wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 03:48 am BST

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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

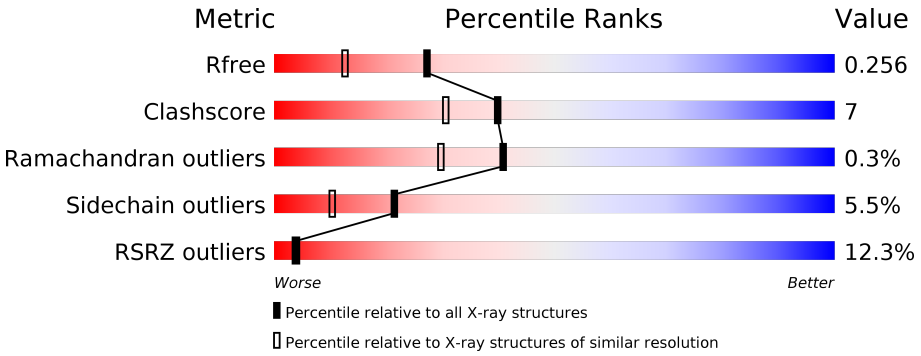
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	2% 83% 15% •
1	B	392	% 82% 16% •
1	C	392	15% 83% 16% •
1	D	392	31% 86% 13% •

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	A	89[B]	-	X	-	-
1	SCY	B	89[A]	-	-	X	-
1	SCY	B	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.

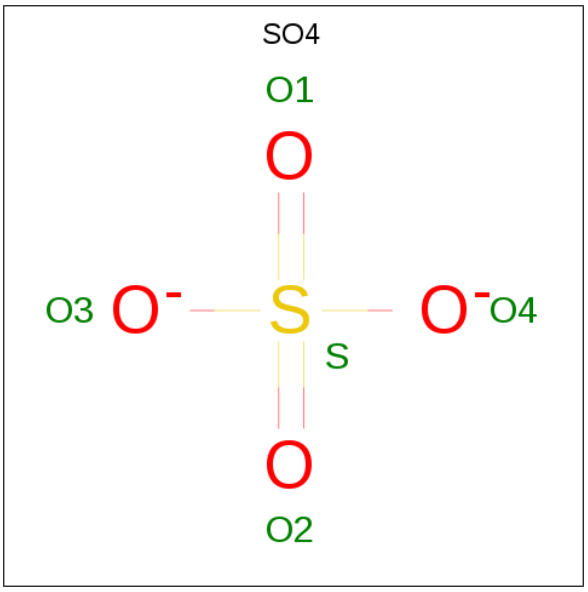
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

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:

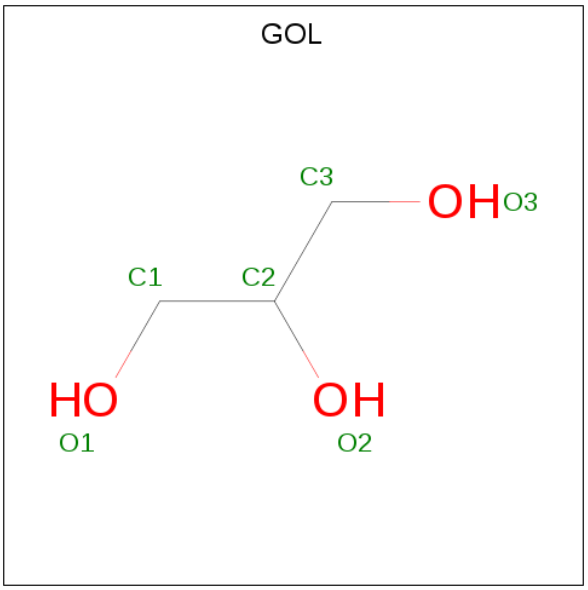
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	SCY	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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

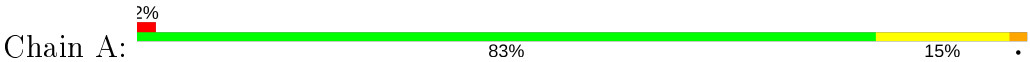
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	420	Total O 420 420	0	0
4	B	427	Total O 427 427	0	0
4	C	116	Total O 116 116	0	0
4	D	131	Total O 131 131	0	0

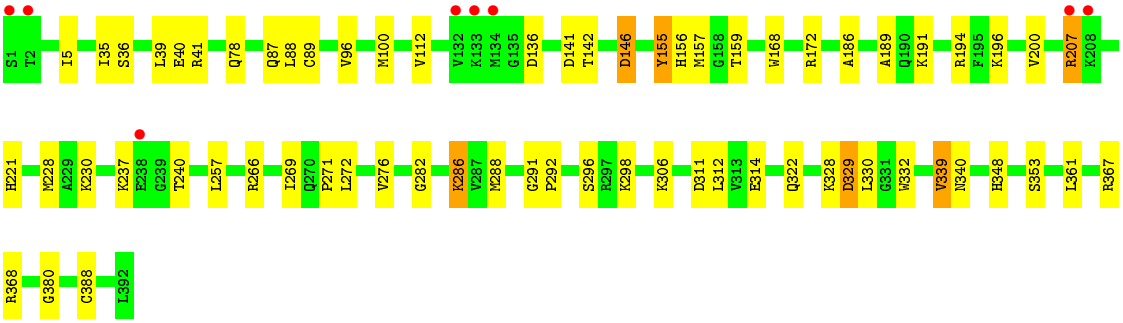
3 Residue-property plots (i)

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

- Molecule 1: Acetyl-CoA acetyltransferase

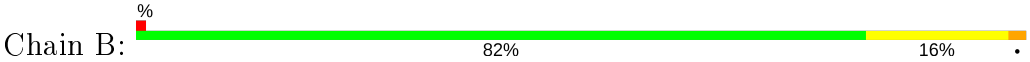
Chain A:

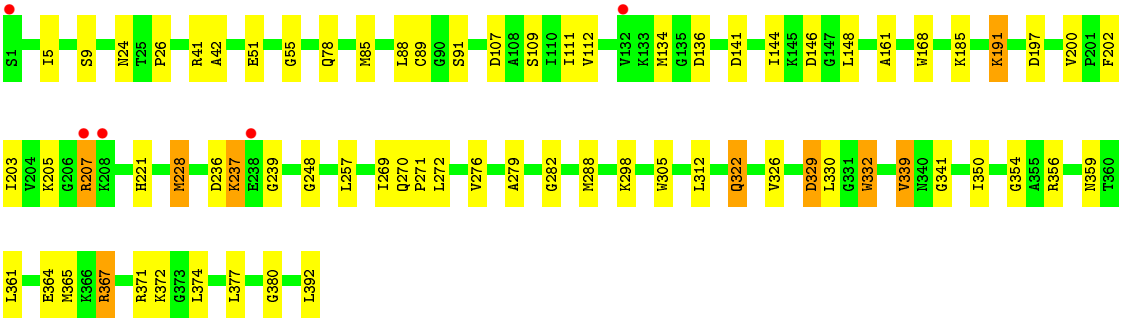




- Molecule 1: Acetyl-CoA acetyltransferase

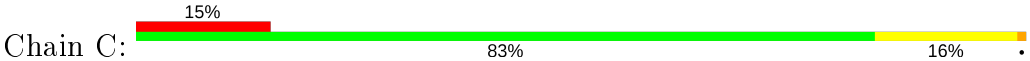
Chain B:

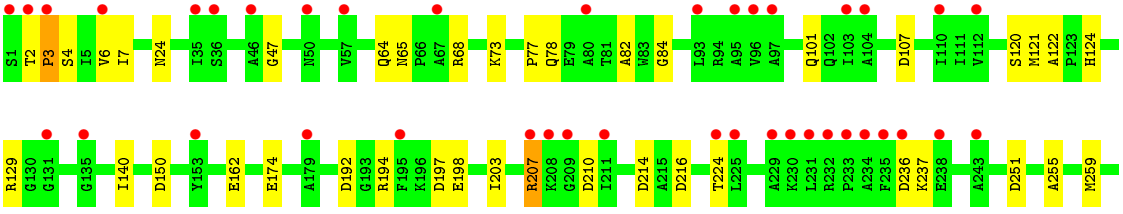


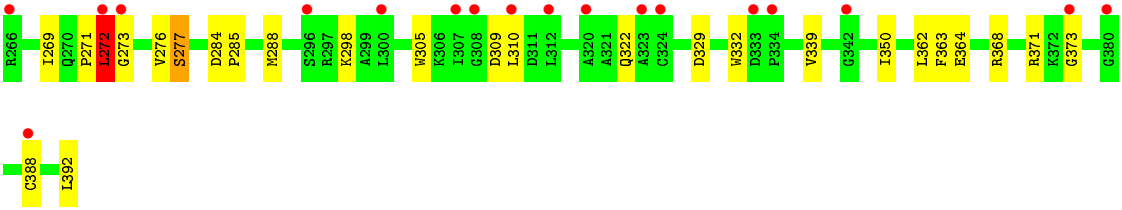


- Molecule 1: Acetyl-CoA acetyltransferase

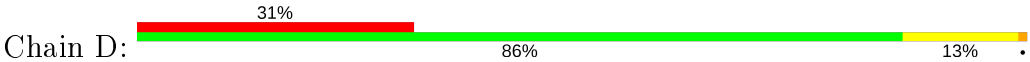
Chain C:

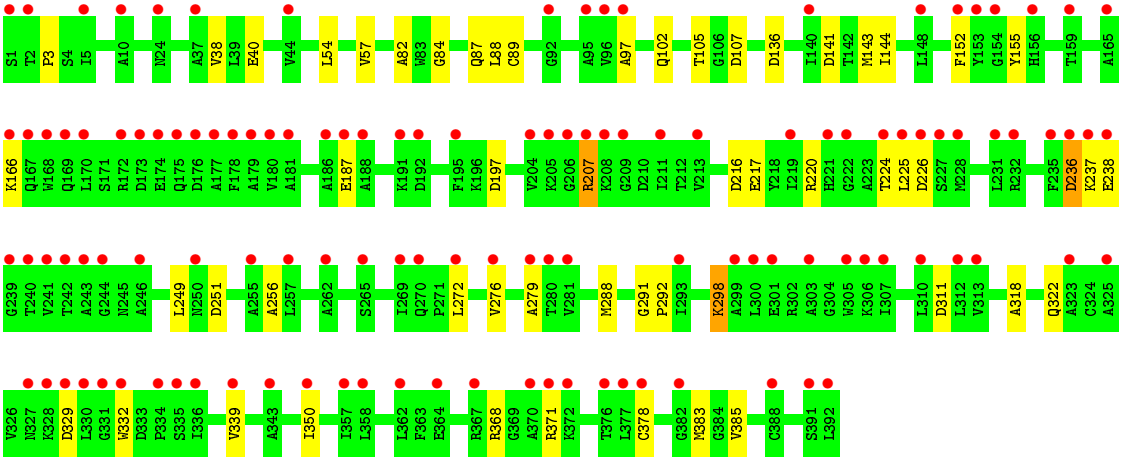






- Molecule 1: Acetyl-CoA acetyltransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.40Å 79.28Å 148.48Å 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
$< I/\sigma(I) >$ [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)	0.34 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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%)

The worst 5 of 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

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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.

The worst 5 of 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

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 (i)

5.3.1 Protein backbone (i)

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%)	41 30
1	C	391/392 (100%)	373 (95%)	15 (4%)	3 (1%)	19 9
1	D	391/392 (100%)	379 (97%)	11 (3%)	1 (0%)	41 30
All	All	1564/1568 (100%)	1495 (96%)	64 (4%)	5 (0%)	41 30

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	280/278 (101%)	263 (94%)	17 (6%)	18 8
1	B	280/278 (101%)	264 (94%)	16 (6%)	20 9
1	C	280/278 (101%)	266 (95%)	14 (5%)	24 13
1	D	280/278 (101%)	265 (95%)	15 (5%)	22 11
All	All	1120/1112 (101%)	1058 (94%)	62 (6%)	21 10

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	298	LYS
1	C	78	GLN
1	D	288	MET
1	B	339	VAL
1	C	203	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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[B]	-	7,5,9	5.76	1 (14%)	3,5,11	5.21	2 (66%)
1	SCY	C	89[A]	-	7,8,9	0.58	0	3,9,11	0.53	0
1	SCY	B	89[A]	-	7,8,9	1.05	0	3,9,11	1.04	0
1	SCY	C	89[B]	-	7,5,9	1.97	1 (14%)	3,5,11	3.48	1 (33%)
1	SCY	A	89[A]	-	7,8,9	0.65	0	3,9,11	0.90	0
1	SCY	B	89[B]	-	7,5,9	6.30	1 (14%)	3,5,11	6.35	2 (66%)
1	SCY	D	89[A]	-	7,8,9	0.62	0	3,9,11	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SCY	D	89[B]	-	7,5,9	2.14	1 (14%)	3,5,11	1.60	1 (33%)

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[B]	-	-	3/5/4/9	-
1	SCY	C	89[A]	-	-	3/5/7/9	-
1	SCY	B	89[A]	-	-	3/5/7/9	-
1	SCY	C	89[B]	-	-	3/5/4/9	-
1	SCY	A	89[A]	-	-	3/5/7/9	-
1	SCY	B	89[B]	-	-	3/5/4/9	-
1	SCY	D	89[A]	-	-	3/5/7/9	-
1	SCY	D	89[B]	-	-	2/5/4/9	-

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	-16.40	0.77	1.75
1	A	89[B]	SCY	CD-SG	-15.11	0.85	1.75
1	D	89[B]	SCY	CD-SG	-5.49	1.42	1.75
1	C	89[B]	SCY	CD-SG	-4.97	1.45	1.75

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89[B]	SCY	CE-CD-SG	-8.17	57.73	114.20
1	A	89[B]	SCY	CE-CD-SG	-7.59	61.68	114.20
1	B	89[B]	SCY	OCD-CD-SG	7.22	154.65	122.60
1	C	89[B]	SCY	CE-CD-SG	-5.73	74.60	114.20
1	A	89[B]	SCY	OCD-CD-SG	4.68	143.39	122.60

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	89[A]	SCY	6	0
1	A	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	B	6393	-	5,5,5	0.75	0	5,5,5	0.95	0
2	SO4	B	9719	-	4,4,4	0.14	0	6,6,6	0.38	0
2	SO4	B	9721	-	4,4,4	0.36	0	6,6,6	0.39	0
3	GOL	A	5393	-	5,5,5	0.52	0	5,5,5	0.44	0
3	GOL	A	5394	-	5,5,5	0.54	0	5,5,5	0.83	0
2	SO4	A	9720	-	4,4,4	0.11	0	6,6,6	0.35	0
3	GOL	B	6394	-	5,5,5	0.42	0	5,5,5	0.59	0
2	SO4	A	9722	-	4,4,4	0.15	0	6,6,6	0.21	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	B	6393	-	-	0/4/4/4	-
3	GOL	B	6394	-	-	2/4/4/4	-
3	GOL	A	5393	-	-	3/4/4/4	-
3	GOL	A	5394	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 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	B	6393	GOL	2	0
3	A	5393	GOL	2	0
3	A	5394	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, 95^{th} 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%)	-0.29	8 (2%) 65 67	6, 11, 28, 54	0
1	B	391/392 (99%)	-0.36	5 (1%) 77 79	5, 11, 30, 53	0
1	C	391/392 (99%)	0.99	58 (14%) 2 2	2, 9, 23, 40	0
1	D	391/392 (99%)	1.66	121 (30%) 0 0	2, 10, 26, 41	0
All	All	1564/1568 (99%)	0.50	192 (12%) 4 4	2, 11, 26, 54	0

The worst 5 of 192 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	ALA	10.1
1	C	36	SER	8.3
1	D	226	ASP	8.2
1	D	232	ARG	8.1
1	D	1	SER	7.5

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. The B-factors column lists the minimum, median, 95^{th} 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	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
1	SCY	C	89[A]	9/10	0.92	0.13	5,8,9,11	5
1	SCY	C	89[B]	6/10	0.92	0.13	2,5,8,9	2
1	SCY	A	89[B]	6/10	0.95	0.11	10,12,13,14	2
1	SCY	A	89[A]	9/10	0.95	0.11	12,13,22,24	5
1	SCY	B	89[A]	9/10	0.97	0.10	8,11,18,24	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SCY	B	89[B]	6/10	0.97	0.10	8,9,9,11	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. The B-factors column lists the minimum, median, 95^{th} 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
3	GOL	B	6393	6/6	0.85	0.15	39,41,44,46	0
3	GOL	A	5393	6/6	0.89	0.20	28,29,31,34	0
3	GOL	A	5394	6/6	0.89	0.20	19,29,32,32	0
2	SO4	B	9719	5/5	0.90	0.15	76,76,77,77	0
2	SO4	A	9722	5/5	0.92	0.11	70,72,73,75	0
3	GOL	B	6394	6/6	0.95	0.18	11,27,27,28	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 (i)

There are no such residues in this entry.