



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:40 am GMT

PDB ID : 2HW5
Title : The crystal structure of human enoyl-coenzyme A (CoA) hydratase short chain 1, ECHS1
Authors : Turnbull, A.P.; Salah, E.; Niesen, F.; Debreczeni, J.; Ugochukwu, E.; Pike, A.C.W.; Kavanagh, K.; Gileadi, O.; Gorrec, F.; Umeano, C.; von Delft, F.; Weigelt, J.; Edwards, A.; Arrowsmith, C.; Sundstrom, M.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2006-07-31
Resolution : 2.55 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

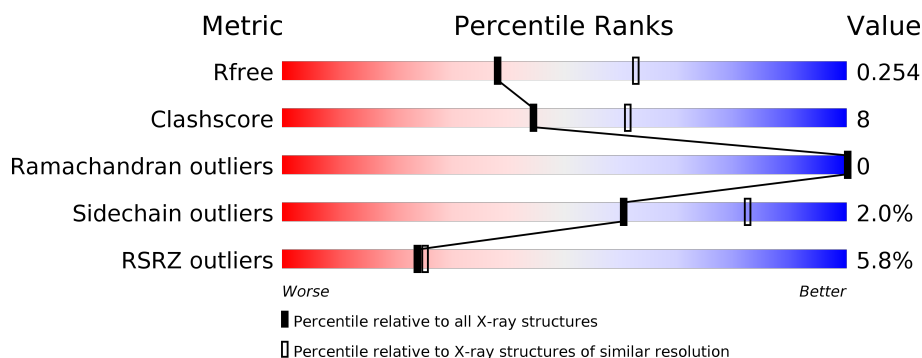
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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	286	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	286	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	286	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	286	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	286	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	286	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>•</div> <div>9%</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	MG	A	291	-	-	-	X
2	MG	C	291	-	-	-	X
2	MG	C	292	-	-	-	X
2	MG	D	291	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11556 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 Enoyl-CoA hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1924	1216	320	374	14			
1	B	260	Total	C	N	O	S	0	2	0
			1934	1228	323	369	14			
1	C	260	Total	C	N	O	S	0	0	0
			1916	1213	321	368	14			
1	D	260	Total	C	N	O	S	0	1	0
			1924	1217	323	370	14			
1	E	260	Total	C	N	O	S	0	0	0
			1872	1185	309	364	14			
1	F	260	Total	C	N	O	S	0	1	0
			1912	1206	320	372	14			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	INITIATING METHIONINE	UNP P30084
A	6	HIS	-	EXPRESSION TAG	UNP P30084
A	7	HIS	-	EXPRESSION TAG	UNP P30084
A	8	HIS	-	EXPRESSION TAG	UNP P30084
A	9	HIS	-	EXPRESSION TAG	UNP P30084
A	10	HIS	-	EXPRESSION TAG	UNP P30084
A	11	HIS	-	EXPRESSION TAG	UNP P30084
A	12	SER	-	CLONING ARTIFACT	UNP P30084
A	13	SER	-	CLONING ARTIFACT	UNP P30084
A	14	GLY	-	CLONING ARTIFACT	UNP P30084
A	15	VAL	-	CLONING ARTIFACT	UNP P30084
A	16	ASP	-	CLONING ARTIFACT	UNP P30084
A	17	LEU	-	CLONING ARTIFACT	UNP P30084
A	18	GLY	-	CLONING ARTIFACT	UNP P30084
A	19	THR	-	CLONING ARTIFACT	UNP P30084
A	20	GLU	-	CLONING ARTIFACT	UNP P30084
A	21	ASN	-	CLONING ARTIFACT	UNP P30084

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	LEU	-	CLONING ARTIFACT	UNP P30084
A	23	TYR	-	CLONING ARTIFACT	UNP P30084
A	24	PHE	-	CLONING ARTIFACT	UNP P30084
A	25	GLN	-	CLONING ARTIFACT	UNP P30084
A	26	SER	-	CLONING ARTIFACT	UNP P30084
A	27	MET	-	CLONING ARTIFACT	UNP P30084
A	75	ILE	THR	VARIANT	UNP P30084
B	5	MET	-	INITIATING METHIONINE	UNP P30084
B	6	HIS	-	EXPRESSION TAG	UNP P30084
B	7	HIS	-	EXPRESSION TAG	UNP P30084
B	8	HIS	-	EXPRESSION TAG	UNP P30084
B	9	HIS	-	EXPRESSION TAG	UNP P30084
B	10	HIS	-	EXPRESSION TAG	UNP P30084
B	11	HIS	-	EXPRESSION TAG	UNP P30084
B	12	SER	-	CLONING ARTIFACT	UNP P30084
B	13	SER	-	CLONING ARTIFACT	UNP P30084
B	14	GLY	-	CLONING ARTIFACT	UNP P30084
B	15	VAL	-	CLONING ARTIFACT	UNP P30084
B	16	ASP	-	CLONING ARTIFACT	UNP P30084
B	17	LEU	-	CLONING ARTIFACT	UNP P30084
B	18	GLY	-	CLONING ARTIFACT	UNP P30084
B	19	THR	-	CLONING ARTIFACT	UNP P30084
B	20	GLU	-	CLONING ARTIFACT	UNP P30084
B	21	ASN	-	CLONING ARTIFACT	UNP P30084
B	22	LEU	-	CLONING ARTIFACT	UNP P30084
B	23	TYR	-	CLONING ARTIFACT	UNP P30084
B	24	PHE	-	CLONING ARTIFACT	UNP P30084
B	25	GLN	-	CLONING ARTIFACT	UNP P30084
B	26	SER	-	CLONING ARTIFACT	UNP P30084
B	27	MET	-	CLONING ARTIFACT	UNP P30084
B	75	ILE	THR	VARIANT	UNP P30084
C	5	MET	-	INITIATING METHIONINE	UNP P30084
C	6	HIS	-	EXPRESSION TAG	UNP P30084
C	7	HIS	-	EXPRESSION TAG	UNP P30084
C	8	HIS	-	EXPRESSION TAG	UNP P30084
C	9	HIS	-	EXPRESSION TAG	UNP P30084
C	10	HIS	-	EXPRESSION TAG	UNP P30084
C	11	HIS	-	EXPRESSION TAG	UNP P30084
C	12	SER	-	CLONING ARTIFACT	UNP P30084
C	13	SER	-	CLONING ARTIFACT	UNP P30084
C	14	GLY	-	CLONING ARTIFACT	UNP P30084
C	15	VAL	-	CLONING ARTIFACT	UNP P30084

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	ASP	-	CLONING ARTIFACT	UNP P30084
C	17	LEU	-	CLONING ARTIFACT	UNP P30084
C	18	GLY	-	CLONING ARTIFACT	UNP P30084
C	19	THR	-	CLONING ARTIFACT	UNP P30084
C	20	GLU	-	CLONING ARTIFACT	UNP P30084
C	21	ASN	-	CLONING ARTIFACT	UNP P30084
C	22	LEU	-	CLONING ARTIFACT	UNP P30084
C	23	TYR	-	CLONING ARTIFACT	UNP P30084
C	24	PHE	-	CLONING ARTIFACT	UNP P30084
C	25	GLN	-	CLONING ARTIFACT	UNP P30084
C	26	SER	-	CLONING ARTIFACT	UNP P30084
C	27	MET	-	CLONING ARTIFACT	UNP P30084
C	75	ILE	THR	VARIANT	UNP P30084
D	5	MET	-	INITIATING METHIONINE	UNP P30084
D	6	HIS	-	EXPRESSION TAG	UNP P30084
D	7	HIS	-	EXPRESSION TAG	UNP P30084
D	8	HIS	-	EXPRESSION TAG	UNP P30084
D	9	HIS	-	EXPRESSION TAG	UNP P30084
D	10	HIS	-	EXPRESSION TAG	UNP P30084
D	11	HIS	-	EXPRESSION TAG	UNP P30084
D	12	SER	-	CLONING ARTIFACT	UNP P30084
D	13	SER	-	CLONING ARTIFACT	UNP P30084
D	14	GLY	-	CLONING ARTIFACT	UNP P30084
D	15	VAL	-	CLONING ARTIFACT	UNP P30084
D	16	ASP	-	CLONING ARTIFACT	UNP P30084
D	17	LEU	-	CLONING ARTIFACT	UNP P30084
D	18	GLY	-	CLONING ARTIFACT	UNP P30084
D	19	THR	-	CLONING ARTIFACT	UNP P30084
D	20	GLU	-	CLONING ARTIFACT	UNP P30084
D	21	ASN	-	CLONING ARTIFACT	UNP P30084
D	22	LEU	-	CLONING ARTIFACT	UNP P30084
D	23	TYR	-	CLONING ARTIFACT	UNP P30084
D	24	PHE	-	CLONING ARTIFACT	UNP P30084
D	25	GLN	-	CLONING ARTIFACT	UNP P30084
D	26	SER	-	CLONING ARTIFACT	UNP P30084
D	27	MET	-	CLONING ARTIFACT	UNP P30084
D	75	ILE	THR	VARIANT	UNP P30084
E	5	MET	-	INITIATING METHIONINE	UNP P30084
E	6	HIS	-	EXPRESSION TAG	UNP P30084
E	7	HIS	-	EXPRESSION TAG	UNP P30084
E	8	HIS	-	EXPRESSION TAG	UNP P30084
E	9	HIS	-	EXPRESSION TAG	UNP P30084

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	HIS	-	EXPRESSION TAG	UNP P30084
E	11	HIS	-	EXPRESSION TAG	UNP P30084
E	12	SER	-	CLONING ARTIFACT	UNP P30084
E	13	SER	-	CLONING ARTIFACT	UNP P30084
E	14	GLY	-	CLONING ARTIFACT	UNP P30084
E	15	VAL	-	CLONING ARTIFACT	UNP P30084
E	16	ASP	-	CLONING ARTIFACT	UNP P30084
E	17	LEU	-	CLONING ARTIFACT	UNP P30084
E	18	GLY	-	CLONING ARTIFACT	UNP P30084
E	19	THR	-	CLONING ARTIFACT	UNP P30084
E	20	GLU	-	CLONING ARTIFACT	UNP P30084
E	21	ASN	-	CLONING ARTIFACT	UNP P30084
E	22	LEU	-	CLONING ARTIFACT	UNP P30084
E	23	TYR	-	CLONING ARTIFACT	UNP P30084
E	24	PHE	-	CLONING ARTIFACT	UNP P30084
E	25	GLN	-	CLONING ARTIFACT	UNP P30084
E	26	SER	-	CLONING ARTIFACT	UNP P30084
E	27	MET	-	CLONING ARTIFACT	UNP P30084
E	75	ILE	THR	VARIANT	UNP P30084
F	5	MET	-	INITIATING METHIONINE	UNP P30084
F	6	HIS	-	EXPRESSION TAG	UNP P30084
F	7	HIS	-	EXPRESSION TAG	UNP P30084
F	8	HIS	-	EXPRESSION TAG	UNP P30084
F	9	HIS	-	EXPRESSION TAG	UNP P30084
F	10	HIS	-	EXPRESSION TAG	UNP P30084
F	11	HIS	-	EXPRESSION TAG	UNP P30084
F	12	SER	-	CLONING ARTIFACT	UNP P30084
F	13	SER	-	CLONING ARTIFACT	UNP P30084
F	14	GLY	-	CLONING ARTIFACT	UNP P30084
F	15	VAL	-	CLONING ARTIFACT	UNP P30084
F	16	ASP	-	CLONING ARTIFACT	UNP P30084
F	17	LEU	-	CLONING ARTIFACT	UNP P30084
F	18	GLY	-	CLONING ARTIFACT	UNP P30084
F	19	THR	-	CLONING ARTIFACT	UNP P30084
F	20	GLU	-	CLONING ARTIFACT	UNP P30084
F	21	ASN	-	CLONING ARTIFACT	UNP P30084
F	22	LEU	-	CLONING ARTIFACT	UNP P30084
F	23	TYR	-	CLONING ARTIFACT	UNP P30084
F	24	PHE	-	CLONING ARTIFACT	UNP P30084
F	25	GLN	-	CLONING ARTIFACT	UNP P30084
F	26	SER	-	CLONING ARTIFACT	UNP P30084
F	27	MET	-	CLONING ARTIFACT	UNP P30084

Continued on next page...

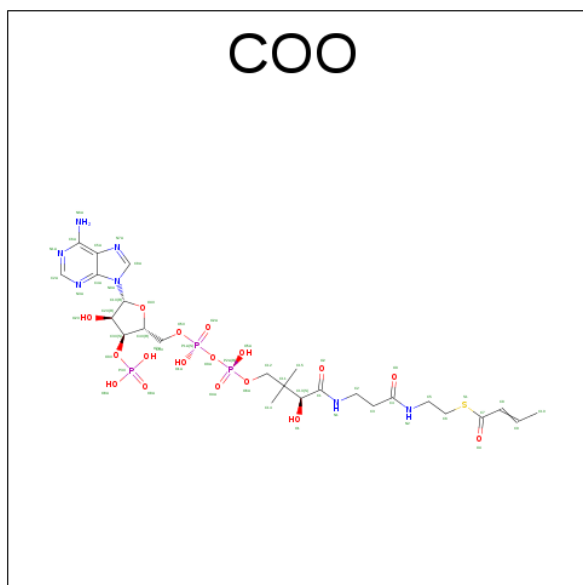
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	75	ILE	THR	VARIANT	UNP P30084

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	2	Total Mg 2 2	0	0

- Molecule 3 is CROTONYL COENZYME A (three-letter code: COO) (formula: C₂₅H₄₀N₇O₁₇P₃S).

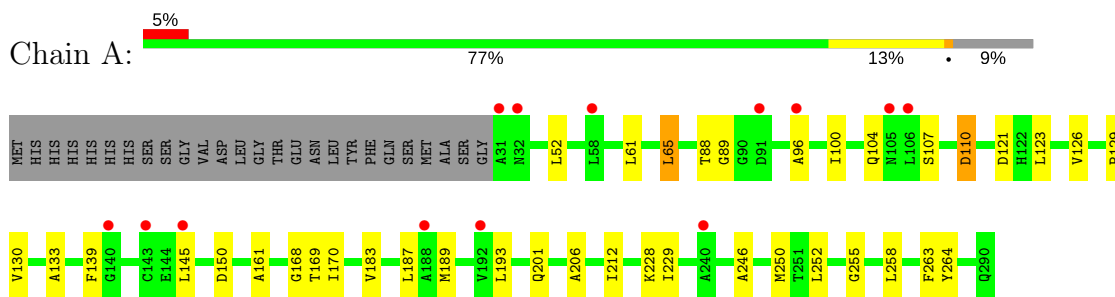


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 35 14 5 13 3	0	0
3	C	1	Total C N O P 35 14 5 13 3	0	0

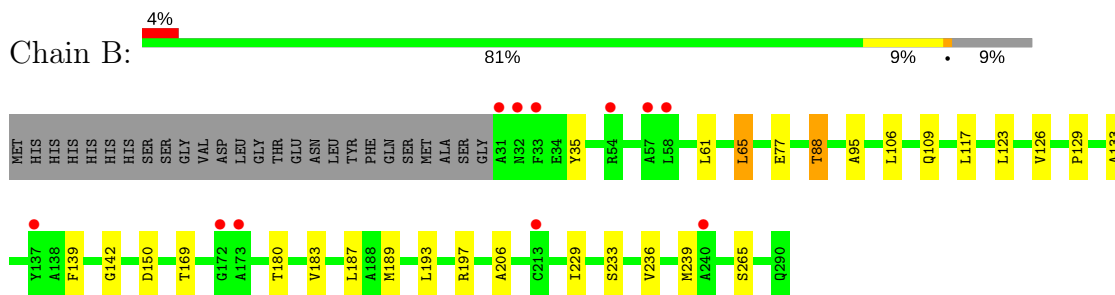
3 Residue-property plots [i](#)

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.

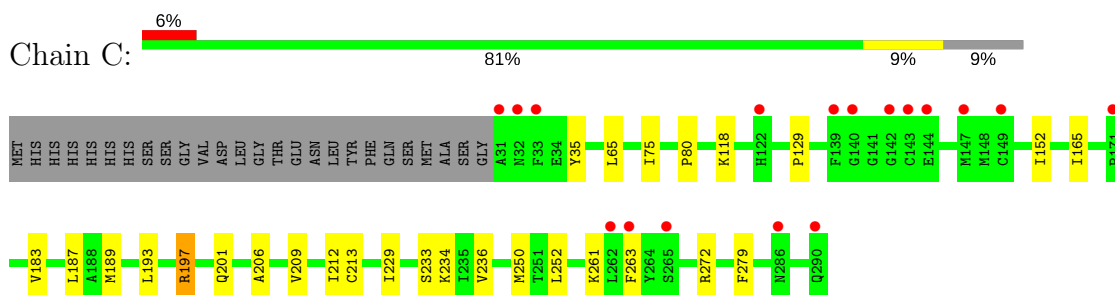
- Molecule 1: Enoyl-CoA hydratase



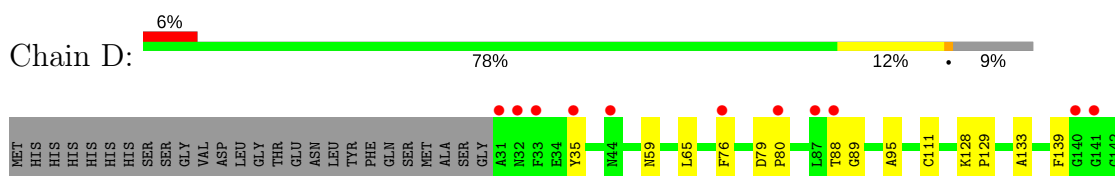
- Molecule 1: Enoyl-CoA hydratase



- Molecule 1: Enoyl-CoA hydratase

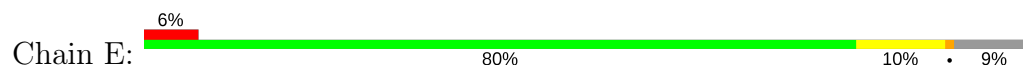


- Molecule 1: Enoyl-CoA hydratase

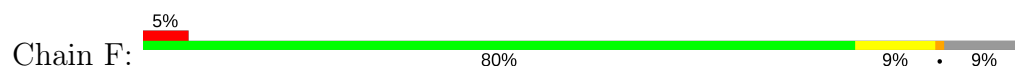




● Molecule 1: Enoyl-CoA hydratase



● Molecule 1: Enoyl-CoA hydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.55Å 97.34Å 231.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.55 29.57 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.60-2.55) 97.4 (29.57-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.252 0.214 , 0.254	Depositor DCC
R_{free} test set	3359 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11556	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, COO

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	0.52	0/1949	0.60	0/2630
1	B	0.48	0/1966	0.57	0/2651
1	C	0.45	0/1942	0.57	1/2622 (0.0%)
1	D	0.46	0/1954	0.56	0/2639
1	E	0.40	0/1896	0.54	0/2566
1	F	0.41	0/1942	0.53	0/2628
All	All	0.46	0/11649	0.56	1/15736 (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	A	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	ARG	NE-CZ-NH1	5.33	122.96	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	F	114	SER	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	1924	0	1893	45	0
1	B	1934	0	1914	31	0
1	C	1916	0	1881	22	0
1	D	1924	0	1886	28	0
1	E	1872	0	1780	35	0
1	F	1912	0	1849	29	0
2	A	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	B	35	0	17	0	0
3	C	35	0	17	2	0
All	All	11556	0	11237	171	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 8.

All (171) 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:183:VAL:CG1	1:B:187:LEU:HD23	1.78	1.13
1:B:183:VAL:HG11	1:B:187:LEU:HD23	1.14	1.13
1:D:246:ALA:HB1	1:D:250:MET:HE1	1.42	0.98
1:C:189:MET:CE	1:C:193:LEU:HD11	1.97	0.95
1:D:189:MET:HE3	1:D:193:LEU:HD11	1.49	0.91
1:D:246:ALA:HB1	1:D:250:MET:CE	1.99	0.90
1:B:183:VAL:HG13	1:B:206:ALA:HB1	1.55	0.89
1:B:183:VAL:HG11	1:B:187:LEU:CD2	2.03	0.84
1:B:35:TYR:HB3	1:B:65:LEU:HD12	1.62	0.82
1:A:250:MET:HE1	1:A:258:LEU:HD22	1.62	0.81
1:F:250:MET:CE	1:F:255:GLY:HA2	2.11	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD22	1:A:65:LEU:HD11	1.65	0.79
1:C:183:VAL:HG22	1:C:206:ALA:HB1	1.64	0.79
1:D:189:MET:CE	1:D:193:LEU:HD11	2.14	0.78
1:C:35:TYR:HB3	1:C:65:LEU:HD13	1.65	0.77
1:A:189:MET:HE3	1:A:193:LEU:HD11	1.65	0.77
1:A:189:MET:CE	1:A:193:LEU:HD11	2.16	0.76
1:F:250:MET:HE3	1:F:255:GLY:HA2	1.71	0.73
1:B:189:MET:CE	1:B:193:LEU:HD11	2.22	0.69
1:D:233:SER:HB3	1:D:236:VAL:HG12	1.75	0.68
1:B:189:MET:HE1	1:B:193:LEU:HD11	1.75	0.68
1:A:88:THR:HG22	1:A:89:GLY:N	2.08	0.67
1:A:183:VAL:CG1	1:A:187:LEU:HB3	2.24	0.67
1:C:189:MET:HE1	1:C:193:LEU:HD11	1.76	0.67
1:C:233:SER:HB3	1:C:236:VAL:HG12	1.77	0.67
1:E:183:VAL:HG13	1:E:187:LEU:HB3	1.77	0.66
1:F:250:MET:HE3	1:F:255:GLY:CA	2.25	0.66
1:B:88:THR:HG23	1:B:133:ALA:O	1.96	0.66
1:C:189:MET:CE	1:C:193:LEU:CD1	2.73	0.65
1:A:250:MET:HE1	1:A:258:LEU:CD2	2.25	0.65
1:A:129:PRO:HG2	1:A:229:ILE:HG21	1.78	0.65
1:D:88:THR:HG23	1:D:133:ALA:O	1.97	0.64
1:C:183:VAL:HG13	1:C:187:LEU:HB3	1.78	0.64
1:E:183:VAL:HG22	1:E:206:ALA:HB1	1.80	0.64
1:E:189:MET:CE	1:E:193:LEU:HD11	2.28	0.62
1:F:250:MET:HE1	1:F:255:GLY:HA2	1.80	0.62
1:B:183:VAL:HG12	1:B:183:VAL:O	1.99	0.62
1:E:88:THR:HG22	1:E:89:GLY:N	2.15	0.62
1:B:233:SER:HB3	1:B:236:VAL:CG1	2.31	0.61
1:D:183:VAL:CG1	1:D:187:LEU:HB3	2.31	0.60
1:A:183:VAL:HG22	1:A:206:ALA:HB1	1.83	0.60
1:A:88:THR:OG1	1:A:133:ALA:HB3	2.02	0.60
1:D:183:VAL:HG13	1:D:187:LEU:HD23	1.84	0.60
1:D:183:VAL:HG22	1:D:206:ALA:HB1	1.83	0.60
1:E:233:SER:HB3	1:E:236:VAL:HG12	1.85	0.59
1:F:88:THR:HG22	1:F:89:GLY:N	2.18	0.59
1:B:129:PRO:HG2	1:B:229:ILE:HG21	1.85	0.59
1:E:183:VAL:CG1	1:E:187:LEU:HB3	2.33	0.59
1:C:183:VAL:HG22	1:C:206:ALA:CB	2.33	0.59
1:A:169:THR:HG22	1:A:170:ILE:H	1.68	0.58
1:C:189:MET:HE2	1:C:193:LEU:HD11	1.83	0.58
1:A:88:THR:HG22	1:A:89:GLY:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:PHE:HA	1:D:272:ARG:HD2	1.85	0.58
1:D:76:PHE:O	1:D:128:LYS:NZ	2.36	0.58
1:B:233:SER:HB3	1:B:236:VAL:HG12	1.86	0.57
1:E:189:MET:HE2	1:E:193:LEU:HD11	1.85	0.57
1:E:233:SER:CB	1:E:236:VAL:HG12	2.34	0.57
1:A:183:VAL:CG1	1:A:187:LEU:HD23	2.35	0.56
1:C:183:VAL:CG1	1:C:187:LEU:HB3	2.36	0.55
1:B:117:LEU:HB2	1:E:260:LYS:NZ	2.22	0.55
1:C:261:LYS:CD	1:F:258:LEU:HD11	2.35	0.55
1:C:80:PRO:O	1:C:234:LYS:NZ	2.39	0.55
1:E:189:MET:HE2	1:E:193:LEU:CD1	2.37	0.55
1:A:88:THR:CG2	1:A:89:GLY:N	2.69	0.55
1:A:183:VAL:HG13	1:A:187:LEU:HD23	1.89	0.54
1:D:139:PHE:CD1	1:D:161:ALA:HB3	2.42	0.54
1:E:88:THR:HG22	1:E:89:GLY:O	2.07	0.54
1:A:250:MET:HE3	1:A:258:LEU:HB3	1.90	0.53
1:A:65:LEU:HD12	1:A:65:LEU:O	2.08	0.53
1:E:233:SER:HB3	1:E:236:VAL:CG1	2.38	0.53
1:A:104:GLN:OE1	1:F:277:THR:HG22	2.09	0.52
1:A:110:ASP:N	1:A:110:ASP:OD1	2.43	0.52
1:D:35:TYR:HB3	1:D:65:LEU:HD13	1.92	0.51
1:B:239:MET:HE1	1:B:265:SER:HB3	1.91	0.51
1:B:61:LEU:HD23	1:B:65:LEU:CD2	2.41	0.51
1:B:189:MET:HE3	1:B:193:LEU:HD11	1.92	0.50
1:B:189:MET:HE3	1:E:150:ASP:HB3	1.93	0.50
1:A:263:PHE:CE1	1:D:169:THR:HG21	2.48	0.49
1:B:95:ALA:HB3	1:B:142:GLY:CA	2.43	0.49
1:C:263:PHE:CE1	1:E:169:THR:HG21	2.48	0.48
1:B:77:GLU:OE1	1:B:126:VAL:HG13	2.13	0.48
1:E:152:ILE:CG2	1:E:209:VAL:HG12	2.43	0.48
1:E:88:THR:OG1	1:E:133:ALA:HB3	2.14	0.48
1:C:189:MET:HE3	1:C:193:LEU:HG	1.96	0.48
1:A:169:THR:HG22	1:A:170:ILE:N	2.28	0.48
1:F:35:TYR:HB3	1:F:65:LEU:HD13	1.95	0.48
1:A:169:THR:HG21	1:F:263:PHE:CE1	2.48	0.47
1:A:150:ASP:HB3	1:D:189:MET:HE2	1.95	0.47
1:A:252:LEU:HB3	1:D:249:GLU:OE2	2.13	0.47
1:A:201:GLN:HA	1:A:212:ILE:HD11	1.96	0.47
1:C:152:ILE:CG2	1:C:209:VAL:HG12	2.45	0.47
1:A:228:LYS:NZ	1:D:196:ASP:OD2	2.47	0.47
1:A:183:VAL:HG22	1:A:206:ALA:CB	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:MET:CE	1:E:193:LEU:CD1	2.93	0.47
1:A:123:LEU:O	1:A:126:VAL:HG22	2.14	0.47
1:A:168:GLY:O	1:F:272:ARG:HB2	2.15	0.47
1:F:169:THR:HG22	1:F:170:ILE:H	1.79	0.47
1:A:126:VAL:HG21	1:A:130:VAL:CG2	2.45	0.47
1:F:152:ILE:HG21	1:F:209:VAL:HG12	1.97	0.47
1:B:183:VAL:O	1:B:183:VAL:CG1	2.63	0.46
1:E:183:VAL:HG22	1:E:206:ALA:CB	2.44	0.46
1:B:189:MET:CE	1:E:150:ASP:HB3	2.45	0.46
1:A:264:TYR:CD1	1:D:111:CYS:HB3	2.51	0.46
1:F:43:LYS:N	1:F:227:GLU:OE2	2.47	0.46
1:F:88:THR:HG23	1:F:133:ALA:O	2.16	0.46
1:B:129:PRO:HA	1:B:150:ASP:OD2	2.16	0.45
1:A:189:MET:HE2	1:A:193:LEU:HD11	1.95	0.45
1:E:95:ALA:HB3	1:E:142:GLY:HA3	1.97	0.45
1:F:61:LEU:HA	1:F:65:LEU:HD23	1.99	0.45
1:F:183:VAL:HG13	1:F:187:LEU:HB3	1.99	0.45
1:F:250:MET:HE3	1:F:255:GLY:N	2.32	0.45
1:A:250:MET:CE	1:A:255:GLY:HA2	2.46	0.45
1:D:183:VAL:HG22	1:D:206:ALA:CB	2.46	0.45
1:A:250:MET:HE3	1:A:258:LEU:CB	2.46	0.45
1:B:180:THR:OG1	1:E:244:VAL:HG13	2.16	0.45
1:E:267:PHE:HA	1:E:272:ARG:HD3	1.98	0.45
1:D:273:LYS:O	1:D:277:THR:HG23	2.17	0.45
1:F:217:THR:O	1:F:221:GLU:HG2	2.17	0.44
1:B:123:LEU:O	1:B:123:LEU:HD23	2.18	0.44
1:B:183:VAL:HG13	1:B:206:ALA:CB	2.37	0.44
1:F:183:VAL:HG22	1:F:206:ALA:HB1	1.99	0.44
1:B:139:PHE:CZ	1:B:197:ARG:HD2	2.53	0.44
1:E:95:ALA:HB3	1:E:142:GLY:CA	2.48	0.44
1:E:152:ILE:HG21	1:E:209:VAL:HG12	1.99	0.44
1:F:126:VAL:HG21	1:F:130:VAL:CG2	2.47	0.44
1:A:100:ILE:HD12	1:A:100:ILE:H	1.83	0.44
1:B:95:ALA:HB3	1:B:142:GLY:HA2	2.00	0.44
3:C:2:COO:O5X	3:C:2:COO:H2X	2.18	0.44
1:B:109:GLN:NE2	1:D:290:GLN:OXT	2.41	0.44
1:E:36:ILE:HG22	1:E:52:LEU:HA	2.00	0.44
3:C:2:COO:O5X	3:C:2:COO:C2X	2.66	0.43
1:A:189:MET:HE2	1:F:150:ASP:HB3	2.00	0.43
1:E:88:THR:CG2	1:E:89:GLY:N	2.81	0.43
1:F:183:VAL:CG1	1:F:187:LEU:HB3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:PRO:HG2	1:C:229:ILE:HG21	2.01	0.43
1:E:267:PHE:HA	1:E:272:ARG:CD	2.48	0.43
1:A:123:LEU:HD23	1:A:145:LEU:HD12	2.00	0.43
1:F:88:THR:CG2	1:F:89:GLY:N	2.82	0.43
1:A:246:ALA:HB1	1:A:250:MET:CE	2.49	0.42
1:C:252:LEU:HB3	1:E:249:GLU:OE2	2.19	0.42
1:E:256:SER:O	1:E:260:LYS:HG2	2.19	0.42
1:F:152:ILE:CG2	1:F:209:VAL:HG12	2.49	0.42
1:C:152:ILE:HG21	1:C:209:VAL:HG12	2.02	0.42
1:A:104:GLN:CG	1:F:277:THR:HG22	2.49	0.42
1:D:129:PRO:HG2	1:D:229:ILE:HG21	2.02	0.42
1:E:35:TYR:HB3	1:E:65:LEU:HD13	2.00	0.42
1:A:61:LEU:HD13	1:A:145:LEU:HD22	2.00	0.42
1:A:183:VAL:HG11	1:A:187:LEU:HB3	2.01	0.42
1:C:201:GLN:HA	1:C:212:ILE:HD11	2.02	0.42
1:D:262:LEU:O	1:D:266:THR:HG23	2.20	0.41
1:D:88:THR:HG22	1:D:89:GLY:N	2.34	0.41
1:C:233:SER:HB3	1:C:236:VAL:CG1	2.49	0.41
1:A:139:PHE:CD1	1:A:161:ALA:HB3	2.56	0.41
1:B:233:SER:CB	1:B:236:VAL:HG12	2.49	0.41
1:D:189:MET:HE2	1:D:189:MET:HB3	1.90	0.41
1:D:263:PHE:CE1	1:F:169:THR:HG21	2.55	0.41
1:E:233:SER:OG	1:E:236:VAL:HG12	2.19	0.41
1:A:250:MET:HE2	1:A:255:GLY:HA2	2.02	0.41
1:E:171:PRO:HG2	1:E:176:THR:HG23	2.02	0.41
1:F:114:SER:O	1:F:115:LYS:C	2.59	0.41
1:F:95:ALA:HB3	1:F:142:GLY:HA2	2.03	0.41
1:B:95:ALA:HB3	1:B:142:GLY:HA3	2.02	0.41
1:C:279:PHE:CE2	1:E:100:ILE:HD12	2.56	0.41
1:F:123:LEU:O	1:F:126:VAL:HG22	2.21	0.41
1:E:145:LEU:HD12	1:E:145:LEU:HA	1.98	0.40
1:A:189:MET:O	1:A:193:LEU:HG	2.21	0.40
1:D:59:ASN:HB2	1:D:95:ALA:HA	2.04	0.40
1:D:79:ASP:HA	1:D:80:PRO:HD3	1.99	0.40
1:E:189:MET:HE1	1:E:193:LEU:HD11	2.03	0.40
1:A:183:VAL:HG11	1:A:187:LEU:HD23	2.04	0.40
1:B:236:VAL:HG22	1:C:165:ILE:HD12	2.02	0.40

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	258/286 (90%)	248 (96%)	10 (4%)	0	100	100
1	B	260/286 (91%)	256 (98%)	4 (2%)	0	100	100
1	C	258/286 (90%)	254 (98%)	4 (2%)	0	100	100
1	D	259/286 (91%)	256 (99%)	3 (1%)	0	100	100
1	E	258/286 (90%)	251 (97%)	7 (3%)	0	100	100
1	F	259/286 (91%)	249 (96%)	10 (4%)	0	100	100
All	All	1552/1716 (90%)	1514 (98%)	38 (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	191/227 (84%)	187 (98%)	4 (2%)	59	81
1	B	190/227 (84%)	186 (98%)	4 (2%)	59	81
1	C	188/227 (83%)	182 (97%)	6 (3%)	44	69
1	D	190/227 (84%)	188 (99%)	2 (1%)	78	91
1	E	177/227 (78%)	174 (98%)	3 (2%)	66	85
1	F	188/227 (83%)	185 (98%)	3 (2%)	68	86
All	All	1124/1362 (82%)	1102 (98%)	22 (2%)	60	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	107	SER
1	A	110	ASP
1	A	121	ASP
1	B	65	LEU
1	B	88	THR
1	B	106	LEU
1	B	169	THR
1	C	75	ILE
1	C	118	LYS
1	C	197	ARG
1	C	213	CYS
1	C	250	MET
1	C	272	ARG
1	D	169	THR
1	D	272	ARG
1	E	75	ILE
1	E	169	THR
1	E	272	ARG
1	F	169	THR
1	F	183	VAL
1	F	272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	162	GLN

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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	COO	B	1	-	32,37,55	1.50	4 (12%)	34,57,81	1.75	3 (8%)
3	COO	C	2	-	32,37,55	1.33	5 (15%)	34,57,81	1.67	3 (8%)

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	COO	B	1	-	-	0/23/43/70	0/3/3/3
3	COO	C	2	-	-	0/23/43/70	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	COO	P2A-O5A	2.37	1.67	1.55
3	C	2	COO	O4X-C1X	2.46	1.44	1.41
3	C	2	COO	P2A-O4A	2.57	1.60	1.50
3	C	2	COO	P1A-O2A	3.22	1.63	1.50
3	C	2	COO	P3X-O9A	3.26	1.61	1.50
3	B	1	COO	P2A-O4A	3.26	1.63	1.50
3	B	1	COO	O4X-C1X	3.47	1.46	1.41
3	B	1	COO	P3X-O9A	3.47	1.62	1.50
3	B	1	COO	P1A-O2A	3.96	1.65	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	COO	N3A-C2A-N1A	-8.30	121.63	128.86
3	C	2	COO	N3A-C2A-N1A	-7.84	122.03	128.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	COO	C4A-C5A-N7A	-2.70	106.80	109.41
3	C	2	COO	C5X-C4X-C3X	-2.63	105.37	114.30
3	C	2	COO	C4A-C5A-N7A	-2.52	106.97	109.41
3	B	1	COO	O1A-P1A-O5X	2.37	119.35	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	COO	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

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	260/286 (90%)	0.18	13 (5%) 30 32	69, 76, 88, 92	0
1	B	260/286 (90%)	0.19	11 (4%) 37 40	70, 77, 86, 91	0
1	C	260/286 (90%)	0.26	17 (6%) 20 21	70, 77, 86, 92	0
1	D	260/286 (90%)	0.35	17 (6%) 20 21	71, 76, 85, 88	0
1	E	260/286 (90%)	0.39	18 (6%) 18 18	69, 77, 85, 89	0
1	F	260/286 (90%)	0.35	14 (5%) 26 28	70, 77, 85, 92	0
All	All	1560/1716 (90%)	0.29	90 (5%) 24 25	69, 77, 86, 92	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	ALA	6.5
1	B	31	ALA	6.4
1	A	31	ALA	5.3
1	C	31	ALA	4.7
1	E	33	PHE	4.6
1	F	285	ALA	4.5
1	D	33	PHE	4.4
1	D	32	ASN	4.3
1	C	290	GLN	4.0
1	A	58	LEU	3.9
1	E	35	TYR	3.9
1	B	58	LEU	3.9
1	C	140	GLY	3.9
1	D	145	LEU	3.9
1	E	281	GLU	3.8
1	B	32	ASN	3.8
1	E	279	PHE	3.7
1	A	32	ASN	3.7
1	D	87	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	283	ARG	3.6
1	B	57	ALA	3.5
1	F	31	ALA	3.5
1	F	286	ASN	3.5
1	B	137	TYR	3.3
1	B	213	CYS	3.2
1	E	57	ALA	3.2
1	D	279	PHE	3.1
1	B	54	ARG	3.1
1	A	106	LEU	3.1
1	C	143	CYS	3.0
1	F	81	ALA	2.9
1	C	144	GLU	2.9
1	D	146	ALA	2.8
1	E	58	LEU	2.8
1	B	173	ALA	2.8
1	C	286	ASN	2.8
1	C	265	SER	2.7
1	B	33	PHE	2.7
1	E	137	TYR	2.7
1	D	44	ASN	2.7
1	E	143	CYS	2.7
1	C	147	MET	2.7
1	F	86	VAL	2.6
1	E	277	THR	2.6
1	E	282	LYS	2.6
1	A	96	ALA	2.6
1	E	278	ALA	2.6
1	D	35	TYR	2.5
1	C	263	PHE	2.4
1	F	238	ALA	2.4
1	A	145	LEU	2.4
1	E	151	ILE	2.4
1	E	139	PHE	2.4
1	D	141	GLY	2.4
1	D	280	VAL	2.4
1	A	140	GLY	2.4
1	E	156	GLU	2.4
1	F	79	ASP	2.3
1	D	80	PRO	2.3
1	F	287	PHE	2.3
1	A	143	CYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	262	LEU	2.3
1	C	122	HIS	2.3
1	E	285	ALA	2.3
1	C	171	PRO	2.2
1	C	149	CYS	2.2
1	D	76	PHE	2.2
1	E	287	PHE	2.2
1	F	268	ALA	2.2
1	D	140	GLY	2.2
1	C	139	PHE	2.2
1	D	147	MET	2.1
1	A	240	ALA	2.1
1	C	142	GLY	2.1
1	A	188	ALA	2.1
1	F	132	ALA	2.1
1	D	88	THR	2.1
1	E	116	PHE	2.1
1	A	192	VAL	2.1
1	C	33	PHE	2.1
1	F	119	HIS	2.1
1	F	283	ARG	2.1
1	F	58	LEU	2.1
1	A	105	ASN	2.1
1	B	172	GLY	2.1
1	D	143	CYS	2.1
1	B	240	ALA	2.0
1	C	32	ASN	2.0
1	F	152	ILE	2.0
1	A	91	ASP	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 ⓘ

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	MG	C	292	1/1	0.75	0.72	31.10	105,105,105,105	0
2	MG	D	291	1/1	0.68	0.89	15.22	87,87,87,87	0
2	MG	A	291	1/1	0.88	0.55	6.92	87,87,87,87	0
2	MG	C	291	1/1	0.72	0.67	4.16	80,80,80,80	0
3	COO	C	2	35/53	0.92	0.18	0.25	72,80,87,89	0
3	COO	B	1	35/53	0.93	0.16	-0.85	75,81,86,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.