



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 03:48 PM EDT

PDB ID : 1NL7
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
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) : 2.35

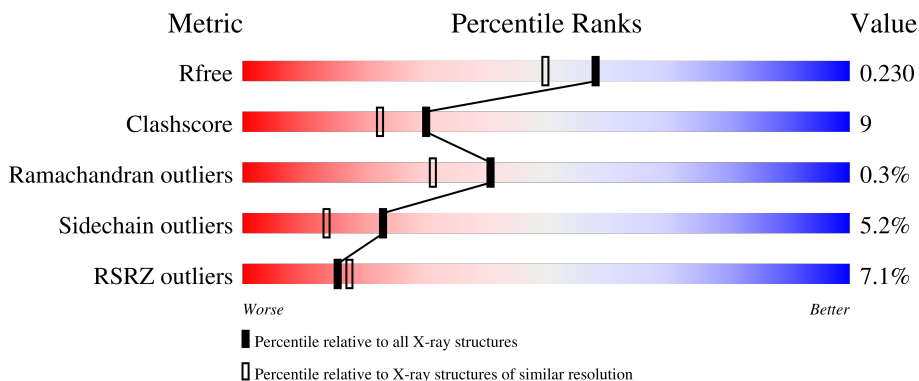
1 Overall quality at a glance

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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	 87% 11% ..
1	B	392	 85% 13% ..
1	C	392	 6% 84% 14% ..
1	D	392	 20% 76% 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 [i](#)

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
			Total	C	N	O	S			
1	A	390	2825	1754	510	540	21	0	1	0
1	B	390	2825	1754	510	540	21	0	1	0
1	C	390	2825	1754	510	540	21	0	1	0
1	D	390	2825	1754	510	540	21	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

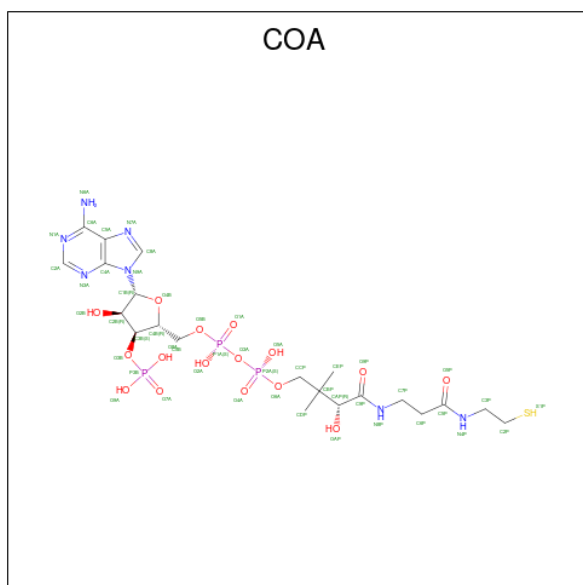
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	insertion	UNP P07097
A	89	SCY	CYS	modified residue	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	10	ALA	-	insertion	UNP P07097
B	89	SCY	CYS	modified residue	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	10	ALA	-	insertion	UNP P07097
C	89	SCY	CYS	modified residue	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	10	ALA	-	insertion	UNP P07097
D	89	SCY	CYS	modified residue	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 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 COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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


- Molecule 4 is water.

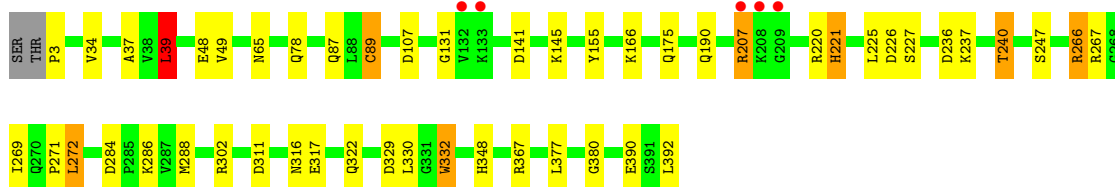
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	443	Total	O	0	0
			443	443		
4	B	446	Total	O	0	0
			446	446		
4	C	190	Total	O	0	0
			190	190		
4	D	196	Total	O	0	0
			196	196		

3 Residue-property plots [i](#)


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.

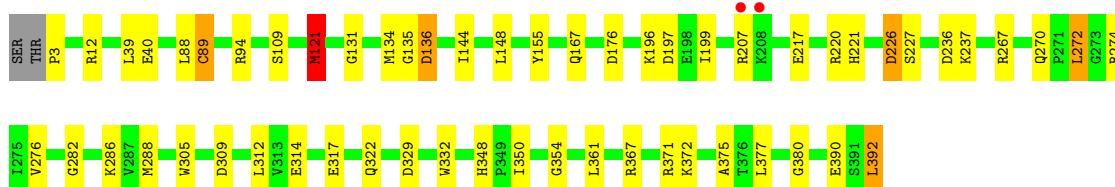
- Molecule 1: Acetyl-CoA acetyltransferase

Chain A: 




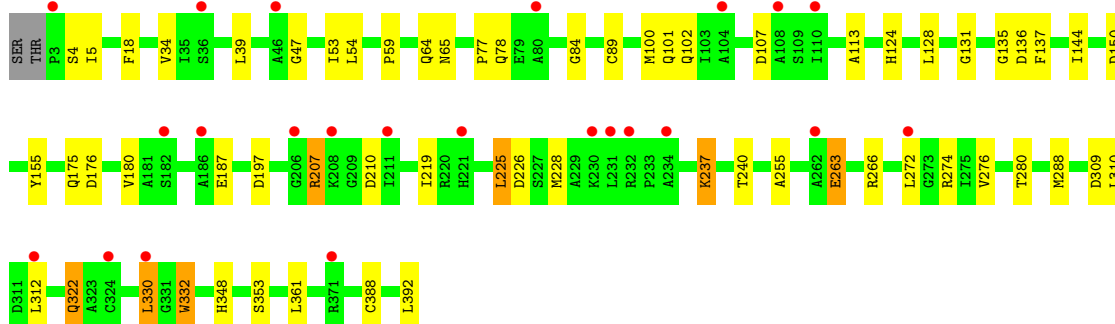
- Molecule 1: Acetyl-CoA acetyltransferase

Chain B: 




- Molecule 1: Acetyl-CoA acetyltransferase

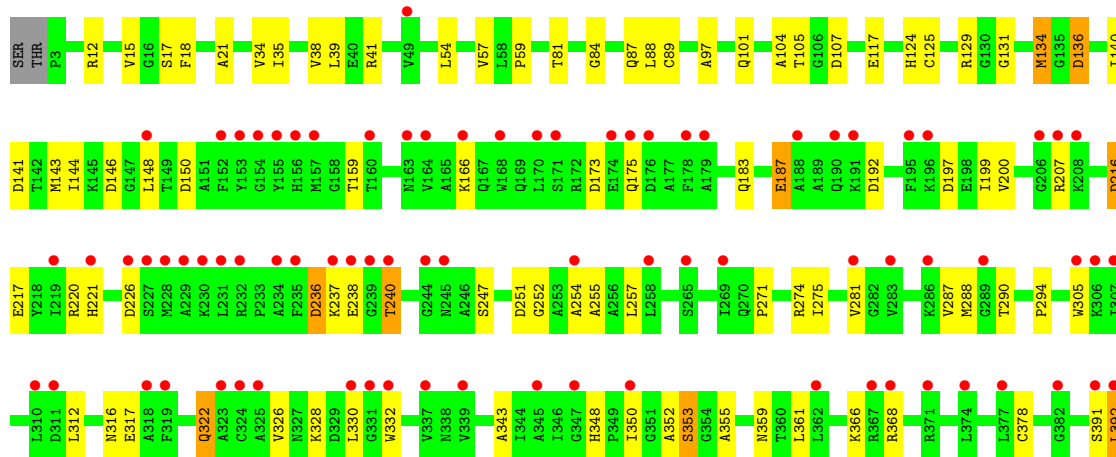
Chain C: 



- 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 27.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-1.90) 85.1 (27.08-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.91Å)	Xtrriage
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	Xtrriage
Anisotropy	0.702	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.124 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12691	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	3/2861 (0.1%)	1.03	17/3861 (0.4%)
1	B	1.02	2/2861 (0.1%)	0.97	12/3861 (0.3%)
1	C	0.66	0/2861	0.83	7/3861 (0.2%)
1	D	0.61	0/2861	0.83	10/3861 (0.3%)
All	All	0.85	5/11444 (0.0%)	0.92	46/15444 (0.3%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	VAL	CB-CG1	-7.47	1.37	1.52
1	B	317	GLU	CD-OE1	6.98	1.33	1.25
1	A	317	GLU	CD-OE1	6.50	1.32	1.25
1	B	109	SER	CB-OG	-6.37	1.33	1.42
1	A	37	ALA	CA-CB	5.28	1.63	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	NE-CZ-NH2	-14.97	112.82	120.30
1	B	309	ASP	CB-CG-OD2	8.83	126.25	118.30
1	A	141	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	266	ARG	NE-CZ-NH1	8.25	124.43	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ASP	CB-CG-OD2	7.68	125.21	118.30
1	D	146	ASP	CB-CG-OD2	7.15	124.74	118.30
1	A	272	LEU	CB-CG-CD1	7.01	122.92	111.00
1	B	121	MET	CG-SD-CE	6.72	110.95	100.20
1	D	107	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	302	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	272	LEU	CB-CG-CD1	6.55	122.14	111.00
1	B	272	LEU	CA-CB-CG	6.54	130.34	115.30
1	B	267	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	329	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	226	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	367	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	367	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	197	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	266	ARG	CG-CD-NE	-5.89	99.42	111.80
1	A	284	ASP	CB-CG-OD1	5.89	123.60	118.30
1	C	150	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	251	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	107	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	176	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	173	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	216	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	107	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	226	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	302	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	236	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	94	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	367	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	D	236	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	272	LEU	CA-CB-CG	5.25	127.36	115.30
1	A	329	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	210	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	226	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	311	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	136	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	192	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	197	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	236	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	309	ASP	CB-CG-OD2	5.09	122.89	118.30
1	C	176	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	39	LEU	CB-CG-CD1	5.04	119.57	111.00
1	D	226	ASP	CB-CG-OD2	5.01	122.81	118.30

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 [i](#)

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	46	0
1	B	2825	0	2830	49	0
1	C	2825	0	2830	42	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	29	0
4	B	446	0	0	31	0
4	C	190	0	0	18	0
4	D	196	0	0	45	0
All	All	12691	0	11384	212	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 9.

All (212) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:227:SER:OG	4:A:9911:HOH:O	1.84	0.91
1:B:392:LEU:HD12	4:B:9839:HOH:O	1.72	0.89
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
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: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:305:TRP:C	4:D:536:HOH:O	2.29	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:C:276:VAL:HG22	1:C:388:CYS:C	2.23	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:145:LYS:NZ	4:A:9881:HOH:O	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:A:498:HOH:O	1:D:134:MET:HE1	2.07	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: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:C:348:HIS:ND1	1:C:353:SER:OG	2.40	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: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: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:183:GLN:CD	4:D:429:HOH:O	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:322:GLN:C	1:C:322:GLN:NE2	2.67	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:C:102:GLN:NE2	4:C:439:HOH:O	2.46	0.47
1:D:87:GLN:O	1:D:88:LEU:C	2.53	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: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
1:C:64:GLN:O	1:C:65:ASN:C	2.53	0.46
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: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:B:220:ARG:NH2	3:B:5939:COA:N1A	2.65	0.44
1:D:257:LEU:C	1:D:257:LEU:HD23	2.36	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:57:VAL:C	1:D:59:PRO:HD3	2.39	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: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:A:39:LEU:HD11	1:A:49:VAL:CG2	2.50	0.41
4:A:498:HOH:O	1:D:134:MET:CE	2.68	0.41
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.55	0.41
1:D:166:LYS:NZ	4:D:416:HOH:O	2.24	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:D:348:HIS:CE1	1:D:353:SER:HG	2.39	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:C:228:MET:HE2	4:C:419: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%)	41	31
1	B	388/392 (99%)	378 (97%)	9 (2%)	1 (0%)	41	31
1	C	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	41	31
1	D	388/392 (99%)	369 (95%)	18 (5%)	1 (0%)	41	31
All	All	1552/1568 (99%)	1486 (96%)	62 (4%)	4 (0%)	41	31

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 [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	277/278 (100%)	265 (96%)	12 (4%)	29	19
1	B	277/278 (100%)	263 (95%)	14 (5%)	24	14
1	C	277/278 (100%)	264 (95%)	13 (5%)	26	16
1	D	277/278 (100%)	259 (94%)	18 (6%)	17	8
All	All	1108/1112 (100%)	1051 (95%)	57 (5%)	23	14

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	207	ARG
1	A	221	HIS
1	A	225	LEU
1	A	237	LYS
1	A	240	THR
1	A	272	LEU
1	A	288	MET
1	A	322	GLN
1	A	332	TRP
1	A	392	LEU
1	B	39	LEU
1	B	121	MET
1	B	134	MET
1	B	155	TYR
1	B	167	GLN
1	B	207	ARG
1	B	221	HIS
1	B	237	LYS
1	B	272	LEU
1	B	276	VAL
1	B	288	MET
1	B	322	GLN
1	B	332	TRP
1	B	392	LEU
1	C	39	LEU
1	C	78	GLN
1	C	155	TYR
1	C	207	ARG
1	C	225	LEU
1	C	237	LYS
1	C	263	GLU
1	C	272	LEU
1	C	288	MET
1	C	322	GLN
1	C	330	LEU
1	C	332	TRP
1	C	392	LEU
1	D	17	SER
1	D	39	LEU
1	D	134	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	187	GLU
1	D	207	ARG
1	D	217	GLU
1	D	220	ARG
1	D	236	ASP
1	D	237	LYS
1	D	238	GLU
1	D	240	THR
1	D	288	MET
1	D	322	GLN
1	D	328	LYS
1	D	332	TRP
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	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	184	ASN
1	D	221	HIS
1	D	316	ASN
1	D	322	GLN

5.3.3 RNA [i](#)

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	D	89	1	7,8,9	0.84	0	3,9,11	1.04	0
1	SCY	C	89	1	7,8,9	0.65	0	3,9,11	0.98	0
1	SCY	B	89	1	7,8,9	1.14	1 (14%)	3,9,11	1.90	1 (33%)
1	SCY	A	89	1	7,8,9	1.24	1 (14%)	3,9,11	2.17	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	D	89	1	-	3/5/7/9	-
1	SCY	C	89	1	-	2/5/7/9	-
1	SCY	B	89	1	-	2/5/7/9	-
1	SCY	A	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	-2.50	1.60	1.75
1	B	89	SCY	CD-SG	-2.03	1.63	1.75

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	SCY	OCD-CD-CE	3.17	136.06	123.07
1	B	89	SCY	OCD-CD-SG	-2.71	110.57	122.60

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	D	89	SCY	6	0
1	C	89	SCY	5	0
1	B	89	SCY	9	0
1	A	89	SCY	8	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	0.18	0	6,6,6	0.44	0
2	SO4	A	9720	-	4,4,4	0.35	0	6,6,6	0.52	0
2	SO4	B	9721	-	4,4,4	0.39	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COA	B	5939	-	41,50,50	1.45	5 (12%)	52,75,75	1.32	5 (9%)
2	SO4	B	9719	-	4,4,4	0.16	0	6,6,6	0.32	0
3	COA	A	1393	-	41,50,50	1.39	4 (9%)	52,75,75	1.20	5 (9%)

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	B	5939	-	-	8/44/64/64	0/3/3/3
3	COA	A	1393	-	-	8/44/64/64	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1393	COA	P3B-O8A	4.33	1.71	1.54
3	B	5939	COA	P3B-O8A	4.28	1.71	1.54
3	B	5939	COA	P3B-O9A	4.20	1.71	1.54
3	A	1393	COA	P3B-O9A	4.12	1.70	1.54
3	B	5939	COA	P2A-O5A	3.57	1.72	1.55
3	B	5939	COA	P1A-O2A	3.35	1.71	1.55
3	A	1393	COA	P1A-O2A	3.31	1.70	1.55
3	A	1393	COA	P2A-O5A	3.17	1.70	1.55
3	B	5939	COA	C5A-C4A	2.09	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5939	COA	C1B-N9A-C4A	-5.26	117.40	126.64
3	A	1393	COA	N3A-C2A-N1A	-4.15	122.19	128.68
3	B	5939	COA	N3A-C2A-N1A	-3.57	123.10	128.68
3	A	1393	COA	C1B-N9A-C4A	-3.03	121.32	126.64
3	B	5939	COA	C5A-C6A-N6A	2.85	124.68	120.35
3	A	1393	COA	N6A-C6A-N1A	2.77	124.31	118.57
3	B	5939	COA	P2A-O3A-P1A	-2.73	123.44	132.83
3	B	5939	COA	C2A-N1A-C6A	2.69	123.35	118.75
3	A	1393	COA	P2A-O3A-P1A	-2.64	123.76	132.83
3	A	1393	COA	C2A-N1A-C6A	2.22	122.54	118.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

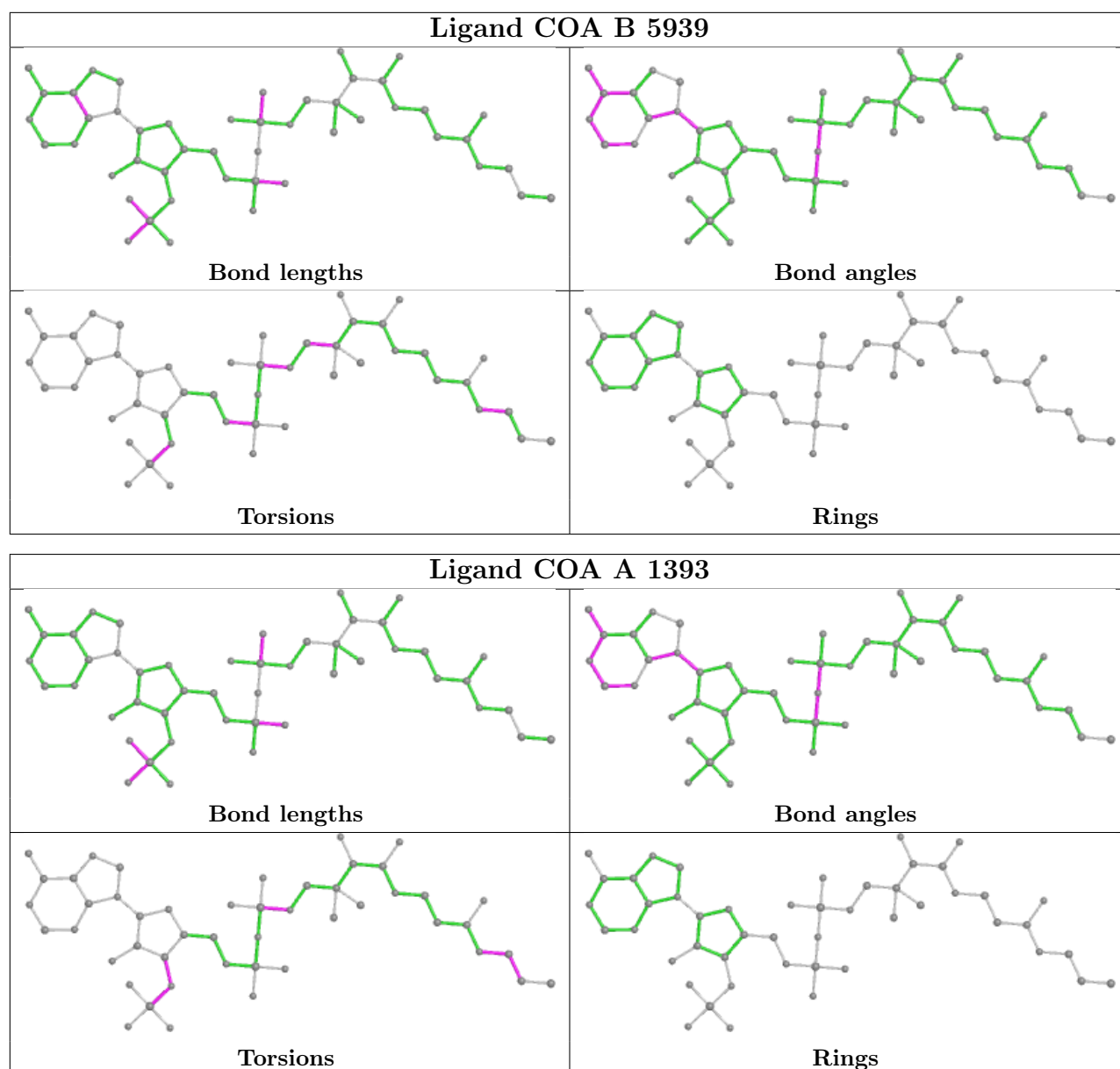
Mol	Chain	Res	Type	Atoms
3	A	1393	COA	C3B-O3B-P3B-O7A
3	A	1393	COA	CCP-O6A-P2A-O3A
3	A	1393	COA	C2P-C3P-N4P-C5P
3	B	5939	COA	C5B-O5B-P1A-O3A
3	B	5939	COA	CCP-O6A-P2A-O3A
3	B	5939	COA	CCP-O6A-P2A-O4A
3	B	5939	COA	C2P-C3P-N4P-C5P
3	A	1393	COA	C4B-C3B-O3B-P3B
3	A	1393	COA	S1P-C2P-C3P-N4P
3	A	1393	COA	CCP-O6A-P2A-O4A
3	A	1393	COA	CCP-O6A-P2A-O5A
3	B	5939	COA	C5B-O5B-P1A-O2A
3	B	5939	COA	CAP-CBP-CCP-O6A
3	B	5939	COA	CEP-CBP-CCP-O6A
3	A	1393	COA	C2B-C3B-O3B-P3B
3	B	5939	COA	C3B-O3B-P3B-O9A

There are no ring outliers.

4 monomers are involved in 12 short contacts:

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

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	389/392 (99%)	-0.34	5 (1%) 77 79	10, 15, 30, 54	0
1	B	389/392 (99%)	-0.34	2 (0%) 91 92	10, 15, 30, 59	0
1	C	389/392 (99%)	0.45	23 (5%) 22 25	3, 17, 26, 51	0
1	D	389/392 (99%)	1.08	80 (20%) 1 1	4, 17, 32, 50	0
All	All	1556/1568 (99%)	0.21	110 (7%) 16 17	3, 16, 30, 59	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	392	LEU	7.2
1	D	331	GLY	7.2
1	D	153	TYR	7.0
1	D	238	GLU	6.5
1	D	221	HIS	5.8
1	D	170	LEU	5.4
1	B	208	LYS	5.1
1	D	228	MET	5.1
1	D	206	GLY	5.0
1	D	332	TRP	5.0
1	D	232	ARG	5.0
1	A	132	VAL	4.9
1	D	371	ARG	4.9
1	D	229	ALA	4.9
1	D	154	GLY	4.9
1	C	206	GLY	4.7
1	D	226	ASP	4.5
1	B	207	ARG	4.4
1	D	240	THR	4.4
1	D	178	PHE	4.2
1	D	325	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	152	PHE	4.0
1	C	80	ALA	4.0
1	D	171	SER	3.9
1	D	207	ARG	3.8
1	C	312	LEU	3.7
1	D	235	PHE	3.6
1	C	46	ALA	3.4
1	A	208	LYS	3.3
1	D	269	ILE	3.3
1	C	104	ALA	3.3
1	D	310	LEU	3.3
1	C	232	ARG	3.2
1	D	166	LYS	3.2
1	D	227	SER	3.1
1	A	207	ARG	3.1
1	D	283	VAL	3.1
1	C	221	HIS	3.0
1	D	307	ILE	3.0
1	D	319	PHE	3.0
1	D	179	ALA	3.0
1	C	230	LYS	2.9
1	D	156	HIS	2.9
1	D	330	LEU	2.8
1	D	231	LEU	2.8
1	D	382	GLY	2.8
1	D	160	THR	2.8
1	C	108	ALA	2.7
1	C	186	ALA	2.7
1	A	209	GLY	2.7
1	D	323	ALA	2.7
1	D	318	ALA	2.7
1	D	324	CYS	2.7
1	D	176	ASP	2.6
1	D	281	VAL	2.6
1	D	245	ASN	2.6
1	C	211	ILE	2.6
1	C	208	LYS	2.6
1	D	157	MET	2.6
1	D	239	GLY	2.6
1	D	367	ARG	2.5
1	D	168	TRP	2.5
1	C	234	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	262	ALA	2.5
1	D	49	VAL	2.5
1	D	289	GLY	2.5
1	C	3	PRO	2.5
1	D	163	ASN	2.5
1	D	377	LEU	2.4
1	D	237	LYS	2.4
1	D	347	GLY	2.4
1	D	337	VAL	2.4
1	D	362	LEU	2.4
1	C	371	ARG	2.4
1	D	155	TYR	2.3
1	D	234	ALA	2.3
1	D	219	ILE	2.3
1	D	191	LYS	2.3
1	D	368	ARG	2.3
1	D	196	LYS	2.3
1	D	306	LYS	2.3
1	D	391	SER	2.3
1	D	174	GLU	2.3
1	D	148	LEU	2.3
1	D	286	LYS	2.2
1	C	36	SER	2.2
1	D	175	GLN	2.2
1	D	230	LYS	2.2
1	D	244	GLY	2.2
1	D	350	ILE	2.2
1	D	305	TRP	2.2
1	D	374	LEU	2.1
1	D	190	GLN	2.1
1	D	164	VAL	2.1
1	A	133	LYS	2.1
1	D	188	ALA	2.1
1	D	345	ALA	2.1
1	C	231	LEU	2.1
1	D	195	PHE	2.1
1	C	324	CYS	2.1
1	C	272	LEU	2.1
1	C	330	LEU	2.1
1	D	311	ASP	2.1
1	C	110	ILE	2.1
1	D	265	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	258	LEU	2.0
1	D	208	LYS	2.0
1	D	339	VAL	2.0
1	D	254	ALA	2.0
1	C	182	SER	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. 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	C	89	9/10	0.89	0.20	15,19,38,41	0
1	SCY	D	89	9/10	0.93	0.13	9,14,27,30	0
1	SCY	A	89	9/10	0.94	0.10	12,17,31,35	0
1	SCY	B	89	9/10	0.95	0.10	11,15,33,37	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

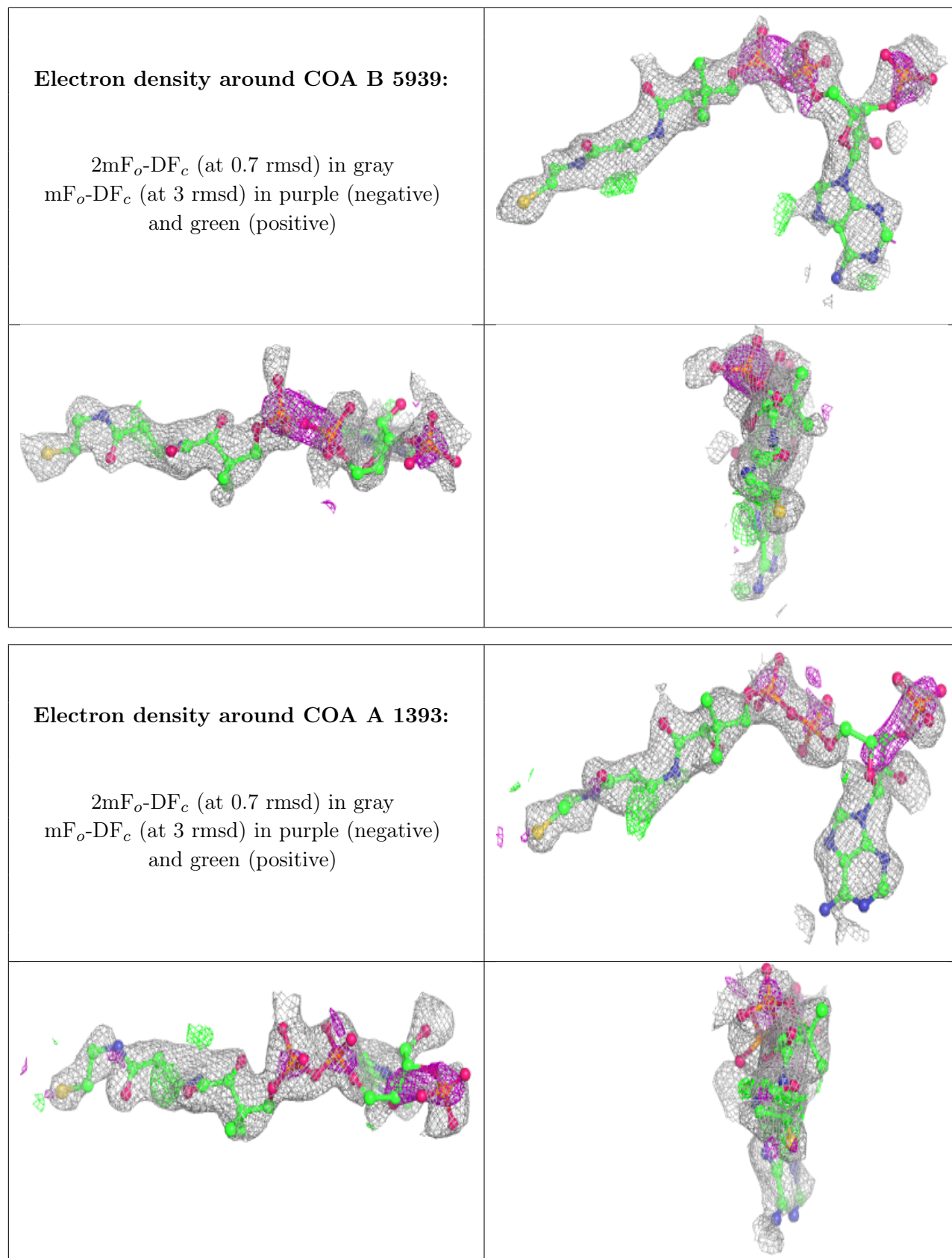
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COA	B	5939	48/48	0.60	0.26	60,75,82,83	0
3	COA	A	1393	48/48	0.65	0.25	60,73,82,83	0
2	SO4	A	9722	5/5	0.94	0.11	66,67,67,68	0
2	SO4	B	9719	5/5	0.96	0.14	77,78,79,79	0
2	SO4	B	9721	5/5	0.97	0.11	45,46,47,50	0
2	SO4	A	9720	5/5	0.99	0.09	47,48,51,51	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.