-OG	11.53	1.57	1.42
1	C	109	SER	C-O	6.63	1.35	1.23
1	D	272	LEU	C-O	6.45	1.35	1.23
1	C	260	SER	CB-OG	6.26	1.50	1.42
1	B	189	ALA	CA-CB	5.49	1.64	1.52
1	A	276	VAL	CB-CG2	-5.38	1.41	1.52
1	B	228	MET	SD-CE	-5.33	1.48	1.77
1	D	6	VAL	C-O	5.15	1.33	1.23
1	B	217	GLU	CD-OE2	-5.09	1.20	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	ASP	CB-CG-OD2	10.02	127.31	118.30
1	A	284	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	266	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	A	107	ASP	CB-CG-OD2	7.15	124.73	118.30
1	A	302	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	311	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	257	LEU	CB-CG-CD2	-6.87	99.33	111.00
1	B	367	ARG	NE-CZ-NH2	-6.69	116.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	146	ASP	CB-CG-OD2	6.69	124.32	118.30
1	B	302	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	266	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	272	LEU	CB-CG-CD1	6.13	121.42	111.00
1	D	226	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	367	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	B	367	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	146	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	225	LEU	CA-CB-CG	5.73	128.48	115.30
1	B	41	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	367	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	216	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	311	ASP	CB-CG-OD2	5.63	123.36	118.30
1	C	329	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	226	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	228	MET	CG-SD-CE	5.41	108.86	100.20
1	C	251	ASP	CB-CG-OD2	5.41	123.16	118.30
1	C	284	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	107	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	392	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	192	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	311	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	251	ASP	CB-CG-OD2	5.34	123.10	118.30
1	D	173	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	107	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	136	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	192	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	216	ASP	CB-CG-OD2	5.00	122.80	118.30

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	2827	0	2833	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2827	0	2833	33	0
1	C	2822	0	2826	66	0
1	D	2822	0	2826	70	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	6	0	7	1	0
3	B	6	0	8	1	0
4	A	403	0	0	23	2
4	B	406	0	0	16	1
4	C	144	0	0	43	0
4	D	138	0	0	42	0
All	All	12421	0	11333	207	2

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 9.

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:A:387:MET:SD	4:A:9864:HOH:O	1.90	1.23
1:D:378:CYS:SG	4:D:499:HOH:O	2.02	1.17
4:C:491:HOH:O	1:D:383:MET:SD	2.07	1.12
1:D:388:CYS:SG	4:D:514:HOH:O	2.09	1.08
1:D:377:LEU:HD11	4:D:471:HOH:O	1.60	1.01
1:A:299:ALA:HB3	4:A:501:HOH:O	1.65	0.96
1:C:294:PRO:HG2	4:C:528:HOH:O	1.67	0.95
1:D:120:SER:HA	4:D:520:HOH:O	1.67	0.94
1:A:71:ALA:HA	4:A:494:HOH:O	1.72	0.88
1:C:72:MET:SD	4:C:534:HOH:O	2.34	0.86
1:C:87:GLN:NE2	4:C:485:HOH:O	2.10	0.84
1:D:51:GLU:C	4:D:484:HOH:O	2.16	0.84
4:C:433:HOH:O	1:D:64:GLN:HG3	1.78	0.83
1:A:200:VAL:HG12	4:A:475:HOH:O	1.79	0.80
1:D:80:ALA:HB3	4:D:476:HOH:O	1.80	0.80
1:A:11:ALA:HB1	4:A:475:HOH:O	1.81	0.80
1:D:108:ALA:HB3	4:D:426:HOH:O	1.84	0.78
1:C:277:SER:OG	1:C:303:ALA:HB2	1.84	0.78
1:B:197:ASP:OD1	4:B:422:HOH:O	2.02	0.78
1:A:225:LEU:HD12	4:A:9891:HOH:O	1.84	0.76
1:D:188:ALA:HA	4:D:523:HOH:O	1.86	0.76
1:A:29:GLU:HG2	4:A:517:HOH:O	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.51	0.75
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.00	0.74
1:D:288:MET:SD	4:D:499:HOH:O	2.47	0.73
1:B:263:GLU:CD	4:B:9888:HOH:O	2.26	0.73
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.53	0.73
1:A:35:ILE:HD13	4:A:494:HOH:O	1.88	0.72
1:B:314:GLU:HG2	4:B:487:HOH:O	1.90	0.72
1:D:19:ASN:OD1	4:D:520:HOH:O	2.08	0.72
1:D:280:THR:HB	4:D:481:HOH:O	1.90	0.71
1:C:65:ASN:ND2	4:C:507:HOH:O	2.24	0.70
1:D:385:VAL:HG23	4:D:481:HOH:O	1.91	0.70
1:C:89:CY4:SG	4:C:498:HOH:O	2.49	0.70
1:B:392:LEU:HB2	4:B:9835:HOH:O	1.90	0.70
1:B:263:GLU:OE2	4:B:9888:HOH:O	2.10	0.69
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.04	0.69
1:B:392:LEU:HD21	4:B:468:HOH:O	1.93	0.69
1:A:214:ASP:HA	4:A:514:HOH:O	1.91	0.69
1:B:257:LEU:HG	4:B:504:HOH:O	1.92	0.69
1:C:96:VAL:HG21	4:C:511:HOH:O	1.94	0.67
1:A:390:GLU:OE2	4:A:9792:HOH:O	2.12	0.67
1:C:316:ASN:HD21	1:C:348:HIS:CE1	2.12	0.67
1:A:93:LEU:HD11	1:A:387:MET:HE1	1.76	0.67
1:C:129:ARG:HD2	4:D:520:HOH:O	1.93	0.66
1:D:354:GLY:HA2	4:D:471:HOH:O	1.94	0.66
1:B:191:LYS:HB3	1:B:191:LYS:NZ	2.10	0.66
1:D:89:CY4:HB2	4:D:475:HOH:O	1.96	0.65
1:C:59:PRO:O	4:C:425:HOH:O	2.15	0.65
1:A:14:ALA:HB2	4:A:514:HOH:O	1.96	0.65
1:B:200:VAL:HG23	3:B:6394:GOL:H2	1.80	0.64
1:D:68:ARG:NH2	4:D:459:HOH:O	2.30	0.64
1:C:28:HIS:HB3	4:C:483:HOH:O	1.97	0.64
1:A:339:VAL:HG21	1:A:368:ARG:HH22	1.62	0.64
1:C:247[B]:SER:OG	4:C:522:HOH:O	2.15	0.64
1:D:352:ALA:HB1	4:D:496:HOH:O	1.98	0.63
1:C:383:MET:HB2	4:C:475:HOH:O	1.99	0.63
1:A:339:VAL:HG21	1:A:368:ARG:NH2	2.15	0.61
1:D:290:THR:HA	4:D:513:HOH:O	2.00	0.60
1:C:58:LEU:CD1	4:C:405:HOH:O	2.49	0.60
1:B:161:ALA:HA	4:B:518:HOH:O	2.01	0.59
1:D:51:GLU:CA	4:D:484:HOH:O	2.48	0.59
1:A:40:GLU:HG3	4:A:9949:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HB3	4:C:486:HOH:O	2.01	0.59
1:A:36:SER:O	1:A:40:GLU:HG3	2.02	0.59
1:C:342:GLY:C	4:C:489:HOH:O	2.41	0.59
1:D:52:VAL:N	4:D:484:HOH:O	2.35	0.59
1:B:298:LYS:HA	1:B:298:LYS:HE3	1.85	0.58
1:C:58:LEU:HD13	4:C:405:HOH:O	2.01	0.58
1:B:298:LYS:O	1:B:298:LYS:HD3	2.03	0.58
1:D:52:VAL:HG13	4:D:510:HOH:O	2.03	0.58
1:C:77:PRO:HD3	4:C:438:HOH:O	2.03	0.58
1:B:392:LEU:HD12	4:B:9835:HOH:O	2.03	0.58
1:C:203:ILE:HG23	4:C:532:HOH:O	2.04	0.58
1:A:196:LYS:NZ	4:A:9977:HOH:O	2.36	0.57
1:D:6:VAL:HG23	1:D:6:VAL:O	2.04	0.57
1:C:388:CYS:N	4:C:446:HOH:O	2.37	0.57
1:D:290:THR:O	1:D:294:PRO:HD2	2.04	0.57
1:C:346:ILE:HD12	4:C:489:HOH:O	2.04	0.57
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.35	0.57
1:C:358:LEU:HA	4:C:519:HOH:O	2.05	0.57
1:C:267:ARG:HB3	4:C:521:HOH:O	2.04	0.56
1:A:312:LEU:HD23	1:A:361:LEU:HD12	1.87	0.56
4:C:507:HOH:O	1:D:87:GLN:HA	2.06	0.56
1:A:35:ILE:HG21	4:A:494:HOH:O	2.06	0.55
1:C:383:MET:HB3	4:C:485:HOH:O	2.06	0.55
1:C:107:ASP:HB2	4:C:436:HOH:O	2.07	0.55
1:C:241:VAL:O	4:C:437:HOH:O	2.18	0.55
1:A:225:LEU:CD1	4:A:9891:HOH:O	2.51	0.55
1:D:21:ALA:HB3	4:D:517:HOH:O	2.06	0.55
1:A:3:PRO:N	4:A:508:HOH:O	2.39	0.54
1:C:343:ALA:O	4:C:522:HOH:O	2.18	0.54
1:D:111:ILE:HG22	1:D:112:VAL:N	2.22	0.54
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.90	0.54
1:D:123:PRO:O	4:D:508:HOH:O	2.17	0.53
1:C:299:ALA:HB1	4:C:446:HOH:O	2.09	0.53
1:C:358:LEU:HD12	4:C:511:HOH:O	2.07	0.53
1:C:8:ALA:HB1	1:C:269:ILE:HG21	1.91	0.53
1:A:237:LYS:N	1:A:237:LYS:HD3	2.24	0.53
1:D:162:GLU:HG3	4:D:521:HOH:O	2.07	0.53
1:D:217:GLU:HA	4:D:442:HOH:O	2.08	0.53
1:D:141:ASP:HA	4:D:508:HOH:O	2.08	0.52
1:D:26:PRO:HB2	4:D:495:HOH:O	2.09	0.52
1:D:34:VAL:HA	4:D:482:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:CG	4:A:9891:HOH:O	2.57	0.52
1:D:33:THR:HG1	1:D:202:PHE:HD1	1.58	0.51
1:D:257:LEU:HD23	1:D:258:LEU:N	2.25	0.51
1:C:105:THR:HG21	1:D:101:GLN:HG2	1.93	0.51
1:D:8:ALA:HB1	1:D:269:ILE:HG21	1.93	0.50
1:D:51:GLU:HA	4:D:484:HOH:O	2.09	0.50
1:C:119:MET:HA	4:C:405:HOH:O	2.11	0.50
1:B:392:LEU:CG	4:B:9835:HOH:O	2.59	0.49
1:D:7:ILE:HD13	1:D:362:LEU:HD11	1.94	0.49
1:D:50:ASN:O	1:D:80:ALA:HB1	2.11	0.49
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.30	0.49
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.76	0.49
1:C:285:PRO:HD3	4:D:459:HOH:O	2.11	0.49
1:D:16:GLY:HA3	4:D:517:HOH:O	2.13	0.49
1:C:348:HIS:ND1	1:C:353:SER:OG	2.43	0.48
1:B:3:PRO:N	4:B:409:HOH:O	2.46	0.48
1:D:156:HIS:HD1	1:D:158:GLY:H	1.61	0.48
1:C:183:GLN:NE2	1:C:220:ARG:HG3	2.28	0.48
1:A:200:VAL:CG1	4:A:475:HOH:O	2.50	0.48
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.96	0.48
1:C:207:ARG:HH11	1:C:207:ARG:HG2	1.78	0.47
1:B:205:LYS:NZ	4:B:413:HOH:O	2.45	0.47
1:D:371:ARG:O	1:D:390:GLU:HG3	2.15	0.47
1:C:83:TRP:HZ2	4:C:450:HOH:O	1.97	0.47
1:D:111:ILE:CG2	1:D:112:VAL:N	2.79	0.46
1:C:275:ILE:HG13	4:C:496:HOH:O	2.15	0.46
1:A:276:VAL:CG2	1:A:388:CYS:HB2	2.45	0.46
1:C:312:LEU:HD23	1:C:361:LEU:HD12	1.96	0.46
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.51	0.46
1:B:191:LYS:HZ2	1:B:191:LYS:HB3	1.78	0.46
1:D:111:ILE:HG12	4:D:426:HOH:O	2.15	0.46
1:B:205:LYS:CE	4:B:413:HOH:O	2.64	0.46
1:D:356:ARG:NH2	1:D:357:ILE:HG22	2.30	0.46
1:B:76:VAL:HG13	1:B:77:PRO:HD2	1.97	0.46
1:A:339:VAL:CG2	4:A:9902:HOH:O	2.64	0.45
1:C:102:GLN:NE2	4:C:450:HOH:O	2.49	0.45
1:D:111:ILE:HD11	4:D:426:HOH:O	2.16	0.45
1:D:39:LEU:HD21	1:D:49:VAL:CG2	2.46	0.45
1:A:76:VAL:HG21	4:A:494:HOH:O	2.15	0.45
1:C:96:VAL:HG13	1:C:258:LEU:HD21	1.97	0.45
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:VAL:HG22	4:D:482:HOH:O	2.15	0.45
1:B:334:PRO:HA	4:B:513:HOH:O	2.17	0.45
1:A:191:LYS:CB	1:A:191:LYS:NZ	2.79	0.45
1:B:8:ALA:HB3	1:B:257:LEU:HD22	1.98	0.45
1:D:348:HIS:CD2	4:D:498:HOH:O	2.70	0.45
1:D:148:LEU:HB3	1:D:156:HIS:NE2	2.32	0.44
1:C:287:VAL:O	1:C:287:VAL:HG23	2.17	0.44
1:B:361:LEU:HD12	4:B:487:HOH:O	2.17	0.44
1:D:352:ALA:CB	4:D:496:HOH:O	2.59	0.44
1:C:269:ILE:HG22	1:C:270:GLN:N	2.33	0.44
1:A:348:HIS:CE1	1:A:353:SER:HG	2.31	0.44
1:B:298:LYS:HD3	1:B:298:LYS:C	2.38	0.44
1:A:248:GLY:HA2	4:A:471:HOH:O	2.17	0.44
1:A:276:VAL:HG23	1:A:388:CYS:HB2	1.99	0.44
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.37	0.44
1:C:66:PRO:HB3	4:C:483:HOH:O	2.18	0.44
1:C:269:ILE:HG22	1:C:270:GLN:H	1.83	0.44
1:D:112:VAL:HG12	4:D:452:HOH:O	2.17	0.43
1:D:292:PRO:HG3	1:D:377:LEU:C	2.38	0.43
1:D:52:VAL:HG23	4:D:484:HOH:O	2.19	0.43
1:B:269:ILE:O	1:B:271:PRO:HD3	2.19	0.42
1:C:66:PRO:CB	4:C:483:HOH:O	2.67	0.42
1:C:76:VAL:CG1	1:C:77:PRO:HD2	2.49	0.42
1:C:211:ILE:C	4:C:532:HOH:O	2.56	0.42
1:C:283:VAL:HG22	1:C:382:GLY:C	2.40	0.42
1:C:116:MET:HE3	4:C:483:HOH:O	2.18	0.42
1:D:100:MET:HE3	4:D:474:HOH:O	2.20	0.42
1:B:392:LEU:CB	4:B:9835:HOH:O	2.57	0.42
1:D:349:PRO:O	1:D:353:SER:N	2.53	0.42
1:A:228:MET:HE2	1:A:228:MET:HA	2.01	0.42
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.32	0.42
1:D:377:LEU:HB3	4:D:475:HOH:O	2.20	0.42
1:C:284:ASP:OD1	1:C:285:PRO:HD2	2.20	0.42
1:D:100:MET:C	1:D:100:MET:SD	2.98	0.42
1:A:330:LEU:HD12	1:A:332:TRP:CZ2	2.54	0.42
1:D:111:ILE:CG1	4:D:426:HOH:O	2.68	0.41
1:D:110:ILE:HG23	1:D:257:LEU:HD21	2.02	0.41
1:C:300:LEU:HB3	4:C:473:HOH:O	2.18	0.41
1:A:233:PRO:HB2	1:A:236:ASP:O	2.21	0.41
1:C:236:ASP:HB3	1:C:239:GLY:HA3	2.01	0.41
1:B:257:LEU:C	1:B:257:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD12	1:B:332:TRP:CZ2	2.56	0.41
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.54	0.41
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.86	0.41
1:B:144:ILE:HD13	1:B:148:LEU:HD12	2.02	0.41
1:C:387:MET:HA	4:C:446:HOH:O	2.20	0.41
1:A:225:LEU:HG	4:A:9891:HOH:O	2.20	0.41
1:C:191:LYS:NZ	4:C:478:HOH:O	2.54	0.41
1:C:103:ILE:HA	1:C:108:ALA:O	2.21	0.41
1:C:143:MET:HG3	4:C:405:HOH:O	2.21	0.41
1:D:367:ARG:HG2	4:D:424:HOH:O	2.21	0.41
1:A:200:VAL:HG23	3:A:5394:GOL:H2	2.02	0.41
1:C:356:ARG:NH2	4:C:489:HOH:O	2.54	0.41
1:C:280:THR:HG23	1:D:81:THR:HG21	2.03	0.41
1:C:263:GLU:HG3	1:C:267:ARG:HD2	2.03	0.40
1:C:187:GLU:HA	4:C:462:HOH:O	2.21	0.40
1:A:29:GLU:CG	4:A:517:HOH:O	2.56	0.40
1:C:7:ILE:HG23	1:C:256:ALA:HB1	2.02	0.40
1:C:86:ASN:C	1:C:86:ASN:OD1	2.60	0.40
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.70	0.40
1:D:198:GLU:OE1	1:D:360:THR:HA	2.22	0.40
1:D:295:ALA:O	1:D:386:ALA:HB3	2.21	0.40

All (2) 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:A:400:HOH:O	4:A:407:HOH:O[2_655]	2.03	0.17
4:A:417:HOH:O	4:B:440:HOH:O[2_645]	2.19	0.01

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	388/392 (99%)	376 (97%)	12 (3%)	0	100	100
1	B	388/392 (99%)	373 (96%)	15 (4%)	0	100	100
1	C	388/392 (99%)	372 (96%)	14 (4%)	2 (0%)	34	16
1	D	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	46	28
All	All	1552/1568 (99%)	1488 (96%)	61 (4%)	3 (0%)	52	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	240	THR
1	D	266	ARG
1	C	291	GLY

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	277/278 (100%)	261 (94%)	16 (6%)	25	8
1	B	277/278 (100%)	264 (95%)	13 (5%)	32	13
1	C	277/278 (100%)	257 (93%)	20 (7%)	18	5
1	D	277/278 (100%)	260 (94%)	17 (6%)	23	7
All	All	1108/1112 (100%)	1042 (94%)	66 (6%)	24	8

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	MET
1	A	155	TYR
1	A	191	LYS
1	A	207	ARG
1	A	225	LEU
1	A	232	ARG
1	A	237	LYS
1	A	238	GLU

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Mol	Chain	Res	Type
1	A	272	LEU
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	367	ARG
1	A	392	LEU
1	B	155	TYR
1	B	207	ARG
1	B	220	ARG
1	B	232	ARG
1	B	237	LYS
1	B	257	LEU
1	B	263	GLU
1	B	272	LEU
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	328	LYS
1	B	332	TRP
1	C	40	GLU
1	C	102	GLN
1	C	155	TYR
1	C	171	SER
1	C	207	ARG
1	C	220	ARG
1	C	225	LEU
1	C	263	GLU
1	C	270	GLN
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	328	LYS
1	C	332	TRP
1	C	339	VAL
1	C	348	HIS
1	C	350	ILE
1	C	358	LEU
1	C	367	ARG
1	D	134	MET

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Mol	Chain	Res	Type
1	D	155	TYR
1	D	167	GLN
1	D	187	GLU
1	D	207	ARG
1	D	227	SER
1	D	232	ARG
1	D	270	GLN
1	D	272	LEU
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	328	LYS
1	D	332	TRP
1	D	358	LEU
1	D	368	ARG
1	D	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	175	GLN
1	A	184	ASN
1	A	221	HIS
1	B	78	GLN
1	B	175	GLN
1	B	184	ASN
1	B	221	HIS
1	C	175	GLN
1	C	184	ASN
1	C	316	ASN
1	D	78	GLN
1	D	175	GLN
1	D	184	ASN
1	D	316	ASN
1	D	340	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	CY4	A	89	1	9,10,11	1.30	1 (11%)	6,11,13	2.13	2 (33%)
1	CY4	B	89	1	9,10,11	1.79	2 (22%)	6,11,13	3.02	2 (33%)
1	CY4	C	89	1	4,5,11	0.40	0	3,5,13	1.31	1 (33%)
1	CY4	D	89	1	4,5,11	0.46	0	3,5,13	1.38	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
1	CY4	A	89	1	-	0/8/10/12	0/0/0/0
1	CY4	B	89	1	-	0/8/10/12	0/0/0/0
1	CY4	C	89	1	-	0/1/4/12	0/0/0/0
1	CY4	D	89	1	-	0/1/4/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	CY4	CA2-CA1	3.00	1.54	1.50
1	A	89	CY4	CA2-CA1	3.01	1.54	1.50
1	B	89	CY4	CB-SG	3.32	1.86	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	CY4	OA1-CA1-CA2	-5.29	120.30	123.94
1	A	89	CY4	OA1-CA1-CA2	-4.05	121.15	123.94
1	A	89	CY4	O-C-CA	-2.09	120.04	125.49
1	C	89	CY4	O-C-CA	-2.05	120.15	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	CY4	OA1-CA1-SG	4.48	126.39	122.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	89	CY4	1	0
1	D	89	CY4	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	GOL	A	5394	-	5,5,5	1.07	1 (20%)	5,5,5	0.69	0
2	SO4	A	9720	-	4,4,4	0.47	0	6,6,6	0.31	0
2	SO4	A	9722	-	4,4,4	0.22	0	6,6,6	0.16	0
3	GOL	B	6394	-	5,5,5	0.95	1 (20%)	5,5,5	0.73	0
2	SO4	B	9719	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	B	9721	-	4,4,4	0.50	0	6,6,6	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
3	GOL	A	5394	-	-	0/4/4/4	0/0/0/0
2	SO4	A	9720	-	-	0/0/0/0	0/0/0/0
2	SO4	A	9722	-	-	0/0/0/0	0/0/0/0
3	GOL	B	6394	-	-	0/4/4/4	0/0/0/0
2	SO4	B	9719	-	-	0/0/0/0	0/0/0/0
2	SO4	B	9721	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5394	GOL	O2-C2	-2.24	1.36	1.43
3	B	6394	GOL	O2-C2	-2.09	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5394	GOL	1	0
3	B	6394	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	389/392 (99%)	0.20	8 (2%) 67 66	5, 11, 28, 54	0
1	B	389/392 (99%)	0.20	8 (2%) 67 66	6, 11, 28, 55	0
1	C	389/392 (99%)	2.76	217 (55%) 0 0	2, 11, 28, 42	0
1	D	389/392 (99%)	3.44	242 (62%) 0 0	2, 13, 29, 45	0
All	All	1556/1568 (99%)	1.65	475 (30%) 1 1	2, 11, 29, 55	0

All (475) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	18.0
1	D	229	ALA	15.1
1	D	219	ILE	14.9
1	D	179	ALA	14.4
1	D	244	GLY	13.7
1	D	188	ALA	13.5
1	D	170	LEU	13.2
1	C	234	ALA	12.5
1	C	105	THR	11.5
1	D	228	MET	10.0
1	A	132	VAL	9.9
1	D	233	PRO	9.7
1	D	235	PHE	9.7
1	C	49	VAL	9.5
1	D	108	ALA	9.5
1	D	227	SER	9.4
1	C	370	ALA	9.3
1	D	164	VAL	9.1
1	C	225	LEU	9.0
1	D	310	LEU	9.0
1	C	239	GLY	8.9

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Mol	Chain	Res	Type	RSRZ
1	D	239	GLY	8.9
1	C	80	ALA	8.7
1	D	392	LEU	8.5
1	D	240	THR	8.5
1	B	207	ARG	8.5
1	C	161	ALA	8.3
1	C	276	VAL	8.2
1	D	178	PHE	8.2
1	D	223	ALA	8.1
1	D	224	THR	8.1
1	C	342	GLY	8.0
1	C	235	PHE	8.0
1	D	265	SER	8.0
1	D	160	THR	8.0
1	D	247[A]	SER	8.0
1	D	159	THR	8.0
1	D	243	ALA	8.0
1	D	168	TRP	7.9
1	D	361	LEU	7.9
1	C	224	THR	7.9
1	D	181	ALA	7.9
1	D	186	ALA	7.8
1	D	295	ALA	7.8
1	D	238	GLU	7.7
1	D	285	PRO	7.7
1	D	153	TYR	7.5
1	C	300	LEU	7.5
1	D	234	ALA	7.5
1	D	319	PHE	7.5
1	D	215	ALA	7.5
1	C	229	ALA	7.4
1	B	208	LYS	7.3
1	D	171	SER	7.3
1	D	330	LEU	7.3
1	D	161	ALA	7.2
1	D	246	ALA	7.2
1	D	332	TRP	7.2
1	D	299	ALA	7.1
1	D	339	VAL	7.0
1	D	279	ALA	7.0
1	D	323	ALA	7.0
1	D	34	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
1	D	275	ILE	6.9
1	C	232	ARG	6.9
1	C	247[A]	SER	6.9
1	D	350	ILE	6.8
1	D	374	LEU	6.8
1	C	34	VAL	6.8
1	C	371	ARG	6.8
1	D	312	LEU	6.8
1	C	283	VAL	6.8
1	C	242	THR	6.7
1	D	272	LEU	6.7
1	C	336	ILE	6.6
1	C	67	ALA	6.6
1	C	293	ILE	6.6
1	C	240	THR	6.6
1	D	335	SER	6.6
1	D	305	TRP	6.6
1	C	279	ALA	6.5
1	D	343	ALA	6.5
1	D	290	THR	6.4
1	C	238	GLU	6.4
1	D	326	VAL	6.4
1	D	6	VAL	6.3
1	C	106	GLY	6.3
1	C	270	GLN	6.2
1	C	392	LEU	6.2
1	D	300	LEU	6.2
1	C	266	ARG	6.2
1	C	221	HIS	6.1
1	C	313	VAL	6.1
1	D	336	ILE	6.1
1	C	208	LYS	6.1
1	C	268	GLY	6.1
1	D	377	LEU	6.1
1	D	245	ASN	6.1
1	C	96	VAL	6.0
1	C	226	ASP	6.0
1	D	207	ARG	6.0
1	D	232	ARG	6.0
1	C	331	GLY	6.0
1	D	357	ILE	5.9
1	C	246	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	207	ARG	5.9
1	C	113	ALA	5.8
1	D	370	ALA	5.8
1	D	230	LYS	5.7
1	C	177	ALA	5.7
1	D	218	TYR	5.6
1	D	269	ILE	5.6
1	D	257	LEU	5.6
1	C	75	GLY	5.6
1	D	157	MET	5.6
1	C	103	ILE	5.6
1	C	203	ILE	5.6
1	D	241	VAL	5.6
1	C	319	PHE	5.5
1	D	222	GLY	5.5
1	C	366	LYS	5.5
1	D	391	SER	5.5
1	D	155	TYR	5.5
1	C	269	ILE	5.5
1	D	291	GLY	5.4
1	D	253	ALA	5.4
1	D	365	MET	5.4
1	D	363	PHE	5.4
1	C	207	ARG	5.4
1	C	231	LEU	5.4
1	C	301	GLU	5.4
1	D	270	GLN	5.4
1	D	271	PRO	5.3
1	D	327	ASN	5.3
1	D	331	GLY	5.3
1	D	325	ALA	5.2
1	D	340	ASN	5.2
1	C	307	ILE	5.1
1	C	378	CYS	5.1
1	D	208	LYS	5.1
1	D	368	ARG	5.0
1	D	169	GLN	5.0
1	C	152	PHE	5.0
1	C	104	ALA	5.0
1	D	369	GLY	5.0
1	D	226	ASP	5.0
1	D	382	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	276	VAL	4.9
1	D	151	ALA	4.9
1	C	335	SER	4.9
1	D	15	VAL	4.9
1	C	305	TRP	4.8
1	D	172	ARG	4.8
1	D	163	ASN	4.8
1	D	225	LEU	4.8
1	C	389	ILE	4.8
1	C	204	VAL	4.8
1	D	320	ALA	4.8
1	C	206	GLY	4.8
1	C	228	MET	4.8
1	C	243	ALA	4.7
1	C	211	ILE	4.7
1	C	57	VAL	4.7
1	D	213	VAL	4.7
1	D	281	VAL	4.7
1	A	208	LYS	4.7
1	D	318	ALA	4.7
1	C	244	GLY	4.7
1	D	358	LEU	4.7
1	D	307	ILE	4.7
1	B	132	VAL	4.7
1	D	304	GLY	4.7
1	C	272	LEU	4.7
1	D	44	VAL	4.7
1	D	112	VAL	4.7
1	C	222	GLY	4.6
1	C	290	THR	4.6
1	C	40	GLU	4.6
1	D	104	ALA	4.6
1	D	4	SER	4.6
1	C	110	ILE	4.6
1	D	262	ALA	4.6
1	D	371	ARG	4.6
1	D	107	ASP	4.6
1	C	215	ALA	4.5
1	C	363	PHE	4.5
1	D	221	HIS	4.5
1	C	170	LEU	4.5
1	D	359	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	287	VAL	4.5
1	D	311	ASP	4.5
1	C	315	ALA	4.4
1	D	152	PHE	4.4
1	D	342	GLY	4.4
1	D	280	THR	4.4
1	C	180	VAL	4.4
1	C	218	TYR	4.4
1	C	4	SER	4.3
1	A	206	GLY	4.3
1	D	180	VAL	4.3
1	C	277	SER	4.3
1	D	7	ILE	4.3
1	D	49	VAL	4.3
1	C	108	ALA	4.3
1	C	258	LEU	4.3
1	C	38	VAL	4.3
1	C	93	LEU	4.2
1	D	385	VAL	4.2
1	C	21	ALA	4.2
1	D	22	PHE	4.2
1	C	376	THR	4.2
1	D	346	ILE	4.2
1	D	165	ALA	4.2
1	C	388	CYS	4.1
1	C	169	GLN	4.1
1	C	195	PHE	4.1
1	C	310	LEU	4.1
1	D	379	ILE	4.0
1	D	220	ARG	4.0
1	D	266	ARG	4.0
1	C	14	ALA	4.0
1	C	227	SER	4.0
1	D	237	LYS	4.0
1	C	175	GLN	4.0
1	D	197	ASP	4.0
1	C	265	SER	4.0
1	D	75	GLY	4.0
1	D	190	GLN	3.9
1	D	352	ALA	4.0
1	D	288	MET	3.9
1	D	40	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	179	ALA	3.9
1	C	264	ALA	3.9
1	C	303	ALA	3.9
1	C	79	GLU	3.9
1	C	168	TRP	3.9
1	C	332	TRP	3.9
1	D	297	ARG	3.9
1	C	287	VAL	3.9
1	C	71	ALA	3.9
1	C	275	ILE	3.9
1	D	83	TRP	3.8
1	D	201	PRO	3.8
1	C	88	LEU	3.8
1	C	7	ILE	3.8
1	C	296	SER	3.8
1	D	35	ILE	3.8
1	C	191	LYS	3.8
1	C	83	TRP	3.8
1	C	10	ALA	3.7
1	C	23	ALA	3.7
1	D	25	THR	3.7
1	C	213	VAL	3.7
1	D	308	GLY	3.7
1	C	391	SER	3.7
1	D	236	ASP	3.7
1	B	206	GLY	3.7
1	C	27	ALA	3.7
1	D	92	GLY	3.7
1	C	358	LEU	3.7
1	C	176	ASP	3.6
1	C	312	LEU	3.6
1	C	262	ALA	3.6
1	C	233	PRO	3.6
1	D	175	GLN	3.6
1	C	280	THR	3.5
1	D	378	CYS	3.5
1	C	299	ALA	3.5
1	D	268	GLY	3.5
1	D	372	LYS	3.5
1	C	374	LEU	3.5
1	C	278	TRP	3.5
1	D	200	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	289	GLY	3.5
1	C	167	GLN	3.5
1	C	320	ALA	3.5
1	D	42	ALA	3.5
1	C	115	GLY	3.4
1	C	309	ASP	3.4
1	D	177	ALA	3.4
1	C	155	TYR	3.4
1	C	325	ALA	3.4
1	D	264	ALA	3.4
1	B	237	LYS	3.4
1	C	114	GLY	3.4
1	C	281	VAL	3.3
1	C	178	PHE	3.3
1	C	308	GLY	3.3
1	C	382	GLY	3.3
1	D	255	ALA	3.3
1	C	133	LYS	3.3
1	C	74	ALA	3.3
1	B	134	MET	3.3
1	D	167	GLN	3.3
1	C	131	GLY	3.3
1	D	309	ASP	3.3
1	C	76	VAL	3.3
1	C	249	LEU	3.3
1	D	88	LEU	3.3
1	C	259	MET	3.3
1	D	13	THR	3.3
1	D	156	HIS	3.3
1	D	3	PRO	3.2
1	D	306	LYS	3.2
1	D	93	LEU	3.2
1	D	211	ILE	3.2
1	C	236	ASP	3.2
1	C	156	HIS	3.2
1	D	242	THR	3.2
1	D	202	PHE	3.2
1	D	174	GLU	3.2
1	C	237	LYS	3.2
1	D	248	GLY	3.1
1	C	70	ALA	3.1
1	C	274	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	367	ARG	3.1
1	D	353	SER	3.1
1	C	362	LEU	3.1
1	D	5	ILE	3.1
1	C	352	ALA	3.1
1	D	21	ALA	3.1
1	D	375	ALA	3.1
1	C	109	SER	3.0
1	C	153	TYR	3.0
1	C	348	HIS	3.0
1	D	322	GLN	3.0
1	C	256	ALA	3.0
1	D	111	ILE	3.0
1	D	119	MET	3.0
1	D	45	ALA	3.0
1	D	277	SER	3.0
1	D	206	GLY	3.0
1	D	98	LEU	3.0
1	D	362	LEU	3.0
1	D	189	ALA	3.0
1	C	321	ALA	2.9
1	D	203	ILE	2.9
1	D	286	LYS	2.9
1	C	223	ALA	2.9
1	C	112	VAL	2.9
1	C	220	ARG	2.9
1	D	367	ARG	2.9
1	C	271	PRO	2.9
1	D	284	ASP	2.8
1	C	334	PRO	2.8
1	C	188	ALA	2.8
1	C	386	ALA	2.8
1	D	321	ALA	2.8
1	D	176	ASP	2.8
1	C	84	GLY	2.8
1	D	90	GLY	2.8
1	D	303	ALA	2.8
1	C	324	CYS	2.8
1	D	100	MET	2.8
1	D	301	GLU	2.8
1	D	194	ARG	2.8
1	D	57	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	392	LEU	2.7
1	C	377	LEU	2.7
1	D	18	PHE	2.7
1	C	181	ALA	2.7
1	D	337	VAL	2.7
1	D	199	ILE	2.7
1	C	192	ASP	2.7
1	D	316	ASN	2.7
1	A	232	ARG	2.7
1	C	252	GLY	2.7
1	D	11	ALA	2.7
1	D	274	ARG	2.7
1	D	144	ILE	2.6
1	D	333	ASP	2.6
1	C	345	ALA	2.6
1	C	304	GLY	2.6
1	D	204	VAL	2.6
1	C	140	ILE	2.6
1	D	39	LEU	2.6
1	D	205	LYS	2.6
1	D	278	TRP	2.6
1	C	219	ILE	2.6
1	D	389	ILE	2.6
1	C	209	GLY	2.6
1	D	260	SER	2.5
1	D	360	THR	2.5
1	C	286	LYS	2.5
1	D	191	LYS	2.5
1	D	328	LYS	2.5
1	C	375	ALA	2.5
1	C	144	ILE	2.5
1	C	384	GLY	2.5
1	C	165	ALA	2.5
1	D	38	VAL	2.5
1	D	212	THR	2.5
1	C	174	GLU	2.5
1	C	186	ALA	2.5
1	C	323	ALA	2.5
1	D	71	ALA	2.5
1	C	6	VAL	2.5
1	C	329	ASP	2.5
1	D	148	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	354	GLY	2.5
1	C	260	SER	2.5
1	D	182	SER	2.5
1	C	166	LYS	2.5
1	D	344	ILE	2.5
1	D	110	ILE	2.4
1	D	390	GLU	2.4
1	D	91	SER	2.4
1	D	302	ARG	2.4
1	C	98	LEU	2.4
1	D	273	GLY	2.4
1	A	237	LYS	2.4
1	C	196	LYS	2.4
1	C	302	ARG	2.4
1	C	368	ARG	2.4
1	D	122	ALA	2.4
1	C	297	ARG	2.4
1	D	314	GLU	2.3
1	C	111	ILE	2.3
1	C	311	ASP	2.3
1	D	254	ALA	2.3
1	C	15	VAL	2.3
1	D	19	ASN	2.3
1	D	249	LEU	2.3
1	C	289	GLY	2.3
1	D	46	ALA	2.3
1	C	48	GLU	2.3
1	D	217	GLU	2.3
1	C	205	LYS	2.3
1	C	387	MET	2.3
1	C	171	SER	2.3
1	C	130	GLY	2.3
1	D	147	GLY	2.3
1	D	32	ALA	2.3
1	C	298	LYS	2.2
1	C	60	ALA	2.2
1	D	14	ALA	2.2
1	C	116	MET	2.2
1	C	354	GLY	2.2
1	D	334	PRO	2.2
1	D	348	HIS	2.2
1	C	50	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	254	ALA	2.2
1	D	345	ALA	2.2
1	D	53	ILE	2.2
1	D	77	PRO	2.2
1	D	96	VAL	2.2
1	C	18	PHE	2.2
1	C	360	THR	2.2
1	C	53	ILE	2.2
1	C	288	MET	2.2
1	A	392	LEU	2.2
1	C	119	MET	2.2
1	D	355	ALA	2.2
1	C	132	VAL	2.2
1	C	339	VAL	2.2
1	B	131	GLY	2.1
1	C	58	LEU	2.1
1	C	158	GLY	2.1
1	C	212	THR	2.1
1	C	337	VAL	2.1
1	A	168	TRP	2.1
1	D	187	GLU	2.1
1	C	330	LEU	2.1
1	C	42	ALA	2.1
1	D	80	ALA	2.1
1	C	248	GLY	2.1
1	C	318	ALA	2.1
1	C	267	ARG	2.1
1	D	192	ASP	2.1
1	D	250	ASN	2.0
1	C	189	ALA	2.0
1	C	261	GLU	2.0
1	C	364	GLU	2.0
1	D	214	ASP	2.0
1	D	33	THR	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	CY4	B	89	11/12	0.94	0.12	-	8,10,26,28	0
1	CY4	C	89	6/12	0.89	0.10	-	8,10,11,15	0
1	CY4	A	89	11/12	0.95	0.13	-	9,12,30,31	0
1	CY4	D	89	6/12	0.74	0.14	-	2,4,4,6	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	6394	6/6	0.85	0.16	2.31	18,26,30,38	0
3	GOL	A	5394	6/6	0.90	0.13	0.71	20,31,33,33	0
2	SO4	A	9722	5/5	0.90	0.20	-	74,74,75,75	0
2	SO4	B	9721	5/5	0.96	0.10	-	47,48,50,51	0
2	SO4	A	9720	5/5	0.97	0.10	-	45,50,50,51	0
2	SO4	B	9719	5/5	0.95	0.18	-	76,77,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.