



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:03 AM UTC

PDB ID : 3HB7 / pdb_00003hb7
Title : The Crystal Structure of an Isochorismatase-like Hydrolase from *Alkaliphilus metalliredigens* to 2.3Å
Authors : Stein, A.J.; Xu, X.; Cui, H.; Ng, J.; Edwards, A.; Savchenko, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-05-04
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

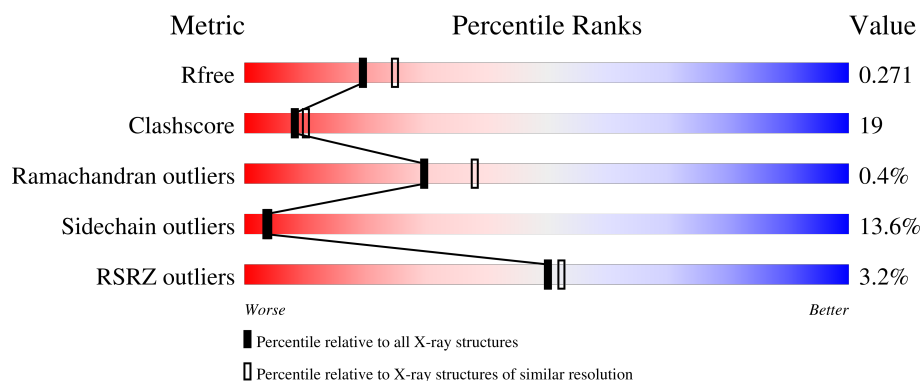
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	204	3% 62% 25% • 8%
1	B	204	4% 59% 25% • 12%
1	C	204	% 50% 31% 6% 13%
1	D	204	% 55% 26% 6% 12%
1	E	204	3% 58% 27% 8% 7%

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Mol	Chain	Length	Quality of chain
1	F	204	3% 57% 30% 10%
1	G	204	2% 57% 25% 8% 11%
1	H	204	4% 35% 33% 15% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11682 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 Isochorismatase hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	Se	0	2	0
			1478	945	254	274	2	3			
1	C	178	Total	C	N	O	S	Se	0	0	0
			1396	887	240	264	2	3			
1	B	179	Total	C	N	O	S	Se	0	1	0
			1419	908	239	267	2	3			
1	D	179	Total	C	N	O	S	Se	0	0	0
			1398	890	241	262	2	3			
1	E	189	Total	C	N	O	S	Se	0	0	0
			1474	935	253	281	2	3			
1	F	183	Total	C	N	O	S	Se	0	0	0
			1437	914	246	272	2	3			
1	G	182	Total	C	N	O	S	Se	0	0	0
			1423	907	242	269	2	3			
1	H	171	Total	C	N	O	S	Se	0	0	0
			1309	835	226	243	2	3			

There are 32 discrepancies between the modelled and reference sequences:

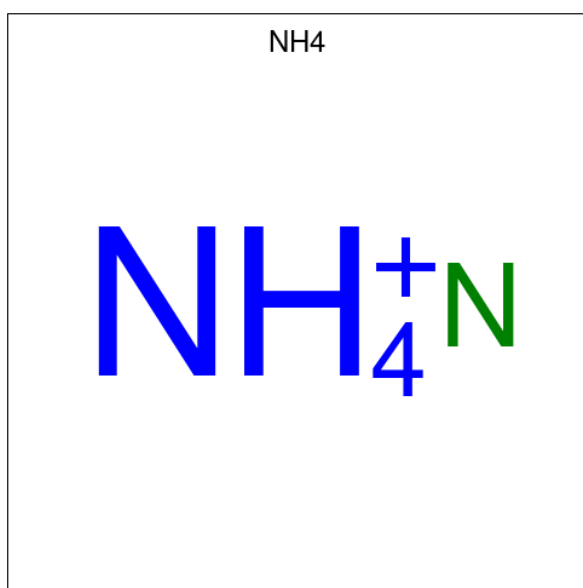
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP A6TWT6
A	-2	PHE	-	expression tag	UNP A6TWT6
A	-1	GLN	-	expression tag	UNP A6TWT6
A	0	GLY	-	expression tag	UNP A6TWT6
C	-3	TYR	-	expression tag	UNP A6TWT6
C	-2	PHE	-	expression tag	UNP A6TWT6
C	-1	GLN	-	expression tag	UNP A6TWT6
C	0	GLY	-	expression tag	UNP A6TWT6
B	-3	TYR	-	expression tag	UNP A6TWT6
B	-2	PHE	-	expression tag	UNP A6TWT6
B	-1	GLN	-	expression tag	UNP A6TWT6
B	0	GLY	-	expression tag	UNP A6TWT6
D	-3	TYR	-	expression tag	UNP A6TWT6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PHE	-	expression tag	UNP A6TWT6
D	-1	GLN	-	expression tag	UNP A6TWT6
D	0	GLY	-	expression tag	UNP A6TWT6
E	-3	TYR	-	expression tag	UNP A6TWT6
E	-2	PHE	-	expression tag	UNP A6TWT6
E	-1	GLN	-	expression tag	UNP A6TWT6
E	0	GLY	-	expression tag	UNP A6TWT6
F	-3	TYR	-	expression tag	UNP A6TWT6
F	-2	PHE	-	expression tag	UNP A6TWT6
F	-1	GLN	-	expression tag	UNP A6TWT6
F	0	GLY	-	expression tag	UNP A6TWT6
G	-3	TYR	-	expression tag	UNP A6TWT6
G	-2	PHE	-	expression tag	UNP A6TWT6
G	-1	GLN	-	expression tag	UNP A6TWT6
G	0	GLY	-	expression tag	UNP A6TWT6
H	-3	TYR	-	expression tag	UNP A6TWT6
H	-2	PHE	-	expression tag	UNP A6TWT6
H	-1	GLN	-	expression tag	UNP A6TWT6
H	0	GLY	-	expression tag	UNP A6TWT6

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total N 1 1	0	0
2	D	1	Total N 1 1	0	0
2	E	1	Total N 1 1	0	0
2	H	1	Total N 1 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0

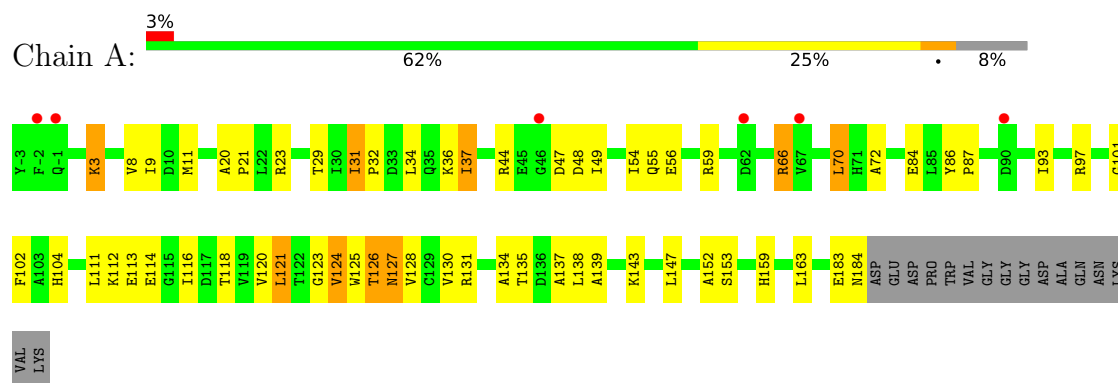
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	C	52	Total O 52 52	0	0
4	B	67	Total O 67 67	0	0
4	D	38	Total O 38 38	0	0
4	E	19	Total O 19 19	0	0
4	F	44	Total O 44 44	0	0
4	G	35	Total O 35 35	0	0
4	H	13	Total O 13 13	0	0

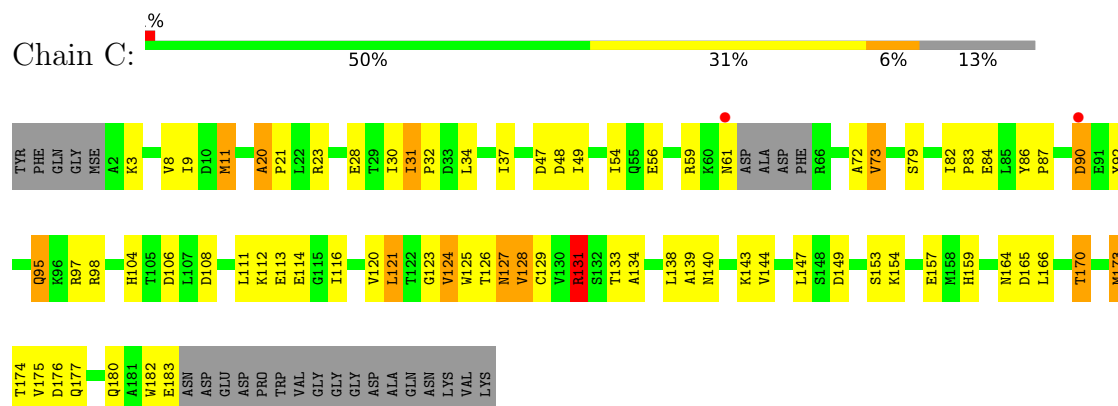
3 Residue-property plots [i](#)

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.

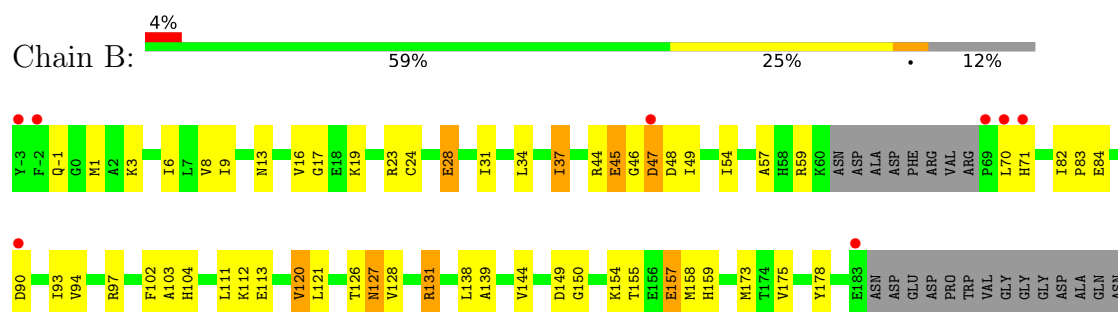
• Molecule 1: Isochorismatase hydrolase



• Molecule 1: Isochorismatase hydrolase



• Molecule 1: Isochorismatase hydrolase



LYS
VAL
LYS

• Molecule 1: Isochorismatase hydrolase



TYR PHE GLN GLY G0 K3 K4 A5 V8 M11 G17 E18 K19 A20 P21 C24 E28 I31 P32 D33 L34 Q35 K36 I37 V40 V41 D47 D48 I54 A57 H58 R59 K60 N61 ASP ALA ASP PHE ARG V67 I82 P83 E84 I85 Y86 P87 V94 Q95

K96 R97 F102 A103 H104 K112 E113 I116 V120 L121 T122 G123 V124 A20 M125 T126 M127 R131 S132 T133 A134 A137 L138 D139 A140 A141 V144 I145 T146 L147 S153 K154 E157 M158 H159 L166 T170 K171 V172 M173 T174 V175 D176 Q177 E183 ASN ASP GLU ASP

PRO TRP VAL GLY GLY ASP ALA GLN LYS LYS VAL LYS

• Molecule 1: Isochorismatase hydrolase



TYR PHE GLN MSE A2 K3 H4 A5 I6 I9 D10 M11 L12 G17 R23 G26 G27 E28 T29 T30 I31 P32 L34 I37 W40 V41 R44 E45 D48 I49 K60 ASN ASP ALA ASP PHE ARG VAL ARG PRO L70 H71 A72 V73 K74 Y86 P87 Q88

E89 D90 E91 H99 S100 G101 H104 L109 V110 L111 K112 T116 D117 V118 V119 V120 V124 W125 T126 M127 V128 C129 P130 R131 D136 A137 L138 A139 T146 L147 H159 L163 N164 D165 L166 S167 I168 K171 V172 M173 T174 V175 D176 Q177 V178 I179 Q180 E183 M184

D185 P188 W189 V190 G193 D194 M197 K198 V199 LYS

• Molecule 1: Isochorismatase hydrolase



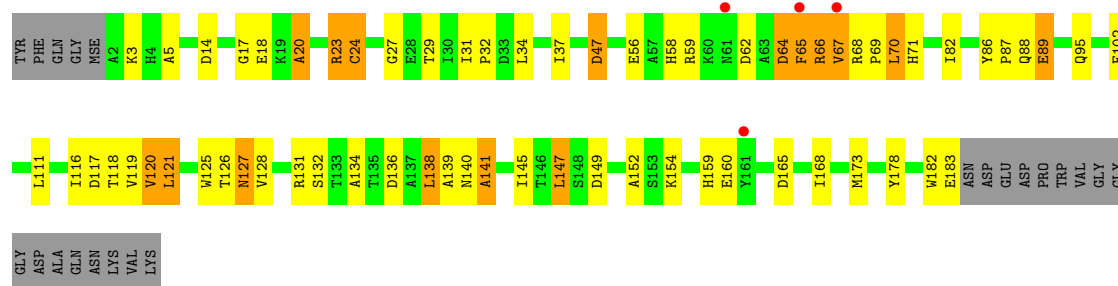
TYR PHE GLN M1 A2 K3 H4 A5 V8 I9 D14 F15 V16 A20 P21 C24 P25 E28 T29 I30 I31 D33 K36 I37 E45 G46 D47 D48 I49 I54 Q55 E56 A57 H58 R59 K60 N61 D62 F65 R66 V67 R68 P69 L70 S79 D80 F81 Q177

Y86 P87 D90 V94 Q95 K96 R97 H104 L107 L111 I116 V120 L121 T122 G123 V124 W125 T126 M127 T133 L138 A139 V144 I145 T146 L147 S148 D149 G150 T151 A152 S153 K154 E157 M158 Y161 M164 D165 L166 T170 M173 D176 Q177

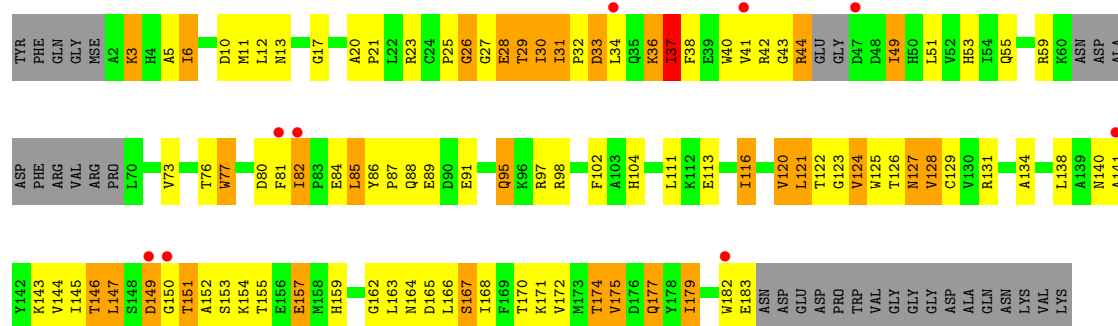
Y178 E183 ASN ASP GLU ASP PRO TRP VAL GLY GLY ASP ALA GLN ASN LYS VAL LYS

• Molecule 1: Isochorismatase hydrolase





• Molecule 1: Isochorismatase hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.65Å 105.42Å 106.27Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	46.32 – 2.30 46.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.32-2.30) 99.5 (46.32-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.29Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0054	Depositor
R, R_{free}	0.196 , 0.238 0.230 , 0.271	Depositor DCC
R_{free} test set	4054 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11682	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NA, NH4

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	2.01	14/1515 (0.9%)	1.14	7/2057 (0.3%)
1	B	2.08	13/1451 (0.9%)	1.16	7/1965 (0.4%)
1	C	1.88	11/1424 (0.8%)	1.06	5/1934 (0.3%)
1	D	1.85	8/1425 (0.6%)	1.05	6/1932 (0.3%)
1	E	1.73	6/1504 (0.4%)	1.02	7/2042 (0.3%)
1	F	1.96	11/1467 (0.7%)	1.04	4/1992 (0.2%)
1	G	1.88	4/1453 (0.3%)	1.04	9/1974 (0.5%)
1	H	1.66	2/1334 (0.1%)	1.15	12/1813 (0.7%)
All	All	1.89	69/11573 (0.6%)	1.08	57/15709 (0.4%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9[A]	ILE	N-CA	-19.66	1.23	1.46
1	B	9[B]	ILE	N-CA	-19.66	1.23	1.46
1	A	9[A]	ILE	N-CA	-14.77	1.27	1.46
1	A	9[B]	ILE	N-CA	-14.77	1.27	1.46
1	F	150	GLY	C-O	-9.22	1.17	1.24
1	A	135[A]	THR	N-CA	-6.90	1.38	1.46
1	A	135[B]	THR	N-CA	-6.90	1.38	1.46
1	E	31	ILE	CA-CB	-6.75	1.50	1.54
1	B	57	ALA	CA-CB	-6.66	1.44	1.53
1	H	31	ILE	CA-CB	-6.62	1.49	1.53
1	F	24	CYS	C-O	-6.47	1.19	1.25
1	F	57	ALA	CA-CB	-6.35	1.44	1.53
1	A	31	ILE	CA-CB	-6.15	1.51	1.54
1	B	93	ILE	C-O	-6.03	1.17	1.24
1	B	150	GLY	C-O	-5.99	1.18	1.24
1	C	31	ILE	CA-CB	-5.96	1.49	1.53
1	A	31	ILE	C-O	-5.92	1.19	1.24
1	A	54	ILE	C-O	-5.86	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	VAL	CA-CB	-5.84	1.47	1.54
1	C	108	ASP	C-O	-5.67	1.17	1.24
1	E	116	ILE	CA-CB	-5.66	1.47	1.54
1	C	54	ILE	C-O	-5.63	1.18	1.24
1	F	49	ILE	C-O	-5.58	1.18	1.24
1	B	144	VAL	C-O	-5.49	1.18	1.24
1	C	8	VAL	C-O	-5.47	1.18	1.24
1	C	131	ARG	C-O	-5.40	1.17	1.24
1	C	140	ASN	C-O	-5.39	1.17	1.24
1	C	11	MSE	SE-CE	-5.38	1.79	1.95
1	C	129	CYS	C-O	-5.38	1.17	1.24
1	G	119	VAL	C-O	-5.38	1.18	1.24
1	A	128	VAL	C-O	-5.36	1.17	1.24
1	D	175	VAL	CA-CB	-5.36	1.47	1.54
1	E	101	GLY	C-O	-5.34	1.17	1.23
1	F	94	VAL	C-O	-5.33	1.18	1.24
1	G	141	ALA	CA-CB	-5.33	1.46	1.53
1	A	93	ILE	C-O	-5.32	1.18	1.24
1	B	6	ILE	C-O	-5.30	1.18	1.24
1	D	133	THR	C-O	-5.28	1.18	1.24
1	C	133	THR	C-O	-5.27	1.18	1.24
1	A	123	GLY	C-O	-5.27	1.18	1.24
1	B	120	VAL	C-O	-5.27	1.18	1.24
1	D	94	VAL	C-O	-5.21	1.18	1.24
1	G	136	ASP	C-O	-5.21	1.18	1.24
1	D	138	LEU	C-O	-5.20	1.18	1.24
1	F	8	VAL	C-O	-5.19	1.18	1.24
1	E	109	LEU	C-O	-5.17	1.18	1.24
1	E	136	ASP	C-O	-5.16	1.18	1.24
1	F	145	ILE	C-O	-5.16	1.18	1.24
1	D	141	ALA	CA-CB	-5.16	1.46	1.53
1	B	128	VAL	C-O	-5.15	1.18	1.24
1	D	57	ALA	CA-CB	-5.15	1.46	1.53
1	B	54	ILE	C-O	-5.14	1.18	1.24
1	A	137	ALA	C-O	-5.14	1.18	1.24
1	B	94	VAL	C-O	-5.13	1.18	1.24
1	A	101	GLY	C-O	-5.11	1.17	1.23
1	F	107	LEU	C-O	-5.10	1.18	1.24
1	F	16	VAL	C-O	-5.09	1.18	1.24
1	D	137	ALA	C-O	-5.09	1.18	1.24
1	D	131	ARG	C-O	-5.08	1.18	1.24
1	H	134	ALA	CA-CB	-5.07	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	VAL	CA-CB	-5.06	1.48	1.54
1	A	118	THR	C-O	-5.05	1.18	1.24
1	G	132	SER	C-O	-5.04	1.18	1.24
1	B	13	ASN	C-O	-5.04	1.18	1.24
1	C	128	VAL	C-O	-5.04	1.18	1.24
1	F	148	SER	C-O	-5.02	1.18	1.24
1	B	103	ALA	CA-CB	-5.02	1.46	1.53
1	F	133	THR	C-O	-5.02	1.18	1.24
1	A	55	GLN	C-O	-5.02	1.18	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9[A]	ILE	CA-C-O	9.09	131.28	120.74
1	B	9[B]	ILE	CA-C-O	9.09	131.28	120.74
1	A	8	VAL	CA-C-N	8.05	134.06	123.11
1	A	8	VAL	C-N-CA	8.05	134.06	123.11
1	B	102	PHE	N-CA-C	7.54	120.56	111.82
1	B	8	VAL	CA-C-N	7.36	132.57	122.93
1	B	8	VAL	C-N-CA	7.36	132.57	122.93
1	H	31	ILE	CB-CA-C	-7.36	106.55	114.35
1	C	20	ALA	CA-C-N	6.54	126.48	119.28
1	C	20	ALA	C-N-CA	6.54	126.48	119.28
1	F	144	VAL	N-CA-C	6.53	117.52	108.12
1	H	89	GLU	CB-CA-C	-6.50	109.08	116.63
1	D	102	PHE	N-CA-C	6.37	119.21	111.82
1	C	31	ILE	CB-CA-C	-6.31	107.66	114.35
1	H	149	ASP	N-CA-C	-6.16	105.77	113.28
1	H	26	GLY	N-CA-C	-6.13	106.15	113.99
1	G	102	PHE	N-CA-C	6.06	118.85	111.82
1	H	102	PHE	N-CA-C	5.95	118.72	111.82
1	F	31	ILE	CB-CA-C	-5.94	108.05	114.35
1	G	67	VAL	N-CA-C	5.86	116.64	110.72
1	H	82	ILE	CA-C-N	5.84	125.54	119.05
1	H	82	ILE	C-N-CA	5.84	125.54	119.05
1	E	175	VAL	CB-CA-C	-5.81	104.29	112.14
1	F	25	PRO	N-CA-C	-5.80	105.82	113.65
1	A	9[A]	ILE	CA-C-O	5.79	127.44	120.66
1	A	9[B]	ILE	CA-C-O	5.79	127.44	120.66
1	H	36	LYS	N-CA-C	-5.75	104.91	111.07
1	E	49	ILE	N-CA-C	5.72	116.10	107.75
1	H	37	ILE	CB-CA-C	-5.71	104.66	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	175	VAL	CB-CA-C	-5.70	104.68	111.97
1	C	144	VAL	N-CA-C	5.63	116.00	108.11
1	G	65	PHE	N-CA-C	-5.58	105.57	112.38
1	A	9[A]	ILE	N-CA-CB	5.58	118.69	111.67
1	A	9[B]	ILE	N-CA-CB	5.58	118.69	111.67
1	H	162	GLY	N-CA-C	-5.57	106.05	112.73
1	C	9	ILE	N-CA-C	5.56	115.86	107.80
1	A	102	PHE	N-CA-C	5.42	118.11	111.82
1	E	99	HIS	N-CA-C	5.39	116.84	111.07
1	G	20	ALA	CA-C-N	5.38	125.20	119.28
1	G	20	ALA	C-N-CA	5.38	125.20	119.28
1	H	10	ASP	N-CA-C	5.28	119.00	112.24
1	G	82	ILE	CA-C-N	5.24	124.86	119.05
1	G	82	ILE	C-N-CA	5.24	124.86	119.05
1	G	66	ARG	N-CA-C	-5.22	105.59	111.28
1	D	144	VAL	N-CA-C	5.21	115.41	108.11
1	E	17	GLY	N-CA-C	5.20	116.89	111.95
1	D	20	ALA	CA-C-N	5.17	124.78	119.05
1	D	20	ALA	C-N-CA	5.17	124.78	119.05
1	E	9	ILE	N-CA-C	5.13	114.96	107.37
1	E	190	VAL	N-CA-C	5.13	116.29	109.37
1	F	9	ILE	N-CA-C	5.11	115.21	107.80
1	G	27	GLY	N-CA-C	-5.10	106.61	112.73
1	D	24	CYS	CA-C-N	5.08	124.87	119.28
1	D	24	CYS	C-N-CA	5.08	124.87	119.28
1	B	16	VAL	N-CA-C	5.07	115.15	107.80
1	E	10	ASP	N-CA-C	5.02	118.66	112.24
1	B	31	ILE	CB-CA-C	-5.00	109.05	114.35

There are no chirality outliers.

There are no planarity outliers.

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	1478	0	1424	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1419	0	1377	40	0
1	C	1396	0	1341	59	0
1	D	1398	0	1352	58	0
1	E	1474	0	1409	63	0
1	F	1437	0	1385	33	1
1	G	1423	0	1367	47	0
1	H	1309	0	1242	117	1
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	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	69	0	0	0	0
4	B	67	0	0	1	0
4	C	52	0	0	3	0
4	D	38	0	0	2	0
4	E	19	0	0	0	0
4	F	44	0	0	2	0
4	G	35	0	0	0	0
4	H	13	0	0	2	0
All	All	11682	0	10897	427	1

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 19.

All (427) 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:H:13:ASN:ND2	1:H:77:TRP:CE3	1.68	1.55
1:E:174:THR:CG2	1:E:177:GLN:HG3	1.34	1.53
1:H:82:ILE:HD11	1:H:85:LEU:CD1	1.53	1.35
1:H:146:THR:OG1	1:H:170:THR:HG21	1.26	1.32
1:H:13:ASN:ND2	1:H:77:TRP:CZ3	1.95	1.31
1:H:49:ILE:HD11	1:H:182:TRP:CZ2	1.67	1.27
1:A:126:THR:HG21	1:A:159:HIS:HD2	1.05	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:THR:CG2	1:E:177:GLN:CG	2.25	1.14
1:A:126:THR:HG21	1:A:159:HIS:CD2	1.83	1.13
1:C:11:MSE:HE1	1:C:30:ILE:HD11	1.26	1.12
1:H:11:MSE:HE2	1:H:123:GLY:HA2	1.17	1.12
1:B:154:LYS:HB3	1:B:158:MSE:CE	1.78	1.12
1:H:13:ASN:CG	1:H:77:TRP:CZ3	2.26	1.11
1:B:154:LYS:HB3	1:B:158:MSE:HE1	1.19	1.11
1:E:171:LYS:NZ	1:E:190:VAL:O	1.83	1.10
1:E:193:GLY:HA3	1:F:67:VAL:CG2	1.82	1.10
1:A:112:LYS:HE2	1:D:112:LYS:HE3	1.33	1.09
1:H:146:THR:OG1	1:H:170:THR:CG2	2.01	1.09
1:B:131:ARG:NH2	1:D:127:ASN:O	1.85	1.09
1:C:23:ARG:NH1	1:C:28:GLU:OE1	1.86	1.09
1:E:174:THR:HG23	1:E:177:GLN:HG3	1.10	1.05
1:G:70:LEU:CD1	1:G:70:LEU:C	2.30	1.04
1:C:11:MSE:CE	1:C:123:GLY:HA2	1.87	1.04
1:G:70:LEU:C	1:G:70:LEU:HD13	1.83	1.02
1:C:11:MSE:HE2	1:C:123:GLY:CA	1.89	1.02
1:H:149:ASP:OD1	1:H:175:VAL:HG23	1.61	1.01
1:E:171:LYS:CG	1:E:173:MSE:CE	2.40	1.00
1:H:82:ILE:HD11	1:H:85:LEU:HD12	1.41	1.00
1:H:82:ILE:CD1	1:H:85:LEU:CD1	2.40	1.00
1:E:171:LYS:HG2	1:E:173:MSE:CE	1.91	0.99
1:B:127:ASN:H	1:B:127:ASN:HD22	1.05	0.99
1:E:174:THR:HG22	1:E:177:GLN:HG3	1.45	0.99
1:E:193:GLY:HA3	1:F:67:VAL:HG23	1.41	0.98
1:D:166:LEU:O	1:D:170:THR:HB	1.64	0.98
1:H:11:MSE:HE1	1:H:30:ILE:CD1	1.95	0.96
1:F:127:ASN:H	1:F:127:ASN:HD22	1.01	0.95
1:H:82:ILE:CD1	1:H:85:LEU:HD12	1.97	0.95
1:H:146:THR:HG1	1:H:170:THR:HG21	1.31	0.95
1:H:13:ASN:ND2	1:H:77:TRP:HE3	1.59	0.94
1:D:127:ASN:H	1:D:127:ASN:HD22	1.10	0.94
1:H:124:VAL:HG13	1:H:125:TRP:CD1	2.04	0.93
1:C:11:MSE:HE2	1:C:123:GLY:HA2	0.95	0.93
1:E:127:ASN:HD22	1:E:127:ASN:H	1.18	0.92
1:H:163:LEU:O	1:H:167:SER:OG	1.87	0.92
1:G:70:LEU:HD12	1:G:70:LEU:O	1.69	0.91
1:H:127:ASN:HD22	1:H:127:ASN:H	1.14	0.91
1:H:88:GLN:N	1:H:91:GLU:OE1	2.04	0.90
1:E:171:LYS:HG2	1:E:173:MSE:HE1	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ASN:HD22	1:C:127:ASN:H	0.92	0.90
1:C:11:MSE:CE	1:C:30:ILE:HD11	2.01	0.89
1:H:88:GLN:O	1:H:91:GLU:HG3	1.72	0.89
1:H:11:MSE:HE1	1:H:30:ILE:HD11	1.53	0.88
1:E:174:THR:HG21	1:E:177:GLN:HG3	1.55	0.88
1:H:82:ILE:HD11	1:H:85:LEU:HD13	1.55	0.88
1:E:174:THR:HG23	1:E:177:GLN:CG	1.96	0.88
1:C:127:ASN:H	1:C:127:ASN:ND2	1.65	0.88
1:H:124:VAL:HG13	1:H:125:TRP:HD1	1.40	0.86
1:F:124:VAL:HG13	1:F:125:TRP:HD1	1.38	0.86
1:C:127:ASN:HD22	1:C:127:ASN:N	1.73	0.86
1:E:23:ARG:HH12	1:E:28:GLU:CD	1.84	0.86
1:H:53:HIS:CD2	1:H:87:PRO:HB3	2.11	0.86
1:H:166:LEU:O	1:H:170:THR:HB	1.76	0.86
1:C:83:PRO:HD2	1:C:84:GLU:OE1	1.76	0.85
1:A:121:LEU:HD21	1:A:134:ALA:HB2	1.58	0.85
1:E:171:LYS:HG3	1:E:173:MSE:CE	2.06	0.85
1:H:82:ILE:CG1	1:H:85:LEU:HD12	2.07	0.85
1:G:56:GLU:OE1	1:G:58:HIS:NE2	2.10	0.84
1:H:11:MSE:CE	1:H:123:GLY:HA2	2.05	0.83
1:A:112:LYS:CE	1:D:112:LYS:HE3	2.09	0.83
1:H:124:VAL:CG1	1:H:125:TRP:HD1	1.92	0.83
1:H:82:ILE:HD11	1:H:85:LEU:HD11	1.59	0.82
1:H:13:ASN:HB3	1:H:77:TRP:CH2	2.16	0.81
1:H:11:MSE:HE3	1:H:34:LEU:HD11	1.62	0.81
1:H:49:ILE:HD11	1:H:182:TRP:CE2	2.16	0.80
1:F:166:LEU:O	1:F:170:THR:HB	1.81	0.80
1:B:154:LYS:CB	1:B:158:MSE:HE1	2.09	0.80
1:A:126:THR:CG2	1:A:159:HIS:HD2	1.92	0.79
1:B:126:THR:OG1	1:B:159:HIS:HD2	1.66	0.79
1:C:112:LYS:HE3	1:B:112:LYS:HE3	1.65	0.78
1:G:70:LEU:CD1	1:G:70:LEU:O	2.30	0.78
1:F:127:ASN:H	1:F:127:ASN:ND2	1.79	0.78
1:H:40:TRP:HH2	1:H:182:TRP:CD1	2.01	0.78
1:G:127:ASN:H	1:G:127:ASN:HD22	1.31	0.77
1:A:104:HIS:HE1	1:C:139:ALA:O	1.67	0.76
1:F:33:ASP:OD2	4:F:219:HOH:O	2.03	0.76
1:H:49:ILE:CD1	1:H:182:TRP:CZ2	2.60	0.76
1:G:17:GLY:O	1:G:23:ARG:HD2	1.87	0.75
1:E:23:ARG:NH1	1:E:28:GLU:OE2	2.19	0.75
1:A:183:GLU:O	1:A:184:ASN:C	2.30	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:TRP:C	1:C:183:GLU:OE2	2.30	0.75
1:G:182:TRP:C	1:G:183:GLU:OE1	2.31	0.74
1:E:174:THR:HG22	1:E:177:GLN:CG	2.05	0.74
1:D:84:GLU:H	1:D:84:GLU:CD	1.92	0.74
1:H:26:GLY:HA3	1:H:152:ALA:HB1	1.70	0.73
1:F:124:VAL:HG13	1:F:125:TRP:CD1	2.23	0.73
1:E:174:THR:HG22	1:E:177:GLN:CD	2.13	0.73
1:A:127:ASN:HD22	1:A:127:ASN:H	1.36	0.73
1:H:127:ASN:H	1:H:127:ASN:ND2	1.85	0.73
1:D:127:ASN:H	1:D:127:ASN:ND2	1.80	0.72
1:B:104:HIS:HE1	1:D:139:ALA:O	1.74	0.71
1:F:36:LYS:NZ	1:F:176:ASP:OD1	2.23	0.71
1:E:173:MSE:HE1	1:E:188:PRO:O	1.91	0.71
1:H:124:VAL:CG1	1:H:125:TRP:CD1	2.72	0.71
1:D:3:LYS:NZ	1:D:47:ASP:O	2.24	0.71
1:H:6:ILE:HG13	1:H:120:VAL:HG13	1.72	0.71
1:H:17:GLY:O	1:H:23:ARG:HD3	1.91	0.70
1:H:43:GLY:O	1:H:44:ARG:CB	2.38	0.70
1:H:13:ASN:HB3	1:H:77:TRP:CZ2	2.27	0.70
1:E:127:ASN:H	1:E:127:ASN:ND2	1.91	0.69
1:A:112:LYS:HE2	1:D:112:LYS:CE	2.16	0.69
1:G:70:LEU:HD13	1:G:71:HIS:N	2.08	0.69
1:D:126:THR:OG1	1:D:159:HIS:HD2	1.73	0.69
1:H:11:MSE:HE1	1:H:30:ILE:HD12	1.72	0.69
1:E:171:LYS:CG	1:E:173:MSE:HE2	2.24	0.68
1:H:40:TRP:CE2	1:H:179:ILE:HG23	2.29	0.68
1:F:127:ASN:HD22	1:F:127:ASN:N	1.83	0.68
1:H:80:ASP:OD1	1:H:81:PHE:N	2.27	0.67
1:C:166:LEU:O	1:C:170:THR:HB	1.93	0.67
1:D:124:VAL:HG13	1:D:125:TRP:HD1	1.60	0.67
1:H:49:ILE:HD11	1:H:182:TRP:HZ2	1.52	0.67
1:H:40:TRP:CH2	1:H:182:TRP:CD1	2.82	0.67
1:H:175:VAL:O	1:H:179:ILE:HG13	1.95	0.67
1:C:113:GLU:OE2	1:D:97:ARG:NH2	2.26	0.67
1:B:127:ASN:H	1:B:127:ASN:ND2	1.82	0.67
1:E:44:ARG:NH1	1:E:48:ASP:HB2	2.10	0.67
1:E:171:LYS:HG3	1:E:173:MSE:HE2	1.76	0.67
1:E:171:LYS:CG	1:E:173:MSE:HE3	2.24	0.66
1:H:82:ILE:HG13	1:H:85:LEU:HD12	1.75	0.66
1:A:121:LEU:CD2	1:A:134:ALA:HB2	2.23	0.66
1:H:43:GLY:O	1:H:44:ARG:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:ASN:HD22	1:H:127:ASN:N	1.91	0.66
1:G:126:THR:OG1	1:G:159:HIS:HD2	1.78	0.66
1:D:183:GLU:N	1:D:183:GLU:OE2	2.30	0.65
1:B:154:LYS:HB3	1:B:158:MSE:HE3	1.74	0.65
1:C:97:ARG:NH2	1:D:113:GLU:OE2	2.26	0.64
1:E:171:LYS:HG3	1:E:173:MSE:HE3	1.79	0.64
1:H:11:MSE:CE	1:H:30:ILE:HD12	2.27	0.64
1:G:183:GLU:OE1	1:G:183:GLU:N	2.30	0.64
1:D:127:ASN:HD22	1:D:127:ASN:N	1.90	0.64
1:H:40:TRP:CD2	1:H:179:ILE:HG23	2.32	0.64
1:E:174:THR:HG23	1:E:177:GLN:H	1.62	0.63
1:C:86:TYR:CD1	1:C:87:PRO:HD2	2.34	0.63
1:E:124:VAL:HG13	1:E:125:TRP:HD1	1.64	0.63
1:C:84:GLU:OE1	1:C:84:GLU:N	2.29	0.63
1:D:174:THR:OG1	1:D:177:GLN:HG3	1.98	0.63
1:C:23:ARG:HH12	1:C:28:GLU:CD	2.07	0.63
1:G:3:LYS:HE3	1:G:47:ASP:O	1.99	0.63
1:E:139:ALA:O	1:F:104:HIS:HE1	1.81	0.63
1:A:124:VAL:HG13	1:A:125:TRP:HD1	1.63	0.62
1:C:83:PRO:CD	1:C:84:GLU:OE1	2.46	0.62
1:B:17:GLY:O	1:B:23:ARG:CD	2.47	0.62
1:F:146:THR:OG1	1:F:170:THR:HG21	1.98	0.62
1:H:53:HIS:HD2	1:H:87:PRO:HB3	1.61	0.62
1:C:11:MSE:HE3	1:C:34:LEU:HD11	1.81	0.62
1:E:126:THR:OG1	1:E:159:HIS:HD2	1.83	0.62
1:C:23:ARG:NH1	1:C:28:GLU:CD	2.58	0.62
1:H:33:ASP:OD2	1:H:33:ASP:N	2.29	0.62
1:E:193:GLY:HA3	1:F:67:VAL:HG22	1.81	0.62
1:B:37:ILE:HD12	1:B:175:VAL:HG13	1.82	0.61
1:G:5:ALA:HB2	1:G:116:ILE:HD13	1.82	0.61
1:A:124:VAL:HG13	1:A:125:TRP:CD1	2.35	0.61
1:E:171:LYS:HE2	1:E:173:MSE:HE2	1.83	0.61
1:C:28:GLU:HG3	4:C:272:HOH:O	2.00	0.61
1:C:90:ASP:OD2	1:C:90:ASP:N	2.29	0.61
1:E:159:HIS:CE1	1:E:163:LEU:HD11	2.35	0.61
1:D:36:LYS:NZ	1:D:176:ASP:OD1	2.33	0.60
1:A:84:GLU:OE1	1:A:84:GLU:N	2.30	0.60
1:D:59:ARG:HD2	4:D:229:HOH:O	2.01	0.60
1:D:82:ILE:HD12	1:D:84:GLU:HG2	1.82	0.60
1:H:121:LEU:CD2	1:H:144:VAL:CG1	2.79	0.60
1:H:38:PHE:CE1	1:H:85:LEU:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:CG1	1:A:125:TRP:HD1	2.15	0.60
1:D:84:GLU:CD	1:D:84:GLU:N	2.60	0.60
1:A:126:THR:HG22	1:A:152:ALA:C	2.26	0.59
1:E:86:TYR:CD1	1:E:87:PRO:HD2	2.37	0.59
1:G:126:THR:OG1	1:G:159:HIS:CD2	2.55	0.59
1:B:127:ASN:HD22	1:B:127:ASN:N	1.86	0.59
1:A:114:GLU:HB2	1:A:116:ILE:HD12	1.85	0.59
1:G:56:GLU:OE1	1:G:58:HIS:CD2	2.56	0.59
1:G:64:ASP:O	1:G:67:VAL:N	2.34	0.59
1:G:139:ALA:HA	1:H:98:ARG:HG3	1.84	0.59
1:H:37:ILE:HG22	1:H:38:PHE:N	2.17	0.58
1:H:40:TRP:CE2	1:H:179:ILE:CG2	2.86	0.58
1:F:173:MSE:HE2	1:F:178:TYR:HA	1.86	0.58
1:H:182:TRP:HB2	1:H:183:GLU:OE2	2.04	0.58
1:A:139:ALA:HA	1:C:98:ARG:HG3	1.86	0.58
1:H:123:GLY:O	1:H:151:THR:HG22	2.04	0.58
1:D:40:TRP:CE3	1:D:41:VAL:HG23	2.38	0.58
1:H:170:THR:HG22	1:H:171:LYS:N	2.17	0.58
1:H:13:ASN:CB	1:H:77:TRP:CZ3	2.86	0.58
1:B:154:LYS:HD3	1:B:158:MSE:HE1	1.85	0.57
1:E:104:HIS:HE1	1:F:139:ALA:O	1.86	0.57
1:G:127:ASN:H	1:G:127:ASN:ND2	2.01	0.57
1:D:84:GLU:N	1:D:84:GLU:OE1	2.30	0.57
1:D:146:THR:OG1	1:D:170:THR:HG21	2.03	0.57
1:C:92:TYR:CE1	1:D:59:ARG:HD3	2.39	0.57
1:B:84:GLU:OE1	1:B:84:GLU:N	2.30	0.57
1:B:155:THR:H	1:B:158:MSE:HE3	1.69	0.57
1:G:139:ALA:O	1:H:104:HIS:HE1	1.87	0.57
1:E:199:VAL:HB	1:F:158:MSE:HE1	1.85	0.57
1:A:139:ALA:O	1:C:104:HIS:HE1	1.88	0.57
1:E:159:HIS:NE2	1:E:163:LEU:HD11	2.20	0.56
1:G:24:CYS:HG	1:G:125:TRP:CD1	2.23	0.56
1:H:6:ILE:HG13	1:H:120:VAL:CG1	2.35	0.56
1:H:11:MSE:CE	1:H:30:ILE:CD1	2.78	0.56
1:H:84:GLU:C	1:H:85:LEU:HG	2.29	0.56
1:A:113:GLU:CD	1:B:97:ARG:HH22	2.12	0.56
1:F:96:LYS:HD2	1:F:98:ARG:O	2.05	0.56
1:C:124:VAL:HG13	1:C:125:TRP:CD1	2.41	0.56
1:E:44:ARG:HH12	1:E:48:ASP:HB2	1.70	0.56
1:H:95:GLN:HG2	4:H:323:HOH:O	2.06	0.56
1:E:168:ILE:HG12	1:E:199:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:GLN:HB3	1:F:81:PHE:CZ	2.41	0.56
1:H:126:THR:OG1	1:H:159:HIS:HD2	1.89	0.56
1:C:124:VAL:HG13	1:C:125:TRP:HD1	1.70	0.55
1:A:97:ARG:NH2	1:B:113:GLU:OE2	2.38	0.55
1:H:153:SER:OG	1:H:154:LYS:N	2.35	0.55
1:A:121:LEU:HD21	1:A:134:ALA:CB	2.33	0.55
1:D:5:ALA:HB2	1:D:116:ILE:HD13	1.89	0.55
1:E:174:THR:HG22	1:E:177:GLN:OE1	2.06	0.55
1:D:170:THR:CG2	1:D:171:LYS:N	2.67	0.55
1:C:59:ARG:HD2	4:C:228:HOH:O	2.05	0.55
1:B:139:ALA:O	1:D:104:HIS:HE1	1.90	0.55
1:D:86:TYR:CD1	1:D:87:PRO:HD2	2.42	0.55
1:A:20:ALA:HB3	1:A:23:ARG:HB2	1.90	0.54
1:C:121:LEU:HD21	1:C:134:ALA:HB2	1.90	0.54
1:C:97:ARG:HH22	1:D:113:GLU:CD	2.13	0.54
1:B:45:GLU:HG2	1:B:46:GLY:N	2.21	0.53
1:A:113:GLU:OE1	1:B:97:ARG:NH2	2.41	0.53
1:B:155:THR:HG23	1:B:158:MSE:HE2	1.89	0.53
1:C:149:ASP:OD1	1:C:175:VAL:HG23	2.08	0.53
1:E:31:ILE:N	1:E:32:PRO:CD	2.72	0.53
1:H:128:VAL:HG12	1:H:129:CYS:N	2.23	0.53
1:B:23:ARG:NH1	1:B:28:GLU:OE1	2.41	0.53
1:G:88:GLN:O	1:G:89:GLU:C	2.50	0.53
1:C:113:GLU:CD	1:D:97:ARG:NH2	2.67	0.52
1:B:157:GLU:H	1:B:157:GLU:CD	2.15	0.52
1:H:40:TRP:O	1:H:43:GLY:O	2.26	0.52
1:F:5:ALA:HB2	1:F:116:ILE:HD13	1.91	0.52
1:G:140:ASN:O	1:G:141:ALA:HB3	2.09	0.52
1:H:53:HIS:CD2	1:H:87:PRO:CB	2.90	0.52
1:C:126:THR:OG1	1:C:159:HIS:HD2	1.93	0.52
1:C:121:LEU:CD2	1:C:134:ALA:HB2	2.41	0.51
1:H:164:ASN:HA	1:H:167:SER:OG	2.10	0.51
1:C:56:GLU:HG2	1:C:72:ALA:HB3	1.91	0.51
1:D:171:LYS:HD3	1:D:173:MSE:CE	2.40	0.51
1:G:120:VAL:HA	1:G:145:ILE:O	2.10	0.51
1:A:127:ASN:H	1:A:127:ASN:ND2	2.07	0.51
1:C:131:ARG:NH2	1:C:165:ASP:OD2	2.44	0.51
1:F:158:MSE:HA	1:F:161:TYR:CE2	2.46	0.51
1:C:97:ARG:NH2	1:D:113:GLU:CD	2.69	0.51
1:G:121:LEU:CD2	1:G:134:ALA:HB2	2.41	0.51
1:H:174:THR:HG23	1:H:177:GLN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:HA	1:A:130:VAL:HB	1.92	0.51
1:D:140:ASN:O	1:D:141:ALA:HB3	2.10	0.50
1:G:59:ARG:O	1:G:62:ASP:HB2	2.10	0.50
1:A:31:ILE:N	1:A:32:PRO:CD	2.73	0.50
1:E:127:ASN:HD22	1:E:127:ASN:N	1.96	0.50
1:G:65:PHE:CD1	1:G:70:LEU:HA	2.47	0.50
1:H:146:THR:HG21	1:H:166:LEU:HD13	1.93	0.50
1:H:175:VAL:O	1:H:179:ILE:CG1	2.60	0.50
1:A:183:GLU:O	1:A:184:ASN:O	2.30	0.50
1:E:131:ARG:NH2	1:F:127:ASN:O	2.43	0.50
1:E:194:ASP:OD2	1:E:199:VAL:HG22	2.12	0.50
1:H:31:ILE:N	1:H:32:PRO:CD	2.75	0.50
1:C:61:ASN:OD1	1:C:61:ASN:O	2.30	0.50
1:E:34:LEU:O	1:E:37:ILE:HG22	2.12	0.50
1:B:17:GLY:O	1:B:23:ARG:HD2	2.11	0.49
1:E:171:LYS:HE2	1:E:173:MSE:CE	2.42	0.49
1:G:120:VAL:HB	1:G:145:ILE:HB	1.93	0.49
1:H:26:GLY:O	1:H:29:THR:HG23	2.12	0.49
1:H:147:LEU:HB3	1:H:150:GLY:HA3	1.93	0.49
1:C:113:GLU:CD	1:D:97:ARG:HH22	2.17	0.49
1:E:40:TRP:CE3	1:E:41:VAL:HG23	2.48	0.48
1:H:13:ASN:CB	1:H:77:TRP:CH2	2.90	0.48
1:E:131:ARG:NH2	1:E:165:ASP:OD2	2.45	0.48
1:H:40:TRP:HH2	1:H:182:TRP:NE1	2.10	0.48
1:C:31:ILE:N	1:C:32:PRO:CD	2.76	0.48
1:D:82:ILE:HD12	1:D:84:GLU:CG	2.43	0.48
1:A:48:ASP:C	1:A:49:ILE:HG13	2.37	0.48
1:C:113:GLU:OE1	1:D:97:ARG:NH2	2.47	0.48
1:G:152:ALA:HA	1:G:159:HIS:CD2	2.49	0.48
1:D:17:GLY:HA2	1:D:28:GLU:OE2	2.14	0.48
1:D:28:GLU:H	1:D:28:GLU:HG2	1.50	0.48
1:F:96:LYS:HB2	4:F:328:HOH:O	2.12	0.47
1:H:121:LEU:HD22	1:H:144:VAL:CG1	2.44	0.47
1:H:73:VAL:O	1:H:76:THR:HG23	2.14	0.47
1:C:106:ASP:OD1	1:D:97:ARG:NH1	2.40	0.47
1:D:31:ILE:O	1:D:35:GLN:HG3	2.14	0.47
1:C:20:ALA:HA	1:C:21:PRO:HD3	1.77	0.47
1:H:140:ASN:O	1:H:141:ALA:HB3	2.15	0.47
1:H:86:TYR:CD1	1:H:87:PRO:HD2	2.49	0.47
1:H:174:THR:H	1:H:177:GLN:CD	2.22	0.47
1:B:173:MSE:CE	1:B:178:TYR:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:CD1	1:D:84:GLU:HG2	2.44	0.47
1:D:170:THR:HG22	1:D:171:LYS:N	2.30	0.47
1:E:6:ILE:HG12	1:E:120:VAL:HG22	1.96	0.47
1:F:70:LEU:C	1:F:70:LEU:HD23	2.40	0.47
1:G:64:ASP:C	1:G:66:ARG:N	2.72	0.47
1:E:180:GLN:O	1:E:180:GLN:HG3	2.13	0.47
1:G:149:ASP:OD1	1:G:149:ASP:N	2.40	0.47
1:B:126:THR:OG1	1:B:159:HIS:CD2	2.58	0.46
1:H:26:GLY:CA	1:H:152:ALA:HB1	2.42	0.46
1:B:173:MSE:HE1	1:B:178:TYR:HA	1.96	0.46
1:E:194:ASP:OD2	1:E:197:ASN:HA	2.15	0.46
1:A:31:ILE:N	1:A:32:PRO:HD3	2.29	0.46
1:A:56:GLU:HG2	1:A:72:ALA:HB3	1.97	0.46
1:B:3:LYS:NZ	1:B:47:ASP:O	2.48	0.46
1:E:88:GLN:O	1:E:91:GLU:HG3	2.14	0.46
1:G:173:MSE:HE2	1:G:178:TYR:HA	1.97	0.46
1:E:31:ILE:HB	1:E:32:PRO:HD3	1.96	0.46
1:G:121:LEU:HD21	1:G:134:ALA:HB2	1.98	0.46
1:A:11:MSE:HE2	1:A:34:LEU:HD12	1.96	0.46
1:C:182:TRP:O	1:C:183:GLU:OE2	2.34	0.46
1:E:146:THR:HG21	1:E:166:LEU:HD13	1.97	0.46
1:A:47:ASP:OD1	1:A:47:ASP:O	2.35	0.45
1:E:128:VAL:HG12	1:E:129:CYS:N	2.31	0.45
1:H:31:ILE:HB	1:H:32:PRO:HD3	1.98	0.45
1:D:20:ALA:HA	1:D:21:PRO:HD3	1.76	0.45
1:G:14:ASP:O	1:G:20:ALA:HB1	2.17	0.45
1:H:149:ASP:CG	1:H:175:VAL:HG23	2.37	0.45
1:H:170:THR:CG2	1:H:171:LYS:N	2.78	0.45
4:C:202:HOH:O	1:D:104:HIS:CD2	2.69	0.45
1:D:153:SER:OG	1:D:154:LYS:N	2.50	0.45
1:B:17:GLY:O	1:B:23:ARG:HD3	2.16	0.45
1:B:155:THR:N	1:B:158:MSE:HE3	2.31	0.45
1:B:48:ASP:C	1:B:49:ILE:HG13	2.41	0.45
1:H:34:LEU:O	1:H:37:ILE:HB	2.17	0.45
1:H:20:ALA:HA	1:H:21:PRO:HD3	1.90	0.45
1:H:25:PRO:C	1:H:27:GLY:N	2.72	0.45
1:H:97:ARG:HG3	4:H:212:HOH:O	2.16	0.45
1:B:155:THR:HG23	1:B:158:MSE:CE	2.46	0.45
1:H:41:VAL:HG22	1:H:49:ILE:HG21	1.98	0.45
1:H:155:THR:OG1	1:H:157:GLU:HG2	2.16	0.44
1:A:127:ASN:ND2	1:A:153:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:LEU:HD23	1:E:163:LEU:HA	1.84	0.44
1:G:65:PHE:CE1	1:G:70:LEU:HA	2.52	0.44
1:A:20:ALA:HA	1:A:21:PRO:HD3	1.82	0.44
1:D:86:TYR:HA	1:D:87:PRO:HD3	1.89	0.44
1:F:153:SER:OG	1:F:154:LYS:N	2.51	0.44
1:C:95:GLN:H	1:C:95:GLN:HG2	1.56	0.44
1:E:4:HIS:CD2	1:E:118:THR:HB	2.53	0.44
1:C:31:ILE:HB	1:C:32:PRO:HD3	2.00	0.44
1:C:153:SER:OG	1:C:154:LYS:N	2.50	0.44
1:C:176:ASP:O	1:C:180:GLN:HB3	2.18	0.44
1:D:40:TRP:CZ3	1:D:41:VAL:HG23	2.53	0.44
1:G:125:TRP:CH2	1:G:154:LYS:HD2	2.53	0.44
1:C:48:ASP:C	1:C:49:ILE:HG13	2.42	0.44
1:A:97:ARG:HH22	1:B:113:GLU:CD	2.23	0.44
1:D:8:VAL:HA	1:D:122:THR:OG1	2.18	0.43
1:D:82:ILE:HA	1:D:83:PRO:HD3	1.81	0.43
1:H:146:THR:OG1	1:H:170:THR:HG22	2.06	0.43
1:C:86:TYR:HA	1:C:87:PRO:HD3	1.81	0.43
1:D:86:TYR:CG	1:D:87:PRO:HD2	2.52	0.43
1:D:95:GLN:H	1:D:95:GLN:HG2	1.67	0.43
1:D:121:LEU:HD21	1:D:134:ALA:HB2	2.00	0.43
1:A:66:ARG:H	1:A:66:ARG:HG2	1.09	0.43
1:F:98:ARG:HD3	1:F:98:ARG:HA	1.85	0.43
1:E:10:ASP:C	1:E:12:LEU:HG	2.44	0.43
1:E:174:THR:HG23	1:E:177:GLN:CB	2.46	0.43
1:H:163:LEU:HD23	1:H:163:LEU:HA	1.68	0.43
1:D:95:GLN:HG2	4:D:209:HOH:O	2.19	0.43
1:G:117:ASP:OD2	1:G:118:THR:OG1	2.32	0.43
1:H:30:ILE:HG22	1:H:149:ASP:O	2.19	0.43
1:H:165:ASP:O	1:H:168:ILE:HG13	2.20	0.42
1:E:26:GLY:O	1:E:29:THR:HG23	2.18	0.42
1:G:31:ILE:HB	1:G:32:PRO:HD3	2.01	0.42
1:A:70:LEU:HA	1:A:70:LEU:HD12	1.71	0.42
1:F:14:ASP:C	1:F:20:ALA:HB1	2.44	0.42
1:A:34:LEU:O	1:A:37:ILE:HG22	2.19	0.42
1:A:86:TYR:HA	1:A:87:PRO:HD3	1.91	0.42
1:G:86:TYR:HA	1:G:87:PRO:HD3	1.78	0.42
1:G:127:ASN:HD22	1:G:127:ASN:N	2.08	0.42
1:C:82:ILE:HA	1:C:83:PRO:HD3	1.87	0.42
1:G:31:ILE:N	1:G:32:PRO:CD	2.82	0.42
1:G:34:LEU:O	1:G:37:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:LEU:HD23	1:G:138:LEU:HA	1.84	0.42
1:C:73:VAL:O	1:C:79:SER:HB2	2.19	0.42
1:B:59:ARG:HD2	4:B:252:HOH:O	2.19	0.42
1:E:73:VAL:HG12	1:E:74:LYS:N	2.35	0.42
1:G:165:ASP:O	1:G:168:ILE:HB	2.20	0.42
1:F:124:VAL:CG1	1:F:125:TRP:HD1	2.20	0.42
1:H:86:TYR:HA	1:H:87:PRO:HD3	1.78	0.42
1:H:125:TRP:CD1	1:H:125:TRP:N	2.88	0.42
1:H:95:GLN:HG2	1:H:95:GLN:H	1.39	0.41
1:F:20:ALA:HA	1:F:21:PRO:HD3	1.81	0.41
1:F:124:VAL:HG22	1:F:152:ALA:O	2.21	0.41
1:C:114:GLU:HB2	1:C:116:ILE:HD12	2.02	0.41
1:C:173:MSE:HE3	1:C:173:MSE:HB3	1.96	0.41
1:C:174:THR:HG23	1:C:177:GLN:OE1	2.20	0.41
1:B:-1:GLN:O	1:B:1:MSE:N	2.50	0.41
1:F:86:TYR:HA	1:F:87:PRO:HD3	1.90	0.41
1:G:59:ARG:HH11	1:G:59:ARG:HD2	1.73	0.41
1:H:147:LEU:O	1:H:150:GLY:CA	2.68	0.41
1:H:147:LEU:O	1:H:150:GLY:HA3	2.20	0.41
1:F:59:ARG:O	1:F:62:ASP:HB2	2.21	0.41
1:H:25:PRO:C	1:H:27:GLY:H	2.27	0.41
1:H:121:LEU:C	1:H:122:THR:CG2	2.93	0.41
1:E:88:GLN:O	1:E:89:GLU:C	2.61	0.41
1:F:122:THR:HG22	1:F:147:LEU:HD12	2.03	0.41
1:G:65:PHE:O	1:G:68:ARG:O	2.38	0.41
1:G:147:LEU:HA	1:G:173:MSE:O	2.20	0.41
1:H:73:VAL:HB	1:H:76:THR:HG21	2.02	0.41
1:A:97:ARG:NH2	1:B:113:GLU:CD	2.79	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.87	0.41
1:H:41:VAL:CG2	1:H:49:ILE:HG21	2.51	0.41
1:D:157:GLU:H	1:D:157:GLU:CD	2.29	0.41
1:C:183:GLU:OE2	1:C:183:GLU:N	2.52	0.41
1:B:82:ILE:HA	1:B:83:PRO:HD3	1.90	0.41
1:D:120:VAL:HA	1:D:145:ILE:O	2.21	0.41
1:E:126:THR:OG1	1:E:159:HIS:CD2	2.69	0.41
1:G:68:ARG:CB	1:G:69:PRO:CD	2.99	0.41
1:H:13:ASN:HB3	1:H:77:TRP:CZ3	2.49	0.41
1:H:28:GLU:O	1:H:31:ILE:HG13	2.21	0.41
1:H:124:VAL:HG12	1:H:125:TRP:HD1	1.79	0.41
1:H:182:TRP:CB	1:H:183:GLU:OE2	2.69	0.41
1:D:11:MSE:HE2	1:D:34:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ILE:N	1:D:32:PRO:CD	2.84	0.40
1:A:3:LYS:HE3	1:A:114:GLU:O	2.21	0.40
1:F:65:PHE:CE1	1:F:70:LEU:HA	2.56	0.40
1:B:149:ASP:OD1	1:B:149:ASP:N	2.50	0.40
1:H:5:ALA:HB2	1:H:116:ILE:HD12	2.02	0.40
1:H:97:ARG:O	1:H:98:ARG:HD3	2.21	0.40
1:C:11:MSE:HE3	1:C:34:LEU:CD1	2.49	0.40
1:B:34:LEU:O	1:B:37:ILE:HG22	2.22	0.40
1:E:189:TRP:O	1:E:189:TRP:CG	2.75	0.40
1:H:3:LYS:HB3	1:H:116:ILE:HA	2.04	0.40

All (1) 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)
1:F:97:ARG:NH2	1:H:113:GLU:OE1[1_655]	2.15	0.05

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	188/204 (92%)	185 (98%)	3 (2%)	0	100	100
1	B	176/204 (86%)	172 (98%)	4 (2%)	0	100	100
1	C	174/204 (85%)	170 (98%)	3 (2%)	1 (1%)	21	27
1	D	175/204 (86%)	171 (98%)	4 (2%)	0	100	100
1	E	185/204 (91%)	179 (97%)	5 (3%)	1 (0%)	24	31
1	F	181/204 (89%)	178 (98%)	3 (2%)	0	100	100
1	G	180/204 (88%)	176 (98%)	2 (1%)	2 (1%)	11	13
1	H	165/204 (81%)	160 (97%)	4 (2%)	1 (1%)	21	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1424/1632 (87%)	1391 (98%)	28 (2%)	5 (0%)	30	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	89	GLU
1	E	128	VAL
1	H	128	VAL
1	C	128	VAL
1	G	128	VAL

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	153/170 (90%)	135 (88%)	18 (12%)	5	6
1	B	150/170 (88%)	133 (89%)	17 (11%)	5	7
1	C	147/170 (86%)	129 (88%)	18 (12%)	5	5
1	D	146/170 (86%)	133 (91%)	13 (9%)	9	12
1	E	154/170 (91%)	133 (86%)	21 (14%)	3	4
1	F	151/170 (89%)	131 (87%)	20 (13%)	4	4
1	G	149/170 (88%)	133 (89%)	16 (11%)	6	8
1	H	133/170 (78%)	96 (72%)	37 (28%)	0	0
All	All	1183/1360 (87%)	1023 (86%)	160 (14%)	3	4

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	29	THR
1	A	36	LYS
1	A	37	ILE
1	A	44	ARG

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	66	ARG
1	A	70	LEU
1	A	111	LEU
1	A	120	VAL
1	A	121	LEU
1	A	124	VAL
1	A	126	THR
1	A	127	ASN
1	A	131	ARG
1	A	138	LEU
1	A	143	LYS
1	A	147	LEU
1	C	3	LYS
1	C	37	ILE
1	C	47	ASP
1	C	90	ASP
1	C	95	GLN
1	C	111	LEU
1	C	120	VAL
1	C	121	LEU
1	C	124	VAL
1	C	127	ASN
1	C	131	ARG
1	C	138	LEU
1	C	143	LYS
1	C	147	LEU
1	C	157	GLU
1	C	164	ASN
1	C	170	THR
1	C	173	MSE
1	B	19	LYS
1	B	24	CYS
1	B	28	GLU
1	B	37	ILE
1	B	44	ARG
1	B	45	GLU
1	B	47	ASP
1	B	70	LEU
1	B	71	HIS
1	B	90	ASP
1	B	111	LEU

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Mol	Chain	Res	Type
1	B	120	VAL
1	B	121	LEU
1	B	127	ASN
1	B	131	ARG
1	B	138	LEU
1	B	157	GLU
1	D	28	GLU
1	D	37	ILE
1	D	54	ILE
1	D	84	GLU
1	D	95	GLN
1	D	112	LYS
1	D	120	VAL
1	D	121	LEU
1	D	124	VAL
1	D	127	ASN
1	D	138	LEU
1	D	147	LEU
1	D	170	THR
1	E	29	THR
1	E	37	ILE
1	E	41	VAL
1	E	44	ARG
1	E	45	GLU
1	E	70	LEU
1	E	88	GLN
1	E	90	ASP
1	E	111	LEU
1	E	112	LYS
1	E	119	VAL
1	E	120	VAL
1	E	124	VAL
1	E	127	ASN
1	E	131	ARG
1	E	138	LEU
1	E	147	LEU
1	E	174	THR
1	E	183	GLU
1	E	198	LYS
1	E	199	VAL
1	F	3	LYS
1	F	28	GLU

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Mol	Chain	Res	Type
1	F	29	THR
1	F	37	ILE
1	F	45	GLU
1	F	47	ASP
1	F	54	ILE
1	F	70	LEU
1	F	79	SER
1	F	111	LEU
1	F	116	ILE
1	F	120	VAL
1	F	121	LEU
1	F	124	VAL
1	F	127	ASN
1	F	138	LEU
1	F	157	GLU
1	F	164	ASN
1	F	170	THR
1	F	183	GLU
1	G	18	GLU
1	G	23	ARG
1	G	24	CYS
1	G	29	THR
1	G	47	ASP
1	G	64	ASP
1	G	70	LEU
1	G	95	GLN
1	G	111	LEU
1	G	120	VAL
1	G	121	LEU
1	G	127	ASN
1	G	131	ARG
1	G	138	LEU
1	G	147	LEU
1	G	160	GLU
1	H	3	LYS
1	H	6	ILE
1	H	12	LEU
1	H	28	GLU
1	H	29	THR
1	H	30	ILE
1	H	33	ASP
1	H	36	LYS

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Mol	Chain	Res	Type
1	H	37	ILE
1	H	42	ARG
1	H	44	ARG
1	H	49	ILE
1	H	51	LEU
1	H	55	GLN
1	H	59	ARG
1	H	77	TRP
1	H	85	LEU
1	H	95	GLN
1	H	111	LEU
1	H	116	ILE
1	H	120	VAL
1	H	121	LEU
1	H	124	VAL
1	H	127	ASN
1	H	131	ARG
1	H	138	LEU
1	H	143	LYS
1	H	145	ILE
1	H	146	THR
1	H	147	LEU
1	H	151	THR
1	H	157	GLU
1	H	167	SER
1	H	172	VAL
1	H	174	THR
1	H	177	GLN
1	H	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	58	HIS
1	A	61	ASN
1	A	71	HIS
1	A	104	HIS
1	A	127	ASN
1	A	159	HIS
1	A	164	ASN
1	C	55	GLN

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Mol	Chain	Res	Type
1	C	61	ASN
1	C	71	HIS
1	C	104	HIS
1	C	127	ASN
1	C	159	HIS
1	B	13	ASN
1	B	35	GLN
1	B	55	GLN
1	B	95	GLN
1	B	104	HIS
1	B	127	ASN
1	B	159	HIS
1	B	164	ASN
1	D	55	GLN
1	D	58	HIS
1	D	71	HIS
1	D	95	GLN
1	D	104	HIS
1	D	127	ASN
1	D	159	HIS
1	E	104	HIS
1	E	127	ASN
1	E	159	HIS
1	E	180	GLN
1	E	196	GLN
1	F	58	HIS
1	F	71	HIS
1	F	104	HIS
1	F	127	ASN
1	G	55	GLN
1	G	127	ASN
1	G	159	HIS
1	H	53	HIS
1	H	55	GLN
1	H	58	HIS
1	H	95	GLN
1	H	104	HIS
1	H	127	ASN
1	H	159	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are modelled with single atom and 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	184/204 (90%)	0.04	6 (3%)	49	51	8, 21, 30, 56	2 (1%)
1	B	175/204 (85%)	0.14	8 (4%)	37	39	8, 23, 32, 64	1 (0%)
1	C	175/204 (85%)	0.06	2 (1%)	78	79	14, 24, 30, 36	0
1	D	175/204 (85%)	0.11	3 (1%)	69	70	15, 24, 31, 55	0
1	E	186/204 (91%)	0.36	7 (3%)	44	46	19, 28, 49, 66	0
1	F	179/204 (87%)	0.20	6 (3%)	48	50	14, 23, 29, 38	0
1	G	179/204 (87%)	0.17	4 (2%)	62	64	11, 24, 39, 62	0
1	H	168/204 (82%)	0.73	9 (5%)	31	33	17, 30, 38, 40	0
All	All	1421/1632 (87%)	0.22	45 (3%)	50	52	8, 24, 36, 66	3 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	199	VAL	3.4
1	B	69	PRO	3.4
1	F	62	ASP	3.4
1	B	-2	PHE	3.3
1	H	47	ASP	3.2
1	F	61	ASN	3.1
1	F	161	TYR	3.0
1	G	65	PHE	3.0
1	E	197	ASN	3.0
1	C	90	ASP	2.9
1	B	70	LEU	2.8
1	G	161	TYR	2.8
1	A	-2	PHE	2.8
1	E	190	VAL	2.7
1	E	185	ASP	2.7
1	F	69	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	-3	TYR	2.6
1	F	90	ASP	2.6
1	G	67	VAL	2.6
1	D	47	ASP	2.6
1	A	-1	GLN	2.5
1	F	176	ASP	2.5
1	B	71	HIS	2.5
1	D	48	ASP	2.4
1	E	188	PRO	2.4
1	H	150	GLY	2.4
1	C	61	ASN	2.4
1	A	67	VAL	2.4
1	H	182	TRP	2.4
1	B	90	ASP	2.3
1	H	149	ASP	2.3
1	H	41	VAL	2.2
1	A	62	ASP	2.2
1	H	81	PHE	2.2
1	E	71	HIS	2.2
1	D	19	LYS	2.1
1	H	34	LEU	2.1
1	B	47	ASP	2.1
1	E	179	ILE	2.1
1	B	183	GLU	2.0
1	A	90	ASP	2.0
1	G	61	ASN	2.0
1	A	46	GLY	2.0
1	H	141	ALA	2.0
1	H	82	ILE	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 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(Å ²)	Q<0.9
2	NH4	D	201	1/1	0.87	0.40	25,25,25,25	0
2	NH4	E	201	1/1	0.87	0.28	30,30,30,30	0
2	NH4	C	201	1/1	0.89	0.43	28,28,28,28	0
3	NA	G	201	1/1	0.91	0.26	49,49,49,49	0
2	NH4	H	201	1/1	0.94	0.26	27,27,27,27	0
2	NH4	A	201	1/1	0.94	0.26	20,20,20,20	0
3	NA	F	201	1/1	0.95	0.32	29,29,29,29	0
2	NH4	B	201	1/1	0.96	0.37	26,26,26,26	0
3	NA	E	202	1/1	0.96	0.28	41,41,41,41	0
3	NA	B	202	1/1	0.97	0.29	31,31,31,31	0
3	NA	A	202	1/1	0.98	0.25	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.