



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 10:00 PM EDT

PDB ID : 1M3E
Title : Succinyl-CoA:3-ketoacid CoA transferase from pig heart (selenomethionine)
Authors : Bateman, K.S.; Brownie, E.R.; Wolodko, W.T.; Fraser, M.E.
Deposited on : unknown
Resolution : 2.50 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

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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

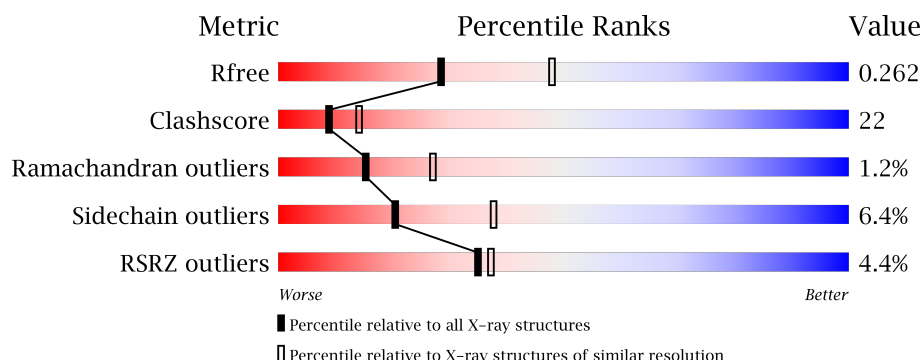
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	481	<div> <div>8%</div> <div> <div></div> <div>60%</div> <div>34%</div> <div>5%</div> </div> </div>
1	B	481	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div></div> </div> </div>
1	C	481	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>5%</div> </div> </div>
1	D	481	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>34%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15308 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 SUCCINYL-COA:3-KETOACID-COENZYME A TRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	Se	0	1	0
			3607	2284	616	689	5	13			
1	B	473	Total	C	N	O	S	Se	0	2	0
			3616	2288	620	690	5	13			
1	C	473	Total	C	N	O	S	Se	0	3	0
			3619	2289	620	692	5	13			
1	D	472	Total	C	N	O	S	Se	0	1	0
			3607	2284	616	689	5	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	195	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	278	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	298	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	349	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	359	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	363	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	375	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	384	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	388	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	402	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	414	MSE	MET	MODIFIED RESIDUE	UNP Q29551
A	476	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	72	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	195	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	278	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	298	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	349	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	359	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	363	MSE	MET	MODIFIED RESIDUE	UNP Q29551

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Chain	Residue	Modelled	Actual	Comment	Reference
B	375	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	384	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	388	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	402	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	414	MSE	MET	MODIFIED RESIDUE	UNP Q29551
B	476	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	72	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	195	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	278	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	298	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	349	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	359	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	363	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	375	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	384	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	388	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	402	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	414	MSE	MET	MODIFIED RESIDUE	UNP Q29551
C	476	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	72	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	195	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	278	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	298	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	349	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	359	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	363	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	375	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	384	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	388	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	402	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	414	MSE	MET	MODIFIED RESIDUE	UNP Q29551
D	476	MSE	MET	MODIFIED RESIDUE	UNP Q29551

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	167	Total O 167 167	0	0
2	B	269	Total O 269 269	0	0
2	C	256	Total O 256 256	0	0

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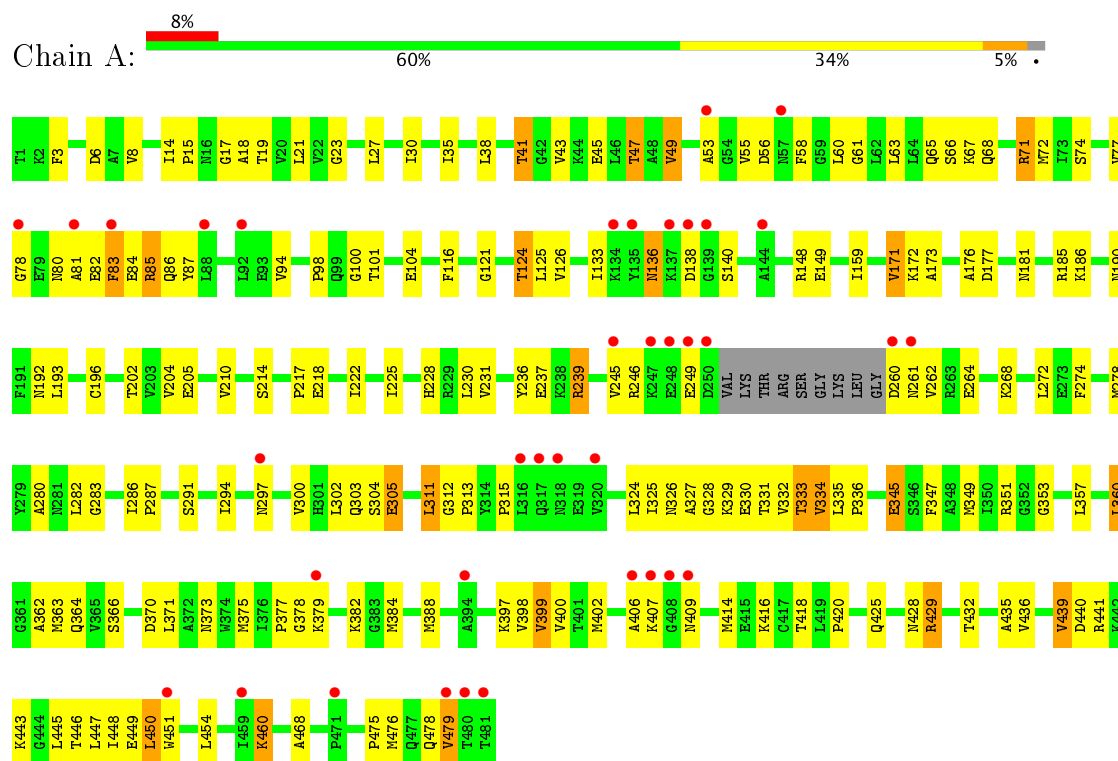
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	167	Total	O	0	0
			167	167		

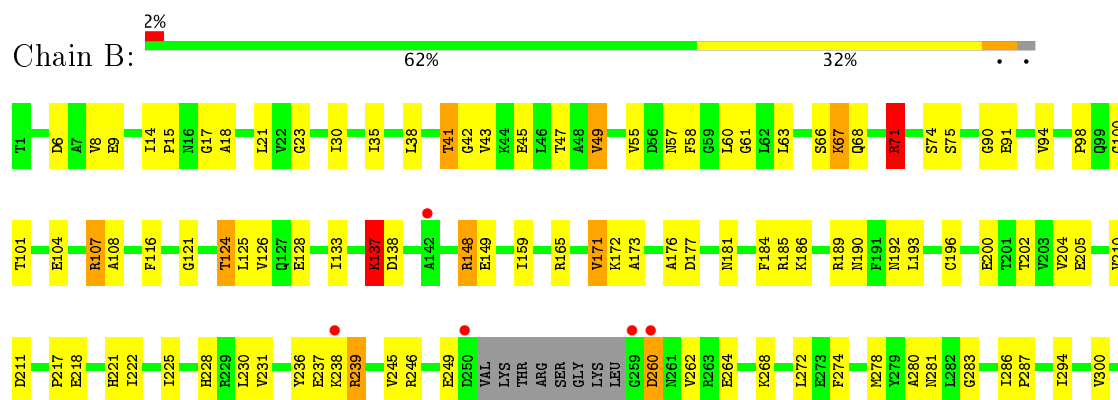
3 Residue-property plots

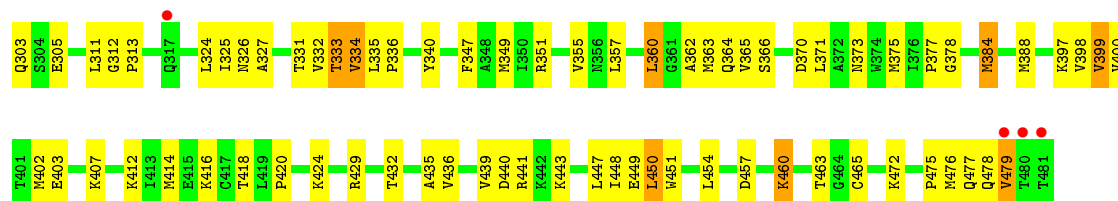
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: SUCCINYL-COA:3-KETOACID-COENZYME A TRANSFERASE

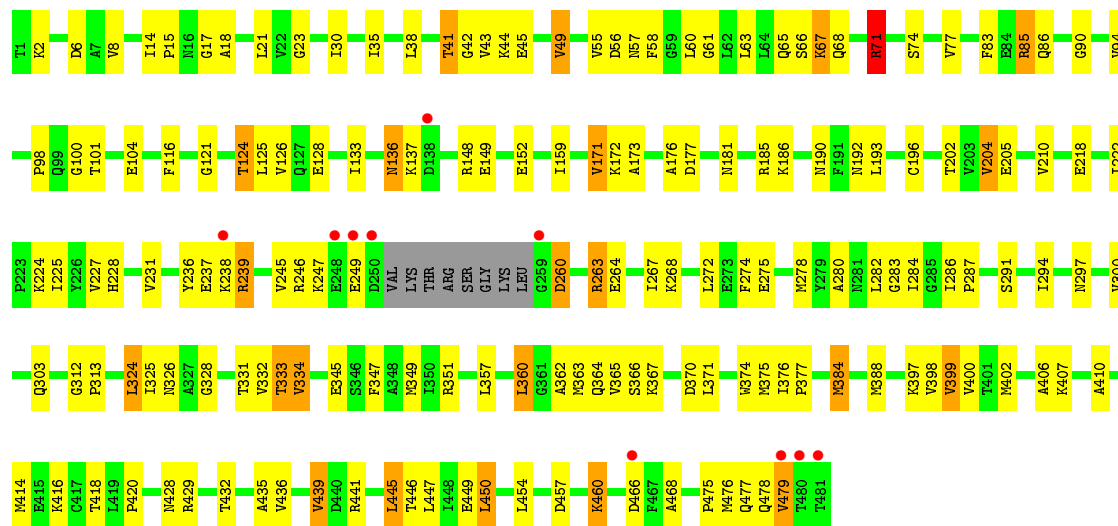


- Molecule 1: SUCCINYL-COA:3-KETOACID-COENZYME A TRANSFERASE

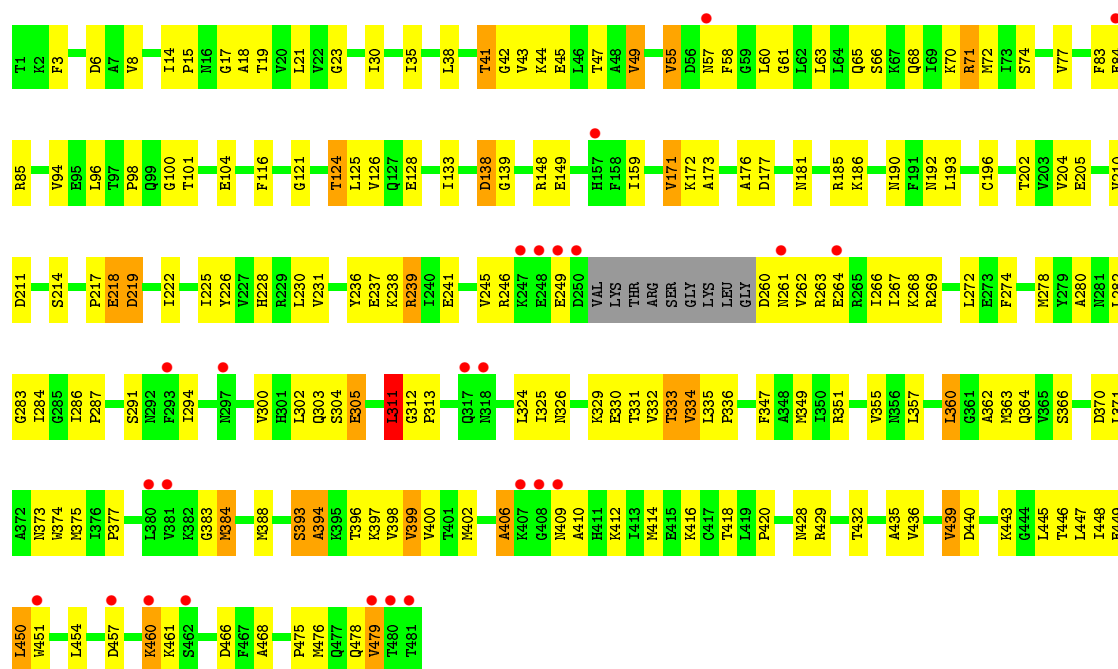




● Molecule 1: SUCCINYL-COA:3-KETOACID-COENZYME A TRANSFERASE



● Molecule 1: SUCCINYL-COA:3-KETOACID-COENZYME A TRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.17Å 264.32Å 62.69Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.50) 96.7 (29.89-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.17 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.265 0.219 , 0.262	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	1.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15308	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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](#)

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	0.36	0/3657	0.87	9/4913 (0.2%)
1	B	0.37	0/3672	0.80	6/4932 (0.1%)
1	C	0.35	0/3680	0.68	6/4943 (0.1%)
1	D	0.35	0/3656	0.67	8/4912 (0.2%)
All	All	0.36	0/14665	0.76	29/19700 (0.1%)

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	NE-CZ-NH2	-22.72	108.94	120.30
1	B	148	ARG	NE-CZ-NH2	-21.89	109.36	120.30
1	A	71	ARG	NE-CZ-NH1	21.54	131.07	120.30
1	B	148	ARG	NE-CZ-NH1	21.07	130.84	120.30
1	A	429	ARG	NE-CZ-NH2	-16.93	111.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3607	0	3665	167	0
1	B	3616	0	3673	170	0
1	C	3619	0	3669	165	0
1	D	3607	0	3663	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	167	0	0	8	0
2	B	269	0	0	22	0
2	C	256	0	0	18	0
2	D	167	0	0	12	0
All	All	15308	0	14670	655	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 22.

The worst 5 of 655 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:B:436:VAL:HG23	1:B:476:MSE:HE2	1.38	1.06
1:D:436:VAL:HG23	1:D:476:MSE:HE2	1.38	1.05
1:A:436:VAL:HG23	1:A:476:MSE:HE2	1.39	1.04
1:C:436:VAL:HG23	1:C:476:MSE:HE2	1.40	1.04
1:A:332:VAL:HG12	1:A:333:THR:H	1.24	0.99

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	469/481 (98%)	441 (94%)	25 (5%)	3 (1%)	28	48
1	B	471/481 (98%)	451 (96%)	14 (3%)	6 (1%)	14	25
1	C	472/481 (98%)	450 (95%)	17 (4%)	5 (1%)	17	29
1	D	469/481 (98%)	440 (94%)	21 (4%)	8 (2%)	11	18
All	All	1881/1924 (98%)	1782 (95%)	77 (4%)	22 (1%)	15	27

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	LYS
1	D	384	MSE
1	D	393	SER
1	D	406	ALA
1	D	138	ASP

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	387/380 (102%)	358 (92%)	29 (8%)	16	29
1	B	388/380 (102%)	365 (94%)	23 (6%)	23	42
1	C	389/380 (102%)	362 (93%)	27 (7%)	18	34
1	D	387/380 (102%)	365 (94%)	22 (6%)	24	44
All	All	1551/1520 (102%)	1450 (94%)	101 (6%)	20	37

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	384	MSE
1	C	74	SER
1	D	334	VAL
1	B	399	VAL
1	B	460	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	292	ASN
1	C	136	ASN
1	D	292	ASN
1	B	477	GLN
1	C	228	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/481 (95%)	0.37	37 (8%) 13 12	7, 27, 60, 104	0
1	B	460/481 (95%)	0.11	9 (1%) 65 67	4, 24, 51, 104	0
1	C	460/481 (95%)	0.01	10 (2%) 62 64	6, 25, 50, 105	0
1	D	459/481 (95%)	0.31	25 (5%) 26 27	9, 28, 53, 105	0
All	All	1838/1924 (95%)	0.20	81 (4%) 35 37	4, 26, 53, 105	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	480	THR	6.9
1	D	250	ASP	6.5
1	C	259	GLY	6.4
1	A	480	THR	6.2
1	A	138	ASP	5.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.