



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:49 PM GMT

PDB ID : 1M4S
Title : Biosynthetic thiolase, Cys89 acetylated, unliganded form
Authors : Kursula, P.; Ojala, J.; Lambeir, A.-M.; Wierenga, R.K.
Deposited on : 2002-07-03
Resolution : 1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

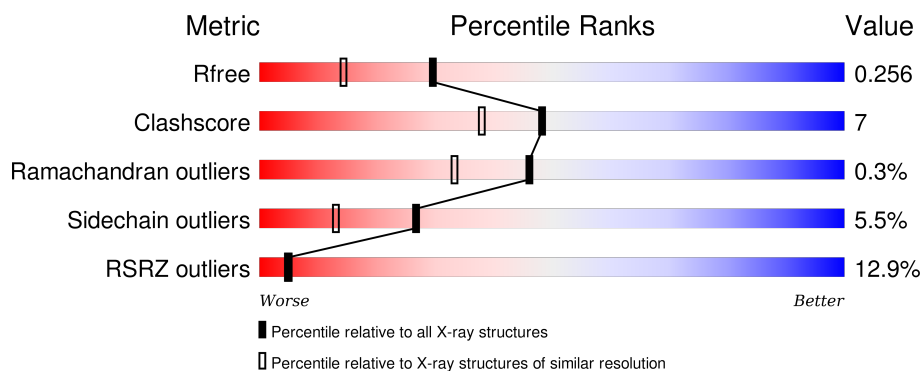
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	B	392	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	C	392	<div> <div>16%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	D	392	<div> <div>32%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SCY	A	89[A]	-	-	X	-
1	SCY	B	89[A]	-	-	X	-
3	GOL	A	5393	-	-	-	X
3	GOL	A	5394	-	-	-	X
3	GOL	B	6393	-	-	-	X
3	GOL	B	6394	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12506 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	392	Total	C	N	O	S	0	3	0
			2842	1763	512	545	22			
1	B	392	Total	C	N	O	S	0	3	0
			2842	1763	512	545	22			
1	C	392	Total	C	N	O	S	0	3	0
			2842	1763	512	545	22			
1	D	392	Total	C	N	O	S	0	3	0
			2842	1763	512	545	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	10	ALA	-	INSERTION	UNP P07097
D	89	SCY	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	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

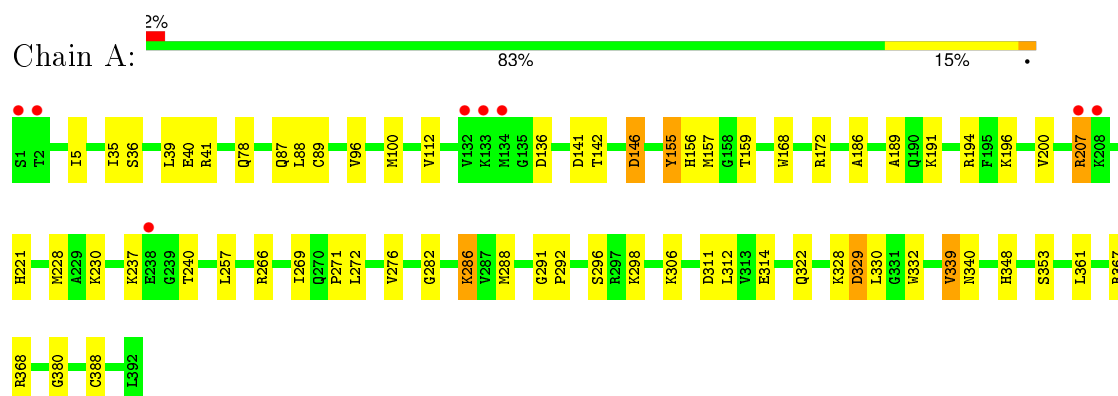
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	420	Total	O	0	0
			420	420		
4	B	427	Total	O	0	0
			427	427		
4	C	116	Total	O	0	0
			116	116		
4	D	131	Total	O	0	0
			131	131		

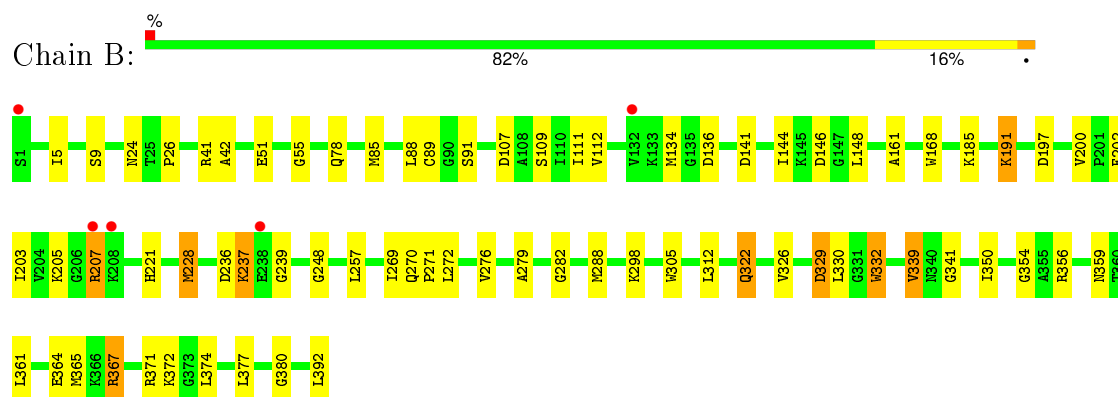
3 Residue-property plots [i](#)

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.

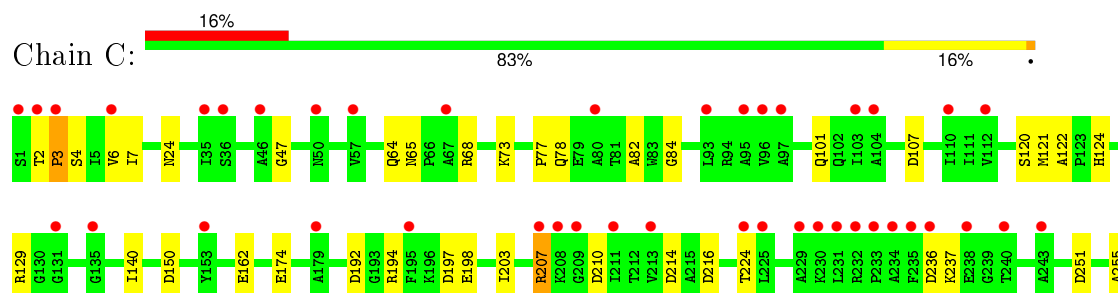
• Molecule 1: Acetyl-CoA acetyltransferase

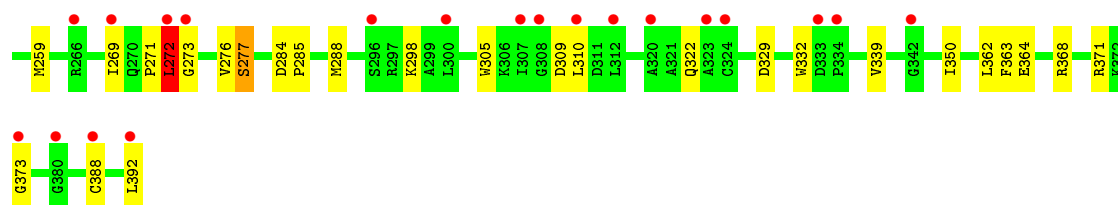


• Molecule 1: Acetyl-CoA acetyltransferase

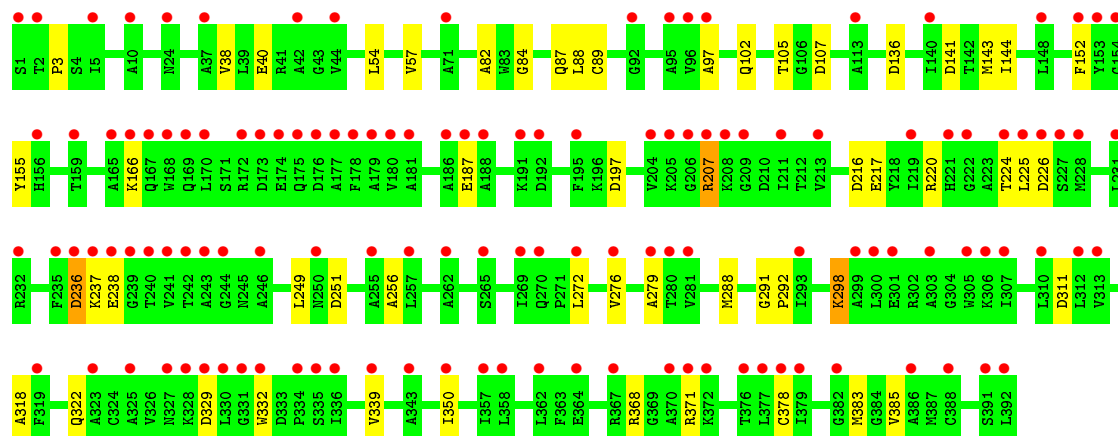
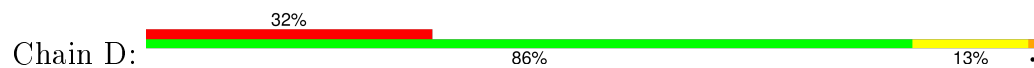


• Molecule 1: Acetyl-CoA acetyltransferase





• Molecule 1: Acetyl-CoA acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.40 Å 79.28 Å 148.48 Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	20.00 – 1.87 37.23 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-1.87) 87.8 (37.23-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 1.87 Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.206 , 0.247 0.218 , 0.256	Depositor DCC
R_{free} test set	7187 reflections (4.76%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.0	EDS
Estimated twinning fraction	0.158 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 158412 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12506	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SCY, 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	0.91	1/2880 (0.0%)	1.00	11/3888 (0.3%)
1	B	0.92	0/2880	0.95	11/3888 (0.3%)
1	C	0.65	6/2880 (0.2%)	0.77	9/3888 (0.2%)
1	D	0.41	0/2880	0.73	9/3888 (0.2%)
All	All	0.75	7/11520 (0.1%)	0.87	40/15552 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	277	SER	CB-OG	11.94	1.57	1.42
1	C	373	GLY	C-O	8.56	1.37	1.23
1	C	273	GLY	C-O	6.12	1.33	1.23
1	C	310	LEU	C-O	5.94	1.34	1.23
1	C	310	LEU	C-N	5.23	1.46	1.34
1	A	96	VAL	CB-CG2	5.08	1.63	1.52
1	C	272	LEU	C-O	5.07	1.32	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	A	141	ASP	CB-CG-OD2	8.85	126.26	118.30
1	A	266	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	A	367	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	266	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	367	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	D	136	ASP	CB-CG-OD2	6.31	123.97	118.30
1	B	41	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	146	ASP	CB-CG-OD2	6.18	123.86	118.30
1	D	251	ASP	CB-CG-OD2	6.12	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	141	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	107	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	107	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	146	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	210	ASP	CB-CG-OD2	5.93	123.63	118.30
1	B	41	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	329	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	197	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	136	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	311	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	329	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	339	VAL	CG1-CB-CG2	5.61	119.87	110.90
1	D	141	ASP	CB-CG-OD2	5.59	123.34	118.30
1	C	309	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	311	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	41	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	C	150	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	236	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	107	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	136	ASP	CB-CG-OD2	5.28	123.06	118.30
1	D	216	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	329	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	197	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	339	VAL	N-CA-CB	-5.22	100.02	111.50
1	B	85	MET	CA-CB-CG	5.17	122.10	113.30
1	C	192	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	329	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	214	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	216	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2842	0	2849	50	0
1	B	2842	0	2849	58	0
1	C	2842	0	2849	29	0
1	D	2842	0	2849	30	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	12	0	16	4	0
3	B	12	0	16	4	0
4	A	420	0	0	29	1
4	B	427	0	0	31	0
4	C	116	0	0	6	0
4	D	131	0	0	18	0
All	All	12506	0	11428	167	1

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 7.

All (167) 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:B:89[A]:SCY:HE1	1:B:380:GLY:H	1.02	1.11
1:A:100:MET:HG3	4:A:468:HOH:O	1.50	1.08
1:A:314:GLU:HB2	4:A:504:HOH:O	1.57	1.03
1:A:296:SER:HB2	4:A:528:HOH:O	1.60	1.01
1:B:257:LEU:HA	4:B:530:HOH:O	1.63	0.97
1:B:89[A]:SCY:HE1	1:B:380:GLY:N	1.78	0.96
1:A:276:VAL:HB	4:A:534:HOH:O	1.68	0.93
1:B:359:ASN:HB2	4:B:481:HOH:O	1.73	0.88
1:B:312:LEU:HB3	4:B:501:HOH:O	1.73	0.88
1:A:89[A]:SCY:HE1	1:A:380:GLY:H	1.42	0.83
1:B:89[A]:SCY:CE	1:B:380:GLY:H	1.88	0.82
1:B:112:VAL:HG22	4:B:530:HOH:O	1.80	0.81
1:D:144:ILE:HG12	4:D:484:HOH:O	1.81	0.81
1:C:276:VAL:HG22	1:C:388:CYS:O	1.83	0.79
3:B:6394:GOL:O3	4:B:9911:HOH:O	1.98	0.77
1:A:189:ALA:HB1	4:A:531:HOH:O	1.84	0.77
1:D:87:GLN:HB3	4:D:523:HOH:O	1.86	0.76
1:B:237:LYS:NZ	4:B:9964:HOH:O	2.20	0.74
1:B:191:LYS:HB3	1:B:191:LYS:NZ	2.02	0.73
1:B:356:ARG:HA	4:B:481:HOH:O	1.89	0.73
1:A:100:MET:CE	4:A:468:HOH:O	2.36	0.72
1:D:385:VAL:HG22	4:D:478:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89[A]:SCY:SG	1:A:348:HIS:NE2	2.64	0.71
1:B:228:MET:HE3	4:B:524:HOH:O	1.90	0.70
1:C:255:ALA:HB3	4:C:457:HOH:O	1.91	0.70
3:B:6393:GOL:H12	4:B:468:HOH:O	1.92	0.69
1:B:185:LYS:HE3	4:B:525:HOH:O	1.90	0.68
1:B:89[A]:SCY:HE2	1:B:89[A]:SCY:H	1.58	0.68
1:B:202:PHE:CD1	4:B:517:HOH:O	2.46	0.68
1:A:35:ILE:HG23	4:A:495:HOH:O	1.93	0.68
1:B:322:GLN:HB3	4:B:476:HOH:O	1.93	0.68
1:A:100:MET:SD	4:A:468:HOH:O	2.51	0.68
1:B:341:GLY:HA2	4:B:525:HOH:O	1.92	0.68
1:B:361:LEU:HD11	4:B:501:HOH:O	1.93	0.67
1:A:87:GLN:C	4:A:464:HOH:O	2.33	0.66
1:D:38:VAL:HG21	4:D:518:HOH:O	1.95	0.66
1:B:203:ILE:HG23	4:B:502:HOH:O	1.96	0.65
1:A:89[A]:SCY:H	1:A:89[A]:SCY:HE2	1.62	0.64
1:B:257:LEU:CA	4:B:530:HOH:O	2.34	0.62
1:A:339:VAL:HG11	1:A:368:ARG:NH2	2.16	0.60
3:A:5393:GOL:H2	4:A:498:HOH:O	2.02	0.60
1:A:89[A]:SCY:CE	1:A:380:GLY:H	2.14	0.60
1:B:202:PHE:CE1	4:B:517:HOH:O	2.54	0.60
1:A:39:LEU:HG	4:A:495:HOH:O	2.03	0.59
1:C:277:SER:OG	1:C:388:CYS:HB2	2.02	0.59
1:C:120:SER:OG	1:C:251:ASP:OD2	2.13	0.59
1:D:256:ALA:C	4:D:518:HOH:O	2.41	0.58
1:B:191:LYS:HB3	1:B:191:LYS:HZ1	1.67	0.58
1:B:89[A]:SCY:HE1	1:B:380:GLY:CA	2.34	0.57
1:C:68:ARG:HG3	1:D:152:PHE:HZ	1.69	0.57
1:B:269:ILE:O	1:B:271:PRO:HD3	2.05	0.57
1:D:143:MET:HB3	4:D:484:HOH:O	2.04	0.56
1:D:225:LEU:N	4:D:423:HOH:O	2.37	0.56
1:B:88:LEU:HB3	1:B:89[A]:SCY:HE2	1.88	0.55
1:C:101:GLN:OE1	1:D:102:GLN:NE2	2.37	0.55
1:D:97:ALA:HA	4:D:497:HOH:O	2.06	0.55
1:A:112:VAL:HG21	4:A:495:HOH:O	2.06	0.54
1:A:286:LYS:HD3	4:A:9759:HOH:O	2.08	0.54
1:B:374:LEU:C	1:B:374:LEU:HD23	2.28	0.54
1:A:88:LEU:HD22	4:A:456:HOH:O	2.08	0.54
1:C:162:GLU:HG3	1:C:236:ASP:HB2	1.90	0.54
1:D:217:GLU:HA	4:D:433:HOH:O	2.06	0.54
1:C:122:ALA:HA	4:C:473:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ALA:HB1	4:B:537:HOH:O	2.08	0.53
1:B:112:VAL:HA	4:B:530:HOH:O	2.08	0.53
1:D:144:ILE:N	4:D:484:HOH:O	2.41	0.53
1:B:203:ILE:HD12	4:B:502:HOH:O	2.09	0.53
1:B:161:ALA:HA	4:B:476:HOH:O	2.08	0.53
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.90	0.53
1:A:88:LEU:HD13	4:A:456:HOH:O	2.08	0.52
1:A:361:LEU:HD22	4:A:504:HOH:O	2.09	0.52
1:B:197:ASP:OD1	4:B:531:HOH:O	2.19	0.52
1:C:6:VAL:HG22	1:C:259:MET:O	2.10	0.52
1:D:166:LYS:HB3	4:D:500:HOH:O	2.09	0.52
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.45	0.51
1:B:270:GLN:NE2	1:B:392:LEU:OXT	2.43	0.51
1:A:269:ILE:O	1:A:271:PRO:HD3	2.10	0.50
1:A:36:SER:O	1:A:40:GLU:HG3	2.11	0.50
1:D:143:MET:HE2	4:D:484:HOH:O	2.11	0.50
1:D:40:GLU:HB3	4:D:459:HOH:O	2.12	0.49
1:D:291:GLY:N	1:D:292:PRO:CD	2.75	0.49
1:A:207:ARG:H	1:A:207:ARG:HD3	1.77	0.49
1:B:392:LEU:HD21	4:B:445:HOH:O	2.13	0.48
1:A:5:ILE:N	1:A:5:ILE:HD12	2.28	0.48
1:D:224:THR:C	4:D:423:HOH:O	2.51	0.48
3:A:5393:GOL:H32	4:A:524:HOH:O	2.12	0.48
1:A:194:ARG:HB2	4:A:531:HOH:O	2.14	0.47
1:C:82:ALA:HB2	4:C:469:HOH:O	2.14	0.47
1:D:339:VAL:HG11	1:D:368:ARG:NH2	2.30	0.47
1:C:272:LEU:O	1:C:362:LEU:HD22	2.14	0.47
1:B:26:PRO:HD3	4:B:444:HOH:O	2.14	0.47
1:D:238:GLU:C	4:D:520:HOH:O	2.53	0.47
1:A:40:GLU:HG3	4:A:9946:HOH:O	2.15	0.47
1:C:207:ARG:H	1:C:207:ARG:HD3	1.79	0.47
1:A:257:LEU:HD23	1:A:257:LEU:C	2.35	0.46
1:B:365:MET:CG	4:B:501:HOH:O	2.63	0.46
1:B:9:SER:HB3	1:B:42:ALA:HB2	1.97	0.46
1:D:383:MET:N	4:D:507:HOH:O	2.47	0.46
1:A:89[A]:SCY:HE1	1:A:380:GLY:N	2.21	0.46
1:B:200:VAL:HG23	3:B:6394:GOL:H2	1.98	0.46
1:A:282:GLY:HA3	1:B:78:GLN:O	2.15	0.46
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.45	0.46
1:A:172:ARG:HB2	1:A:240:THR:HG22	1.97	0.46
1:C:194:ARG:O	4:C:494:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLU:OE1	1:B:367:ARG:HD2	2.15	0.46
1:B:322:GLN:O	1:B:326:VAL:HG23	2.16	0.46
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.50	0.46
1:C:339:VAL:HG11	1:C:368:ARG:NH2	2.31	0.46
1:C:24:ASN:HA	1:C:121:MET:SD	2.56	0.46
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.98	0.45
1:C:284:ASP:OD1	1:C:285:PRO:HD2	2.17	0.45
1:C:269:ILE:O	1:C:271:PRO:HD3	2.15	0.45
1:B:248:GLY:O	3:B:6393:GOL:O1	2.34	0.45
1:C:198:GLU:HB3	1:C:363:PHE:CD2	2.51	0.45
1:B:205:LYS:HD2	4:B:456:HOH:O	2.17	0.45
1:D:318:ALA:HB1	4:D:461:HOH:O	2.17	0.45
1:A:330:LEU:HD21	4:A:528:HOH:O	2.17	0.45
1:B:88:LEU:HD12	1:B:380:GLY:O	2.17	0.44
1:A:286:LYS:CE	4:A:9759:HOH:O	2.64	0.44
1:A:200:VAL:HG23	3:A:5394:GOL:H2	1.98	0.44
1:A:286:LYS:CD	4:A:9759:HOH:O	2.65	0.44
1:B:305:TRP:CE2	1:B:372:LYS:HD3	2.53	0.44
1:A:157:MET:HB2	4:A:498:HOH:O	2.18	0.44
1:C:2:THR:HA	1:C:3:PRO:HD2	1.87	0.44
1:B:51:GLU:HB3	1:B:111:ILE:CD1	2.48	0.44
1:C:174:GLU:HG3	4:C:488:HOH:O	2.17	0.44
1:B:257:LEU:HD23	1:B:257:LEU:C	2.38	0.43
1:A:312:LEU:HD23	1:A:361:LEU:HD12	2.01	0.43
1:A:156:HIS:CE1	4:A:498:HOH:O	2.71	0.43
1:C:124:HIS:HA	1:C:140:ILE:O	2.18	0.43
1:B:24:ASN:C	4:B:444:HOH:O	2.56	0.43
1:C:84:GLY:HA3	4:C:403:HOH:O	2.18	0.43
1:A:291:GLY:N	1:A:292:PRO:CD	2.81	0.43
1:C:276:VAL:HG22	1:C:388:CYS:C	2.38	0.43
1:B:207:ARG:HD3	1:B:207:ARG:N	2.33	0.43
1:B:185:LYS:CE	4:B:525:HOH:O	2.58	0.43
1:A:306:LYS:NZ	4:A:523:HOH:O	2.51	0.42
1:A:78:GLN:O	1:B:282:GLY:HA3	2.19	0.42
1:D:82:ALA:HB2	4:D:394:HOH:O	2.18	0.42
1:A:196:LYS:NZ	4:A:9896:HOH:O	2.53	0.42
1:B:354:GLY:HA2	1:B:377:LEU:HD11	2.02	0.42
1:A:35:ILE:CG2	4:A:495:HOH:O	2.62	0.42
1:B:236:ASP:O	1:B:239:GLY:N	2.50	0.42
1:D:292:PRO:HD3	1:D:378:CYS:HB3	2.00	0.42
1:C:305:TRP:CZ3	1:C:388:CYS:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:HB3	1:D:89[B]:SCY:H	1.54	0.42
1:D:54:LEU:O	1:D:84:GLY:HA2	2.20	0.41
1:D:88:LEU:HB3	1:D:89[A]:SCY:H	1.55	0.41
1:C:64:GLN:O	1:C:65:ASN:C	2.58	0.41
1:A:276:VAL:CG2	4:A:534:HOH:O	2.67	0.41
1:B:26:PRO:CD	4:B:444:HOH:O	2.68	0.41
1:B:55:GLY:HA3	1:B:91:SER:HB3	2.02	0.41
1:C:47:GLY:HA2	1:C:77:PRO:HG3	2.03	0.41
1:D:207:ARG:HD3	1:D:207:ARG:N	2.35	0.41
1:B:203:ILE:N	4:B:517:HOH:O	2.52	0.41
1:A:186:ALA:HA	1:A:340:ASN:O	2.21	0.41
1:A:276:VAL:CG2	1:A:388:CYS:HB2	2.51	0.41
1:B:392:LEU:HD22	4:B:493:HOH:O	2.21	0.41
1:D:279:ALA:CB	1:D:298:LYS:HB3	2.51	0.41
1:A:142:THR:O	1:A:146:ASP:HB2	2.21	0.41
1:A:89[A]:SCY:SG	1:A:348:HIS:CE1	3.14	0.40
1:C:101:GLN:HG2	1:D:105:THR:HG21	2.03	0.40
1:C:364:GLU:O	1:C:368:ARG:HG2	2.22	0.40
1:A:155:TYR:CD2	1:A:159:THR:HG21	2.57	0.40
1:A:155:TYR:CG	1:A:159:THR:HG21	2.56	0.40
3:A:5394:GOL:H12	4:A:407:HOH:O	2.20	0.40
1:B:330:LEU:HD12	1:B:332:TRP:CZ2	2.57	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	Interatomic distance (Å)	Clash overlap (Å)
4:A:408:HOH:O	4:A:9967:HOH:O[2_645]	2.00	0.20

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%)	376 (96%)	15 (4%)	0	100	100
1	B	391/392 (100%)	367 (94%)	23 (6%)	1 (0%)	46	33
1	C	391/392 (100%)	373 (95%)	15 (4%)	3 (1%)	24	10
1	D	391/392 (100%)	379 (97%)	11 (3%)	1 (0%)	46	33
All	All	1564/1568 (100%)	1495 (96%)	64 (4%)	5 (0%)	46	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	PRO
1	C	350	ILE
1	D	3	PRO
1	B	350	ILE
1	C	4	SER

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	280/278 (101%)	263 (94%)	17 (6%)	23	10
1	B	280/278 (101%)	264 (94%)	16 (6%)	25	12
1	C	280/278 (101%)	266 (95%)	14 (5%)	30	16
1	D	280/278 (101%)	265 (95%)	15 (5%)	27	14
All	All	1120/1112 (101%)	1058 (94%)	62 (6%)	27	13

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	TYR
1	A	191	LYS
1	A	207	ARG
1	A	221	HIS
1	A	228	MET
1	A	230	LYS

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Mol	Chain	Res	Type
1	A	237	LYS
1	A	272	LEU
1	A	286	LYS
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	339	VAL
1	A	353[A]	SER
1	A	353[B]	SER
1	B	5	ILE
1	B	109	SER
1	B	134	MET
1	B	191	LYS
1	B	207	ARG
1	B	221	HIS
1	B	228	MET
1	B	237	LYS
1	B	272	LEU
1	B	276	VAL
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	339	VAL
1	B	371	ARG
1	C	73	LYS
1	C	78	GLN
1	C	129	ARG
1	C	203	ILE
1	C	207	ARG
1	C	224	THR
1	C	237	LYS
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	371	ARG
1	C	392	LEU
1	D	155	TYR

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Mol	Chain	Res	Type
1	D	187	GLU
1	D	207	ARG
1	D	220	ARG
1	D	226	ASP
1	D	236	ASP
1	D	237	LYS
1	D	249	LEU
1	D	272	LEU
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	SCY	A	89[A]	-	7,8,9	0.67	0	4,9,11	1.52	1 (25%)
1	SCY	A	89[B]	-	4,5,9	1.07	0	3,5,11	2.05	2 (66%)
1	SCY	B	89[A]	-	7,8,9	1.02	0	4,9,11	1.53	1 (25%)
1	SCY	B	89[B]	-	4,5,9	1.61	0	3,5,11	1.51	1 (33%)
1	SCY	C	89[A]	-	7,8,9	0.53	0	4,9,11	1.15	1 (25%)
1	SCY	C	89[B]	-	4,5,9	0.80	0	3,5,11	1.30	1 (33%)
1	SCY	D	89[A]	-	7,8,9	0.56	0	4,9,11	1.03	0
1	SCY	D	89[B]	-	4,5,9	0.58	0	3,5,11	1.15	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	SCY	A	89[A]	-	-	1/5/7/9	0/0/0/0
1	SCY	A	89[B]	-	-	0/1/4/9	0/0/0/0
1	SCY	B	89[A]	-	-	0/5/7/9	0/0/0/0
1	SCY	B	89[B]	-	-	0/1/4/9	0/0/0/0
1	SCY	C	89[A]	-	-	0/5/7/9	0/0/0/0
1	SCY	C	89[B]	-	-	0/1/4/9	0/0/0/0
1	SCY	D	89[A]	-	-	0/5/7/9	0/0/0/0
1	SCY	D	89[B]	-	-	0/1/4/9	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89[B]	SCY	O-C-CA	-2.70	118.45	125.49
1	A	89[A]	SCY	O-C-CA	-2.70	118.45	125.49
1	B	89[A]	SCY	O-C-CA	-2.59	118.75	125.49
1	B	89[B]	SCY	O-C-CA	-2.59	118.75	125.49
1	C	89[A]	SCY	O-C-CA	-2.19	119.78	125.49
1	C	89[B]	SCY	O-C-CA	-2.19	119.78	125.49
1	A	89[B]	SCY	CB-CA-C	-2.12	106.28	111.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	89[A]	SCY	OCD-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	89[A]	SCY	6	0
1	B	89[A]	SCY	6	0
1	D	89[A]	SCY	1	0
1	D	89[B]	SCY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	0.52	0	5,5,5	0.47	0
3	GOL	A	5394	-	5,5,5	0.53	0	5,5,5	0.82	0
2	SO4	A	9720	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	A	9722	-	4,4,4	0.25	0	6,6,6	0.20	0
3	GOL	B	6393	-	5,5,5	0.76	0	5,5,5	0.97	0
3	GOL	B	6394	-	5,5,5	0.42	0	5,5,5	0.60	0
2	SO4	B	9719	-	4,4,4	0.24	0	6,6,6	0.46	0
2	SO4	B	9721	-	4,4,4	0.66	0	6,6,6	0.62	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
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
3	GOL	B	6393	-	-	0/4/4/4	0/0/0/0
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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5393	GOL	2	0
3	A	5394	GOL	2	0
3	B	6393	GOL	2	0
3	B	6394	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	391/392 (99%)	-0.26	8 (2%) 68 70	6, 11, 28, 54	0
1	B	391/392 (99%)	-0.33	5 (1%) 79 81	5, 11, 30, 53	0
1	C	391/392 (99%)	1.04	62 (15%) 3 3	2, 9, 23, 40	0
1	D	391/392 (99%)	1.71	127 (32%) 1 0	2, 10, 26, 41	0
All	All	1564/1568 (99%)	0.54	202 (12%) 5 5	2, 11, 26, 54	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	ALA	10.3
1	C	36	SER	8.5
1	D	226	ASP	8.4
1	D	232	ARG	8.1
1	D	1	SER	7.6
1	D	170	LEU	7.6
1	D	331	GLY	7.5
1	D	330	LEU	6.5
1	A	132	VAL	6.5
1	C	1	SER	6.3
1	D	2	THR	6.2
1	D	231	LEU	6.2
1	D	228	MET	6.1
1	D	237	LYS	5.9
1	C	232	ARG	5.9
1	D	224	THR	5.8
1	D	235	PHE	5.4
1	D	180	VAL	5.2
1	D	382	GLY	5.1
1	D	279	ALA	5.0
1	C	234	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	308	GLY	4.8
1	D	332	TRP	4.8
1	A	2	THR	4.8
1	D	392	LEU	4.7
1	D	328	LYS	4.6
1	D	186	ALA	4.6
1	D	178	PHE	4.5
1	D	175	GLN	4.4
1	D	165	ALA	4.3
1	C	388	CYS	4.3
1	D	343	ALA	4.3
1	D	325	ALA	4.2
1	D	195	PHE	4.2
1	D	173	ASP	4.2
1	D	238	GLU	4.2
1	C	2	THR	4.2
1	D	358	LEU	4.2
1	D	236	ASP	4.2
1	D	5	ILE	4.1
1	D	303	ALA	4.1
1	D	336	ILE	4.0
1	D	350	ILE	4.0
1	D	246	ALA	4.0
1	C	208	LYS	3.9
1	D	207	ARG	3.9
1	D	313	VAL	3.8
1	A	208	LYS	3.8
1	C	235	PHE	3.8
1	C	323	ALA	3.8
1	D	310	LEU	3.7
1	D	208	LYS	3.7
1	C	80	ALA	3.7
1	D	240	THR	3.6
1	D	140	ILE	3.6
1	A	1	SER	3.6
1	C	67	ALA	3.6
1	D	191	LYS	3.6
1	D	227	SER	3.6
1	D	276	VAL	3.5
1	D	241	VAL	3.5
1	D	152	PHE	3.4
1	C	153	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	166	LYS	3.4
1	D	307	ILE	3.4
1	D	272	LEU	3.3
1	C	225	LEU	3.3
1	D	323	ALA	3.3
1	C	272	LEU	3.3
1	D	371	ARG	3.3
1	C	230	LYS	3.3
1	D	378	CYS	3.2
1	D	206	GLY	3.2
1	D	209	GLY	3.2
1	D	370	ALA	3.2
1	D	211	ILE	3.2
1	C	209	GLY	3.2
1	D	92	GLY	3.2
1	D	376	THR	3.1
1	C	320	ALA	3.1
1	C	211	ILE	3.1
1	D	391	SER	3.1
1	D	187	GLU	3.1
1	D	221	HIS	3.0
1	C	307	ILE	3.0
1	D	335	SER	3.0
1	C	236	ASP	3.0
1	C	93	LEU	3.0
1	D	306	LYS	2.9
1	C	224	THR	2.9
1	C	334	PRO	2.9
1	D	388	CYS	2.9
1	D	96	VAL	2.9
1	D	339	VAL	2.9
1	D	204	VAL	2.9
1	C	131	GLY	2.9
1	D	156	HIS	2.8
1	C	104	ALA	2.8
1	D	153	TYR	2.8
1	D	242	THR	2.8
1	C	207	ARG	2.8
1	B	132	VAL	2.8
1	C	243	ALA	2.8
1	D	244	GLY	2.7
1	C	96	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	177	ALA	2.7
1	C	273	GLY	2.7
1	C	310	LEU	2.7
1	D	225	LEU	2.7
1	D	329	ASP	2.7
1	C	231	LEU	2.7
1	C	110	ILE	2.7
1	D	192	ASP	2.7
1	D	357	ILE	2.7
1	D	281	VAL	2.7
1	C	95	ALA	2.7
1	D	377	LEU	2.7
1	D	148	LEU	2.6
1	D	174	GLU	2.6
1	D	159	THR	2.6
1	D	280	THR	2.6
1	C	103	ILE	2.6
1	D	243	ALA	2.6
1	C	373	GLY	2.6
1	D	265	SER	2.6
1	D	372	LYS	2.5
1	D	97	ALA	2.5
1	D	10	ALA	2.5
1	D	95	ALA	2.5
1	D	181	ALA	2.5
1	C	324	CYS	2.5
1	D	269	ILE	2.5
1	B	1	SER	2.5
1	B	208	LYS	2.5
1	D	154	GLY	2.5
1	D	179	ALA	2.5
1	C	333	ASP	2.5
1	A	134	MET	2.4
1	D	219	ILE	2.4
1	D	172	ARG	2.4
1	D	362	LEU	2.4
1	C	179	ALA	2.4
1	D	239	GLY	2.4
1	D	299	ALA	2.4
1	D	169	GLN	2.4
1	C	300	LEU	2.4
1	D	334	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	207	ARG	2.4
1	D	168	TRP	2.4
1	D	327	ASN	2.4
1	C	46	ALA	2.3
1	C	35	ILE	2.3
1	D	176	ASP	2.3
1	C	238	GLU	2.3
1	D	250	ASN	2.3
1	D	257	LEU	2.3
1	A	133	LYS	2.3
1	C	380	GLY	2.3
1	D	364	GLU	2.3
1	C	97	ALA	2.3
1	C	6	VAL	2.3
1	D	24	ASN	2.3
1	C	3	PRO	2.3
1	D	167	GLN	2.3
1	D	270	GLN	2.3
1	C	266	ARG	2.2
1	C	342	GLY	2.2
1	B	238	GLU	2.2
1	D	37	ALA	2.2
1	C	296	SER	2.2
1	D	305	TRP	2.2
1	C	229	ALA	2.2
1	D	255	ALA	2.2
1	C	195	PHE	2.2
1	A	207	ARG	2.2
1	C	312	LEU	2.2
1	C	57	VAL	2.2
1	D	213	VAL	2.2
1	D	222	GLY	2.1
1	D	300	LEU	2.1
1	C	112	VAL	2.1
1	D	44	VAL	2.1
1	D	205	LYS	2.1
1	C	135	GLY	2.1
1	D	262	ALA	2.1
1	A	238	GLU	2.1
1	D	293	ILE	2.1
1	D	312	LEU	2.1
1	C	50	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	233	PRO	2.1
1	C	392	LEU	2.1
1	D	113	ALA	2.1
1	D	367	ARG	2.1
1	D	301	GLU	2.0
1	D	42	ALA	2.0
1	D	386	ALA	2.0
1	D	319	PHE	2.0
1	C	240	THR	2.0
1	C	213	VAL	2.0
1	D	71	ALA	2.0
1	C	269	ILE	2.0
1	D	379	ILE	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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SCY	A	89[B]	6/10	0.95	0.11	-	10,12,13,14	2
1	SCY	C	89[A]	9/10	0.92	0.13	-	5,8,9,11	5
1	SCY	B	89[A]	9/10	0.97	0.10	-	8,11,18,24	5
1	SCY	C	89[B]	6/10	0.92	0.13	-	2,5,8,9	2
1	SCY	A	89[A]	9/10	0.95	0.11	-	12,13,22,24	5
1	SCY	B	89[B]	6/10	0.97	0.10	-	8,9,9,11	2
1	SCY	D	89[A]	9/10	0.88	0.14	-	5,6,9,10	5
1	SCY	D	89[B]	6/10	0.88	0.14	-	2,6,6,6	2

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	6394	6/6	0.95	0.18	6.34	11,27,27,28	0
3	GOL	A	5393	6/6	0.89	0.20	3.65	28,29,31,34	0
3	GOL	B	6393	6/6	0.85	0.15	3.24	39,41,44,46	0
3	GOL	A	5394	6/6	0.89	0.20	2.41	19,29,32,32	0
2	SO4	B	9719	5/5	0.90	0.15	1.45	76,76,77,77	0
2	SO4	A	9722	5/5	0.92	0.11	0.40	70,72,73,75	0
2	SO4	B	9721	5/5	0.96	0.09	-	48,49,51,54	0
2	SO4	A	9720	5/5	0.98	0.09	-	50,53,54,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.