



# Full wwPDB X-ray Structure Validation Report i

May 16, 2020 – 09:03 pm BST

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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.1.3  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

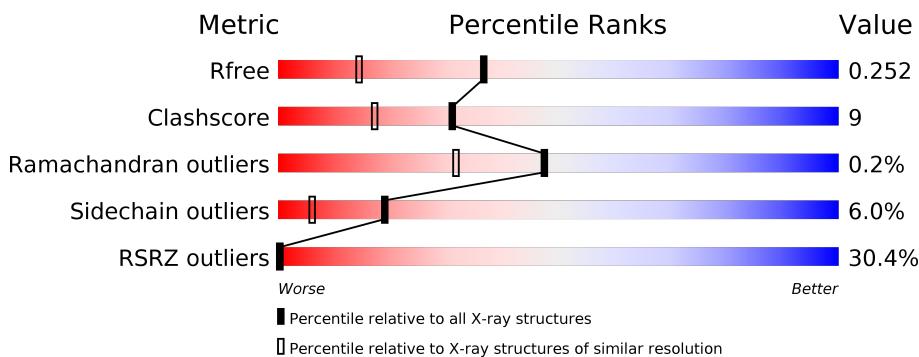
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

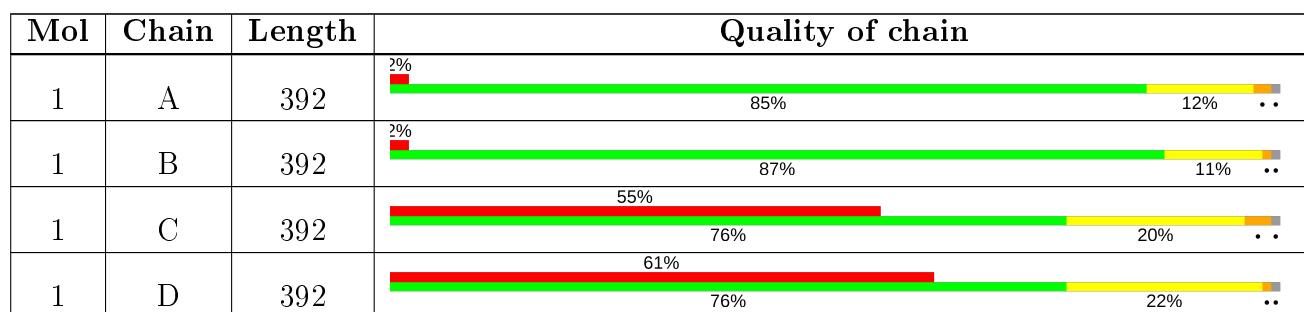
The reported resolution of this entry is 1.77 Å.

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))
$R_{free}$	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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.



## 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.

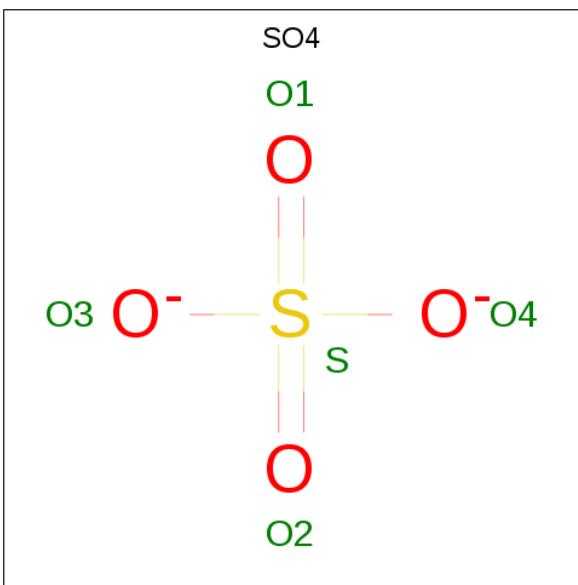
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

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:

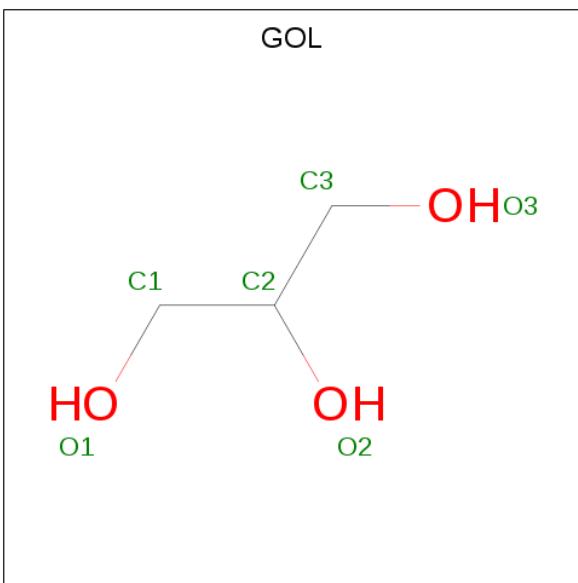
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	CY4	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	CY4	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	CY4	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<sub>4</sub>S).



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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

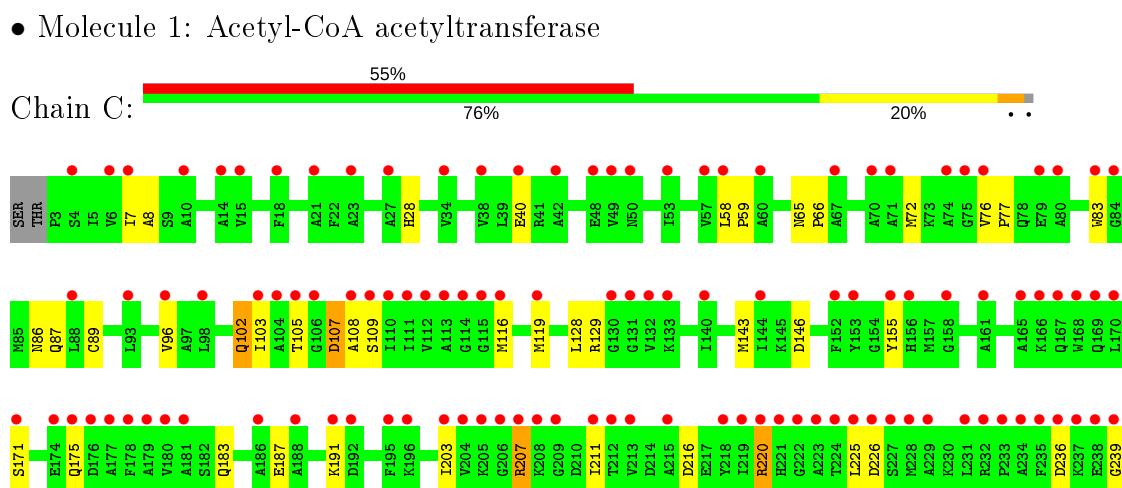
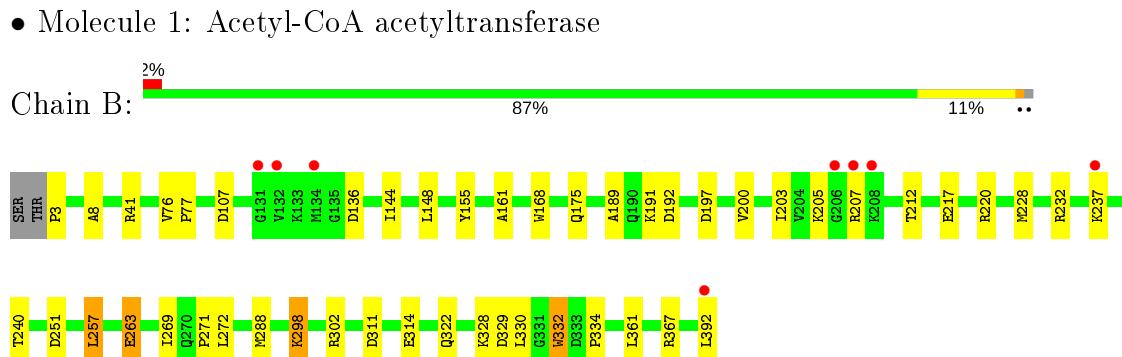
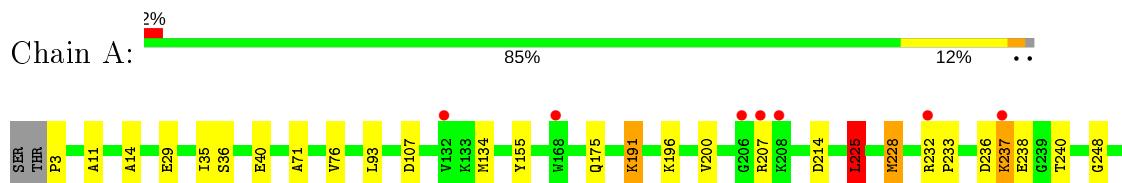
- Molecule 4 is water.

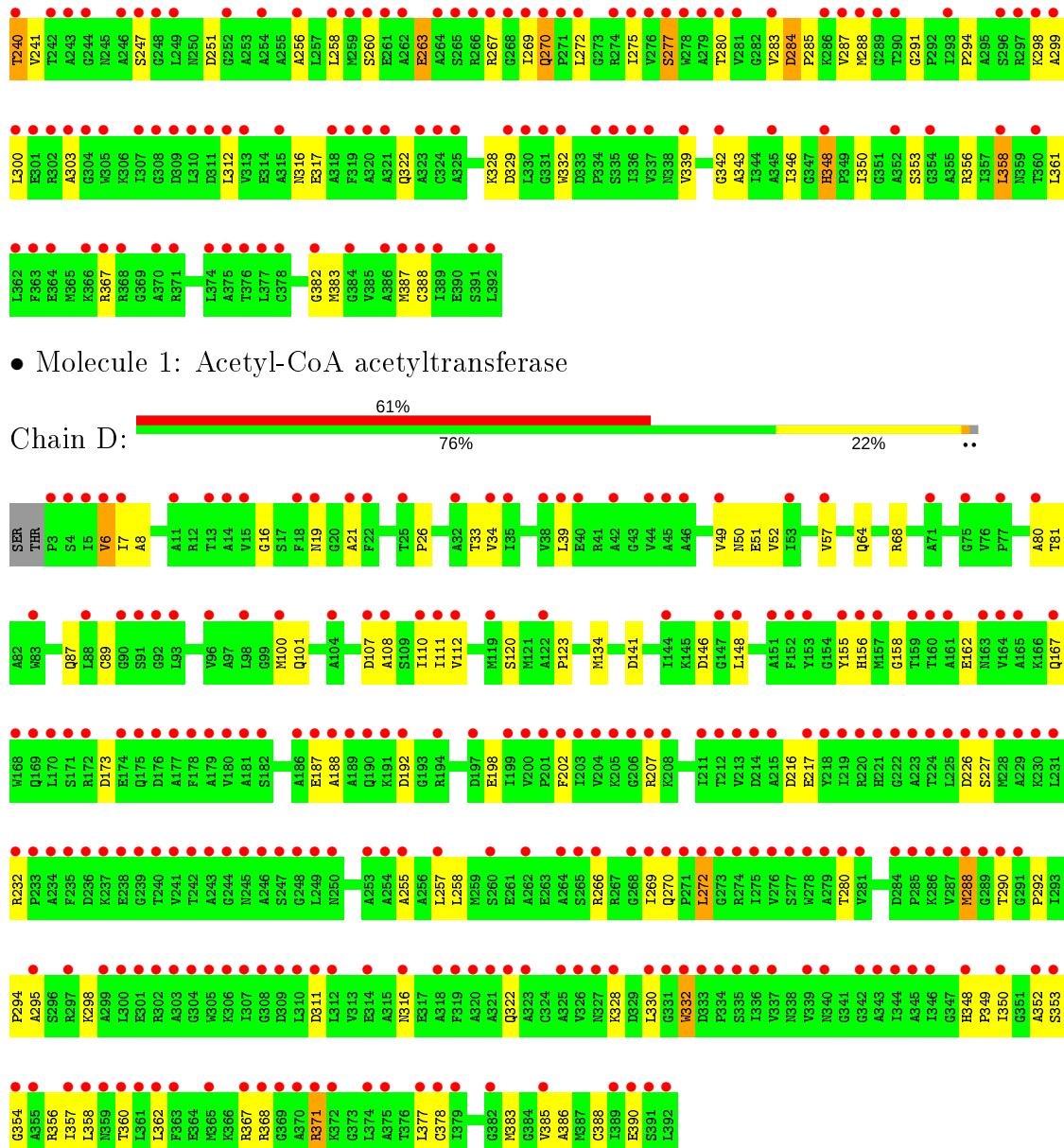
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	403	Total O 403 403	0	0
4	B	406	Total O 406 406	0	0
4	C	144	Total O 144 144	0	0
4	D	138	Total O 138 138	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.35Å    79.31Å    147.32Å 90.00°    93.97°    90.00°	Depositor
Resolution (Å)	20.00 – 1.77 37.17 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-1.77) 80.8 (37.17-1.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	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 (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.4	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.38$ , $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12421	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 6.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>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: GOL, SO4, CY4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.02	1/2861 (0.0%)	1.02	13/3861 (0.3%)
1	B	1.00	3/2861 (0.1%)	0.99	9/3861 (0.2%)
1	C	0.57	3/2861 (0.1%)	0.77	7/3861 (0.2%)
1	D	0.52	2/2861 (0.1%)	0.77	7/3861 (0.2%)
All	All	0.81	9/11444 (0.1%)	0.90	36/15444 (0.2%)

All (9) bond length outliers are listed below:

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

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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(°)	Ideal(°)
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:HA	1:B:298:LYS:HE3	1.85	0.58
1:C:58:LEU:HD13	4:C:405:HOH:O	2.01	0.58
1:B:298:LYS:O	1:B:298:LYS:HD3	2.03	0.58
1: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:316:ASN:HD21	1:D:348:HIS:CE1	2.30	0.49
1:D:50:ASN:O	1:D:80:ALA:HB1	2.11	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:HZ2	1:B:191:LYS:HB3	1.78	0.46
1:B:205:LYS:CE	4:B:413:HOH:O	2.64	0.46
1:B:76:VAL:HG13	1:B:77:PRO:HD2	1.97	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:O	1:C:287:VAL:HG23	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:269:ILE:HG22	1:C:270:GLN:H	1.83	0.44
1:C:66:PRO:HB3	4:C:483:HOH:O	2.18	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:211:ILE:C	4:C:532:HOH:O	2.56	0.42
1:C:76:VAL:CG1	1:C:77:PRO:HD2	2.49	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:HE2	1:A:228:MET:HA	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:C	1:B:257:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD12	1:B:332:TRP:CZ2	2.56	0.41
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.54	0.41
1: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:356:ARG:NH2	4:C:489:HOH:O	2.54	0.41
1:C:280:THR:HG23	1:D:81:THR:HG21	2.03	0.41
1:C: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

### 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%)	29	14
1	D	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	41	25
All	All	1552/1568 (99%)	1488 (96%)	61 (4%)	3 (0%)	47	32

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%)	20	6
1	B	277/278 (100%)	264 (95%)	13 (5%)	26	10
1	C	277/278 (100%)	257 (93%)	20 (7%)	14	4
1	D	277/278 (100%)	260 (94%)	17 (6%)	18	6
All	All	1108/1112 (100%)	1042 (94%)	66 (6%)	19	6

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

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

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

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

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

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

### 5.3.3 RNA [\(i\)](#)

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	B	89	1	9,10,11	1.64	2 (22%)	6,11,13	2.21	3 (50%)
1	CY4	C	89	1	4,5,11	0.45	0	1,5,13	0.02	0
1	CY4	A	89	1	9,10,11	1.36	1 (11%)	6,11,13	1.77	2 (33%)
1	CY4	D	89	1	4,5,11	0.51	0	1,5,13	1.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CY4	B	89	1	-	2/8/10/12	-
1	CY4	C	89	1	-	0/1/4/12	-
1	CY4	A	89	1	-	3/8/10/12	-
1	CY4	D	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	3.28	1.54	1.50
1	B	89	CY4	CA2-CA1	3.26	1.54	1.50
1	B	89	CY4	CB-SG	2.03	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	100.84
1	B	89	CY4	CB-SG-CA1	-3.14	96.45	100.84
1	B	89	CY4	OA1-CA1-CA2	-3.12	120.30	123.99
1	B	89	CY4	OA1-CA1-SG	2.90	126.39	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	89	CY4	OA1-CA1-CA2	-2.40	121.15	123.99

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	C	89	CY4	1	0
1	D	89	CY4	1	0

## 5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [\(i\)](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	9721	-	4,4,4	0.23	0	6,6,6	0.37	0
2	SO4	B	9719	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	A	9722	-	4,4,4	0.16	0	6,6,6	0.20	0
3	GOL	B	6394	-	5,5,5	0.94	1 (20%)	5,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	9720	-	4,4,4	0.17	0	6,6,6	0.44	0
3	GOL	A	5394	-	5,5,5	1.07	1 (20%)	5,5,5	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	5394	-	-	2/4/4/4	-
3	GOL	B	6394	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5394	GOL	O2-C2	-2.21	1.36	1.43
3	B	6394	GOL	O2-C2	-2.06	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	B	6394	GOL	O1-C1-C2-C3
3	A	5394	GOL	O1-C1-C2-C3
3	B	6394	GOL	O1-C1-C2-O2
3	A	5394	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 (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, 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	389/392 (99%)	0.17	8 (2%) 63 63	5, 11, 28, 54	0
1	B	389/392 (99%)	0.18	8 (2%) 63 63	6, 11, 28, 55	0
1	C	389/392 (99%)	2.73	216 (55%) 0 0	2, 11, 28, 42	0
1	D	389/392 (99%)	3.41	241 (61%) 0 0	2, 13, 29, 45	0
All	All	1556/1568 (99%)	1.62	473 (30%) 0 0	2, 11, 29, 55	0

All (473) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	17.8
1	D	229	ALA	15.0
1	D	219	ILE	14.8
1	D	179	ALA	14.2
1	D	244	GLY	13.6
1	D	188	ALA	13.3
1	D	170	LEU	13.1
1	C	234	ALA	12.4
1	C	105	THR	11.5
1	D	228	MET	10.0
1	A	132	VAL	9.8
1	D	235	PHE	9.7
1	D	233	PRO	9.7
1	C	49	VAL	9.6
1	D	108	ALA	9.4
1	D	227	SER	9.3
1	C	370	ALA	9.2
1	D	164	VAL	9.1
1	C	225	LEU	8.9
1	D	310	LEU	8.9
1	C	239	GLY	8.9

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Mol	Chain	Res	Type	RSRZ
1	D	239	GLY	8.8
1	C	80	ALA	8.6
1	B	207	ARG	8.5
1	D	392	LEU	8.5
1	D	240	THR	8.5
1	C	161	ALA	8.3
1	D	178	PHE	8.2
1	C	276	VAL	8.2
1	D	224	THR	8.1
1	D	223	ALA	8.1
1	C	235	PHE	8.0
1	D	160	THR	8.0
1	D	265	SER	8.0
1	C	342	GLY	7.9
1	D	247[A]	SER	7.9
1	D	159	THR	7.9
1	C	224	THR	7.9
1	D	243	ALA	7.9
1	D	361	LEU	7.8
1	D	181	ALA	7.8
1	D	168	TRP	7.8
1	D	186	ALA	7.7
1	D	295	ALA	7.7
1	D	238	GLU	7.7
1	D	285	PRO	7.7
1	D	153	TYR	7.5
1	D	319	PHE	7.5
1	C	300	LEU	7.4
1	D	234	ALA	7.4
1	B	208	LYS	7.4
1	C	229	ALA	7.4
1	D	215	ALA	7.4
1	D	171	SER	7.2
1	D	330	LEU	7.2
1	D	161	ALA	7.2
1	D	246	ALA	7.2
1	D	332	TRP	7.1
1	D	299	ALA	7.0
1	D	339	VAL	7.0
1	D	34	VAL	6.9
1	C	232	ARG	6.9
1	D	279	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
1	D	323	ALA	6.9
1	D	275	ILE	6.8
1	C	371	ARG	6.8
1	C	247[A]	SER	6.8
1	C	34	VAL	6.8
1	D	350	ILE	6.8
1	D	374	LEU	6.7
1	C	283	VAL	6.7
1	C	242	THR	6.7
1	D	312	LEU	6.7
1	D	272	LEU	6.6
1	C	336	ILE	6.6
1	C	240	THR	6.6
1	C	293	ILE	6.5
1	D	335	SER	6.5
1	C	67	ALA	6.5
1	D	305	TRP	6.5
1	C	238	GLU	6.4
1	D	290	THR	6.4
1	C	279	ALA	6.4
1	D	343	ALA	6.4
1	D	326	VAL	6.3
1	D	6	VAL	6.3
1	C	270	GLN	6.2
1	C	106	GLY	6.2
1	C	266	ARG	6.2
1	C	392	LEU	6.1
1	D	300	LEU	6.1
1	C	208	LYS	6.1
1	C	313	VAL	6.1
1	C	221	HIS	6.1
1	D	336	ILE	6.0
1	C	268	GLY	6.0
1	D	245	ASN	6.0
1	C	226	ASP	6.0
1	C	96	VAL	6.0
1	D	207	ARG	6.0
1	D	232	ARG	6.0
1	D	377	LEU	6.0
1	C	331	GLY	5.9
1	A	207	ARG	5.9
1	D	357	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	246	ALA	5.8
1	D	370	ALA	5.7
1	D	230	LYS	5.7
1	C	113	ALA	5.7
1	D	218	TYR	5.6
1	D	157	MET	5.6
1	C	366	LYS	5.6
1	D	257	LEU	5.6
1	D	241	VAL	5.6
1	C	75	GLY	5.6
1	D	269	ILE	5.6
1	C	177	ALA	5.6
1	C	319	PHE	5.5
1	C	103	ILE	5.5
1	C	203	ILE	5.5
1	D	222	GLY	5.5
1	D	391	SER	5.5
1	D	155	TYR	5.4
1	D	270	GLN	5.4
1	C	269	ILE	5.4
1	D	365	MET	5.4
1	C	207	ARG	5.4
1	D	363	PHE	5.4
1	D	291	GLY	5.4
1	C	301	GLU	5.4
1	D	271	PRO	5.3
1	C	231	LEU	5.3
1	D	327	ASN	5.3
1	D	253	ALA	5.3
1	D	331	GLY	5.2
1	D	340	ASN	5.2
1	D	325	ALA	5.1
1	C	307	ILE	5.1
1	D	208	LYS	5.1
1	D	169	GLN	5.1
1	D	368	ARG	5.0
1	C	378	CYS	5.0
1	C	152	PHE	5.0
1	D	226	ASP	4.9
1	C	104	ALA	4.9
1	D	369	GLY	4.9
1	D	276	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	382	GLY	4.9
1	D	151	ALA	4.9
1	D	172	ARG	4.8
1	C	335	SER	4.8
1	D	15	VAL	4.8
1	D	163	ASN	4.8
1	C	204	VAL	4.8
1	C	228	MET	4.8
1	C	305	TRP	4.8
1	D	225	LEU	4.8
1	C	389	ILE	4.8
1	A	208	LYS	4.7
1	D	320	ALA	4.7
1	C	206	GLY	4.7
1	C	57	VAL	4.7
1	C	211	ILE	4.7
1	D	213	VAL	4.7
1	D	281	VAL	4.7
1	C	243	ALA	4.7
1	B	132	VAL	4.7
1	C	244	GLY	4.7
1	D	358	LEU	4.7
1	D	307	ILE	4.6
1	D	304	GLY	4.6
1	D	318	ALA	4.6
1	C	272	LEU	4.6
1	D	44	VAL	4.6
1	D	112	VAL	4.6
1	C	40	GLU	4.6
1	C	290	THR	4.6
1	C	222	GLY	4.6
1	D	371	ARG	4.6
1	D	107	ASP	4.6
1	D	4	SER	4.6
1	D	104	ALA	4.5
1	C	110	ILE	4.5
1	C	363	PHE	4.5
1	D	262	ALA	4.5
1	D	311	ASP	4.5
1	D	221	HIS	4.5
1	C	215	ALA	4.5
1	D	359	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	287	VAL	4.5
1	C	170	LEU	4.4
1	D	152	PHE	4.4
1	D	280	THR	4.4
1	C	315	ALA	4.4
1	D	342	GLY	4.4
1	C	180	VAL	4.4
1	C	218	TYR	4.3
1	C	4	SER	4.3
1	A	206	GLY	4.3
1	C	277	SER	4.3
1	D	180	VAL	4.3
1	D	49	VAL	4.3
1	D	7	ILE	4.2
1	C	38	VAL	4.2
1	C	258	LEU	4.2
1	C	108	ALA	4.2
1	D	385	VAL	4.2
1	D	22	PHE	4.2
1	C	93	LEU	4.2
1	C	376	THR	4.2
1	C	21	ALA	4.2
1	D	346	ILE	4.1
1	C	169	GLN	4.1
1	D	165	ALA	4.1
1	C	195	PHE	4.1
1	C	388	CYS	4.0
1	D	237	LYS	4.0
1	D	220	ARG	4.0
1	D	266	ARG	4.0
1	C	310	LEU	4.0
1	C	175	GLN	4.0
1	D	197	ASP	4.0
1	D	379	ILE	4.0
1	C	227	SER	4.0
1	D	190	GLN	4.0
1	C	14	ALA	4.0
1	D	288	MET	4.0
1	D	40	GLU	3.9
1	C	265	SER	3.9
1	D	75	GLY	3.9
1	C	79	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	297	ARG	3.9
1	C	264	ALA	3.9
1	C	303	ALA	3.9
1	D	352	ALA	3.9
1	C	332	TRP	3.9
1	C	179	ALA	3.8
1	C	287	VAL	3.8
1	C	168	TRP	3.8
1	C	71	ALA	3.8
1	C	275	ILE	3.8
1	D	201	PRO	3.8
1	D	83	TRP	3.8
1	C	191	LYS	3.8
1	D	35	ILE	3.7
1	C	7	ILE	3.7
1	C	88	LEU	3.7
1	C	296	SER	3.7
1	D	25	THR	3.7
1	C	10	ALA	3.7
1	C	23	ALA	3.7
1	D	236	ASP	3.7
1	C	213	VAL	3.7
1	D	308	GLY	3.7
1	C	83	TRP	3.7
1	C	391	SER	3.7
1	B	206	GLY	3.6
1	C	176	ASP	3.6
1	D	92	GLY	3.6
1	C	27	ALA	3.6
1	C	358	LEU	3.6
1	D	175	GLN	3.5
1	C	233	PRO	3.5
1	C	280	THR	3.5
1	C	312	LEU	3.5
1	D	372	LYS	3.5
1	C	262	ALA	3.5
1	C	167	GLN	3.5
1	D	268	GLY	3.5
1	C	299	ALA	3.5
1	D	378	CYS	3.5
1	C	374	LEU	3.4
1	D	200	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	309	ASP	3.4
1	C	278	TRP	3.4
1	B	237	LYS	3.4
1	D	289	GLY	3.4
1	C	155	TYR	3.4
1	C	320	ALA	3.4
1	D	42	ALA	3.4
1	C	115	GLY	3.4
1	D	177	ALA	3.4
1	C	325	ALA	3.3
1	D	264	ALA	3.3
1	C	114	GLY	3.3
1	C	133	LYS	3.3
1	C	178	PHE	3.3
1	C	281	VAL	3.3
1	C	308	GLY	3.3
1	C	382	GLY	3.3
1	D	167	GLN	3.3
1	B	134	MET	3.3
1	D	255	ALA	3.3
1	D	306	LYS	3.3
1	C	259	MET	3.3
1	D	309	ASP	3.3
1	D	13	THR	3.2
1	C	76	VAL	3.2
1	D	88	LEU	3.2
1	C	74	ALA	3.2
1	C	131	GLY	3.2
1	D	156	HIS	3.2
1	D	3	PRO	3.2
1	C	236	ASP	3.2
1	C	249	LEU	3.2
1	D	211	ILE	3.2
1	C	156	HIS	3.2
1	C	237	LYS	3.2
1	D	174	GLU	3.2
1	D	93	LEU	3.2
1	D	202	PHE	3.2
1	D	242	THR	3.2
1	C	274	ARG	3.1
1	C	367	ARG	3.1
1	D	248	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	70	ALA	3.1
1	D	353	SER	3.1
1	D	5	ILE	3.0
1	C	352	ALA	3.0
1	D	21	ALA	3.0
1	D	375	ALA	3.0
1	C	362	LEU	3.0
1	D	322	GLN	3.0
1	C	109	SER	3.0
1	C	153	TYR	3.0
1	C	348	HIS	3.0
1	D	119	MET	3.0
1	D	111	ILE	3.0
1	C	256	ALA	2.9
1	D	277	SER	2.9
1	D	206	GLY	2.9
1	D	45	ALA	2.9
1	D	286	LYS	2.9
1	D	362	LEU	2.9
1	D	189	ALA	2.9
1	C	220	ARG	2.9
1	D	367	ARG	2.9
1	C	321	ALA	2.9
1	C	112	VAL	2.9
1	D	98	LEU	2.9
1	D	203	ILE	2.9
1	D	284	ASP	2.8
1	C	271	PRO	2.8
1	C	223	ALA	2.8
1	D	176	ASP	2.8
1	C	334	PRO	2.8
1	C	188	ALA	2.8
1	C	386	ALA	2.8
1	D	321	ALA	2.8
1	D	100	MET	2.8
1	C	84	GLY	2.8
1	D	90	GLY	2.8
1	C	324	CYS	2.8
1	D	194	ARG	2.7
1	D	301	GLU	2.7
1	D	303	ALA	2.7
1	D	57	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	392	LEU	2.7
1	C	377	LEU	2.7
1	D	18	PHE	2.7
1	A	232	ARG	2.7
1	D	337	VAL	2.7
1	C	192	ASP	2.7
1	C	181	ALA	2.6
1	D	274	ARG	2.6
1	D	316	ASN	2.6
1	D	199	ILE	2.6
1	C	252	GLY	2.6
1	D	333	ASP	2.6
1	D	205	LYS	2.6
1	D	11	ALA	2.6
1	C	140	ILE	2.6
1	C	304	GLY	2.6
1	D	144	ILE	2.6
1	D	204	VAL	2.6
1	C	345	ALA	2.6
1	D	39	LEU	2.6
1	C	286	LYS	2.5
1	D	191	LYS	2.5
1	D	328	LYS	2.5
1	D	278	TRP	2.5
1	C	219	ILE	2.5
1	D	389	ILE	2.5
1	D	360	THR	2.5
1	D	260	SER	2.5
1	C	209	GLY	2.5
1	C	375	ALA	2.5
1	C	384	GLY	2.5
1	C	174	GLU	2.5
1	C	144	ILE	2.5
1	D	38	VAL	2.5
1	C	329	ASP	2.5
1	C	166	LYS	2.5
1	D	212	THR	2.5
1	C	6	VAL	2.5
1	D	354	GLY	2.5
1	C	165	ALA	2.4
1	C	186	ALA	2.4
1	C	323	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	71	ALA	2.4
1	C	260	SER	2.4
1	D	182	SER	2.4
1	D	148	LEU	2.4
1	D	390	GLU	2.4
1	D	344	ILE	2.4
1	D	302	ARG	2.4
1	A	237	LYS	2.4
1	C	196	LYS	2.4
1	D	110	ILE	2.4
1	C	302	ARG	2.4
1	C	368	ARG	2.4
1	D	91	SER	2.4
1	D	273	GLY	2.4
1	C	297	ARG	2.3
1	C	98	LEU	2.3
1	D	314	GLU	2.3
1	D	122	ALA	2.3
1	C	311	ASP	2.3
1	C	205	LYS	2.3
1	D	19	ASN	2.3
1	C	111	ILE	2.3
1	C	48	GLU	2.3
1	D	217	GLU	2.3
1	C	387	MET	2.3
1	C	289	GLY	2.3
1	C	15	VAL	2.3
1	D	46	ALA	2.3
1	D	254	ALA	2.3
1	C	130	GLY	2.3
1	C	298	LYS	2.3
1	C	171	SER	2.2
1	D	249	LEU	2.2
1	D	147	GLY	2.2
1	C	116	MET	2.2
1	D	32	ALA	2.2
1	D	334	PRO	2.2
1	D	348	HIS	2.2
1	C	50	ASN	2.2
1	C	354	GLY	2.2
1	D	14	ALA	2.2
1	D	77	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	360	THR	2.2
1	C	18	PHE	2.2
1	C	60	ALA	2.2
1	C	254	ALA	2.2
1	D	345	ALA	2.2
1	C	288	MET	2.2
1	D	96	VAL	2.2
1	D	53	ILE	2.2
1	C	119	MET	2.1
1	C	53	ILE	2.1
1	D	355	ALA	2.1
1	C	132	VAL	2.1
1	C	339	VAL	2.1
1	C	212	THR	2.1
1	D	187	GLU	2.1
1	B	131	GLY	2.1
1	C	158	GLY	2.1
1	C	337	VAL	2.1
1	A	392	LEU	2.1
1	C	42	ALA	2.1
1	C	58	LEU	2.1
1	C	267	ARG	2.1
1	A	168	TRP	2.1
1	D	80	ALA	2.1
1	C	248	GLY	2.1
1	C	330	LEU	2.1
1	C	318	ALA	2.0
1	D	192	ASP	2.0
1	C	261	GLU	2.0
1	D	250	ASN	2.0
1	C	364	GLU	2.0
1	D	214	ASP	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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CY4	D	89	6/12	0.74	0.14	2,4,4,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CY4	C	89	6/12	0.89	0.10	8,10,11,15	0
1	CY4	B	89	11/12	0.94	0.12	8,10,26,28	0
1	CY4	A	89	11/12	0.95	0.13	9,12,30,31	0

### 6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	6394	6/6	0.85	0.16	18,26,30,38	0
2	SO4	A	9722	5/5	0.90	0.20	74,74,75,75	0
3	GOL	A	5394	6/6	0.90	0.13	20,31,33,33	0
2	SO4	B	9719	5/5	0.95	0.18	76,77,78,78	0
2	SO4	B	9721	5/5	0.96	0.10	47,48,50,51	0
2	SO4	A	9720	5/5	0.97	0.10	45,50,50,51	0

### 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.