



wwPDB X-ray Structure Validation Summary Report

May 29, 2014 – 02:43 AM EDT

PDB ID : 4LCM
Title : Simvastatin Synthase (LOVD), from Aspergillus Terreus, LovD9 mutant (simh9014)
Authors : Gao, X.; Sawaya, M.R.; Yeates, T.O.; Tang, Y.
Deposited on : 2013-06-21
Resolution : 3.19 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

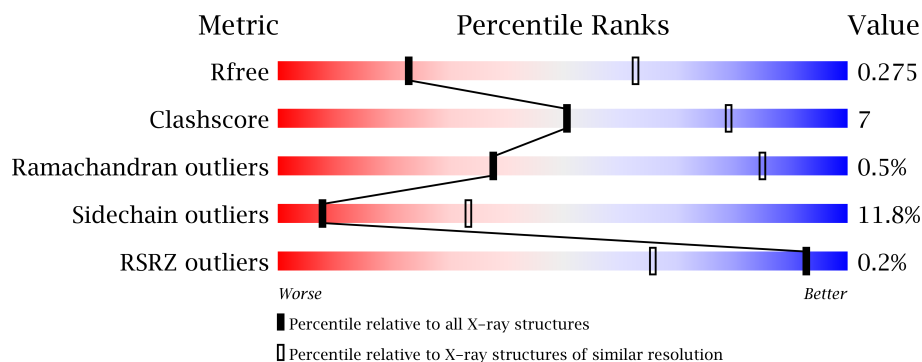
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 3.19 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	
1	C	421	
1	D	421	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12356 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3086	1942	555	565	24			
1	B	393	Total	C	N	O	S	0	0	0
			3086	1942	555	565	24			
1	C	393	Total	C	N	O	S	0	0	0
			3086	1942	555	565	24			
1	D	393	Total	C	N	O	S	0	0	0
			3086	1942	555	565	24			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLU	LYS	ENGINEERED MUTATION	UNP Q9Y7D1
A	28	SER	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
A	35	LEU	ILE	ENGINEERED MUTATION	UNP Q9Y7D1
A	40	ALA	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
A	43	ARG	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
A	60	ASN	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
A	96	ARG	ASP	ENGINEERED MUTATION	UNP Q9Y7D1
A	109	CYS	SER	ENGINEERED MUTATION	UNP Q9Y7D1
A	123	PRO	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
A	157	VAL	MET	ENGINEERED MUTATION	UNP Q9Y7D1
A	164	GLY	SER	ENGINEERED MUTATION	UNP Q9Y7D1
A	172	ASN	SER	ENGINEERED MUTATION	UNP Q9Y7D1
A	174	PHE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
A	178	LEU	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
A	191	GLY	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
A	192	ILE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
A	241	MET	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
A	247	SER	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
A	250	LYS	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
A	256	THR	SER	ENGINEERED MUTATION	UNP Q9Y7D1
A	275	SER	GLY	ENGINEERED MUTATION	UNP Q9Y7D1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLY	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
A	335	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
A	361	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
A	370	ILE	VAL	ENGINEERED MUTATION	UNP Q9Y7D1
A	383	VAL	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
A	391	SER	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
A	404	LYS	HIS	ENGINEERED MUTATION	UNP Q9Y7D1
B	26	GLU	LYS	ENGINEERED MUTATION	UNP Q9Y7D1
B	28	SER	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
B	35	LEU	ILE	ENGINEERED MUTATION	UNP Q9Y7D1
B	40	ALA	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
B	43	ARG	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
B	60	ASN	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
B	96	ARG	ASP	ENGINEERED MUTATION	UNP Q9Y7D1
B	109	CYS	SER	ENGINEERED MUTATION	UNP Q9Y7D1
B	123	PRO	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
B	157	VAL	MET	ENGINEERED MUTATION	UNP Q9Y7D1
B	164	GLY	SER	ENGINEERED MUTATION	UNP Q9Y7D1
B	172	ASN	SER	ENGINEERED MUTATION	UNP Q9Y7D1
B	174	PHE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
B	178	LEU	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
B	191	GLY	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
B	192	ILE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
B	241	MET	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
B	247	SER	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
B	250	LYS	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
B	256	THR	SER	ENGINEERED MUTATION	UNP Q9Y7D1
B	275	SER	GLY	ENGINEERED MUTATION	UNP Q9Y7D1
B	297	GLY	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
B	335	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
B	361	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
B	370	ILE	VAL	ENGINEERED MUTATION	UNP Q9Y7D1
B	383	VAL	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
B	391	SER	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
B	404	LYS	HIS	ENGINEERED MUTATION	UNP Q9Y7D1
C	26	GLU	LYS	ENGINEERED MUTATION	UNP Q9Y7D1
C	28	SER	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
C	35	LEU	ILE	ENGINEERED MUTATION	UNP Q9Y7D1
C	40	ALA	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
C	43	ARG	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
C	60	ASN	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
C	96	ARG	ASP	ENGINEERED MUTATION	UNP Q9Y7D1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	109	CYS	SER	ENGINEERED MUTATION	UNP Q9Y7D1
C	123	PRO	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
C	157	VAL	MET	ENGINEERED MUTATION	UNP Q9Y7D1
C	164	GLY	SER	ENGINEERED MUTATION	UNP Q9Y7D1
C	172	ASN	SER	ENGINEERED MUTATION	UNP Q9Y7D1
C	174	PHE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
C	178	LEU	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
C	191	GLY	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
C	192	ILE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
C	241	MET	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
C	247	SER	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
C	250	LYS	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
C	256	THR	SER	ENGINEERED MUTATION	UNP Q9Y7D1
C	275	SER	GLY	ENGINEERED MUTATION	UNP Q9Y7D1
C	297	GLY	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
C	335	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
C	361	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
C	370	ILE	VAL	ENGINEERED MUTATION	UNP Q9Y7D1
C	383	VAL	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
C	391	SER	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
C	404	LYS	HIS	ENGINEERED MUTATION	UNP Q9Y7D1
D	26	GLU	LYS	ENGINEERED MUTATION	UNP Q9Y7D1
D	28	SER	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
D	35	LEU	ILE	ENGINEERED MUTATION	UNP Q9Y7D1
D	40	ALA	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
D	43	ARG	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
D	60	ASN	CYS	ENGINEERED MUTATION	UNP Q9Y7D1
D	96	ARG	ASP	ENGINEERED MUTATION	UNP Q9Y7D1
D	109	CYS	SER	ENGINEERED MUTATION	UNP Q9Y7D1
D	123	PRO	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
D	157	VAL	MET	ENGINEERED MUTATION	UNP Q9Y7D1
D	164	GLY	SER	ENGINEERED MUTATION	UNP Q9Y7D1
D	172	ASN	SER	ENGINEERED MUTATION	UNP Q9Y7D1
D	174	PHE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
D	178	LEU	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
D	191	GLY	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
D	192	ILE	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
D	241	MET	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
D	247	SER	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
D	250	LYS	ARG	ENGINEERED MUTATION	UNP Q9Y7D1
D	256	THR	SER	ENGINEERED MUTATION	UNP Q9Y7D1
D	275	SER	GLY	ENGINEERED MUTATION	UNP Q9Y7D1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	297	GLY	GLN	ENGINEERED MUTATION	UNP Q9Y7D1
D	335	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
D	361	MET	LEU	ENGINEERED MUTATION	UNP Q9Y7D1
D	370	ILE	VAL	ENGINEERED MUTATION	UNP Q9Y7D1
D	383	VAL	ALA	ENGINEERED MUTATION	UNP Q9Y7D1
D	391	SER	ASN	ENGINEERED MUTATION	UNP Q9Y7D1
D	404	LYS	HIS	ENGINEERED MUTATION	UNP Q9Y7D1

- Molecule 2 is water.

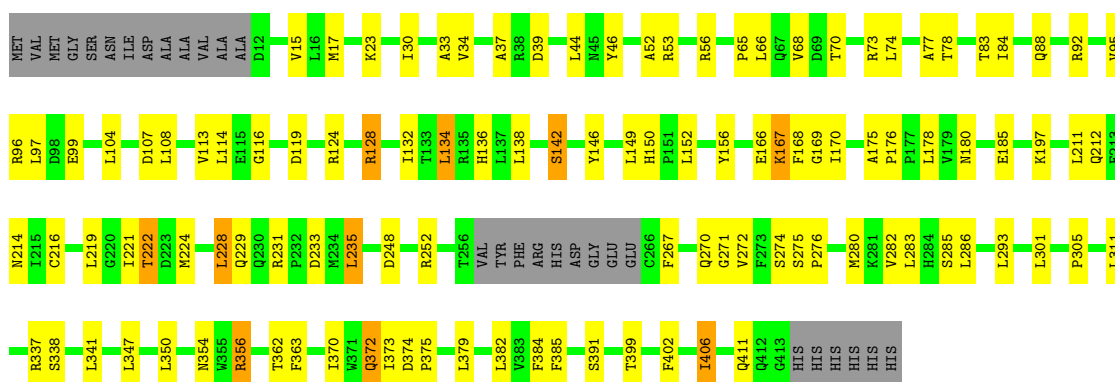
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	2	Total O 2 2	0	0
2	C	4	Total O 4 4	0	0
2	D	3	Total O 3 3	0	0

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 errors 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.

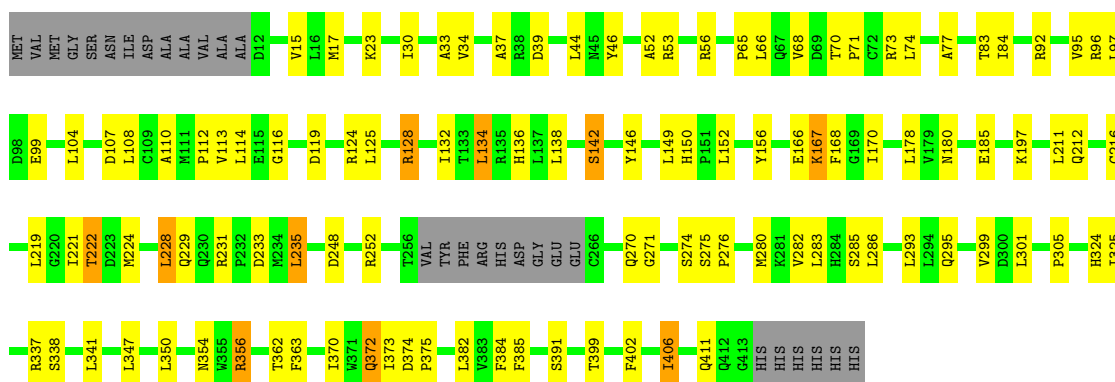
• Molecule 1: Transesterase

Chain A:



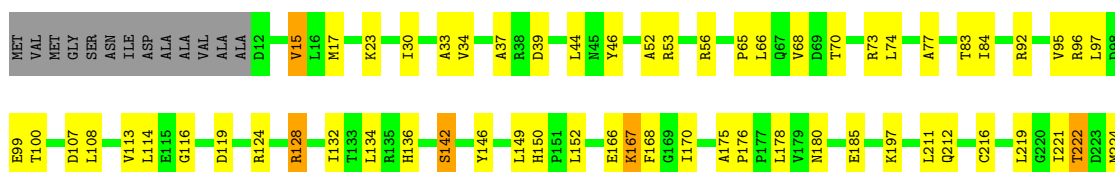
• Molecule 1: Transesterase

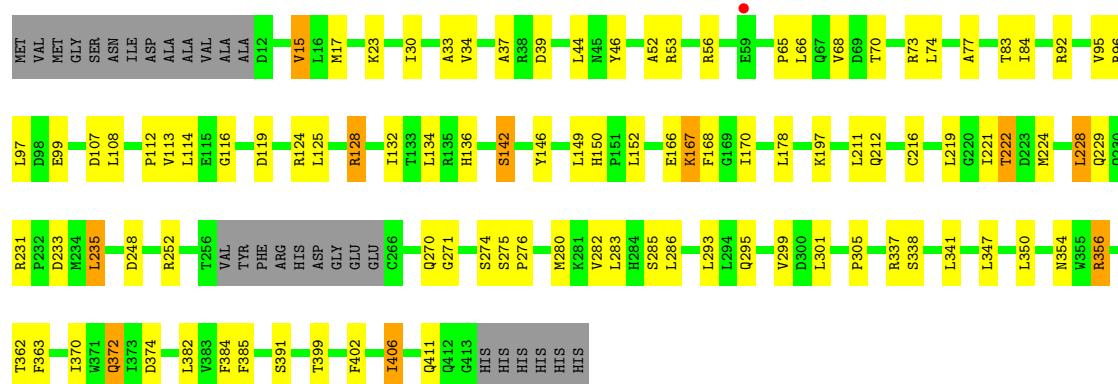
Chain B:



• Molecule 1: Transesterase

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.31Å 83.94Å 99.20Å 102.56° 89.02° 107.64°	Depositor
Resolution (Å)	19.66 – 3.19 19.66 – 3.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.66-3.19) 92.7 (19.66-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.22Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.208 , 0.252 0.224 , 0.275	Depositor DCC
R_{free} test set	1301 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.4	EDS
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 25938 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12356	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 23.64 % 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 4.4796e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.53	0/3152	0.79	0/4264
1	B	0.51	0/3152	0.78	0/4264
1	C	0.51	0/3152	0.78	0/4264
1	D	0.52	0/3152	0.78	0/4264
All	All	0.52	0/12608	0.78	0/17056

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3086	0	3069	51	0
1	B	3086	0	3069	50	0
1	C	3086	0	3069	43	0
1	D	3086	0	3069	43	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
All	All	12356	0	12276	183	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 183 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:ARG:HB3	1:A:99:GLU:HB2	1.56	0.87
1:C:96:ARG:HB3	1:C:99:GLU:HB2	1.56	0.87
1:B:96:ARG:HB3	1:B:99:GLU:HB2	1.56	0.86
1:D:96:ARG:HB3	1:D:99:GLU:HB2	1.57	0.85
1:C:15:VAL:HG11	1:D:15:VAL:HG11	1.59	0.82

There are no symmetry-related clashes.

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	389/421 (92%)	358 (92%)	29 (8%)	2 (0%)	38	85
1	B	389/421 (92%)	358 (92%)	29 (8%)	2 (0%)	38	85
1	C	389/421 (92%)	358 (92%)	29 (8%)	2 (0%)	38	85
1	D	389/421 (92%)	359 (92%)	28 (7%)	2 (0%)	38	85
All	All	1556/1684 (92%)	1433 (92%)	115 (7%)	8 (0%)	38	85

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	GLY
1	B	271	GLY
1	C	271	GLY
1	D	271	GLY
1	A	356	ARG

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	330/352 (94%)	290 (88%)	40 (12%)	7	32
1	B	330/352 (94%)	291 (88%)	39 (12%)	8	33
1	C	330/352 (94%)	291 (88%)	39 (12%)	8	33
1	D	330/352 (94%)	292 (88%)	38 (12%)	8	35
All	All	1320/1408 (94%)	1164 (88%)	156 (12%)	8	33

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	301	LEU
1	C	97	LEU
1	D	248	ASP
1	B	341	LEU
1	C	15	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	372	GLN
1	C	212	GLN
1	D	212	GLN
1	B	295	GLN
1	D	229	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	393/421 (93%)	-0.22	0	100 100	14, 42, 75, 105	0
1	B	393/421 (93%)	-0.12	0	100 100	18, 51, 84, 115	0
1	C	393/421 (93%)	-0.16	2 (0%)	88 46	22, 49, 87, 114	0
1	D	393/421 (93%)	-0.18	1 (0%)	91 58	19, 46, 76, 116	0
All	All	1572/1684 (93%)	-0.17	3 (0%)	93 66	14, 48, 81, 116	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	413	GLY	2.4
1	C	412	GLN	2.1
1	D	59	GLU	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.