



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:24 am GMT

PDB ID : 2F2S  
Title : Human mitochondrial acetoacetyl-CoA thiolase  
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Deposited on : 2005-11-17  
Resolution : 2.00 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	:	1.7.2 (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

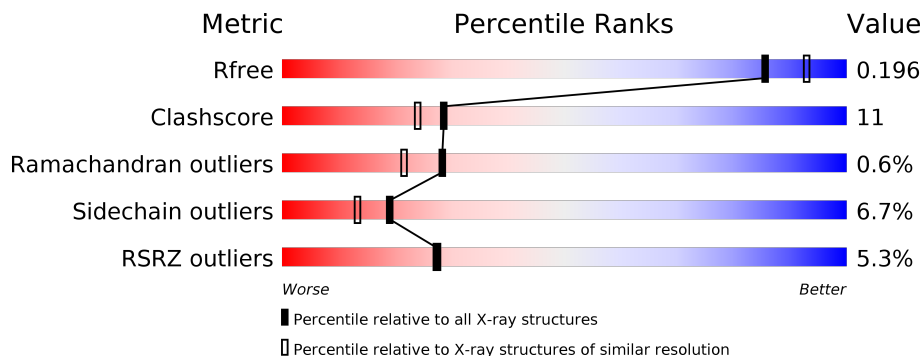
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	406	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• • •</div> </div> </div>
1	B	406	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	C	406	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	406	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>20%</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
1	SCY	A	126	-	-	X	-
1	SCY	B	126	-	-	X	-
1	SCY	C	126	-	-	X	-
1	SCY	D	126	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12020 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2834	1783	486	544	21			
1	B	386	Total	C	N	O	S	0	0	0
			2818	1773	484	540	21			
1	C	388	Total	C	N	O	S	0	0	0
			2841	1789	487	544	21			
1	D	382	Total	C	N	O	S	0	0	0
			2801	1765	478	537	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	CLONING ARTIFACT	UNP P24752
A	23	GLY	-	CLONING ARTIFACT	UNP P24752
A	24	SER	-	CLONING ARTIFACT	UNP P24752
A	25	SER	-	CLONING ARTIFACT	UNP P24752
A	26	HIS	-	EXPRESSION TAG	UNP P24752
A	27	HIS	-	EXPRESSION TAG	UNP P24752
A	28	HIS	-	EXPRESSION TAG	UNP P24752
A	29	HIS	-	EXPRESSION TAG	UNP P24752
A	30	HIS	-	EXPRESSION TAG	UNP P24752
A	31	HIS	-	EXPRESSION TAG	UNP P24752
A	32	SER	-	CLONING ARTIFACT	UNP P24752
A	33	SER	-	CLONING ARTIFACT	UNP P24752
A	34	GLY	-	CLONING ARTIFACT	UNP P24752
A	35	LEU	-	CLONING ARTIFACT	UNP P24752
A	36	VAL	-	CLONING ARTIFACT	UNP P24752
A	37	PRO	-	CLONING ARTIFACT	UNP P24752
A	38	ARG	-	CLONING ARTIFACT	UNP P24752
A	39	GLY	-	CLONING ARTIFACT	UNP P24752
A	40	SER	-	CLONING ARTIFACT	UNP P24752
A	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752
B	22	MET	-	CLONING ARTIFACT	UNP P24752

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	GLY	-	CLONING ARTIFACT	UNP P24752
B	24	SER	-	CLONING ARTIFACT	UNP P24752
B	25	SER	-	CLONING ARTIFACT	UNP P24752
B	26	HIS	-	EXPRESSION TAG	UNP P24752
B	27	HIS	-	EXPRESSION TAG	UNP P24752
B	28	HIS	-	EXPRESSION TAG	UNP P24752
B	29	HIS	-	EXPRESSION TAG	UNP P24752
B	30	HIS	-	EXPRESSION TAG	UNP P24752
B	31	HIS	-	EXPRESSION TAG	UNP P24752
B	32	SER	-	CLONING ARTIFACT	UNP P24752
B	33	SER	-	CLONING ARTIFACT	UNP P24752
B	34	GLY	-	CLONING ARTIFACT	UNP P24752
B	35	LEU	-	CLONING ARTIFACT	UNP P24752
B	36	VAL	-	CLONING ARTIFACT	UNP P24752
B	37	PRO	-	CLONING ARTIFACT	UNP P24752
B	38	ARG	-	CLONING ARTIFACT	UNP P24752
B	39	GLY	-	CLONING ARTIFACT	UNP P24752
B	40	SER	-	CLONING ARTIFACT	UNP P24752
B	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752
C	22	MET	-	CLONING ARTIFACT	UNP P24752
C	23	GLY	-	CLONING ARTIFACT	UNP P24752
C	24	SER	-	CLONING ARTIFACT	UNP P24752
C	25	SER	-	CLONING ARTIFACT	UNP P24752
C	26	HIS	-	EXPRESSION TAG	UNP P24752
C	27	HIS	-	EXPRESSION TAG	UNP P24752
C	28	HIS	-	EXPRESSION TAG	UNP P24752
C	29	HIS	-	EXPRESSION TAG	UNP P24752
C	30	HIS	-	EXPRESSION TAG	UNP P24752
C	31	HIS	-	EXPRESSION TAG	UNP P24752
C	32	SER	-	CLONING ARTIFACT	UNP P24752
C	33	SER	-	CLONING ARTIFACT	UNP P24752
C	34	GLY	-	CLONING ARTIFACT	UNP P24752
C	35	LEU	-	CLONING ARTIFACT	UNP P24752
C	36	VAL	-	CLONING ARTIFACT	UNP P24752
C	37	PRO	-	CLONING ARTIFACT	UNP P24752
C	38	ARG	-	CLONING ARTIFACT	UNP P24752
C	39	GLY	-	CLONING ARTIFACT	UNP P24752
C	40	SER	-	CLONING ARTIFACT	UNP P24752
C	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752
D	22	MET	-	CLONING ARTIFACT	UNP P24752
D	23	GLY	-	CLONING ARTIFACT	UNP P24752
D	24	SER	-	CLONING ARTIFACT	UNP P24752

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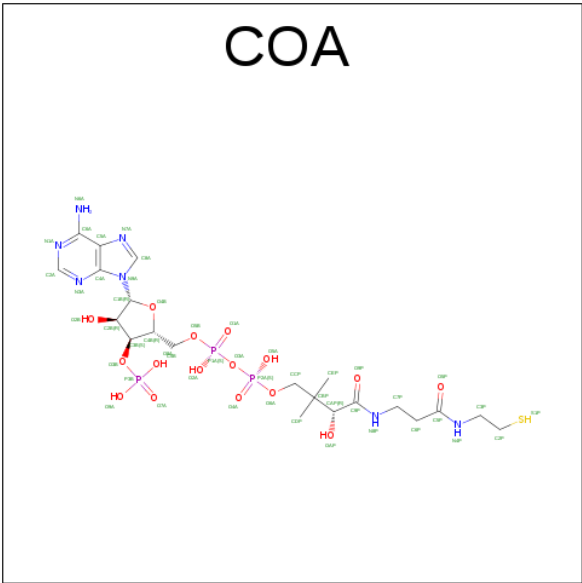
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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	SER	-	CLONING ARTIFACT	UNP P24752
D	26	HIS	-	EXPRESSION TAG	UNP P24752
D	27	HIS	-	EXPRESSION TAG	UNP P24752
D	28	HIS	-	EXPRESSION TAG	UNP P24752
D	29	HIS	-	EXPRESSION TAG	UNP P24752
D	30	HIS	-	EXPRESSION TAG	UNP P24752
D	31	HIS	-	EXPRESSION TAG	UNP P24752
D	32	SER	-	CLONING ARTIFACT	UNP P24752
D	33	SER	-	CLONING ARTIFACT	UNP P24752
D	34	GLY	-	CLONING ARTIFACT	UNP P24752
D	35	LEU	-	CLONING ARTIFACT	UNP P24752
D	36	VAL	-	CLONING ARTIFACT	UNP P24752
D	37	PRO	-	CLONING ARTIFACT	UNP P24752
D	38	ARG	-	CLONING ARTIFACT	UNP P24752
D	39	GLY	-	CLONING ARTIFACT	UNP P24752
D	40	SER	-	CLONING ARTIFACT	UNP P24752
D	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



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

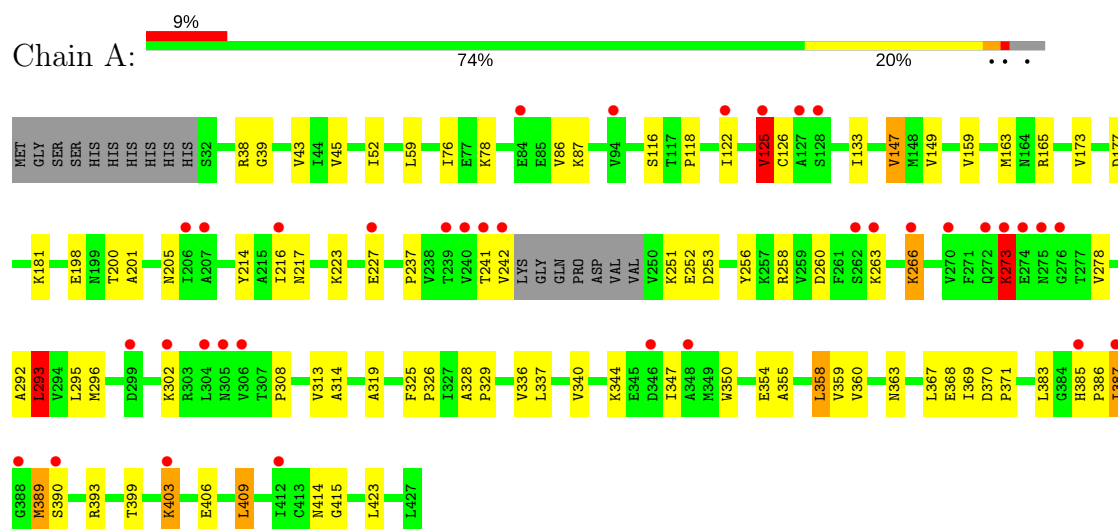
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total 99	O 99	0	0
4	B	172	Total 172	O 172	0	0
4	C	137	Total 137	O 137	0	0
4	D	123	Total 123	O 123	0	0

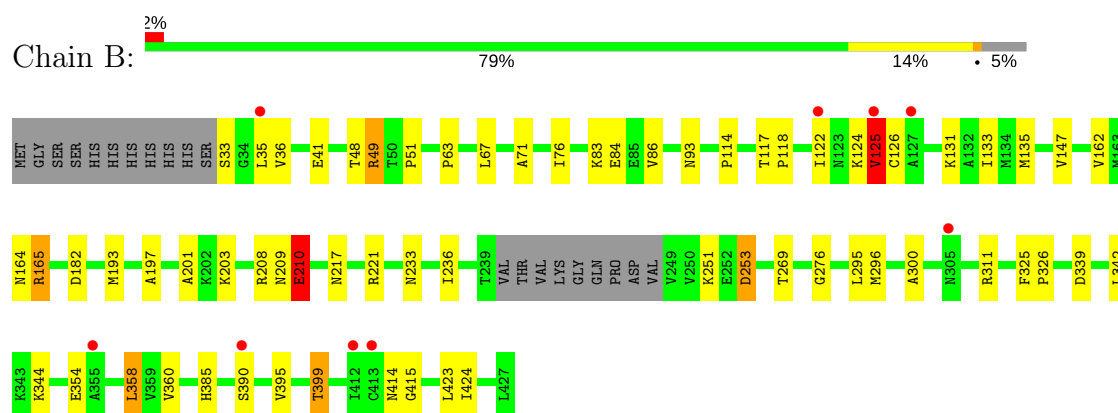
### 3 Residue-property plots [i](#)

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.

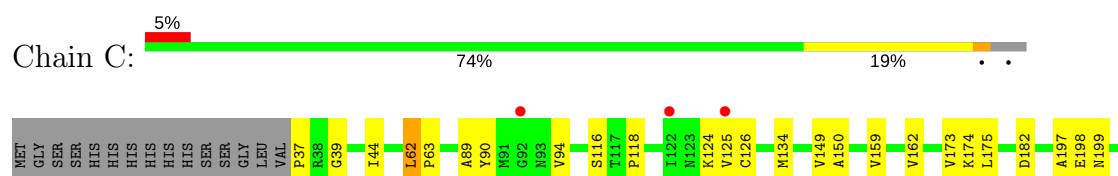
- Molecule 1: Acetyl-CoA acetyltransferase, mitochondrial



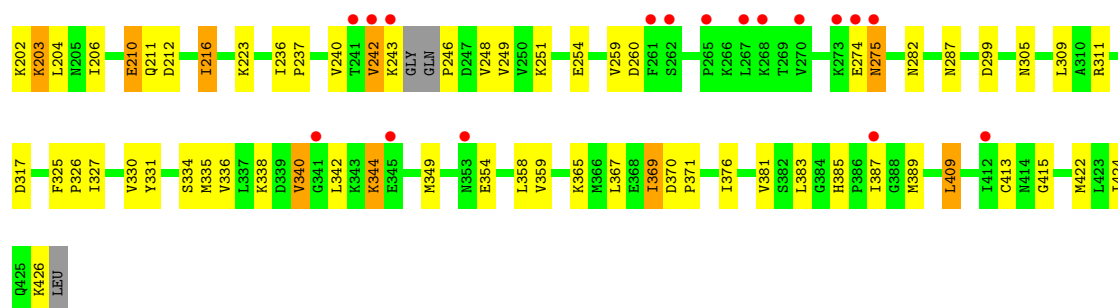
- Molecule 1: Acetyl-CoA acetyltransferase, mitochondrial



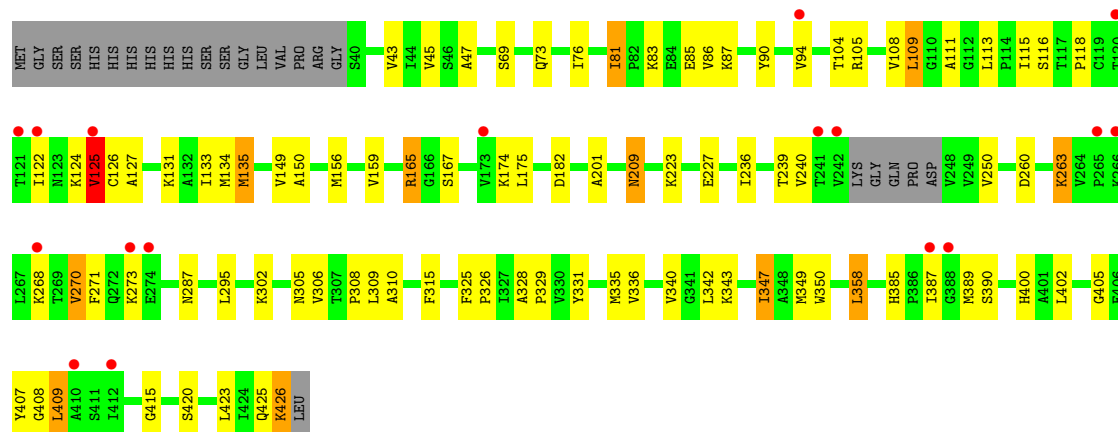
- Molecule 1: Acetyl-CoA acetyltransferase, mitochondrial







- Molecule 1: Acetyl-CoA acetyltransferase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.99Å 126.64Å 111.86Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	33.80 – 2.00 33.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (33.80-2.00) 99.0 (33.78-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.257 0.202 , 0.196	Depositor DCC
$R_{free}$ test set	5269 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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: COA, SCY, CL

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	0.78	0/2864	0.87	5/3876 (0.1%)
1	B	0.98	3/2848 (0.1%)	0.95	8/3851 (0.2%)
1	C	0.90	0/2871	0.87	3/3883 (0.1%)
1	D	0.82	0/2830	0.84	5/3828 (0.1%)
All	All	0.87	3/11413 (0.0%)	0.88	21/15438 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CG-CD	7.71	1.63	1.51
1	B	210	GLU	CB-CG	6.04	1.63	1.52
1	B	71	ALA	CA-CB	5.93	1.64	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ARG	NE-CZ-NH2	-14.14	113.23	120.30
1	A	165	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	B	49	ARG	NE-CZ-NH1	12.89	126.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	D	165	ARG	NE-CZ-NH2	-7.06	116.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	386	PRO	Peptide
1	B	125	VAL	Mainchain
1	D	425	GLN	Peptide

## 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	2834	0	2887	59	0
1	B	2818	0	2882	61	0
1	C	2841	0	2910	62	0
1	D	2801	0	2869	80	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	5	0
3	C	48	0	32	2	0
3	D	48	0	32	0	0
4	A	99	0	0	0	0
4	B	172	0	0	7	0
4	C	137	0	0	5	0
4	D	123	0	0	6	0
All	All	12020	0	11676	252	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 11.

The worst 5 of 252 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:125:VAL:C	1:A:126:SCY:H2	1.21	1.44
1:B:131:LYS:HG3	1:B:135:MET:HE2	1.08	1.07
1:B:131:LYS:HG3	1:B:135:MET:CE	1.86	1.06
1:D:426:LYS:O	1:D:426:LYS:HD3	1.58	1.03
1:D:309:LEU:O	1:D:426:LYS:HG2	1.66	0.96

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	384/406 (95%)	370 (96%)	11 (3%)	3 (1%)	22	15
1	B	381/406 (94%)	369 (97%)	10 (3%)	2 (0%)	32	26
1	C	383/406 (94%)	362 (94%)	18 (5%)	3 (1%)	22	15
1	D	377/406 (93%)	367 (97%)	9 (2%)	1 (0%)	44	40
All	All	1525/1624 (94%)	1468 (96%)	48 (3%)	9 (1%)	28	21

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	VAL
1	A	340	VAL
1	C	203	LYS
1	A	273	LYS
1	C	242	VAL

### 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	296/317 (93%)	269 (91%)	27 (9%)	11	6
1	B	296/317 (93%)	287 (97%)	9 (3%)	46	46
1	C	299/317 (94%)	277 (93%)	22 (7%)	16	10
1	D	295/317 (93%)	273 (92%)	22 (8%)	16	10
All	All	1186/1268 (94%)	1106 (93%)	80 (7%)	19	13

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	62	LEU
1	C	240	VAL
1	D	302	LYS
1	C	173	VAL
1	C	198	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	385	HIS
1	C	275	ASN
1	D	287	ASN
1	B	377	ASN
1	D	377	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SCY	A	126	1	8,8,9	1.70	1 (12%)	4,9,11	1.14	1 (25%)
1	SCY	B	126	1	8,8,9	1.41	1 (12%)	4,9,11	0.97	0
1	SCY	C	126	1	8,8,9	1.37	1 (12%)	4,9,11	1.42	1 (25%)
1	SCY	D	126	1	8,8,9	1.39	1 (12%)	4,9,11	1.42	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	A	126	1	-	1/5/7/9	0/0/0/0
1	SCY	B	126	1	-	0/5/7/9	0/0/0/0
1	SCY	C	126	1	-	0/5/7/9	0/0/0/0
1	SCY	D	126	1	-	0/5/7/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	SCY	CB-SG	-4.33	1.76	1.81
1	C	126	SCY	CB-SG	-3.55	1.77	1.81
1	D	126	SCY	CB-SG	-3.42	1.77	1.81
1	B	126	SCY	CB-SG	-3.34	1.77	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	SCY	O-C-CA	-2.55	117.97	125.02
1	C	126	SCY	O-C-CA	-2.48	118.18	125.02
1	A	126	SCY	O-C-CA	-2.28	118.73	125.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	126	SCY	OCD-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	126	SCY	10	0
1	B	126	SCY	9	0
1	C	126	SCY	7	0
1	D	126	SCY	11	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
3	COA	A	1001	-	43,50,50	1.66	3 (6%)	48,75,75	1.67	3 (6%)
3	COA	B	1002	-	43,50,50	1.64	3 (6%)	48,75,75	1.82	6 (12%)
3	COA	C	1003	-	43,50,50	1.65	3 (6%)	48,75,75	1.83	2 (4%)
3	COA	D	1004	-	43,50,50	1.69	4 (9%)	48,75,75	1.66	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	1001	-	-	0/44/64/64	0/3/3/3
3	COA	B	1002	-	-	0/44/64/64	0/3/3/3
3	COA	C	1003	-	-	0/44/64/64	0/3/3/3
3	COA	D	1004	-	-	0/44/64/64	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1004	COA	CCP-CBP	2.07	1.55	1.52
3	A	1001	COA	C2A-N1A	2.43	1.38	1.33
3	B	1002	COA	C2A-N1A	2.53	1.38	1.33
3	D	1004	COA	C2A-N1A	2.64	1.38	1.33
3	C	1003	COA	C2A-N1A	2.82	1.39	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	COA	N3A-C2A-N1A	-10.80	119.46	128.86
3	D	1004	COA	N3A-C2A-N1A	-9.84	120.29	128.86
3	A	1001	COA	N3A-C2A-N1A	-9.68	120.43	128.86
3	B	1002	COA	N3A-C2A-N1A	-9.46	120.62	128.86
3	B	1002	COA	C7P-C6P-C5P	-4.07	105.68	112.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	COA	2	0
3	B	1002	COA	5	0
3	C	1003	COA	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	388/406 (95%)	0.42	36 (9%) 9 9	30, 48, 69, 80	0
1	B	385/406 (94%)	0.04	9 (2%) 61 60	21, 34, 49, 55	0
1	C	387/406 (95%)	0.23	20 (5%) 28 28	23, 38, 60, 71	0
1	D	381/406 (93%)	0.10	17 (4%) 34 34	30, 41, 58, 67	0
All	All	1541/1624 (94%)	0.20	82 (5%) 27 27	21, 41, 63, 80	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	VAL	5.9
1	A	242	VAL	5.4
1	A	387	ILE	4.4
1	C	241	THR	4.0
1	D	273	LYS	4.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
1	SCY	D	126	9/10	0.95	0.19	-	32,34,48,50	0
1	SCY	C	126	9/10	0.90	0.22	-	31,33,48,56	0
1	SCY	B	126	9/10	0.89	0.22	-	25,28,42,51	0
1	SCY	A	126	9/10	0.81	0.29	-	43,46,53,54	0

### 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
3	COA	C	1003	48/48	0.75	0.24	1.27	69,81,93,93	0
3	COA	D	1004	48/48	0.82	0.19	1.21	57,67,78,79	0
3	COA	B	1002	48/48	0.84	0.17	0.81	44,62,71,73	0
3	COA	A	1001	48/48	0.77	0.20	0.57	71,98,105,106	0
2	CL	B	2001	1/1	1.00	0.16	0.41	29,29,29,29	0
2	CL	A	2003	1/1	0.98	0.12	-0.19	42,42,42,42	0
2	CL	B	2002	1/1	0.99	0.14	-0.22	34,34,34,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.