



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:16 pm BST

PDB ID : 2AZ1
Title : Structure of a halophilic nucleoside diphosphate kinase from Halobacterium salinarum
Authors : Besir, H.; Zeth, K.; Bracher, A.; Heider, U.; Ishibashi, M.; Tokunaga, M.; Oesterhelt, D.
Deposited on : 2005-09-09
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

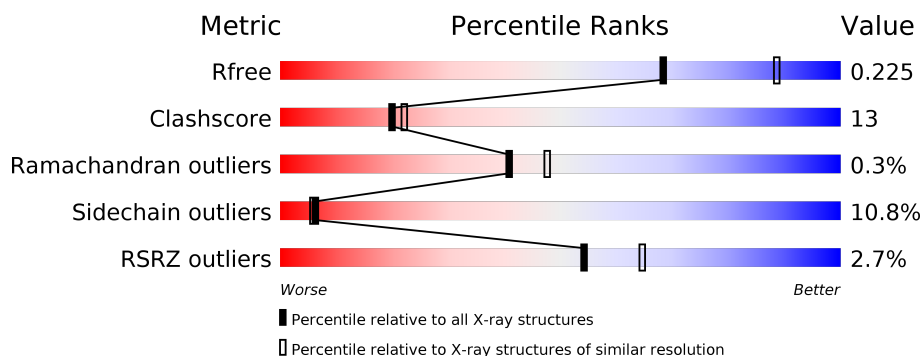
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	181	<div> <div>0%</div> <div> <div>60%</div> <div>22%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	181	<div> <div>3%</div> <div> <div>56%</div> <div>23%</div> <div>• •</div> <div>17%</div> </div> </div>
1	C	181	<div> <div>0%</div> <div> <div>60%</div> <div>20%</div> <div>5%</div> <div>14%</div> </div> </div>
1	D	181	<div> <div>2%</div> <div> <div>60%</div> <div>23%</div> <div>•</div> <div>14%</div> </div> </div>
1	E	181	<div> <div>5%</div> <div> <div>54%</div> <div>27%</div> <div>• •</div> <div>15%</div> </div> </div>
1	F	181	<div> <div>3%</div> <div> <div>56%</div> <div>22%</div> <div>6%</div> <div>17%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7204 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1204	753	210	236	5			
1	B	151	Total	C	N	O	S	0	0	0
			1157	726	204	222	5			
1	C	155	Total	C	N	O	S	0	0	0
			1204	752	209	238	5			
1	D	155	Total	C	N	O	S	0	0	0
			1196	747	208	236	5			
1	E	154	Total	C	N	O	S	0	0	0
			1164	731	205	223	5			
1	F	151	Total	C	N	O	S	0	0	0
			1169	730	206	228	5			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP P61136
A	-18	GLY	-	CLONING ARTIFACT	UNP P61136
A	-17	SER	-	CLONING ARTIFACT	UNP P61136
A	-16	SER	-	CLONING ARTIFACT	UNP P61136
A	-15	HIS	-	CLONING ARTIFACT	UNP P61136
A	-14	HIS	-	CLONING ARTIFACT	UNP P61136
A	-13	HIS	-	CLONING ARTIFACT	UNP P61136
A	-12	HIS	-	CLONING ARTIFACT	UNP P61136
A	-11	HIS	-	CLONING ARTIFACT	UNP P61136
A	-10	HIS	-	CLONING ARTIFACT	UNP P61136
A	-9	SER	-	CLONING ARTIFACT	UNP P61136
A	-8	SER	-	CLONING ARTIFACT	UNP P61136
A	-7	GLY	-	CLONING ARTIFACT	UNP P61136
A	-6	LEU	-	CLONING ARTIFACT	UNP P61136
A	-5	VAL	-	CLONING ARTIFACT	UNP P61136
A	-4	PRO	-	CLONING ARTIFACT	UNP P61136
A	-3	ARG	-	CLONING ARTIFACT	UNP P61136

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P61136
A	-1	SER	-	CLONING ARTIFACT	UNP P61136
A	0	HIS	-	CLONING ARTIFACT	UNP P61136
B	-19	MET	-	CLONING ARTIFACT	UNP P61136
B	-18	GLY	-	CLONING ARTIFACT	UNP P61136
B	-17	SER	-	CLONING ARTIFACT	UNP P61136
B	-16	SER	-	CLONING ARTIFACT	UNP P61136
B	-15	HIS	-	CLONING ARTIFACT	UNP P61136
B	-14	HIS	-	CLONING ARTIFACT	UNP P61136
B	-13	HIS	-	CLONING ARTIFACT	UNP P61136
B	-12	HIS	-	CLONING ARTIFACT	UNP P61136
B	-11	HIS	-	CLONING ARTIFACT	UNP P61136
B	-10	HIS	-	CLONING ARTIFACT	UNP P61136
B	-9	SER	-	CLONING ARTIFACT	UNP P61136
B	-8	SER	-	CLONING ARTIFACT	UNP P61136
B	-7	GLY	-	CLONING ARTIFACT	UNP P61136
B	-6	LEU	-	CLONING ARTIFACT	UNP P61136
B	-5	VAL	-	CLONING ARTIFACT	UNP P61136
B	-4	PRO	-	CLONING ARTIFACT	UNP P61136
B	-3	ARG	-	CLONING ARTIFACT	UNP P61136
B	-2	GLY	-	CLONING ARTIFACT	UNP P61136
B	-1	SER	-	CLONING ARTIFACT	UNP P61136
B	0	HIS	-	CLONING ARTIFACT	UNP P61136
C	-19	MET	-	CLONING ARTIFACT	UNP P61136
C	-18	GLY	-	CLONING ARTIFACT	UNP P61136
C	-17	SER	-	CLONING ARTIFACT	UNP P61136
C	-16	SER	-	CLONING ARTIFACT	UNP P61136
C	-15	HIS	-	CLONING ARTIFACT	UNP P61136
C	-14	HIS	-	CLONING ARTIFACT	UNP P61136
C	-13	HIS	-	CLONING ARTIFACT	UNP P61136
C	-12	HIS	-	CLONING ARTIFACT	UNP P61136
C	-11	HIS	-	CLONING ARTIFACT	UNP P61136
C	-10	HIS	-	CLONING ARTIFACT	UNP P61136
C	-9	SER	-	CLONING ARTIFACT	UNP P61136
C	-8	SER	-	CLONING ARTIFACT	UNP P61136
C	-7	GLY	-	CLONING ARTIFACT	UNP P61136
C	-6	LEU	-	CLONING ARTIFACT	UNP P61136
C	-5	VAL	-	CLONING ARTIFACT	UNP P61136
C	-4	PRO	-	CLONING ARTIFACT	UNP P61136
C	-3	ARG	-	CLONING ARTIFACT	UNP P61136
C	-2	GLY	-	CLONING ARTIFACT	UNP P61136
C	-1	SER	-	CLONING ARTIFACT	UNP P61136

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	CLONING ARTIFACT	UNP P61136
D	-19	MET	-	CLONING ARTIFACT	UNP P61136
D	-18	GLY	-	CLONING ARTIFACT	UNP P61136
D	-17	SER	-	CLONING ARTIFACT	UNP P61136
D	-16	SER	-	CLONING ARTIFACT	UNP P61136
D	-15	HIS	-	CLONING ARTIFACT	UNP P61136
D	-14	HIS	-	CLONING ARTIFACT	UNP P61136
D	-13	HIS	-	CLONING ARTIFACT	UNP P61136
D	-12	HIS	-	CLONING ARTIFACT	UNP P61136
D	-11	HIS	-	CLONING ARTIFACT	UNP P61136
D	-10	HIS	-	CLONING ARTIFACT	UNP P61136
D	-9	SER	-	CLONING ARTIFACT	UNP P61136
D	-8	SER	-	CLONING ARTIFACT	UNP P61136
D	-7	GLY	-	CLONING ARTIFACT	UNP P61136
D	-6	LEU	-	CLONING ARTIFACT	UNP P61136
D	-5	VAL	-	CLONING ARTIFACT	UNP P61136
D	-4	PRO	-	CLONING ARTIFACT	UNP P61136
D	-3	ARG	-	CLONING ARTIFACT	UNP P61136
D	-2	GLY	-	CLONING ARTIFACT	UNP P61136
D	-1	SER	-	CLONING ARTIFACT	UNP P61136
D	0	HIS	-	CLONING ARTIFACT	UNP P61136
E	-19	MET	-	CLONING ARTIFACT	UNP P61136
E	-18	GLY	-	CLONING ARTIFACT	UNP P61136
E	-17	SER	-	CLONING ARTIFACT	UNP P61136
E	-16	SER	-	CLONING ARTIFACT	UNP P61136
E	-15	HIS	-	CLONING ARTIFACT	UNP P61136
E	-14	HIS	-	CLONING ARTIFACT	UNP P61136
E	-13	HIS	-	CLONING ARTIFACT	UNP P61136
E	-12	HIS	-	CLONING ARTIFACT	UNP P61136
E	-11	HIS	-	CLONING ARTIFACT	UNP P61136
E	-10	HIS	-	CLONING ARTIFACT	UNP P61136
E	-9	SER	-	CLONING ARTIFACT	UNP P61136
E	-8	SER	-	CLONING ARTIFACT	UNP P61136
E	-7	GLY	-	CLONING ARTIFACT	UNP P61136
E	-6	LEU	-	CLONING ARTIFACT	UNP P61136
E	-5	VAL	-	CLONING ARTIFACT	UNP P61136
E	-4	PRO	-	CLONING ARTIFACT	UNP P61136
E	-3	ARG	-	CLONING ARTIFACT	UNP P61136
E	-2	GLY	-	CLONING ARTIFACT	UNP P61136
E	-1	SER	-	CLONING ARTIFACT	UNP P61136
E	0	HIS	-	CLONING ARTIFACT	UNP P61136
F	-19	MET	-	CLONING ARTIFACT	UNP P61136

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	CLONING ARTIFACT	UNP P61136
F	-17	SER	-	CLONING ARTIFACT	UNP P61136
F	-16	SER	-	CLONING ARTIFACT	UNP P61136
F	-15	HIS	-	CLONING ARTIFACT	UNP P61136
F	-14	HIS	-	CLONING ARTIFACT	UNP P61136
F	-13	HIS	-	CLONING ARTIFACT	UNP P61136
F	-12	HIS	-	CLONING ARTIFACT	UNP P61136
F	-11	HIS	-	CLONING ARTIFACT	UNP P61136
F	-10	HIS	-	CLONING ARTIFACT	UNP P61136
F	-9	SER	-	CLONING ARTIFACT	UNP P61136
F	-8	SER	-	CLONING ARTIFACT	UNP P61136
F	-7	GLY	-	CLONING ARTIFACT	UNP P61136
F	-6	LEU	-	CLONING ARTIFACT	UNP P61136
F	-5	VAL	-	CLONING ARTIFACT	UNP P61136
F	-4	PRO	-	CLONING ARTIFACT	UNP P61136
F	-3	ARG	-	CLONING ARTIFACT	UNP P61136
F	-2	GLY	-	CLONING ARTIFACT	UNP P61136
F	-1	SER	-	CLONING ARTIFACT	UNP P61136
F	0	HIS	-	CLONING ARTIFACT	UNP P61136

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	13	Total O 13 13	0	0
3	C	24	Total O 24 24	0	0
3	D	20	Total O 20 20	0	0
3	E	11	Total O 11 11	0	0

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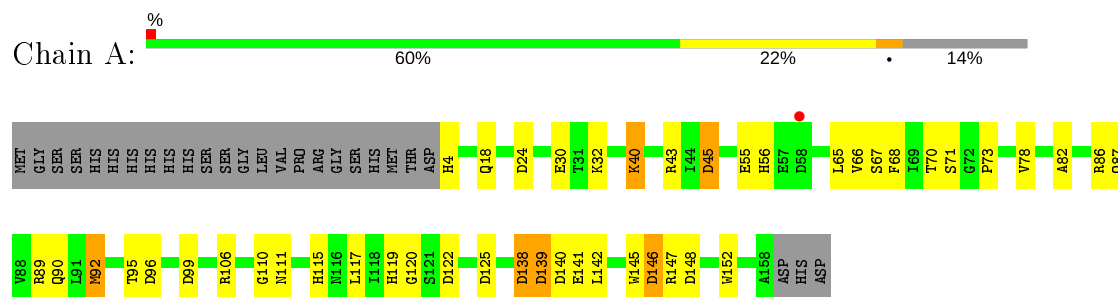
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	18	Total	O	0	0
			18	18		

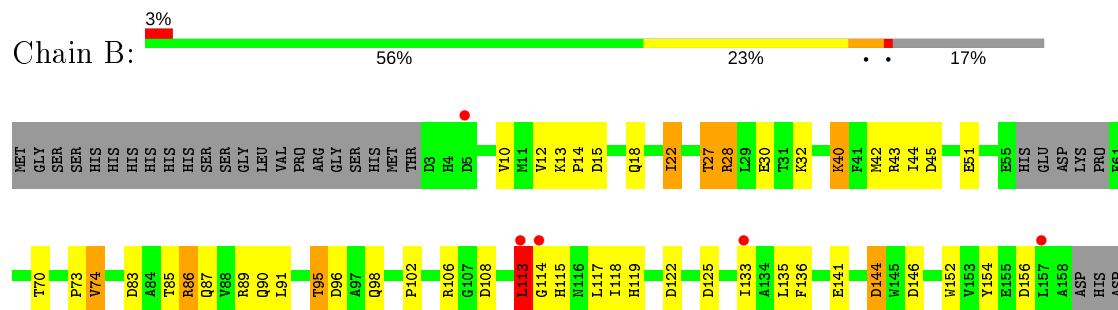
3 Residue-property plots [i](#)

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.

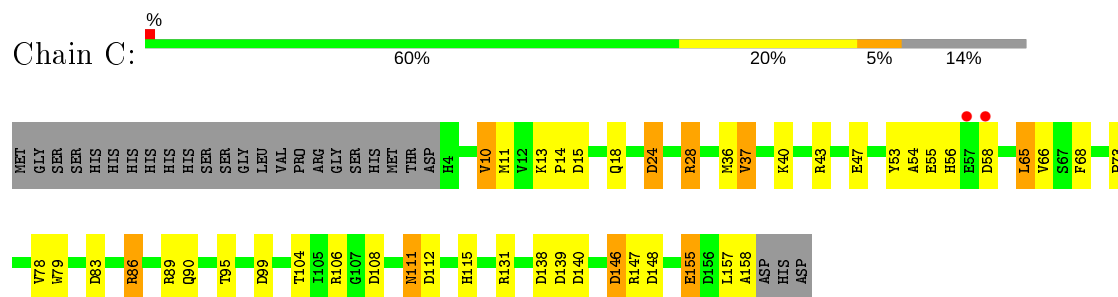
- Molecule 1: Nucleoside diphosphate kinase



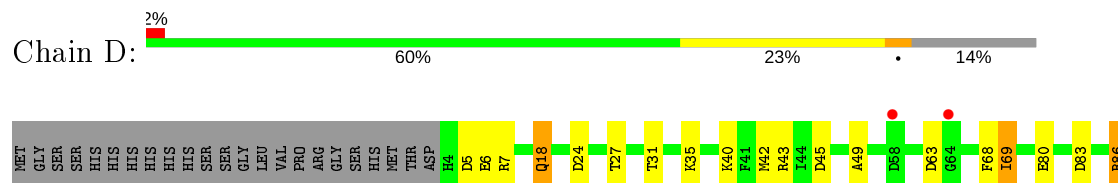
- Molecule 1: Nucleoside diphosphate kinase

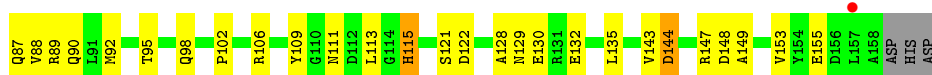


- Molecule 1: Nucleoside diphosphate kinase

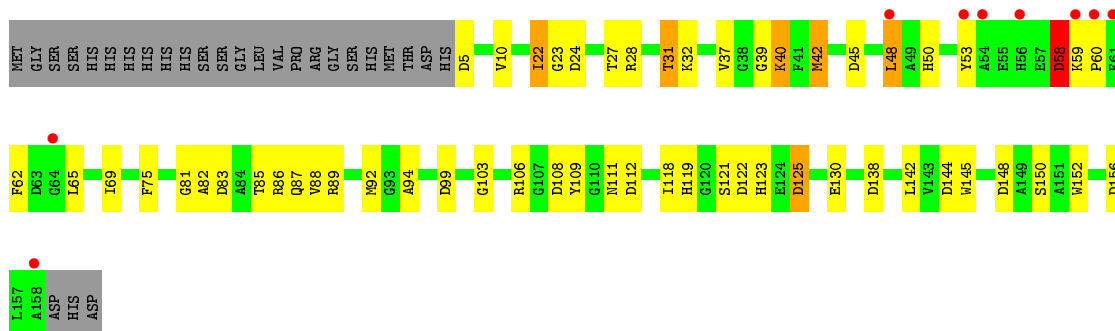


- Molecule 1: Nucleoside diphosphate kinase

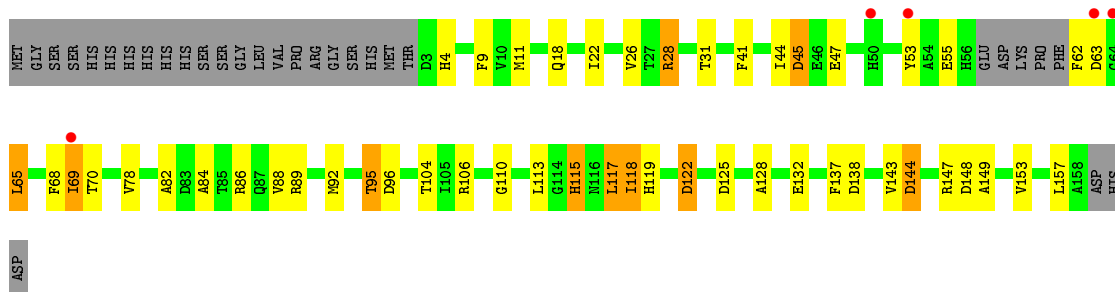




- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.28Å 108.70Å 119.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 80.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.35) 99.4 (80.46-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.289 0.221 , 0.225	Depositor DCC
R_{free} test set	2004 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.1	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	7204	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 24.08 % 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 4.1081e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.93	1/1231 (0.1%)	1.07	9/1667 (0.5%)
1	B	0.88	0/1181	1.11	10/1597 (0.6%)
1	C	1.03	0/1230	1.14	14/1664 (0.8%)
1	D	0.91	0/1222	1.04	4/1655 (0.2%)
1	E	0.88	0/1190	1.07	9/1613 (0.6%)
1	F	0.96	0/1193	1.12	7/1613 (0.4%)
All	All	0.93	1/7247 (0.0%)	1.09	53/9809 (0.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	MET	SD-CE	-5.49	1.47	1.77

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	45	ASP	CB-CG-OD2	8.31	125.78	118.30
1	E	24	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	125	ASP	CB-CG-OD2	8.12	125.61	118.30
1	C	15	ASP	CB-CG-OD2	7.87	125.38	118.30
1	E	58	ASP	CB-CG-OD2	7.63	125.17	118.30
1	F	144	ASP	CB-CG-OD2	7.28	124.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	ASP	CB-CG-OD1	7.08	124.67	118.30
1	C	108	ASP	CB-CG-OD2	7.02	124.62	118.30
1	E	125	ASP	CB-CG-OD2	6.98	124.58	118.30
1	F	138	ASP	CB-CG-OD2	6.94	124.55	118.30
1	B	15	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	45	ASP	CB-CG-OD2	6.83	124.44	118.30
1	D	63	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	144	ASP	CB-CG-OD2	6.60	124.24	118.30
1	C	28	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	F	63	ASP	CB-CG-OD2	6.36	124.02	118.30
1	C	28	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	138	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	28	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	86	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	146	ASP	CB-CG-OD2	5.96	123.67	118.30
1	E	45	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	24	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	146	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	108	ASP	CB-CG-OD2	5.87	123.58	118.30
1	E	99	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	45	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	99	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	96	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	28	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	E	108	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	96	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	148	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	45	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	122	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	86	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	E	148	ASP	CB-CG-OD2	5.35	123.12	118.30
1	F	86	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	146	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	140	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	96	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	28	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	139	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	89	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	138	ASP	CB-CG-OD2	5.11	122.90	118.30
1	E	138	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	139	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	122	ASP	CB-CG-OD1	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	LEU	CA-CB-CG	5.07	126.97	115.30
1	C	112	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	140	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	89	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	E	156	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	157	LEU	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	1204	0	1107	28	0
1	B	1157	0	1065	38	0
1	C	1204	0	1108	32	0
1	D	1196	0	1093	31	0
1	E	1164	0	1062	37	0
1	F	1169	0	1080	39	0
2	A	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	19	0	0	5	0
3	B	13	0	0	3	0
3	C	24	0	0	3	0
3	D	20	0	0	3	0
3	E	11	0	0	4	0
3	F	18	0	0	1	0
All	All	7204	0	6515	172	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 13.

All (172) 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:D:35:LYS:NZ	1:D:80:GLU:OE2	1.99	0.95
1:B:125:ASP:OD1	3:B:170:HOH:O	1.93	0.84
1:B:12:VAL:HA	1:B:118:ILE:HG22	1.61	0.83
1:D:24:ASP:OD2	3:D:210:HOH:O	1.97	0.83
1:E:112:ASP:OD2	3:E:167:HOH:O	1.96	0.83
1:D:7:ARG:NH1	1:D:80:GLU:OE1	2.13	0.82
1:A:4:HIS:N	3:A:211:HOH:O	2.13	0.80
1:C:147:ARG:HD3	3:C:228:HOH:O	1.80	0.80
1:F:147:ARG:HD3	3:F:178:HOH:O	1.81	0.80
1:F:65:LEU:O	1:F:69:ILE:HD13	1.80	0.79
1:E:27:THR:O	1:E:31:THR:HG23	1.82	0.79
1:D:27:THR:O	1:D:31:THR:HG23	1.88	0.73
1:A:55:GLU:HG2	1:A:56:HIS:CD2	2.23	0.73
1:C:18:GLN:HE22	1:F:147:ARG:HA	1.54	0.73
1:C:146:ASP:HB3	3:C:227:HOH:O	1.87	0.73
1:C:18:GLN:NE2	1:F:148:ASP:H	1.89	0.71
1:F:53:TYR:CE2	1:F:69:ILE:HD12	2.26	0.70
1:A:147:ARG:HD3	3:A:221:HOH:O	1.91	0.69
1:A:66:VAL:O	1:A:70:THR:HG22	1.92	0.69
1:F:117:LEU:HB3	1:F:118:ILE:HG22	1.73	0.69
1:A:24:ASP:OD2	3:A:215:HOH:O	2.11	0.68
1:F:53:TYR:HE2	1:F:69:ILE:HD12	1.58	0.67
1:C:55:GLU:HG3	1:C:56:HIS:CD2	2.30	0.66
1:E:53:TYR:CE2	1:E:69:ILE:HD13	2.32	0.65
1:E:28:ARG:NH1	1:E:109:TYR:HE2	1.94	0.65
1:D:155:GLU:N	3:E:167:HOH:O	2.29	0.65
1:B:86:ARG:NH1	1:B:90:GLN:HE22	1.96	0.64
1:A:111:ASN:HD21	1:B:87:GLN:HG3	1.61	0.64
1:E:28:ARG:HH11	1:E:109:TYR:HE2	1.43	0.64
1:A:18:GLN:O	3:A:217:HOH:O	2.15	0.64
1:C:155:GLU:O	1:C:158:ALA:C	2.36	0.63
1:B:27:THR:HG21	3:E:172:HOH:O	1.98	0.63
3:A:217:HOH:O	1:D:147:ARG:CZ	2.47	0.63
1:E:28:ARG:NH2	1:E:103:GLY:O	2.32	0.63
1:E:65:LEU:O	1:E:69:ILE:HD12	1.98	0.63
1:D:149:ALA:O	1:D:153:VAL:HG23	1.99	0.62
1:F:44:ILE:O	1:F:70:THR:HG22	1.99	0.61
1:B:86:ARG:HH11	1:B:90:GLN:HE22	1.46	0.61
1:C:36:MET:HE3	1:F:41:PHE:HB2	1.82	0.61
1:E:92:MET:HE2	1:E:118:ILE:HG23	1.82	0.61
1:C:13:LYS:HB3	1:C:14:PRO:CD	2.31	0.61
1:E:59:LYS:HB3	1:E:60:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TRP:CD1	1:C:18:GLN:HG2	2.36	0.60
1:B:27:THR:HG22	1:E:23:GLY:HA3	1.85	0.59
1:F:65:LEU:C	1:F:69:ILE:HD13	2.23	0.59
1:B:22:ILE:HD12	1:B:22:ILE:C	2.23	0.58
1:C:148:ASP:H	1:F:18:GLN:HE22	1.51	0.58
1:A:148:ASP:H	1:D:18:GLN:HE22	1.50	0.58
1:E:40:LYS:CG	1:E:42:MET:HG2	2.34	0.58
1:C:18:GLN:NE2	1:F:147:ARG:HA	2.19	0.57
1:E:88:VAL:O	1:E:88:VAL:HG12	2.04	0.56
1:E:89:ARG:HD2	1:E:122:ASP:HA	1.87	0.56
1:B:44:ILE:HD11	1:B:136:PHE:HE2	1.71	0.56
1:E:83:ASP:OD2	1:E:86:ARG:HB3	2.07	0.55
1:A:145:TRP:CZ3	1:A:147:ARG:HB2	2.42	0.55
1:F:117:LEU:CB	1:F:118:ILE:HG22	2.36	0.54
1:F:89:ARG:NH2	1:F:122:ASP:OD1	2.40	0.54
1:F:11:MET:HE1	1:F:44:ILE:HD11	1.88	0.54
1:F:22:ILE:O	1:F:26:VAL:HG23	2.06	0.54
1:E:32:LYS:NZ	1:E:87:GLN:OE1	2.39	0.53
1:F:84:ALA:O	1:F:88:VAL:HG23	2.08	0.53
1:E:58:ASP:N	1:E:58:ASP:OD1	2.42	0.52
1:A:40:LYS:HD3	1:A:141:GLU:OE2	2.10	0.52
1:B:43:ARG:NH2	1:E:144:ASP:O	2.41	0.52
1:D:92:MET:CE	1:D:106:ARG:NH2	2.73	0.52
1:B:117:LEU:O	1:B:118:ILE:CG2	2.59	0.51
1:B:95:THR:HG23	3:B:173:HOH:O	2.10	0.51
1:F:4:HIS:HD2	1:F:82:ALA:HB2	1.75	0.51
1:D:87:GLN:HG3	1:E:111:ASN:HD21	1.73	0.51
1:D:88:VAL:O	1:D:92:MET:HG3	2.10	0.51
1:B:30:GLU:OE1	1:E:22:ILE:HG22	2.11	0.51
1:C:10:VAL:HG13	1:C:79:TRP:CD1	2.45	0.51
1:F:95:THR:HA	1:F:106:ARG:NH1	2.26	0.50
1:B:102:PRO:HG2	1:C:104:THR:HG22	1.94	0.50
1:B:40:LYS:HE3	1:B:141:GLU:OE2	2.12	0.50
1:B:86:ARG:HD2	1:B:90:GLN:NE2	2.27	0.50
1:A:111:ASN:ND2	1:B:87:GLN:HG3	2.25	0.50
1:A:86:ARG:NH1	1:A:90:GLN:HE22	2.09	0.50
1:C:54:ALA:C	1:C:56:HIS:H	2.15	0.50
1:A:110:GLY:O	1:B:32:LYS:NZ	2.41	0.49
1:E:50:HIS:HD2	1:E:62:PHE:CZ	2.30	0.49
1:F:119:HIS:NE2	1:F:132:GLU:OE1	2.25	0.49
1:C:18:GLN:HE22	1:F:148:ASP:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:THR:CG2	3:E:172:HOH:O	2.56	0.49
1:D:49:ALA:HB1	1:D:69:ILE:HD11	1.93	0.48
1:C:10:VAL:HG13	1:C:79:TRP:HD1	1.79	0.48
1:B:44:ILE:HD11	1:B:136:PHE:CE2	2.49	0.48
1:D:68:PHE:CD1	1:D:115:HIS:CE1	3.02	0.48
1:B:10:VAL:HA	1:B:119:HIS:O	2.14	0.48
1:D:102:PRO:HG2	1:F:104:THR:HG22	1.96	0.48
1:A:87:GLN:HG3	1:C:111:ASN:HD21	1.79	0.47
1:B:113:LEU:HD22	1:B:114:GLY:N	2.28	0.47
1:D:83:ASP:OD2	1:D:86:ARG:NE	2.47	0.47
1:E:106:ARG:NH2	1:E:118:ILE:O	2.47	0.47
1:A:4:HIS:CD2	1:A:82:ALA:HB2	2.49	0.47
1:A:43:ARG:NH2	1:D:144:ASP:O	2.47	0.47
1:B:117:LEU:O	1:B:118:ILE:HG23	2.14	0.47
1:E:94:ALA:O	1:E:106:ARG:HD3	2.15	0.47
1:F:117:LEU:C	1:F:118:ILE:HG22	2.35	0.47
1:D:89:ARG:HD2	1:D:122:ASP:HA	1.97	0.47
1:E:88:VAL:O	1:E:88:VAL:CG1	2.63	0.47
1:D:95:THR:HA	1:D:106:ARG:NH1	2.30	0.46
1:D:87:GLN:HG3	1:E:111:ASN:ND2	2.29	0.46
1:D:128:ALA:O	1:D:132:GLU:HG3	2.15	0.46
1:D:43:ARG:NH2	3:D:206:HOH:O	2.46	0.46
1:B:83:ASP:OD1	1:B:86:ARG:HB2	2.15	0.46
1:C:24:ASP:O	1:C:28:ARG:HG2	2.16	0.46
1:C:37:VAL:HG12	1:C:78:VAL:HB	1.97	0.46
1:A:89:ARG:NH1	1:A:120:GLY:O	2.49	0.46
1:A:73:PRO:HB3	1:D:143:VAL:HG11	1.98	0.46
1:E:32:LYS:HE2	1:F:110:GLY:O	2.17	0.45
1:B:14:PRO:HD3	1:B:74:VAL:HG23	1.99	0.45
1:E:10:VAL:HA	1:E:119:HIS:O	2.16	0.45
1:A:152:TRP:CG	1:C:18:GLN:HG2	2.52	0.45
1:D:49:ALA:CB	1:D:69:ILE:HD11	2.46	0.45
1:D:7:ARG:NE	3:D:208:HOH:O	2.50	0.45
1:E:69:ILE:HG22	1:E:69:ILE:O	2.17	0.45
1:F:62:PHE:C	1:F:62:PHE:CD2	2.90	0.45
1:C:68:PHE:CD1	1:C:115:HIS:CE1	3.05	0.45
1:D:98:GLN:HG2	1:D:111:ASN:HB2	1.99	0.45
1:D:6:GLU:O	1:D:80:GLU:HA	2.17	0.44
1:A:55:GLU:CG	1:A:56:HIS:CD2	2.97	0.44
1:B:44:ILE:HB	3:B:171:HOH:O	2.17	0.44
1:C:18:GLN:HG3	3:C:207:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TYR:CE2	1:C:65:LEU:HD22	2.53	0.44
1:E:85:THR:HG22	1:E:123:HIS:HB3	1.99	0.44
1:A:95:THR:HA	1:A:106:ARG:NH1	2.33	0.44
1:E:48:LEU:O	1:E:48:LEU:HD12	2.17	0.44
1:B:13:LYS:HB3	1:B:14:PRO:HD2	2.00	0.44
1:A:32:LYS:HE3	1:A:87:GLN:HE21	1.82	0.44
1:F:45:ASP:N	1:F:45:ASP:OD1	2.51	0.43
1:F:92:MET:SD	1:F:118:ILE:HG12	2.58	0.43
1:B:22:ILE:HD12	1:B:22:ILE:O	2.18	0.43
1:F:9:PHE:HZ	1:F:11:MET:HE3	1.83	0.43
1:D:86:ARG:HH11	1:D:90:GLN:HE22	1.66	0.43
1:E:152:TRP:O	1:F:115:HIS:HD2	2.01	0.43
1:C:18:GLN:NE2	1:F:148:ASP:N	2.64	0.43
1:E:22:ILE:HD11	1:E:75:PHE:CE2	2.54	0.43
1:E:81:GLY:O	1:E:82:ALA:C	2.56	0.43
1:B:113:LEU:HD22	1:B:114:GLY:H	1.83	0.43
1:C:13:LYS:HB3	1:C:14:PRO:HD2	2.01	0.43
1:B:113:LEU:H	1:B:113:LEU:HD13	1.83	0.42
1:F:89:ARG:HD2	1:F:92:MET:CE	2.49	0.42
1:F:78:VAL:HG23	1:F:137:PHE:CE2	2.55	0.42
1:A:152:TRP:CE2	1:C:18:GLN:HG2	2.54	0.42
1:B:40:LYS:HA	1:E:39:GLY:O	2.20	0.42
1:E:59:LYS:HB3	1:E:60:PRO:CD	2.49	0.42
1:E:22:ILE:HD11	1:E:75:PHE:CD2	2.55	0.42
1:C:86:ARG:O	1:C:90:GLN:HG3	2.20	0.42
1:F:4:HIS:CD2	1:F:82:ALA:HB2	2.55	0.42
1:A:115:HIS:HD2	1:B:152:TRP:O	2.02	0.42
1:F:68:PHE:CD1	1:F:115:HIS:CE1	3.08	0.42
1:A:68:PHE:O	1:A:71:SER:OG	2.30	0.41
1:F:149:ALA:O	1:F:153:VAL:HG23	2.19	0.41
1:B:32:LYS:O	1:B:32:LYS:HG3	2.20	0.41
1:E:40:LYS:HG3	1:E:42:MET:HG2	2.01	0.41
1:A:92:MET:HE1	1:A:119:HIS:C	2.41	0.41
1:B:95:THR:HA	1:B:106:ARG:NH1	2.36	0.41
1:D:121:SER:OG	1:D:129:ASN:HA	2.20	0.41
1:C:54:ALA:C	1:C:56:HIS:N	2.74	0.41
1:D:92:MET:O	1:D:106:ARG:HG3	2.21	0.41
1:C:95:THR:HA	1:C:106:ARG:NH1	2.36	0.41
1:B:73:PRO:HG2	1:E:145:TRP:CD2	2.56	0.41
1:C:73:PRO:HB3	1:F:143:VAL:HG11	2.03	0.41
1:B:98:GLN:HE22	1:C:83:ASP:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:VAL:HG21	1:A:142:LEU:HD21	2.02	0.40
1:B:117:LEU:C	1:B:118:ILE:HG23	2.42	0.40
1:D:111:ASN:CG	1:D:111:ASN:O	2.59	0.40
1:B:98:GLN:NE2	1:C:83:ASP:HB3	2.37	0.40
1:F:122:ASP:HB3	1:F:125:ASP:HB3	2.03	0.40
1:F:128:ALA:O	1:F:132:GLU:HG3	2.21	0.40
1:D:109:TYR:HD1	1:F:31:THR:HG22	1.85	0.40

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	153/181 (84%)	146 (95%)	7 (5%)	0	100	100
1	B	147/181 (81%)	136 (92%)	11 (8%)	0	100	100
1	C	153/181 (84%)	145 (95%)	8 (5%)	0	100	100
1	D	153/181 (84%)	144 (94%)	9 (6%)	0	100	100
1	E	152/181 (84%)	136 (90%)	14 (9%)	2 (1%)	12	10
1	F	147/181 (81%)	138 (94%)	8 (5%)	1 (1%)	22	23
All	All	905/1086 (83%)	845 (93%)	57 (6%)	3 (0%)	41	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	55	GLU
1	E	121	SER
1	E	125	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	120/148 (81%)	111 (92%)	9 (8%)	13	13
1	B	112/148 (76%)	91 (81%)	21 (19%)	1	1
1	C	120/148 (81%)	108 (90%)	12 (10%)	7	6
1	D	118/148 (80%)	108 (92%)	10 (8%)	10	10
1	E	111/148 (75%)	100 (90%)	11 (10%)	8	7
1	F	116/148 (78%)	104 (90%)	12 (10%)	7	6
All	All	697/888 (78%)	622 (89%)	75 (11%)	6	6

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	40	LYS
1	A	45	ASP
1	A	65	LEU
1	A	67	SER
1	A	117	LEU
1	A	138	ASP
1	A	139	ASP
1	A	146	ASP
1	B	18	GLN
1	B	22	ILE
1	B	27	THR
1	B	28	ARG
1	B	40	LYS
1	B	42	MET
1	B	51	GLU
1	B	70	THR
1	B	74	VAL
1	B	85	THR
1	B	86	ARG
1	B	89	ARG
1	B	91	LEU

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Mol	Chain	Res	Type
1	B	95	THR
1	B	113	LEU
1	B	115	HIS
1	B	133	ILE
1	B	135	LEU
1	B	144	ASP
1	B	154	TYR
1	B	156	ASP
1	C	10	VAL
1	C	11	MET
1	C	37	VAL
1	C	40	LYS
1	C	43	ARG
1	C	47	GLU
1	C	58	ASP
1	C	65	LEU
1	C	66	VAL
1	C	111	ASN
1	C	131	ARG
1	C	155	GLU
1	D	5	ASP
1	D	18	GLN
1	D	40	LYS
1	D	42	MET
1	D	69	ILE
1	D	113	LEU
1	D	115	HIS
1	D	130	GLU
1	D	135	LEU
1	D	144	ASP
1	E	5	ASP
1	E	22	ILE
1	E	31	THR
1	E	37	VAL
1	E	40	LYS
1	E	42	MET
1	E	48	LEU
1	E	58	ASP
1	E	130	GLU
1	E	142	LEU
1	E	150	SER
1	F	28	ARG

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Mol	Chain	Res	Type
1	F	47	GLU
1	F	65	LEU
1	F	69	ILE
1	F	95	THR
1	F	113	LEU
1	F	115	HIS
1	F	117	LEU
1	F	118	ILE
1	F	122	ASP
1	F	144	ASP
1	F	157	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	56	HIS
1	A	87	GLN
1	A	90	GLN
1	A	111	ASN
1	A	115	HIS
1	B	4	HIS
1	B	18	GLN
1	B	87	GLN
1	B	90	GLN
1	B	98	GLN
1	C	18	GLN
1	C	56	HIS
1	C	90	GLN
1	C	111	ASN
1	D	18	GLN
1	D	90	GLN
1	D	115	HIS
1	E	18	GLN
1	E	50	HIS
1	E	52	HIS
1	E	56	HIS
1	E	111	ASN
1	F	4	HIS
1	F	18	GLN
1	F	50	HIS
1	F	52	HIS

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Mol	Chain	Res	Type
1	F	115	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](#)

Of 5 ligands modelled in this entry, 5 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 [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	155/181 (85%)	0.12	1 (0%) 89 93	35, 47, 66, 72	0
1	B	151/181 (83%)	0.31	5 (3%) 46 59	35, 53, 69, 72	0
1	C	155/181 (85%)	0.18	2 (1%) 77 84	32, 43, 64, 71	0
1	D	155/181 (85%)	0.17	3 (1%) 66 76	35, 47, 69, 74	0
1	E	154/181 (85%)	0.39	9 (5%) 23 33	41, 54, 70, 77	0
1	F	151/181 (83%)	0.27	5 (3%) 46 59	33, 48, 67, 76	0
All	All	921/1086 (84%)	0.24	25 (2%) 54 64	32, 49, 68, 77	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	53	TYR	4.0
1	F	69	ILE	4.0
1	D	64	GLY	3.8
1	B	113	LEU	3.4
1	E	64	GLY	3.2
1	C	57	GLU	3.2
1	E	61	PHE	3.1
1	D	157	LEU	3.0
1	C	58	ASP	3.0
1	B	5	ASP	3.0
1	E	60	PRO	2.9
1	F	53	TYR	2.8
1	F	50	HIS	2.8
1	D	58	ASP	2.7
1	E	56	HIS	2.7
1	E	158	ALA	2.6
1	B	133	ILE	2.6
1	A	58	ASP	2.6
1	E	59	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	64	GLY	2.3
1	B	157	LEU	2.2
1	F	63	ASP	2.2
1	E	48	LEU	2.1
1	B	114	GLY	2.0
1	E	54	ALA	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 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. 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(Å ²)	Q<0.9
2	CA	C	204	1/1	0.75	0.10	72,72,72,72	0
2	CA	D	205	1/1	0.90	0.22	78,78,78,78	0
2	CA	A	203	1/1	0.96	0.08	71,71,71,71	0
2	CA	C	201	1/1	0.96	0.11	52,52,52,52	0
2	CA	D	202	1/1	0.98	0.10	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.