



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 10, 2017 – 05:44 PM EST

PDB ID : 5LOT  
Title : Crystal structure of SCP2 thiolase from Leishmania mexicana. Complex of the C123A mutant with acetyl-CoA.  
Authors : Harijan, R.K.; Kiema, T.-R.; Wierenga, R.K.  
Deposited on : 2016-08-09  
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

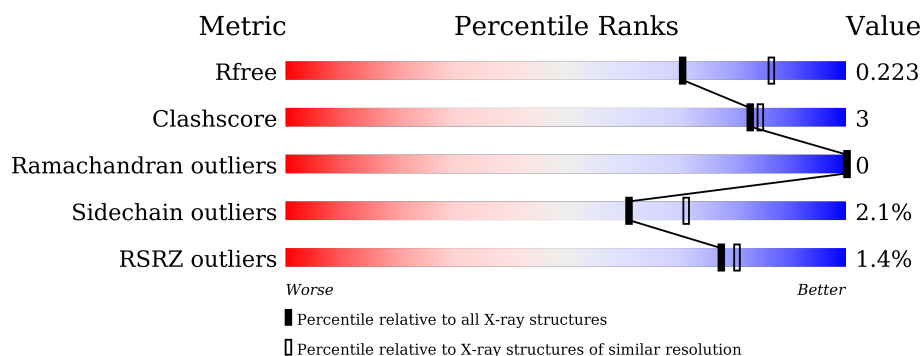
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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  $\geq 3$ , 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	457	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	457	<div> <div></div> <div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	457	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>
1	D	457	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>6%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACO	A	501	-	-	-	X
2	ACO	D	501	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13679 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 3-ketoacyl-CoA thiolase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			
1	B	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			
1	C	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			
1	D	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP E9AW84
A	-14	HIS	-	expression tag	UNP E9AW84
A	-13	HIS	-	expression tag	UNP E9AW84
A	-12	HIS	-	expression tag	UNP E9AW84
A	-11	HIS	-	expression tag	UNP E9AW84
A	-10	HIS	-	expression tag	UNP E9AW84
A	-9	SER	-	expression tag	UNP E9AW84
A	-8	SER	-	expression tag	UNP E9AW84
A	-7	GLY	-	expression tag	UNP E9AW84
A	-6	LEU	-	expression tag	UNP E9AW84
A	-5	VAL	-	expression tag	UNP E9AW84
A	-4	PRO	-	expression tag	UNP E9AW84
A	-3	ARG	-	expression tag	UNP E9AW84
A	-2	GLY	-	expression tag	UNP E9AW84
A	-1	SER	-	expression tag	UNP E9AW84
A	0	HIS	-	expression tag	UNP E9AW84
A	6	LEU	MET	conflict	UNP E9AW84
A	12	ALA	THR	conflict	UNP E9AW84
A	31	PRO	LYS	conflict	UNP E9AW84
A	34	ILE	VAL	conflict	UNP E9AW84
A	45	LYS	GLN	conflict	UNP E9AW84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	HIS	conflict	UNP E9AW84
A	61	MET	ILE	conflict	UNP E9AW84
A	63	HIS	ASN	conflict	UNP E9AW84
A	64	SER	VAL	conflict	UNP E9AW84
A	65	GLY	SER	conflict	UNP E9AW84
A	67	SER	LYS	conflict	UNP E9AW84
A	69	ARG	LYS	conflict	UNP E9AW84
A	71	GLY	ASP	conflict	UNP E9AW84
A	107	SER	ALA	conflict	UNP E9AW84
A	112	MET	ILE	conflict	UNP E9AW84
A	123	ALA	CYS	conflict	UNP E9AW84
A	134	MET	THR	conflict	UNP E9AW84
A	139	SER	ALA	conflict	UNP E9AW84
A	145	THR	VAL	conflict	UNP E9AW84
A	157	SER	THR	conflict	UNP E9AW84
A	176	GLN	LYS	conflict	UNP E9AW84
A	229	THR	SER	conflict	UNP E9AW84
A	268	VAL	ALA	conflict	UNP E9AW84
A	277	ARG	LYS	conflict	UNP E9AW84
A	327	ILE	VAL	conflict	UNP E9AW84
A	356	GLU	ASP	conflict	UNP E9AW84
A	368	ASP	GLU	conflict	UNP E9AW84
A	398	ILE	VAL	conflict	UNP E9AW84
A	410	GLU	GLY	conflict	UNP E9AW84
B	-15	HIS	-	expression tag	UNP E9AW84
B	-14	HIS	-	expression tag	UNP E9AW84
B	-13	HIS	-	expression tag	UNP E9AW84
B	-12	HIS	-	expression tag	UNP E9AW84
B	-11	HIS	-	expression tag	UNP E9AW84
B	-10	HIS	-	expression tag	UNP E9AW84
B	-9	SER	-	expression tag	UNP E9AW84
B	-8	SER	-	expression tag	UNP E9AW84
B	-7	GLY	-	expression tag	UNP E9AW84
B	-6	LEU	-	expression tag	UNP E9AW84
B	-5	VAL	-	expression tag	UNP E9AW84
B	-4	PRO	-	expression tag	UNP E9AW84
B	-3	ARG	-	expression tag	UNP E9AW84
B	-2	GLY	-	expression tag	UNP E9AW84
B	-1	SER	-	expression tag	UNP E9AW84
B	0	HIS	-	expression tag	UNP E9AW84
B	6	LEU	MET	conflict	UNP E9AW84
B	12	ALA	THR	conflict	UNP E9AW84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	PRO	LYS	conflict	UNP E9AW84
B	34	ILE	VAL	conflict	UNP E9AW84
B	45	LYS	GLN	conflict	UNP E9AW84
B	59	GLY	HIS	conflict	UNP E9AW84
B	61	MET	ILE	conflict	UNP E9AW84
B	63	HIS	ASN	conflict	UNP E9AW84
B	64	SER	VAL	conflict	UNP E9AW84
B	65	GLY	SER	conflict	UNP E9AW84
B	67	SER	LYS	conflict	UNP E9AW84
B	69	ARG	LYS	conflict	UNP E9AW84
B	71	GLY	ASP	conflict	UNP E9AW84
B	107	SER	ALA	conflict	UNP E9AW84
B	112	MET	ILE	conflict	UNP E9AW84
B	123	ALA	CYS	conflict	UNP E9AW84
B	134	MET	THR	conflict	UNP E9AW84
B	139	SER	ALA	conflict	UNP E9AW84
B	145	THR	VAL	conflict	UNP E9AW84
B	157	SER	THR	conflict	UNP E9AW84
B	176	GLN	LYS	conflict	UNP E9AW84
B	229	THR	SER	conflict	UNP E9AW84
B	268	VAL	ALA	conflict	UNP E9AW84
B	277	ARG	LYS	conflict	UNP E9AW84
B	327	ILE	VAL	conflict	UNP E9AW84
B	356	GLU	ASP	conflict	UNP E9AW84
B	368	ASP	GLU	conflict	UNP E9AW84
B	398	ILE	VAL	conflict	UNP E9AW84
B	410	GLU	GLY	conflict	UNP E9AW84
C	-15	HIS	-	expression tag	UNP E9AW84
C	-14	HIS	-	expression tag	UNP E9AW84
C	-13	HIS	-	expression tag	UNP E9AW84
C	-12	HIS	-	expression tag	UNP E9AW84
C	-11	HIS	-	expression tag	UNP E9AW84
C	-10	HIS	-	expression tag	UNP E9AW84
C	-9	SER	-	expression tag	UNP E9AW84
C	-8	SER	-	expression tag	UNP E9AW84
C	-7	GLY	-	expression tag	UNP E9AW84
C	-6	LEU	-	expression tag	UNP E9AW84
C	-5	VAL	-	expression tag	UNP E9AW84
C	-4	PRO	-	expression tag	UNP E9AW84
C	-3	ARG	-	expression tag	UNP E9AW84
C	-2	GLY	-	expression tag	UNP E9AW84
C	-1	SER	-	expression tag	UNP E9AW84

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP E9AW84
C	6	LEU	MET	conflict	UNP E9AW84
C	12	ALA	THR	conflict	UNP E9AW84
C	31	PRO	LYS	conflict	UNP E9AW84
C	34	ILE	VAL	conflict	UNP E9AW84
C	45	LYS	GLN	conflict	UNP E9AW84
C	59	GLY	HIS	conflict	UNP E9AW84
C	61	MET	ILE	conflict	UNP E9AW84
C	63	HIS	ASN	conflict	UNP E9AW84
C	64	SER	VAL	conflict	UNP E9AW84
C	65	GLY	SER	conflict	UNP E9AW84
C	67	SER	LYS	conflict	UNP E9AW84
C	69	ARG	LYS	conflict	UNP E9AW84
C	71	GLY	ASP	conflict	UNP E9AW84
C	107	SER	ALA	conflict	UNP E9AW84
C	112	MET	ILE	conflict	UNP E9AW84
C	123	ALA	CYS	conflict	UNP E9AW84
C	134	MET	THR	conflict	UNP E9AW84
C	139	SER	ALA	conflict	UNP E9AW84
C	145	THR	VAL	conflict	UNP E9AW84
C	157	SER	THR	conflict	UNP E9AW84
C	176	GLN	LYS	conflict	UNP E9AW84
C	229	THR	SER	conflict	UNP E9AW84
C	268	VAL	ALA	conflict	UNP E9AW84
C	277	ARG	LYS	conflict	UNP E9AW84
C	327	ILE	VAL	conflict	UNP E9AW84
C	356	GLU	ASP	conflict	UNP E9AW84
C	368	ASP	GLU	conflict	UNP E9AW84
C	398	ILE	VAL	conflict	UNP E9AW84
C	410	GLU	GLY	conflict	UNP E9AW84
D	-15	HIS	-	expression tag	UNP E9AW84
D	-14	HIS	-	expression tag	UNP E9AW84
D	-13	HIS	-	expression tag	UNP E9AW84
D	-12	HIS	-	expression tag	UNP E9AW84
D	-11	HIS	-	expression tag	UNP E9AW84
D	-10	HIS	-	expression tag	UNP E9AW84
D	-9	SER	-	expression tag	UNP E9AW84
D	-8	SER	-	expression tag	UNP E9AW84
D	-7	GLY	-	expression tag	UNP E9AW84
D	-6	LEU	-	expression tag	UNP E9AW84
D	-5	VAL	-	expression tag	UNP E9AW84
D	-4	PRO	-	expression tag	UNP E9AW84

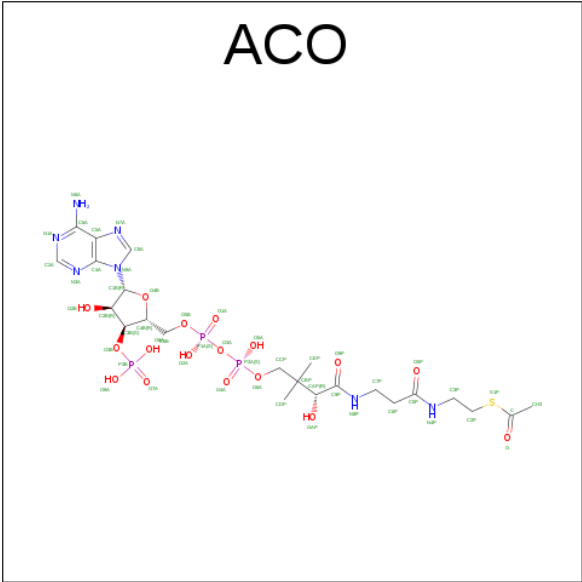
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP E9AW84
D	-2	GLY	-	expression tag	UNP E9AW84
D	-1	SER	-	expression tag	UNP E9AW84
D	0	HIS	-	expression tag	UNP E9AW84
D	6	LEU	MET	conflict	UNP E9AW84
D	12	ALA	THR	conflict	UNP E9AW84
D	31	PRO	LYS	conflict	UNP E9AW84
D	34	ILE	VAL	conflict	UNP E9AW84
D	45	LYS	GLN	conflict	UNP E9AW84
D	59	GLY	HIS	conflict	UNP E9AW84
D	61	MET	ILE	conflict	UNP E9AW84
D	63	HIS	ASN	conflict	UNP E9AW84
D	64	SER	VAL	conflict	UNP E9AW84
D	65	GLY	SER	conflict	UNP E9AW84
D	67	SER	LYS	conflict	UNP E9AW84
D	69	ARG	LYS	conflict	UNP E9AW84
D	71	GLY	ASP	conflict	UNP E9AW84
D	107	SER	ALA	conflict	UNP E9AW84
D	112	MET	ILE	conflict	UNP E9AW84
D	123	ALA	CYS	conflict	UNP E9AW84
D	134	MET	THR	conflict	UNP E9AW84
D	139	SER	ALA	conflict	UNP E9AW84
D	145	THR	VAL	conflict	UNP E9AW84
D	157	SER	THR	conflict	UNP E9AW84
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D	277	ARG	LYS	conflict	UNP E9AW84
D	327	ILE	VAL	conflict	UNP E9AW84
D	356	GLU	ASP	conflict	UNP E9AW84
D	368	ASP	GLU	conflict	UNP E9AW84
D	398	ILE	VAL	conflict	UNP E9AW84
D	410	GLU	GLY	conflict	UNP E9AW84

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).





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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	197	Total	O	0	0
			197	197		
3	C	151	Total	O	0	0
			151	151		
3	D	164	Total	O	0	0
			164	164		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.70Å 89.89Å 126.33Å 90.00° 105.78° 90.00°	Depositor
Resolution (Å)	47.30 – 2.25 47.26 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.30-2.25) 98.2 (47.26-2.25)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.213 , 0.255 0.221 , 0.223	Depositor DCC
$R_{free}$ test set	3952 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ACO

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	0.60	0/3276	0.73	3/4417 (0.1%)
1	B	0.69	2/3276 (0.1%)	0.78	7/4417 (0.2%)
1	C	0.64	1/3276 (0.0%)	0.75	4/4417 (0.1%)
1	D	0.61	0/3276	0.73	4/4417 (0.1%)
All	All	0.64	3/13104 (0.0%)	0.75	18/17668 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	GLU	CD-OE1	9.43	1.36	1.25
1	C	84	GLU	CD-OE2	5.05	1.31	1.25
1	B	84	GLU	CD-OE2	5.04	1.31	1.25

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	118	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	118	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	C	118	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	118	ARG	NE-CZ-NH2	-7.35	116.62	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3223	0	3202	25	0
1	B	3223	0	3202	20	0
1	C	3223	0	3202	21	0
1	D	3223	0	3202	14	0
2	A	51	0	34	3	0
2	B	51	0	34	1	0
2	D	51	0	34	3	0
3	A	122	0	0	5	0
3	B	197	0	0	6	0
3	C	151	0	0	6	0
3	D	164	0	0	6	0
All	All	13679	0	12910	80	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 3.

The worst 5 of 80 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:A:441:ILE:C	3:A:632:HOH:O	1.83	1.17
1:C:410:GLU:HG3	3:C:614:HOH:O	1.80	0.82
2:A:501:ACO:H8A	2:A:501:ACO:O5B	1.82	0.79
1:A:18:VAL:O	1:A:287:ARG:NH1	2.17	0.78
1:D:374:ARG:HD2	3:D:722:HOH:O	1.85	0.77

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	428/457 (94%)	420 (98%)	8 (2%)	0	100	100
1	B	428/457 (94%)	418 (98%)	10 (2%)	0	100	100
1	C	428/457 (94%)	420 (98%)	8 (2%)	0	100	100
1	D	428/457 (94%)	419 (98%)	9 (2%)	0	100	100
All	All	1712/1828 (94%)	1677 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/362 (93%)	331 (98%)	7 (2%)	61	71
1	B	338/362 (93%)	332 (98%)	6 (2%)	66	77
1	C	338/362 (93%)	330 (98%)	8 (2%)	57	67
1	D	338/362 (93%)	331 (98%)	7 (2%)	61	71
All	All	1352/1448 (93%)	1324 (98%)	28 (2%)	61	71

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	386	PHE
1	C	118	ARG
1	D	319	GLN
1	C	13	SER
1	C	45	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	316	GLN
1	C	80	ASN
1	D	316	GLN

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Mol	Chain	Res	Type
1	B	319	GLN
1	C	38	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	ACO	A	501	-	44,53,53	0.96	2 (4%)	54,79,79	1.94	12 (22%)
2	ACO	B	501	-	44,53,53	1.00	2 (4%)	54,79,79	2.00	10 (18%)
2	ACO	D	501	-	44,53,53	0.87	1 (2%)	54,79,79	2.22	15 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	A	501	-	-	0/47/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	B	501	-	-	0/47/67/67	0/3/3/3
2	ACO	D	501	-	-	3/47/67/67	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ACO	C2B-C3B	-2.87	1.46	1.53
2	A	501	ACO	P3B-O8A	-2.08	1.47	1.54
2	A	501	ACO	C5A-C4A	2.67	1.46	1.40
2	B	501	ACO	C5A-C4A	3.14	1.47	1.40
2	D	501	ACO	C5A-C4A	3.20	1.47	1.40

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	ACO	N3A-C2A-N1A	-9.42	121.47	128.87
2	A	501	ACO	N3A-C2A-N1A	-7.43	123.03	128.87
2	B	501	ACO	N3A-C2A-N1A	-7.16	123.25	128.87
2	B	501	ACO	C3P-C2P-S1P	-5.53	96.78	111.47
2	B	501	ACO	C1B-N9A-C4A	-5.12	121.09	126.81

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	ACO	CH3-C-S1P-C2P
2	D	501	ACO	O-C-S1P-C2P
2	D	501	ACO	CAP-C9P-N8P-C7P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ACO	3	0
2	B	501	ACO	1	0
2	D	501	ACO	3	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	430/457 (94%)	0.14	13 (3%) 54 58	15, 31, 59, 99	0
1	B	430/457 (94%)	-0.18	1 (0%) 95 96	12, 22, 42, 77	0
1	C	430/457 (94%)	0.11	6 (1%) 78 80	13, 28, 59, 90	0
1	D	430/457 (94%)	-0.07	4 (0%) 85 87	14, 26, 51, 89	0
All	All	1720/1828 (94%)	0.00	24 (1%) 78 80	12, 26, 54, 99	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	LYS	4.1
1	A	103	GLY	4.1
1	A	41	PHE	3.2
1	A	12	ALA	3.2
1	A	237	ASP	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	ACO	A	501	51/51	0.70	0.35	5.68	42,97,126,131	0
2	ACO	D	501	51/51	0.85	0.20	2.69	45,64,78,83	0
2	ACO	B	501	51/51	0.96	0.11	-0.50	16,21,28,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.