



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:48 PM UTC

PDB ID : 1M4T / pdb_00001m4t
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

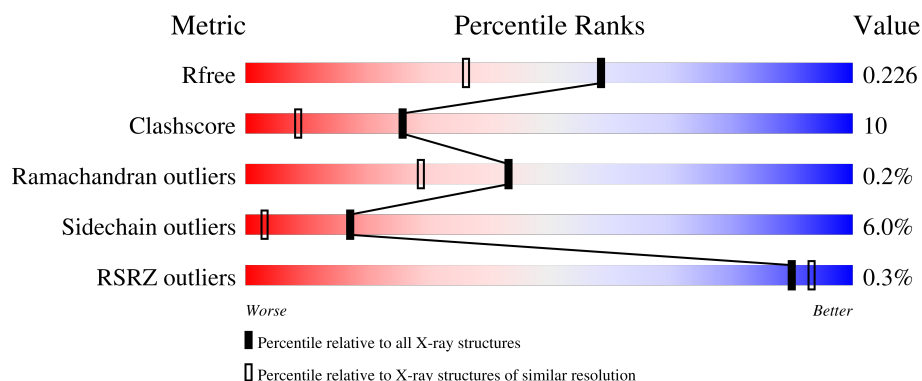
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	85% 13% ..
1	B	392	87% 11% ..
1	C	392	% 77% 20% ..
1	D	392	78% 20% ..

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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

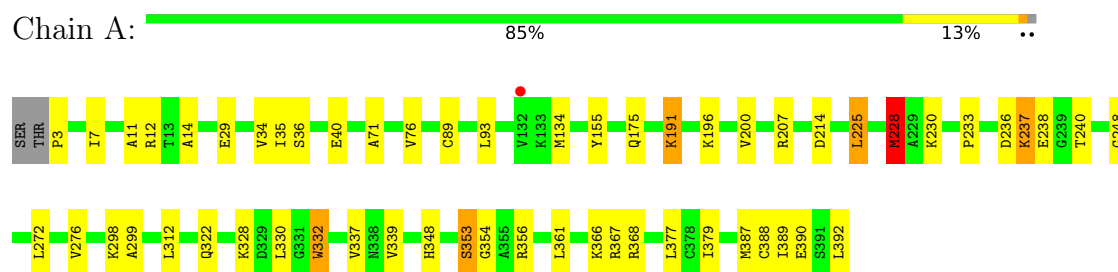
- Molecule 4 is water.

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

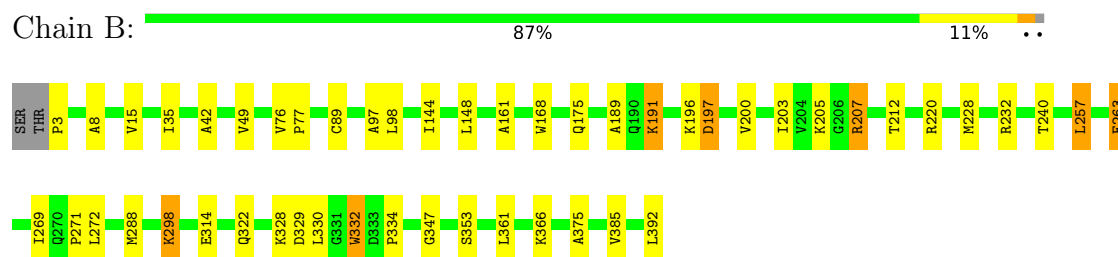
3 Residue-property plots

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.

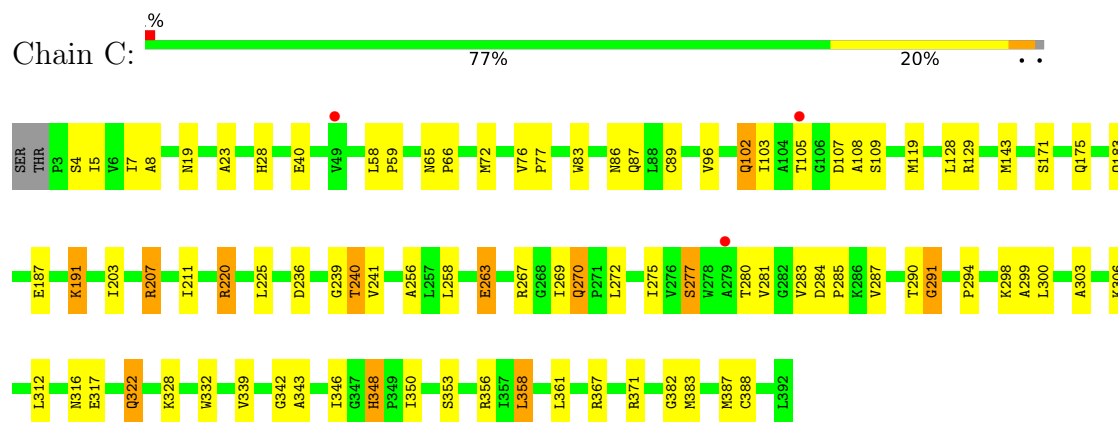
- Molecule 1: Acetyl-CoA acetyltransferase



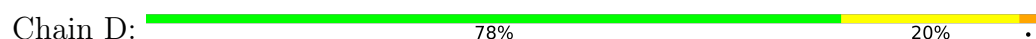
- Molecule 1: Acetyl-CoA acetyltransferase

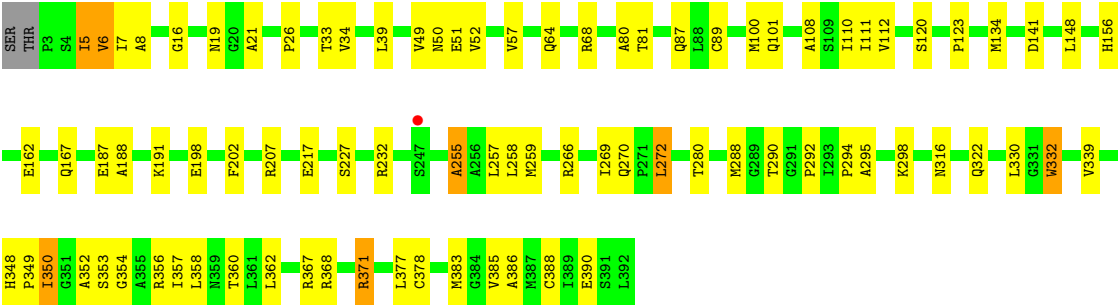


- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.242 (Not available) , 0.226	Depositor DCC
R_{free} test set	8648 reflections (4.62%)	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 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CY4, 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	1.32	6/2861 (0.2%)	1.18	3/3861 (0.1%)
1	B	1.32	11/2861 (0.4%)	1.16	5/3861 (0.1%)
1	C	0.74	2/2861 (0.1%)	0.94	0/3861
1	D	0.74	3/2861 (0.1%)	0.93	2/3861 (0.1%)
All	All	1.07	22/11444 (0.2%)	1.06	10/15444 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	MET	SD-CE	-12.62	1.48	1.79
1	D	272	LEU	C-O	9.21	1.35	1.24
1	D	6	VAL	C-O	8.72	1.33	1.24
1	C	109	SER	C-O	8.59	1.35	1.23
1	C	277	SER	CB-OG	7.54	1.57	1.42
1	A	228	MET	SD-CE	-7.16	1.61	1.79
1	B	49	VAL	C-O	-7.14	1.16	1.24
1	B	189	ALA	CA-CB	6.85	1.64	1.53
1	B	353	SER	C-O	-6.53	1.16	1.24
1	A	366	LYS	C-O	6.29	1.31	1.24
1	A	7	ILE	CA-CB	6.11	1.60	1.53
1	A	337	VAL	C-O	6.10	1.31	1.24
1	B	375	ALA	C-O	6.03	1.31	1.24
1	B	98	LEU	N-CA	5.63	1.53	1.46
1	B	288	MET	SD-CE	-5.57	1.65	1.79
1	B	35	ILE	CA-CB	5.49	1.60	1.54
1	A	353	SER	C-O	-5.47	1.17	1.24
1	B	97	ALA	CA-CB	5.30	1.61	1.53
1	B	42	ALA	CA-CB	-5.22	1.44	1.53
1	A	12	ARG	CD-NE	5.21	1.53	1.46
1	D	259	MET	SD-CE	-5.08	1.66	1.79
1	B	385	VAL	C-O	5.04	1.29	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ALA	N-CA-C	6.95	117.41	108.24
1	B	347	GLY	N-CA-C	6.04	118.21	112.04
1	B	15	VAL	CA-C-N	5.77	127.23	120.71
1	B	15	VAL	C-N-CA	5.77	127.23	120.71
1	B	197	ASP	N-CA-C	-5.63	105.06	111.14
1	D	350	ILE	N-CA-C	5.61	116.06	110.23
1	A	34	VAL	N-CA-C	5.51	116.24	110.62
1	A	379	ILE	CA-C-N	5.38	125.08	119.92
1	A	379	ILE	C-N-CA	5.38	125.08	119.92
1	B	207	ARG	N-CA-C	-5.03	105.38	112.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	42	0
1	B	2827	0	2833	34	0
1	C	2822	0	2826	69	0
1	D	2822	0	2826	72	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	6	0	7	2	0
3	B	6	0	8	1	0
4	A	403	0	0	24	2
4	B	406	0	0	16	1
4	C	144	0	0	42	0
4	D	138	0	0	43	0
All	All	12421	0	11333	216	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 10.

All (216) 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
4:C:491:HOH:O	1:D:383:MET:SD	2.07	1.12
1:D:378:CYS:SG	4:D:499:HOH:O	2.02	1.09
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:D:51:GLU:C	4:D:484:HOH:O	2.16	0.89
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
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:263:GLU:CD	4:B:9888:HOH:O	2.26	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
1:A:387:MET:HE3	1:A:389:ILE:HD11	1.68	0.75
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:342:GLY:C	4:C:489:HOH:O	2.41	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:D:148:LEU:HD13	1:D:156:HIS:HE2	1.64	0.61
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
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: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: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:93:LEU:HD11	1:A:387:MET:HE2	1.88	0.56
1:A:312:LEU:HD23	1:A:361:LEU:HD12	1.87	0.56
1:D:6:VAL:HG23	1:D:6:VAL:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:225:LEU:CG	4:A:9891:HOH:O	2.57	0.52
1:D:52:VAL:N	4:D:484:HOH:O	2.35	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:33:THR:HG1	1:D:202:PHE:HD1	1.59	0.50
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:D:292:PRO:HG3	1:D:377:LEU:C	2.38	0.49
1:B:298:LYS:HD3	1:B:298:LYS:C	2.38	0.49
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.37	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLN:NE2	1:C:220:ARG:HG3	2.28	0.48
1:C:211:ILE:C	4:C:532:HOH:O	2.56	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:C:283:VAL:HG22	1:C:382:GLY:C	2.40	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:100:MET:C	1:D:100:MET:SD	2.98	0.47
1:A:228:MET:HA	1:A:228:MET:HE2	1.96	0.46
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:257:LEU:HD23	1:B:257:LEU:C	2.41	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
1:D:34:VAL:HG22	4:D:482:HOH:O	2.15	0.45
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.97	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:86:ASN:OD1	1:C:86:ASN:C	2.60	0.45
1:A:356:ARG:HD2	1:A:356:ARG:C	2.42	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:C:306:LYS:C	4:C:473:HOH:O	2.60	0.44
1:D:352:ALA:CB	4:D:496:HOH:O	2.59	0.44
1:C:4:SER:C	1:C:5:ILE:HD13	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:C	4:D:497:HOH:O	2.60	0.44
1:A:276:VAL:HG23	1:A:388:CYS:HB2	1.99	0.44
1:B:196:LYS:NZ	4:B:9975:HOH:O	2.48	0.44
1:A:348:HIS:ND1	1:A:353:SER:OG	2.41	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:B:191:LYS:HB3	1:B:191:LYS:HZ1	1.81	0.43
1:C:287:VAL:O	1:C:287:VAL:HG23	2.17	0.43
1:D:148:LEU:CD1	1:D:156:HIS:HE2	2.30	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
3:A:5394:GOL:O3	4:A:9857:HOH:O	2.22	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: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: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:19:ASN:C	1:C:23:ALA:HB2	2.45	0.42
1:C:284:ASP:OD1	1:C:285:PRO:HD2	2.20	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: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:C:322:GLN:C	1:C:322:GLN:NE2	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:NH2	4:C:489:HOH:O	2.54	0.41
1:C:290:THR:O	1:C:291:GLY:C	2.64	0.40
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:B:191:LYS:HB3	1:B:191:LYS:HZ2	1.83	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: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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	24	11
1	D	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	36	22
All	All	1552/1568 (99%)	1488 (96%)	61 (4%)	3 (0%)	43	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 ⓘ

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%)	18	3
1	B	277/278 (100%)	265 (96%)	12 (4%)	26	7
1	C	277/278 (100%)	256 (92%)	21 (8%)	12	1
1	D	277/278 (100%)	260 (94%)	17 (6%)	17	3
All	All	1108/1112 (100%)	1042 (94%)	66 (6%)	17	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	228	MET
1	A	230	LYS
1	A	237	LYS
1	A	238	GLU
1	A	272	LEU
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	191	LYS
1	B	207	ARG
1	B	220	ARG

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Mol	Chain	Res	Type
1	B	232	ARG
1	B	257	LEU
1	B	263	GLU
1	B	272	LEU
1	B	298	LYS
1	B	322	GLN
1	B	328	LYS
1	B	332	TRP
1	B	366	LYS
1	C	40	GLU
1	C	102	GLN
1	C	171	SER
1	C	191	LYS
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	281	VAL
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	C	371	ARG
1	D	5	ILE
1	D	134	MET
1	D	167	GLN
1	D	187	GLU
1	D	191	LYS
1	D	207	ARG
1	D	227	SER
1	D	232	ARG
1	D	270	GLN
1	D	272	LEU
1	D	298	LYS
1	D	322	GLN

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Mol	Chain	Res	Type
1	D	332	TRP
1	D	339	VAL
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 (18) 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	78	GLN
1	C	175	GLN
1	C	184	ASN
1	C	316	ASN
1	D	65	ASN
1	D	78	GLN
1	D	127	HIS
1	D	175	GLN
1	D	184	ASN
1	D	316	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	B	89	1	9,10,11	1.68	2 (22%)	7,11,13	2.06	3 (42%)
1	CY4	A	89	1	9,10,11	1.38	1 (11%)	7,11,13	1.65	2 (28%)
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	B	89	1	-	2/8/10/12	-
1	CY4	A	89	1	-	3/8/10/12	-
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(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms
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
3	GOL	A	5394	-	5,5,5	1.09	1 (20%)	5,5,5	0.76	0
2	SO4	B	9719	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	A	9722	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	A	9720	-	4,4,4	0.12	0	6,6,6	0.39	0
2	SO4	B	9721	-	4,4,4	0.23	0	6,6,6	0.39	0
3	GOL	B	6394	-	5,5,5	0.96	1 (20%)	5,5,5	0.71	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5394	GOL	2	0
3	B	6394	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	-0.99	1 (0%) 90 93	5, 11, 28, 54	1 (0%)
1	B	389/392 (99%)	-1.00	0 100 100	6, 11, 28, 55	1 (0%)
1	C	389/392 (99%)	-0.40	3 (0%) 82 87	2, 11, 28, 42	1 (0%)
1	D	389/392 (99%)	-0.31	1 (0%) 90 93	2, 13, 29, 45	1 (0%)
All	All	1556/1568 (99%)	-0.68	5 (0%) 90 93	2, 11, 29, 55	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	VAL	3.1
1	C	105	THR	2.7
1	C	49	VAL	2.1
1	C	279	ALA	2.0
1	D	247[A]	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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($\text{\AA}^2$)	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 [i](#)

There are no such residues in this entry.