Full wwPDB X-ray Structure Validation Report (i)

Mar 19, 2025 – 06:06 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

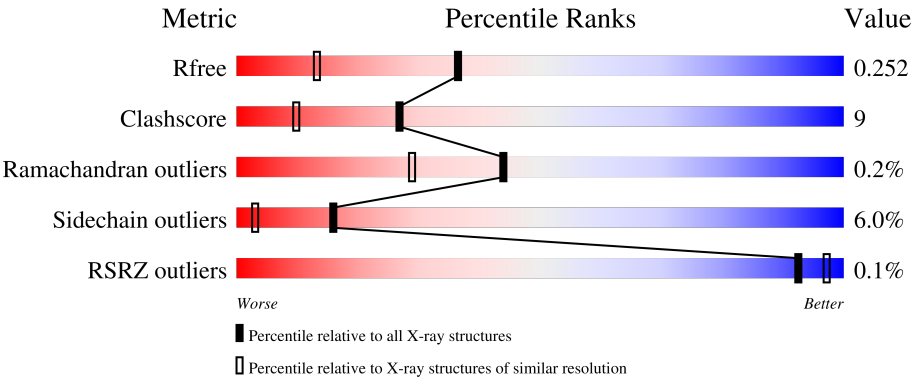
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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}	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	392	85% 12%
1	B	392	87% 11%
1	C	392	76% 20%
1	D	392	76% 22%

2 Entry composition (i)

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.

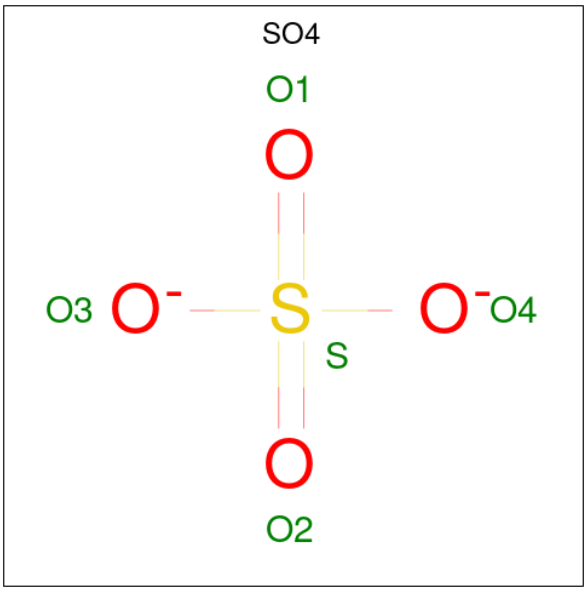
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

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:

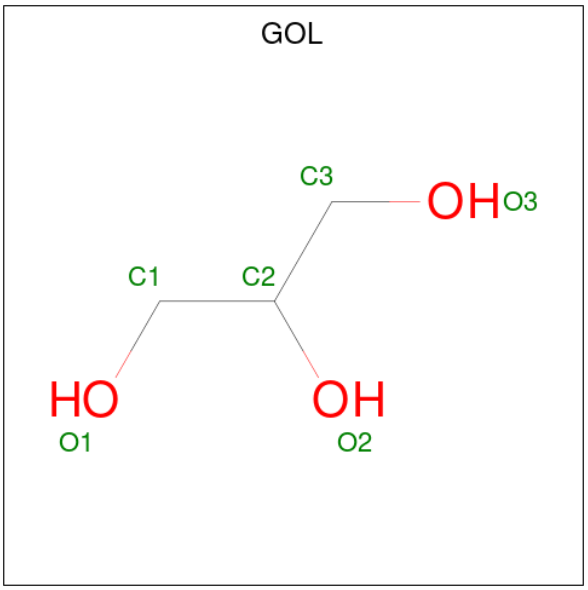
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	insertion	UNP P07097
A	89	CY4	CYS	modified residue	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	10	ALA	-	insertion	UNP P07097
B	89	CY4	CYS	modified residue	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	10	ALA	-	insertion	UNP P07097
C	89	CY4	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.

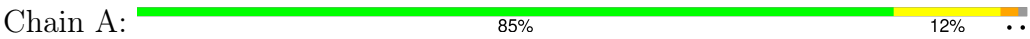
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	403	Total O 403 403	0	0
4	B	406	Total O 406 406	0	0
4	C	144	Total O 144 144	0	0
4	D	138	Total O 138 138	0	0

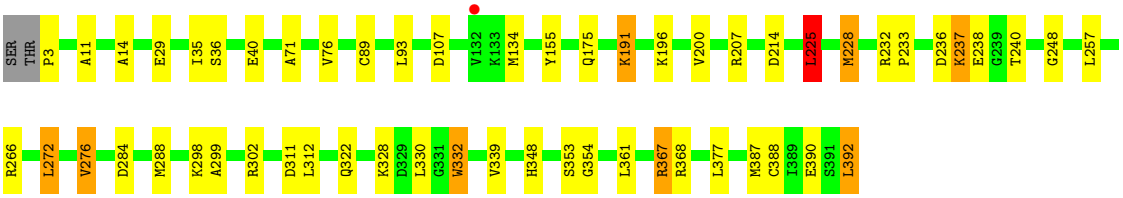
3 Residue-property plots (i)

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

• Molecule 1: Acetyl-CoA acetyltransferase

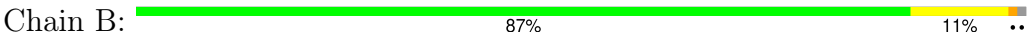
Chain A:

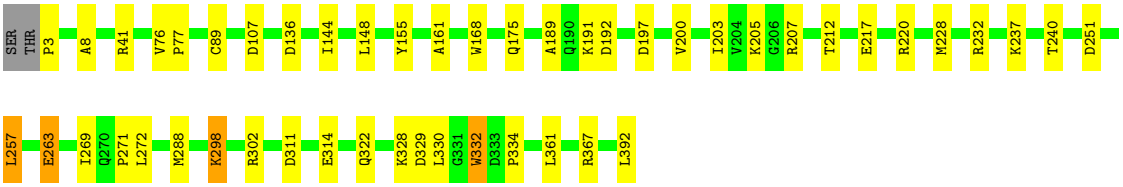




• Molecule 1: Acetyl-CoA acetyltransferase

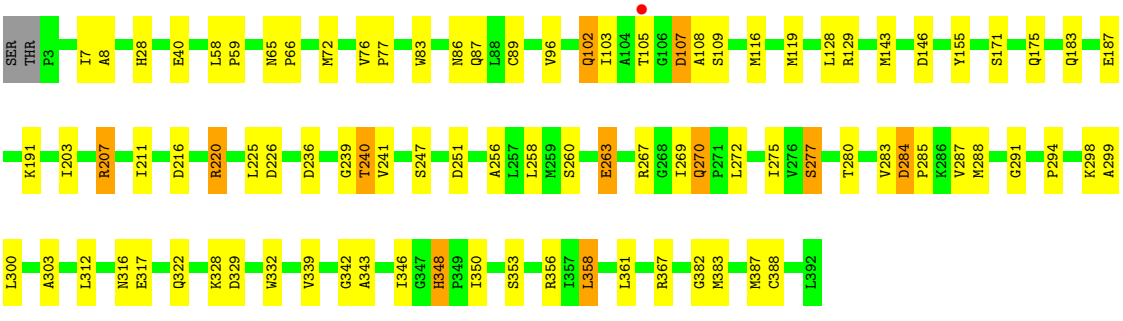
Chain B:





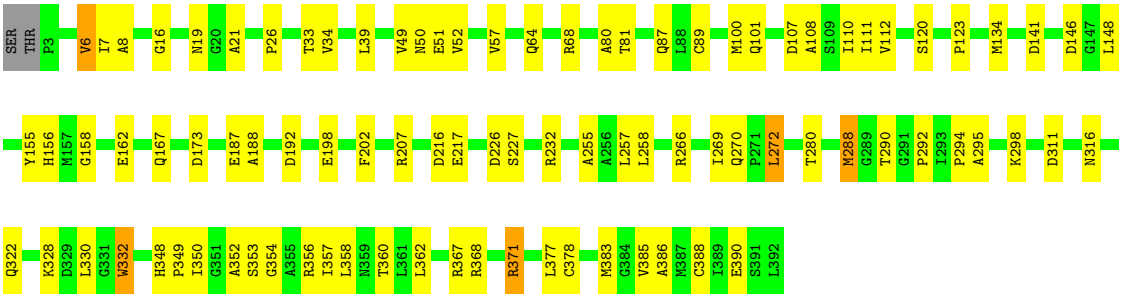
• Molecule 1: Acetyl-CoA acetyltransferase

Chain C:



• Molecule 1: Acetyl-CoA acetyltransferase

Chain D:


SER THR P3 V6 I7 A8 G16 N19 G20 A21 P26 T33 V34 L39 V49 N50 E51 V52 V57 Q64 R68 A80 T81 Q87 L88 C89 M100 Q101 D107 A108 S109 I110 I111 V112 S120 P123 M134 D141 D146 G147 L148
Y155 H156 M157 G158 E162 Q167 D173 E187 A188 D192 E198 F202 R207 D216 E217 D226 S227 R232 A255 A256 L257 L258 R266 I269 Q270 P271 L272 T280 M288 G289 T290 G291 P292 I293 P294 A295 K298 D311 N316
Q322 K328 D329 L330 G331 W332 H348 P349 I350 G351 A352 S353 G354 A355 R356 I357 L358 N359 T360 L361 L362 R367 R368 R371 L377 C378 M383 G384 V385 A386 M387 C388 I389 E390 S391 L392

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 20.00 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-1.77) 80.8 (20.00-1.77)	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	Depositor
R, R_{free}	0.206 , 0.242 0.221 , 0.252	Depositor DCC
R_{free} test set	8648 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CY4, SO4, GOL

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:B:197:ASP:OD1	4:B:422:HOH:O	2.02	0.78
1:C:277:SER:OG	1:C:303:ALA:HB2	1.84	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:A:214:ASP:HA	4:A:514:HOH:O	1.91	0.69
1:B:392:LEU:HD21	4:B:468:HOH:O	1.93	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:A:40:GLU:HG3	4:A:9949:HOH:O	2.02	0.59
1:D:51:GLU:CA	4:D:484:HOH:O	2.48	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:HE3	1:B:298:LYS:HA	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:C:77:PRO:HD3	4:C:438:HOH:O	2.03	0.58
1:D:52:VAL:HG13	4:D:510: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:C:388:CYS:N	4:C:446:HOH:O	2.37	0.57
1:D:6:VAL:HG23	1:D:6:VAL:O	2.04	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:107:ASP:HB2	4:C:436:HOH:O	2.07	0.55
1:C:383:MET:HB3	4:C:485:HOH:O	2.06	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:A:237:LYS:N	1:A:237:LYS:HD3	2.24	0.53
1:C:8:ALA:HB1	1:C:269:ILE:HG21	1.91	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:A:276:VAL:CG2	1:A:388:CYS:HB2	2.45	0.46
1:C:275:ILE:HG13	4:C:496:HOH:O	2.15	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:HB3	1:B:191:LYS:HZ2	1.78	0.46
1:B:76:VAL:HG13	1:B:77:PRO:HD2	1.97	0.46
1:B:205:LYS:CE	4:B:413:HOH:O	2.64	0.46
1:D:111:ILE:HG12	4:D:426:HOH:O	2.15	0.46
1:D:356:ARG:NH2	1:D:357:ILE:HG22	2.30	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:B:334:PRO:HA	4:B:513:HOH:O	2.17	0.45
1:C:96:VAL:HG13	1:C:258:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.97	0.45
1:D:34:VAL:HG22	4:D:482:HOH:O	2.15	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:C:287:VAL:HG23	1:C:287:VAL:O	2.17	0.44
1:D:148:LEU:HB3	1:D:156:HIS:NE2	2.32	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:A:348:HIS:CE1	1:A:353:SER:HG	2.31	0.44
1:C:269:ILE:HG22	1:C:270:GLN:N	2.33	0.44
1:A:248:GLY:HA2	4:A:471:HOH:O	2.17	0.44
1:B:298:LYS:HD3	1:B:298:LYS:C	2.38	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:A:228:MET:HA	1:A:228:MET:HE2	2.01	0.42
1:B:392:LEU:CB	4:B:9835:HOH:O	2.57	0.42
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.32	0.42
1:D:349:PRO:O	1:D:353:SER:N	2.53	0.42
1:A:330:LEU:HD12	1:A:332:TRP:CZ2	2.54	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:D:377:LEU:HB3	4:D:475:HOH:O	2.20	0.42
1:D:111:ILE:CG1	4:D:426:HOH:O	2.68	0.41
1:C:300:LEU:HB3	4:C:473:HOH:O	2.18	0.41
1:D:110:ILE:HG23	1:D:257:LEU:HD21	2.02	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:HD23	1:B:257:LEU:C	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:B:144:ILE:HD13	1:B:148:LEU:HD12	2.02	0.41
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.86	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:103:ILE:HA	1:C:108:ALA:O	2.21	0.41
1:C:191:LYS:NZ	4:C:478:HOH:O	2.54	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:280:THR:HG23	1:D:81:THR:HG21	2.03	0.41
1:C:356:ARG:NH2	4:C:489:HOH:O	2.54	0.41
1:C:187:GLU:HA	4:C:462:HOH:O	2.21	0.40
1:C:263:GLU:HG3	1:C:267:ARG:HD2	2.03	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:B:203:ILE:CD1	1:B:212:THR:OG1	2.70	0.40
1:C:86:ASN:C	1:C:86:ASN:OD1	2.60	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%)	25	11
1	D	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	37	23
All	All	1552/1568 (99%)	1488 (96%)	61 (4%)	3 (0%)	44	29

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%)	17	3
1	B	277/278 (100%)	264 (95%)	13 (5%)	22	5
1	C	277/278 (100%)	257 (93%)	20 (7%)	12	1
1	D	277/278 (100%)	260 (94%)	17 (6%)	15	3
All	All	1108/1112 (100%)	1042 (94%)	66 (6%)	16	3

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

Sometimes 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	D	89	1	4,5,11	0.53	0	1,5,13	1.41	0
1	CY4	A	89	1	9,10,11	1.38	1 (11%)	7,11,13	1.65	2 (28%)
1	CY4	B	89	1	9,10,11	1.68	2 (22%)	7,11,13	2.06	3 (42%)
1	CY4	C	89	1	4,5,11	0.46	0	1,5,13	0.04	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	D	89	1	-	0/1/4/12	-
1	CY4	A	89	1	-	3/8/10/12	-
1	CY4	B	89	1	-	2/8/10/12	-
1	CY4	C	89	1	-	0/1/4/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	CY4	CA2-CA1	3.33	1.54	1.50
1	B	89	CY4	CA2-CA1	3.31	1.54	1.50
1	B	89	CY4	CB-SG	2.08	1.86	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	CY4	CB-SG-CA1	-3.24	96.31	100.76
1	B	89	CY4	OA1-CA1-CA2	-3.19	120.30	123.98
1	B	89	CY4	CB-SG-CA1	-3.14	96.45	100.76
1	B	89	CY4	OA1-CA1-SG	2.91	126.39	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	CY4	OA1-CA1-CA2	-2.45	121.15	123.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	89	CY4	SG-CA1-CA2-CA3
1	A	89	CY4	OA1-CA1-CA2-CA3
1	A	89	CY4	CA1-CA2-CA3-CA4
1	B	89	CY4	SG-CA1-CA2-CA3
1	B	89	CY4	OA1-CA1-CA2-CA3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
2	SO4	A	9722	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	B	9721	-	4,4,4	0.23	0	6,6,6	0.39	0
2	SO4	B	9719	-	4,4,4	0.26	0	6,6,6	0.18	0
3	GOL	B	6394	-	5,5,5	0.96	1 (20%)	5,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	5394	-	5,5,5	1.09	1 (20%)	5,5,5	0.76	0
2	SO4	A	9720	-	4,4,4	0.12	0	6,6,6	0.39	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	B	6394	-	-	4/4/4/4	-
3	GOL	A	5394	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5394	GOL	O2-C2	-2.26	1.36	1.43
3	B	6394	GOL	O2-C2	-2.11	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5394	GOL	O1-C1-C2-C3
3	B	6394	GOL	O1-C1-C2-C3
3	A	5394	GOL	O1-C1-C2-O2
3	B	6394	GOL	O1-C1-C2-O2
3	B	6394	GOL	C1-C2-C3-O3
3	B	6394	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6394	GOL	1	0
3	A	5394	GOL	1	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	389/392 (99%)	-1.05	1 (0%) 90 93	5, 11, 28, 54	1 (0%)
1	B	389/392 (99%)	-1.06	0 100 100	6, 11, 28, 55	1 (0%)
1	C	389/392 (99%)	-0.47	1 (0%) 90 93	2, 11, 28, 42	1 (0%)
1	D	389/392 (99%)	-0.38	0 100 100	2, 13, 29, 45	1 (0%)
All	All	1556/1568 (99%)	-0.74	2 (0%) 92 97	2, 11, 29, 55	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	VAL	3.0
1	C	105	THR	2.6

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

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
1	CY4	D	89	6/12	0.97	0.06	2,4,4,6	0
1	CY4	B	89	11/12	0.99	0.04	8,10,26,28	0
1	CY4	C	89	6/12	0.99	0.03	8,10,11,15	0
1	CY4	A	89	11/12	0.99	0.04	9,12,30,31	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	SO4	B	9719	5/5	0.94	0.10	76,77,78,78	0
2	SO4	A	9722	5/5	0.97	0.10	74,74,75,75	0
3	GOL	A	5394	6/6	0.97	0.06	20,31,33,33	0
3	GOL	B	6394	6/6	0.97	0.07	18,26,30,38	0
2	SO4	A	9720	5/5	0.98	0.05	45,50,50,51	0
2	SO4	B	9721	5/5	0.99	0.05	47,48,50,51	0

6.5 Other polymers

There are no such residues in this entry.