



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:08 PM GMT

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

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

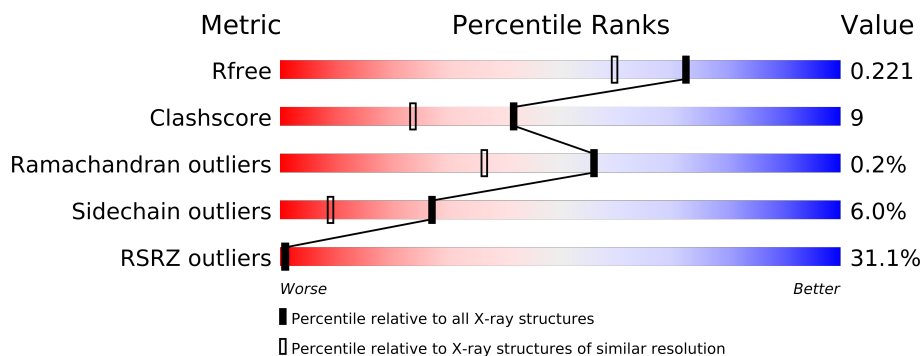
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.77 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}	66092	4987 (1.80-1.76)
Clashscore	79885	6152 (1.80-1.76)
Ramachandran outliers	78287	6074 (1.80-1.76)
Sidechain outliers	78261	6073 (1.80-1.76)
RSRZ outliers	66119	4990 (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. 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	9722	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12421 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	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: 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 (three-letter code: GOL) (formula: C₃H₈O₃).



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.

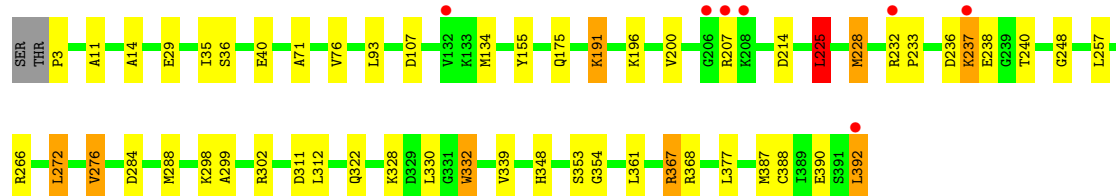
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	403	Total	O	0	0
			403	403		
4	B	406	Total	O	0	0
			406	406		
4	C	144	Total	O	0	0
			144	144		
4	D	138	Total	O	0	0
			138	138		

3 Residue-property plots

These plots are drawn for all protein, RNA 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.

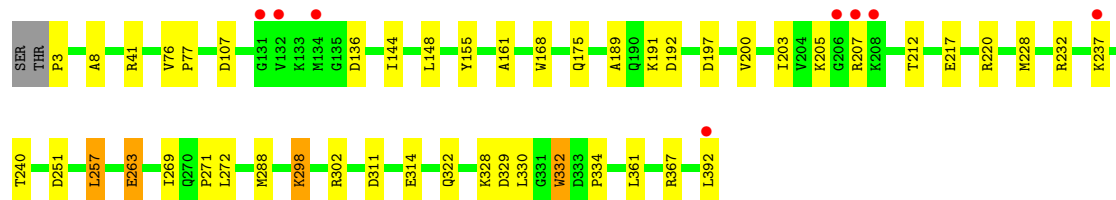
• Molecule 1: Acetyl-CoA acetyltransferase

Chain A: 



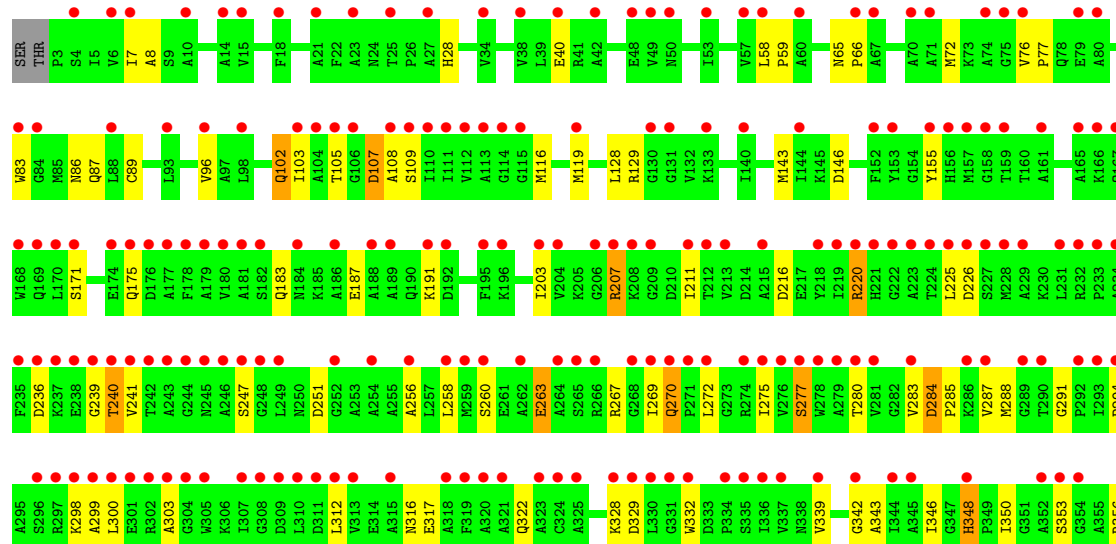
• Molecule 1: Acetyl-CoA acetyltransferase

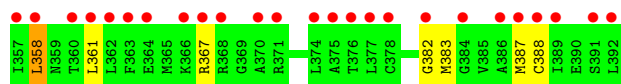
Chain B: 



• Molecule 1: Acetyl-CoA acetyltransferase

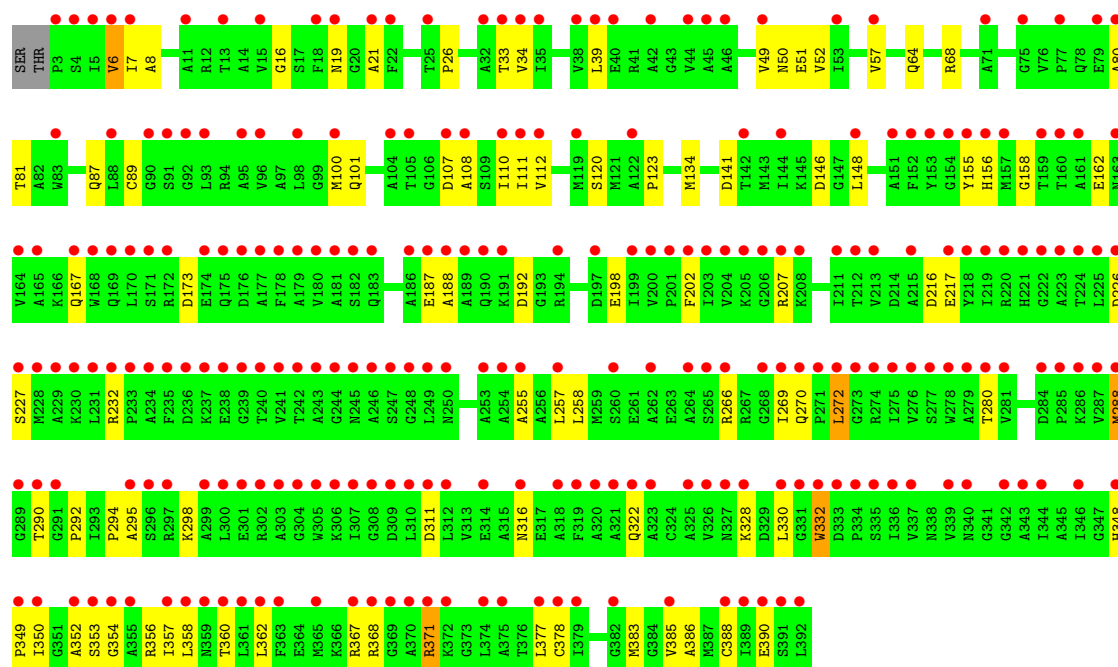
Chain C: 





- 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, α , β , γ	84.35Å 79.31Å 147.32Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	20.00 – 1.77 37.17 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-1.77) 80.8 (37.17-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.206 , 0.242 0.207 , 0.221	Depositor DCC
R_{free} test set	8648 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 187197 reflections	Xtriage
F_o, F_c correlation	0.91	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.

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 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	2827	0	2833	40	0
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

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 9.

All (207) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:387:MET:SD	4:A:9864:HOH:O	1.90	1.23
1:D:378:CYS:SG	4:D:499:HOH:O	2.02	1.17
4:C:491:HOH:O	1:D:383:MET:SD	2.07	1.12
1:D:388:CYS:SG	4:D:514:HOH:O	2.09	1.08
1:D:377:LEU:HD11	4:D:471:HOH:O	1.60	1.01
1:A:299:ALA:HB3	4:A:501:HOH:O	1.65	0.96
1:C:294:PRO:HG2	4:C:528:HOH:O	1.67	0.95
1:D:120:SER:HA	4:D:520:HOH:O	1.67	0.94
1:A:71:ALA:HA	4:A:494:HOH:O	1.72	0.88
1:C:72:MET:SD	4:C:534:HOH:O	2.34	0.86
1:C:87:GLN:NE2	4:C:485:HOH:O	2.10	0.84
1:D:51:GLU:C	4:D:484:HOH:O	2.16	0.84
4:C:433:HOH:O	1:D:64:GLN:HG3	1.78	0.83
1:A:200:VAL:HG12	4:A:475:HOH:O	1.79	0.80
1:D:80:ALA:HB3	4:D:476:HOH:O	1.80	0.80
1:A:11:ALA:HB1	4:A:475:HOH:O	1.81	0.80
1:D:108:ALA:HB3	4:D:426:HOH:O	1.84	0.78
1:C:277:SER:OG	1:C:303:ALA:HB2	1.84	0.78
1:B:197:ASP:OD1	4:B:422:HOH:O	2.02	0.78
1:A:225:LEU:HD12	4:A:9891:HOH:O	1.84	0.76
1:D:188:ALA:HA	4:D:523:HOH:O	1.86	0.76
1:A:29:GLU:HG2	4:A:517:HOH:O	1.83	0.76
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

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

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:8:ALA:HB1	1:D:269:ILE:HG21	1.93	0.50
1:D:51:GLU:HA	4:D:484:HOH:O	2.09	0.50
1:C:119:MET:HA	4:C:405:HOH:O	2.11	0.50
1:B:392:LEU:CG	4:B:9835:HOH:O	2.59	0.49
1:D:7:ILE:HD13	1:D:362:LEU:HD11	1.94	0.49
1:D:50:ASN:O	1:D:80:ALA:HB1	2.11	0.49
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.30	0.49
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.76	0.49
1:C:285:PRO:HD3	4:D:459:HOH:O	2.11	0.49
1:D:16:GLY:HA3	4:D:517:HOH:O	2.13	0.49
1:C:348:HIS:ND1	1:C:353:SER:OG	2.43	0.48
1:B:3:PRO:N	4:B:409:HOH:O	2.46	0.48
1:D:156:HIS:HD1	1:D:158:GLY:H	1.61	0.48
1:C:183:GLN:NE2	1:C:220:ARG:HG3	2.28	0.48
1:A:200:VAL:CG1	4:A:475:HOH:O	2.50	0.48
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.96	0.48
1:C:207:ARG:HH11	1:C:207:ARG:HG2	1.78	0.47
1:B:205:LYS:NZ	4:B:413:HOH:O	2.45	0.47
1:D:371:ARG:O	1:D:390:GLU:HG3	2.15	0.47
1:C:83:TRP:HZ2	4:C:450:HOH:O	1.97	0.47
1:D:111:ILE:CG2	1:D:112:VAL:N	2.79	0.46
1:C:275:ILE:HG13	4:C:496:HOH:O	2.15	0.46
1:A:276:VAL:CG2	1:A:388:CYS:HB2	2.45	0.46
1:C:312:LEU:HD23	1:C:361:LEU:HD12	1.96	0.46
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.51	0.46
1:B:191:LYS:HZ2	1:B:191:LYS:HB3	1.78	0.46
1:D:111:ILE:HG12	4:D:426:HOH:O	2.15	0.46
1:B:205:LYS:CE	4:B:413:HOH:O	2.64	0.46
1:D:356:ARG:NH2	1:D:357:ILE:HG22	2.30	0.46
1:B:76:VAL:HG13	1:B:77:PRO:HD2	1.97	0.46
1:A:339:VAL:CG2	4:A:9902:HOH:O	2.64	0.45
1:C:102:GLN:NE2	4:C:450:HOH:O	2.49	0.45
1:D:111:ILE:HD11	4:D:426:HOH:O	2.16	0.45
1:D:39:LEU:HD21	1:D:49:VAL:CG2	2.46	0.45
1:A:76:VAL:HG21	4:A:494:HOH:O	2.15	0.45
1:C:96:VAL:HG13	1:C:258:LEU:HD21	1.97	0.45
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.97	0.45
1:D:34:VAL:HG22	4:D:482:HOH:O	2.15	0.45
1:B:334:PRO:HA	4:B:513:HOH:O	2.17	0.45
1:A:191:LYS:CB	1:A:191:LYS:NZ	2.79	0.45
1:B:8:ALA:HB3	1:B:257:LEU:HD22	1.98	0.45
1:D:348:HIS:CD2	4:D:498:HOH:O	2.70	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:148:LEU:HB3	1:D:156:HIS:NE2	2.32	0.44
1:C:287:VAL:O	1:C:287:VAL:HG23	2.17	0.44
1:B:361:LEU:HD12	4:B:487:HOH:O	2.17	0.44
1:D:352:ALA:CB	4:D:496:HOH:O	2.59	0.44
1:C:269:ILE:HG22	1:C:270:GLN:N	2.33	0.44
1:A:348:HIS:CE1	1:A:353:SER:HG	2.31	0.44
1:B:298:LYS:HD3	1:B:298:LYS:C	2.38	0.44
1:A:248:GLY:HA2	4:A:471:HOH:O	2.17	0.44
1:A:276:VAL:HG23	1:A:388:CYS:HB2	1.99	0.44
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.37	0.44
1:C:66:PRO:HB3	4:C:483:HOH:O	2.18	0.44
1:C:269:ILE:HG22	1:C:270:GLN:H	1.83	0.44
1:D:112:VAL:HG12	4:D:452:HOH:O	2.17	0.43
1:D:292:PRO:HG3	1:D:377:LEU:C	2.38	0.43
1:D:52:VAL:HG23	4:D:484:HOH:O	2.19	0.43
1:B:269:ILE:O	1:B:271:PRO:HD3	2.19	0.42
1:C:66:PRO:CB	4:C:483:HOH:O	2.67	0.42
1:C:76:VAL:CG1	1:C:77:PRO:HD2	2.49	0.42
1:C:211:ILE:C	4:C:532:HOH:O	2.56	0.42
1:C:283:VAL:HG22	1:C:382:GLY:C	2.40	0.42
1:C:116:MET:HE3	4:C:483:HOH:O	2.18	0.42
1:D:100:MET:HE3	4:D:474:HOH:O	2.20	0.42
1:B:392:LEU:CB	4:B:9835:HOH:O	2.57	0.42
1:D:349:PRO:O	1:D:353:SER:N	2.53	0.42
1:A:228:MET:HE2	1:A:228:MET:HA	2.01	0.42
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.32	0.42
1:D:377:LEU:HB3	4:D:475:HOH:O	2.20	0.42
1:C:284:ASP:OD1	1:C:285:PRO:HD2	2.20	0.42
1:D:100:MET:C	1:D:100:MET:SD	2.98	0.42
1:A:330:LEU:HD12	1:A:332:TRP:CZ2	2.54	0.42
1:D:111:ILE:CG1	4:D:426:HOH:O	2.68	0.41
1:D:110:ILE:HG23	1:D:257:LEU:HD21	2.02	0.41
1:C:300:LEU:HB3	4:C:473:HOH:O	2.18	0.41
1:A:233:PRO:HB2	1:A:236:ASP:O	2.21	0.41
1:C:236:ASP:HB3	1:C:239:GLY:HA3	2.01	0.41
1:B:257:LEU:C	1:B:257:LEU:HD23	2.41	0.41
1:B:330:LEU:HD12	1:B:332:TRP:CZ2	2.56	0.41
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.54	0.41
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.86	0.41
1:B:144:ILE:HD13	1:B:148:LEU:HD12	2.02	0.41
1:C:387:MET:HA	4:C:446:HOH:O	2.20	0.41
1:A:225:LEU:HG	4:A:9891:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:191:LYS:NZ	4:C:478:HOH:O	2.54	0.41
1:C:103:ILE:HA	1:C:108:ALA:O	2.21	0.41
1:C:143:MET:HG3	4:C:405:HOH:O	2.21	0.41
1:D:367:ARG:HG2	4:D:424:HOH:O	2.21	0.41
1:A:200:VAL:HG23	3:A:5394:GOL:H2	2.02	0.41
1:C:356:ARG:NH2	4:C:489:HOH:O	2.54	0.41
1:C:280:THR:HG23	1:D:81:THR:HG21	2.03	0.41
1:C:263:GLU:HG3	1:C:267:ARG:HD2	2.03	0.40
1:C:187:GLU:HA	4:C:462:HOH:O	2.21	0.40
1:A:29:GLU:CG	4:A:517:HOH:O	2.56	0.40
1:C:7:ILE:HG23	1:C:256:ALA:HB1	2.02	0.40
1:C:86:ASN:C	1:C:86:ASN:OD1	2.60	0.40
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.70	0.40
1:D:198:GLU:OE1	1:D:360:THR:HA	2.22	0.40
1:D:295:ALA:O	1:D:386:ALA:HB3	2.21	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(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%)	38	18
1	D	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	50	30
All	All	1552/1568 (99%)	1488 (96%)	61 (4%)	3 (0%)	56	36

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%)	28	9
1	B	277/278 (100%)	264 (95%)	13 (5%)	36	15
1	C	277/278 (100%)	257 (93%)	20 (7%)	21	5
1	D	277/278 (100%)	260 (94%)	17 (6%)	26	8
All	All	1108/1112 (100%)	1042 (94%)	66 (6%)	27	9

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	D	332	TRP
1	D	358	LEU
1	D	368	ARG
1	D	371	ARG

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

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

5.3.3 RNA ⓘ

There are no RNA chains 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	A	89	1	10,10,11	6.63	3 (30%)	9,11,13	2.81	4 (44%)
1	CY4	B	89	1	10,10,11	6.86	4 (40%)	9,11,13	3.04	4 (44%)
1	CY4	C	89	1	5,5,11	7.53	2 (40%)	2,5,13	0.90	0
1	CY4	D	89	1	5,5,11	8.30	2 (40%)	2,5,13	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CY4	A	89	1	-	0/8/10/12	0/0/0/0
1	CY4	B	89	1	-	0/8/10/12	0/0/0/0
1	CY4	C	89	1	-	0/2/4/12	0/0/0/0
1	CY4	D	89	1	-	0/2/4/12	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	CY4	O-C	20.70	1.25	1.11
1	A	89	CY4	O-C	20.47	1.25	1.11
1	D	89	CY4	O-C	18.19	1.23	1.11
1	C	89	CY4	O-C	16.61	1.22	1.11
1	B	89	CY4	CB-SG	3.80	1.86	1.81
1	D	89	CY4	CA-C	3.62	1.55	1.48
1	B	89	CY4	CA-C	3.29	1.54	1.48
1	A	89	CY4	CA2-CA1	3.01	1.54	1.50
1	B	89	CY4	CA2-CA1	3.00	1.54	1.50
1	C	89	CY4	CA-C	2.78	1.53	1.48
1	A	89	CY4	CA-C	2.24	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	CY4	CB-SG-CA1	-6.72	96.31	100.95
1	B	89	CY4	CB-SG-CA1	-6.52	96.45	100.95
1	B	89	CY4	OA1-CA1-CA2	-4.17	120.30	123.95
1	B	89	CY4	OA1-CA1-SG	3.35	126.39	122.85
1	A	89	CY4	OA1-CA1-CA2	-3.19	121.15	123.95
1	B	89	CY4	CA-CB-SG	-2.39	108.08	112.94
1	A	89	CY4	CB-CA-N	-2.22	106.50	110.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	CY4	CA-CB-SG	-2.16	108.55	112.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GOL	A	5394	-	5,5,5	1.04	1 (20%)	5,5,5	0.65	0
2	SO4	A	9720	-	4,4,4	0.46	0	6,6,6	0.31	0
2	SO4	A	9722	-	4,4,4	0.20	0	6,6,6	0.16	0
3	GOL	B	6394	-	5,5,5	0.92	1 (20%)	5,5,5	0.68	0
2	SO4	B	9719	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	B	9721	-	4,4,4	0.50	0	6,6,6	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	5394	-	-	0/4/4/4	0/0/0/0
2	SO4	A	9720	-	-	0/0/0/0	0/0/0/0
2	SO4	A	9722	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	6394	-	-	0/4/4/4	0/0/0/0
2	SO4	B	9719	-	-	0/0/0/0	0/0/0/0
2	SO4	B	9721	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5394	GOL	O2-C2	-2.16	1.36	1.43
3	B	6394	GOL	O2-C2	-2.03	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	390/392 (99%)	0.38	7 (1%) 65 65	5, 11, 28, 54	0
1	B	390/392 (99%)	0.38	8 (2%) 60 59	6, 11, 28, 55	0
1	C	390/392 (99%)	2.83	226 (57%) 0 0	2, 11, 28, 42	0
1	D	390/392 (99%)	3.50	246 (63%) 0 0	2, 13, 29, 45	0
All	All	1560/1568 (99%)	1.77	487 (31%) 1 1	2, 11, 29, 55	0

All (487) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	17.2
1	D	219	ILE	14.8
1	D	229	ALA	14.5
1	D	179	ALA	14.4
1	D	244	GLY	14.1
1	D	188	ALA	13.3
1	D	170	LEU	12.7
1	C	105	THR	11.8
1	C	234	ALA	11.7
1	D	227	SER	10.0
1	D	228	MET	9.6
1	C	239	GLY	9.6
1	A	132	VAL	9.5
1	D	108	ALA	9.5
1	C	225	LEU	9.5
1	D	310	LEU	9.5
1	C	370	ALA	9.2
1	C	49	VAL	9.2
1	D	233	PRO	9.1
1	D	361	LEU	9.1
1	C	342	GLY	9.1

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Mol	Chain	Res	Type	RSRZ
1	C	80	ALA	9.0
1	D	160	THR	9.0
1	D	235	PHE	9.0
1	D	164	VAL	8.9
1	D	224	THR	8.8
1	D	239	GLY	8.8
1	D	159	THR	8.7
1	C	161	ALA	8.6
1	D	265	SER	8.6
1	D	243	ALA	8.6
1	D	181	ALA	8.4
1	C	224	THR	8.4
1	D	240	THR	8.3
1	D	223	ALA	8.2
1	B	207	ARG	8.1
1	D	171	SER	8.0
1	D	247[A]	SER	8.0
1	D	392	LEU	8.0
1	C	229	ALA	7.9
1	D	161	ALA	7.9
1	D	238	GLU	7.9
1	D	186	ALA	7.9
1	C	300	LEU	7.9
1	D	295	ALA	7.8
1	C	276	VAL	7.8
1	D	168	TRP	7.7
1	D	234	ALA	7.6
1	D	285	PRO	7.6
1	D	246	ALA	7.5
1	C	336	ILE	7.4
1	D	330	LEU	7.3
1	C	235	PHE	7.3
1	C	240	THR	7.2
1	D	215	ALA	7.2
1	D	323	ALA	7.2
1	D	319	PHE	7.2
1	D	335	SER	7.2
1	D	299	ALA	7.2
1	C	67	ALA	7.1
1	D	374	LEU	7.0
1	D	178	PHE	7.0
1	D	153	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	283	VAL	7.0
1	D	332	TRP	6.9
1	C	247[A]	SER	6.9
1	D	279	ALA	6.9
1	C	177	ALA	6.9
1	C	371	ARG	6.8
1	B	208	LYS	6.8
1	C	242	THR	6.8
1	C	34	VAL	6.8
1	D	290	THR	6.7
1	D	34	VAL	6.7
1	D	343	ALA	6.7
1	C	293	ILE	6.7
1	C	238	GLU	6.7
1	D	272	LEU	6.7
1	D	339	VAL	6.6
1	C	268	GLY	6.6
1	D	300	LEU	6.6
1	D	350	ILE	6.6
1	C	226	ASP	6.5
1	C	96	VAL	6.5
1	C	279	ALA	6.5
1	C	106	GLY	6.5
1	C	331	GLY	6.5
1	C	270	GLN	6.4
1	D	312	LEU	6.4
1	D	326	VAL	6.3
1	D	336	ILE	6.3
1	C	246	ALA	6.3
1	C	232	ARG	6.3
1	C	208	LYS	6.2
1	D	245	ASN	6.2
1	C	266	ARG	6.2
1	C	113	ALA	6.2
1	C	221	HIS	6.1
1	D	305	TRP	6.1
1	C	392	LEU	6.1
1	C	313	VAL	5.9
1	C	366	LYS	5.9
1	D	391	SER	5.9
1	D	157	MET	5.9
1	D	377	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	6	VAL	5.9
1	D	304	GLY	5.8
1	D	275	ILE	5.8
1	C	75	GLY	5.8
1	D	357	ILE	5.8
1	C	269	ILE	5.7
1	D	363	PHE	5.7
1	C	103	ILE	5.7
1	C	335	SER	5.7
1	D	291	GLY	5.7
1	D	163	ASN	5.7
1	D	218	TYR	5.6
1	D	232	ARG	5.6
1	D	222	GLY	5.6
1	D	327	ASN	5.6
1	D	270	GLN	5.6
1	D	230	LYS	5.5
1	D	340	ASN	5.5
1	D	253	ALA	5.5
1	D	325	ALA	5.5
1	D	365	MET	5.5
1	A	207	ARG	5.4
1	D	241	VAL	5.4
1	D	207	ARG	5.4
1	D	382	GLY	5.4
1	C	243	ALA	5.4
1	D	262	ALA	5.4
1	C	231	LEU	5.4
1	D	269	ILE	5.3
1	D	271	PRO	5.3
1	D	226	ASP	5.3
1	D	331	GLY	5.3
1	D	370	ALA	5.3
1	D	155	TYR	5.3
1	C	301	GLU	5.2
1	D	107	ASP	5.2
1	D	276	VAL	5.2
1	C	244	GLY	5.2
1	D	257	LEU	5.2
1	C	389	ILE	5.2
1	D	359	ASN	5.2
1	C	206	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	307	ILE	5.1
1	C	207	ARG	5.1
1	C	40	GLU	5.1
1	C	203	ILE	5.1
1	C	264	ALA	5.1
1	C	104	ALA	5.0
1	C	376	THR	5.0
1	D	280	THR	5.0
1	D	4	SER	4.9
1	C	319	PHE	4.9
1	D	320	ALA	4.9
1	D	225	LEU	4.9
1	D	221	HIS	4.9
1	C	180	VAL	4.9
1	C	228	MET	4.9
1	D	369	GLY	4.9
1	D	104	ALA	4.9
1	D	15	VAL	4.8
1	D	208	LYS	4.8
1	D	172	ARG	4.8
1	C	378	CYS	4.7
1	D	368	ARG	4.7
1	B	132	VAL	4.7
1	C	290	THR	4.7
1	C	57	VAL	4.7
1	C	204	VAL	4.7
1	D	318	ALA	4.7
1	C	305	TRP	4.6
1	C	93	LEU	4.6
1	D	358	LEU	4.6
1	D	169	GLN	4.6
1	D	165	ALA	4.6
1	C	108	ALA	4.6
1	D	342	GLY	4.6
1	D	311	ASP	4.6
1	D	151	ALA	4.6
1	D	152	PHE	4.6
1	D	281	VAL	4.5
1	D	346	ILE	4.5
1	C	152	PHE	4.5
1	C	222	GLY	4.5
1	C	4	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	296	SER	4.5
1	C	71	ALA	4.5
1	C	227	SER	4.5
1	C	38	VAL	4.4
1	D	49	VAL	4.4
1	D	180	VAL	4.4
1	C	388	CYS	4.4
1	C	265	SER	4.4
1	C	27	ALA	4.4
1	C	110	ILE	4.4
1	C	215	ALA	4.4
1	C	315	ALA	4.4
1	D	197	ASP	4.4
1	D	35	ILE	4.3
1	D	371	ARG	4.3
1	C	272	LEU	4.3
1	C	277	SER	4.3
1	D	190	GLN	4.3
1	C	14	ALA	4.3
1	D	287	VAL	4.2
1	D	236	ASP	4.2
1	A	208	LYS	4.2
1	D	44	VAL	4.2
1	D	40	GLU	4.2
1	C	211	ILE	4.2
1	C	170	LEU	4.2
1	D	288	MET	4.2
1	D	266	ARG	4.2
1	C	262	ALA	4.1
1	A	206	GLY	4.1
1	C	363	PHE	4.1
1	C	79	GLU	4.1
1	C	303	ALA	4.1
1	C	275	ILE	4.1
1	D	385	VAL	4.1
1	D	309	ASP	4.1
1	C	169	GLN	4.1
1	C	299	ALA	4.1
1	D	220	ARG	4.1
1	C	358	LEU	4.0
1	C	374	LEU	4.0
1	C	176	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	237	LYS	4.0
1	C	175	GLN	4.0
1	D	352	ALA	4.0
1	C	391	SER	4.0
1	C	382	GLY	4.0
1	C	325	ALA	4.0
1	C	310	LEU	4.0
1	D	379	ILE	4.0
1	D	289	GLY	4.0
1	D	7	ILE	4.0
1	D	22	PHE	3.9
1	C	21	ALA	3.9
1	C	179	ALA	3.9
1	C	23	ALA	3.9
1	D	201	PRO	3.9
1	C	76	VAL	3.9
1	D	175	GLN	3.9
1	D	92	GLY	3.9
1	D	308	GLY	3.9
1	C	332	TRP	3.8
1	C	218	TYR	3.8
1	D	264	ALA	3.8
1	D	297	ARG	3.8
1	C	188	ALA	3.8
1	D	213	VAL	3.8
1	D	268	GLY	3.8
1	D	75	GLY	3.7
1	D	378	CYS	3.7
1	C	280	THR	3.7
1	C	131	GLY	3.7
1	D	112	VAL	3.7
1	C	155	TYR	3.7
1	D	322	GLN	3.7
1	C	213	VAL	3.6
1	C	287	VAL	3.6
1	C	168	TRP	3.6
1	D	25	THR	3.6
1	C	88	LEU	3.6
1	D	307	ILE	3.6
1	C	320	ALA	3.6
1	C	114	GLY	3.6
1	D	242	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	309	ASP	3.6
1	D	83	TRP	3.6
1	C	167	GLN	3.6
1	B	206	GLY	3.6
1	C	236	ASP	3.6
1	D	13	THR	3.6
1	D	277	SER	3.6
1	D	372	LYS	3.6
1	C	7	ILE	3.5
1	C	10	ALA	3.5
1	C	70	ALA	3.5
1	C	258	LEU	3.5
1	D	284	ASP	3.5
1	C	115	GLY	3.5
1	D	167	GLN	3.4
1	D	177	ALA	3.4
1	D	353	SER	3.4
1	B	237	LYS	3.4
1	C	278	TRP	3.4
1	D	200	VAL	3.4
1	C	362	LEU	3.4
1	C	367	ARG	3.4
1	C	83	TRP	3.4
1	C	195	PHE	3.4
1	C	178	PHE	3.3
1	C	233	PRO	3.3
1	D	156	HIS	3.3
1	D	174	GLU	3.3
1	D	98	LEU	3.3
1	D	42	ALA	3.3
1	D	303	ALA	3.3
1	C	308	GLY	3.3
1	C	249	LEU	3.3
1	D	362	LEU	3.3
1	C	312	LEU	3.3
1	C	191	LYS	3.2
1	C	74	ALA	3.2
1	C	181	ALA	3.2
1	D	255	ALA	3.2
1	C	334	PRO	3.2
1	C	281	VAL	3.2
1	C	348	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	345	ALA	3.2
1	C	192	ASP	3.2
1	D	375	ALA	3.2
1	D	306	LYS	3.2
1	C	219	ILE	3.2
1	D	206	GLY	3.2
1	D	90	GLY	3.1
1	C	186	ALA	3.1
1	C	109	SER	3.1
1	D	211	ILE	3.1
1	C	153	TYR	3.1
1	D	45	ALA	3.1
1	D	248	GLY	3.1
1	D	321	ALA	3.1
1	D	202	PHE	3.0
1	D	278	TRP	3.0
1	D	194	ARG	3.0
1	C	386	ALA	3.0
1	C	220	ARG	3.0
1	C	223	ALA	3.0
1	D	21	ALA	3.0
1	C	133	LYS	3.0
1	D	199	ILE	3.0
1	C	274	ARG	3.0
1	D	333	ASP	3.0
1	C	156	HIS	3.0
1	D	367	ARG	3.0
1	D	111	ILE	3.0
1	D	91	SER	2.9
1	D	176	ASP	2.9
1	C	237	LYS	2.9
1	D	93	LEU	2.9
1	C	324	CYS	2.9
1	C	321	ALA	2.9
1	D	301	GLU	2.9
1	D	71	ALA	2.9
1	C	171	SER	2.9
1	D	360	THR	2.8
1	C	252	GLY	2.8
1	C	271	PRO	2.8
1	D	57	VAL	2.8
1	D	96	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	323	ALA	2.8
1	C	209	GLY	2.8
1	D	3	PRO	2.8
1	D	88	LEU	2.8
1	D	119	MET	2.8
1	C	384	GLY	2.8
1	D	189	ALA	2.8
1	D	316	ASN	2.8
1	D	182	SER	2.8
1	B	134	MET	2.8
1	C	256	ALA	2.7
1	B	392	LEU	2.7
1	D	204	VAL	2.7
1	C	259	MET	2.7
1	C	311	ASP	2.7
1	D	77	PRO	2.7
1	C	84	GLY	2.7
1	D	5	ILE	2.7
1	D	337	VAL	2.7
1	C	368	ARG	2.7
1	C	42	ALA	2.7
1	D	274	ARG	2.7
1	D	38	VAL	2.7
1	D	144	ILE	2.7
1	D	260	SER	2.7
1	C	329	ASP	2.6
1	C	6	VAL	2.6
1	C	304	GLY	2.6
1	D	203	ILE	2.6
1	D	389	ILE	2.6
1	D	11	ALA	2.6
1	D	250	ASN	2.6
1	D	212	THR	2.6
1	C	166	LYS	2.6
1	C	48	GLU	2.6
1	C	352	ALA	2.6
1	D	18	PHE	2.6
1	C	254	ALA	2.6
1	D	80	ALA	2.6
1	C	158	GLY	2.5
1	C	174	GLU	2.5
1	C	184	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	297	ARG	2.5
1	C	360	THR	2.5
1	C	286	LYS	2.5
1	D	328	LYS	2.5
1	D	32	ALA	2.5
1	C	318	ALA	2.5
1	D	122	ALA	2.5
1	C	58	LEU	2.5
1	C	377	LEU	2.5
1	D	148	LEU	2.5
1	D	191	LYS	2.5
1	C	302	ARG	2.5
1	D	46	ALA	2.4
1	D	334	PRO	2.4
1	D	110	ILE	2.4
1	C	130	GLY	2.4
1	C	364	GLU	2.4
1	D	217	GLU	2.4
1	D	390	GLU	2.4
1	D	286	LYS	2.4
1	C	18	PHE	2.4
1	C	241	VAL	2.4
1	C	361	LEU	2.4
1	C	140	ILE	2.4
1	D	53	ILE	2.4
1	D	302	ARG	2.4
1	C	157	MET	2.4
1	D	388	CYS	2.4
1	D	254	ALA	2.3
1	D	348	HIS	2.3
1	D	142	THR	2.3
1	C	375	ALA	2.3
1	C	196	LYS	2.3
1	C	289	GLY	2.3
1	D	154	GLY	2.3
1	D	205	LYS	2.3
1	D	100	MET	2.3
1	C	212	THR	2.3
1	A	232	ARG	2.3
1	D	344	ILE	2.3
1	C	339	VAL	2.3
1	D	39	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	248	GLY	2.3
1	C	354	GLY	2.3
1	D	354	GLY	2.3
1	C	387	MET	2.3
1	C	294	PRO	2.3
1	B	131	GLY	2.3
1	D	19	ASN	2.2
1	D	95	ALA	2.2
1	C	292	PRO	2.2
1	A	237	LYS	2.2
1	D	273	GLY	2.2
1	D	314	GLU	2.2
1	A	392	LEU	2.2
1	C	98	LEU	2.2
1	C	260	SER	2.2
1	C	344	ILE	2.2
1	D	79	GLU	2.2
1	D	355	ALA	2.2
1	C	112	VAL	2.2
1	C	357	ILE	2.2
1	C	328	LYS	2.2
1	D	187	GLU	2.1
1	C	144	ILE	2.1
1	C	182	SER	2.1
1	C	353	SER	2.1
1	D	183	GLN	2.1
1	D	296	SER	2.1
1	C	15	VAL	2.1
1	C	159	THR	2.1
1	C	53	ILE	2.1
1	C	298	LYS	2.1
1	C	25	THR	2.1
1	C	66	PRO	2.1
1	D	33	THR	2.1
1	C	337	VAL	2.1
1	C	50	ASN	2.0
1	C	60	ALA	2.0
1	C	165	ALA	2.0
1	C	111	ILE	2.0
1	C	245	ASN	2.0
1	D	105	THR	2.0
1	C	119	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	330	LEU	2.0
1	C	189	ALA	2.0
1	D	349	PRO	2.0
1	D	249	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CY4	A	89	11/12	0.13	1.46	9,12,30,31	0
1	CY4	B	89	11/12	0.12	1.14	8,10,26,28	0
1	CY4	D	89	6/12	0.14	-1.85	2,4,4,6	0
1	CY4	C	89	6/12	0.11	-2.55	8,10,11,15	0

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	9722	5/5	0.22	2.60	74,74,75,75	0
3	GOL	B	6394	6/6	0.15	1.70	18,26,30,38	0
2	SO4	A	9720	5/5	0.12	1.11	45,50,50,51	0
2	SO4	B	9719	5/5	0.19	0.94	76,77,78,78	0
3	GOL	A	5394	6/6	0.12	0.34	20,31,33,33	0
2	SO4	B	9721	5/5	0.12	-0.93	47,48,50,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.