



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:53 AM UTC

PDB ID : 1NL7 / pdb_00001nl7
Title : Z. ramigera biosynthetic thiolase, acetylated enzyme complexed with CoA at pH 9.5
Authors : Kursula, P.; Wierenga, R.K.
Deposited on : 2003-01-06
Resolution : 1.90 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

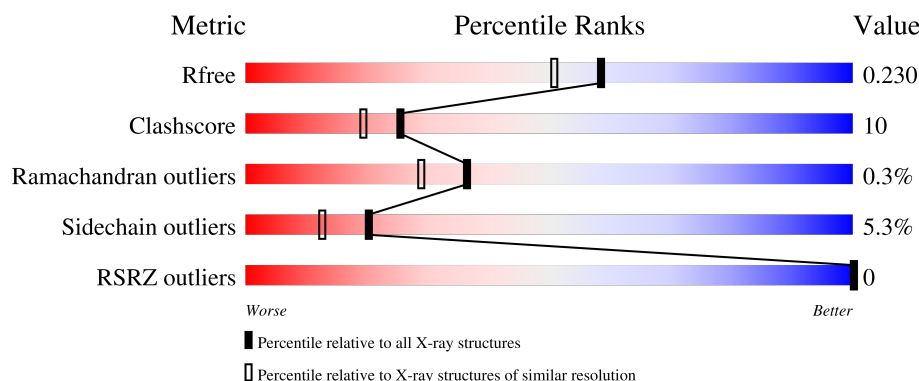
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	 86% 12% ..
1	B	392	 83% 15% ..
1	C	392	 86% 11% ..
1	D	392	 77% 21% ..

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	-	-	X	-
1	SCY	B	89	-	-	X	-
1	SCY	C	89	-	-	X	-
1	SCY	D	89	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12691 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.

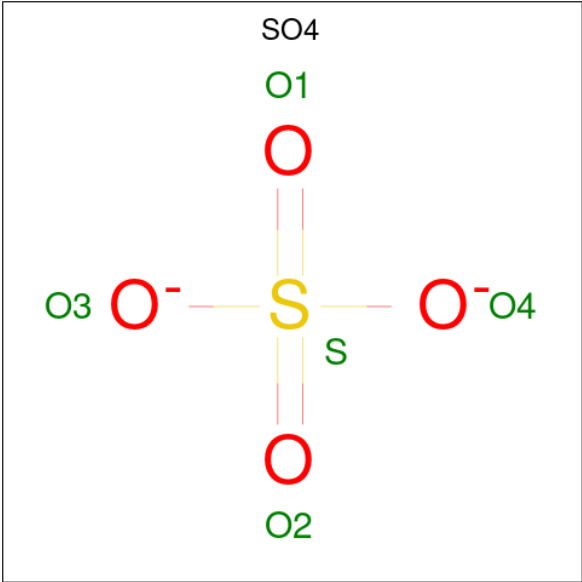
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			
1	B	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			
1	C	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			
1	D	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			

There are 12 discrepancies between the modelled and reference sequences:

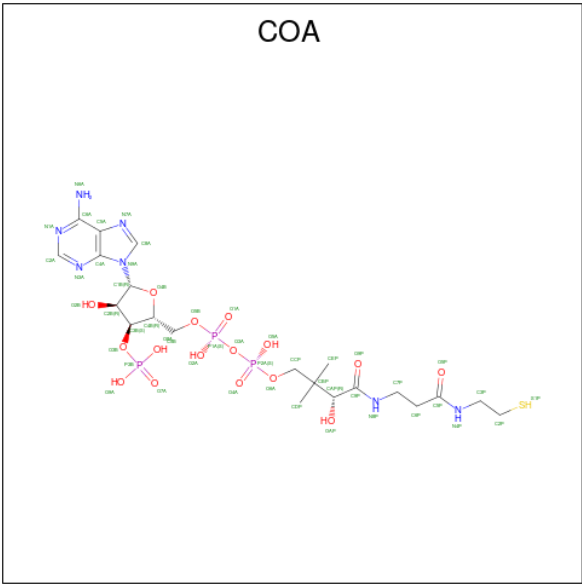
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	insertion	UNP P07097
A	89	SCY	CYS	modified residue	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	10	ALA	-	insertion	UNP P07097
B	89	SCY	CYS	modified residue	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	10	ALA	-	insertion	UNP P07097
C	89	SCY	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 COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 4 is water.

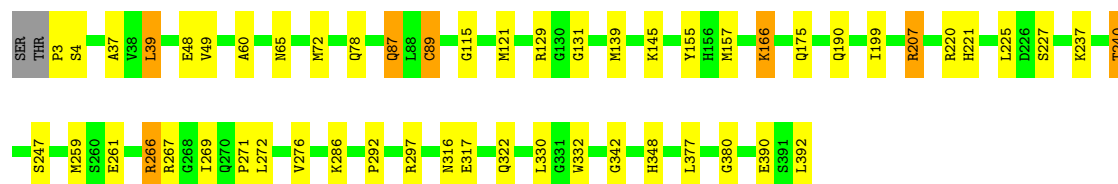
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	443	Total 443	O 443	0	0
4	B	446	Total 446	O 446	0	0
4	C	190	Total 190	O 190	0	0
4	D	196	Total 196	O 196	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

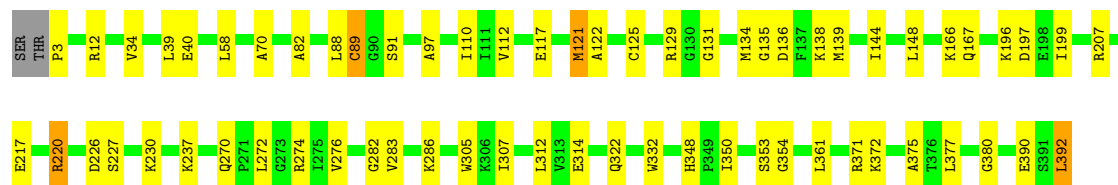
- Molecule 1: Acetyl-CoA acetyltransferase

Chain A: 



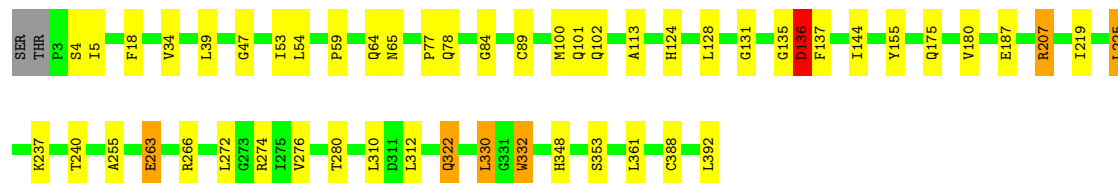
- Molecule 1: Acetyl-CoA acetyltransferase

Chain B: 



- Molecule 1: Acetyl-CoA acetyltransferase

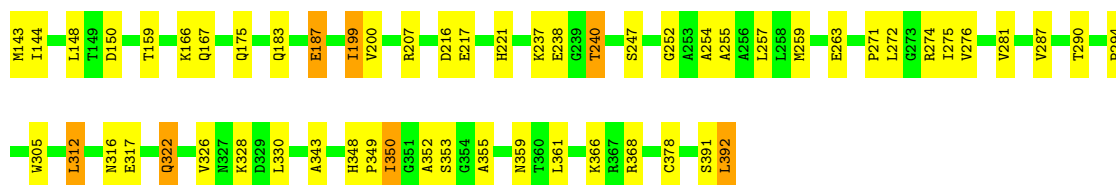
Chain C: 



- Molecule 1: Acetyl-CoA acetyltransferase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 79.06Å 148.88Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-1.90) 85.1 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.223 0.191 , 0.230	Depositor DCC
R_{free} test set	6714 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.124 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12691	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: SCY, SO4, COA

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	1.35	8/2861 (0.3%)	1.13	5/3861 (0.1%)
1	B	1.33	9/2861 (0.3%)	1.10	4/3861 (0.1%)
1	C	0.91	1/2861 (0.0%)	0.99	0/3861
1	D	0.83	0/2861	0.99	0/3861
All	All	1.13	18/11444 (0.2%)	1.05	9/15444 (0.1%)

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	C	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	ASP	N-CA	7.64	1.56	1.46
1	B	117	GLU	CA-C	-6.88	1.44	1.52
1	B	82	ALA	CA-CB	-6.85	1.42	1.53
1	A	37	ALA	CA-CB	6.45	1.63	1.53
1	B	58	LEU	C-O	-6.40	1.16	1.24
1	A	72	MET	SD-CE	-6.28	1.63	1.79
1	B	70	ALA	CA-CB	-6.25	1.43	1.53
1	B	112	VAL	CA-CB	6.14	1.61	1.54
1	A	121	MET	SD-CE	-6.03	1.64	1.79
1	A	115	GLY	CA-C	-5.74	1.45	1.51
1	B	283	VAL	CA-C	5.58	1.57	1.52
1	A	259	MET	SD-CE	5.37	1.93	1.79
1	B	307	ILE	CA-CB	5.24	1.60	1.54
1	B	122	ALA	CA-C	5.17	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	ARG	C-O	-5.12	1.18	1.24
1	B	97	ALA	CA-CB	5.10	1.61	1.53
1	A	292	PRO	C-O	-5.04	1.17	1.24
1	A	60	ALA	CA-CB	-5.01	1.45	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	B	353	SER	N-CA-C	6.04	118.64	111.33
1	A	199	ILE	N-CA-C	5.98	116.77	109.30
1	A	266	ARG	CG-CD-NE	-5.72	99.42	112.00
1	B	91	SER	N-CA-C	5.69	117.15	111.07
1	A	129	ARG	N-CA-C	5.60	117.38	111.28
1	B	129	ARG	N-CA-C	5.37	117.21	111.36
1	B	125	CYS	N-CA-C	5.12	116.77	109.14
1	A	87	GLN	N-CA-C	-5.12	104.33	110.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	135	GLY	Peptide,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	2825	0	2830	50	0
1	B	2825	0	2830	53	0
1	C	2825	0	2830	41	0
1	D	2825	0	2830	76	0
2	A	10	0	0	1	0
2	B	10	0	0	1	0
3	A	48	0	32	5	0
3	B	48	0	32	5	0
4	A	443	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	446	0	0	34	0
4	C	190	0	0	17	0
4	D	196	0	0	45	0
All	All	12691	0	11384	218	0

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 10.

All (218) 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:D:89:SCY:CD	4:D:393:HOH:O	1.64	1.32
1:C:89:SCY:CD	4:C:393:HOH:O	1.89	1.20
1:B:121:MET:SD	4:B:487:HOH:O	1.98	1.18
1:B:314:GLU:HB2	4:B:551:HOH:O	1.46	1.14
1:A:89:SCY:HE1	1:A:380:GLY:H	1.03	1.13
1:B:89:SCY:HE1	1:B:380:GLY:H	0.96	1.10
1:B:348:HIS:HE1	4:B:458:HOH:O	1.29	1.10
1:B:3:PRO:N	4:B:9942:HOH:O	1.84	1.09
1:B:89:SCY:HE2	1:B:89:SCY:H	1.14	1.07
1:D:18:PHE:HA	4:D:463:HOH:O	1.57	1.04
1:B:392:LEU:HB2	4:B:9839:HOH:O	1.60	1.00
1:A:87:GLN:NE2	4:A:558:HOH:O	1.77	0.99
1:D:125:CYS:SG	4:D:412:HOH:O	2.21	0.97
1:B:89:SCY:HE1	1:B:380:GLY:N	1.80	0.95
1:A:89:SCY:HE2	1:A:89:SCY:H	1.28	0.95
1:D:101:GLN:HA	4:D:566:HOH:O	1.67	0.94
1:D:326:VAL:HG22	4:D:576:HOH:O	1.69	0.93
1:B:392:LEU:HD12	4:B:9839:HOH:O	1.72	0.89
1:A:227:SER:OG	4:A:9911:HOH:O	1.84	0.87
1:A:89:SCY:HE1	1:A:380:GLY:N	1.88	0.87
1:C:136:ASP:OD1	4:C:559:HOH:O	1.94	0.86
1:D:89:SCY:HE2	4:D:393:HOH:O	1.66	0.85
1:D:89:SCY:SG	4:D:393:HOH:O	2.22	0.82
1:D:378:CYS:SG	4:D:588:HOH:O	2.38	0.82
1:A:348:HIS:HE1	4:A:515:HOH:O	1.62	0.80
3:A:1393:COA:N6A	4:A:9858:HOH:O	2.14	0.80
1:A:3:PRO:N	4:A:9915:HOH:O	2.15	0.79
1:D:104:ALA:HB3	4:D:566:HOH:O	1.83	0.78
1:D:117:GLU:HB3	4:D:534:HOH:O	1.84	0.78
1:D:221:HIS:CE1	4:D:531:HOH:O	2.37	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1393:COA:O5A	4:A:409:HOH:O	2.03	0.76
1:D:359:ASN:ND2	4:D:409:HOH:O	2.19	0.74
1:D:305:TRP:C	4:D:536:HOH:O	2.29	0.73
1:B:390:GLU:OE1	4:B:539:HOH:O	2.06	0.73
1:D:252:GLY:HA3	4:D:571:HOH:O	1.89	0.72
1:A:89:SCY:HB2	4:A:515:HOH:O	1.89	0.72
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.02	0.72
1:B:89:SCY:HE2	1:B:89:SCY:N	1.98	0.72
1:B:371:ARG:CZ	4:B:477:HOH:O	2.38	0.71
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.08	0.71
1:A:247[A]:SER:OG	4:A:513:HOH:O	2.09	0.71
1:B:89:SCY:CE	1:B:380:GLY:H	1.90	0.70
1:D:144:ILE:HA	4:D:509:HOH:O	1.91	0.70
1:C:89:SCY:SG	4:C:393:HOH:O	2.42	0.70
1:D:305:TRP:O	4:D:536:HOH:O	2.09	0.70
1:D:166:LYS:NZ	4:D:416:HOH:O	2.24	0.69
1:B:196:LYS:HB2	4:B:542:HOH:O	1.91	0.69
1:A:390:GLU:OE2	4:A:9910:HOH:O	2.10	0.69
1:D:148:LEU:HD12	4:D:509:HOH:O	1.94	0.68
1:B:89:SCY:HB2	4:B:458:HOH:O	1.95	0.67
1:A:220:ARG:NH1	4:A:481:HOH:O	2.28	0.66
1:C:237:LYS:HB3	4:C:541:HOH:O	1.95	0.66
1:D:352:ALA:HB1	4:D:541:HOH:O	1.94	0.66
1:D:316:ASN:HA	4:D:554:HOH:O	1.96	0.66
1:A:286:LYS:HE3	4:A:9871:HOH:O	1.96	0.65
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.62	0.65
1:A:286:LYS:CE	4:A:9871:HOH:O	2.45	0.64
1:D:140:ILE:HB	4:D:412:HOH:O	1.98	0.64
1:A:89:SCY:CE	1:A:380:GLY:H	1.95	0.63
1:B:197:ASP:OD1	4:B:543:HOH:O	2.15	0.63
1:B:226:ASP:HB3	4:B:9858:HOH:O	1.97	0.62
1:C:276:VAL:HG22	1:C:388:CYS:C	2.23	0.62
1:D:326:VAL:HG12	1:D:330:LEU:HD12	1.81	0.62
1:B:227:SER:OG	4:B:467:HOH:O	2.16	0.62
1:B:375:ALA:HB2	4:B:551:HOH:O	1.98	0.62
1:A:286:LYS:NZ	4:A:9871:HOH:O	2.34	0.61
1:A:89:SCY:HE2	1:A:89:SCY:N	2.10	0.60
1:B:348:HIS:CE1	4:B:458:HOH:O	2.19	0.60
1:C:187:GLU:HB2	4:C:538:HOH:O	2.00	0.60
1:B:121:MET:CG	4:B:487:HOH:O	2.41	0.59
1:C:276:VAL:HG22	1:C:388:CYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247[B]:SER:HB3	4:A:513:HOH:O	2.03	0.59
1:C:101:GLN:HG2	1:D:105:THR:HG21	1.84	0.59
4:A:498:HOH:O	1:D:134:MET:HE2	2.02	0.59
1:C:59:PRO:CG	4:C:512:HOH:O	2.51	0.59
1:C:89:SCY:CE	4:C:393:HOH:O	2.39	0.58
1:C:312:LEU:HD23	1:C:361:LEU:HD12	1.83	0.58
1:D:89:SCY:CE	4:D:393:HOH:O	1.98	0.58
1:B:89:SCY:H	1:B:89:SCY:CE	2.04	0.58
1:B:371:ARG:NH2	4:B:477:HOH:O	2.38	0.57
1:D:366:LYS:HD3	4:D:548:HOH:O	2.04	0.57
1:A:266:ARG:NH2	2:A:9720:SO4:O4	2.36	0.57
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.86	0.56
1:C:207:ARG:N	1:C:207:ARG:HD3	2.21	0.56
1:B:88:LEU:HB3	1:B:89:SCY:HE2	1.87	0.56
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.87	0.56
1:C:180:VAL:HG21	1:C:225:LEU:HA	1.88	0.56
1:D:175:GLN:NE2	1:D:240:THR:OG1	2.38	0.55
1:A:175:GLN:NE2	1:A:240:THR:HG23	2.20	0.55
1:D:159:THR:N	4:D:552:HOH:O	2.39	0.55
1:D:15:VAL:HB	4:D:579:HOH:O	2.07	0.55
1:D:150:ASP:HB2	4:D:517:HOH:O	2.07	0.55
1:A:65:ASN:ND2	4:A:553:HOH:O	2.40	0.54
1:D:183:GLN:CD	4:D:429:HOH:O	2.50	0.54
1:C:59:PRO:CD	4:C:512:HOH:O	2.55	0.54
1:D:136:ASP:OD2	4:D:484:HOH:O	2.19	0.54
1:D:254:ALA:HB3	1:D:355:ALA:HB3	1.89	0.54
1:A:131:GLY:HA2	1:C:131:GLY:HA2	1.89	0.54
3:A:1393:COA:C6A	4:A:481:HOH:O	2.55	0.53
1:A:89:SCY:H	1:A:89:SCY:CE	2.10	0.53
1:A:87:GLN:CG	4:A:558:HOH:O	2.56	0.53
1:B:220:ARG:HD3	4:B:9919:HOH:O	2.07	0.53
1:C:322:GLN:C	1:C:322:GLN:NE2	2.67	0.53
1:C:348:HIS:ND1	1:C:353:SER:OG	2.40	0.53
1:D:89:SCY:CB	4:D:393:HOH:O	2.53	0.53
1:A:190:GLN:OE1	1:A:221:HIS:HE1	1.90	0.53
1:B:286:LYS:NZ	4:B:9943:HOH:O	2.41	0.53
1:B:135:GLY:HA2	1:C:144:ILE:HD12	1.90	0.52
1:D:183:GLN:NE2	4:D:429:HOH:O	2.42	0.52
1:A:390:GLU:OE1	4:A:536:HOH:O	2.19	0.52
1:D:322:GLN:O	1:D:326:VAL:HG23	2.10	0.52
1:D:87:GLN:O	1:D:88:LEU:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:NZ	4:A:9881:HOH:O	2.37	0.52
1:D:136:ASP:OD1	4:D:512:HOH:O	2.18	0.52
1:A:269:ILE:O	1:A:271:PRO:HD3	2.10	0.51
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.41	0.51
1:C:263:GLU:O	1:C:266:ARG:HB2	2.10	0.51
1:C:64:GLN:O	1:C:65:ASN:C	2.53	0.51
1:C:219:ILE:CG2	4:C:538:HOH:O	2.59	0.51
1:A:166:LYS:HD3	4:A:511:HOH:O	2.10	0.51
3:A:1393:COA:O5P	3:A:1393:COA:C2P	2.58	0.51
1:D:124:HIS:HA	1:D:140:ILE:O	2.10	0.51
1:A:316:ASN:HB3	4:A:9900:HOH:O	2.12	0.50
1:B:392:LEU:CD1	4:B:9839:HOH:O	2.45	0.50
1:B:375:ALA:CB	4:B:551:HOH:O	2.56	0.50
2:B:9721:SO4:O1	4:B:419:HOH:O	2.19	0.50
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.94	0.50
1:C:310:LEU:HD22	4:C:565:HOH:O	2.12	0.49
1:D:89:SCY:HB2	4:D:434:HOH:O	2.11	0.49
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.47	0.49
1:B:136:ASP:OD1	4:B:456:HOH:O	2.18	0.49
1:D:257:LEU:C	1:D:257:LEU:HD23	2.36	0.49
1:D:287:VAL:O	1:D:290:THR:OG1	2.27	0.49
1:B:270:GLN:HG2	4:B:457:HOH:O	2.11	0.49
1:C:89:SCY:CB	4:C:393:HOH:O	2.60	0.49
1:D:275:ILE:HG21	4:D:546:HOH:O	2.13	0.49
1:D:274:ARG:NH2	4:D:540:HOH:O	2.46	0.49
1:B:270:GLN:CG	4:B:457:HOH:O	2.61	0.48
1:D:312:LEU:HD23	1:D:361:LEU:HD12	1.95	0.48
1:B:40:GLU:HG3	4:B:536:HOH:O	2.13	0.48
1:D:317:GLU:O	1:D:343:ALA:HB3	2.12	0.48
1:D:41:ARG:NH2	1:D:200:VAL:HB	2.29	0.48
1:C:274:ARG:HD3	4:C:536:HOH:O	2.14	0.47
1:A:139:MET:HE1	1:B:139:MET:HE1	1.97	0.47
1:C:102:GLN:NE2	4:C:439:HOH:O	2.46	0.47
1:A:157:MET:HA	1:A:157:MET:HE2	1.97	0.47
1:D:12:ARG:O	1:D:199:ILE:HA	2.15	0.47
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.76	0.47
1:C:219:ILE:HG22	4:C:538:HOH:O	2.14	0.47
1:D:57:VAL:C	1:D:59:PRO:HD3	2.39	0.47
1:A:166:LYS:CD	4:A:511:HOH:O	2.63	0.47
1:C:47:GLY:HA2	1:C:77:PRO:HG3	1.96	0.47
1:D:15:VAL:HA	4:D:571:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:NZ	4:B:9889:HOH:O	2.48	0.47
1:B:88:LEU:HB3	1:B:89:SCY:CE	2.44	0.46
1:B:274:ARG:NH2	1:B:392:LEU:HD21	2.30	0.46
1:B:305:TRP:CE2	1:B:372:LYS:HD3	2.51	0.46
1:B:375:ALA:HA	4:B:551:HOH:O	2.16	0.46
1:A:4:SER:OG	1:A:261:GLU:OE1	2.30	0.45
1:A:87:GLN:HG2	4:A:558:HOH:O	2.17	0.45
1:C:280:THR:HG23	1:D:81:THR:HG21	1.98	0.45
1:C:330:LEU:HD13	1:C:332:TRP:CH2	2.52	0.45
1:D:255:ALA:N	4:D:409:HOH:O	2.50	0.45
1:D:257:LEU:HD22	1:D:259:MET:HE3	1.98	0.45
1:B:220:ARG:NH2	3:B:5939:COA:N1A	2.65	0.44
1:D:281:VAL:HG11	1:D:294:PRO:HB2	1.99	0.44
1:D:352:ALA:CB	4:D:541:HOH:O	2.60	0.44
1:B:131:GLY:HA2	1:D:131:GLY:HA2	1.99	0.44
1:D:312:LEU:HD13	1:D:368:ARG:HD2	1.99	0.44
1:C:89:SCY:HE2	4:C:393:HOH:O	2.09	0.44
1:D:35:ILE:O	1:D:38:VAL:HG22	2.18	0.44
1:B:312:LEU:HD23	1:B:361:LEU:HD12	2.00	0.44
1:A:317:GLU:CD	1:A:342:GLY:HA3	2.43	0.43
1:A:348:HIS:CE1	4:A:515:HOH:O	2.50	0.43
1:A:190:GLN:OE1	1:A:221:HIS:CE1	2.70	0.43
1:B:226:ASP:CB	4:B:9858:HOH:O	2.63	0.43
1:C:53:ILE:O	1:C:113:ALA:HA	2.19	0.43
1:A:247[B]:SER:OG	1:A:348:HIS:HB2	2.18	0.43
1:A:316:ASN:HD21	1:A:348:HIS:CE1	2.36	0.43
1:B:217:GLU:HG2	4:B:522:HOH:O	2.18	0.43
4:C:502:HOH:O	1:D:59:PRO:HB2	2.19	0.43
1:C:54:LEU:O	1:C:84:GLY:HA2	2.19	0.43
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.32	0.42
1:D:97:ALA:HA	4:D:546:HOH:O	2.19	0.42
1:D:271:PRO:HB2	4:D:562:HOH:O	2.18	0.42
1:A:220:ARG:NH2	4:A:418:HOH:O	2.51	0.42
4:A:553:HOH:O	1:B:88:LEU:HG	2.19	0.42
1:B:230:LYS:NZ	4:B:9858:HOH:O	2.53	0.42
1:A:48:GLU:OE1	1:A:267:ARG:NH2	2.48	0.42
1:B:375:ALA:CA	4:B:551:HOH:O	2.68	0.42
3:B:5939:COA:O5P	3:B:5939:COA:C2P	2.68	0.42
1:D:322:GLN:HB3	4:D:444:HOH:O	2.19	0.42
1:A:89:SCY:OCD	3:A:1393:COA:S1P	2.77	0.42
3:B:5939:COA:H52A	4:B:534:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:CG1	4:D:509:HOH:O	2.67	0.42
3:B:5939:COA:O5P	3:B:5939:COA:H21	2.19	0.42
1:D:21:ALA:HA	4:D:564:HOH:O	2.20	0.42
1:B:354:GLY:HA2	1:B:377:LEU:HD11	2.02	0.42
1:D:54:LEU:O	1:D:84:GLY:HA2	2.19	0.42
1:D:349:PRO:O	1:D:350:ILE:C	2.63	0.42
1:B:12:ARG:O	1:B:199:ILE:HA	2.20	0.41
1:A:78:GLN:O	1:B:282:GLY:HA3	2.20	0.41
1:B:121:MET:HE2	4:B:9951:HOH:O	2.20	0.41
1:A:39:LEU:HD11	1:A:49:VAL:CG2	2.50	0.41
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.55	0.41
1:D:247[B]:SER:OG	1:D:348:HIS:HB2	2.20	0.41
1:C:18:PHE:CZ	1:D:129:ARG:HD3	2.55	0.41
1:D:392:LEU:HD12	4:D:562:HOH:O	2.20	0.41
1:A:377:LEU:HD23	4:A:515:HOH:O	2.21	0.41
1:D:216:ASP:HB3	4:D:579:HOH:O	2.20	0.41
1:B:227:SER:HB2	3:B:5939:COA:H2A	2.01	0.41
1:C:5:ILE:CG1	1:C:100:MET:HG2	2.50	0.41
1:C:124:HIS:O	1:D:125:CYS:HA	2.21	0.41
1:D:141:ASP:OD1	1:D:143:MET:HB3	2.21	0.41
1:D:187:GLU:HG2	4:D:531:HOH:O	2.21	0.40
1:C:310:LEU:HD13	4:C:565:HOH:O	2.21	0.40
1:A:131:GLY:HA2	1:C:131:GLY:CA	2.51	0.40
1:D:240:THR:OG1	1:D:240:THR:O	2.37	0.40

There are no symmetry-related clashes.

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	388/392 (99%)	372 (96%)	15 (4%)	1 (0%)	36 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	388/392 (99%)	378 (97%)	9 (2%)	1 (0%)	36	29
1	C	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	36	29
1	D	388/392 (99%)	369 (95%)	18 (5%)	1 (0%)	36	29
All	All	1552/1568 (99%)	1486 (96%)	62 (4%)	4 (0%)	36	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	350	ILE
1	A	207	ARG
1	C	4	SER
1	B	350	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/278 (100%)	266 (96%)	11 (4%)	28	20
1	B	277/278 (100%)	262 (95%)	15 (5%)	20	12
1	C	277/278 (100%)	265 (96%)	12 (4%)	26	18
1	D	277/278 (100%)	256 (92%)	21 (8%)	12	5
All	All	1108/1112 (100%)	1049 (95%)	59 (5%)	20	12

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	166	LYS
1	A	207	ARG
1	A	225	LEU
1	A	237	LYS
1	A	240	THR

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Mol	Chain	Res	Type
1	A	272	LEU
1	A	276	VAL
1	A	322	GLN
1	A	392	LEU
1	B	34	VAL
1	B	39	LEU
1	B	110	ILE
1	B	121	MET
1	B	134	MET
1	B	166	LYS
1	B	167	GLN
1	B	207	ARG
1	B	220	ARG
1	B	237	LYS
1	B	272	LEU
1	B	276	VAL
1	B	322	GLN
1	B	332	TRP
1	B	392	LEU
1	C	39	LEU
1	C	78	GLN
1	C	136	ASP
1	C	155	TYR
1	C	207	ARG
1	C	225	LEU
1	C	263	GLU
1	C	272	LEU
1	C	322	GLN
1	C	330	LEU
1	C	332	TRP
1	C	392	LEU
1	D	6	VAL
1	D	17	SER
1	D	39	LEU
1	D	134	MET
1	D	167	GLN
1	D	187	GLU
1	D	199	ILE
1	D	207	ARG
1	D	217	GLU
1	D	237	LYS
1	D	238	GLU

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Mol	Chain	Res	Type
1	D	240	THR
1	D	263	GLU
1	D	272	LEU
1	D	276	VAL
1	D	312	LEU
1	D	322	GLN
1	D	328	LYS
1	D	353	SER
1	D	391	SER
1	D	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	175	GLN
1	A	221	HIS
1	A	316	ASN
1	B	78	GLN
1	B	184	ASN
1	B	221	HIS
1	C	78	GLN
1	C	175	GLN
1	C	184	ASN
1	C	221	HIS
1	C	322	GLN
1	D	78	GLN
1	D	175	GLN
1	D	221	HIS
1	D	316	ASN
1	D	322	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	SCY	C	89	1	7,8,9	0.67	0	4,9,11	1.04	0
1	SCY	A	89	1	7,8,9	1.28	1 (14%)	4,9,11	2.26	3 (75%)
1	SCY	B	89	1	7,8,9	1.17	1 (14%)	4,9,11	1.81	1 (25%)
1	SCY	D	89	1	7,8,9	0.86	0	4,9,11	1.05	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	1	-	2/5/7/9	-
1	SCY	A	89	1	-	3/5/7/9	-
1	SCY	B	89	1	-	2/5/7/9	-
1	SCY	D	89	1	-	3/5/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	SCY	CD-SG	-2.72	1.60	1.75
1	B	89	SCY	CD-SG	-2.22	1.63	1.75

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	SCY	OCD-CD-CE	3.34	136.06	123.12
1	B	89	SCY	OCD-CD-SG	-2.99	110.57	122.65
1	A	89	SCY	OCD-CD-SG	-2.10	114.15	122.65
1	A	89	SCY	CB-CA-C	-2.09	105.13	110.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	89	SCY	5	0
1	A	89	SCY	8	0
1	B	89	SCY	9	0
1	D	89	SCY	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	9722	-	4,4,4	0.28	0	6,6,6	0.42	0
2	SO4	B	9721	-	4,4,4	0.36	0	6,6,6	0.59	0
3	COA	B	5939	-	47,50,50	1.77	11 (23%)	69,75,75	1.55	12 (17%)
3	COA	A	1393	-	47,50,50	1.59	9 (19%)	69,75,75	1.58	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	9719	-	4,4,4	0.27	0	6,6,6	0.34	0
2	SO4	A	9720	-	4,4,4	0.24	0	6,6,6	0.44	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	COA	A	1393	-	-	8/48/64/64	0/3/3/3
3	COA	B	5939	-	-	10/48/64/64	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1393	COA	P3B-O8A	4.51	1.71	1.54
3	B	5939	COA	P3B-O8A	4.45	1.71	1.54
3	B	5939	COA	P3B-O9A	4.37	1.71	1.54
3	A	1393	COA	P3B-O9A	4.29	1.70	1.54
3	B	5939	COA	C5A-C4A	4.13	1.46	1.39
3	B	5939	COA	P1A-O3A	3.77	1.63	1.59
3	B	5939	COA	P2A-O5A	3.61	1.72	1.55
3	A	1393	COA	C5A-N7A	-3.49	1.32	1.39
3	B	5939	COA	P1A-O2A	3.39	1.71	1.55
3	A	1393	COA	P1A-O2A	3.34	1.70	1.55
3	B	5939	COA	P2A-O3A	3.25	1.63	1.59
3	A	1393	COA	P2A-O5A	3.21	1.70	1.55
3	B	5939	COA	C5A-C6A	3.19	1.49	1.41
3	A	1393	COA	C5A-C4A	3.13	1.44	1.39
3	A	1393	COA	C4A-N9A	-2.81	1.31	1.37
3	B	5939	COA	C4A-N9A	-2.63	1.32	1.37
3	A	1393	COA	P1A-O3A	2.55	1.62	1.59
3	B	5939	COA	C8A-N7A	2.55	1.36	1.31
3	B	5939	COA	C5A-N7A	-2.46	1.34	1.39
3	A	1393	COA	P2A-O3A	2.29	1.62	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1393	COA	N3A-C4A-N9A	5.80	137.03	127.17
3	A	1393	COA	C5A-C4A-N3A	-5.03	119.79	126.72
3	B	5939	COA	C5A-C4A-N3A	-4.67	120.29	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1393	COA	N3A-C2A-N1A	-4.22	122.19	128.58
3	A	1393	COA	C4A-N9A-C8A	4.11	110.05	105.74
3	B	5939	COA	N3A-C4A-N9A	3.98	133.94	127.17
3	B	5939	COA	C4A-N9A-C1B	-3.95	117.40	126.63
3	B	5939	COA	N3A-C2A-N1A	-3.62	123.10	128.58
3	A	1393	COA	C2A-N3A-C4A	3.56	120.53	111.83
3	B	5939	COA	C2A-N3A-C4A	3.40	120.14	111.83
3	B	5939	COA	C4A-N9A-C8A	3.38	109.29	105.74
3	B	5939	COA	O4B-C1B-N9A	2.82	113.50	108.09
3	B	5939	COA	C2A-N1A-C6A	2.81	123.35	118.73
3	B	5939	COA	C1B-N9A-C8A	2.80	133.31	127.09
3	A	1393	COA	N6A-C6A-N1A	2.67	124.31	118.38
3	B	5939	COA	N9A-C8A-N7A	-2.46	110.45	113.94
3	A	1393	COA	C5A-C4A-N9A	-2.42	103.17	105.81
3	A	1393	COA	C2A-N1A-C6A	2.32	122.54	118.73
3	B	5939	COA	C4A-C5A-N7A	-2.30	107.95	110.58
3	A	1393	COA	C4A-N9A-C1B	-2.27	121.32	126.63
3	B	5939	COA	C4B-O4B-C1B	-2.24	104.53	109.47
3	A	1393	COA	N9A-C8A-N7A	-2.19	110.83	113.94

There are no chirality outliers.

All (18) torsion outliers are listed below:

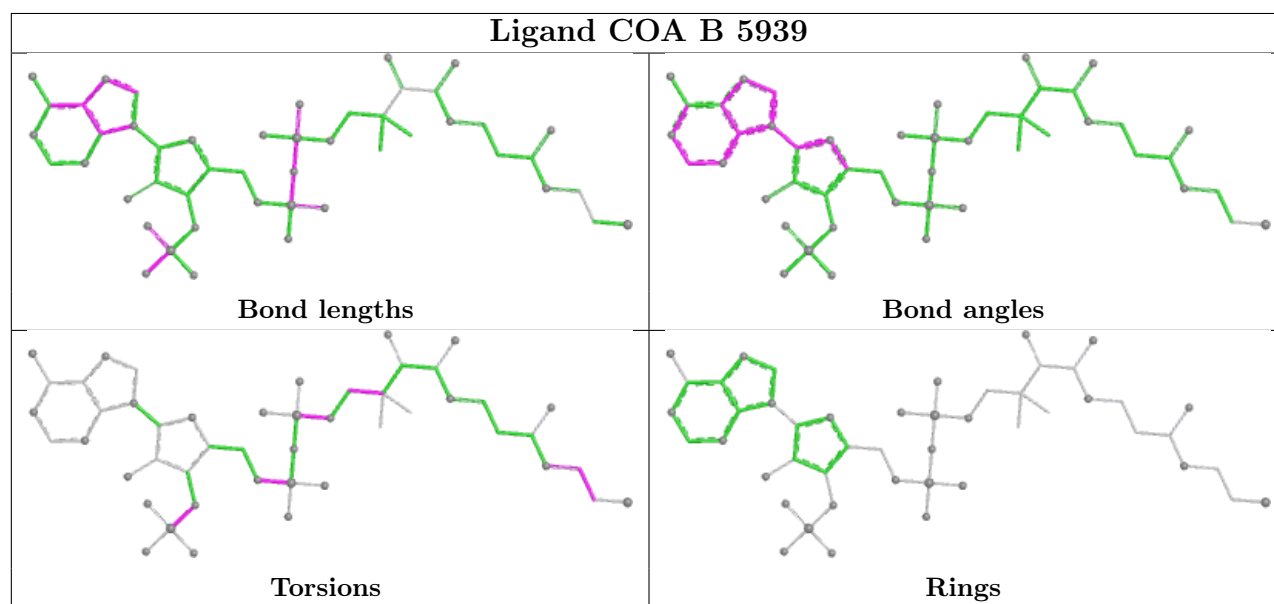
Mol	Chain	Res	Type	Atoms
3	A	1393	COA	CCP-O6A-P2A-O3A
3	A	1393	COA	CCP-O6A-P2A-O5A
3	A	1393	COA	C2P-C3P-N4P-C5P
3	B	5939	COA	C5B-O5B-P1A-O2A
3	B	5939	COA	C5B-O5B-P1A-O3A
3	B	5939	COA	CCP-O6A-P2A-O3A
3	B	5939	COA	CCP-O6A-P2A-O4A
3	B	5939	COA	C2P-C3P-N4P-C5P
3	A	1393	COA	C4B-C3B-O3B-P3B
3	B	5939	COA	CEP-CBP-CCP-O6A
3	A	1393	COA	C3B-O3B-P3B-O7A
3	A	1393	COA	S1P-C2P-C3P-N4P
3	B	5939	COA	CAP-CBP-CCP-O6A
3	B	5939	COA	S1P-C2P-C3P-N4P
3	A	1393	COA	CCP-O6A-P2A-O4A
3	B	5939	COA	C3B-O3B-P3B-O7A
3	A	1393	COA	C2B-C3B-O3B-P3B
3	B	5939	COA	CDP-CBP-CCP-O6A

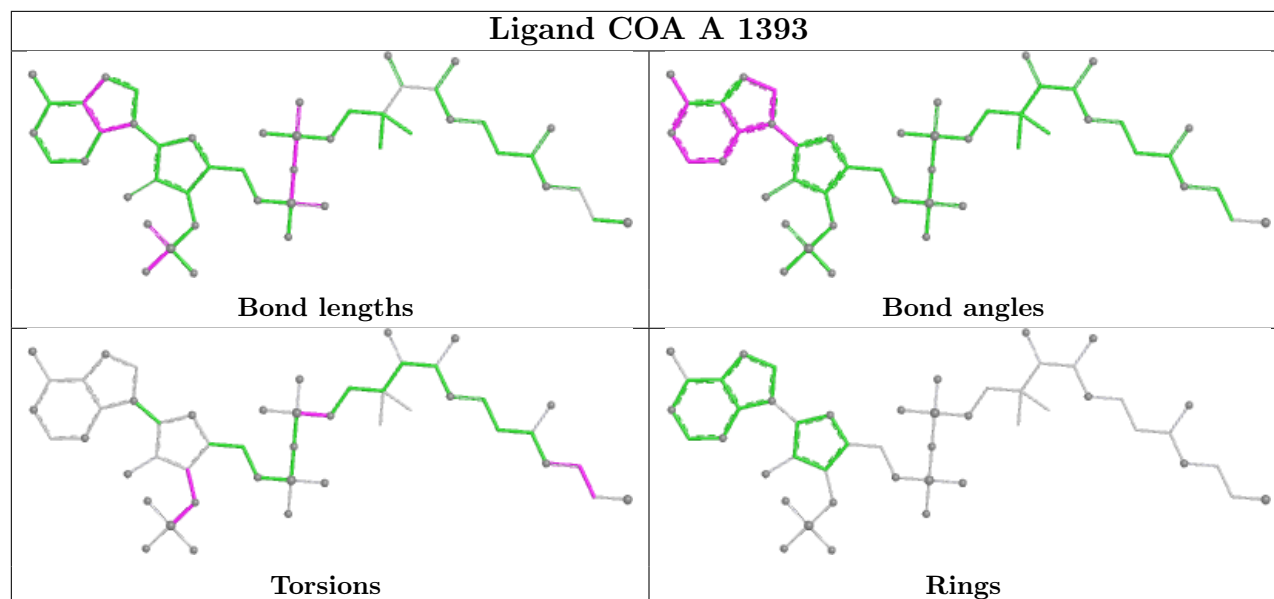
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9721	SO4	1	0
3	B	5939	COA	5	0
3	A	1393	COA	5	0
2	A	9720	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [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	389/392 (99%)	-1.30	0 100 100	10, 15, 30, 54	1 (0%)
1	B	389/392 (99%)	-1.26	0 100 100	10, 15, 30, 59	1 (0%)
1	C	389/392 (99%)	-1.09	0 100 100	3, 17, 26, 51	1 (0%)
1	D	389/392 (99%)	-0.98	0 100 100	4, 17, 32, 50	1 (0%)
All	All	1556/1568 (99%)	-1.16	0 100 100	3, 16, 30, 59	4 (0%)

There are no RSRZ outliers to report.

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	9/10	0.99	0.03	12,17,31,35	0
1	SCY	C	89	9/10	0.99	0.04	15,19,38,41	0
1	SCY	D	89	9/10	0.99	0.04	9,14,27,30	0
1	SCY	B	89	9/10	1.00	0.03	11,15,33,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

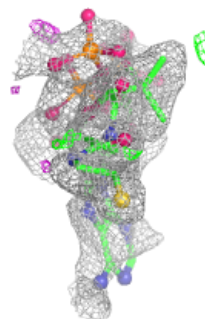
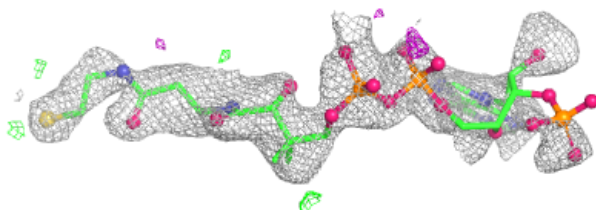
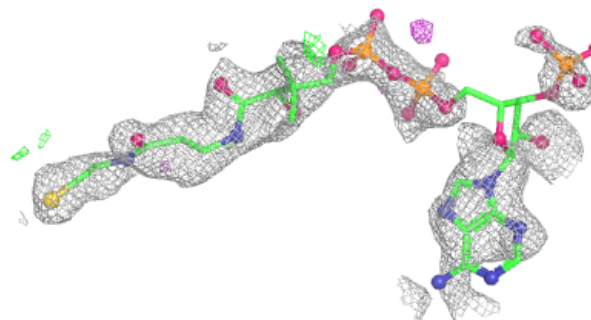
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COA	A	1393	48/48	0.96	0.08	60,73,82,83	0
3	COA	B	5939	48/48	0.96	0.08	60,75,82,83	0
2	SO4	A	9722	5/5	0.97	0.06	66,67,67,68	0
2	SO4	B	9719	5/5	0.98	0.05	77,78,79,79	0
2	SO4	A	9720	5/5	0.99	0.03	47,48,51,51	0
2	SO4	B	9721	5/5	0.99	0.04	45,46,47,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

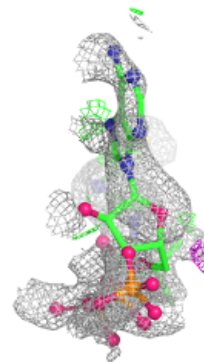
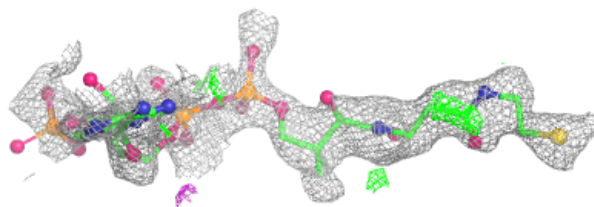
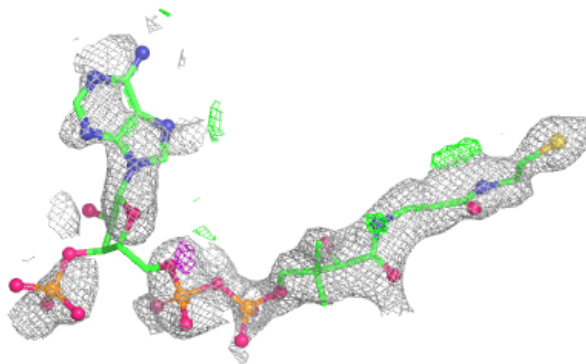
Electron density around COA A 1393:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COA B 5939:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.