



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:04 PM UTC

PDB ID : 6QZ2 / pdb_00006qz2
Title : Structure of MHETase from Ideonella sakaiensis
Authors : Allen, M.D.; Johnson, C.W.; Knott, B.C.; Beckham, G.T.; McGeehan, J.E.
Deposited on : 2019-03-10
Resolution : 1.90 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

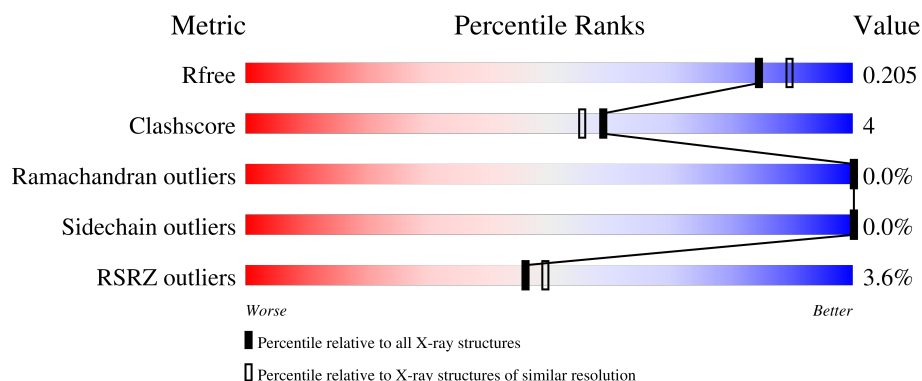
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	611	% 87% 5% 8%
1	B	611	% 88% . 8%
1	C	611	% 86% 6% 8%
1	D	611	% 88% . 8%
1	E	611	% 85% 7% 8%

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Mol	Chain	Length	Quality of chain
1	F	611	% 87% 5% 8%
1	G	611	% 85% 7% 8%
1	H	611	3% 84% 8% 8%
1	I	611	7% 82% 10% 8%
1	J	611	16% 72% 19% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47549 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4147	2597	729	793	28			
1	B	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	C	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	D	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	E	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	F	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	G	562	Total	C	N	O	S	0	0	0
			4147	2597	729	793	28			
1	H	562	Total	C	N	O	S	0	0	0
			4147	2597	729	793	28			
1	I	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	J	560	Total	C	N	O	S	0	0	0
			4133	2587	727	791	28			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	LEU	-	expression tag	UNP A0A0K8P8E7
A	605	GLU	-	expression tag	UNP A0A0K8P8E7
A	606	HIS	-	expression tag	UNP A0A0K8P8E7
A	607	HIS	-	expression tag	UNP A0A0K8P8E7
A	608	HIS	-	expression tag	UNP A0A0K8P8E7
A	609	HIS	-	expression tag	UNP A0A0K8P8E7
A	610	HIS	-	expression tag	UNP A0A0K8P8E7
A	611	HIS	-	expression tag	UNP A0A0K8P8E7
B	604	LEU	-	expression tag	UNP A0A0K8P8E7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	605	GLU	-	expression tag	UNP A0A0K8P8E7
B	606	HIS	-	expression tag	UNP A0A0K8P8E7
B	607	HIS	-	expression tag	UNP A0A0K8P8E7
B	608	HIS	-	expression tag	UNP A0A0K8P8E7
B	609	HIS	-	expression tag	UNP A0A0K8P8E7
B	610	HIS	-	expression tag	UNP A0A0K8P8E7
B	611	HIS	-	expression tag	UNP A0A0K8P8E7
C	604	LEU	-	expression tag	UNP A0A0K8P8E7
C	605	GLU	-	expression tag	UNP A0A0K8P8E7
C	606	HIS	-	expression tag	UNP A0A0K8P8E7
C	607	HIS	-	expression tag	UNP A0A0K8P8E7
C	608	HIS	-	expression tag	UNP A0A0K8P8E7
C	609	HIS	-	expression tag	UNP A0A0K8P8E7
C	610	HIS	-	expression tag	UNP A0A0K8P8E7
C	611	HIS	-	expression tag	UNP A0A0K8P8E7
D	604	LEU	-	expression tag	UNP A0A0K8P8E7
D	605	GLU	-	expression tag	UNP A0A0K8P8E7
D	606	HIS	-	expression tag	UNP A0A0K8P8E7
D	607	HIS	-	expression tag	UNP A0A0K8P8E7
D	608	HIS	-	expression tag	UNP A0A0K8P8E7
D	609	HIS	-	expression tag	UNP A0A0K8P8E7
D	610	HIS	-	expression tag	UNP A0A0K8P8E7
D	611	HIS	-	expression tag	UNP A0A0K8P8E7
E	604	LEU	-	expression tag	UNP A0A0K8P8E7
E	605	GLU	-	expression tag	UNP A0A0K8P8E7
E	606	HIS	-	expression tag	UNP A0A0K8P8E7
E	607	HIS	-	expression tag	UNP A0A0K8P8E7
E	608	HIS	-	expression tag	UNP A0A0K8P8E7
E	609	HIS	-	expression tag	UNP A0A0K8P8E7
E	610	HIS	-	expression tag	UNP A0A0K8P8E7
E	611	HIS	-	expression tag	UNP A0A0K8P8E7
F	604	LEU	-	expression tag	UNP A0A0K8P8E7
F	605	GLU	-	expression tag	UNP A0A0K8P8E7
F	606	HIS	-	expression tag	UNP A0A0K8P8E7
F	607	HIS	-	expression tag	UNP A0A0K8P8E7
F	608	HIS	-	expression tag	UNP A0A0K8P8E7
F	609	HIS	-	expression tag	UNP A0A0K8P8E7
F	610	HIS	-	expression tag	UNP A0A0K8P8E7
F	611	HIS	-	expression tag	UNP A0A0K8P8E7
G	604	LEU	-	expression tag	UNP A0A0K8P8E7
G	605	GLU	-	expression tag	UNP A0A0K8P8E7
G	606	HIS	-	expression tag	UNP A0A0K8P8E7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	607	HIS	-	expression tag	UNP A0A0K8P8E7
G	608	HIS	-	expression tag	UNP A0A0K8P8E7
G	609	HIS	-	expression tag	UNP A0A0K8P8E7
G	610	HIS	-	expression tag	UNP A0A0K8P8E7
G	611	HIS	-	expression tag	UNP A0A0K8P8E7
H	604	LEU	-	expression tag	UNP A0A0K8P8E7
H	605	GLU	-	expression tag	UNP A0A0K8P8E7
H	606	HIS	-	expression tag	UNP A0A0K8P8E7
H	607	HIS	-	expression tag	UNP A0A0K8P8E7
H	608	HIS	-	expression tag	UNP A0A0K8P8E7
H	609	HIS	-	expression tag	UNP A0A0K8P8E7
H	610	HIS	-	expression tag	UNP A0A0K8P8E7
H	611	HIS	-	expression tag	UNP A0A0K8P8E7
I	604	LEU	-	expression tag	UNP A0A0K8P8E7
I	605	GLU	-	expression tag	UNP A0A0K8P8E7
I	606	HIS	-	expression tag	UNP A0A0K8P8E7
I	607	HIS	-	expression tag	UNP A0A0K8P8E7
I	608	HIS	-	expression tag	UNP A0A0K8P8E7
I	609	HIS	-	expression tag	UNP A0A0K8P8E7
I	610	HIS	-	expression tag	UNP A0A0K8P8E7
I	611	HIS	-	expression tag	UNP A0A0K8P8E7
J	604	LEU	-	expression tag	UNP A0A0K8P8E7
J	605	GLU	-	expression tag	UNP A0A0K8P8E7
J	606	HIS	-	expression tag	UNP A0A0K8P8E7
J	607	HIS	-	expression tag	UNP A0A0K8P8E7
J	608	HIS	-	expression tag	UNP A0A0K8P8E7
J	609	HIS	-	expression tag	UNP A0A0K8P8E7
J	610	HIS	-	expression tag	UNP A0A0K8P8E7
J	611	HIS	-	expression tag	UNP A0A0K8P8E7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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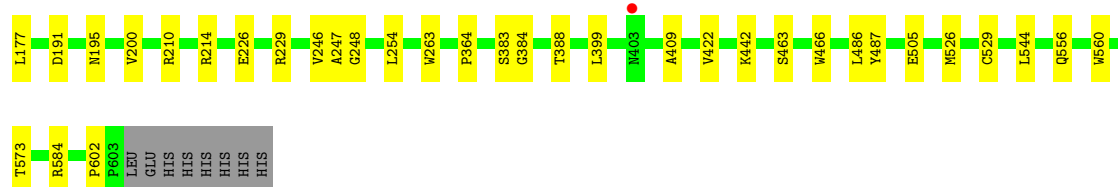
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	Ca 1	0	0
2	G	1	Total 1	Ca 1	0	0
2	H	1	Total 1	Ca 1	0	0
2	I	1	Total 1	Ca 1	0	0
2	J	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

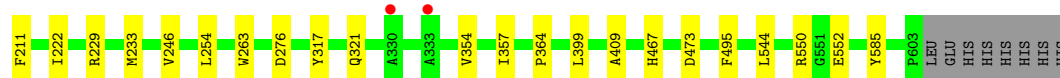
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	777	Total 777	O 777	0	0
3	B	759	Total 759	O 759	0	0
3	C	785	Total 785	O 785	0	0
3	D	706	Total 706	O 706	0	0
3	E	724	Total 724	O 724	0	0
3	F	773	Total 773	O 773	0	0
3	G	567	Total 567	O 567	0	0
3	H	461	Total 461	O 461	0	0
3	I	341	Total 341	O 341	0	0
3	J	232	Total 232	O 232	0	0



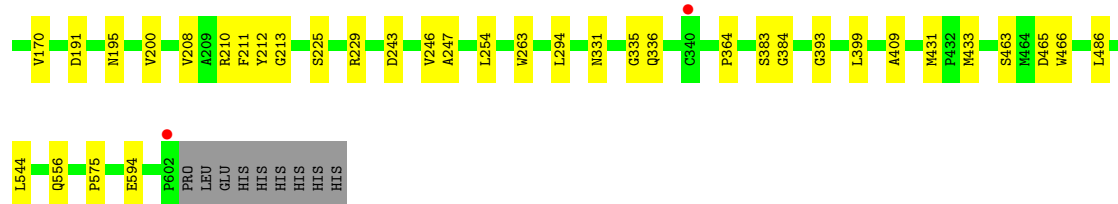
- Chain E:  85% 7% 8%
- | Residue | Count | Percentage |
|---------|-------|------------|
| MET | 1 | 1% |
| GLN | 1 | 1% |
| THR | 1 | 1% |
| VAL | 1 | 1% |
| THR | 1 | 1% |
| MET | 1 | 1% |
| LEU | 1 | 1% |
| LEU | 1 | 1% |
| ALA | 1 | 1% |
| SER | 1 | 1% |
| VAL | 1 | 1% |
| ALA | 1 | 1% |
| LEU | 1 | 1% |
| ALA | 1 | 1% |
| CYS | 1 | 1% |
| ALA | 1 | 1% |
| GLY | 1 | 1% |
| GLY | 1 | 1% |
| GLY | 1 | 1% |
| SER | 1 | 1% |
| THR | 1 | 1% |
| PRO | 1 | 1% |
| LEU | 1 | 1% |
| PRO | 1 | 1% |
| LEU | 1 | 1% |
| PRO | 1 | 1% |
| GLN | 1 | 1% |
| GLN | 1 | 1% |
| GLN | 1 | 1% |
| PRO | 1 | 1% |
| PRO | 1 | 1% |
| PRO | 1 | 1% |
| PRO | 1 | 1% |
| PRO | 1 | 1% |
| PRO | 1 | 1% |
| V43 | 1 | 1% |
| E52 | 1 | 1% |
| G57 | 1 | 1% |
| D60 | 1 | 1% |
| K100 | 1 | 1% |
| P108 | 1 | 1% |
| S131 | 1 | 1% |
| T162 | 1 | 1% |
| V170 | 1 | 1% |



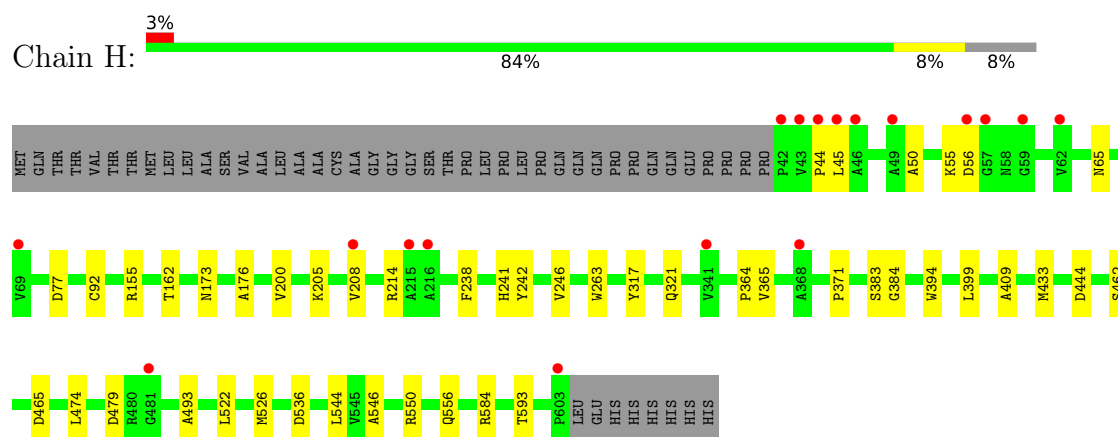
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 MET GLN THR THR VAL THR THR MET LEU LEU ALA SER VAL ALA LEU LEU ALA ALA CYS GLY GLY GLY SER THR PRO PRO PRO PRO GLN GLN GLN PRO PRO PRO PRO PRO PRO PRO V43 P44 L45 A46 D86 G57 N58 G59 D80 N156 D191 N195 P210



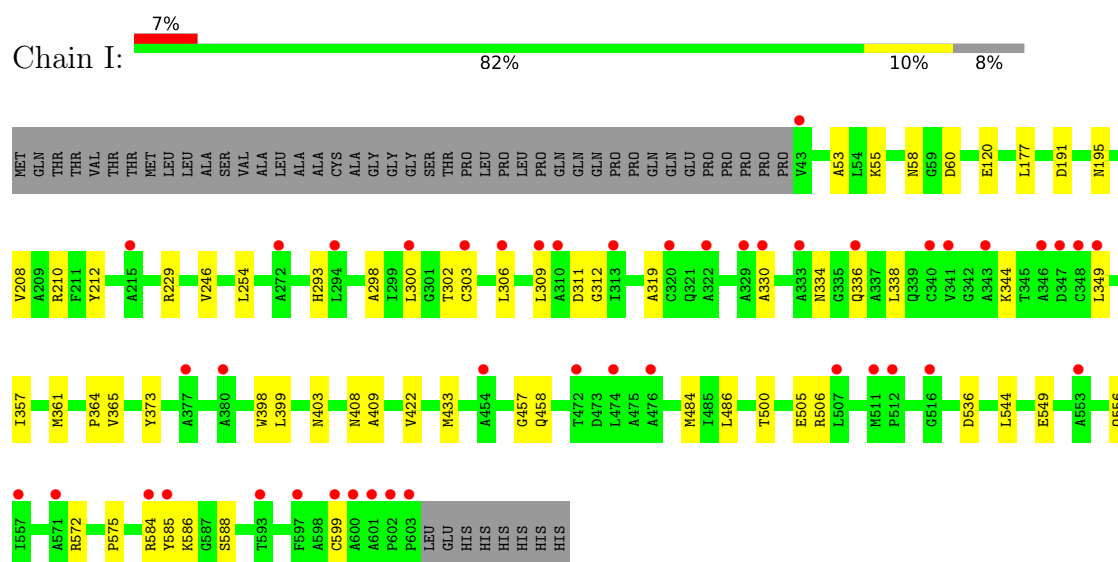
- Chain G: 
- | Residue | Category |
|---------|----------|
| MET | Green |
| GLN | Green |
| THR | Green |
| THR | Green |
| VAL | Green |
| THR | Green |
| THR | Green |
| MET | Green |
| MET | Green |
| LEU | Green |
| LEU | Green |
| ALA | Green |
| ALA | Green |
| CYS | Green |
| GLY | Green |
| GLY | Green |
| GLY | Green |
| SER | Green |
| THR | Green |
| PRO | Green |
| LEU | Green |
| PRO | Green |
| PRO | Green |
| LEU | Green |
| PRO | Green |
| GLN | Green |
| GLN | Green |
| GLN | Green |
| PRO | Green |
| PRO | Green |
| PRO | Green |
| PRO | Green |
| PRO | Green |
| PRO | Green |
| PRO | Green |
| P41 | Green |
| A46 | Yellow |
| K55 | Yellow |
| D56 | Yellow |
| G57 | Yellow |
| I58 | Yellow |
| G59 | Yellow |
| D60 | Yellow |
| M61 | Yellow |
| V62 | Yellow |
| T102 | Grey |
| M127 | Grey |
| R156 | Grey |
| T180 | Grey |



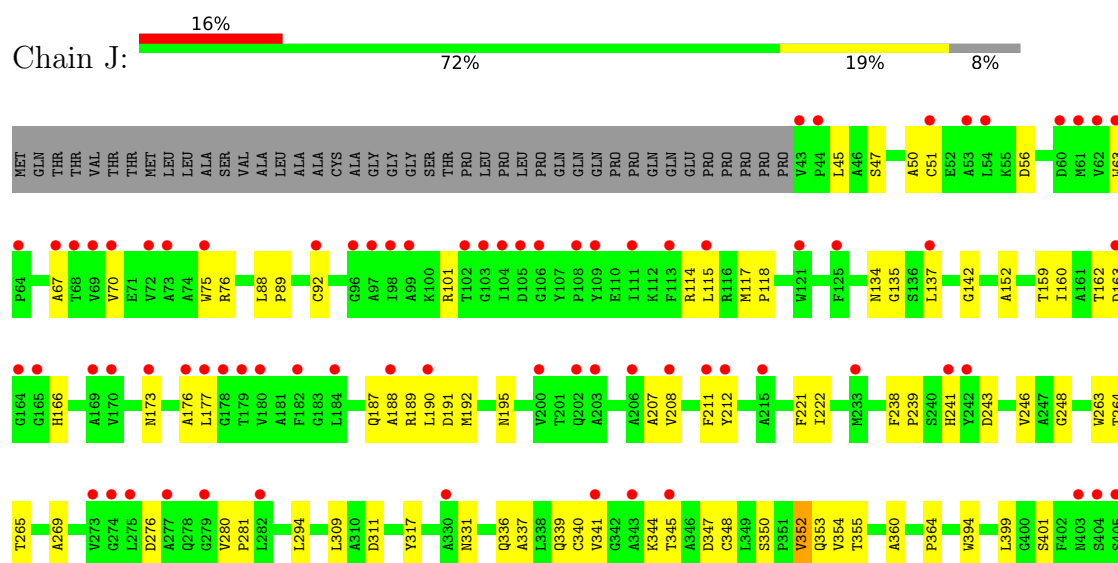
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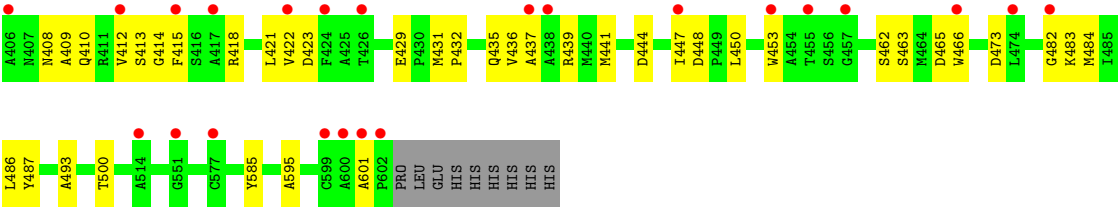


- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.49Å 135.63Å 138.15Å 83.09° 67.91° 67.57°	Depositor
Resolution (Å)	57.62 – 1.90 57.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (57.62-1.90) 93.7 (57.62-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.185 , 0.205 0.186 , 0.205	Depositor DCC
R_{free} test set	24892 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h,l,h-k 0.016 for h,h-l,k 0.023 for h,h-k,h-l 0.017 for -h,-h+k,-l 0.017 for -h,-k,-h+l 0.023 for -h,-l,-k 0.055 for -h,-h+l,-h+k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	47549	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: 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	0.14	0/4256	0.35	0/5796
1	B	0.14	0/4248	0.35	0/5785
1	C	0.14	0/4248	0.36	0/5785
1	D	0.13	0/4248	0.34	0/5785
1	E	0.13	0/4248	0.34	0/5785
1	F	0.13	0/4248	0.34	0/5785
1	G	0.13	0/4256	0.33	1/5796 (0.0%)
1	H	0.13	0/4256	0.32	0/5796
1	I	0.17	0/4248	0.35	0/5785
1	J	0.18	0/4240	0.38	0/5773
All	All	0.14	0/42496	0.35	1/57871 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	225	SER	CB-CA-C	-5.10	110.29	117.23

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	4147	0	3937	21	0
1	B	4140	0	3929	18	0
1	C	4140	0	3929	24	0
1	D	4140	0	3929	25	0
1	E	4140	0	3929	30	0
1	F	4140	0	3929	23	0
1	G	4147	0	3937	33	0
1	H	4147	0	3937	33	0
1	I	4140	0	3929	54	0
1	J	4133	0	3922	94	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
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	777	0	0	7	4
3	B	759	0	0	7	1
3	C	785	0	0	11	3
3	D	706	0	0	14	3
3	E	724	0	0	15	8
3	F	773	0	0	8	1
3	G	567	0	0	16	4
3	H	461	0	0	14	3
3	I	341	0	0	26	0
3	J	232	0	0	29	1
All	All	47549	0	39307	353	14

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 4.

All (353) 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:92:CYS:SG	3:H:1295:HOH:O	2.21	0.98
1:J:345:THR:HG23	1:J:347:ASP:H	1.26	0.98
1:E:602:PRO:O	3:E:901:HOH:O	1.87	0.91
1:G:58:ASN:N	3:G:901:HOH:O	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:GLY:N	3:F:902:HOH:O	2.05	0.89
1:D:345:THR:HG23	1:D:347:ASP:H	1.37	0.87
1:I:549:GLU:OE2	3:I:901:HOH:O	1.93	0.86
1:J:117:MET:SD	3:J:1108:HOH:O	2.33	0.86
1:I:336:GLN:NE2	3:I:902:HOH:O	1.94	0.85
1:F:354:VAL:O	3:F:901:HOH:O	1.96	0.84
1:B:442:LYS:CE	3:B:924:HOH:O	2.26	0.83
1:J:317:TYR:OH	3:J:901:HOH:O	1.96	0.82
1:J:422:VAL:O	3:J:902:HOH:O	1.97	0.81
1:I:588:SER:O	3:I:904:HOH:O	1.98	0.81
1:E:131:SER:HA	3:E:907:HOH:O	1.83	0.79
1:I:536:ASP:OD2	3:I:903:HOH:O	1.97	0.79
1:H:526:MET:HE3	1:H:536:ASP:HB2	1.64	0.79
1:C:473:ASP:OD2	3:C:902:HOH:O	1.99	0.79
1:D:60:ASP:O	1:D:210:ARG:NH2	2.16	0.79
1:J:473:ASP:OD1	3:J:903:HOH:O	2.01	0.79
1:J:101:ARG:NE	3:J:912:HOH:O	2.17	0.77
1:J:190:LEU:N	3:J:910:HOH:O	2.16	0.76
1:J:177:LEU:HD12	1:J:422:VAL:HG23	1.66	0.76
1:J:221:PHE:O	3:J:904:HOH:O	2.04	0.75
1:J:134:ASN:HB2	1:J:192:MET:HE1	1.67	0.75
1:C:48:ARG:NH1	3:C:901:HOH:O	1.90	0.75
1:J:337:ALA:O	3:J:905:HOH:O	2.06	0.73
1:I:506:ARG:NH1	3:I:915:HOH:O	2.22	0.73
1:G:55:LYS:O	3:G:901:HOH:O	2.05	0.73
1:H:77:ASP:O	3:H:901:HOH:O	2.06	0.73
1:H:45:LEU:O	3:H:902:HOH:O	2.06	0.73
1:G:56:ASP:OD2	3:G:903:HOH:O	2.06	0.73
1:G:393:GLY:HA3	3:G:1138:HOH:O	1.88	0.72
1:G:335:GLY:O	3:G:902:HOH:O	2.06	0.72
1:H:546:ALA:HA	1:H:550:ARG:HH21	1.56	0.71
1:J:246:VAL:N	3:J:904:HOH:O	2.18	0.71
1:I:120:GLU:OE2	3:I:905:HOH:O	2.08	0.70
1:J:191:ASP:HA	1:J:195:ASN:HB3	1.74	0.70
1:I:556:GLN:HG2	1:I:599:CYS:SG	2.31	0.70
1:J:340:CYS:O	3:J:907:HOH:O	2.09	0.69
1:I:229:ARG:HD3	1:I:254:LEU:HD12	1.72	0.69
1:C:429:GLU:OE2	3:C:903:HOH:O	2.10	0.69
1:G:213:GLY:N	3:G:905:HOH:O	2.19	0.69
1:F:585:TYR:OH	3:F:903:HOH:O	2.10	0.69
1:E:226:GLU:N	3:E:907:HOH:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:303:CYS:HA	1:I:306:LEU:HD13	1.75	0.67
1:J:188:ALA:C	3:J:910:HOH:O	2.36	0.67
1:F:473:ASP:OD1	3:F:904:HOH:O	2.13	0.67
1:J:345:THR:HG23	1:J:347:ASP:N	2.04	0.67
1:B:403:ASN:OD1	3:B:901:HOH:O	2.10	0.67
1:J:429:GLU:OE1	3:J:908:HOH:O	2.13	0.67
1:I:330:ALA:O	3:I:906:HOH:O	2.12	0.67
1:A:71:GLU:OE2	3:A:903:HOH:O	2.11	0.67
1:D:405:SER:OG	3:D:901:HOH:O	1.86	0.67
1:H:479:ASP:OD2	3:H:904:HOH:O	2.13	0.66
1:D:407:ASN:ND2	3:D:905:HOH:O	2.28	0.66
1:G:556:GLN:OE1	3:G:904:HOH:O	2.13	0.66
1:I:408:ASN:O	3:I:907:HOH:O	2.13	0.66
1:I:457:GLY:HA3	3:I:931:HOH:O	1.95	0.66
1:B:550:ARG:HB2	1:B:552:GLU:HG3	1.78	0.66
1:J:500:THR:OG1	3:J:906:HOH:O	2.09	0.66
1:C:403:ASN:ND2	3:C:909:HOH:O	2.24	0.66
1:J:115:LEU:HB2	1:J:160:ILE:HD13	1.78	0.66
1:I:549:GLU:O	3:I:908:HOH:O	2.14	0.66
1:C:556:GLN:NE2	3:C:914:HOH:O	2.29	0.66
1:E:388:THR:N	3:E:902:HOH:O	1.92	0.66
1:B:442:LYS:HE3	3:B:924:HOH:O	1.89	0.65
1:E:214:ARG:NH1	3:E:903:HOH:O	2.00	0.65
1:J:56:ASP:OD1	3:J:909:HOH:O	2.15	0.65
1:G:246:VAL:HG23	1:G:544:LEU:HD22	1.77	0.65
1:J:409:ALA:HB3	1:J:412:VAL:HG22	1.79	0.64
1:B:210:ARG:NH1	3:B:903:HOH:O	2.28	0.64
1:D:246:VAL:HG23	1:D:544:LEU:HD22	1.79	0.64
1:B:60:ASP:O	3:B:903:HOH:O	2.16	0.64
1:F:357:ILE:N	3:F:901:HOH:O	2.30	0.64
1:J:345:THR:HG22	1:J:348:CYS:SG	2.38	0.64
1:B:229:ARG:HD3	1:B:254:LEU:HD12	1.80	0.63
1:J:281:PRO:HD2	1:J:441:MET:HE3	1.80	0.63
1:C:336:GLN:OE1	3:C:906:HOH:O	2.16	0.63
1:D:214:ARG:NE	3:D:903:HOH:O	2.23	0.63
1:E:229:ARG:HD3	1:E:254:LEU:HD12	1.81	0.63
1:C:473:ASP:OD1	3:C:905:HOH:O	2.15	0.63
1:I:584:ARG:HH22	1:I:586:LYS:HA	1.64	0.63
1:J:309:LEU:HD12	1:J:585:TYR:HB2	1.81	0.63
1:I:309:LEU:HD12	1:I:585:TYR:HB2	1.81	0.62
1:G:229:ARG:HD3	1:G:254:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:GLU:OE1	3:E:904:HOH:O	2.16	0.62
1:I:246:VAL:HG23	1:I:544:LEU:HD22	1.81	0.62
1:J:191:ASP:N	3:J:910:HOH:O	2.33	0.62
1:A:458:GLN:NE2	3:A:912:HOH:O	2.33	0.62
1:E:246:VAL:HG23	1:E:544:LEU:HD22	1.82	0.62
1:J:309:LEU:HD22	1:J:311:ASP:HB3	1.82	0.61
1:I:458:GLN:NE2	3:I:924:HOH:O	2.33	0.61
1:D:214:ARG:NH2	3:D:903:HOH:O	2.17	0.61
1:J:483:LYS:NZ	3:J:919:HOH:O	2.27	0.61
1:B:48:ARG:NH2	3:B:902:HOH:O	2.11	0.60
1:F:246:VAL:HG23	1:F:544:LEU:HD22	1.83	0.60
1:H:546:ALA:HA	1:H:550:ARG:NH2	2.15	0.60
1:I:364:PRO:O	3:I:909:HOH:O	2.17	0.59
1:C:155:ARG:NH1	3:C:918:HOH:O	2.34	0.59
1:G:336:GLN:NE2	3:G:914:HOH:O	2.35	0.59
1:F:550:ARG:NH1	3:F:911:HOH:O	2.34	0.59
1:A:214:ARG:NH2	3:A:907:HOH:O	2.26	0.59
1:E:210:ARG:NH1	3:E:911:HOH:O	2.36	0.59
1:J:453:TRP:O	3:J:911:HOH:O	2.17	0.59
1:J:47:SER:H	1:J:211:PHE:HE1	1.49	0.59
1:D:590:ASP:OD2	3:D:902:HOH:O	2.16	0.58
1:A:294:LEU:HD11	1:A:346:ALA:O	2.03	0.58
1:B:246:VAL:HG23	1:B:544:LEU:HD22	1.86	0.58
1:J:117:MET:HE3	1:J:211:PHE:HD2	1.68	0.58
1:A:60:ASP:O	1:A:210:ARG:NH2	2.35	0.58
1:E:247:ALA:HB3	1:E:486:LEU:HD23	1.84	0.58
1:I:484:MET:HE3	1:I:486:LEU:HD11	1.85	0.58
1:J:462:SER:HB3	1:J:465:ASP:HB2	1.85	0.58
1:D:556:GLN:NE2	3:D:909:HOH:O	2.37	0.58
1:A:246:VAL:HG23	1:A:544:LEU:HD22	1.87	0.57
1:C:214:ARG:NH1	3:C:920:HOH:O	2.37	0.57
1:A:573:THR:HB	3:A:1168:HOH:O	2.04	0.57
1:F:222:ILE:HG12	1:F:246:VAL:HB	1.86	0.56
1:I:584:ARG:HG2	1:I:584:ARG:HH21	1.70	0.56
1:H:321:GLN:O	3:H:905:HOH:O	2.18	0.56
1:D:214:ARG:NH1	3:D:910:HOH:O	2.37	0.56
1:F:229:ARG:NE	1:F:467:HIS:CE1	2.74	0.56
1:J:173:ASN:HB3	1:J:176:ALA:HB3	1.87	0.56
1:D:345:THR:HG22	1:D:348:CYS:SG	2.45	0.55
1:J:269:ALA:HB2	1:J:441:MET:HE1	1.88	0.55
1:D:214:ARG:NH2	3:D:910:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:ASP:OD1	1:I:210:ARG:NH2	2.38	0.55
1:J:189:ARG:NE	3:J:902:HOH:O	2.27	0.55
1:H:205:LYS:HA	1:H:208:VAL:HG22	1.87	0.55
1:H:214:ARG:HD2	3:H:916:HOH:O	2.07	0.55
1:E:226:GLU:HB3	3:E:907:HOH:O	2.07	0.55
1:J:412:VAL:HG23	1:J:413:SER:H	1.72	0.55
1:C:246:VAL:HG23	1:C:544:LEU:HD22	1.89	0.54
1:H:556:GLN:O	3:H:906:HOH:O	2.19	0.54
1:E:100:LYS:NZ	3:E:910:HOH:O	2.35	0.54
1:I:306:LEU:HD23	1:I:319:ALA:HB1	1.89	0.53
1:J:177:LEU:HD22	1:J:418:ARG:HG2	1.90	0.53
1:D:403:ASN:ND2	3:D:914:HOH:O	2.40	0.53
1:E:556:GLN:NE2	3:E:905:HOH:O	2.21	0.53
1:J:177:LEU:HD12	1:J:422:VAL:CG2	2.37	0.53
1:I:338:LEU:O	1:I:349:LEU:N	2.42	0.53
1:G:210:ARG:C	3:G:905:HOH:O	2.52	0.53
1:J:399:LEU:C	1:J:409:ALA:HB2	2.33	0.53
1:E:442:LYS:HE2	3:E:1188:HOH:O	2.09	0.53
1:I:584:ARG:NH2	1:I:585:TYR:O	2.42	0.53
1:F:276:ASP:HB2	3:F:1330:HOH:O	2.08	0.52
1:I:311:ASP:HB2	1:I:572:ARG:HH12	1.75	0.52
1:C:229:ARG:HD3	1:C:254:LEU:HD12	1.91	0.52
1:E:100:LYS:HG3	3:E:1284:HOH:O	2.10	0.52
1:C:438:ALA:O	1:C:442:LYS:HG3	2.09	0.52
1:G:247:ALA:HB3	1:G:486:LEU:HD23	1.92	0.52
1:A:552:GLU:OE2	3:A:905:HOH:O	2.19	0.52
1:H:246:VAL:HG23	1:H:544:LEU:HD22	1.92	0.52
1:F:254:LEU:HD21	1:F:495:PHE:CZ	2.45	0.52
1:J:67:ALA:O	3:J:914:HOH:O	2.19	0.52
1:A:214:ARG:NH1	3:A:902:HOH:O	2.10	0.51
1:J:187:GLN:O	3:J:910:HOH:O	2.19	0.51
1:D:133:THR:HG23	3:D:923:HOH:O	2.10	0.51
1:J:601:ALA:HB1	3:J:933:HOH:O	2.11	0.51
1:G:465:ASP:O	3:G:906:HOH:O	2.19	0.51
1:H:162:THR:HB	1:H:200:VAL:HG21	1.93	0.50
1:J:421:LEU:HD21	1:J:439:ARG:HG2	1.92	0.50
1:G:393:GLY:CA	3:G:1138:HOH:O	2.51	0.50
1:H:242:TYR:N	3:H:903:HOH:O	2.12	0.50
1:J:92:CYS:CB	1:J:211:PHE:HE2	2.24	0.50
1:C:403:ASN:ND2	3:C:924:HOH:O	2.44	0.50
1:I:55:LYS:HE3	3:I:1108:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:GLN:NE2	3:D:912:HOH:O	2.39	0.50
1:I:365:VAL:O	3:I:911:HOH:O	2.19	0.50
1:J:447:ILE:HA	1:J:450:LEU:HD12	1.93	0.50
1:H:444:ASP:OD2	3:H:908:HOH:O	2.20	0.50
1:J:135:GLY:HA2	1:J:166:HIS:O	2.12	0.49
1:J:264:THR:HG22	1:J:360:ALA:HB1	1.95	0.49
1:E:60:ASP:CB	1:E:210:ARG:HH12	2.26	0.49
1:E:162:THR:HB	1:E:200:VAL:HG21	1.94	0.48
1:I:309:LEU:HD22	1:I:311:ASP:HB3	1.93	0.48
1:A:108:PRO:HG2	1:A:170:VAL:HG11	1.95	0.48
1:A:439:ARG:HA	1:A:442:LYS:HE3	1.96	0.48
1:J:341:VAL:C	3:J:907:HOH:O	2.55	0.48
1:A:263:TRP:CD2	1:A:364:PRO:HA	2.49	0.48
1:J:222:ILE:HG12	1:J:246:VAL:HB	1.95	0.48
1:G:383:SER:OG	1:G:384:GLY:N	2.47	0.48
1:J:208:VAL:HA	3:J:1108:HOH:O	2.14	0.48
1:J:63:TRP:CH2	1:J:207:ALA:HB2	2.49	0.48
1:I:373:TYR:OH	3:I:912:HOH:O	2.20	0.48
1:F:263:TRP:CD2	1:F:364:PRO:HA	2.49	0.47
1:E:442:LYS:HG2	3:E:1188:HOH:O	2.13	0.47
1:C:480:ARG:NH2	3:C:904:HOH:O	2.14	0.47
1:E:52:GLU:HG3	3:E:1023:HOH:O	2.14	0.47
1:F:156:ASN:ND2	3:F:925:HOH:O	2.47	0.47
1:F:399:LEU:C	1:F:409:ALA:HB2	2.40	0.47
1:G:208:VAL:HG13	1:G:212:TYR:HD2	1.78	0.47
1:I:575:PRO:O	3:I:913:HOH:O	2.20	0.47
1:J:263:TRP:CD2	1:J:364:PRO:HA	2.50	0.47
1:H:263:TRP:HB2	1:H:364:PRO:HB3	1.95	0.47
1:H:263:TRP:CD2	1:H:364:PRO:HA	2.50	0.47
1:J:45:LEU:HD23	1:J:212:TYR:O	2.15	0.47
1:D:263:TRP:CD2	1:D:364:PRO:HA	2.50	0.47
1:H:474:LEU:HA	3:H:1141:HOH:O	2.13	0.47
1:A:399:LEU:C	1:A:409:ALA:HB2	2.40	0.47
1:H:55:LYS:HE3	1:H:56:ASP:HB2	1.97	0.47
1:I:293:HIS:CE1	3:I:935:HOH:O	2.68	0.46
1:I:506:ARG:CZ	3:I:915:HOH:O	2.62	0.46
1:J:344:LYS:NZ	1:J:345:THR:O	2.40	0.46
1:D:162:THR:HB	1:D:200:VAL:HG21	1.96	0.46
1:A:162:THR:HB	1:A:200:VAL:HG21	1.97	0.46
1:D:480:ARG:NH2	3:D:904:HOH:O	2.19	0.46
1:J:88:LEU:HA	1:J:89:PRO:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:595:ALA:HB2	3:J:987:HOH:O	2.15	0.46
1:H:44:PRO:O	1:H:50:ALA:HB2	2.16	0.46
1:J:276:ASP:CG	1:J:280:VAL:HG22	2.41	0.46
1:C:110:GLU:OE2	1:C:112:LYS:NZ	2.45	0.46
1:C:162:THR:HB	1:C:200:VAL:HG21	1.97	0.46
1:D:210:ARG:HH21	1:F:210:ARG:HH12	1.63	0.46
1:I:300:LEU:HD22	1:I:312:GLY:HA2	1.96	0.46
1:J:118:PRO:O	1:J:212:TYR:OH	2.33	0.46
1:I:344:LYS:NZ	1:I:349:LEU:HA	2.32	0.45
1:J:401:SER:N	1:J:408:ASN:OD1	2.46	0.45
1:B:46:ALA:HA	1:B:211:PHE:CZ	2.51	0.45
1:C:46:ALA:HA	1:C:211:PHE:CZ	2.52	0.45
1:J:114:ARG:O	1:J:160:ILE:HD12	2.16	0.45
1:E:560:TRP:HB3	1:E:573:THR:HG22	1.99	0.45
1:H:462:SER:O	1:H:465:ASP:HB2	2.16	0.45
1:J:56:ASP:OD2	1:J:70:VAL:N	2.48	0.45
1:J:431:MET:HE3	1:J:435:GLN:HB2	1.99	0.45
1:E:383:SER:OG	1:E:384:GLY:N	2.46	0.45
1:J:248:GLY:HA3	1:J:487:TYR:CZ	2.51	0.45
1:D:229:ARG:HD3	1:D:254:LEU:HD12	1.98	0.45
1:H:593:THR:HG21	3:H:1283:HOH:O	2.17	0.45
1:C:294:LEU:HD21	1:C:347:ASP:C	2.42	0.45
1:I:53:ALA:HB3	3:I:971:HOH:O	2.16	0.45
1:J:412:VAL:HG23	1:J:413:SER:N	2.30	0.45
1:D:399:LEU:C	1:D:409:ALA:HB2	2.41	0.45
1:F:550:ARG:HB2	1:F:552:GLU:HG3	1.99	0.45
1:G:433:MET:HG3	3:G:1098:HOH:O	2.16	0.45
1:J:294:LEU:HD21	1:J:347:ASP:C	2.41	0.45
1:H:65:ASN:HB2	3:H:1139:HOH:O	2.16	0.44
1:H:399:LEU:C	1:H:409:ALA:HB2	2.41	0.44
1:I:298:ALA:O	1:I:302:THR:HG23	2.17	0.44
1:I:500:THR:HG22	3:I:996:HOH:O	2.16	0.44
1:J:162:THR:OG1	1:J:163:ASP:N	2.50	0.44
1:J:238:PHE:HB3	1:J:241:HIS:CD2	2.52	0.44
1:G:399:LEU:C	1:G:409:ALA:HB2	2.42	0.44
1:I:177:LEU:C	1:I:433:MET:HE2	2.42	0.44
1:I:505:GLU:OE2	3:I:914:HOH:O	2.21	0.44
1:C:317:TYR:O	1:C:321:GLN:HG2	2.18	0.44
1:D:210:ARG:NH1	3:D:938:HOH:O	2.51	0.44
1:D:294:LEU:HD21	1:D:347:ASP:C	2.43	0.44
1:G:57:GLY:N	3:G:901:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:357:ILE:O	1:I:361:MET:HG2	2.18	0.44
1:E:399:LEU:C	1:E:409:ALA:HB2	2.43	0.44
1:I:344:LYS:HZ1	1:I:349:LEU:HA	1.82	0.44
1:J:423:ASP:HA	3:J:902:HOH:O	2.17	0.44
1:G:243:ASP:HA	3:G:938:HOH:O	2.17	0.44
1:H:394:TRP:CD1	1:H:493:ALA:HB2	2.53	0.44
1:G:191:ASP:HA	1:G:195:ASN:HB3	2.00	0.44
1:G:46:ALA:HA	1:G:211:PHE:CZ	2.52	0.44
1:A:526:MET:HE3	1:A:536:ASP:HA	2.00	0.43
1:A:587:GLY:O	1:G:170:VAL:HG22	2.18	0.43
1:G:162:THR:HB	1:G:200:VAL:HG21	2.00	0.43
1:D:214:ARG:CZ	3:D:910:HOH:O	2.66	0.43
1:F:263:TRP:HB2	1:F:364:PRO:HB3	2.00	0.43
1:J:331:ASN:N	1:J:336:GLN:O	2.47	0.43
1:J:410:GLN:OE1	1:J:415:PHE:HB2	2.18	0.43
1:J:410:GLN:HA	1:J:414:GLY:HA3	2.00	0.43
1:B:222:ILE:HG12	1:B:246:VAL:HB	1.98	0.43
1:I:398:TRP:CD1	1:I:398:TRP:N	2.85	0.43
1:I:506:ARG:NH2	3:I:940:HOH:O	2.43	0.43
1:J:142:GLY:HA3	1:J:152:ALA:HB3	1.99	0.43
3:A:1460:HOH:O	1:G:102:THR:HG21	2.18	0.43
1:B:294:LEU:HD21	1:B:347:ASP:C	2.44	0.43
1:E:526:MET:HE3	1:E:529:CYS:C	2.44	0.43
1:H:155:ARG:NH1	3:H:915:HOH:O	2.38	0.43
1:I:334:ASN:HA	3:I:1003:HOH:O	2.18	0.43
1:H:383:SER:OG	1:H:384:GLY:N	2.49	0.43
1:E:108:PRO:HG2	1:E:170:VAL:HG11	2.00	0.43
1:J:463:SER:HA	1:J:466:TRP:CE2	2.54	0.43
1:C:263:TRP:HB2	1:C:364:PRO:HB3	2.01	0.42
1:C:365:VAL:HG12	1:C:371:PRO:HA	2.01	0.42
1:E:177:LEU:HD12	1:E:422:VAL:HG23	2.01	0.42
1:H:584:ARG:NE	3:H:920:HOH:O	2.42	0.42
1:J:115:LEU:HD12	1:J:159:THR:O	2.18	0.42
1:E:463:SER:HA	1:E:466:TRP:CE2	2.54	0.42
1:G:127:MET:HE2	3:G:1021:HOH:O	2.17	0.42
1:J:394:TRP:CD1	1:J:493:ALA:HB2	2.53	0.42
1:A:46:ALA:HA	1:A:211:PHE:CZ	2.54	0.42
1:G:263:TRP:CD2	1:G:364:PRO:HA	2.54	0.42
1:J:339:GLN:HG3	1:J:354:VAL:HG21	2.01	0.42
1:J:432:PRO:HD2	1:J:435:GLN:OE1	2.19	0.42
1:A:191:ASP:HA	1:A:195:ASN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:575:PRO:HD3	1:G:594:GLU:HG3	2.01	0.42
1:I:208:VAL:HG13	1:I:212:TYR:HD2	1.85	0.42
1:I:53:ALA:HA	1:I:58:ASN:HB3	2.02	0.42
1:J:166:HIS:HE1	3:J:972:HOH:O	2.03	0.42
1:J:444:ASP:O	1:J:448:ASP:HB2	2.19	0.42
1:H:238:PHE:HB3	1:H:241:HIS:CD2	2.55	0.42
1:J:177:LEU:HD13	1:J:418:ARG:HA	2.00	0.42
1:I:191:ASP:HA	1:I:195:ASN:HB3	2.01	0.42
1:I:403:ASN:HB3	3:I:925:HOH:O	2.20	0.42
1:J:134:ASN:HB3	1:J:163:ASP:O	2.20	0.42
1:J:189:ARG:NH2	3:J:902:HOH:O	2.49	0.42
1:J:265:THR:HG23	1:J:412:VAL:HG12	2.01	0.42
1:H:433:MET:HE2	1:H:433:MET:HB3	1.94	0.41
1:E:191:ASP:HA	1:E:195:ASN:HB3	2.01	0.41
1:E:248:GLY:HA3	1:E:487:TYR:CZ	2.56	0.41
1:I:336:GLN:NE2	3:I:921:HOH:O	2.25	0.41
1:J:51:CYS:HB2	1:J:211:PHE:CE2	2.55	0.41
1:J:421:LEU:HD23	1:J:421:LEU:HA	1.95	0.41
1:F:46:ALA:HA	1:F:211:PHE:CZ	2.56	0.41
1:F:191:ASP:HA	1:F:195:ASN:HB3	2.01	0.41
1:I:433:MET:HE3	3:I:1215:HOH:O	2.20	0.41
1:I:311:ASP:OD1	1:I:311:ASP:N	2.54	0.41
1:B:442:LYS:NZ	3:B:924:HOH:O	2.49	0.41
1:C:399:LEU:C	1:C:409:ALA:HB2	2.46	0.41
1:G:294:LEU:HD11	1:G:331:ASN:ND2	2.36	0.41
1:I:177:LEU:HD12	1:I:422:VAL:HG23	2.02	0.41
1:J:421:LEU:HD12	1:J:436:VAL:HG13	2.02	0.41
1:B:399:LEU:C	1:B:409:ALA:HB2	2.45	0.41
1:D:263:TRP:HB2	1:D:364:PRO:HB3	2.03	0.41
1:G:463:SER:HA	1:G:466:TRP:CE2	2.56	0.41
1:E:263:TRP:CD2	1:E:364:PRO:HA	2.55	0.41
1:H:173:ASN:HB3	1:H:176:ALA:HB3	2.02	0.41
1:J:239:PRO:HB3	3:J:977:HOH:O	2.20	0.41
1:J:352:VAL:HA	1:J:355:THR:HG22	2.02	0.41
1:A:526:MET:HE1	1:A:538:PHE:CZ	2.55	0.41
1:B:366:ASN:HB2	1:B:446:ASP:OD1	2.21	0.41
1:C:191:ASP:HA	1:C:195:ASN:HB3	2.02	0.41
1:E:584:ARG:HD3	3:E:1427:HOH:O	2.21	0.41
1:G:155:ARG:NH1	3:G:939:HOH:O	2.53	0.41
1:G:263:TRP:HB2	1:G:364:PRO:HB3	2.03	0.41
1:I:208:VAL:HG13	1:I:212:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:399:LEU:C	1:I:409:ALA:HB2	2.45	0.41
1:J:114:ARG:HB2	1:J:137:LEU:HD21	2.02	0.41
1:B:208:VAL:HG13	1:B:212:TYR:HD2	1.85	0.41
1:B:263:TRP:CD2	1:B:364:PRO:HA	2.56	0.41
1:J:280:VAL:HG21	1:J:437:ALA:HB1	2.03	0.41
1:A:248:GLY:HA3	1:A:487:TYR:CZ	2.56	0.40
1:F:43:VAL:HA	1:F:44:PRO:HD3	1.94	0.40
1:F:233:MET:HE3	1:F:233:MET:HB3	2.02	0.40
1:F:254:LEU:CD2	1:F:495:PHE:CE1	3.04	0.40
1:G:431:MET:HE2	1:G:431:MET:HB3	1.92	0.40
1:J:75:TRP:C	1:J:76:ARG:HD3	2.47	0.40
1:A:263:TRP:HB2	1:A:364:PRO:HB3	2.03	0.40
1:B:191:ASP:HA	1:B:195:ASN:HB3	2.02	0.40
1:C:379:ASP:OD2	1:C:491:SER:OG	2.34	0.40
1:H:317:TYR:CZ	1:H:522:LEU:HD12	2.56	0.40
1:F:317:TYR:O	1:F:321:GLN:HG2	2.22	0.40
1:H:365:VAL:HG12	1:H:371:PRO:HA	2.04	0.40
1:J:350:SER:HB2	1:J:353:GLN:H	1.87	0.40
1:J:208:VAL:HG22	3:J:1108:HOH:O	2.21	0.40
1:J:243:ASP:O	1:J:482:GLY:HA2	2.21	0.40
1:J:484:MET:SD	1:J:486:LEU:HD21	2.62	0.40

All (14) 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:E:1449:HOH:O	3:H:1218:HOH:O[1_655]	1.83	0.37
3:D:1450:HOH:O	3:E:1566:HOH:O[1_455]	1.92	0.28
3:A:1307:HOH:O	3:G:1262:HOH:O[1_655]	1.93	0.27
3:A:1530:HOH:O	3:G:1310:HOH:O[1_655]	2.01	0.19
3:D:1176:HOH:O	3:E:1039:HOH:O[1_455]	2.02	0.18
3:E:1548:HOH:O	3:H:1292:HOH:O[1_655]	2.02	0.18
3:C:1669:HOH:O	3:D:1586:HOH:O[1_645]	2.05	0.15
3:C:1188:HOH:O	3:E:1226:HOH:O[1_545]	2.06	0.14
3:B:1369:HOH:O	3:F:1518:HOH:O[1_556]	2.08	0.12
3:E:1591:HOH:O	3:H:1342:HOH:O[1_655]	2.09	0.11
3:E:904:HOH:O	3:J:1039:HOH:O[1_655]	2.13	0.07
3:C:1261:HOH:O	3:E:1262:HOH:O[1_545]	2.18	0.02
3:A:1307:HOH:O	3:G:1372:HOH:O[1_655]	2.19	0.01
3:A:1480:HOH:O	3:G:1347:HOH:O[1_655]	2.19	0.01

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	560/611 (92%)	544 (97%)	16 (3%)	0	100	100
1	B	559/611 (92%)	543 (97%)	16 (3%)	0	100	100
1	C	559/611 (92%)	544 (97%)	15 (3%)	0	100	100
1	D	559/611 (92%)	541 (97%)	18 (3%)	0	100	100
1	E	559/611 (92%)	545 (98%)	14 (2%)	0	100	100
1	F	559/611 (92%)	544 (97%)	15 (3%)	0	100	100
1	G	560/611 (92%)	547 (98%)	13 (2%)	0	100	100
1	H	560/611 (92%)	544 (97%)	16 (3%)	0	100	100
1	I	559/611 (92%)	540 (97%)	19 (3%)	0	100	100
1	J	558/611 (91%)	536 (96%)	21 (4%)	1 (0%)	43	36
All	All	5592/6110 (92%)	5428 (97%)	163 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	50	ALA

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	408/449 (91%)	407 (100%)	1 (0%)	87	90
1	B	407/449 (91%)	407 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	407/449 (91%)	407 (100%)	0	100	100
1	D	407/449 (91%)	407 (100%)	0	100	100
1	E	407/449 (91%)	407 (100%)	0	100	100
1	F	407/449 (91%)	407 (100%)	0	100	100
1	G	408/449 (91%)	408 (100%)	0	100	100
1	H	408/449 (91%)	408 (100%)	0	100	100
1	I	407/449 (91%)	407 (100%)	0	100	100
1	J	406/449 (90%)	405 (100%)	1 (0%)	87	90
All	All	4072/4490 (91%)	4070 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	J	352	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	297	GLN
1	A	336	GLN
1	A	458	GLN
1	B	156	ASN
1	C	156	ASN
1	C	403	ASN
1	C	461	GLN
1	C	581	GLN
1	D	339	GLN
1	D	458	GLN
1	D	556	GLN
1	E	297	GLN
1	F	581	GLN
1	G	297	GLN
1	H	187	GLN
1	H	297	GLN
1	H	339	GLN
1	H	556	GLN

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Mol	Chain	Res	Type
1	I	156	ASN
1	I	336	GLN
1	I	435	GLN
1	J	241	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 10 ligands modelled in this entry, 10 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	562/611 (91%)	-0.35	6 (1%) 78 80	13, 20, 33, 63	0
1	B	561/611 (91%)	-0.33	7 (1%) 76 79	12, 19, 31, 57	0
1	C	561/611 (91%)	-0.33	7 (1%) 76 79	11, 19, 31, 53	0
1	D	561/611 (91%)	-0.26	5 (0%) 81 83	14, 21, 33, 61	0
1	E	561/611 (91%)	-0.27	4 (0%) 84 86	14, 21, 33, 59	0
1	F	561/611 (91%)	-0.25	6 (1%) 78 80	11, 20, 33, 57	0
1	G	562/611 (91%)	0.04	9 (1%) 70 74	18, 27, 38, 66	0
1	H	562/611 (91%)	0.34	18 (3%) 50 54	21, 31, 50, 70	0
1	I	561/611 (91%)	0.83	45 (8%) 18 19	26, 41, 59, 72	0
1	J	560/611 (91%)	1.19	97 (17%) 4 4	28, 49, 64, 80	0
All	All	5612/6110 (91%)	0.06	204 (3%) 46 49	11, 24, 54, 80	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	57	GLY	6.3
1	H	43	VAL	6.2
1	B	57	GLY	4.6
1	F	57	GLY	4.6
1	H	42	PRO	4.5
1	H	44	PRO	4.3
1	A	42	PRO	4.3
1	C	57	GLY	4.2
1	J	177	LEU	4.2
1	J	51	CYS	4.0
1	H	45	LEU	3.9
1	J	63	TRP	3.8
1	J	44	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	164	GLY	3.7
1	C	58	ASN	3.5
1	I	349	LEU	3.5
1	J	188	ALA	3.5
1	H	57	GLY	3.5
1	J	279	GLY	3.5
1	I	341	VAL	3.4
1	J	341	VAL	3.4
1	A	60	ASP	3.4
1	B	601	ALA	3.4
1	I	553	ALA	3.4
1	J	99	ALA	3.4
1	J	211	PHE	3.4
1	J	601	ALA	3.4
1	J	92	CYS	3.4
1	D	57	GLY	3.3
1	J	176	ALA	3.3
1	I	43	VAL	3.3
1	F	56	ASP	3.2
1	I	377	ALA	3.2
1	G	57	GLY	3.2
1	C	60	ASP	3.2
1	D	60	ASP	3.2
1	D	59	GLY	3.2
1	J	165	GLY	3.1
1	C	56	ASP	3.1
1	J	455	THR	3.1
1	I	343	ALA	3.1
1	H	216	ALA	3.1
1	J	600	ALA	3.1
1	J	104	ILE	3.0
1	J	43	VAL	3.0
1	J	170	VAL	3.0
1	J	273	VAL	3.0
1	B	603	PRO	3.0
1	J	184	LEU	3.0
1	J	412	VAL	3.0
1	A	57	GLY	3.0
1	G	41	PRO	3.0
1	I	309	LEU	2.9
1	H	208	VAL	2.9
1	J	69	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	206	ALA	2.9
1	J	466	TRP	2.9
1	I	306	LEU	2.9
1	I	322	ALA	2.9
1	J	103	GLY	2.9
1	H	62	VAL	2.8
1	J	179	THR	2.8
1	I	585	TYR	2.8
1	J	208	VAL	2.8
1	J	53	ALA	2.8
1	J	54	LEU	2.8
1	J	111	ILE	2.8
1	J	422	VAL	2.8
1	I	511	MET	2.8
1	J	274	GLY	2.8
1	I	512	PRO	2.8
1	J	437	ALA	2.7
1	B	59	GLY	2.7
1	E	60	ASP	2.7
1	I	330	ALA	2.7
1	J	275	LEU	2.7
1	E	403	ASN	2.7
1	J	277	ALA	2.7
1	G	340	CYS	2.7
1	J	178	GLY	2.6
1	A	56	ASP	2.6
1	J	453	TRP	2.6
1	J	113	PHE	2.6
1	J	182	PHE	2.6
1	I	600	ALA	2.6
1	J	105	ASP	2.6
1	J	203	ALA	2.6
1	G	62	VAL	2.6
1	J	169	ALA	2.6
1	I	347	ASP	2.6
1	I	215	ALA	2.6
1	J	68	THR	2.6
1	B	60	ASP	2.5
1	F	60	ASP	2.5
1	G	56	ASP	2.5
1	F	58	ASN	2.5
1	J	403	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	180	VAL	2.5
1	J	242	TYR	2.5
1	J	424	PHE	2.5
1	D	403	ASN	2.5
1	J	163	ASP	2.5
1	J	173	ASN	2.5
1	F	333	ALA	2.5
1	J	64	PRO	2.5
1	I	599	CYS	2.4
1	A	58	ASN	2.4
1	J	190	LEU	2.4
1	J	282	LEU	2.4
1	H	368	ALA	2.4
1	J	97	ALA	2.4
1	J	96	GLY	2.4
1	J	212	TYR	2.4
1	I	557	ILE	2.4
1	H	215	ALA	2.4
1	J	215	ALA	2.4
1	H	603	PRO	2.4
1	J	108	PRO	2.4
1	J	62	VAL	2.4
1	J	106	GLY	2.4
1	J	109	TYR	2.4
1	I	603	PRO	2.4
1	J	474	LEU	2.3
1	J	415	PHE	2.3
1	J	102	THR	2.3
1	I	272	ALA	2.3
1	J	98	ILE	2.3
1	J	330	ALA	2.3
1	J	447	ILE	2.3
1	B	602	PRO	2.3
1	D	341	VAL	2.3
1	I	320	CYS	2.3
1	J	75	TRP	2.3
1	I	507	LEU	2.3
1	J	345	THR	2.3
1	I	602	PRO	2.3
1	J	233	MET	2.3
1	J	404	SER	2.3
1	J	200	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	49	ALA	2.3
1	J	417	ALA	2.3
1	C	59	GLY	2.3
1	H	59	GLY	2.3
1	I	329	ALA	2.2
1	J	457	GLY	2.2
1	G	58	ASN	2.2
1	I	584	ARG	2.2
1	J	426	THR	2.2
1	I	474	LEU	2.2
1	I	336	GLN	2.2
1	J	551	GLY	2.2
1	C	333	ALA	2.2
1	F	330	ALA	2.2
1	J	514	ALA	2.2
1	I	597	PHE	2.2
1	I	348	CYS	2.2
1	G	59	GLY	2.2
1	H	56	ASP	2.2
1	J	405	SER	2.2
1	I	310	ALA	2.2
1	I	333	ALA	2.2
1	I	346	ALA	2.2
1	I	380	ALA	2.2
1	J	406	ALA	2.2
1	J	61	MET	2.2
1	J	70	VAL	2.2
1	I	303	CYS	2.2
1	J	599	CYS	2.2
1	I	294	LEU	2.2
1	J	482	GLY	2.2
1	I	571	ALA	2.2
1	J	343	ALA	2.2
1	J	121	TRP	2.1
1	B	56	ASP	2.1
1	G	60	ASP	2.1
1	H	341	VAL	2.1
1	G	602	PRO	2.1
1	J	241	HIS	2.1
1	I	454	ALA	2.1
1	J	73	ALA	2.1
1	J	125	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	340	CYS	2.1
1	I	300	LEU	2.1
1	J	115	LEU	2.1
1	I	476	ALA	2.1
1	J	438	ALA	2.1
1	I	313	ILE	2.1
1	I	472	THR	2.1
1	H	481	GLY	2.1
1	C	403	ASN	2.1
1	J	137	LEU	2.1
1	J	577	CYS	2.1
1	I	601	ALA	2.1
1	J	67	ALA	2.1
1	I	593	THR	2.0
1	A	387	GLY	2.0
1	I	516	GLY	2.0
1	E	43	VAL	2.0
1	H	69	VAL	2.0
1	J	602	PRO	2.0
1	H	46	ALA	2.0
1	J	60	ASP	2.0
1	J	202	GLN	2.0
1	J	72	VAL	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	I	801	1/1	0.94	0.08	47,47,47,47	0
2	CA	B	801	1/1	0.97	0.22	51,51,51,51	0
2	CA	J	801	1/1	0.98	0.05	44,44,44,44	0
2	CA	D	801	1/1	0.99	0.04	20,20,20,20	0
2	CA	E	801	1/1	0.99	0.01	21,21,21,21	0
2	CA	F	801	1/1	0.99	0.03	23,23,23,23	0
2	CA	G	801	1/1	0.99	0.02	25,25,25,25	0
2	CA	H	801	1/1	0.99	0.03	26,26,26,26	0
2	CA	A	801	1/1	0.99	0.03	21,21,21,21	0
2	CA	C	801	1/1	0.99	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.