



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:55 PM GMT

PDB ID : 4UBV
Title : Structure of the 3-ketoacyl-CoA thiolase FadA5 from *M. tuberculosis* with an partially acetylated cysteine in complex with acetyl-CoA and CoA
Authors : Schaefer, C.M.; Kisker, C.
Deposited on : 2014-08-13
Resolution : 1.95 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

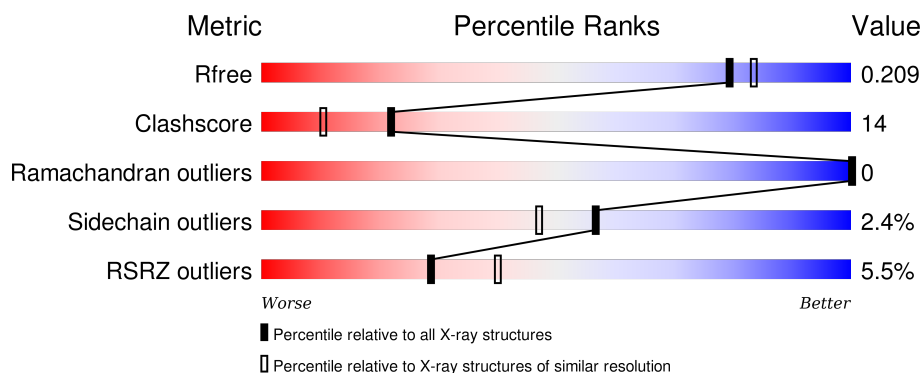
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	400	
1	B	400	

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
2	ACO	A	401	-	-	X	X
3	COA	A	402	-	-	-	X
3	COA	B	401[A]	-	-	-	X
3	COA	B	401[B]	-	-	-	X
4	SO4	A	403	-	-	-	X
4	SO4	A	404	-	-	-	X
5	DIO	A	406	-	-	-	X
5	DIO	B	403	-	-	X	X
6	GOL	A	408	-	-	-	X
6	GOL	A	409	-	-	-	X
6	GOL	B	408	-	-	-	X
6	GOL	B	410	-	-	-	X
6	GOL	B	413	-	-	-	X
6	GOL	B	415	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6504 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 FadA5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	11	0
			2961	1839	547	560	15			
1	B	392	Total	C	N	O	S	0	5	0
			2938	1822	538	563	15			

There are 18 discrepancies between the modelled and reference sequences:

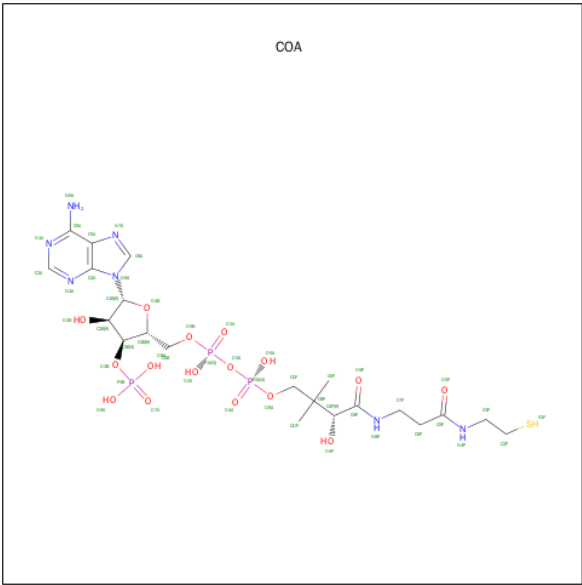
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP I6XHI4
A	-6	HIS	-	expression tag	UNP I6XHI4
A	-5	HIS	-	expression tag	UNP I6XHI4
A	-4	HIS	-	expression tag	UNP I6XHI4
A	-3	HIS	-	expression tag	UNP I6XHI4
A	-2	HIS	-	expression tag	UNP I6XHI4
A	-1	GLY	-	expression tag	UNP I6XHI4
A	0	SER	-	expression tag	UNP I6XHI4
A	93	SCY	CYS	Microheterogeneity	UNP I6XHI4
B	-7	HIS	-	expression tag	UNP I6XHI4
B	-6	HIS	-	expression tag	UNP I6XHI4
B	-5	HIS	-	expression tag	UNP I6XHI4
B	-4	HIS	-	expression tag	UNP I6XHI4
B	-3	HIS	-	expression tag	UNP I6XHI4
B	-2	HIS	-	expression tag	UNP I6XHI4
B	-1	GLY	-	expression tag	UNP I6XHI4
B	0	SER	-	expression tag	UNP I6XHI4
B	93	SCY	CYS	Microheterogeneity	UNP I6XHI4

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	51	23	7	17	3	1	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



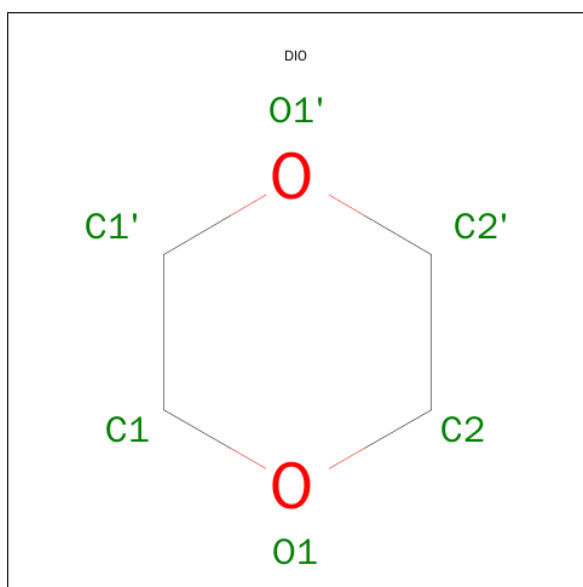
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	48	21	7	16	3	1	0	0
3	B	1	96	42	14	32	6	2	0	1

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



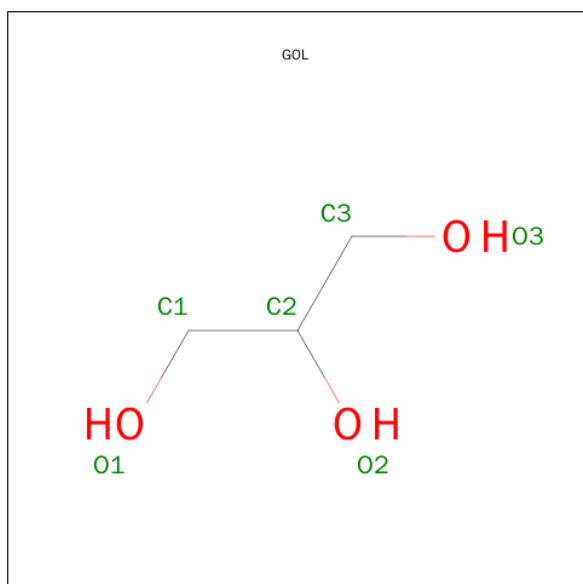
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

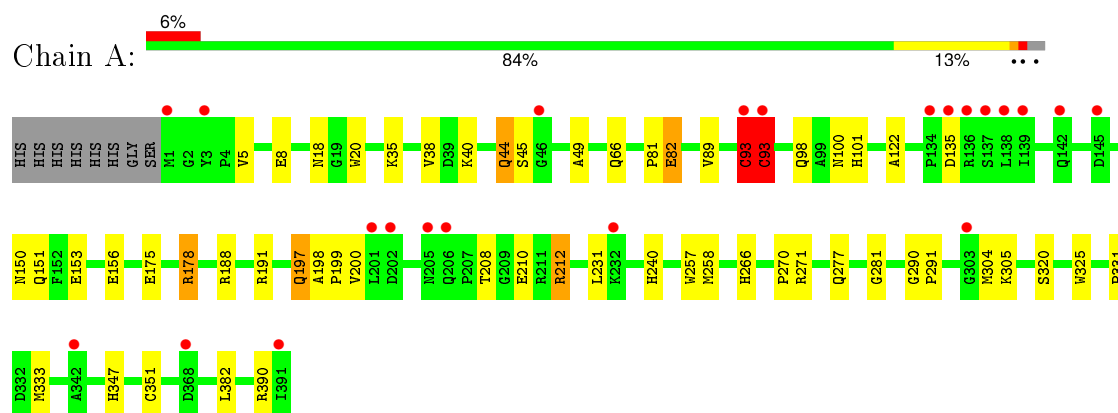
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	B	157	Total	O	0	0
			157	157		

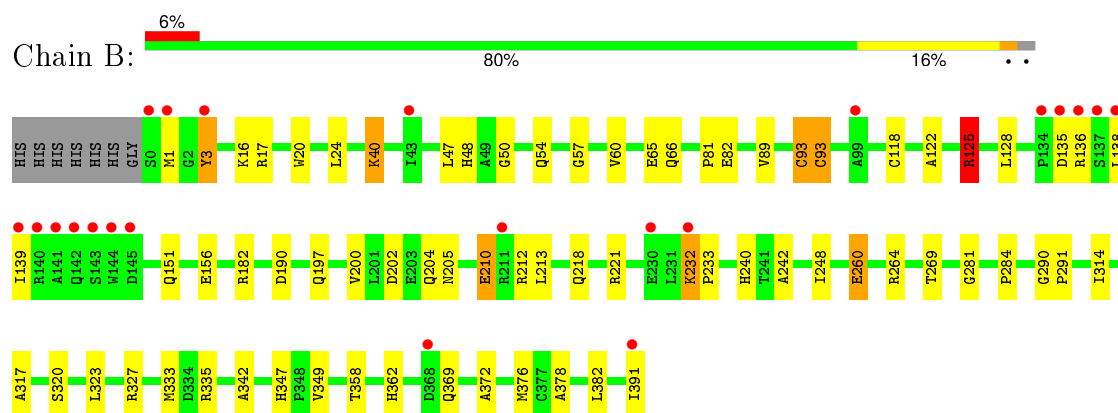
3 Residue-property plots [i](#)

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 FadA5



- Molecule 1: Acetyl-CoA acetyltransferase FadA5



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.68Å 124.68Å 124.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.99 – 1.95 35.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.99-1.95) 100.0 (35.99-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.231 0.172 , 0.209	Depositor DCC
R_{free} test set	3640 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.3	EDS
Estimated twinning fraction	0.016 for -h,l,k 0.008 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 71930 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6504	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.22% 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, DIO, ACO, COA, 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	0.53	0/3026	0.66	0/4098
1	B	0.56	0/2985	0.68	1/4047 (0.0%)
All	All	0.55	0/6011	0.67	1/8145 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ARG	NE-CZ-NH1	-12.47	114.06	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ARG	Sidechain
1	A	93[A]	SCY	Mainchain
1	B	125	ARG	Sidechain
1	B	24	LEU	Mainchain
1	B	314	ILE	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	372	ALA	Mainchain
1	B	93[A]	SCY	Mainchain

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	2961	0	2989	48	0
1	B	2938	0	2937	68	0
2	A	51	0	25	30	0
3	A	48	0	21	18	0
3	B	96	0	64	24	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	12	0	16	1	0
5	B	30	0	40	9	0
6	A	24	0	32	6	0
6	B	48	0	64	4	0
7	A	124	0	0	4	1
7	B	157	0	0	8	1
All	All	6504	0	6188	152	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 14.

All (152) 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)
2:A:401:ACO:CDP	3:A:402:COA:O9P	1.68	1.42
2:A:401:ACO:H51A	3:A:402:COA:O3A	1.35	1.22
1:A:81:PRO:HB3	6:A:408:GOL:H31	1.27	1.10
1:A:208:THR:OG1	1:A:210:GLU:HG3	1.53	1.08
1:B:242:ALA:HB1	3:B:401[B]:COA:H8A	1.36	1.07
2:A:401:ACO:C5B	3:A:402:COA:O3A	2.11	0.99
2:A:401:ACO:H4B	2:A:401:ACO:O8A	1.61	0.97
3:B:401[A]:COA:O8A	3:B:401[A]:COA:O2B	1.81	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93[B]:CYS:SG	2:A:401:ACO:O	2.24	0.95
2:A:401:ACO:H132	3:A:402:COA:O9P	0.77	0.95
1:B:20:TRP:HE1	5:B:407:DIO:H21	1.33	0.93
2:A:401:ACO:H51A	3:A:402:COA:P1A	2.09	0.92
2:A:401:ACO:H132	3:A:402:COA:C9P	1.98	0.90
1:B:151:GLN:OE1	3:B:401[A]:COA:H31	1.71	0.90
1:B:242:ALA:HB1	3:B:401[B]:COA:C8A	2.03	0.88
3:B:401[B]:COA:H51A	7:B:633:HOH:O	1.73	0.88
1:B:242:ALA:CB	3:B:401[B]:COA:C8A	2.52	0.87
1:B:128:LEU:HD11	3:B:401[B]:COA:H32	1.55	0.87
1:B:65:GLU:OE1	1:B:125:ARG:HD2	1.78	0.84
1:B:260:GLU:OE2	1:B:264:ARG:NH2	2.10	0.83
1:B:221:ARG:HH12	3:B:401[A]:COA:H2B	1.43	0.81
1:B:20:TRP:H	1:B:218:GLN:HE22	1.27	0.80
1:A:188:ARG:O	1:A:191[A]:ARG:NH2	2.14	0.80
1:B:20:TRP:NE1	5:B:407:DIO:H21	1.98	0.79
1:B:240:HIS:HE1	1:B:320:SER:H	1.30	0.78
1:A:151:GLN:OE1	2:A:401:ACO:HH32	1.82	0.77
1:A:35[A]:LYS:HE2	7:A:536:HOH:O	1.85	0.77
1:A:40[B]:LYS:NZ	7:A:605:HOH:O	2.16	0.77
1:B:248:ILE:CD1	3:B:401[B]:COA:H10	2.15	0.76
1:B:242:ALA:CB	3:B:401[B]:COA:H8A	2.14	0.75
1:B:93[B]:CYS:SG	1:B:376:MET:HE2	2.26	0.75
1:B:248:ILE:HD11	3:B:401[B]:COA:H10	1.66	0.75
1:B:182:ARG:HH11	6:B:412:GOL:H2	1.52	0.74
1:A:100:ASN:ND2	1:A:257:TRP:HE1	1.85	0.74
1:A:20:TRP:HE1	6:A:407:GOL:H2	1.52	0.74
1:A:100:ASN:HD22	1:A:257:TRP:HE1	1.34	0.73
1:B:66:GLN:NE2	1:B:122:ALA:H	1.87	0.72
1:A:240:HIS:HE1	1:A:320:SER:H	1.38	0.71
2:A:401:ACO:O8A	2:A:401:ACO:C4B	2.37	0.71
1:B:200:VAL:HG21	1:B:210:GLU:HG3	1.73	0.71
1:B:182:ARG:NH1	6:B:412:GOL:H2	2.06	0.70
1:B:242:ALA:HB3	3:B:401[B]:COA:C8A	2.20	0.70
1:A:81:PRO:CB	6:A:408:GOL:H31	2.16	0.69
1:B:81:PRO:HB3	6:B:408:GOL:H2	1.75	0.68
1:B:82[B]:GLU:OE2	7:B:501:HOH:O	2.12	0.67
1:B:66:GLN:HE22	1:B:122:ALA:H	1.40	0.67
1:B:60:VAL:HG21	1:B:349:VAL:CG1	2.25	0.67
1:A:66:GLN:NE2	1:A:122:ALA:H	1.93	0.67
2:A:401:ACO:H4B	3:A:402:COA:O8A	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:ACO:C4B	3:A:402:COA:O8A	2.44	0.66
1:B:317:ALA:HB1	3:B:401[A]:COA:H32	1.78	0.65
2:A:401:ACO:C3B	3:A:402:COA:O5B	2.15	0.64
1:B:156:GLU:OE2	1:B:240:HIS:HD2	1.81	0.64
1:A:89:VAL:HG12	1:B:89:VAL:HG12	1.79	0.64
2:A:401:ACO:O5B	3:A:402:COA:O4B	2.14	0.64
1:A:66:GLN:HE22	1:A:122:ALA:H	1.45	0.62
1:B:93[B]:CYS:HB3	1:B:378:ALA:HA	1.80	0.62
1:A:150:ASN:OD1	1:A:153:GLU:HG3	1.99	0.62
2:A:401:ACO:O9A	3:A:402:COA:O7A	2.19	0.61
1:A:156:GLU:OE2	1:A:240:HIS:HD2	1.84	0.61
1:A:98:GLN:HE22	1:B:54:GLN:HE22	1.49	0.61
1:A:82[A]:GLU:HG3	6:A:408:GOL:O2	2.01	0.60
1:B:60:VAL:HG21	1:B:349:VAL:HG12	1.83	0.60
1:B:212:ARG:HD2	7:B:631:HOH:O	2.01	0.59
1:B:135:ASP:OD2	1:B:138:LEU:HG	2.03	0.59
1:B:48:HIS:HB3	5:B:403:DIO:H2'1	1.85	0.58
3:B:401[A]:COA:O2B	3:B:401[A]:COA:P3B	2.61	0.57
2:A:401:ACO:C1B	3:A:402:COA:P3B	2.93	0.56
1:B:93[B]:CYS:SG	1:B:376:MET:CE	2.93	0.56
1:A:151:GLN:NE2	2:A:401:ACO:S1P	2.73	0.56
1:B:260:GLU:CD	1:B:264:ARG:HH21	2.09	0.56
1:A:150:ASN:CG	1:A:153:GLU:HG3	2.27	0.55
1:B:323:LEU:O	1:B:327:ARG:HG3	2.05	0.55
1:B:47:LEU:HG	1:B:48:HIS:N	2.22	0.55
1:B:358:THR:O	1:B:362:HIS:HD2	1.90	0.54
1:B:248:ILE:HD11	3:B:401[B]:COA:H72	1.90	0.54
1:B:347:HIS:CD2	3:B:401[A]:COA:H21	2.44	0.53
1:B:333:MET:HE3	7:B:622:HOH:O	2.08	0.52
3:A:402:COA:O5A	3:A:402:COA:O1A	2.26	0.52
1:A:290:GLY:N	1:A:291:PRO:CD	2.73	0.52
1:A:208:THR:OG1	1:A:210:GLU:CG	2.42	0.52
6:A:407:GOL:H31	7:A:624:HOH:O	2.09	0.52
1:B:335:ARG:HH12	1:B:369:GLN:HE22	1.57	0.52
2:A:401:ACO:C5B	2:A:401:ACO:O4A	2.58	0.52
5:B:403:DIO:H1'1	7:B:645:HOH:O	2.09	0.52
1:A:175:GLU:OE2	1:A:178:ARG:NH2	2.40	0.51
1:A:93[B]:CYS:SG	1:A:347:HIS:NE2	2.82	0.51
5:B:403:DIO:C1'	7:B:645:HOH:O	2.59	0.51
1:A:281:GLY:HA2	1:A:382:LEU:HD23	1.92	0.51
1:A:151:GLN:CD	2:A:401:ACO:HH32	2.31	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:HIS:CE1	1:B:320:SER:H	2.20	0.50
1:A:197[A]:GLN:HA	1:A:197[A]:GLN:HE21	1.77	0.50
1:B:40:LYS:HE2	7:B:611:HOH:O	2.13	0.49
1:A:200:VAL:CG2	1:A:212:ARG:HG2	2.43	0.49
2:A:401:ACO:N3A	3:A:402:COA:C2B	2.73	0.49
3:B:401[A]:COA:HO2A	3:B:401[A]:COA:P3B	2.29	0.48
1:B:197:GLN:CD	1:B:213:LEU:HD13	2.34	0.48
1:B:20:TRP:H	1:B:218:GLN:NE2	2.03	0.48
3:B:401[B]:COA:O6A	3:B:401[B]:COA:OAP	2.23	0.48
3:B:401[A]:COA:H141	3:B:401[A]:COA:O9P	2.14	0.48
2:A:401:ACO:CEP	2:A:401:ACO:HN8	2.26	0.47
3:A:402:COA:O9P	3:A:402:COA:H121	2.03	0.47
1:A:304:MET:O	1:A:305:LYS:HD3	2.13	0.47
1:B:60:VAL:HG21	1:B:349:VAL:HG11	1.95	0.47
1:A:191[A]:ARG:HH11	1:A:191[A]:ARG:HG3	1.79	0.47
2:A:401:ACO:O9P	2:A:401:ACO:C6P	2.63	0.47
1:A:258[B]:MET:HE1	1:A:266:HIS:CD2	2.50	0.47
2:A:401:ACO:N3A	3:A:402:COA:O2B	2.47	0.46
1:B:20:TRP:N	1:B:218:GLN:HE22	2.06	0.46
3:B:401[B]:COA:H72	3:B:401[B]:COA:CEP	2.46	0.45
3:B:401[B]:COA:H72	3:B:401[B]:COA:H10	1.69	0.45
1:A:5:VAL:HG21	1:A:270:PRO:HB3	1.98	0.45
1:A:38:VAL:HG11	1:A:49:ALA:HB2	1.98	0.45
1:B:50:GLY:H	5:B:403:DIO:C2'	2.30	0.45
1:A:240:HIS:CE1	1:A:320:SER:H	2.26	0.45
1:A:8:GLU:OE2	1:A:44:GLN:NE2	2.50	0.45
1:B:16:LYS:H	1:B:218:GLN:NE2	2.14	0.45
1:B:342:ALA:HB1	1:B:347:HIS:HB2	1.99	0.45
1:B:20:TRP:HE1	5:B:407:DIO:C2	2.15	0.45
2:A:401:ACO:H10	3:A:402:COA:N8P	2.33	0.44
1:B:136:ARG:O	1:B:139:ILE:HG12	2.17	0.44
1:B:57:GLY:HA2	1:B:118:CYS:O	2.18	0.44
3:B:401[B]:COA:C5B	7:B:633:HOH:O	2.46	0.44
2:A:401:ACO:H141	2:A:401:ACO:N8P	2.32	0.43
1:A:325:TRP:CZ3	1:A:331:PRO:HG3	2.54	0.43
1:B:204:GLN:O	1:B:205:ASN:HB2	2.19	0.43
1:B:17:ARG:NE	3:B:401[B]:COA:O4A	2.51	0.43
1:B:81:PRO:HG3	5:B:403:DIO:H1'1	2.00	0.43
1:B:290:GLY:N	1:B:291:PRO:CD	2.82	0.43
1:A:271:ARG:NH1	7:A:605:HOH:O	2.09	0.42
1:A:333:MET:HG3	6:A:410:GOL:H31	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:ACO:CEP	2:A:401:ACO:N8P	2.82	0.42
1:B:190:ASP:HB3	5:B:406:DIO:H12	2.01	0.42
1:B:232:LYS:HA	1:B:233:PRO:HD3	1.95	0.42
1:B:281:GLY:HA2	1:B:382:LEU:HD23	2.01	0.42
1:B:202:ASP:OD1	1:B:202:ASP:C	2.59	0.41
1:A:151:GLN:HE22	2:A:401:ACO:C2P	2.33	0.41
1:A:82[A]:GLU:OE1	1:B:284:PRO:CD	2.68	0.41
1:B:93[B]:CYS:SG	1:B:93[B]:CYS:O	2.77	0.41
1:A:198:ALA:HA	1:A:199:PRO:HD3	1.87	0.41
3:B:401[B]:COA:O9P	3:B:401[B]:COA:H131	2.18	0.41
1:A:188:ARG:HA	1:A:191[A]:ARG:HH22	1.84	0.41
1:A:45:SER:HB2	1:A:266:HIS:O	2.20	0.41
1:A:18:ASN:O	5:A:405:DIO:H1'1	2.20	0.41
1:A:135:ASP:C	1:A:135:ASP:OD1	2.59	0.41
2:A:401:ACO:H10	3:A:402:COA:C9P	2.51	0.41
1:A:231:LEU:HD11	2:A:401:ACO:C5A	2.51	0.41
1:B:333:MET:HG3	6:B:411:GOL:O2	2.20	0.41
1:A:101:HIS:HB3	1:A:277:GLN:OE1	2.21	0.41
2:A:401:ACO:H141	2:A:401:ACO:HN8	1.85	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)
7:A:514:HOH:O	7:B:526:HOH:O[8_554]	1.55	0.65

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	398/400 (100%)	390 (98%)	8 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	393/400 (98%)	384 (98%)	9 (2%)	0	100	100
All	All	791/800 (99%)	774 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	304/303 (100%)	295 (97%)	9 (3%)	48	36
1	B	300/303 (99%)	292 (97%)	8 (3%)	52	41
All	All	604/606 (100%)	587 (97%)	17 (3%)	57	39

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	82[A]	GLU
1	A	82[B]	GLU
1	A	93[B]	CYS
1	A	197[A]	GLN
1	A	197[B]	GLN
1	A	212	ARG
1	A	351	CYS
1	A	390	ARG
1	B	3[A]	TYR
1	B	3[B]	TYR
1	B	40	LYS
1	B	210	GLU
1	B	232	LYS
1	B	260	GLU
1	B	269	THR
1	B	391	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	100	ASN
1	A	206	GLN
1	A	240	HIS
1	A	266	HIS
1	A	369	GLN
1	B	54	GLN
1	B	62	GLN
1	B	66	GLN
1	B	68	ASN
1	B	218	GLN
1	B	240	HIS
1	B	362	HIS
1	B	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	93[A]	1	7,8,9	2.00	1 (14%)	4,9,11	1.76	2 (50%)
1	SCY	B	93[A]	1	7,8,9	0.70	0	4,9,11	1.92	2 (50%)

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	93[A]	1	-	0/5/7/9	0/0/0/0
1	SCY	B	93[A]	1	-	0/5/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93[A]	SCY	CD-SG	-4.81	1.42	1.74

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93[A]	SCY	O-C-CA	-2.63	118.64	125.49
1	A	93[A]	SCY	OCD-CD-SG	-2.42	109.69	122.43
1	B	93[A]	SCY	OCD-CD-SG	-2.33	110.19	122.43
1	A	93[A]	SCY	O-C-CA	-2.16	119.86	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

26 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	ACO	A	401	-	43,53,53	0.80	1 (2%)	55,79,79	1.52	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COA	A	402	-	40,50,50	0.79	1 (2%)	50,75,75	1.63	5 (10%)
4	SO4	A	403	-	4,4,4	0.40	0	6,6,6	0.15	0
4	SO4	A	404	-	4,4,4	0.45	0	6,6,6	0.15	0
5	DIO	A	405	-	6,6,6	0.47	0	6,6,6	0.48	0
5	DIO	A	406	-	6,6,6	0.48	0	6,6,6	0.52	0
6	GOL	A	407	-	5,5,5	0.24	0	5,5,5	0.17	0
6	GOL	A	408	-	5,5,5	0.32	0	5,5,5	0.40	0
6	GOL	A	409	-	5,5,5	0.26	0	5,5,5	0.22	0
6	GOL	A	410	-	5,5,5	0.35	0	5,5,5	0.46	0
3	COA	B	401[A]	-	40,50,50	0.79	1 (2%)	50,75,75	1.75	7 (14%)
3	COA	B	401[B]	-	40,50,50	0.84	2 (5%)	50,75,75	1.62	4 (8%)
4	SO4	B	402	-	4,4,4	0.38	0	6,6,6	0.08	0
5	DIO	B	403	-	6,6,6	0.42	0	6,6,6	0.44	0
5	DIO	B	404	-	6,6,6	0.56	0	6,6,6	0.65	0
5	DIO	B	405	-	6,6,6	0.49	0	6,6,6	0.49	0
5	DIO	B	406	-	6,6,6	0.48	0	6,6,6	1.11	0
5	DIO	B	407	-	6,6,6	0.51	0	6,6,6	0.45	0
6	GOL	B	408	-	5,5,5	0.38	0	5,5,5	0.66	0
6	GOL	B	409	-	5,5,5	0.26	0	5,5,5	0.19	0
6	GOL	B	410	-	5,5,5	0.27	0	5,5,5	0.36	0
6	GOL	B	411	-	5,5,5	0.27	0	5,5,5	0.18	0
6	GOL	B	412	-	5,5,5	0.25	0	5,5,5	0.21	0
6	GOL	B	413	-	5,5,5	0.31	0	5,5,5	0.25	0
6	GOL	B	414	-	5,5,5	0.27	0	5,5,5	0.19	0
6	GOL	B	415	-	5,5,5	0.33	0	5,5,5	0.33	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
2	ACO	A	401	-	-	0/47/67/67	0/3/3/3
3	COA	A	402	-	-	0/44/64/64	0/3/3/3
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
4	SO4	A	404	-	-	0/0/0/0	0/0/0/0
5	DIO	A	405	-	-	0/0/6/6	0/1/1/1
5	DIO	A	406	-	-	0/0/6/6	0/1/1/1
6	GOL	A	407	-	-	0/4/4/4	0/0/0/0
6	GOL	A	408	-	-	0/4/4/4	0/0/0/0
6	GOL	A	409	-	-	0/4/4/4	0/0/0/0
6	GOL	A	410	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	401[A]	-	-	0/44/64/64	0/3/3/3
3	COA	B	401[B]	-	-	1/44/64/64	0/3/3/3
4	SO4	B	402	-	-	0/0/0/0	0/0/0/0
5	DIO	B	403	-	-	0/0/6/6	0/1/1/1
5	DIO	B	404	-	-	0/0/6/6	0/1/1/1
5	DIO	B	405	-	-	0/0/6/6	0/1/1/1
5	DIO	B	406	-	-	0/0/6/6	0/1/1/1
5	DIO	B	407	-	-	0/0/6/6	0/1/1/1
6	GOL	B	408	-	-	0/4/4/4	0/0/0/0
6	GOL	B	409	-	-	0/4/4/4	0/0/0/0
6	GOL	B	410	-	-	0/4/4/4	0/0/0/0
6	GOL	B	411	-	-	0/4/4/4	0/0/0/0
6	GOL	B	412	-	-	0/4/4/4	0/0/0/0
6	GOL	B	413	-	-	0/4/4/4	0/0/0/0
6	GOL	B	414	-	-	0/4/4/4	0/0/0/0
6	GOL	B	415	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401[B]	COA	O4B-C1B	2.27	1.44	1.41
3	B	401[A]	COA	C5A-C4A	3.01	1.47	1.40
3	A	402	COA	C5A-C4A	3.11	1.47	1.40
2	A	401	ACO	C5A-C4A	3.20	1.47	1.40
3	B	401[B]	COA	C5A-C4A	3.21	1.47	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401[A]	COA	N3A-C2A-N1A	-7.58	123.09	128.89
2	A	401	ACO	N3A-C2A-N1A	-7.25	123.34	128.89
3	A	402	COA	N3A-C2A-N1A	-7.10	123.46	128.89
3	B	401[B]	COA	N3A-C2A-N1A	-6.47	123.94	128.89
3	B	401[A]	COA	P2A-O3A-P1A	-4.84	119.14	132.73
3	B	401[B]	COA	C2B-C1B-N9A	-4.71	107.10	114.29
3	B	401[B]	COA	P2A-O3A-P1A	-4.59	119.85	132.73
3	A	402	COA	P2A-O3A-P1A	-4.51	120.06	132.73
2	A	401	ACO	P2A-O3A-P1A	-4.15	121.08	132.73
3	A	402	COA	C4A-C5A-N7A	-3.74	106.04	109.48
3	B	401[A]	COA	C4A-C5A-N7A	-3.38	106.37	109.48
3	B	401[B]	COA	C4A-C5A-N7A	-3.34	106.41	109.48
2	A	401	ACO	C4A-C5A-N7A	-2.98	106.74	109.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	C2B-C1B-N9A	-2.76	110.08	114.29
3	B	401[A]	COA	C2B-C1B-N9A	-2.29	110.79	114.29
2	A	401	ACO	C7P-C6P-C5P	-2.08	108.88	112.31
3	B	401[A]	COA	O6A-CCP-CBP	-2.04	107.27	110.55
3	B	401[A]	COA	C6P-C5P-N4P	2.41	120.65	116.46
3	B	401[A]	COA	C3B-C2B-C1B	2.48	105.93	99.98
3	A	402	COA	C3B-C2B-C1B	2.67	106.40	99.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401[B]	COA	CAP-C9P-N8P-C7P

There are no ring outliers.

14 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ACO	30	0
3	A	402	COA	18	0
5	A	405	DIO	1	0
6	A	407	GOL	2	0
6	A	408	GOL	3	0
6	A	410	GOL	1	0
3	B	401[A]	COA	8	0
3	B	401[B]	COA	16	0
5	B	403	DIO	5	0
5	B	406	DIO	1	0
5	B	407	DIO	3	0
6	B	408	GOL	1	0
6	B	411	GOL	1	0
6	B	412	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	93[A]:SCY	C	94:GLY	N	1.10

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	390/400 (97%)	0.30	20 (5%) 32 43	14, 26, 47, 87	0
1	B	391/400 (97%)	0.28	22 (5%) 28 39	14, 24, 46, 81	0
All	All	781/800 (97%)	0.29	42 (5%) 29 41	14, 25, 47, 87	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	PRO	6.0
1	B	0	SER	4.6
1	B	135	ASP	4.5
1	B	138	LEU	4.5
1	A	134	PRO	4.2
1	A	303	GLY	4.2
1	A	3	TYR	4.1
1	B	145	ASP	3.7
1	A	205	ASN	3.7
1	A	368	ASP	3.6
1	A	136	ARG	3.6
1	B	43	ILE	3.6
1	A	135	ASP	3.4
1	B	136	ARG	3.4
1	B	142	GLN	3.4
1	A	391	ILE	3.4
1	A	142	GLN	3.4
1	A	138	LEU	3.4
1	B	143	SER	3.3
1	B	140	ARG	3.3
1	B	141	ALA	3.2
1	A	145	ASP	3.1
1	A	1	MET	3.1
1	B	3[A]	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	139	ILE	2.9
1	B	391	ILE	2.9
1	A	137	SER	2.8
1	A	202	ASP	2.8
1	B	1[A]	MET	2.7
1	A	139	ILE	2.7
1	B	232	LYS	2.7
1	B	368	ASP	2.6
1	A	206	GLN	2.5
1	B	144	TRP	2.3
1	A	232	LYS	2.3
1	B	230	GLU	2.3
1	B	99	ALA	2.3
1	A	201	LEU	2.2
1	A	342	ALA	2.2
1	B	211	ARG	2.1
1	B	137	SER	2.1
1	A	46	GLY	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	93[A]	9/10	0.95	0.17	-	15,22,30,45	9
1	SCY	B	93[A]	9/10	0.95	0.18	-	14,19,39,50	9

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	COA	A	402	48/48	0.57	0.55	13.93	20,53,68,77	48
6	GOL	B	415	6/6	0.65	0.35	13.41	67,70,87,87	0
2	ACO	A	401	51/51	0.40	0.52	12.59	25,50,83,92	51
3	COA	B	401[B]	48/48	0.61	0.44	11.64	16,42,67,79	48
6	GOL	A	409	6/6	0.76	0.43	11.35	61,65,78,78	0
5	DIO	B	403	6/6	0.76	0.31	11.29	30,60,74,76	0
6	GOL	B	410	6/6	0.65	0.36	8.87	47,60,63,72	0
3	COA	B	401[A]	48/48	0.61	0.44	8.50	17,33,60,70	48
6	GOL	B	413	6/6	0.77	0.37	6.65	41,69,74,82	0
6	GOL	B	408	6/6	0.80	0.31	6.09	33,46,54,68	0
6	GOL	A	408	6/6	0.83	0.48	5.76	26,47,61,72	0
5	DIO	A	406	6/6	0.90	0.18	4.67	33,37,43,47	0
4	SO4	A	403	5/5	0.86	0.25	4.30	53,64,82,91	0
4	SO4	A	404	5/5	0.78	0.40	3.95	49,83,99,110	0
5	DIO	B	406	6/6	0.89	0.15	1.89	32,37,40,42	0
5	DIO	B	404	6/6	0.96	0.09	-1.00	27,31,33,42	0
6	GOL	B	411	6/6	0.84	0.21	-	36,60,68,77	0
6	GOL	B	412	6/6	0.69	0.24	-	55,76,80,84	0
6	GOL	B	409	6/6	0.62	0.20	-	61,66,80,82	0
6	GOL	B	414	6/6	0.40	0.49	-	89,103,105,105	0
5	DIO	B	407	6/6	0.74	0.17	-	51,56,58,73	0
5	DIO	A	405	6/6	0.76	0.32	-	68,76,95,95	0
6	GOL	A	410	6/6	0.76	0.29	-	34,62,71,79	0
4	SO4	B	402	5/5	0.61	0.67	-	99,108,124,129	0
5	DIO	B	405	6/6	0.63	0.60	-	57,62,85,92	0
6	GOL	A	407	6/6	0.79	0.14	-	65,77,79,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.