



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:14 PM GMT

PDB ID : 1M3K  
Title : biosynthetic thiolase, inactive C89A mutant  
Authors : Kursula, P.; Ojala, J.; Lambeir, A.-M.; Wierenga, R.K.  
Deposited on : 2002-06-28  
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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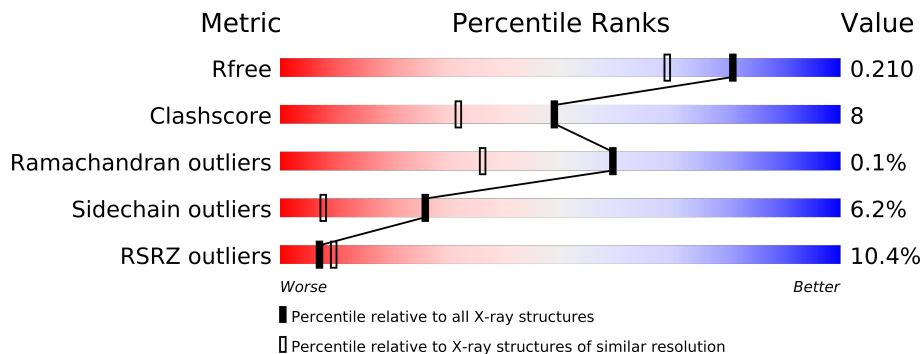
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	392	
1	B	392	
1	C	392	
1	D	392	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	9720	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12527 atoms, of which 0 are hydrogen and 0 are deuterium.

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	392	Total	C	N	O	S	0	1	0
			2834	1759	512	543	20			
1	B	392	Total	C	N	O	S	0	1	0
			2834	1759	512	543	20			
1	C	392	Total	C	N	O	S	0	1	0
			2834	1759	512	543	20			
1	D	392	Total	C	N	O	S	0	1	0
			2834	1759	512	543	20			

There are 12 discrepancies between the modelled and reference sequences:

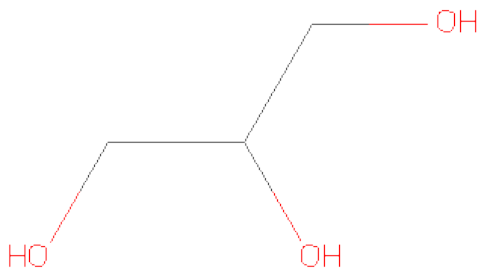
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	ALA	CYS	ENGINEERED	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	ALA	CYS	ENGINEERED	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	ALA	CYS	ENGINEERED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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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.

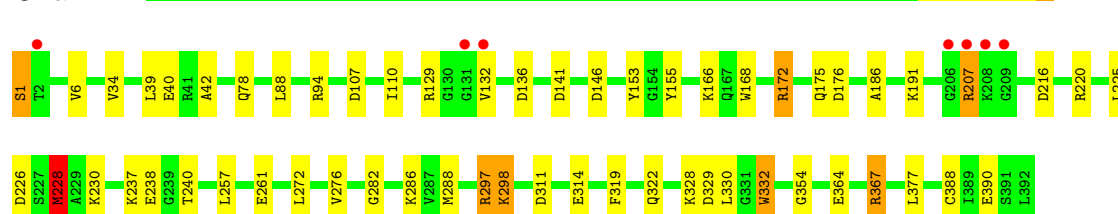
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	416	Total	O	0	0
			416	416		
4	B	425	Total	O	0	0
			425	425		
4	C	152	Total	O	0	0
			152	152		
4	D	166	Total	O	0	0
			166	166		

### 3 Residue-property plots

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

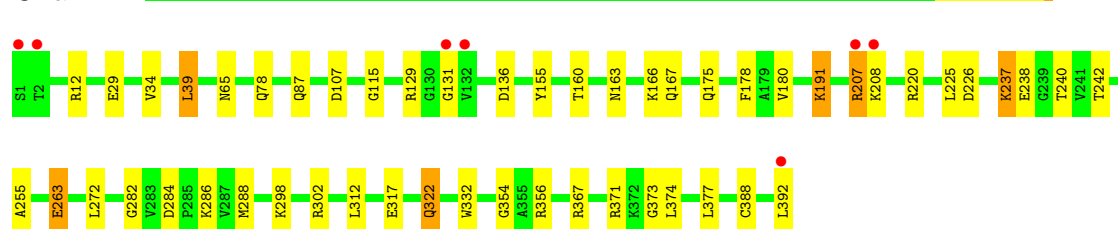
#### • Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



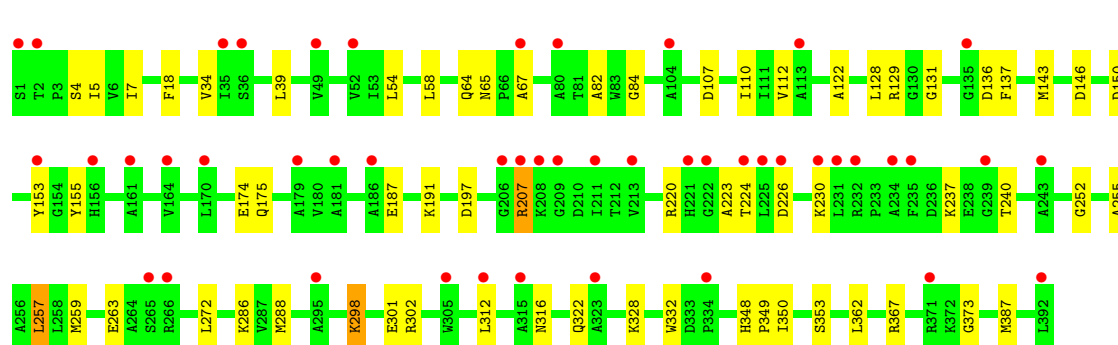
#### • Molecule 1: Acetyl-CoA acetyltransferase

Chain B:



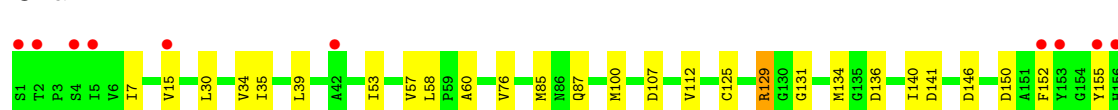
#### • Molecule 1: Acetyl-CoA acetyltransferase

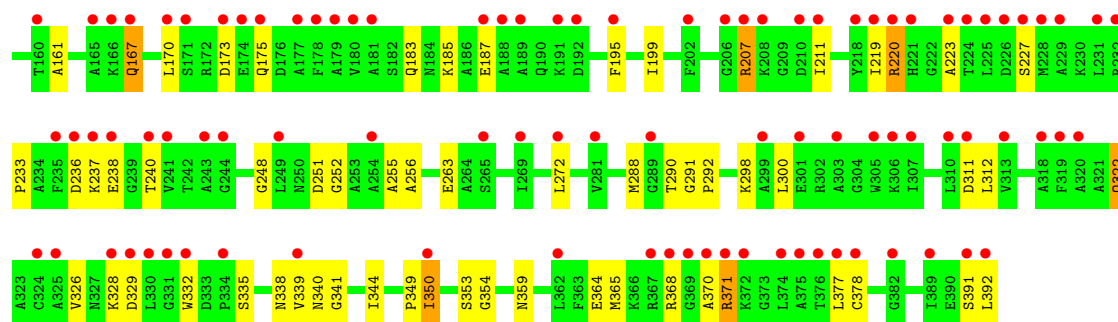
Chain C:



#### • Molecule 1: Acetyl-CoA acetyltransferase

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.37Å 79.20Å 148.86Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.1 (20.00-1.70) 81.4 (19.84-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.199 , 0.243 0.192 , 0.210	Depositor DCC
$R_{free}$ test set	8981 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.7	EDS
Estimated twinning fraction	0.155 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 193695 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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

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	1.06	6/2880 (0.2%)	1.05	11/3890 (0.3%)
1	B	1.03	3/2880 (0.1%)	1.06	9/3890 (0.2%)
1	C	0.61	0/2880	0.83	7/3890 (0.2%)
1	D	0.56	0/2880	0.79	5/3890 (0.1%)
All	All	0.85	9/11520 (0.1%)	0.94	32/15560 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	GLU	CD-OE1	6.37	1.32	1.25
1	A	314	GLU	CD-OE1	6.01	1.32	1.25
1	A	94	ARG	CZ-NH1	-5.66	1.25	1.33
1	B	115	GLY	CA-C	-5.52	1.43	1.51
1	B	178	PHE	CE2-CZ	5.45	1.47	1.37
1	A	34	VAL	CB-CG1	-5.40	1.41	1.52
1	A	319	PHE	CE2-CZ	5.36	1.47	1.37
1	A	186	ALA	CA-CB	-5.13	1.41	1.52
1	A	42	ALA	CA-CB	-5.04	1.41	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	B	367	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	A	107	ASP	CB-CG-OD2	8.45	125.90	118.30
1	A	141	ASP	CB-CG-OD2	7.88	125.39	118.30
1	B	107	ASP	CB-CG-OD2	7.82	125.34	118.30
1	D	146	ASP	CB-CG-OD2	7.30	124.87	118.30
1	D	136	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	311	ASP	CB-CG-OD2	7.00	124.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	MET	CG-SD-CE	6.61	110.78	100.20
1	B	12	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	C	146	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	146	ASP	CB-CG-OD2	6.21	123.88	118.30
1	D	329	ASP	CB-CG-OD2	5.98	123.69	118.30
1	B	284	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	150	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	226	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	94	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	297	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	136	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	302	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	173	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	197	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	107	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	107	ASP	CB-CG-OD2	5.29	123.07	118.30
1	A	176	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	39	LEU	CA-CB-CG	5.23	127.34	115.30
1	C	367	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	216	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	302	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	172	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	129	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	136	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2834	0	2842	31	0
1	B	2834	0	2842	48	0
1	C	2834	0	2842	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2834	0	2842	58	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	A	6	0	7	2	0
3	B	6	0	8	0	0
4	A	416	0	0	17	0
4	B	425	0	0	29	1
4	C	152	0	0	18	0
4	D	166	0	0	36	0
All	All	12527	0	11383	174	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (174) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:225:LEU:HG	4:A:9889:HOH:O	1.51	1.08
1:A:228:MET:SD	4:A:488:HOH:O	2.19	1.00
1:C:353:SER:HA	4:C:505:HOH:O	1.63	0.96
1:A:225:LEU:HD21	4:A:523:HOH:O	1.67	0.95
1:B:371:ARG:HD3	4:B:476:HOH:O	1.69	0.92
4:C:483:HOH:O	1:D:87:GLN:HA	1.70	0.89
1:C:65:ASN:ND2	4:C:483:HOH:O	2.06	0.87
1:D:183:GLN:HG2	4:D:539:HOH:O	1.75	0.85
1:D:252:GLY:HA3	4:D:515:HOH:O	1.75	0.84
4:A:432:HOH:O	1:B:65:ASN:HB2	1.77	0.84
1:B:163:ASN:ND2	4:B:416:HOH:O	2.12	0.83
1:D:141:ASP:HA	4:D:446:HOH:O	1.79	0.82
1:D:125:CYS:SG	4:D:431:HOH:O	2.37	0.81
1:B:191:LYS:HB3	1:B:191:LYS:NZ	1.97	0.80
1:D:185:LYS:O	4:D:409:HOH:O	2.01	0.79
4:A:9993:HOH:O	1:C:131:GLY:HA3	1.82	0.78
1:D:152:PHE:CE2	4:D:503:HOH:O	2.37	0.77
1:A:6:VAL:HG11	4:A:530:HOH:O	1.84	0.76
1:C:110:ILE:HG22	4:C:528:HOH:O	1.86	0.76
1:C:67:ALA:HB1	4:C:524:HOH:O	1.86	0.75
1:D:150:ASP:HB2	4:D:494:HOH:O	1.86	0.73
1:B:160:THR:HA	4:B:416:HOH:O	1.89	0.71
1:B:388:CYS:HA	4:B:444:HOH:O	1.90	0.71
1:D:251:ASP:O	4:D:551:HOH:O	2.07	0.71
1:B:322:GLN:HB3	4:B:524:HOH:O	1.90	0.71
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.74	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:223:ALA:HB3	4:D:487:HOH:O	1.91	0.70
1:C:143:MET:HB2	4:C:399:HOH:O	1.91	0.69
1:A:207:ARG:H	1:A:207:ARG:HD3	1.56	0.69
1:D:53:ILE:HG22	4:D:460:HOH:O	1.93	0.68
1:D:370:ALA:HB1	4:D:538:HOH:O	1.94	0.68
1:D:290:THR:HA	4:D:502:HOH:O	1.93	0.67
1:C:58:LEU:HD13	4:C:399:HOH:O	1.93	0.67
1:D:344:ILE:HG22	4:D:539:HOH:O	1.96	0.65
1:B:388:CYS:SG	4:B:444:HOH:O	2.55	0.65
1:D:340:ASN:ND2	1:D:364:GLU:OE1	2.23	0.64
1:B:191:LYS:HB3	1:B:191:LYS:HZ3	1.62	0.64
1:D:7:ILE:HG23	1:D:256:ALA:HB1	1.81	0.63
1:C:82:ALA:HB1	4:C:524:HOH:O	1.97	0.63
1:C:252:GLY:HA2	4:C:459:HOH:O	2.00	0.62
1:B:87:GLN:C	4:B:9970:HOH:O	2.38	0.61
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.64	0.60
1:D:30:LEU:HD11	4:D:543:HOH:O	2.00	0.60
1:D:15:VAL:HG13	4:D:551:HOH:O	2.01	0.60
1:D:170:LEU:HB3	4:D:496:HOH:O	2.02	0.60
1:B:191:LYS:HB3	4:B:475:HOH:O	2.02	0.59
1:A:228:MET:HG3	4:A:9831:HOH:O	2.02	0.59
1:A:129:ARG:O	4:A:9993:HOH:O	2.16	0.58
3:A:5393:GOL:C1	4:A:511:HOH:O	2.25	0.58
1:B:374:LEU:HB2	4:B:444:HOH:O	2.02	0.58
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.32	0.58
1:B:166:LYS:HG3	4:B:480:HOH:O	2.03	0.58
1:D:233:PRO:HB2	1:D:236:ASP:O	2.04	0.57
1:A:88:LEU:HG	4:A:432:HOH:O	2.04	0.57
1:A:298:LYS:HE3	2:A:9722:SO4:O3	2.05	0.57
1:D:220:ARG:NH1	4:D:479:HOH:O	2.37	0.57
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.18	0.57
1:B:29:GLU:HG2	4:B:497:HOH:O	2.05	0.57
1:D:85:MET:HG3	4:D:460:HOH:O	2.04	0.56
1:A:172:ARG:NH1	4:A:501:HOH:O	2.38	0.56
1:B:34:VAL:HG12	1:B:255:ALA:HB3	1.87	0.56
1:D:338:ASN:HB3	1:D:341:GLY:O	2.05	0.55
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.41	0.55
1:D:392:LEU:HG	4:D:500:HOH:O	2.06	0.55
1:D:251:ASP:C	4:D:551:HOH:O	2.46	0.54
1:B:29:GLU:CG	4:B:497:HOH:O	2.54	0.54
1:A:207:ARG:H	1:A:207:ARG:CD	2.20	0.54
1:B:191:LYS:HD2	4:B:475:HOH:O	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:349:PRO:HG2	4:C:505:HOH:O	2.09	0.53
1:B:191:LYS:HB3	1:B:191:LYS:HZ2	1.73	0.53
1:C:129:ARG:CG	4:C:509:HOH:O	2.57	0.53
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.75	0.52
1:B:374:LEU:CB	4:B:444:HOH:O	2.58	0.52
1:D:140:ILE:HG22	4:D:431:HOH:O	2.10	0.52
1:C:257:LEU:CD1	1:C:259:MET:CE	2.87	0.52
1:B:87:GLN:HA	4:B:9970:HOH:O	2.09	0.52
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.74	0.52
1:B:240:THR:C	4:B:510:HOH:O	2.47	0.52
1:C:257:LEU:CD1	1:C:259:MET:HE2	2.39	0.52
1:D:349:PRO:HB3	4:D:551:HOH:O	2.09	0.51
1:C:122:ALA:HA	4:C:514:HOH:O	2.11	0.51
1:B:87:GLN:CA	4:B:9970:HOH:O	2.59	0.50
1:B:242:THR:CG2	4:B:510:HOH:O	2.59	0.50
1:B:242:THR:HG23	4:B:510:HOH:O	2.12	0.50
1:B:312:LEU:HB3	4:B:479:HOH:O	2.11	0.50
1:D:15:VAL:HG22	4:D:515:HOH:O	2.11	0.50
1:B:225:LEU:HB2	4:B:515:HOH:O	2.11	0.50
1:D:60:ALA:O	4:D:519:HOH:O	2.20	0.50
1:A:228:MET:CE	4:A:488:HOH:O	2.54	0.49
1:A:40:GLU:HG3	4:A:9951:HOH:O	2.12	0.49
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.76	0.49
1:B:226:ASP:HB3	4:B:509:HOH:O	2.12	0.49
1:A:276:VAL:CG2	1:A:388:CYS:HB2	2.42	0.49
1:B:180:VAL:HG11	4:B:515:HOH:O	2.12	0.49
1:C:129:ARG:HG2	4:C:509:HOH:O	2.13	0.48
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.94	0.48
1:A:282:GLY:HA3	1:B:78:GLN:O	2.13	0.48
1:B:263:GLU:OE1	4:B:9846:HOH:O	2.20	0.48
1:D:291:GLY:N	1:D:292:PRO:CD	2.76	0.48
1:A:166:LYS:HB3	4:A:489:HOH:O	2.13	0.48
1:B:286:LYS:NZ	4:B:9815:HOH:O	2.28	0.47
1:B:34:VAL:CG1	1:B:255:ALA:HB3	2.43	0.47
1:B:374:LEU:C	1:B:374:LEU:HD23	2.35	0.47
1:C:112:VAL:HG22	1:C:257:LEU:HD23	1.96	0.47
1:B:207:ARG:HD3	1:B:207:ARG:N	2.29	0.47
1:D:140:ILE:HB	4:D:431:HOH:O	2.15	0.47
1:C:54:LEU:O	1:C:84:GLY:HA2	2.14	0.47
1:A:237:LYS:HD3	1:A:237:LYS:N	2.30	0.47
1:C:64:GLN:O	1:C:65:ASN:C	2.54	0.47
1:B:208:LYS:NZ	4:B:468:HOH:O	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:GLY:HA2	1:D:131:GLY:HA2	1.97	0.47
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.45	0.47
1:C:223:ALA:HB1	4:C:523:HOH:O	2.16	0.46
1:D:219:ILE:HD11	4:D:510:HOH:O	2.15	0.46
4:A:9993:HOH:O	1:C:131:GLY:CA	2.52	0.46
1:B:191:LYS:HZ2	1:B:191:LYS:CB	2.27	0.46
1:A:110:ILE:HG23	1:A:257:LEU:HD21	1.98	0.46
1:D:248:GLY:HA2	4:D:474:HOH:O	2.16	0.46
1:B:356:ARG:HD2	1:B:356:ARG:C	2.37	0.46
1:C:129:ARG:HG3	4:C:509:HOH:O	2.16	0.45
1:C:174:GLU:OE2	1:C:328:LYS:NZ	2.39	0.45
1:A:330:LEU:HD12	1:A:332:TRP:CZ2	2.51	0.45
1:A:261:GLU:HG3	4:A:530:HOH:O	2.17	0.45
1:B:237:LYS:N	1:B:237:LYS:HD2	2.31	0.45
1:A:225:LEU:HD23	1:A:225:LEU:C	2.37	0.45
1:D:322:GLN:O	1:D:326:VAL:HG23	2.16	0.45
1:D:58:LEU:HB3	4:D:441:HOH:O	2.16	0.45
1:D:167:GLN:HB3	4:D:397:HOH:O	2.17	0.45
1:B:373:GLY:CA	4:B:479:HOH:O	2.65	0.44
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.99	0.44
1:C:4:SER:C	1:C:5:ILE:HD13	2.37	0.44
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.52	0.44
1:D:211:ILE:HB	4:D:554:HOH:O	2.17	0.44
1:A:354:GLY:HA2	1:A:377:LEU:HD11	2.00	0.44
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.30	0.44
1:D:76:VAL:HG23	4:D:540:HOH:O	2.16	0.44
1:A:364:GLU:OE1	1:A:367:ARG:HD2	2.18	0.44
1:D:207:ARG:HD3	1:D:207:ARG:N	2.33	0.43
1:A:1:SER:O	1:A:1:SER:OG	2.29	0.43
1:D:175:GLN:NE2	1:D:240:THR:OG1	2.51	0.43
1:D:335:SER:HA	4:D:526:HOH:O	2.18	0.43
1:D:335:SER:O	1:D:339:VAL:HG12	2.19	0.43
1:D:312:LEU:HD13	1:D:368:ARG:HD2	2.00	0.43
1:C:153:TYR:CE2	1:C:286:LYS:HD3	2.53	0.43
1:B:392:LEU:HD23	4:B:471:HOH:O	2.18	0.43
1:D:326:VAL:HG22	4:D:502:HOH:O	2.18	0.43
1:D:292:PRO:HD3	1:D:378:CYS:HB3	2.01	0.43
1:D:300:LEU:HD22	4:D:427:HOH:O	2.19	0.42
1:C:257:LEU:HD13	1:C:259:MET:HE2	1.99	0.42
1:D:365:MET:CE	1:D:371:ARG:O	2.67	0.42
1:A:276:VAL:HG11	1:A:390:GLU:HB2	2.01	0.42
1:C:316:ASN:HD21	1:C:348:HIS:CE1	2.37	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:195:PHE:HB3	1:D:199:ILE:HD12	2.02	0.42
1:C:226:ASP:O	1:C:230:LYS:HG3	2.19	0.42
1:C:312:LEU:O	1:C:373:GLY:HA2	2.20	0.42
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.33	0.42
1:D:354:GLY:HA2	1:D:377:LEU:HD21	2.02	0.41
1:A:297:ARG:NE	4:A:9987:HOH:O	2.53	0.41
1:D:35:ILE:HG12	1:D:112:VAL:HG11	2.02	0.41
1:A:78:GLN:O	1:B:282:GLY:HA3	2.20	0.41
1:C:18:PHE:CZ	1:D:129:ARG:HD3	2.56	0.41
1:D:328:LYS:HA	4:D:520:HOH:O	2.20	0.41
1:D:100:MET:SD	1:D:100:MET:C	2.98	0.41
1:C:387:MET:HB2	4:C:497:HOH:O	2.21	0.41
1:B:312:LEU:CB	4:B:479:HOH:O	2.68	0.41
1:B:354:GLY:HA2	1:B:377:LEU:HD11	2.03	0.41
1:C:298:LYS:HD3	1:C:301:GLU:OE1	2.21	0.40
1:C:65:ASN:CG	4:C:483:HOH:O	2.52	0.40
1:C:207:ARG:HG2	4:C:517:HOH:O	2.20	0.40
1:C:257:LEU:HD11	1:C:259:MET:CE	2.51	0.40
1:A:153:TYR:CE2	1:A:286:LYS:HG3	2.56	0.40
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.86	0.40
1:D:161:ALA:HB2	4:D:415:HOH:O	2.21	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:437:HOH:O	4:B:9890:HOH:O[2_555]	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	391/392 (100%)	378 (97%)	13 (3%)	0	100	100
1	B	391/392 (100%)	380 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	391/392 (100%)	374 (96%)	16 (4%)	1 (0%)	50	27
1	D	391/392 (100%)	371 (95%)	19 (5%)	1 (0%)	50	27
All	All	1564/1568 (100%)	1503 (96%)	59 (4%)	2 (0%)	59	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	350	ILE
1	C	350	ILE

### 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	279/278 (100%)	261 (94%)	18 (6%)	24	7
1	B	279/278 (100%)	265 (95%)	14 (5%)	34	12
1	C	279/278 (100%)	264 (95%)	15 (5%)	31	11
1	D	279/278 (100%)	257 (92%)	22 (8%)	18	4
All	All	1116/1112 (100%)	1047 (94%)	69 (6%)	26	8

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	39	LEU
1	A	132	VAL
1	A	136	ASP
1	A	155	TYR
1	A	191	LYS
1	A	207	ARG
1	A	220	ARG
1	A	228	MET
1	A	230	LYS
1	A	238	GLU
1	A	272	LEU

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Mol	Chain	Res	Type
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	B	39	LEU
1	B	155	TYR
1	B	167	GLN
1	B	191	LYS
1	B	207	ARG
1	B	220	ARG
1	B	237	LYS
1	B	238	GLU
1	B	263	GLU
1	B	272	LEU
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	C	39	LEU
1	C	155	TYR
1	C	187	GLU
1	C	191	LYS
1	C	207	ARG
1	C	220	ARG
1	C	224	THR
1	C	237	LYS
1	C	257	LEU
1	C	263	GLU
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	D	39	LEU
1	D	129	ARG
1	D	134	MET
1	D	155	TYR
1	D	167	GLN
1	D	187	GLU
1	D	207	ARG

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Mol	Chain	Res	Type
1	D	220	ARG
1	D	227	SER
1	D	237	LYS
1	D	238	GLU
1	D	263	GLU
1	D	272	LEU
1	D	288	MET
1	D	298	LYS
1	D	311	ASP
1	D	322	GLN
1	D	332	TRP
1	D	353	SER
1	D	359	ASN
1	D	371	ARG
1	D	391	SER

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

Mol	Chain	Res	Type
1	A	78	GLN
1	A	175	GLN
1	A	184	ASN
1	B	175	GLN
1	B	184	ASN
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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	5393	-	5,5,5	1.05	1 (20%)	5,5,5	1.16	0
2	SO4	A	9720	-	4,4,4	0.18	0	6,6,6	0.29	0
2	SO4	A	9722	-	4,4,4	0.17	0	6,6,6	0.42	0
3	GOL	B	6393	-	5,5,5	0.25	0	5,5,5	1.05	0
2	SO4	B	9719	-	4,4,4	0.24	0	6,6,6	0.21	0
2	SO4	B	9721	-	4,4,4	0.47	0	6,6,6	0.17	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	5393	-	-	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	6393	-	-	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5393	GOL	O3-C3	-2.16	1.32	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	392/392 (100%)	0.05	7 (1%) 65 71	5, 10, 25, 48	0
1	B	392/392 (100%)	0.06	7 (1%) 65 71	5, 10, 25, 51	0
1	C	392/392 (100%)	0.93	47 (11%) 5 7	3, 13, 26, 40	0
1	D	392/392 (100%)	1.52	102 (26%) 1 2	2, 15, 27, 39	0
All	All	1568/1568 (100%)	0.64	163 (10%) 7 9	2, 12, 26, 51	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	SER	8.9
1	D	170	LEU	8.7
1	D	1	SER	8.3
1	D	229	ALA	8.1
1	D	2	THR	7.3
1	D	392	LEU	7.0
1	D	232	ARG	6.5
1	D	188	ALA	6.2
1	B	207	ARG	6.0
1	D	228	MET	5.9
1	C	104	ALA	5.4
1	C	208	LYS	5.3
1	D	226	ASP	5.3
1	C	225	LEU	5.3
1	A	208	LYS	5.1
1	D	237	LYS	5.1
1	D	235	PHE	5.1
1	D	231	LEU	5.0
1	D	240	THR	4.9
1	D	328	LYS	4.8
1	C	2	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	224	THR	4.7
1	D	208	LYS	4.5
1	C	232	ARG	4.5
1	D	207	ARG	4.3
1	C	243	ALA	4.3
1	D	221	HIS	4.3
1	C	206	GLY	4.2
1	C	186	ALA	4.2
1	C	211	ILE	4.2
1	D	219	ILE	4.2
1	D	332	TRP	4.2
1	D	227	SER	4.1
1	D	238	GLU	4.0
1	D	225	LEU	4.0
1	D	377	LEU	3.9
1	D	167	GLN	3.9
1	D	325	ALA	3.9
1	D	371	ARG	3.9
1	A	209	GLY	3.8
1	D	206	GLY	3.8
1	A	132	VAL	3.8
1	D	382	GLY	3.7
1	B	1	SER	3.7
1	C	36	SER	3.6
1	D	152	PHE	3.6
1	D	324	CYS	3.6
1	D	269	ILE	3.5
1	D	223	ALA	3.5
1	C	231	LEU	3.5
1	D	310	LEU	3.5
1	D	330	LEU	3.5
1	C	221	HIS	3.5
1	D	236	ASP	3.4
1	C	234	ALA	3.4
1	D	339	VAL	3.4
1	C	67	ALA	3.4
1	C	80	ALA	3.3
1	B	392	LEU	3.3
1	A	206	GLY	3.3
1	D	173	ASP	3.3
1	D	306	LYS	3.3
1	D	331	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	378	CYS	3.2
1	D	180	VAL	3.2
1	D	289	GLY	3.2
1	D	220	ARG	3.1
1	C	153	TYR	3.1
1	D	350	ILE	3.1
1	D	375	ALA	3.1
1	D	391	SER	3.0
1	D	195	PHE	3.0
1	C	226	ASP	3.0
1	C	224	THR	3.0
1	C	209	GLY	3.0
1	D	281	VAL	3.0
1	C	239	GLY	3.0
1	C	334	PRO	3.0
1	D	303	ALA	3.0
1	D	5	ILE	2.9
1	A	131	GLY	2.9
1	B	132	VAL	2.9
1	D	189	ALA	2.9
1	D	15	VAL	2.9
1	D	241	VAL	2.9
1	D	299	ALA	2.8
1	D	181	ALA	2.8
1	D	311	ASP	2.8
1	C	235	PHE	2.8
1	D	153	TYR	2.7
1	D	155	TYR	2.7
1	D	301	GLU	2.7
1	B	208	LYS	2.7
1	D	307	ILE	2.7
1	D	313	VAL	2.7
1	D	389	ILE	2.7
1	D	178	PHE	2.7
1	C	392	LEU	2.7
1	C	49	VAL	2.7
1	C	135	GLY	2.6
1	D	319	PHE	2.6
1	C	179	ALA	2.6
1	D	370	ALA	2.6
1	D	329	ASP	2.6
1	D	254	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	367	ARG	2.5
1	A	207	ARG	2.5
1	C	181	ALA	2.5
1	D	165	ALA	2.5
1	C	207	ARG	2.5
1	D	175	GLN	2.5
1	D	171	SER	2.5
1	C	265	SER	2.5
1	C	315	ALA	2.5
1	D	272	LEU	2.5
1	D	192	ASP	2.5
1	C	222	GLY	2.4
1	D	191	LYS	2.4
1	C	371	ARG	2.4
1	C	161	ALA	2.4
1	D	243	ALA	2.4
1	C	35	ILE	2.4
1	D	376	THR	2.4
1	D	42	ALA	2.3
1	C	230	LYS	2.3
1	C	156	HIS	2.3
1	D	156	HIS	2.3
1	D	211	ILE	2.3
1	C	170	LEU	2.2
1	D	374	LEU	2.2
1	D	166	LYS	2.2
1	C	164	VAL	2.2
1	D	187	GLU	2.2
1	D	160	THR	2.2
1	C	312	LEU	2.2
1	D	368	ARG	2.2
1	C	295	ALA	2.2
1	D	179	ALA	2.1
1	D	202	PHE	2.1
1	D	249	LEU	2.1
1	D	4	SER	2.1
1	C	52	VAL	2.1
1	D	320	ALA	2.1
1	D	244	GLY	2.1
1	D	372	LYS	2.1
1	C	305	TRP	2.1
1	D	210	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2	THR	2.1
1	D	318	ALA	2.1
1	D	218	TYR	2.1
1	B	131	GLY	2.1
1	D	305	TRP	2.1
1	C	266	ARG	2.1
1	D	362	LEU	2.1
1	C	323	ALA	2.0
1	D	177	ALA	2.0
1	D	369	GLY	2.0
1	D	174	GLU	2.0
1	D	265	SER	2.0
1	A	2	THR	2.0
1	C	113	ALA	2.0
1	D	334	PRO	2.0
1	C	213	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	9720	5/5	0.11	2.33	44,49,52,55	0
3	GOL	B	6393	6/6	0.11	1.26	9,24,30,31	0
2	SO4	A	9722	5/5	0.14	1.13	65,65,68,69	0
3	GOL	A	5393	6/6	0.11	0.64	17,23,28,28	0
2	SO4	B	9721	5/5	0.09	-0.74	42,45,51,54	0
2	SO4	B	9719	5/5	0.08	-1.24	67,67,68,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.