



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:11 PM UTC

PDB ID : 3F0D / pdb_00003f0d
Title : High resolution crystal structure of 2C-methyl-D-erythritol 2,4-cyclodiphosphatase synthase from Burkholderia pseudomallei
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2008-10-24
Resolution : 1.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

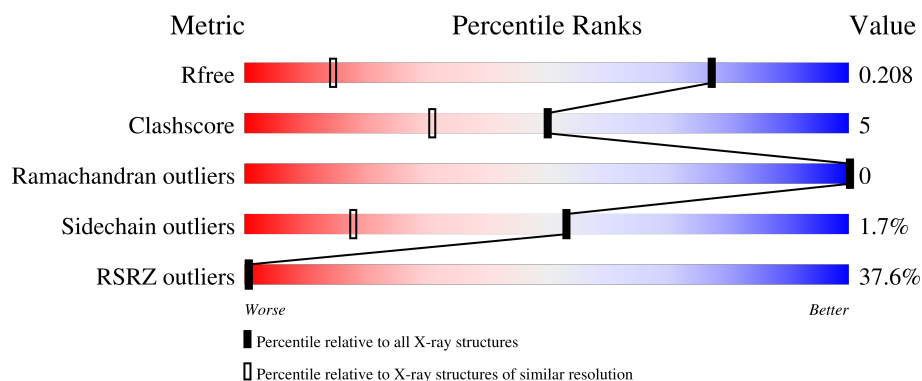
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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.



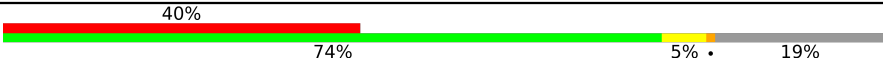
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	183	22% 78% 7% 15%
1	B	183	37% 69% 9% 21%
1	C	183	31% 73% 7% 19%
1	D	183	24% 77% 7% 14%
1	E	183	31% 73% 6% 21%

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Mol	Chain	Length	Quality of chain
1	F	183	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (40%), green (74%), yellow (5%), and grey (19%). The percentages are labeled above or below the segments. The red segment is the largest, followed by green, then yellow, and finally grey.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7315 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	5	0
			1184	752	215	214	3			
1	B	144	Total	C	N	O	S	0	4	0
			1089	692	196	198	3			
1	C	148	Total	C	N	O	S	0	2	0
			1118	706	207	202	3			
1	D	157	Total	C	N	O	S	0	5	0
			1201	761	220	217	3			
1	E	145	Total	C	N	O	S	0	4	0
			1095	694	199	199	3			
1	F	148	Total	C	N	O	S	5	2	0
			1118	706	207	202	3			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q63T71
A	-19	ALA	-	expression tag	UNP Q63T71
A	-18	HIS	-	expression tag	UNP Q63T71
A	-17	HIS	-	expression tag	UNP Q63T71
A	-16	HIS	-	expression tag	UNP Q63T71
A	-15	HIS	-	expression tag	UNP Q63T71
A	-14	HIS	-	expression tag	UNP Q63T71
A	-13	HIS	-	expression tag	UNP Q63T71
A	-12	MET	-	expression tag	UNP Q63T71
A	-11	GLY	-	expression tag	UNP Q63T71
A	-10	THR	-	expression tag	UNP Q63T71
A	-9	LEU	-	expression tag	UNP Q63T71
A	-8	GLU	-	expression tag	UNP Q63T71
A	-7	ALA	-	expression tag	UNP Q63T71
A	-6	GLN	-	expression tag	UNP Q63T71
A	-5	THR	-	expression tag	UNP Q63T71
A	-4	GLN	-	expression tag	UNP Q63T71

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q63T71
A	-2	PRO	-	expression tag	UNP Q63T71
A	-1	GLY	-	expression tag	UNP Q63T71
A	0	SER	-	expression tag	UNP Q63T71
B	-20	MET	-	expression tag	UNP Q63T71
B	-19	ALA	-	expression tag	UNP Q63T71
B	-18	HIS	-	expression tag	UNP Q63T71
B	-17	HIS	-	expression tag	UNP Q63T71
B	-16	HIS	-	expression tag	UNP Q63T71
B	-15	HIS	-	expression tag	UNP Q63T71
B	-14	HIS	-	expression tag	UNP Q63T71
B	-13	HIS	-	expression tag	UNP Q63T71
B	-12	MET	-	expression tag	UNP Q63T71
B	-11	GLY	-	expression tag	UNP Q63T71
B	-10	THR	-	expression tag	UNP Q63T71
B	-9	LEU	-	expression tag	UNP Q63T71
B	-8	GLU	-	expression tag	UNP Q63T71
B	-7	ALA	-	expression tag	UNP Q63T71
B	-6	GLN	-	expression tag	UNP Q63T71
B	-5	THR	-	expression tag	UNP Q63T71
B	-4	GLN	-	expression tag	UNP Q63T71
B	-3	GLY	-	expression tag	UNP Q63T71
B	-2	PRO	-	expression tag	UNP Q63T71
B	-1	GLY	-	expression tag	UNP Q63T71
B	0	SER	-	expression tag	UNP Q63T71
C	-20	MET	-	expression tag	UNP Q63T71
C	-19	ALA	-	expression tag	UNP Q63T71
C	-18	HIS	-	expression tag	UNP Q63T71
C	-17	HIS	-	expression tag	UNP Q63T71
C	-16	HIS	-	expression tag	UNP Q63T71
C	-15	HIS	-	expression tag	UNP Q63T71
C	-14	HIS	-	expression tag	UNP Q63T71
C	-13	HIS	-	expression tag	UNP Q63T71
C	-12	MET	-	expression tag	UNP Q63T71
C	-11	GLY	-	expression tag	UNP Q63T71
C	-10	THR	-	expression tag	UNP Q63T71
C	-9	LEU	-	expression tag	UNP Q63T71
C	-8	GLU	-	expression tag	UNP Q63T71
C	-7	ALA	-	expression tag	UNP Q63T71
C	-6	GLN	-	expression tag	UNP Q63T71
C	-5	THR	-	expression tag	UNP Q63T71
C	-4	GLN	-	expression tag	UNP Q63T71

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q63T71
C	-2	PRO	-	expression tag	UNP Q63T71
C	-1	GLY	-	expression tag	UNP Q63T71
C	0	SER	-	expression tag	UNP Q63T71
D	-20	MET	-	expression tag	UNP Q63T71
D	-19	ALA	-	expression tag	UNP Q63T71
D	-18	HIS	-	expression tag	UNP Q63T71
D	-17	HIS	-	expression tag	UNP Q63T71
D	-16	HIS	-	expression tag	UNP Q63T71
D	-15	HIS	-	expression tag	UNP Q63T71
D	-14	HIS	-	expression tag	UNP Q63T71
D	-13	HIS	-	expression tag	UNP Q63T71
D	-12	MET	-	expression tag	UNP Q63T71
D	-11	GLY	-	expression tag	UNP Q63T71
D	-10	THR	-	expression tag	UNP Q63T71
D	-9	LEU	-	expression tag	UNP Q63T71
D	-8	GLU	-	expression tag	UNP Q63T71
D	-7	ALA	-	expression tag	UNP Q63T71
D	-6	GLN	-	expression tag	UNP Q63T71
D	-5	THR	-	expression tag	UNP Q63T71
D	-4	GLN	-	expression tag	UNP Q63T71
D	-3	GLY	-	expression tag	UNP Q63T71
D	-2	PRO	-	expression tag	UNP Q63T71
D	-1	GLY	-	expression tag	UNP Q63T71
D	0	SER	-	expression tag	UNP Q63T71
E	-20	MET	-	expression tag	UNP Q63T71
E	-19	ALA	-	expression tag	UNP Q63T71
E	-18	HIS	-	expression tag	UNP Q63T71
E	-17	HIS	-	expression tag	UNP Q63T71
E	-16	HIS	-	expression tag	UNP Q63T71
E	-15	HIS	-	expression tag	UNP Q63T71
E	-14	HIS	-	expression tag	UNP Q63T71
E	-13	HIS	-	expression tag	UNP Q63T71
E	-12	MET	-	expression tag	UNP Q63T71
E	-11	GLY	-	expression tag	UNP Q63T71
E	-10	THR	-	expression tag	UNP Q63T71
E	-9	LEU	-	expression tag	UNP Q63T71
E	-8	GLU	-	expression tag	UNP Q63T71
E	-7	ALA	-	expression tag	UNP Q63T71
E	-6	GLN	-	expression tag	UNP Q63T71
E	-5	THR	-	expression tag	UNP Q63T71
E	-4	GLN	-	expression tag	UNP Q63T71

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q63T71
E	-2	PRO	-	expression tag	UNP Q63T71
E	-1	GLY	-	expression tag	UNP Q63T71
E	0	SER	-	expression tag	UNP Q63T71
F	-20	MET	-	expression tag	UNP Q63T71
F	-19	ALA	-	expression tag	UNP Q63T71
F	-18	HIS	-	expression tag	UNP Q63T71
F	-17	HIS	-	expression tag	UNP Q63T71
F	-16	HIS	-	expression tag	UNP Q63T71
F	-15	HIS	-	expression tag	UNP Q63T71
F	-14	HIS	-	expression tag	UNP Q63T71
F	-13	HIS	-	expression tag	UNP Q63T71
F	-12	MET	-	expression tag	UNP Q63T71
F	-11	GLY	-	expression tag	UNP Q63T71
F	-10	THR	-	expression tag	UNP Q63T71
F	-9	LEU	-	expression tag	UNP Q63T71
F	-8	GLU	-	expression tag	UNP Q63T71
F	-7	ALA	-	expression tag	UNP Q63T71
F	-6	GLN	-	expression tag	UNP Q63T71
F	-5	THR	-	expression tag	UNP Q63T71
F	-4	GLN	-	expression tag	UNP Q63T71
F	-3	GLY	-	expression tag	UNP Q63T71
F	-2	PRO	-	expression tag	UNP Q63T71
F	-1	GLY	-	expression tag	UNP Q63T71
F	0	SER	-	expression tag	UNP Q63T71

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

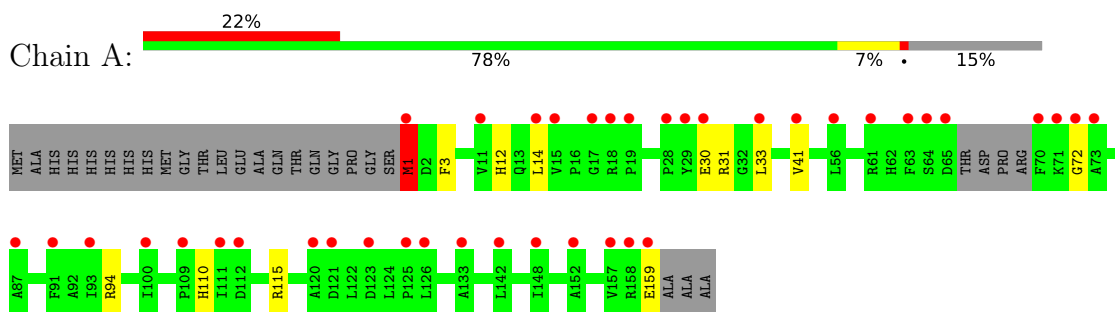
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total 128	O 128	0	0
3	B	62	Total 62	O 62	0	0
3	C	65	Total 65	O 65	0	0
3	D	110	Total 110	O 110	0	0
3	E	81	Total 81	O 81	0	0
3	F	58	Total 58	O 58	0	0

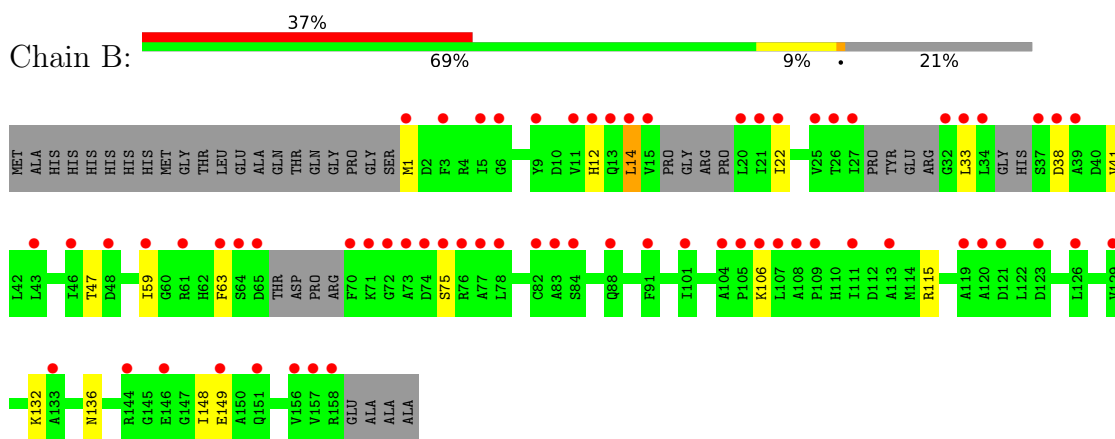
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

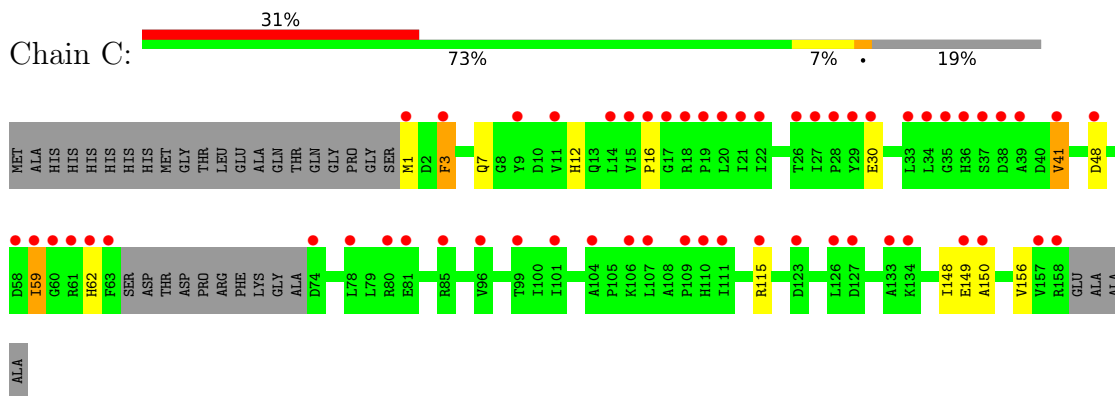
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

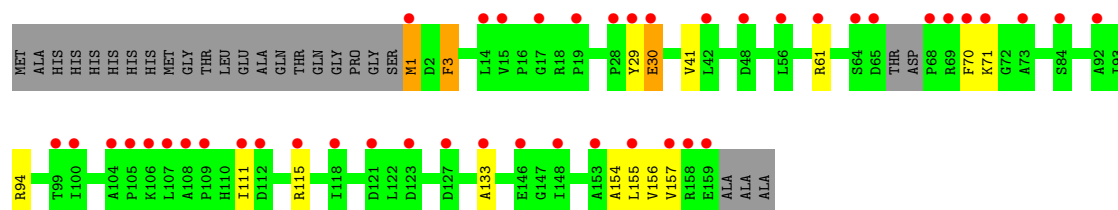


- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



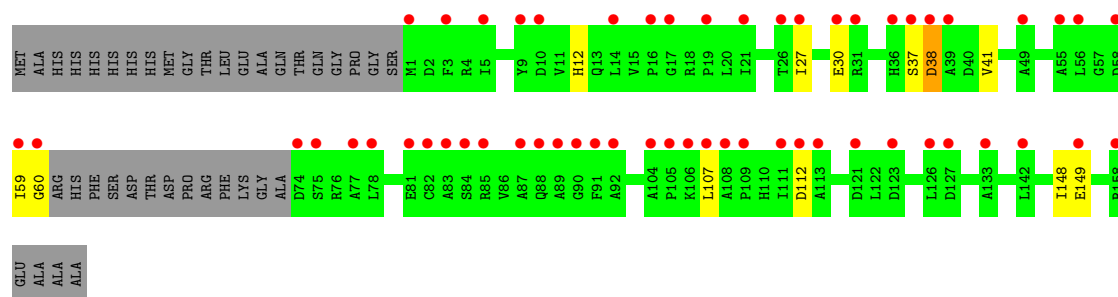
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain D: 



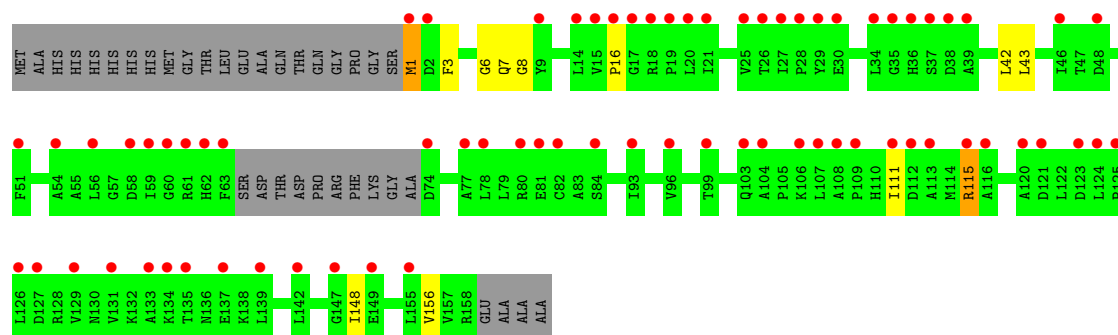
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain E: 



- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.89Å 69.04Å 116.58Å 90.00° 130.15° 90.00°	Depositor
Resolution (Å)	50.00 – 1.20 50.00 – 1.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-1.20) 91.2 (50.00-1.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.5.0035	Depositor
R, R_{free}	0.185 , 0.209 0.186 , 0.208	Depositor DCC
R_{free} test set	13745 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7315	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 39.32 % 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 3.2291e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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

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	1.12	2/1216 (0.2%)	0.97	3/1645 (0.2%)
1	B	1.09	4/1110 (0.4%)	0.87	0/1495
1	C	1.08	7/1140 (0.6%)	0.93	0/1543
1	D	1.20	7/1234 (0.6%)	0.90	0/1668
1	E	1.10	3/1121 (0.3%)	0.90	0/1519
1	F	1.16	10/1140 (0.9%)	0.90	0/1543
All	All	1.13	33/6961 (0.5%)	0.91	3/9413 (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	C	0	1
1	F	0	1
All	All	0	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	148	ILE	C-O	-7.60	1.16	1.24
1	D	154	ALA	C-O	-7.06	1.15	1.23
1	D	156	VAL	C-O	-6.99	1.15	1.23
1	F	8	GLY	C-O	-6.85	1.15	1.23
1	C	156	VAL	C-O	-6.51	1.16	1.23
1	E	149	GLU	C-O	-6.37	1.16	1.23
1	F	42[A]	LEU	C-O	-6.31	1.16	1.24
1	F	42[B]	LEU	C-O	-6.31	1.16	1.24
1	C	150	ALA	C-O	-6.24	1.16	1.23
1	D	155	LEU	C-O	-6.24	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	GLN	C-O	-6.21	1.16	1.23
1	C	3	PHE	C-O	-6.11	1.16	1.23
1	B	132	LYS	C-O	-6.11	1.16	1.23
1	C	48	ASP	C-O	-5.79	1.17	1.24
1	F	7	GLN	C-O	-5.66	1.17	1.23
1	A	31	ARG	CZ-NH2	-5.66	1.26	1.33
1	D	29	TYR	C-O	-5.59	1.16	1.23
1	D	70	PHE	C-O	-5.50	1.16	1.24
1	B	136	ASN	C-O	-5.48	1.16	1.24
1	B	106	LYS	C-O	-5.44	1.17	1.23
1	F	148	ILE	C-O	-5.39	1.18	1.24
1	C	149	GLU	C-O	-5.37	1.17	1.23
1	F	115	ARG	C-O	-5.31	1.18	1.24
1	F	43	LEU	C-O	-5.28	1.18	1.24
1	D	41	VAL	C-O	-5.24	1.18	1.24
1	F	6	GLY	C-O	-5.21	1.16	1.23
1	E	38	ASP	C-O	-5.18	1.17	1.24
1	F	3	PHE	C-O	-5.13	1.17	1.23
1	D	3	PHE	C-O	-5.11	1.17	1.23
1	B	149	GLU	C-O	-5.10	1.17	1.23
1	A	3	PHE	C-O	-5.09	1.17	1.23
1	F	156	VAL	C-O	-5.05	1.17	1.23
1	C	148	ILE	C-O	-5.03	1.19	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14[A]	LEU	CB-CA-C	5.70	119.16	109.75
1	A	14[B]	LEU	CB-CA-C	5.70	119.16	109.75
1	A	1	MET	CB-CA-C	5.16	119.91	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	16	PRO	Peptide
1	F	16	PRO	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	1184	0	1227	15	0
1	B	1089	0	1134	19	0
1	C	1118	0	1151	16	0
1	D	1201	0	1244	22	1
1	E	1095	0	1142	4	1
1	F	1118	0	1151	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	128	0	0	3	1
3	B	62	0	0	1	0
3	C	65	0	0	4	0
3	D	110	0	0	2	1
3	E	81	0	0	0	0
3	F	58	0	0	1	0
All	All	7315	0	7049	73	2

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 5.

All (73) 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:C:59:ILE:HG22	3:C:367:HOH:O	1.11	1.24
1:A:12:HIS:HD2	1:A:41[A]:VAL:HG12	1.03	1.11
1:A:33:LEU:HD13	1:A:41[B]:VAL:HG23	1.33	1.07
1:B:47:THR:HG21	1:B:59[A]:ILE:HD13	1.35	1.07
1:D:1:MET:SD	1:D:1:MET:N	2.29	1.06
1:F:115:ARG:HD2	3:F:353:HOH:O	1.54	1.04
1:A:12:HIS:CD2	1:A:41[A]:VAL:HG12	1.92	1.04
1:B:47:THR:CG2	1:B:59[A]:ILE:HD13	1.88	1.03
1:A:33:LEU:HD13	1:A:41[B]:VAL:CG2	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:PHE:CD1	1:D:157[B]:VAL:CG1	2.52	0.93
1:D:3:PHE:CD1	1:D:157[B]:VAL:HG12	2.03	0.92
1:B:1:MET:HE3	1:C:1:MET:HG3	1.52	0.91
1:D:1:MET:HE1	1:F:1:MET:SD	2.16	0.84
1:B:47:THR:HG21	1:B:59[A]:ILE:CD1	2.06	0.84
1:A:33:LEU:CD1	1:A:41[B]:VAL:HG23	2.08	0.83
1:D:1:MET:HE1	1:F:1:MET:CE	2.12	0.80
1:D:1:MET:SD	1:F:1:MET:HE3	2.21	0.79
1:D:3:PHE:CE1	1:D:157[B]:VAL:CG1	2.68	0.77
1:D:3:PHE:CE1	1:D:157[B]:VAL:HG11	2.21	0.75
1:D:1:MET:SD	1:F:1:MET:CE	2.76	0.73
1:A:12:HIS:HD2	1:A:41[A]:VAL:CG1	1.93	0.72
1:A:12:HIS:CD2	1:A:41[A]:VAL:CG1	2.72	0.70
1:C:12:HIS:HD2	1:C:41[A]:VAL:CG1	2.06	0.69
1:B:1:MET:CE	1:C:1:MET:HG3	2.21	0.68
1:C:59:ILE:CG2	3:C:367:HOH:O	1.89	0.68
1:D:3:PHE:CD1	1:D:157[A]:VAL:HG22	2.29	0.68
1:A:72:GLY:HA2	3:A:449:HOH:O	1.94	0.67
1:B:47:THR:HG22	1:B:59[A]:ILE:HD13	1.75	0.67
1:A:1:MET:HE1	1:C:1:MET:N	2.10	0.66
1:D:1:MET:HE1	1:F:1:MET:HE3	1.81	0.62
1:D:1:MET:CE	1:F:1:MET:HE3	2.30	0.61
1:C:115:ARG:CZ	3:C:257:HOH:O	2.49	0.60
1:D:1:MET:CE	1:F:1:MET:CE	2.78	0.60
1:B:12:HIS:HD2	1:B:41:VAL:HG12	1.66	0.60
1:D:115:ARG:NH2	3:D:419:HOH:O	2.33	0.59
1:B:59[A]:ILE:HD11	1:B:63:PHE:HD2	1.69	0.58
1:C:12:HIS:HD2	1:C:41[A]:VAL:HG13	1.69	0.57
1:B:12:HIS:HD2	1:B:41:VAL:CG1	2.17	0.56
1:C:12:HIS:HD2	1:C:41[A]:VAL:HG12	1.70	0.56
1:B:1:MET:HE3	1:C:1:MET:CG	2.31	0.55
1:D:1:MET:SD	1:F:1:MET:HE1	2.48	0.54
1:D:94:ARG:HH22	1:F:1:MET:CE	2.22	0.53
1:D:1:MET:N	1:D:3:PHE:CE2	2.77	0.52
1:B:38:ASP:OD1	1:B:75:SER:OG	2.20	0.52
1:B:59[A]:ILE:CD1	1:B:63:PHE:HD2	2.23	0.52
1:B:59[A]:ILE:HD11	1:B:63:PHE:CD2	2.46	0.51
1:E:59:ILE:HD12	1:E:60:GLY:N	2.26	0.51
1:A:1:MET:HE3	1:A:94:ARG:HH22	1.75	0.51
1:B:12:HIS:CD2	1:B:41:VAL:HG12	2.43	0.51
1:A:115:ARG:NH2	3:A:287:HOH:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HB2	1:C:3:PHE:CE2	2.47	0.49
1:F:111:ILE:O	1:F:115:ARG:HG3	2.13	0.49
1:C:62:HIS:HE1	3:C:182:HOH:O	1.97	0.48
1:B:59[A]:ILE:CD1	1:B:63:PHE:CD2	2.98	0.47
1:A:110:HIS:HD2	3:A:197:HOH:O	1.98	0.45
1:C:30:GLU:H	1:C:30:GLU:CD	2.23	0.45
1:D:94:ARG:HG2	1:D:157[A]:VAL:HG23	1.99	0.45
1:B:115:ARG:HD2	3:B:175:HOH:O	2.16	0.45
1:E:37:SER:HB3	1:E:38:ASP:H	1.64	0.44
1:A:33:LEU:HD13	1:A:41[A]:VAL:HG13	1.99	0.43
1:B:22:ILE:HD11	1:B:33:LEU:HD11	2.00	0.43
1:D:30:GLU:HG3	3:D:204:HOH:O	2.17	0.43
1:E:27:ILE:HD13	1:E:107:LEU:HD22	2.02	0.42
1:A:1:MET:HE1	1:C:1:MET:H3	1.81	0.42
1:A:33:LEU:CD1	1:A:41[B]:VAL:CG2	2.76	0.42
1:C:12:HIS:CD2	1:C:41[A]:VAL:HG13	2.52	0.42
1:E:12:HIS:HD2	1:E:41[A]:VAL:HG12	1.85	0.42
1:B:14[A]:LEU:HD13	1:B:33:LEU:HD23	2.02	0.42
1:C:12:HIS:CD2	1:C:41[A]:VAL:CG1	2.95	0.42
1:D:94:ARG:HH22	1:F:1:MET:HE1	1.85	0.42
1:D:111:ILE:HD11	1:D:133:ALA:HB2	2.02	0.42
1:B:14[B]:LEU:HD11	1:B:148:ILE:HG13	2.03	0.41
1:D:94:ARG:HH22	1:F:1:MET:HE2	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:433:HOH:O	3:D:327:HOH:O[4_444]	1.68	0.52
1:D:61:ARG:CD	1:E:112:ASP:OD2[2_555]	1.88	0.32

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	156/183 (85%)	153 (98%)	3 (2%)	0	100	100
1	B	138/183 (75%)	137 (99%)	1 (1%)	0	100	100
1	C	146/183 (80%)	143 (98%)	3 (2%)	0	100	100
1	D	158/183 (86%)	156 (99%)	2 (1%)	0	100	100
1	E	145/183 (79%)	144 (99%)	1 (1%)	0	100	100
1	F	146/183 (80%)	144 (99%)	2 (1%)	0	100	100
All	All	889/1098 (81%)	877 (99%)	12 (1%)	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	120/135 (89%)	117 (98%)	3 (2%)	42	8
1	B	110/135 (82%)	108 (98%)	2 (2%)	51	16
1	C	112/135 (83%)	109 (97%)	3 (3%)	39	6
1	D	122/135 (90%)	119 (98%)	3 (2%)	42	8
1	E	111/135 (82%)	110 (99%)	1 (1%)	70	40
1	F	112/135 (83%)	111 (99%)	1 (1%)	70	40
All	All	687/810 (85%)	674 (98%)	13 (2%)	53	13

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	GLU
1	A	159	GLU
1	B	14[A]	LEU
1	B	14[B]	LEU

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Mol	Chain	Res	Type
1	C	41[A]	VAL
1	C	41[B]	VAL
1	C	59	ILE
1	D	1	MET
1	D	30	GLU
1	D	71	LYS
1	E	30	GLU
1	F	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	136	ASN
1	B	13	GLN
1	B	88	GLN
1	B	110	HIS
1	B	136	ASN
1	C	110	HIS
1	C	136	ASN
1	D	36	HIS
1	D	110	HIS
1	D	136	ASN
1	E	88	GLN
1	E	110	HIS
1	F	136	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	155/183 (84%)	1.59	40 (25%)	1 2	8, 16, 25, 36	5 (3%)
1	B	144/183 (78%)	2.13	67 (46%)	0 0	9, 19, 32, 41	4 (2%)
1	C	148/183 (80%)	2.02	57 (38%)	1 0	10, 19, 32, 41	2 (1%)
1	D	157/183 (85%)	1.55	44 (28%)	1 2	10, 16, 26, 34	5 (3%)
1	E	145/183 (79%)	1.92	56 (38%)	1 0	9, 19, 29, 34	4 (2%)
1	F	148/183 (80%)	2.13	73 (49%)	0 0	11, 21, 31, 38	2 (1%)
All	All	897/1098 (81%)	1.88	337 (37%)	1 1	8, 18, 31, 41	22 (2%)

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	PHE	9.5
1	B	34	LEU	8.0
1	C	17	GLY	7.5
1	E	59	ILE	7.4
1	B	27	ILE	7.1
1	F	17	GLY	7.0
1	B	37	SER	6.3
1	D	65	ASP	5.5
1	B	15	VAL	5.5
1	B	70	PHE	5.2
1	C	60	GLY	5.0
1	E	1	MET	5.0
1	A	1	MET	4.9
1	C	59	ILE	4.9
1	A	159	GLU	4.9
1	C	62	HIS	4.9
1	E	56	LEU	4.9
1	D	68	PRO	4.8
1	C	36	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	26	THR	4.7
1	E	75	SER	4.7
1	C	18	ARG	4.5
1	F	19	PRO	4.5
1	F	59	ILE	4.5
1	D	1	MET	4.5
1	D	159	GLU	4.5
1	B	104	ALA	4.5
1	B	65	ASP	4.5
1	F	62	HIS	4.5
1	C	29	TYR	4.4
1	F	63	PHE	4.4
1	E	36	HIS	4.4
1	F	29	TYR	4.3
1	E	37	SER	4.2
1	C	37	SER	4.2
1	B	108	ALA	4.2
1	C	16	PRO	4.1
1	C	101	ILE	4.1
1	F	15	VAL	4.1
1	F	96[A]	VAL	4.1
1	F	112	ASP	4.1
1	A	70	PHE	4.1
1	B	14[A]	LEU	4.0
1	E	78	LEU	4.0
1	C	48	ASP	4.0
1	F	60	GLY	4.0
1	B	1	MET	3.9
1	B	149	GLU	3.9
1	E	74	ASP	3.9
1	B	59[A]	ILE	3.9
1	D	14[A]	LEU	3.9
1	C	78	LEU	3.8
1	A	17	GLY	3.8
1	F	36	HIS	3.8
1	C	30	GLU	3.8
1	C	39	ALA	3.8
1	E	27	ILE	3.8
1	E	60	GLY	3.7
1	B	21	ILE	3.7
1	B	25	VAL	3.7
1	B	38	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	61	ARG	3.7
1	A	111[A]	ILE	3.7
1	F	39	ALA	3.7
1	C	1	MET	3.6
1	B	74	ASP	3.6
1	A	72	GLY	3.6
1	B	20	LEU	3.6
1	E	89	ALA	3.6
1	C	9	TYR	3.6
1	A	158	ARG	3.5
1	E	77	ALA	3.5
1	F	26	THR	3.5
1	C	27	ILE	3.5
1	C	111[A]	ILE	3.5
1	F	111	ILE	3.5
1	F	107	LEU	3.5
1	F	131	VAL	3.5
1	C	74	ASP	3.5
1	C	133	ALA	3.4
1	F	116	ALA	3.4
1	F	37	SER	3.4
1	E	90	GLY	3.4
1	A	73	ALA	3.4
1	C	104	ALA	3.4
1	F	48	ASP	3.4
1	C	127	ASP	3.4
1	A	28	PRO	3.4
1	A	65	ASP	3.3
1	D	15	VAL	3.3
1	E	127	ASP	3.3
1	B	84	SER	3.3
1	B	33	LEU	3.3
1	A	63	PHE	3.3
1	A	133	ALA	3.3
1	B	133	ALA	3.3
1	E	87	ALA	3.3
1	D	69	ARG	3.3
1	C	19	PRO	3.3
1	B	156	VAL	3.3
1	F	133	ALA	3.3
1	C	81	GLU	3.2
1	D	64[A]	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	158	ARG	3.2
1	E	158	ARG	3.2
1	C	15	VAL	3.2
1	E	111	ILE	3.2
1	A	71	LYS	3.2
1	F	16	PRO	3.2
1	F	61	ARG	3.2
1	E	104	ALA	3.2
1	F	54	ALA	3.2
1	B	91	PHE	3.2
1	F	30	GLU	3.2
1	F	77	ALA	3.1
1	E	30	GLU	3.1
1	B	63	PHE	3.1
1	B	22	ILE	3.1
1	E	14[A]	LEU	3.1
1	A	41[A]	VAL	3.1
1	C	38	ASP	3.1
1	F	14	LEU	3.1
1	E	82	CYS	3.1
1	C	26	THR	3.1
1	A	112	ASP	3.1
1	A	121	ASP	3.1
1	E	38	ASP	3.1
1	F	126	LEU	3.0
1	B	73	ALA	3.0
1	D	73	ALA	3.0
1	F	21	ILE	3.0
1	A	123	ASP	3.0
1	D	106	LYS	3.0
1	B	32	GLY	3.0
1	B	39	ALA	3.0
1	E	92	ALA	3.0
1	B	106	LYS	3.0
1	E	126	LEU	3.0
1	F	18	ARG	2.9
1	E	17	GLY	2.9
1	B	9	TYR	2.9
1	E	84	SER	2.9
1	E	133	ALA	2.9
1	D	70	PHE	2.9
1	E	81	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	123	ASP	2.9
1	C	35	GLY	2.9
1	A	30	GLU	2.9
1	C	158	ARG	2.9
1	C	41[A]	VAL	2.9
1	F	28	PRO	2.9
1	D	56	LEU	2.9
1	D	121	ASP	2.9
1	F	1	MET	2.9
1	E	105	PRO	2.9
1	D	108	ALA	2.9
1	F	120	ALA	2.9
1	A	126	LEU	2.8
1	F	46	ILE	2.8
1	A	19	PRO	2.8
1	D	71	LYS	2.8
1	B	64	SER	2.8
1	B	61	ARG	2.8
1	B	82	CYS	2.8
1	F	104	ALA	2.8
1	F	127	ASP	2.8
1	B	78	LEU	2.8
1	F	51	PHE	2.8
1	B	109	PRO	2.8
1	A	87	ALA	2.8
1	B	121	ASP	2.8
1	D	133	ALA	2.8
1	F	108	ALA	2.8
1	A	29	TYR	2.8
1	D	61	ARG	2.8
1	F	20	LEU	2.8
1	C	28	PRO	2.8
1	C	58	ASP	2.8
1	D	111	ILE	2.8
1	B	72	GLY	2.8
1	A	64	SER	2.7
1	D	157[A]	VAL	2.7
1	C	115	ARG	2.7
1	B	101	ILE	2.7
1	E	55	ALA	2.7
1	B	105	PRO	2.7
1	F	106	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	134	LYS	2.7
1	E	88	GLN	2.7
1	A	91	PHE	2.7
1	B	123	ASP	2.7
1	E	39	ALA	2.7
1	B	111	ILE	2.7
1	C	21	ILE	2.7
1	F	80	ARG	2.7
1	B	12	HIS	2.7
1	F	125	PRO	2.7
1	F	25	VAL	2.7
1	B	107	LEU	2.7
1	F	142	LEU	2.7
1	B	5	ILE	2.6
1	F	74	ASP	2.6
1	C	157	VAL	2.6
1	C	107	LEU	2.6
1	D	42	LEU	2.6
1	D	153	ALA	2.6
1	F	123	ASP	2.6
1	B	75	SER	2.6
1	B	71	LYS	2.6
1	D	30	GLU	2.6
1	E	142	LEU	2.6
1	F	124	LEU	2.6
1	D	123	ASP	2.6
1	F	113	ALA	2.6
1	D	105	PRO	2.6
1	B	146	GLU	2.6
1	E	121	ASP	2.5
1	A	56	LEU	2.5
1	B	126[A]	LEU	2.5
1	C	109	PRO	2.5
1	D	28	PRO	2.5
1	E	16	PRO	2.5
1	E	19	PRO	2.5
1	B	3	PHE	2.5
1	D	107	LEU	2.5
1	F	81	GLU	2.5
1	D	99	THR	2.5
1	E	26	THR	2.5
1	F	115	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	109	PRO	2.5
1	E	9	TYR	2.5
1	F	155	LEU	2.5
1	E	106	LYS	2.5
1	E	85	ARG	2.4
1	B	48	ASP	2.4
1	E	10	ASP	2.4
1	F	99	THR	2.4
1	F	149	GLU	2.4
1	B	120	ALA	2.4
1	F	9	TYR	2.4
1	D	48	ASP	2.4
1	B	13	GLN	2.4
1	D	118	ILE	2.4
1	E	113	ALA	2.4
1	D	17	GLY	2.4
1	A	142	LEU	2.4
1	A	18	ARG	2.4
1	B	11	VAL	2.4
1	C	96	VAL	2.4
1	E	31	ARG	2.4
1	E	149	GLU	2.4
1	F	38	ASP	2.4
1	A	120	ALA	2.4
1	B	76	ARG	2.3
1	B	88	GLN	2.3
1	E	58	ASP	2.3
1	F	58	ASP	2.3
1	C	110	HIS	2.3
1	E	91	PHE	2.3
1	F	27	ILE	2.3
1	F	135	THR	2.3
1	C	14	LEU	2.3
1	F	34	LEU	2.3
1	D	29	TYR	2.3
1	D	19	PRO	2.3
1	F	109	PRO	2.3
1	A	152	ALA	2.3
1	B	113	ALA	2.3
1	B	43	LEU	2.3
1	C	123	ASP	2.3
1	C	126	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	107	LEU	2.2
1	F	78	LEU	2.2
1	D	148	ILE	2.2
1	E	5[A]	ILE	2.2
1	C	11	VAL	2.2
1	D	158	ARG	2.2
1	F	121	ASP	2.2
1	A	109	PRO	2.2
1	C	34	LEU	2.2
1	D	155	LEU	2.2
1	A	93	ILE	2.2
1	C	85	ARG	2.2
1	B	119	ALA	2.2
1	D	104	ALA	2.2
1	D	112	ASP	2.2
1	B	151	GLN	2.2
1	C	20	LEU	2.1
1	E	112	ASP	2.1
1	C	149	GLU	2.1
1	A	100[A]	ILE	2.1
1	C	22	ILE	2.1
1	F	93	ILE	2.1
1	B	83	ALA	2.1
1	C	150	ALA	2.1
1	B	157	VAL	2.1
1	F	129	VAL	2.1
1	B	144	ARG	2.1
1	D	146	GLU	2.1
1	F	139	LEU	2.1
1	C	134	LYS	2.1
1	C	3	PHE	2.1
1	A	148	ILE	2.1
1	C	80	ARG	2.1
1	D	115	ARG	2.1
1	F	137	GLU	2.1
1	F	2	ASP	2.1
1	C	106	LYS	2.1
1	B	6	GLY	2.1
1	F	35	GLY	2.1
1	F	84	SER	2.1
1	A	61	ARG	2.1
1	C	33	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	56	LEU	2.1
1	F	103	GLN	2.1
1	B	77	ALA	2.1
1	D	92	ALA	2.1
1	E	3	PHE	2.1
1	E	49	ALA	2.1
1	B	46	ILE	2.1
1	E	21	ILE	2.1
1	A	15	VAL	2.1
1	A	157	VAL	2.1
1	B	129	VAL	2.1
1	D	84	SER	2.0
1	F	147	GLY	2.0
1	A	14[A]	LEU	2.0
1	A	33	LEU	2.0
1	F	82	CYS	2.0
1	E	83	ALA	2.0
1	E	108	ALA	2.0
1	A	125	PRO	2.0
1	E	109	PRO	2.0
1	D	100	ILE	2.0
1	A	11	VAL	2.0
1	D	127	ASP	2.0
1	C	99	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	163	1/1	0.99	0.12	17,17,17,17	0
2	ZN	B	163	1/1	0.99	0.30	28,28,28,28	0
2	ZN	C	163	1/1	0.99	0.32	27,27,27,27	0
2	ZN	D	163	1/1	0.99	0.12	17,17,17,17	0
2	ZN	E	163	1/1	0.99	0.27	26,26,26,26	0
2	ZN	F	163	1/1	1.00	0.16	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.