



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:55 am GMT

PDB ID : 5AB7
Title : Crystal structure of Trypanosoma brucei SCP2-thiolase like protein (TbSLP) in complex with malonyl-CoA.
Authors : Harijan, R.K.; Kiema, T.R.; Wierenga, R.K.
Deposited on : 2015-08-02
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

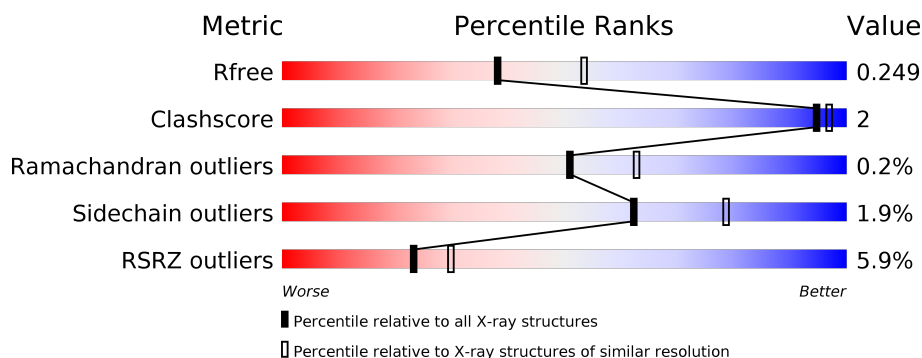
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	425	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	B	425	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	425	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	D	425	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>•</div> <div>7%</div> </div> </div>
1	E	425	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	F	425	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>8%</div> </div> </div>

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	MLC	A	1410	-	-	-	X
2	MLC	B	1410	-	-	-	X
2	MLC	E	1411	-	-	-	X
3	SO4	A	1411	-	-	-	X
3	SO4	C	1412	-	-	-	X
3	SO4	D	1413	-	-	-	X
3	SO4	F	1411	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18248 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 SCP2-THIOLASE LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	1	0
			2921	1850	509	537	25			
1	B	392	Total	C	N	O	S	0	1	0
			2922	1850	511	537	24			
1	C	393	Total	C	N	O	S	0	1	0
			2926	1853	510	538	25			
1	D	396	Total	C	N	O	S	0	1	0
			2948	1864	513	546	25			
1	E	392	Total	C	N	O	S	0	1	0
			2925	1853	511	537	24			
1	F	391	Total	C	N	O	S	0	2	0
			2918	1847	510	536	25			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	EXPRESSION TAG	UNP C9ZUV7
A	-14	HIS	-	EXPRESSION TAG	UNP C9ZUV7
A	-13	HIS	-	EXPRESSION TAG	UNP C9ZUV7
A	-12	HIS	-	EXPRESSION TAG	UNP C9ZUV7
A	-11	HIS	-	EXPRESSION TAG	UNP C9ZUV7
A	-10	HIS	-	EXPRESSION TAG	UNP C9ZUV7
A	-9	SER	-	EXPRESSION TAG	UNP C9ZUV7
A	-8	SER	-	EXPRESSION TAG	UNP C9ZUV7
A	-7	GLY	-	EXPRESSION TAG	UNP C9ZUV7
A	-6	LEU	-	EXPRESSION TAG	UNP C9ZUV7
A	-5	VAL	-	EXPRESSION TAG	UNP C9ZUV7
A	-4	PRO	-	EXPRESSION TAG	UNP C9ZUV7
A	-3	ARG	-	EXPRESSION TAG	UNP C9ZUV7
A	-2	GLY	-	EXPRESSION TAG	UNP C9ZUV7
A	-1	SER	-	EXPRESSION TAG	UNP C9ZUV7
A	0	HIS	-	EXPRESSION TAG	UNP C9ZUV7
B	-15	HIS	-	EXPRESSION TAG	UNP C9ZUV7

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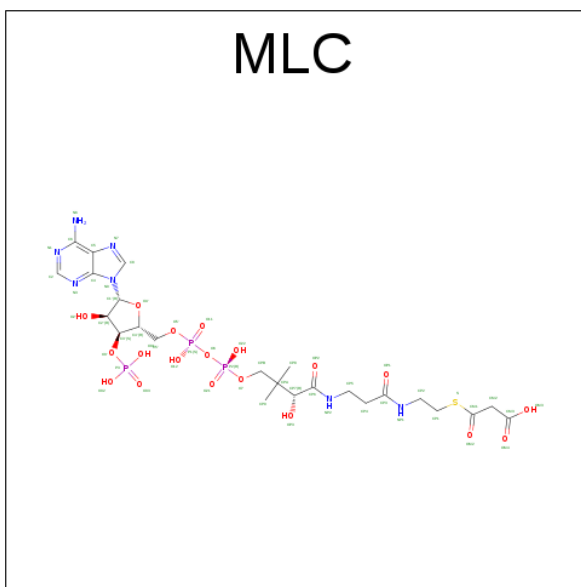
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP C9ZUV7
B	-13	HIS	-	EXPRESSION TAG	UNP C9ZUV7
B	-12	HIS	-	EXPRESSION TAG	UNP C9ZUV7
B	-11	HIS	-	EXPRESSION TAG	UNP C9ZUV7
B	-10	HIS	-	EXPRESSION TAG	UNP C9ZUV7
B	-9	SER	-	EXPRESSION TAG	UNP C9ZUV7
B	-8	SER	-	EXPRESSION TAG	UNP C9ZUV7
B	-7	GLY	-	EXPRESSION TAG	UNP C9ZUV7
B	-6	LEU	-	EXPRESSION TAG	UNP C9ZUV7
B	-5	VAL	-	EXPRESSION TAG	UNP C9ZUV7
B	-4	PRO	-	EXPRESSION TAG	UNP C9ZUV7
B	-3	ARG	-	EXPRESSION TAG	UNP C9ZUV7
B	-2	GLY	-	EXPRESSION TAG	UNP C9ZUV7
B	-1	SER	-	EXPRESSION TAG	UNP C9ZUV7
B	0	HIS	-	EXPRESSION TAG	UNP C9ZUV7
C	-15	HIS	-	EXPRESSION TAG	UNP C9ZUV7
C	-14	HIS	-	EXPRESSION TAG	UNP C9ZUV7
C	-13	HIS	-	EXPRESSION TAG	UNP C9ZUV7
C	-12	HIS	-	EXPRESSION TAG	UNP C9ZUV7
C	-11	HIS	-	EXPRESSION TAG	UNP C9ZUV7
C	-10	HIS	-	EXPRESSION TAG	UNP C9ZUV7
C	-9	SER	-	EXPRESSION TAG	UNP C9ZUV7
C	-8	SER	-	EXPRESSION TAG	UNP C9ZUV7
C	-7	GLY	-	EXPRESSION TAG	UNP C9ZUV7
C	-6	LEU	-	EXPRESSION TAG	UNP C9ZUV7
C	-5	VAL	-	EXPRESSION TAG	UNP C9ZUV7
C	-4	PRO	-	EXPRESSION TAG	UNP C9ZUV7
C	-3	ARG	-	EXPRESSION TAG	UNP C9ZUV7
C	-2	GLY	-	EXPRESSION TAG	UNP C9ZUV7
C	-1	SER	-	EXPRESSION TAG	UNP C9ZUV7
C	0	HIS	-	EXPRESSION TAG	UNP C9ZUV7
D	-15	HIS	-	EXPRESSION TAG	UNP C9ZUV7
D	-14	HIS	-	EXPRESSION TAG	UNP C9ZUV7
D	-13	HIS	-	EXPRESSION TAG	UNP C9ZUV7
D	-12	HIS	-	EXPRESSION TAG	UNP C9ZUV7
D	-11	HIS	-	EXPRESSION TAG	UNP C9ZUV7
D	-10	HIS	-	EXPRESSION TAG	UNP C9ZUV7
D	-9	SER	-	EXPRESSION TAG	UNP C9ZUV7
D	-8	SER	-	EXPRESSION TAG	UNP C9ZUV7
D	-7	GLY	-	EXPRESSION TAG	UNP C9ZUV7
D	-6	LEU	-	EXPRESSION TAG	UNP C9ZUV7
D	-5	VAL	-	EXPRESSION TAG	UNP C9ZUV7

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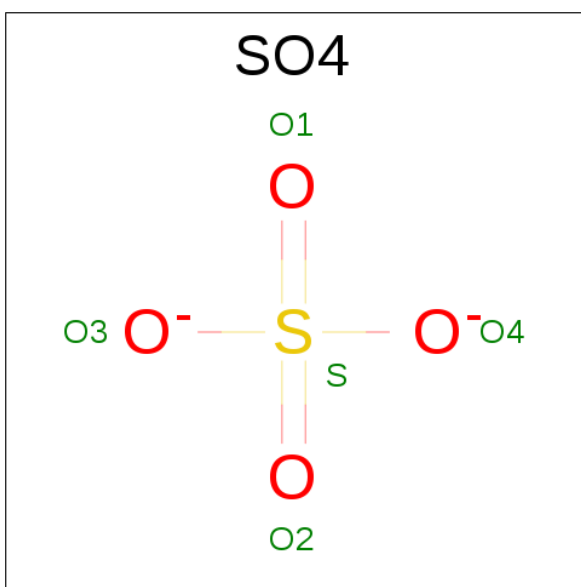
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PRO	-	EXPRESSION TAG	UNP C9ZUV7
D	-3	ARG	-	EXPRESSION TAG	UNP C9ZUV7
D	-2	GLY	-	EXPRESSION TAG	UNP C9ZUV7
D	-1	SER	-	EXPRESSION TAG	UNP C9ZUV7
D	0	HIS	-	EXPRESSION TAG	UNP C9ZUV7
E	-15	HIS	-	EXPRESSION TAG	UNP C9ZUV7
E	-14	HIS	-	EXPRESSION TAG	UNP C9ZUV7
E	-13	HIS	-	EXPRESSION TAG	UNP C9ZUV7
E	-12	HIS	-	EXPRESSION TAG	UNP C9ZUV7
E	-11	HIS	-	EXPRESSION TAG	UNP C9ZUV7
E	-10	HIS	-	EXPRESSION TAG	UNP C9ZUV7
E	-9	SER	-	EXPRESSION TAG	UNP C9ZUV7
E	-8	SER	-	EXPRESSION TAG	UNP C9ZUV7
E	-7	GLY	-	EXPRESSION TAG	UNP C9ZUV7
E	-6	LEU	-	EXPRESSION TAG	UNP C9ZUV7
E	-5	VAL	-	EXPRESSION TAG	UNP C9ZUV7
E	-4	PRO	-	EXPRESSION TAG	UNP C9ZUV7
E	-3	ARG	-	EXPRESSION TAG	UNP C9ZUV7
E	-2	GLY	-	EXPRESSION TAG	UNP C9ZUV7
E	-1	SER	-	EXPRESSION TAG	UNP C9ZUV7
E	0	HIS	-	EXPRESSION TAG	UNP C9ZUV7
F	-15	HIS	-	EXPRESSION TAG	UNP C9ZUV7
F	-14	HIS	-	EXPRESSION TAG	UNP C9ZUV7
F	-13	HIS	-	EXPRESSION TAG	UNP C9ZUV7
F	-12	HIS	-	EXPRESSION TAG	UNP C9ZUV7
F	-11	HIS	-	EXPRESSION TAG	UNP C9ZUV7
F	-10	HIS	-	EXPRESSION TAG	UNP C9ZUV7
F	-9	SER	-	EXPRESSION TAG	UNP C9ZUV7
F	-8	SER	-	EXPRESSION TAG	UNP C9ZUV7
F	-7	GLY	-	EXPRESSION TAG	UNP C9ZUV7
F	-6	LEU	-	EXPRESSION TAG	UNP C9ZUV7
F	-5	VAL	-	EXPRESSION TAG	UNP C9ZUV7
F	-4	PRO	-	EXPRESSION TAG	UNP C9ZUV7
F	-3	ARG	-	EXPRESSION TAG	UNP C9ZUV7
F	-2	GLY	-	EXPRESSION TAG	UNP C9ZUV7
F	-1	SER	-	EXPRESSION TAG	UNP C9ZUV7
F	0	HIS	-	EXPRESSION TAG	UNP C9ZUV7

- Molecule 2 is MALONYL-COENZYME A (three-letter code: MLC) (formula: $C_{24}H_{38}N_7O_{19}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

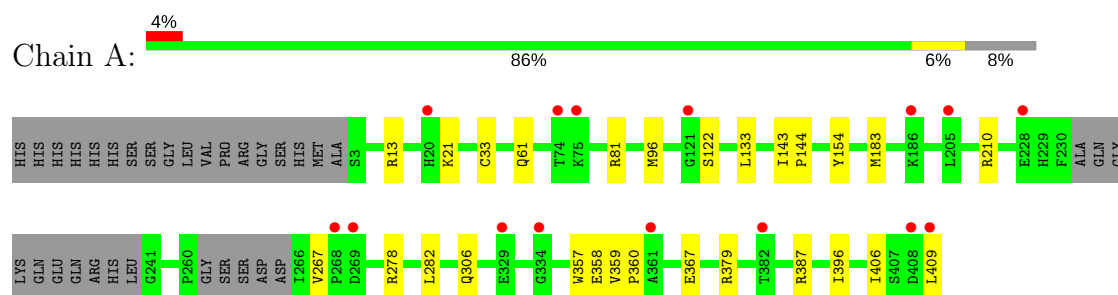
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total 56	O 56	0	0
4	B	60	Total 60	O 60	0	0
4	C	49	Total 49	O 49	0	0
4	D	49	Total 49	O 49	0	0
4	E	44	Total 44	O 44	0	0
4	F	36	Total 36	O 36	0	0

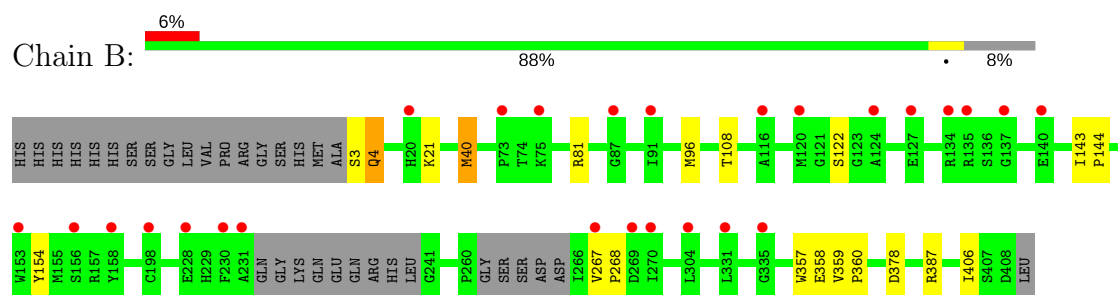
3 Residue-property plots [i](#)

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

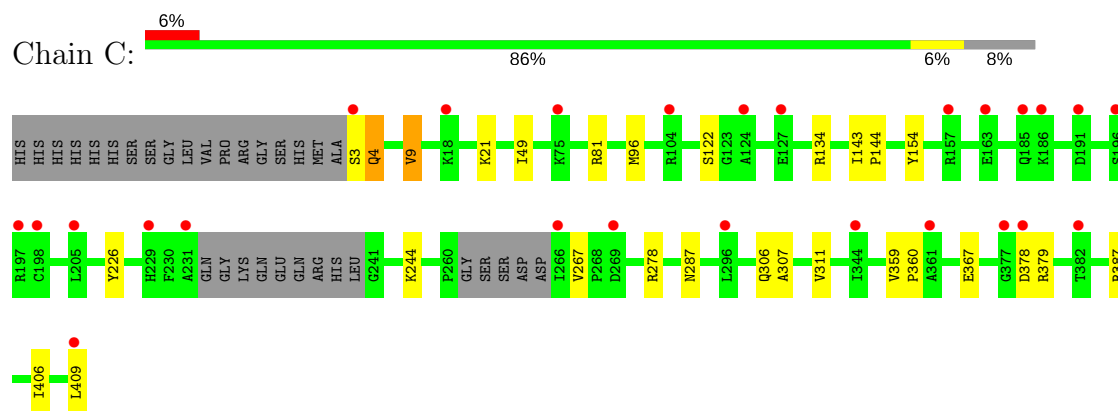
• Molecule 1: SCP2-THIOLASE LIKE PROTEIN



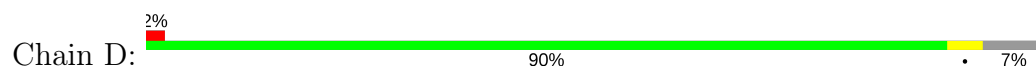
• Molecule 1: SCP2-THIOLASE LIKE PROTEIN

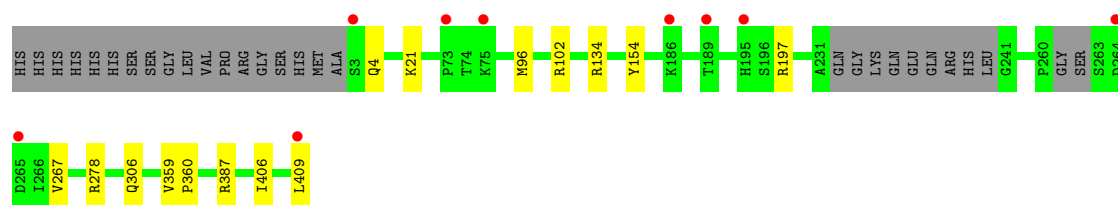


• Molecule 1: SCP2-THIOLASE LIKE PROTEIN

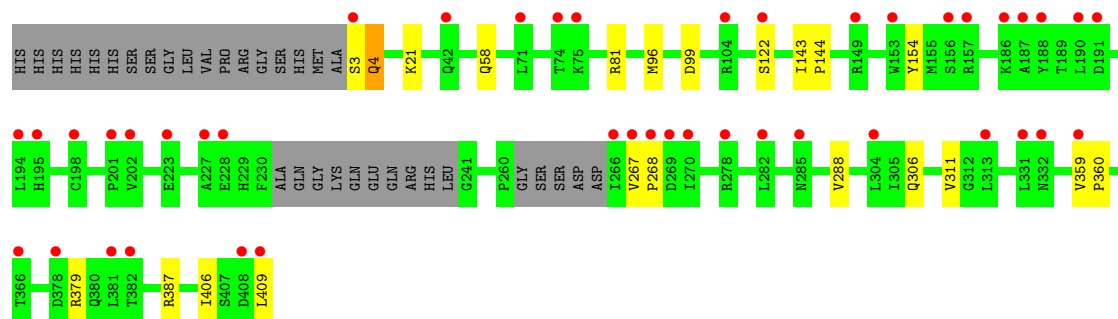
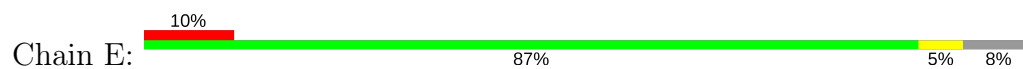


• Molecule 1: SCP2-THIOLASE LIKE PROTEIN

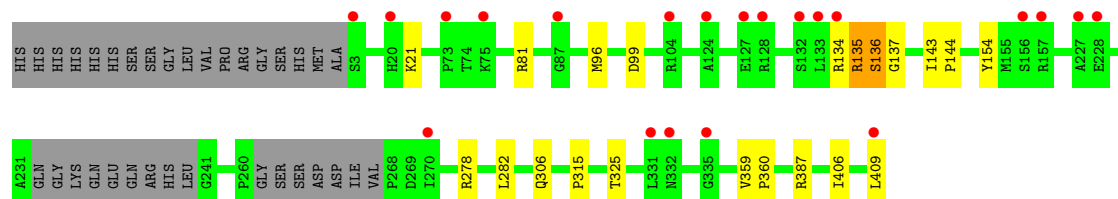
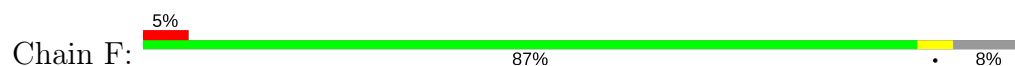




• Molecule 1: SCP2-THIOLASE LIKE PROTEIN



• Molecule 1: SCP2-THIOLASE LIKE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.55Å 66.40Å 159.83Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	29.40 – 2.30 29.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.40-2.30) 94.4 (29.38-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.236 , 0.249 0.235 , 0.249	Depositor DCC
R_{free} test set	5191 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18248	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.52 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.7644e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MLC, 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	0.29	0/2984	0.51	0/4049
1	B	0.29	0/2986	0.51	1/4052 (0.0%)
1	C	0.29	0/2989	0.54	1/4056 (0.0%)
1	D	0.29	0/3011	0.53	1/4086 (0.0%)
1	E	0.30	0/2989	0.52	2/4056 (0.0%)
1	F	0.33	0/2985	0.53	0/4049
All	All	0.30	0/17944	0.52	5/24348 (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	F	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	379	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	40	MET	CG-SD-CE	5.58	109.12	100.20
1	D	134	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	134	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	379	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	134	ARG	Peptide

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	2921	0	2921	16	0
1	B	2922	0	2917	10	0
1	C	2926	0	2926	11	1
1	D	2948	0	2939	6	0
1	E	2925	0	2923	9	0
1	F	2918	0	2914	11	0
2	A	54	0	33	0	0
2	B	54	0	33	0	0
2	C	54	0	33	0	0
2	D	54	0	33	1	0
2	E	54	0	33	0	0
2	F	54	0	33	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
4	A	56	0	0	0	0
4	B	60	0	0	0	0
4	C	49	0	0	0	0
4	D	49	0	0	0	0
4	E	44	0	0	0	0
4	F	36	0	0	0	0
All	All	18248	0	17738	54	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 2.

All (54) 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:4:GLN:O	1:D:102:ARG:NH1	2.10	0.85
1:E:81:ARG:HD3	1:F:96:MET:CE	2.18	0.73
1:A:183:MET:CE	1:A:210:ARG:HG3	2.19	0.71
1:E:96:MET:CE	1:F:81:ARG:HD3	2.23	0.67
1:C:367:GLU:OE2	1:C:379:ARG:NH1	2.32	0.63
1:C:9:VAL:HG21	1:C:226:TYR:CG	2.33	0.63
1:A:133:LEU:HD21	1:A:396:ILE:HD11	1.81	0.62
1:A:367:GLU:OE2	1:A:379:ARG:NH1	2.32	0.62
1:A:183:MET:CE	1:A:210:ARG:CG	2.78	0.60
1:B:40:MET:HE1	1:B:108:THR:HG21	1.84	0.59
1:E:99:ASP:OD1	1:F:99:ASP:OD1	2.20	0.59
1:C:49:ILE:HD13	1:C:96:MET:HE2	1.84	0.59
1:B:267:VAL:HG12	1:B:268:PRO:HD2	1.88	0.54
1:E:267:VAL:HG12	1:E:268:PRO:HD2	1.89	0.54
1:C:9:VAL:HG22	1:C:244:LYS:HD3	1.91	0.53
1:F:135:ARG:HA	1:F:137:GLY:H	1.73	0.53
1:A:183:MET:HE3	1:A:210:ARG:HG3	1.91	0.53
1:A:183:MET:HE3	1:A:210:ARG:CG	2.39	0.52
1:A:33[A]:CYS:SG	1:F:325:THR:HG21	2.50	0.52
1:D:197:ARG:NH2	2:D:1411:MLC:O12	2.39	0.51
1:C:9:VAL:HG21	1:C:226:TYR:CD2	2.45	0.50
1:A:183:MET:HE1	1:A:210:ARG:HG3	1.92	0.49
1:A:96:MET:CE	1:B:81:ARG:HD3	2.43	0.48
1:B:378:ASP:OD2	1:D:278:ARG:NH1	2.48	0.47
1:C:307:ALA:O	1:C:311:VAL:HG23	2.14	0.46
1:A:13:ARG:NH2	1:F:315:PRO:HG3	2.31	0.45
1:A:81:ARG:HD3	1:B:96:MET:CE	2.46	0.45
1:C:387:ARG:HG2	1:C:406:ILE:HG22	2.00	0.43
1:A:387:ARG:HG2	1:A:406:ILE:HG22	2.00	0.43
1:E:3:SER:O	1:E:4:GLN:CB	2.66	0.43
1:B:3:SER:O	1:B:4:GLN:CB	2.66	0.42
1:E:288:VAL:HG22	1:E:311:VAL:O	2.19	0.42
1:F:359:VAL:N	1:F:360:PRO:CD	2.82	0.42
1:B:387:ARG:HG2	1:B:406:ILE:HG22	2.01	0.42
1:D:387:ARG:HG2	1:D:406:ILE:HG22	2.00	0.42
1:C:81:ARG:HD3	1:D:96:MET:CE	2.49	0.42
1:F:387:ARG:HG2	1:F:406:ILE:HG22	2.00	0.42
1:A:359:VAL:N	1:A:360:PRO:CD	2.82	0.42
1:E:387:ARG:HG2	1:E:406:ILE:HG22	2.00	0.42
1:F:135:ARG:HG3	1:F:137:GLY:HA2	2.02	0.42
1:C:3:SER:O	1:C:4:GLN:CB	2.67	0.42
1:B:359:VAL:N	1:B:360:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:VAL:N	1:E:360:PRO:CD	2.83	0.41
1:A:278:ARG:O	1:A:282:LEU:HD13	2.21	0.41
1:B:143:ILE:HB	1:B:144:PRO:HD3	2.03	0.41
1:F:143:ILE:HB	1:F:144:PRO:HD3	2.02	0.41
1:C:143:ILE:HB	1:C:144:PRO:HD3	2.03	0.41
1:A:143:ILE:HB	1:A:144:PRO:HD3	2.03	0.40
1:C:359:VAL:N	1:C:360:PRO:CD	2.85	0.40
1:A:357:TRP:CD1	1:A:358:GLU:HG3	2.56	0.40
1:D:359:VAL:N	1:D:360:PRO:CD	2.84	0.40
1:F:278:ARG:O	1:F:282:LEU:HD13	2.21	0.40
1:B:357:TRP:CD1	1:B:358:GLU:HG3	2.57	0.40
1:E:143:ILE:HB	1:E:144:PRO:HD3	2.03	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)
1:C:278:ARG:NH1	1:C:378:ASP:OD2[2_454]	1.98	0.22

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/425 (91%)	379 (98%)	8 (2%)	0	100	100
1	B	387/425 (91%)	378 (98%)	8 (2%)	1 (0%)	44	55
1	C	388/425 (91%)	380 (98%)	7 (2%)	1 (0%)	44	55
1	D	391/425 (92%)	382 (98%)	9 (2%)	0	100	100
1	E	387/425 (91%)	378 (98%)	8 (2%)	1 (0%)	44	55
1	F	387/425 (91%)	376 (97%)	10 (3%)	1 (0%)	44	55
All	All	2327/2550 (91%)	2273 (98%)	50 (2%)	4 (0%)	51	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	C	4	GLN
1	E	4	GLN
1	F	136	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/332 (92%)	298 (98%)	7 (2%)	56	73
1	B	304/332 (92%)	301 (99%)	3 (1%)	80	90
1	C	305/332 (92%)	297 (97%)	8 (3%)	51	69
1	D	308/332 (93%)	303 (98%)	5 (2%)	68	82
1	E	305/332 (92%)	299 (98%)	6 (2%)	60	77
1	F	304/332 (92%)	298 (98%)	6 (2%)	60	77
All	All	1831/1992 (92%)	1796 (98%)	35 (2%)	62	78

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	61	GLN
1	A	122	SER
1	A	154	TYR
1	A	267	VAL
1	A	306	GLN
1	A	409	LEU
1	B	21	LYS
1	B	122	SER
1	B	154	TYR
1	C	9	VAL
1	C	21	LYS
1	C	122	SER

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Mol	Chain	Res	Type
1	C	154	TYR
1	C	267	VAL
1	C	287	ASN
1	C	306	GLN
1	C	409	LEU
1	D	21	LYS
1	D	154	TYR
1	D	267	VAL
1	D	306	GLN
1	D	409	LEU
1	E	21	LYS
1	E	58	GLN
1	E	122	SER
1	E	154	TYR
1	E	306	GLN
1	E	409	LEU
1	F	21	LYS
1	F	135	ARG
1	F	136	SER
1	F	154	TYR
1	F	306	GLN
1	F	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	B	292	HIS
1	F	64	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

20 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	MLC	A	1410	-	46,56,56	1.07	2 (4%)	53,83,83	1.54	4 (7%)
3	SO4	A	1411	-	4,4,4	0.41	0	6,6,6	0.06	0
3	SO4	B	1409	-	4,4,4	0.38	0	6,6,6	0.12	0
2	MLC	B	1410	-	46,56,56	1.05	2 (4%)	53,83,83	1.92	5 (9%)
3	SO4	B	1411	-	4,4,4	0.42	0	6,6,6	0.09	0
3	SO4	C	1410	-	4,4,4	0.42	0	6,6,6	0.08	0
3	SO4	C	1411	-	4,4,4	0.42	0	6,6,6	0.11	0
3	SO4	C	1412	-	4,4,4	0.40	0	6,6,6	0.09	0
2	MLC	C	1413	-	46,56,56	1.05	2 (4%)	53,83,83	1.61	5 (9%)
3	SO4	D	1410	-	4,4,4	0.40	0	6,6,6	0.10	0
2	MLC	D	1411	-	46,56,56	1.08	2 (4%)	53,83,83	1.62	5 (9%)
3	SO4	D	1412	-	4,4,4	0.42	0	6,6,6	0.09	0
3	SO4	D	1413	-	4,4,4	0.40	0	6,6,6	0.12	0
3	SO4	E	1410	-	4,4,4	0.41	0	6,6,6	0.06	0
2	MLC	E	1411	-	46,56,56	1.05	2 (4%)	53,83,83	1.52	6 (11%)
3	SO4	E	1412	-	4,4,4	0.42	0	6,6,6	0.15	0
3	SO4	F	1410	-	4,4,4	0.41	0	6,6,6	0.12	0
3	SO4	F	1411	-	4,4,4	0.41	0	6,6,6	0.08	0
2	MLC	F	1412	-	46,56,56	1.04	2 (4%)	53,83,83	1.58	5 (9%)
3	SO4	F	1413	-	4,4,4	0.41	0	6,6,6	0.08	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	MLC	A	1410	-	-	0/48/71/71	0/3/3/3
3	SO4	A	1411	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1409	-	-	0/0/0/0	0/0/0/0
2	MLC	B	1410	-	-	0/48/71/71	0/3/3/3
3	SO4	B	1411	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1410	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1411	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1412	-	-	0/0/0/0	0/0/0/0
2	MLC	C	1413	-	-	0/48/71/71	0/3/3/3
3	SO4	D	1410	-	-	0/0/0/0	0/0/0/0
2	MLC	D	1411	-	-	0/48/71/71	0/3/3/3
3	SO4	D	1412	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1413	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1410	-	-	0/0/0/0	0/0/0/0
2	MLC	E	1411	-	-	0/48/71/71	0/3/3/3
3	SO4	E	1412	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1410	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1411	-	-	0/0/0/0	0/0/0/0
2	MLC	F	1412	-	-	0/48/71/71	0/3/3/3
3	SO4	F	1413	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1411	MLC	CM1-S	-4.70	1.66	1.76
2	C	1413	MLC	CM1-S	-4.39	1.67	1.76
2	A	1410	MLC	CM1-S	-4.39	1.67	1.76
2	E	1411	MLC	CM1-S	-4.24	1.67	1.76
2	B	1410	MLC	CM1-S	-4.24	1.67	1.76
2	F	1412	MLC	CM1-S	-4.22	1.67	1.76
2	C	1413	MLC	C5-C4	3.06	1.47	1.40
2	B	1410	MLC	C5-C4	3.10	1.47	1.40
2	A	1410	MLC	C5-C4	3.11	1.47	1.40
2	D	1411	MLC	C5-C4	3.12	1.47	1.40
2	F	1412	MLC	C5-C4	3.15	1.47	1.40
2	E	1411	MLC	C5-C4	3.19	1.47	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1410	MLC	N3-C2-N1	-6.87	122.87	128.86
2	D	1411	MLC	N3-C2-N1	-6.75	122.98	128.86
2	C	1413	MLC	N3-C2-N1	-6.68	123.04	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1410	MLC	N3-C2-N1	-6.58	123.13	128.86
2	F	1412	MLC	N3-C2-N1	-6.53	123.17	128.86
2	E	1411	MLC	N3-C2-N1	-6.15	123.50	128.86
2	B	1410	MLC	OM2-CM1-S	-3.82	118.84	122.84
2	B	1410	MLC	OM2-CM1-CM2	-3.22	118.22	123.08
2	D	1411	MLC	OM2-CM1-S	-3.21	119.48	122.84
2	C	1413	MLC	C4-C5-N7	-3.12	106.39	109.41
2	D	1411	MLC	C4-C5-N7	-3.04	106.47	109.41
2	A	1410	MLC	C4-C5-N7	-2.98	106.53	109.41
2	E	1411	MLC	C4-C5-N7	-2.91	106.60	109.41
2	B	1410	MLC	C4-C5-N7	-2.70	106.80	109.41
2	A	1410	MLC	OM2-CM1-CM2	-2.61	119.15	123.08
2	F	1412	MLC	C4-C5-N7	-2.61	106.89	109.41
2	F	1412	MLC	OM2-CM1-CM2	-2.55	119.23	123.08
2	C	1413	MLC	OM2-CM1-CM2	-2.35	119.53	123.08
2	E	1411	MLC	OM2-CM1-CM2	-2.21	119.74	123.08
2	F	1412	MLC	OM2-CM1-S	-2.06	120.68	122.84
2	E	1411	MLC	CP9-CPA-CP7	2.09	112.45	108.82
2	C	1413	MLC	CP9-CPA-CPB	2.30	111.75	108.37
2	D	1411	MLC	C3'-C2'-C1'	2.34	105.22	99.95
2	E	1411	MLC	C3'-C2'-C1'	2.69	106.00	99.95
2	E	1411	MLC	CM2-CM1-S	5.56	119.31	113.42
2	C	1413	MLC	CM2-CM1-S	5.86	119.64	113.42
2	A	1410	MLC	CM2-CM1-S	5.91	119.68	113.42
2	D	1411	MLC	CM2-CM1-S	6.02	119.81	113.42
2	F	1412	MLC	CM2-CM1-S	6.29	120.09	113.42
2	B	1410	MLC	CM2-CM1-S	8.97	122.94	113.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1411	MLC	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	392/425 (92%)	0.23	15 (3%) 41 48	24, 35, 52, 73	0
1	B	392/425 (92%)	0.27	26 (6%) 19 25	24, 34, 53, 76	0
1	C	393/425 (92%)	0.39	26 (6%) 19 25	25, 40, 58, 73	0
1	D	396/425 (93%)	0.25	9 (2%) 61 67	24, 34, 53, 74	0
1	E	392/425 (92%)	0.61	43 (10%) 6 9	26, 41, 64, 87	0
1	F	391/425 (92%)	0.38	21 (5%) 26 33	25, 36, 60, 86	0
All	All	2356/2550 (92%)	0.36	140 (5%) 23 30	24, 37, 59, 87	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	409	LEU	9.3
1	C	409	LEU	7.8
1	F	75	LYS	6.8
1	D	409	LEU	6.1
1	E	269	ASP	5.7
1	A	228	GLU	5.2
1	A	75	LYS	4.8
1	E	228	GLU	4.8
1	E	268	PRO	4.6
1	E	332	ASN	4.3
1	B	231	ALA	4.3
1	B	267	VAL	4.3
1	B	73	PRO	4.3
1	F	228	GLU	4.1
1	E	187	ALA	4.1
1	E	282	LEU	4.0
1	E	267	VAL	4.0
1	B	127	GLU	4.0
1	A	409	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	264	ASP	3.7
1	D	265	ASP	3.7
1	F	409	LEU	3.7
1	E	156	SER	3.6
1	A	268	PRO	3.6
1	E	75	LYS	3.6
1	B	20	HIS	3.5
1	C	378	ASP	3.5
1	F	270	ILE	3.4
1	C	205	LEU	3.4
1	C	75	LYS	3.4
1	F	124	ALA	3.4
1	F	20	HIS	3.4
1	E	191	ASP	3.3
1	C	124	ALA	3.3
1	F	132	SER	3.3
1	C	3	SER	3.2
1	E	201	PRO	3.2
1	F	104	ARG	3.2
1	E	186	LYS	3.2
1	F	335	GLY	3.2
1	C	163	GLU	3.1
1	E	42	GLN	3.1
1	D	75	LYS	3.1
1	B	331	LEU	3.0
1	B	335	GLY	3.0
1	E	153	TRP	3.0
1	F	227	ALA	2.9
1	C	361	ALA	2.9
1	E	198	CYS	2.9
1	E	270	ILE	2.9
1	D	186	LYS	2.9
1	E	408	ASP	2.9
1	F	3	SER	2.9
1	A	74	THR	2.8
1	F	156	SER	2.8
1	E	366	THR	2.8
1	B	270	ILE	2.8
1	A	408	ASP	2.7
1	E	157	ARG	2.8
1	E	71	LEU	2.7
1	A	20	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	378	ASP	2.7
1	B	228	GLU	2.7
1	A	361	ALA	2.7
1	B	135	ARG	2.7
1	E	190	LEU	2.7
1	B	137	GLY	2.7
1	C	186	LYS	2.7
1	B	304	LEU	2.6
1	C	196	SER	2.6
1	E	188	TYR	2.6
1	C	229	HIS	2.6
1	C	269	ASP	2.6
1	F	332	ASN	2.5
1	F	128	ARG	2.5
1	F	73	PRO	2.5
1	B	140	GLU	2.5
1	E	202	VAL	2.5
1	B	269	ASP	2.5
1	E	285	ASN	2.5
1	A	121	GLY	2.5
1	E	266	ILE	2.5
1	C	382	THR	2.4
1	B	230	PHE	2.4
1	B	134	ARG	2.4
1	C	197	ARG	2.4
1	C	104	ARG	2.4
1	C	296	LEU	2.4
1	E	382	THR	2.4
1	C	266	ILE	2.3
1	F	133	LEU	2.3
1	E	74	THR	2.3
1	C	377	GLY	2.3
1	E	304	LEU	2.3
1	F	157	ARG	2.3
1	C	231	ALA	2.3
1	E	122	SER	2.3
1	A	382	THR	2.2
1	E	194	LEU	2.2
1	A	186	LYS	2.2
1	C	18	LYS	2.2
1	D	73	PRO	2.2
1	B	156	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	381	LEU	2.2
1	C	157	ARG	2.2
1	A	334	GLY	2.2
1	B	116	ALA	2.2
1	C	191	ASP	2.2
1	C	185	GLN	2.2
1	E	104	ARG	2.2
1	F	134	ARG	2.2
1	B	198	CYS	2.2
1	D	3	SER	2.2
1	C	344	ILE	2.2
1	E	3	SER	2.2
1	B	75	LYS	2.1
1	B	158	TYR	2.1
1	A	269	ASP	2.1
1	E	223	GLU	2.1
1	E	227	ALA	2.1
1	B	87	GLY	2.1
1	F	331	LEU	2.1
1	E	149	ARG	2.1
1	A	205	LEU	2.1
1	A	329	GLU	2.1
1	F	127	GLU	2.1
1	B	124	ALA	2.1
1	E	195	HIS	2.1
1	B	153	TRP	2.1
1	E	359	VAL	2.1
1	F	87	GLY	2.1
1	B	91	ILE	2.0
1	E	313	LEU	2.0
1	B	120	MET	2.0
1	D	189	THR	2.0
1	C	198[A]	CYS	2.0
1	E	278	ARG	2.0
1	C	127	GLU	2.0
1	D	195	HIS	2.0
1	E	331	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

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
2	MLC	E	1411	54/54	0.63	0.34	3.44	53,86,101,102	0
3	SO4	F	1411	5/5	0.94	0.36	3.42	65,65,67,67	0
2	MLC	B	1410	54/54	0.78	0.28	3.40	59,80,99,100	0
2	MLC	A	1410	54/54	0.66	0.31	3.27	51,71,81,82	0
3	SO4	A	1411	5/5	0.95	0.28	2.69	66,67,68,68	0
3	SO4	D	1413	5/5	0.91	0.19	2.19	63,63,66,67	0
3	SO4	C	1412	5/5	0.78	0.41	2.03	88,89,90,91	0
2	MLC	C	1413	54/54	0.73	0.27	1.98	53,84,100,103	0
2	MLC	D	1411	54/54	0.71	0.24	1.96	57,73,94,96	0
2	MLC	F	1412	54/54	0.83	0.20	1.20	52,69,84,86	0
3	SO4	B	1409	5/5	0.93	0.31	0.72	57,58,60,60	0
3	SO4	E	1412	5/5	0.86	0.23	0.36	74,76,76,77	0
3	SO4	E	1410	5/5	0.93	0.19	0.16	79,80,80,80	0
3	SO4	F	1413	5/5	0.94	0.13	-0.29	70,70,71,72	0
3	SO4	C	1411	5/5	0.96	0.14	-0.56	56,58,58,58	0
3	SO4	D	1410	5/5	0.96	0.15	-0.90	61,61,62,62	0
3	SO4	B	1411	5/5	0.83	0.32	-	78,78,81,81	0
3	SO4	C	1410	5/5	0.88	0.23	-	84,84,85,86	0
3	SO4	D	1412	5/5	0.83	0.20	-	74,74,77,77	0
3	SO4	F	1410	5/5	0.93	0.19	-	64,65,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.