



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:05 PM UTC

PDB ID : 1M4S / pdb_00001m4s
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

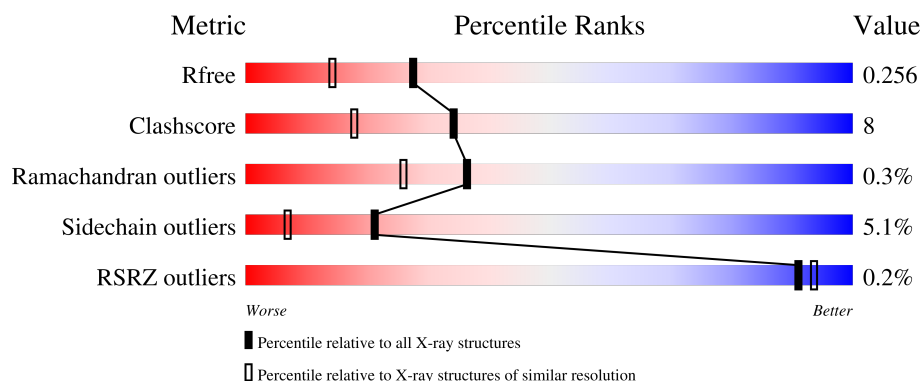
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	 84% 14% .
1	B	392	 80% 18% .
1	C	392	 85% 14% .
1	D	392	 88% 11% .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SCY	A	89[A]	-	-	X	-
1	SCY	A	89[B]	-	X	-	-
1	SCY	B	89[A]	-	-	X	-
1	SCY	B	89[B]	-	X	-	-
1	SCY	C	89[B]	-	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.

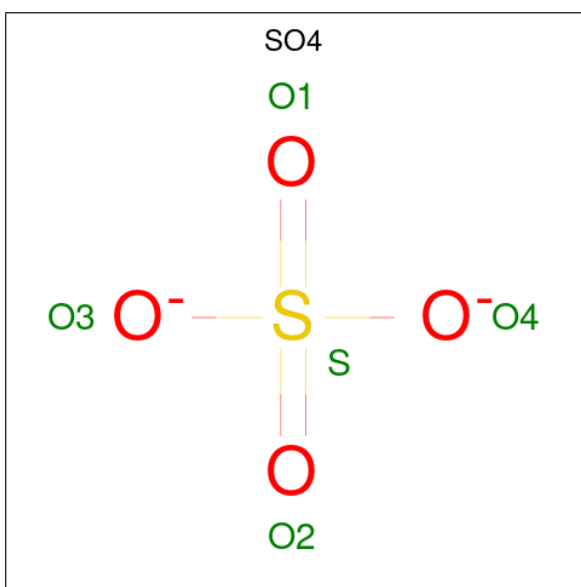
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

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:

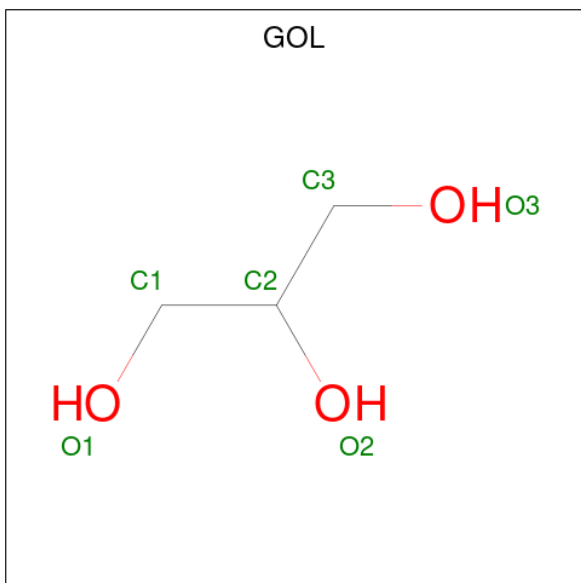
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	insertion	UNP P07097
A	89	SCY	CYS	modified residue	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	10	ALA	-	insertion	UNP P07097
B	89	SCY	CYS	modified residue	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	10	ALA	-	insertion	UNP P07097
C	89	SCY	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 (CCD ID: SO4) (formula: O₄S).



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

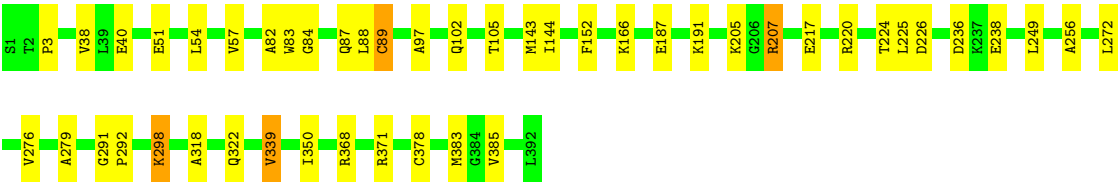
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.40Å 79.28Å 148.48Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	20.00 – 1.87 20.00 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-1.87) 87.8 (20.00-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 1.87Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.247 0.218 , 0.256	Depositor DCC
R_{free} test set	7188 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.158 for h,-k,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, SCY

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	1.21	4/2880 (0.1%)	1.15	1/3888 (0.0%)
1	B	1.22	7/2880 (0.2%)	1.15	7/3888 (0.2%)
1	C	0.85	10/2880 (0.3%)	0.95	1/3888 (0.0%)
1	D	0.60	0/2880	0.86	0/3888
All	All	1.01	21/11520 (0.2%)	1.04	9/15552 (0.1%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	373	GLY	C-O	10.68	1.37	1.23
1	C	373	GLY	C-N	9.03	1.45	1.33
1	C	310	LEU	C-O	8.46	1.34	1.24
1	C	277	SER	CB-OG	7.81	1.57	1.42
1	C	310	LEU	C-N	7.25	1.46	1.33
1	C	273	GLY	C-O	6.89	1.33	1.23
1	C	272	LEU	C-O	6.83	1.32	1.24
1	A	35	ILE	CA-C	6.42	1.60	1.52
1	C	273	GLY	CA-C	6.35	1.58	1.51
1	B	157	MET	SD-CE	-5.89	1.64	1.79
1	C	359	ASN	CG-ND2	5.74	1.45	1.33
1	A	189	ALA	CA-CB	5.61	1.62	1.53
1	A	259	MET	SD-CE	5.55	1.93	1.79
1	A	157	MET	SD-CE	-5.28	1.66	1.79
1	B	385	VAL	CA-C	5.12	1.58	1.52
1	C	135	GLY	C-O	5.12	1.30	1.24
1	B	112	VAL	CA-CB	5.11	1.60	1.54
1	B	186	ALA	CA-CB	-5.07	1.45	1.53
1	B	45	ALA	C-O	-5.05	1.17	1.23
1	B	256	ALA	CA-CB	-5.02	1.43	1.54
1	B	97	ALA	CA-CB	5.01	1.61	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	VAL	N-CA-CB	-6.22	100.02	110.65
1	C	373	GLY	O-C-N	6.21	129.20	123.73
1	A	129	ARG	N-CA-C	6.09	117.72	111.14
1	B	54	LEU	N-CA-C	5.83	117.91	108.41
1	B	207	ARG	N-CA-C	-5.25	105.95	112.93
1	B	338	ASN	CA-C-N	5.16	128.63	120.47
1	B	338	ASN	C-N-CA	5.16	128.63	120.47
1	B	2	THR	N-CA-C	-5.12	97.67	108.73
1	B	34	VAL	N-CA-C	5.02	115.79	110.72

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	53	0
1	B	2842	0	2849	61	0
1	C	2842	0	2849	29	0
1	D	2842	0	2849	31	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	173	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 8.

All (173) 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:A:100:MET:HE2	4:A:468:HOH:O	1.71	0.91
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: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:D:385:VAL:HG22	4:D:478:HOH:O	1.88	0.72
1:A:89[A]:SCY:SG	1:A:348:HIS:NE2	2.64	0.71
1:C:255:ALA:HB3	4:C:457:HOH:O	1.91	0.70
1:A:87:GLN:C	4:A:464:HOH:O	2.33	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: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:HE2	1:A:89[A]:SCY:H	1.62	0.64
1:D:256:ALA:C	4:D:518:HOH:O	2.41	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HG	4:A:495:HOH:O	2.03	0.59
1:A:100:MET:CE	4:A:468:HOH:O	2.36	0.59
1:C:277:SER:OG	1:C:388:CYS:HB2	2.02	0.59
1:B:374:LEU:C	1:B:374:LEU:HD23	2.28	0.59
1:C:120:SER:OG	1:C:251:ASP:OD2	2.13	0.59
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:A:139:MET:HE1	1:B:139:MET:HE1	1.87	0.56
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: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:B:279:ALA:HB1	4:B:537:HOH:O	2.08	0.53
1:C:122:ALA:HA	4:C:473:HOH:O	2.09	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:144:ILE:HD13	1:B:148:LEU:HD12	1.90	0.53
1:B:161:ALA:HA	4:B:476:HOH:O	2.08	0.53
1:B:203:ILE:HD12	4:B:502:HOH:O	2.09	0.53
1:D:224:THR:C	4:D:423:HOH:O	2.51	0.52
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:D:238:GLU:C	4:D:520:HOH:O	2.53	0.51
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:257:LEU:C	1:A:257:LEU:HD23	2.35	0.51
1:B:306:LYS:NZ	4:B:475:HOH:O	2.44	0.50
1:A:36:SER:O	1:A:40:GLU:HG3	2.11	0.50
1:A:269:ILE:O	1:A:271:PRO:HD3	2.10	0.50
1:D:40:GLU:HB3	4:D:459:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:LEU:HD23	1:B:257:LEU:C	2.38	0.48
1:D:143:MET:HE2	4:D:484:HOH:O	2.13	0.48
1:B:392:LEU:HD21	4:B:445:HOH:O	2.13	0.48
1:A:5:ILE:HD12	1:A:5:ILE:N	2.28	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:276:VAL:HG22	1:C:388:CYS:C	2.38	0.47
1:C:82:ALA:HB2	4:C:469:HOH:O	2.14	0.47
1:B:24:ASN:C	4:B:444:HOH:O	2.56	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:A:40:GLU:HG3	4:A:9946:HOH:O	2.15	0.47
1:C:207:ARG:HD3	1:C:207:ARG:H	1.79	0.47
1:B:228:MET:HE1	4:B:524:HOH:O	2.14	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:C:64:GLN:O	1:C:65:ASN:C	2.58	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:A:172:ARG:HB2	1:A:240:THR:HG22	1.97	0.46
1:A:282:GLY:HA3	1:B:78:GLN:O	2.15	0.46
1:B:200:VAL:HG23	3:B:6394:GOL:H2	1.98	0.46
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.45	0.46
1:B:364:GLU:OE1	1:B:367:ARG:HD2	2.15	0.46
1:C:194:ARG:O	4:C:494:HOH:O	2.20	0.46
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.50	0.46
1:B:322:GLN:O	1:B:326:VAL:HG23	2.16	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:A:286:LYS:CE	4:A:9759:HOH:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD12	1:B:380:GLY:O	2.17	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:A:156:HIS:CE1	4:A:498:HOH:O	2.71	0.43
1:A:312:LEU:HD23	1:A:361:LEU:HD12	2.01	0.43
1:C:124:HIS:HA	1:C:140:ILE:O	2.18	0.43
1:D:51:GLU:CD	1:D:83:TRP:HE1	2.27	0.43
1:A:291:GLY:N	1:A:292:PRO:CD	2.81	0.43
1:C:84:GLY:HA3	4:C:403:HOH:O	2.18	0.43
1:B:207:ARG:N	1:B:207:ARG:HD3	2.33	0.43
1:B:185:LYS:CE	4:B:525:HOH:O	2.58	0.43
1:A:78:GLN:O	1:B:282:GLY:HA3	2.19	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:D:82:ALA:HB2	4:D:394:HOH:O	2.18	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
1:D:88:LEU:HB3	1:D:89[B]:SCY:H	1.54	0.42
1:A:157:MET:HA	1:A:157:MET:HE2	2.01	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:A:4:SER:C	1:A:5:ILE:HD12	2.45	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:B:317:GLU:CD	1:B:342:GLY:HA3	2.46	0.41
1:C:47:GLY:HA2	1:C:77:PRO:HG3	2.03	0.41
1:D:207:ARG:N	1:D:207:ARG:HD3	2.35	0.41
1:A:186:ALA:HA	1:A:340:ASN:O	2.21	0.41
1:B:203:ILE:N	4:B:517:HOH:O	2.52	0.41
1:A:276:VAL:CG2	1:A:388:CYS:HB2	2.51	0.41
1:A:142:THR:O	1:A:146:ASP:HB2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:MET:HE2	1:B:85:MET:HB2	1.99	0.40
1:A:89[A]:SCY:SG	1:A:348:HIS:CE1	3.14	0.40
1:A:155:TYR:CD2	1:A:159:THR:HG21	2.57	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: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%)	36	26
1	C	391/392 (100%)	373 (95%)	15 (4%)	3 (1%)	16	5
1	D	391/392 (100%)	379 (97%)	11 (3%)	1 (0%)	36	26
All	All	1564/1568 (100%)	1495 (96%)	64 (4%)	5 (0%)	36	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	PRO
1	C	350	ILE

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Mol	Chain	Res	Type
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%)	17	4
1	B	280/278 (101%)	266 (95%)	14 (5%)	22	7
1	C	280/278 (101%)	267 (95%)	13 (5%)	24	9
1	D	280/278 (101%)	266 (95%)	14 (5%)	22	7
All	All	1120/1112 (101%)	1062 (95%)	58 (5%)	21	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ILE
1	A	132	VAL
1	A	191	LYS
1	A	207	ARG
1	A	228	MET
1	A	230	LYS
1	A	237	LYS
1	A	272	LEU
1	A	286	LYS
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	A	367	ARG
1	B	5	ILE

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Mol	Chain	Res	Type
1	B	109	SER
1	B	134	MET
1	B	166	LYS
1	B	191	LYS
1	B	207	ARG
1	B	228	MET
1	B	272	LEU
1	B	276	VAL
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	187	GLU
1	C	191	LYS
1	C	203	ILE
1	C	207	ARG
1	C	224	THR
1	C	237	LYS
1	C	272	LEU
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	371	ARG
1	C	392	LEU
1	D	187	GLU
1	D	191	LYS
1	D	205	LYS
1	D	207	ARG
1	D	220	ARG
1	D	226	ASP
1	D	236	ASP
1	D	249	LEU
1	D	272	LEU
1	D	276	VAL
1	D	298	LYS
1	D	322	GLN
1	D	339	VAL
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	87	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	C	89[A]	-	7,8,9	0.60	0	4,9,11	0.51	0
1	SCY	D	89[B]	-	7,5,9	2.32	1 (14%)	4,5,11	1.51	1 (25%)
1	SCY	B	89[B]	-	7,5,9	6.83	1 (14%)	4,5,11	6.02	2 (50%)
1	SCY	C	89[B]	-	7,5,9	2.14	1 (14%)	4,5,11	3.29	2 (50%)
1	SCY	A	89[B]	-	7,5,9	6.26	1 (14%)	4,5,11	5.00	2 (50%)
1	SCY	D	89[A]	-	7,8,9	0.65	0	4,9,11	0.53	0
1	SCY	B	89[A]	-	7,8,9	1.09	0	4,9,11	1.10	0
1	SCY	A	89[A]	-	7,8,9	0.68	0	4,9,11	0.83	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	C	89[A]	-	-	3/5/7/9	-
1	SCY	D	89[B]	-	-	2/5/4/9	-
1	SCY	B	89[B]	-	-	3/5/4/9	-
1	SCY	C	89[B]	-	-	3/5/4/9	-
1	SCY	A	89[B]	-	-	3/5/4/9	-
1	SCY	D	89[A]	-	-	3/5/7/9	-
1	SCY	B	89[A]	-	-	3/5/7/9	-
1	SCY	A	89[A]	-	-	3/5/7/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89[B]	SCY	CD-SG	-17.81	0.77	1.75
1	A	89[B]	SCY	CD-SG	-16.42	0.85	1.75
1	D	89[B]	SCY	CD-SG	-5.97	1.42	1.75
1	C	89[B]	SCY	CD-SG	-5.40	1.45	1.75

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89[B]	SCY	CE-CD-SG	-8.92	57.73	114.13
1	A	89[B]	SCY	CE-CD-SG	-8.30	61.68	114.13
1	B	89[B]	SCY	OCD-CD-SG	7.91	154.65	122.65
1	C	89[B]	SCY	CE-CD-SG	-6.25	74.60	114.13
1	A	89[B]	SCY	OCD-CD-SG	5.13	143.39	122.65
1	D	89[B]	SCY	CE-CD-SG	-2.90	95.80	114.13
1	C	89[B]	SCY	OCD-CD-SG	2.02	130.84	122.65

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	B	89[B]	SCY	N-CA-CB-SG
1	C	89[A]	SCY	CA-CB-SG-CD
1	C	89[A]	SCY	OCD-CD-SG-CB
1	C	89[A]	SCY	CE-CD-SG-CB
1	C	89[B]	SCY	N-CA-CB-SG
1	C	89[B]	SCY	OCD-CD-SG-CB
1	D	89[A]	SCY	OCD-CD-SG-CB
1	D	89[B]	SCY	N-CA-CB-SG
1	D	89[B]	SCY	OCD-CD-SG-CB
1	B	89[B]	SCY	OCD-CD-SG-CB
1	D	89[A]	SCY	CE-CD-SG-CB
1	A	89[A]	SCY	CA-CB-SG-CD
1	B	89[A]	SCY	CA-CB-SG-CD
1	C	89[B]	SCY	CA-CB-SG-CD
1	D	89[A]	SCY	CA-CB-SG-CD
1	B	89[B]	SCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 14 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	SO4	A	9720	-	4,4,4	0.21	0	6,6,6	0.33	0
3	GOL	A	5393	-	5,5,5	0.53	0	5,5,5	0.46	0
2	SO4	A	9722	-	4,4,4	0.24	0	6,6,6	0.22	0
3	GOL	A	5394	-	5,5,5	0.55	0	5,5,5	0.90	0
2	SO4	B	9719	-	4,4,4	0.23	0	6,6,6	0.39	0
2	SO4	B	9721	-	4,4,4	0.34	0	6,6,6	0.43	0
3	GOL	B	6394	-	5,5,5	0.43	0	5,5,5	0.65	0
3	GOL	B	6393	-	5,5,5	0.77	0	5,5,5	1.00	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	-	-	1/4/4/4	-
3	GOL	A	5394	-	-	2/4/4/4	-
3	GOL	B	6394	-	-	2/4/4/4	-
3	GOL	B	6393	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5394	GOL	O1-C1-C2-O2
3	A	5394	GOL	O1-C1-C2-C3
3	B	6394	GOL	O1-C1-C2-O2
3	B	6394	GOL	O1-C1-C2-C3
3	A	5393	GOL	O1-C1-C2-O2

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	6394	GOL	2	0
3	B	6393	GOL	2	0

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	391/392 (99%)	-1.21	0	100	100	6, 11, 28, 54	2 (0%)
1	B	391/392 (99%)	-1.23	0	100	100	5, 11, 30, 53	2 (0%)
1	C	391/392 (99%)	-0.74	3 (0%)	82	86	2, 9, 23, 40	2 (0%)
1	D	391/392 (99%)	-0.70	0	100	100	2, 10, 26, 41	2 (0%)
All	All	1564/1568 (99%)	-0.97	3 (0%)	91	93	2, 11, 26, 54	8 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36	SER	3.6
1	C	273	GLY	2.4
1	C	135	GLY	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SCY	A	89[A]	9/10	0.99	0.04	12,13,22,24	5
1	SCY	A	89[B]	6/10	0.99	0.04	10,12,13,14	2
1	SCY	B	89[A]	9/10	0.99	0.04	8,11,18,24	5
1	SCY	B	89[B]	6/10	0.99	0.04	8,9,9,11	2
1	SCY	C	89[A]	9/10	0.99	0.04	5,8,9,11	5
1	SCY	C	89[B]	6/10	0.99	0.04	2,5,8,9	2
1	SCY	D	89[A]	9/10	0.99	0.04	5,6,9,10	5
1	SCY	D	89[B]	6/10	0.99	0.04	2,6,6,6	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	6393	6/6	0.95	0.09	39,41,44,46	0
3	GOL	A	5394	6/6	0.96	0.09	19,29,32,32	0
2	SO4	A	9722	5/5	0.97	0.07	70,72,73,75	0
3	GOL	A	5393	6/6	0.97	0.10	28,29,31,34	0
2	SO4	B	9719	5/5	0.98	0.08	76,76,77,77	0
3	GOL	B	6394	6/6	0.98	0.08	11,27,27,28	0
2	SO4	A	9720	5/5	0.99	0.05	50,53,54,57	0
2	SO4	B	9721	5/5	0.99	0.05	48,49,51,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.