



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 AM UTC

PDB ID : 2BS9 / pdb_00002bs9
Title : Native crystal structure of a GH39 beta-xylosidase XynB1 from *Geobacillus stearothermophilus*
Authors : Czjzek, M.; Bravman, T.; Henrissat, B.; Shoham, Y.
Deposited on : 2005-05-19
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

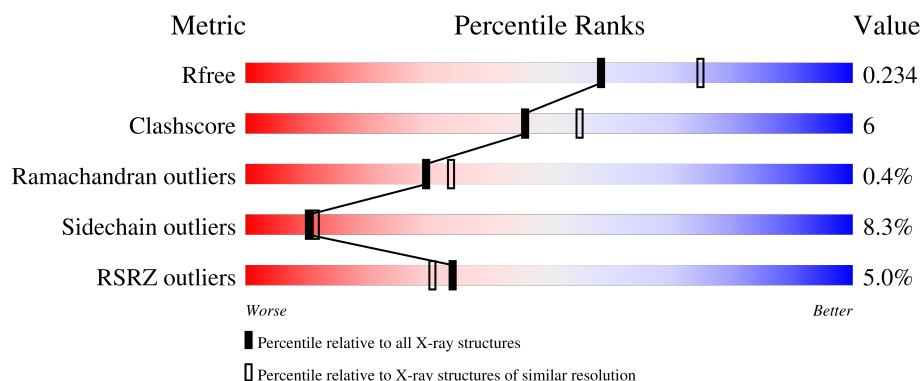
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	503	5% 83% 15% .
1	B	503	6% 82% 14% .
1	C	503	6% 82% 16% .
1	D	503	7% 79% 17% .
1	E	503	4% 84% 13% .

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Mol	Chain	Length	Quality of chain
1	F	503	4% 81% 16%
1	G	503	5% 83% 14%
1	H	503	5% 83% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34099 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 BETA-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	B	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	C	501	Total	C	N	O	S	0	0	0
			4088	2642	693	742	11			
1	D	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	E	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	F	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	G	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	H	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	LYS	conflict	UNP Q9ZFM2
A	?	-	LEU	deletion	UNP Q9ZFM2
A	?	-	GLU	deletion	UNP Q9ZFM2
A	406	GLU	PHE	conflict	UNP Q9ZFM2
A	445	ARG	PRO	conflict	UNP Q9ZFM2
A	446	GLN	-	insertion	UNP Q9ZFM2
A	447	VAL	SER	conflict	UNP Q9ZFM2
B	2	GLY	LYS	conflict	UNP Q9ZFM2
B	?	-	LEU	deletion	UNP Q9ZFM2
B	?	-	GLU	deletion	UNP Q9ZFM2
B	406	GLU	PHE	conflict	UNP Q9ZFM2
B	445	ARG	PRO	conflict	UNP Q9ZFM2
B	446	GLN	-	insertion	UNP Q9ZFM2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	447	VAL	SER	conflict	UNP Q9ZFM2
C	2	GLY	LYS	conflict	UNP Q9ZFM2
C	?	-	LEU	deletion	UNP Q9ZFM2
C	?	-	GLU	deletion	UNP Q9ZFM2
C	406	GLU	PHE	conflict	UNP Q9ZFM2
C	445	ARG	PRO	conflict	UNP Q9ZFM2
C	446	GLN	-	insertion	UNP Q9ZFM2
C	447	VAL	SER	conflict	UNP Q9ZFM2
D	2	GLY	LYS	conflict	UNP Q9ZFM2
D	?	-	LEU	deletion	UNP Q9ZFM2
D	?	-	GLU	deletion	UNP Q9ZFM2
D	406	GLU	PHE	conflict	UNP Q9ZFM2
D	445	ARG	PRO	conflict	UNP Q9ZFM2
D	446	GLN	-	insertion	UNP Q9ZFM2
D	447	VAL	SER	conflict	UNP Q9ZFM2
E	2	GLY	LYS	conflict	UNP Q9ZFM2
E	?	-	LEU	deletion	UNP Q9ZFM2
E	?	-	GLU	deletion	UNP Q9ZFM2
E	406	GLU	PHE	conflict	UNP Q9ZFM2
E	445	ARG	PRO	conflict	UNP Q9ZFM2
E	446	GLN	-	insertion	UNP Q9ZFM2
E	447	VAL	SER	conflict	UNP Q9ZFM2
F	2	GLY	LYS	conflict	UNP Q9ZFM2
F	?	-	LEU	deletion	UNP Q9ZFM2
F	?	-	GLU	deletion	UNP Q9ZFM2
F	406	GLU	PHE	conflict	UNP Q9ZFM2
F	445	ARG	PRO	conflict	UNP Q9ZFM2
F	446	GLN	-	insertion	UNP Q9ZFM2
F	447	VAL	SER	conflict	UNP Q9ZFM2
G	2	GLY	LYS	conflict	UNP Q9ZFM2
G	?	-	LEU	deletion	UNP Q9ZFM2
G	?	-	GLU	deletion	UNP Q9ZFM2
G	406	GLU	PHE	conflict	UNP Q9ZFM2
G	445	ARG	PRO	conflict	UNP Q9ZFM2
G	446	GLN	-	insertion	UNP Q9ZFM2
G	447	VAL	SER	conflict	UNP Q9ZFM2
H	2	GLY	LYS	conflict	UNP Q9ZFM2
H	?	-	LEU	deletion	UNP Q9ZFM2
H	?	-	GLU	deletion	UNP Q9ZFM2
H	406	GLU	PHE	conflict	UNP Q9ZFM2
H	445	ARG	PRO	conflict	UNP Q9ZFM2
H	446	GLN	-	insertion	UNP Q9ZFM2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	447	VAL	SER	conflict	UNP Q9ZFM2

- 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	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
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

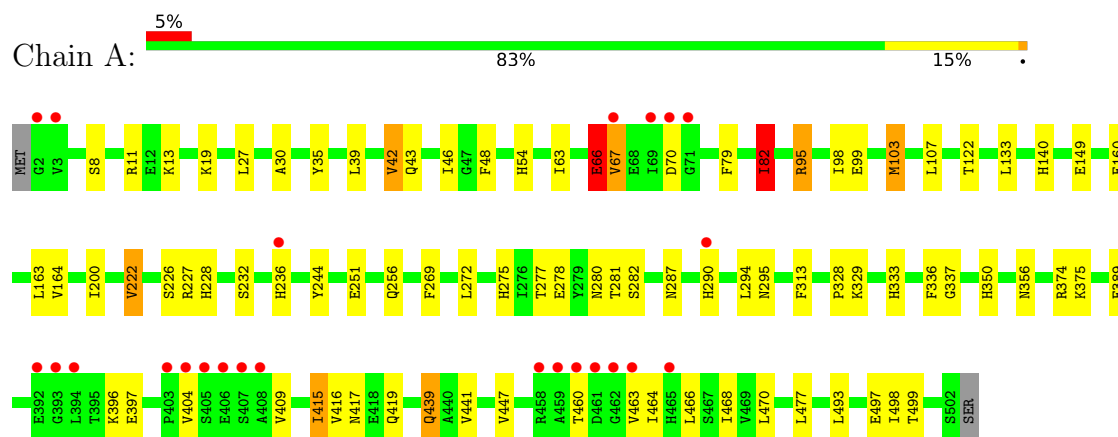
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	170	Total O 170 170	0	0
3	B	161	Total O 161 161	0	0
3	C	177	Total O 177 177	0	0
3	D	172	Total O 172 172	0	0
3	E	180	Total O 180 180	0	0
3	F	140	Total O 140 140	0	0
3	G	179	Total O 179 179	0	0
3	H	188	Total O 188 188	0	0

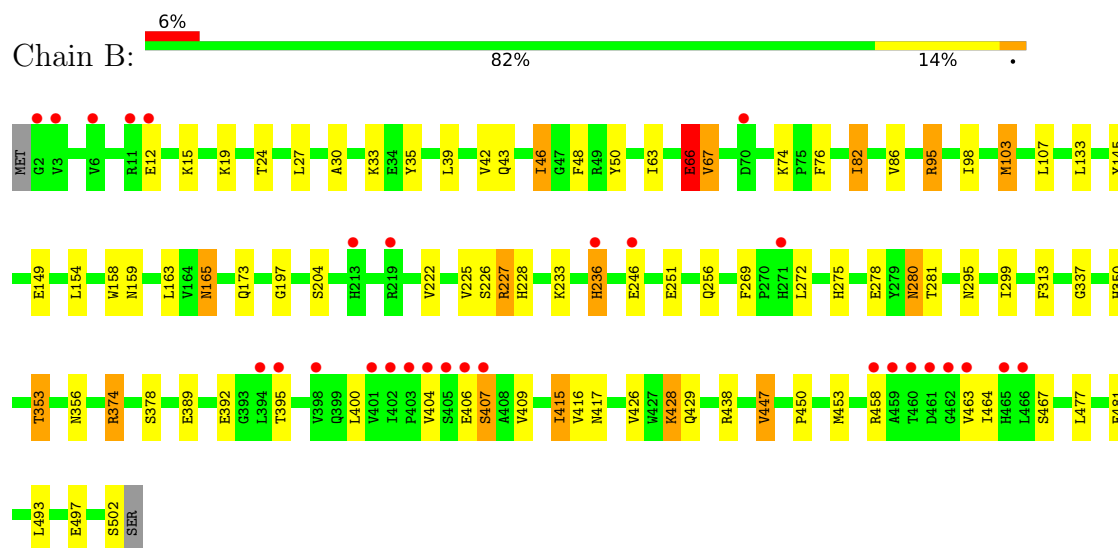
3 Residue-property plots [i](#)

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.

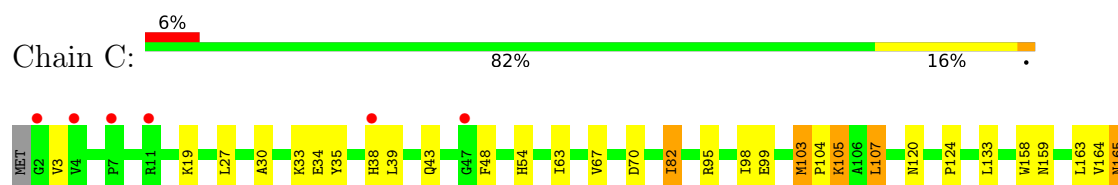
• Molecule 1: BETA-XYLOSIDASE

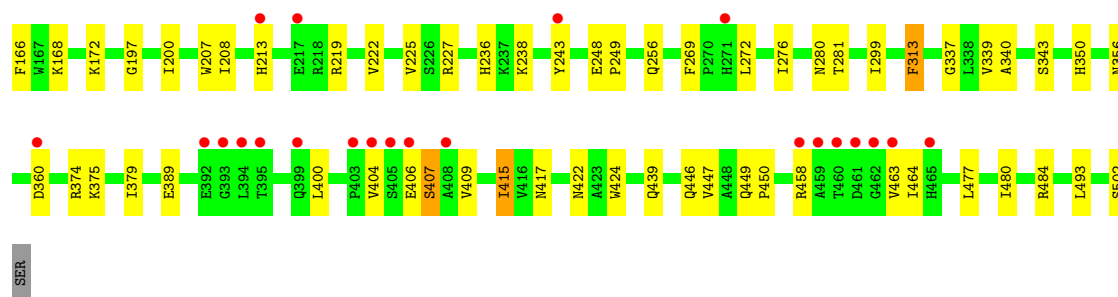


• Molecule 1: BETA-XYLOSIDASE

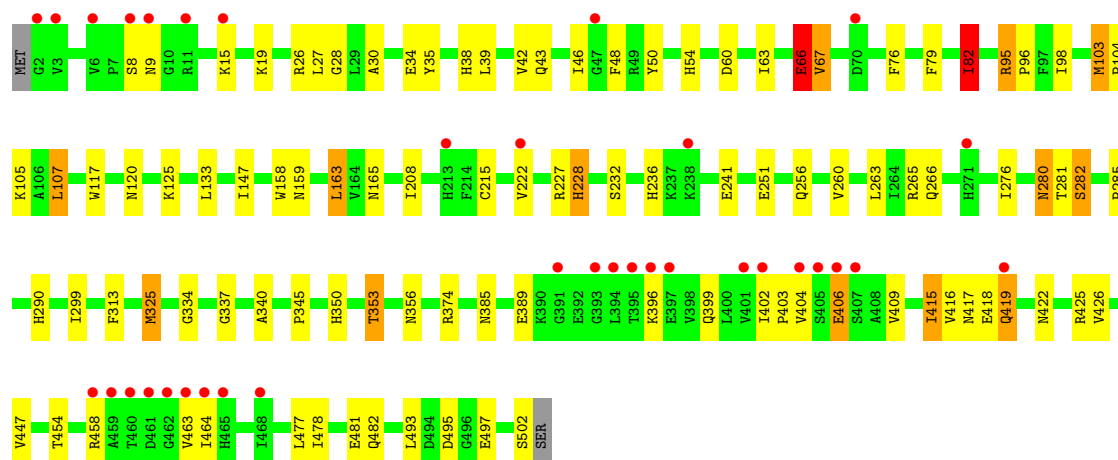
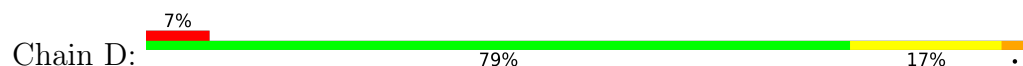


• Molecule 1: BETA-XYLOSIDASE

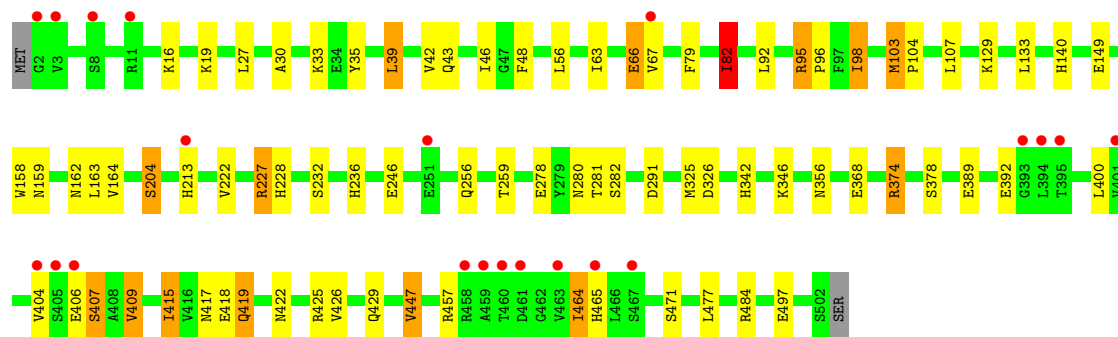
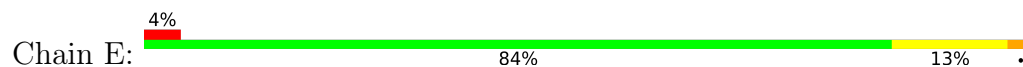




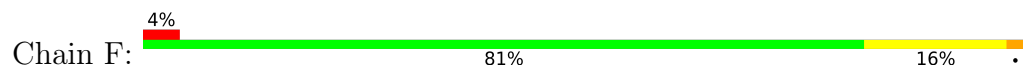
• Molecule 1: BETA-XYLOSIDASE

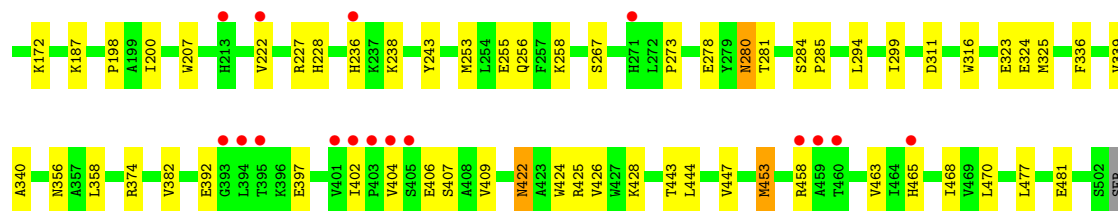


• Molecule 1: BETA-XYLOSIDASE

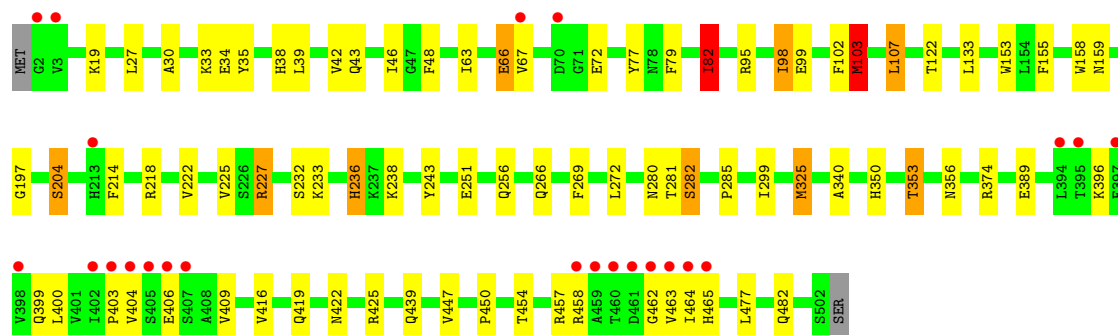
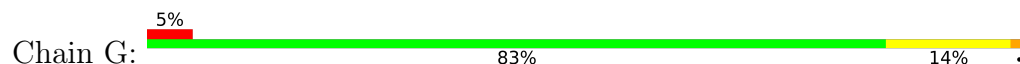


• Molecule 1: BETA-XYLOSIDASE

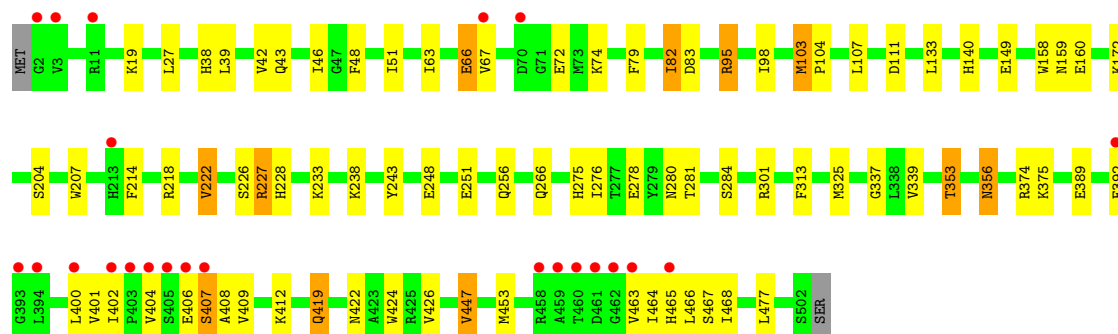
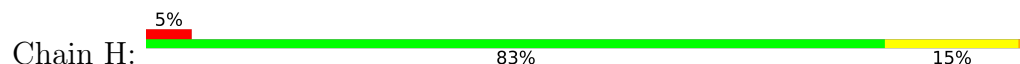




● Molecule 1: BETA-XYLOSIDASE



● Molecule 1: BETA-XYLOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.67Å 165.74Å 311.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.20) 98.0 (50.00-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.259 (Not available) , 0.234	Depositor DCC
R_{free} test set	13754 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34099	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 23.07 % 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 5.0212e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.77	1/4206 (0.0%)	0.93	7/5710 (0.1%)
1	B	0.75	1/4206 (0.0%)	0.93	5/5710 (0.1%)
1	C	0.76	1/4203 (0.0%)	0.91	1/5706 (0.0%)
1	D	0.77	2/4206 (0.0%)	0.93	5/5710 (0.1%)
1	E	0.77	2/4206 (0.0%)	0.93	3/5710 (0.1%)
1	F	0.71	2/4206 (0.0%)	0.93	3/5710 (0.1%)
1	G	0.76	1/4206 (0.0%)	0.93	5/5710 (0.1%)
1	H	0.78	1/4206 (0.0%)	0.95	4/5710 (0.1%)
All	All	0.76	11/33645 (0.0%)	0.93	33/45676 (0.1%)

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	E	0	1
1	H	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	103	MET	SD-CE	-14.71	1.42	1.79
1	E	103	MET	SD-CE	-12.32	1.48	1.79
1	G	103	MET	SD-CE	-12.25	1.49	1.79
1	B	103	MET	SD-CE	-8.49	1.58	1.79
1	D	103	MET	SD-CE	-8.00	1.59	1.79
1	C	103	MET	SD-CE	-7.89	1.59	1.79
1	F	103	MET	SD-CE	-7.55	1.60	1.79
1	A	103	MET	SD-CE	-7.42	1.61	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	453	MET	SD-CE	6.10	1.94	1.79
1	E	325	MET	SD-CE	5.87	1.94	1.79
1	D	147	ILE	CA-CB	5.65	1.61	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	GLU	CA-C-N	8.46	136.93	121.70
1	G	66	GLU	C-N-CA	8.46	136.93	121.70
1	B	46	ILE	N-CA-C	-8.10	96.37	108.85
1	H	66	GLU	CA-C-N	7.87	135.86	121.70
1	H	66	GLU	C-N-CA	7.87	135.86	121.70
1	D	337	GLY	N-CA-C	7.63	120.70	111.93
1	D	66	GLU	CA-C-N	7.61	135.40	121.70
1	D	66	GLU	C-N-CA	7.61	135.40	121.70
1	F	66	GLU	CA-C-N	7.51	135.22	121.70
1	F	66	GLU	C-N-CA	7.51	135.22	121.70
1	B	66	GLU	CA-C-N	7.44	135.09	121.70
1	B	66	GLU	C-N-CA	7.44	135.09	121.70
1	A	66	GLU	CA-C-N	6.98	134.26	121.70
1	A	66	GLU	C-N-CA	6.98	134.26	121.70
1	H	337	GLY	N-CA-C	6.55	119.46	111.93
1	E	82	ILE	CB-CA-C	-5.98	102.57	112.26
1	G	66	GLU	O-C-N	-5.70	116.32	123.27
1	A	337	GLY	N-CA-C	5.69	118.02	111.36
1	C	337	GLY	N-CA-C	5.66	117.98	111.36
1	A	222	VAL	CB-CA-C	-5.62	101.84	110.50
1	D	82	ILE	CB-CA-C	-5.60	103.18	112.26
1	G	82	ILE	CB-CA-C	-5.58	103.23	112.26
1	B	337	GLY	N-CA-C	5.55	118.32	111.93
1	E	66	GLU	CA-C-N	5.50	131.88	121.97
1	E	66	GLU	C-N-CA	5.50	131.88	121.97
1	A	66	GLU	N-CA-C	-5.48	100.73	109.23
1	F	66	GLU	O-C-N	-5.36	117.05	123.27
1	A	66	GLU	O-C-N	-5.31	117.11	123.27
1	D	241	GLU	N-CA-CB	-5.20	103.67	110.59
1	G	82	ILE	N-CA-CB	5.11	120.02	110.77
1	B	407	SER	N-CA-C	5.11	121.67	110.80
1	A	82	ILE	CB-CA-C	-5.07	104.04	112.26
1	H	222	VAL	CB-CA-C	-5.03	102.75	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	66	GLU	Peptide
1	H	66	GLU	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	4091	0	4001	46	0
1	B	4091	0	4001	47	0
1	C	4088	0	3999	47	0
1	D	4091	0	4001	57	0
1	E	4091	0	4001	42	0
1	F	4091	0	4001	50	0
1	G	4091	0	4001	39	0
1	H	4091	0	4001	54	0
2	A	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
3	A	170	0	0	4	0
3	B	161	0	0	2	0
3	C	177	0	0	3	0
3	D	172	0	0	5	0
3	E	180	0	0	5	0
3	F	140	0	0	2	0
3	G	179	0	0	4	0
3	H	188	0	0	8	0
All	All	34099	0	32006	372	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 6.

All (372) 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:227:ARG:HH12	1:D:256:GLN:HE21	1.12	0.93
1:F:426:VAL:HG21	1:F:447:VAL:HG11	1.51	0.91
1:B:227:ARG:HH12	1:B:256:GLN:HE21	1.09	0.91
1:B:42:VAL:O	1:B:46:ILE:O	1.89	0.90
1:D:280:ASN:HD22	1:D:281:THR:H	1.19	0.88
1:C:280:ASN:HD22	1:C:281:THR:H	1.18	0.87
1:A:227:ARG:HH12	1:A:256:GLN:HE21	1.16	0.87
1:E:103:MET:SD	3:E:2062:HOH:O	2.31	0.86
1:C:227:ARG:HH12	1:C:256:GLN:HE21	1.25	0.85
1:H:280:ASN:HD22	1:H:281:THR:H	1.23	0.85
1:H:19:LYS:NZ	1:H:356:ASN:HD21	1.73	0.84
1:G:227:ARG:HH12	1:G:256:GLN:HE21	1.26	0.84
1:F:103:MET:HE1	1:F:107:LEU:HB3	1.57	0.83
1:F:19:LYS:NZ	1:F:356:ASN:HD21	1.78	0.81
1:D:426:VAL:HG21	1:D:447:VAL:HG11	1.61	0.81
1:B:502:SER:C	3:B:2160:HOH:O	2.23	0.80
1:D:353:THR:HG21	3:D:2131:HOH:O	1.81	0.80
1:H:19:LYS:HZ2	1:H:356:ASN:HD21	1.24	0.80
1:G:465:HIS:HB2	3:G:2161:HOH:O	1.81	0.80
1:H:233:LYS:NZ	1:H:248:GLU:OE2	2.15	0.79
1:H:426:VAL:HG21	1:H:447:VAL:HG11	1.65	0.79
1:G:353:THR:HG21	3:G:2125:HOH:O	1.83	0.78
1:B:103:MET:HE1	1:B:107:LEU:HB3	1.64	0.78
1:E:280:ASN:HD22	1:E:281:THR:H	1.28	0.78
1:E:227:ARG:HH12	1:E:256:GLN:HE21	1.28	0.78
1:G:280:ASN:HD22	1:G:281:THR:H	1.30	0.78
1:H:227:ARG:HH12	1:H:256:GLN:HE21	1.29	0.78
1:H:227:ARG:HH12	1:H:256:GLN:NE2	1.82	0.77
1:B:280:ASN:HD22	1:B:281:THR:H	1.31	0.76
1:E:422:ASN:ND2	3:E:2148:HOH:O	2.19	0.75
1:D:227:ARG:NH1	1:D:256:GLN:HE21	1.83	0.75
1:F:103:MET:HG3	1:F:122:THR:O	1.87	0.75
1:H:111:ASP:HB2	3:H:2064:HOH:O	1.87	0.74
1:A:287:ASN:O	1:A:290:HIS:HD2	1.69	0.74
1:F:280:ASN:HD22	1:F:281:THR:H	1.37	0.73
1:B:227:ARG:HH12	1:B:256:GLN:NE2	1.85	0.72
1:D:215:CYS:SG	1:D:222:VAL:HG21	2.30	0.72
1:A:280:ASN:HD22	1:A:281:THR:H	1.35	0.72
1:B:236:HIS:NE2	1:D:497:GLU:OE1	2.20	0.72
1:E:406:GLU:O	1:E:407:SER:HB3	1.90	0.72
1:B:228:HIS:CE1	1:B:278:GLU:CD	2.68	0.71
1:C:422:ASN:C	1:C:422:ASN:HD22	1.98	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:GLN:HG2	3:E:2147:HOH:O	1.90	0.71
1:A:227:ARG:HH12	1:A:256:GLN:NE2	1.89	0.70
1:A:287:ASN:O	1:A:290:HIS:CD2	2.44	0.70
1:F:19:LYS:HZ3	1:F:356:ASN:HD21	1.37	0.70
1:C:34:GLU:O	1:C:38:HIS:HD2	1.74	0.70
1:D:38:HIS:HE1	1:D:340:ALA:O	1.75	0.70
1:F:38:HIS:HE1	1:F:340:ALA:O	1.75	0.69
1:B:103:MET:CE	1:B:107:LEU:HB3	2.22	0.69
1:B:227:ARG:NH1	1:B:256:GLN:HE21	1.89	0.69
1:G:103:MET:HE1	1:G:107:LEU:HB3	1.75	0.69
1:F:34:GLU:O	1:F:38:HIS:HD2	1.77	0.68
1:A:290:HIS:CG	3:A:2109:HOH:O	2.45	0.68
1:C:54:HIS:ND1	1:C:99:GLU:OE2	2.24	0.68
1:A:63:ILE:HD11	1:A:82:ILE:HG12	1.75	0.67
1:A:439:GLN:H	1:A:439:GLN:HE21	1.42	0.67
1:G:42:VAL:O	1:G:46:ILE:O	2.12	0.67
1:F:227:ARG:NH1	1:F:256:GLN:HE21	1.93	0.67
1:H:280:ASN:ND2	1:H:281:THR:H	1.93	0.66
1:A:103:MET:HG3	1:A:122:THR:O	1.95	0.66
1:H:103:MET:HE3	1:H:107:LEU:HB2	1.77	0.66
1:B:353:THR:HG21	3:B:2120:HOH:O	1.95	0.66
1:B:43:GLN:HE22	1:B:48:PHE:H	1.44	0.66
1:F:34:GLU:O	1:F:38:HIS:CD2	2.49	0.65
1:C:280:ASN:HD22	1:C:281:THR:N	1.92	0.65
1:E:103:MET:CE	1:E:107:LEU:HB3	2.26	0.65
1:H:19:LYS:NZ	1:H:356:ASN:ND2	2.44	0.65
1:H:95:ARG:NH2	3:H:2056:HOH:O	2.29	0.65
1:D:502:SER:C	3:D:2171:HOH:O	2.39	0.65
1:E:429:GLN:NE2	1:G:454:THR:OG1	2.25	0.64
1:H:419:GLN:HG2	3:H:2151:HOH:O	1.97	0.64
1:F:227:ARG:HH12	1:F:256:GLN:HE21	1.46	0.64
1:H:280:ASN:HD22	1:H:281:THR:N	1.96	0.63
1:E:497:GLU:OE1	1:G:236:HIS:NE2	2.30	0.63
1:A:328:PRO:HG3	1:A:333:HIS:CE1	2.33	0.63
1:A:497:GLU:OE1	1:C:236:HIS:HE1	1.82	0.63
1:G:280:ASN:ND2	1:G:281:THR:H	1.97	0.63
1:E:63:ILE:HD11	1:E:82:ILE:HG12	1.80	0.62
1:E:426:VAL:HG21	1:E:447:VAL:HG11	1.81	0.62
1:H:19:LYS:HZ2	1:H:356:ASN:ND2	1.95	0.62
1:D:103:MET:CE	1:D:107:LEU:HB3	2.30	0.62
1:H:422:ASN:C	1:H:422:ASN:HD22	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:MET:HE2	1:E:107:LEU:HB3	1.81	0.61
1:H:43:GLN:HE22	1:H:48:PHE:H	1.48	0.61
1:E:236:HIS:HD2	3:E:2089:HOH:O	1.83	0.61
1:G:350:HIS:ND1	1:G:450:PRO:HG3	2.16	0.61
1:D:422:ASN:ND2	3:D:2144:HOH:O	2.34	0.61
1:H:63:ILE:HD11	1:H:82:ILE:HG12	1.82	0.60
1:H:103:MET:CE	1:H:107:LEU:HB2	2.31	0.60
1:H:158:TRP:CD1	1:H:159:ASN:H	2.20	0.60
1:A:54:HIS:HD2	1:A:99:GLU:OE2	1.84	0.59
1:B:95:ARG:HD3	1:B:149:GLU:OE2	2.02	0.59
1:D:103:MET:HE3	1:D:104:PRO:HD2	1.83	0.59
1:D:426:VAL:CG2	1:D:447:VAL:HG11	2.32	0.59
1:B:19:LYS:NZ	1:B:356:ASN:HD21	2.01	0.59
1:B:63:ILE:HD11	1:B:82:ILE:HG12	1.84	0.59
1:G:63:ILE:HD11	1:G:82:ILE:HG12	1.83	0.59
1:C:34:GLU:O	1:C:38:HIS:CD2	2.54	0.58
1:A:290:HIS:ND1	1:A:336:PHE:HA	2.18	0.58
1:H:140:HIS:HE1	3:H:2048:HOH:O	1.87	0.58
1:A:42:VAL:O	1:A:46:ILE:O	2.21	0.58
1:C:38:HIS:HE1	1:C:340:ALA:O	1.86	0.58
1:D:43:GLN:HE22	1:D:48:PHE:H	1.52	0.58
1:C:63:ILE:HD11	1:C:82:ILE:HG12	1.86	0.58
1:C:158:TRP:CD1	1:C:159:ASN:H	2.22	0.58
1:D:105:LYS:NZ	1:D:120:ASN:HD22	2.01	0.58
1:G:34:GLU:O	1:G:38:HIS:HD2	1.86	0.57
1:H:227:ARG:NH1	1:H:256:GLN:HE21	2.01	0.57
1:H:406:GLU:O	1:H:408:ALA:N	2.37	0.56
1:A:95:ARG:HD3	1:A:149:GLU:OE2	2.05	0.56
1:B:426:VAL:HG21	1:B:447:VAL:HG21	1.86	0.56
1:D:158:TRP:CD1	1:D:159:ASN:H	2.24	0.56
1:F:19:LYS:NZ	1:F:356:ASN:ND2	2.51	0.56
1:D:63:ILE:HD11	1:D:82:ILE:HG12	1.88	0.56
1:G:422:ASN:ND2	3:G:2139:HOH:O	2.38	0.56
1:G:19:LYS:NZ	1:G:356:ASN:HD21	2.03	0.56
1:A:160:GLU:OE2	1:A:228:HIS:HD2	1.89	0.56
1:B:66:GLU:HA	1:B:67:VAL:HB	1.88	0.56
1:D:34:GLU:O	1:D:38:HIS:HD2	1.89	0.56
1:D:280:ASN:HD22	1:D:281:THR:N	1.97	0.56
1:C:38:HIS:CE1	1:C:339:VAL:HG12	2.41	0.56
1:D:419:GLN:HB3	3:D:2142:HOH:O	2.05	0.55
1:F:422:ASN:C	1:F:422:ASN:HD22	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:LYS:HZ3	1:F:356:ASN:ND2	2.04	0.55
1:H:228:HIS:CE1	1:H:278:GLU:HG3	2.41	0.55
1:D:493:LEU:C	1:D:493:LEU:HD23	2.32	0.55
1:H:42:VAL:O	1:H:46:ILE:O	2.25	0.55
1:F:468:ILE:HG22	1:F:470:LEU:HD12	1.89	0.55
1:H:160:GLU:HG2	1:H:228:HIS:HD2	1.71	0.54
1:F:228:HIS:CE1	1:F:278:GLU:HG3	2.43	0.54
1:A:280:ASN:ND2	1:A:281:THR:H	2.05	0.54
1:D:227:ARG:HH12	1:D:256:GLN:NE2	1.94	0.54
1:G:34:GLU:O	1:G:38:HIS:CD2	2.61	0.54
1:G:43:GLN:HE22	1:G:48:PHE:H	1.55	0.54
1:F:106:ALA:O	1:F:125:LYS:NZ	2.40	0.54
1:E:42:VAL:O	1:E:46:ILE:O	2.24	0.54
1:B:228:HIS:HE1	1:B:278:GLU:OE2	1.91	0.54
1:D:345:PRO:HB2	1:D:350:HIS:CE1	2.43	0.54
1:B:228:HIS:CE1	1:B:278:GLU:OE2	2.61	0.53
1:B:493:LEU:HD23	1:B:493:LEU:C	2.33	0.53
1:E:232:SER:HB3	1:E:282:SER:HA	1.91	0.53
1:G:285:PRO:HG2	1:G:325:MET:HG3	1.89	0.53
1:H:228:HIS:CE1	1:H:278:GLU:CD	2.87	0.53
1:C:38:HIS:ND1	1:C:339:VAL:CG1	2.72	0.53
1:B:350:HIS:CE1	1:B:450:PRO:HD3	2.43	0.53
1:C:238:LYS:HE2	1:C:243:TYR:CZ	2.44	0.53
1:D:34:GLU:O	1:D:38:HIS:CD2	2.61	0.53
1:A:43:GLN:HE22	1:A:48:PHE:H	1.57	0.53
1:C:269:PHE:HB3	1:C:272:LEU:HG	1.91	0.53
1:B:228:HIS:ND1	1:B:278:GLU:CD	2.67	0.52
1:C:406:GLU:O	1:C:407:SER:CB	2.56	0.52
1:D:263:LEU:HA	1:D:266:GLN:HE21	1.75	0.52
1:E:43:GLN:HE22	1:E:48:PHE:H	1.55	0.52
1:G:19:LYS:HZ3	1:G:356:ASN:HD21	1.58	0.52
1:H:426:VAL:CG2	1:H:447:VAL:HG11	2.37	0.52
1:G:227:ARG:HH12	1:G:256:GLN:NE2	2.02	0.52
1:H:79:PHE:CD2	1:H:140:HIS:CD2	2.97	0.52
1:H:301:ARG:HB2	3:H:2112:HOH:O	2.09	0.52
1:D:285:PRO:HG2	1:D:325:MET:HG3	1.92	0.52
1:F:172:LYS:HA	1:F:207:TRP:CH2	2.45	0.52
1:G:38:HIS:HE1	1:G:340:ALA:O	1.92	0.52
1:G:269:PHE:HB3	1:G:272:LEU:HG	1.92	0.51
1:B:33:LYS:HG3	1:C:33:LYS:HG3	1.92	0.51
1:A:66:GLU:HA	1:A:67:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASN:HD22	1:B:281:THR:N	2.03	0.50
1:H:158:TRP:CG	1:H:159:ASN:H	2.29	0.50
1:A:228:HIS:CE1	1:A:278:GLU:HG3	2.46	0.50
1:G:280:ASN:HD22	1:G:281:THR:N	2.03	0.50
1:B:228:HIS:CE1	1:B:278:GLU:CG	2.95	0.50
1:E:422:ASN:HD22	1:E:422:ASN:C	2.19	0.50
1:E:415:ILE:HD11	1:E:417:ASN:ND2	2.26	0.50
1:H:238:LYS:HE2	1:H:243:TYR:CZ	2.47	0.50
1:D:215:CYS:SG	1:D:222:VAL:CG2	2.98	0.50
1:D:415:ILE:CD1	1:D:417:ASN:ND2	2.75	0.50
1:A:200:ILE:HD12	3:A:2084:HOH:O	2.12	0.49
1:F:19:LYS:HZ2	1:F:356:ASN:HD21	1.55	0.49
1:G:98:ILE:HD13	1:G:155:PHE:CE2	2.46	0.49
1:E:280:ASN:HD22	1:E:281:THR:N	2.04	0.49
1:E:374:ARG:HD3	1:E:378:SER:OG	2.11	0.49
1:G:79:PHE:HA	1:G:82:ILE:HD11	1.94	0.49
1:H:227:ARG:O	1:H:276:ILE:HA	2.12	0.49
1:C:19:LYS:NZ	1:C:356:ASN:HD21	2.10	0.49
1:C:280:ASN:ND2	1:C:281:THR:H	1.99	0.49
1:D:26:ARG:HD3	1:D:117:TRP:CD2	2.48	0.49
1:D:30:ALA:HA	1:D:35:TYR:CG	2.48	0.49
1:D:30:ALA:HA	1:D:35:TYR:CD2	2.47	0.49
1:A:350:HIS:CG	1:A:416:VAL:HG11	2.48	0.49
1:D:79:PHE:HD2	1:D:82:ILE:HD11	1.78	0.49
1:B:158:TRP:CD1	1:B:159:ASN:H	2.30	0.49
1:B:350:HIS:HE1	1:B:450:PRO:HD3	1.77	0.49
1:F:30:ALA:HA	1:F:35:TYR:CD2	2.48	0.49
1:D:227:ARG:O	1:D:276:ILE:HA	2.13	0.49
1:C:197:GLY:O	1:C:225:VAL:HA	2.13	0.48
1:A:329:LYS:HB3	1:D:76:PHE:CZ	2.48	0.48
1:B:374:ARG:HD3	1:B:378:SER:OG	2.13	0.48
1:D:96:PRO:HB2	1:D:98:ILE:HG13	1.94	0.48
1:D:208:ILE:HD13	1:D:260:VAL:HG13	1.94	0.48
1:B:43:GLN:HE22	1:B:48:PHE:N	2.08	0.48
1:C:43:GLN:HE22	1:C:48:PHE:HB2	1.79	0.48
1:H:79:PHE:CG	1:H:140:HIS:CD2	3.01	0.48
1:G:98:ILE:HD11	1:G:153:TRP:CE3	2.48	0.48
1:B:226:SER:HA	1:B:275:HIS:O	2.14	0.48
1:F:406:GLU:O	1:F:407:SER:HB3	2.12	0.48
1:B:19:LYS:HZ3	1:B:356:ASN:HD21	1.61	0.48
1:C:38:HIS:CE1	1:C:343:SER:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:TRP:CD1	1:F:159:ASN:H	2.31	0.48
1:G:103:MET:HG3	1:G:122:THR:O	2.13	0.48
1:H:79:PHE:HD2	1:H:82:ILE:HD11	1.79	0.48
1:H:103:MET:HE3	1:H:104:PRO:HD2	1.96	0.48
1:E:228:HIS:CE1	1:E:278:GLU:CD	2.92	0.48
1:E:19:LYS:NZ	1:E:356:ASN:HD21	2.12	0.47
1:E:158:TRP:CD1	1:E:159:ASN:H	2.32	0.47
1:G:419:GLN:HG2	3:G:2137:HOH:O	2.12	0.47
1:H:103:MET:CE	1:H:107:LEU:CB	2.92	0.47
1:C:103:MET:HE3	1:C:104:PRO:HD2	1.97	0.47
1:C:406:GLU:O	1:C:407:SER:HB3	2.14	0.47
1:F:422:ASN:ND2	1:F:425:ARG:H	2.12	0.47
1:B:95:ARG:CD	1:B:149:GLU:OE2	2.61	0.47
1:C:422:ASN:HD21	1:C:424:TRP:HB3	1.80	0.47
1:E:39:LEU:HD12	1:E:92:LEU:HD12	1.96	0.47
1:E:418:GLU:O	1:E:425:ARG:HD2	2.15	0.47
1:G:158:TRP:CD1	1:G:159:ASN:H	2.33	0.47
1:H:228:HIS:CE1	1:H:278:GLU:CG	2.97	0.47
1:C:493:LEU:C	1:C:493:LEU:HD23	2.40	0.47
1:G:238:LYS:HE2	1:G:243:TYR:CZ	2.50	0.47
1:A:280:ASN:HD22	1:A:281:THR:N	2.10	0.47
1:C:165:ASN:HB2	3:C:2080:HOH:O	2.15	0.47
1:C:415:ILE:CD1	1:C:417:ASN:ND2	2.78	0.47
1:D:38:HIS:CE1	1:D:340:ALA:O	2.61	0.47
1:D:232:SER:HB3	1:D:282:SER:HA	1.96	0.47
1:E:107:LEU:HD21	1:E:129:LYS:HB3	1.97	0.47
1:F:426:VAL:CG2	1:F:447:VAL:HG11	2.35	0.47
1:A:281:THR:OG1	1:A:295:ASN:ND2	2.47	0.46
1:C:158:TRP:CG	1:C:159:ASN:H	2.33	0.46
1:F:316:TRP:O	1:F:336:PHE:HB3	2.14	0.46
1:A:95:ARG:CD	1:A:149:GLU:OE2	2.63	0.46
1:G:406:GLU:HG2	1:G:482:GLN:HE21	1.81	0.46
1:C:407:SER:O	1:C:458:ARG:HG2	2.15	0.46
1:A:290:HIS:HE1	1:A:336:PHE:CD2	2.34	0.46
1:A:328:PRO:HB3	1:A:333:HIS:CE1	2.50	0.46
1:E:30:ALA:HA	1:E:35:TYR:CD2	2.50	0.46
1:C:30:ALA:HA	1:C:35:TYR:CD2	2.51	0.46
1:B:228:HIS:CE1	1:B:278:GLU:HG3	2.51	0.46
1:E:228:HIS:CE1	1:E:278:GLU:OE2	2.69	0.46
1:C:38:HIS:CE1	1:C:343:SER:HA	2.51	0.45
1:F:30:ALA:HA	1:F:35:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:GLU:HA	1:F:67:VAL:HB	1.98	0.45
1:F:165:ASN:H	1:F:165:ASN:HD22	1.63	0.45
1:F:38:HIS:CE1	1:F:339:VAL:HG12	2.52	0.45
1:F:253:MET:O	1:F:256:GLN:HB2	2.16	0.45
1:A:30:ALA:HA	1:A:35:TYR:CD2	2.52	0.45
1:D:103:MET:HE3	1:D:107:LEU:HB3	1.97	0.45
1:G:197:GLY:O	1:G:225:VAL:HA	2.16	0.45
1:H:422:ASN:HD21	1:H:424:TRP:HB3	1.80	0.45
1:E:16:LYS:HD3	3:E:2007:HOH:O	2.17	0.45
1:F:43:GLN:HE22	1:F:48:PHE:H	1.64	0.45
1:A:269:PHE:HB3	1:A:272:LEU:HG	1.99	0.45
1:B:415:ILE:CD1	1:B:417:ASN:ND2	2.80	0.45
1:B:428:LYS:HE3	1:D:495:ASP:OD2	2.16	0.45
1:D:158:TRP:CG	1:D:159:ASN:H	2.34	0.45
1:F:54:HIS:HD2	3:F:2089:HOH:O	2.00	0.45
1:F:228:HIS:ND1	1:F:278:GLU:HB2	2.32	0.45
1:H:172:LYS:HA	1:H:207:TRP:CH2	2.52	0.45
1:B:30:ALA:HA	1:B:35:TYR:CG	2.52	0.45
1:C:236:HIS:HD2	3:C:2088:HOH:O	2.00	0.45
1:E:409:VAL:HG11	1:E:464:ILE:HD13	1.99	0.45
1:E:415:ILE:CD1	1:E:417:ASN:ND2	2.80	0.45
1:C:63:ILE:HD11	1:C:82:ILE:CG1	2.47	0.44
1:F:358:LEU:HD21	1:F:382:VAL:HG23	1.99	0.44
1:G:79:PHE:HD2	1:G:82:ILE:HD11	1.81	0.44
1:A:30:ALA:HA	1:A:35:TYR:CG	2.52	0.44
1:C:350:HIS:CE1	1:C:450:PRO:HD3	2.53	0.44
1:D:66:GLU:HA	1:D:67:VAL:HB	1.99	0.44
1:A:19:LYS:NZ	1:A:356:ASN:HD21	2.16	0.44
1:A:290:HIS:CD2	1:A:290:HIS:H	2.36	0.44
1:B:86:VAL:HB	1:B:145:TYR:OH	2.17	0.44
1:C:103:MET:CE	1:C:107:LEU:HB3	2.47	0.44
1:C:163:LEU:HD23	1:C:166:PHE:CD1	2.53	0.44
1:C:276:ILE:HB	1:C:313:PHE:HA	2.00	0.43
1:H:83:ASP:OD1	1:H:140:HIS:NE2	2.36	0.43
1:F:443:THR:HG23	1:H:412:LYS:HE3	2.00	0.43
1:H:19:LYS:HZ3	1:H:356:ASN:ND2	2.16	0.43
1:A:103:MET:HE1	1:A:107:LEU:CB	2.48	0.43
1:B:415:ILE:HD11	1:B:417:ASN:ND2	2.33	0.43
1:G:19:LYS:NZ	1:G:356:ASN:ND2	2.65	0.43
1:B:497:GLU:OE1	1:D:236:HIS:HE1	2.01	0.43
1:C:172:LYS:HA	1:C:207:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:MET:HE3	1:E:104:PRO:HD2	1.99	0.43
1:F:285:PRO:CG	1:F:325:MET:HG3	2.49	0.43
1:A:236:HIS:CE1	1:A:244:TYR:HB3	2.54	0.43
1:E:43:GLN:HE22	1:E:48:PHE:N	2.16	0.43
1:F:28:GLY:HA3	1:F:60:ASP:OD2	2.18	0.43
1:B:269:PHE:HB3	1:B:272:LEU:HG	2.00	0.43
1:D:418:GLU:C	1:D:419:GLN:NE2	2.77	0.43
1:E:96:PRO:HB2	1:E:98:ILE:HG13	2.01	0.43
1:A:232:SER:HB3	1:A:282:SER:HA	2.01	0.42
1:D:163:LEU:HD22	1:D:165:ASN:HD22	1.83	0.42
1:F:273:PRO:HA	1:F:311:ASP:OD2	2.19	0.42
1:D:19:LYS:NZ	1:D:356:ASN:HD21	2.16	0.42
1:F:51:ILE:O	1:F:51:ILE:HG23	2.19	0.42
1:A:350:HIS:CD2	1:A:416:VAL:HG11	2.54	0.42
1:B:50:TYR:HA	1:B:95:ARG:O	2.20	0.42
1:H:422:ASN:C	1:H:422:ASN:ND2	2.76	0.42
1:B:163:LEU:HD22	1:B:165:ASN:ND2	2.35	0.42
1:H:400:LEU:HD23	1:H:402:ILE:HD11	2.02	0.42
1:E:140:HIS:HE1	3:H:2154:HOH:O	2.02	0.42
1:F:444:LEU:HD23	1:F:444:LEU:HA	1.92	0.42
1:D:28:GLY:HA3	1:D:60:ASP:OD2	2.19	0.42
1:D:50:TYR:HA	1:D:95:ARG:O	2.19	0.42
1:E:79:PHE:CG	1:E:140:HIS:CD2	3.07	0.42
1:E:426:VAL:CG2	1:E:447:VAL:HG11	2.48	0.42
1:F:163:LEU:HD22	1:F:165:ASN:HD22	1.85	0.42
1:A:468:ILE:HG22	1:A:470:LEU:HD23	2.02	0.42
1:B:281:THR:OG1	1:B:295:ASN:ND2	2.52	0.42
1:C:200:ILE:HD11	1:C:208:ILE:CD1	2.50	0.42
1:E:162:ASN:HD22	1:E:204:SER:HB3	1.84	0.42
1:F:79:PHE:HD2	1:F:82:ILE:HD11	1.85	0.42
1:G:232:SER:HB3	1:G:282:SER:HA	2.01	0.42
1:C:227:ARG:NH1	1:C:256:GLN:HE21	2.05	0.42
1:C:379:ILE:HB	1:C:480:ILE:HB	2.01	0.42
1:E:426:VAL:HG21	1:E:447:VAL:HG21	2.01	0.42
1:F:198:PRO:HG2	1:F:200:ILE:HG12	2.02	0.42
1:F:323:GLU:O	1:F:324:GLU:C	2.62	0.42
1:F:447:VAL:CG1	3:F:2109:HOH:O	2.67	0.42
1:G:30:ALA:HA	1:G:35:TYR:CG	2.55	0.42
1:H:401:VAL:HG22	1:H:465:HIS:CE1	2.54	0.42
1:A:415:ILE:CD1	1:A:417:ASN:ND2	2.83	0.41
1:D:425:ARG:NE	3:D:2145:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:LYS:HG2	1:F:243:TYR:CD2	2.55	0.41
1:F:422:ASN:HD21	1:F:424:TRP:HB3	1.85	0.41
1:G:158:TRP:CG	1:G:159:ASN:H	2.39	0.41
1:H:95:ARG:CD	1:H:149:GLU:OE2	2.68	0.41
1:C:449:GLN:NE2	3:C:2156:HOH:O	2.48	0.41
1:H:38:HIS:CE1	1:H:339:VAL:HG12	2.54	0.41
1:H:228:HIS:ND1	1:H:278:GLU:HB2	2.34	0.41
1:D:227:ARG:HD3	1:D:228:HIS:O	2.20	0.41
1:E:291:ASP:HA	1:E:346:LYS:HD3	2.02	0.41
1:H:214:PHE:CE1	1:H:218:ARG:HD3	2.55	0.41
1:A:236:HIS:HD2	3:A:2090:HOH:O	2.04	0.41
1:C:248:GLU:HB3	1:C:249:PRO:HD2	2.02	0.41
1:F:38:HIS:ND1	1:F:339:VAL:CG1	2.84	0.41
1:B:158:TRP:CG	1:B:159:ASN:H	2.38	0.41
1:D:8:SER:HA	1:D:403:PRO:HG2	2.02	0.41
1:D:290:HIS:HD2	1:D:334:GLY:O	2.04	0.41
1:G:403:PRO:HA	1:G:462:GLY:O	2.21	0.41
1:H:251:GLU:HB2	3:H:2103:HOH:O	2.20	0.41
1:B:67:VAL:HG21	1:B:76:PHE:CB	2.50	0.41
1:C:103:MET:HE1	1:C:124:PRO:HB3	2.02	0.41
1:H:353:THR:HG21	3:H:2140:HOH:O	2.19	0.41
1:D:103:MET:HE1	1:D:107:LEU:HD13	2.02	0.41
1:B:197:GLY:O	1:B:225:VAL:HA	2.21	0.41
1:D:42:VAL:O	1:D:46:ILE:O	2.38	0.41
1:D:385:ASN:HD22	1:D:396:LYS:NZ	2.18	0.41
1:F:280:ASN:HD22	1:F:281:THR:N	2.11	0.41
1:H:226:SER:HA	1:H:275:HIS:O	2.21	0.41
1:C:38:HIS:ND1	1:C:339:VAL:HG12	2.34	0.41
1:G:214:PHE:CE1	1:G:218:ARG:HD3	2.56	0.41
1:F:187:LYS:HA	1:F:187:LYS:HD3	1.94	0.41
1:B:429:GLN:NE2	1:D:454:THR:OG1	2.48	0.40
1:G:63:ILE:O	1:G:77:TYR:HA	2.21	0.40
1:A:290:HIS:CE1	3:A:2109:HOH:O	2.75	0.40
1:A:493:LEU:C	1:A:493:LEU:HD23	2.46	0.40
1:D:406:GLU:OE1	1:D:482:GLN:HB2	2.21	0.40
1:A:79:PHE:CD1	1:A:140:HIS:ND1	2.90	0.40
1:A:226:SER:HA	1:A:275:HIS:O	2.22	0.40
1:E:30:ALA:HA	1:E:35:TYR:CG	2.57	0.40
1:E:95:ARG:HD2	1:E:149:GLU:OE2	2.22	0.40
1:A:43:GLN:HE22	1:A:48:PHE:N	2.18	0.40
1:A:498:ILE:O	1:A:499:THR:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LYS:NZ	1:C:120:ASN:HD22	2.19	0.40
1:H:160:GLU:CG	1:H:228:HIS:CD2	3.05	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	499/503 (99%)	473 (95%)	24 (5%)	2 (0%)	30	34
1	B	499/503 (99%)	476 (95%)	21 (4%)	2 (0%)	30	34
1	C	499/503 (99%)	477 (96%)	21 (4%)	1 (0%)	43	51
1	D	499/503 (99%)	474 (95%)	23 (5%)	2 (0%)	30	34
1	E	499/503 (99%)	476 (95%)	19 (4%)	4 (1%)	16	16
1	F	499/503 (99%)	476 (95%)	22 (4%)	1 (0%)	43	51
1	G	499/503 (99%)	476 (95%)	20 (4%)	3 (1%)	21	23
1	H	499/503 (99%)	473 (95%)	24 (5%)	2 (0%)	30	34
All	All	3992/4024 (99%)	3801 (95%)	174 (4%)	17 (0%)	30	34

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	B	407	SER
1	D	67	VAL
1	E	67	VAL
1	E	407	SER
1	F	67	VAL
1	G	67	VAL
1	H	67	VAL

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Mol	Chain	Res	Type
1	H	407	SER
1	B	67	VAL
1	C	407	SER
1	A	70	ASP
1	D	406	GLU
1	E	326	ASP
1	G	204	SER
1	E	204	SER
1	G	102	PHE

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	440/442 (100%)	405 (92%)	35 (8%)	11	13
1	B	440/442 (100%)	395 (90%)	45 (10%)	7	7
1	C	439/442 (99%)	404 (92%)	35 (8%)	11	13
1	D	440/442 (100%)	404 (92%)	36 (8%)	10	12
1	E	440/442 (100%)	408 (93%)	32 (7%)	13	15
1	F	440/442 (100%)	403 (92%)	37 (8%)	10	11
1	G	440/442 (100%)	401 (91%)	39 (9%)	9	10
1	H	440/442 (100%)	406 (92%)	34 (8%)	12	13
All	All	3519/3536 (100%)	3226 (92%)	293 (8%)	10	11

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	11	ARG
1	A	13	LYS
1	A	27	LEU
1	A	39	LEU
1	A	42	VAL

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Mol	Chain	Res	Type
1	A	66	GLU
1	A	82	ILE
1	A	95	ARG
1	A	98	ILE
1	A	133	LEU
1	A	163	LEU
1	A	164	VAL
1	A	222	VAL
1	A	251	GLU
1	A	277	THR
1	A	294	LEU
1	A	313	PHE
1	A	374	ARG
1	A	375	LYS
1	A	389	GLU
1	A	396	LYS
1	A	397	GLU
1	A	404	VAL
1	A	409	VAL
1	A	415	ILE
1	A	419	GLN
1	A	439	GLN
1	A	441	VAL
1	A	447	VAL
1	A	460	THR
1	A	463	VAL
1	A	464	ILE
1	A	466	LEU
1	A	477	LEU
1	B	12	GLU
1	B	15	LYS
1	B	24	THR
1	B	27	LEU
1	B	39	LEU
1	B	66	GLU
1	B	74	LYS
1	B	82	ILE
1	B	95	ARG
1	B	98	ILE
1	B	133	LEU
1	B	154	LEU
1	B	165	ASN

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Mol	Chain	Res	Type
1	B	173	GLN
1	B	204	SER
1	B	222	VAL
1	B	227	ARG
1	B	233	LYS
1	B	236	HIS
1	B	246	GLU
1	B	251	GLU
1	B	280	ASN
1	B	299	ILE
1	B	313	PHE
1	B	353	THR
1	B	374	ARG
1	B	389	GLU
1	B	392	GLU
1	B	395	THR
1	B	400	LEU
1	B	404	VAL
1	B	406	GLU
1	B	409	VAL
1	B	415	ILE
1	B	416	VAL
1	B	428	LYS
1	B	438	ARG
1	B	447	VAL
1	B	453	MET
1	B	458	ARG
1	B	463	VAL
1	B	464	ILE
1	B	467	SER
1	B	477	LEU
1	B	481	GLU
1	C	3	VAL
1	C	27	LEU
1	C	39	LEU
1	C	67	VAL
1	C	70	ASP
1	C	82	ILE
1	C	95	ARG
1	C	98	ILE
1	C	105	LYS
1	C	107	LEU

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Mol	Chain	Res	Type
1	C	133	LEU
1	C	164	VAL
1	C	165	ASN
1	C	168	LYS
1	C	213	HIS
1	C	219	ARG
1	C	222	VAL
1	C	299	ILE
1	C	313	PHE
1	C	360	ASP
1	C	374	ARG
1	C	375	LYS
1	C	389	GLU
1	C	400	LEU
1	C	404	VAL
1	C	409	VAL
1	C	415	ILE
1	C	439	GLN
1	C	446	GLN
1	C	447	VAL
1	C	463	VAL
1	C	464	ILE
1	C	477	LEU
1	C	484	ARG
1	C	502	SER
1	D	9	ASN
1	D	15	LYS
1	D	27	LEU
1	D	39	LEU
1	D	54	HIS
1	D	66	GLU
1	D	82	ILE
1	D	95	ARG
1	D	107	LEU
1	D	125	LYS
1	D	133	LEU
1	D	163	LEU
1	D	228	HIS
1	D	251	GLU
1	D	265	ARG
1	D	280	ASN
1	D	282	SER

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Mol	Chain	Res	Type
1	D	299	ILE
1	D	313	PHE
1	D	325	MET
1	D	353	THR
1	D	374	ARG
1	D	389	GLU
1	D	399	GLN
1	D	402	ILE
1	D	404	VAL
1	D	409	VAL
1	D	415	ILE
1	D	416	VAL
1	D	419	GLN
1	D	458	ARG
1	D	463	VAL
1	D	464	ILE
1	D	477	LEU
1	D	478	ILE
1	D	481	GLU
1	E	27	LEU
1	E	33	LYS
1	E	39	LEU
1	E	56	LEU
1	E	82	ILE
1	E	95	ARG
1	E	98	ILE
1	E	133	LEU
1	E	163	LEU
1	E	164	VAL
1	E	213	HIS
1	E	222	VAL
1	E	227	ARG
1	E	246	GLU
1	E	259	THR
1	E	342	HIS
1	E	368	GLU
1	E	374	ARG
1	E	389	GLU
1	E	392	GLU
1	E	400	LEU
1	E	404	VAL
1	E	409	VAL

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Mol	Chain	Res	Type
1	E	415	ILE
1	E	419	GLN
1	E	447	VAL
1	E	457	ARG
1	E	464	ILE
1	E	465	HIS
1	E	471	SER
1	E	477	LEU
1	E	484	ARG
1	F	3	VAL
1	F	8	SER
1	F	24	THR
1	F	39	LEU
1	F	82	ILE
1	F	95	ARG
1	F	98	ILE
1	F	107	LEU
1	F	125	LYS
1	F	133	LEU
1	F	163	LEU
1	F	164	VAL
1	F	165	ASN
1	F	168	LYS
1	F	222	VAL
1	F	236	HIS
1	F	255	GLU
1	F	258	LYS
1	F	267	SER
1	F	280	ASN
1	F	284	SER
1	F	294	LEU
1	F	299	ILE
1	F	374	ARG
1	F	392	GLU
1	F	397	GLU
1	F	402	ILE
1	F	404	VAL
1	F	409	VAL
1	F	422	ASN
1	F	428	LYS
1	F	453	MET
1	F	458	ARG

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Mol	Chain	Res	Type
1	F	463	VAL
1	F	465	HIS
1	F	477	LEU
1	F	481	GLU
1	G	27	LEU
1	G	33	LYS
1	G	39	LEU
1	G	66	GLU
1	G	72	GLU
1	G	82	ILE
1	G	95	ARG
1	G	98	ILE
1	G	99	GLU
1	G	103	MET
1	G	107	LEU
1	G	133	LEU
1	G	204	SER
1	G	222	VAL
1	G	227	ARG
1	G	233	LYS
1	G	236	HIS
1	G	251	GLU
1	G	266	GLN
1	G	282	SER
1	G	299	ILE
1	G	325	MET
1	G	353	THR
1	G	374	ARG
1	G	389	GLU
1	G	396	LYS
1	G	399	GLN
1	G	400	LEU
1	G	404	VAL
1	G	409	VAL
1	G	416	VAL
1	G	425	ARG
1	G	439	GLN
1	G	447	VAL
1	G	457	ARG
1	G	458	ARG
1	G	463	VAL
1	G	464	ILE

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Mol	Chain	Res	Type
1	G	477	LEU
1	H	27	LEU
1	H	39	LEU
1	H	51	ILE
1	H	72	GLU
1	H	74	LYS
1	H	82	ILE
1	H	95	ARG
1	H	98	ILE
1	H	133	LEU
1	H	204	SER
1	H	222	VAL
1	H	227	ARG
1	H	266	GLN
1	H	284	SER
1	H	313	PHE
1	H	325	MET
1	H	353	THR
1	H	356	ASN
1	H	374	ARG
1	H	375	LYS
1	H	389	GLU
1	H	392	GLU
1	H	404	VAL
1	H	407	SER
1	H	409	VAL
1	H	419	GLN
1	H	447	VAL
1	H	453	MET
1	H	463	VAL
1	H	464	ILE
1	H	466	LEU
1	H	467	SER
1	H	468	ILE
1	H	477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	54	HIS
1	A	165	ASN

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Mol	Chain	Res	Type
1	A	228	HIS
1	A	236	HIS
1	A	256	GLN
1	A	280	ASN
1	A	290	HIS
1	A	295	ASN
1	A	333	HIS
1	A	356	ASN
1	A	385	ASN
1	A	414	GLN
1	A	419	GLN
1	A	422	ASN
1	A	429	GLN
1	A	439	GLN
1	A	449	GLN
1	B	5	ASN
1	B	43	GLN
1	B	112	GLN
1	B	165	ASN
1	B	192	HIS
1	B	194	GLN
1	B	256	GLN
1	B	266	GLN
1	B	280	ASN
1	B	295	ASN
1	B	356	ASN
1	B	385	ASN
1	B	422	ASN
1	B	429	GLN
1	B	439	GLN
1	C	38	HIS
1	C	43	GLN
1	C	120	ASN
1	C	165	ASN
1	C	236	HIS
1	C	256	GLN
1	C	280	ASN
1	C	290	HIS
1	C	295	ASN
1	C	356	ASN
1	C	385	ASN
1	C	399	GLN

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Mol	Chain	Res	Type
1	C	422	ASN
1	C	429	GLN
1	C	439	GLN
1	C	446	GLN
1	D	5	ASN
1	D	38	HIS
1	D	43	GLN
1	D	112	GLN
1	D	120	ASN
1	D	165	ASN
1	D	213	HIS
1	D	236	HIS
1	D	256	GLN
1	D	266	GLN
1	D	280	ASN
1	D	356	ASN
1	D	385	ASN
1	D	414	GLN
1	D	419	GLN
1	D	422	ASN
1	D	429	GLN
1	E	43	GLN
1	E	213	HIS
1	E	236	HIS
1	E	256	GLN
1	E	280	ASN
1	E	295	ASN
1	E	356	ASN
1	E	385	ASN
1	E	399	GLN
1	E	422	ASN
1	E	429	GLN
1	F	43	GLN
1	F	54	HIS
1	F	112	GLN
1	F	165	ASN
1	F	213	HIS
1	F	256	GLN
1	F	266	GLN
1	F	280	ASN
1	F	290	HIS
1	F	295	ASN

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Mol	Chain	Res	Type
1	F	356	ASN
1	F	385	ASN
1	F	419	GLN
1	F	422	ASN
1	F	429	GLN
1	F	456	GLN
1	G	43	GLN
1	G	54	HIS
1	G	165	ASN
1	G	256	GLN
1	G	266	GLN
1	G	280	ASN
1	G	290	HIS
1	G	356	ASN
1	G	385	ASN
1	G	422	ASN
1	G	429	GLN
1	G	439	GLN
1	H	5	ASN
1	H	43	GLN
1	H	165	ASN
1	H	228	HIS
1	H	256	GLN
1	H	266	GLN
1	H	280	ASN
1	H	290	HIS
1	H	295	ASN
1	H	356	ASN
1	H	385	ASN
1	H	419	GLN
1	H	422	ASN
1	H	429	GLN
1	H	451	HIS
1	H	482	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	501/503 (99%)	0.26	24 (4%)	35	32	10, 16, 39, 45	0
1	B	501/503 (99%)	0.26	29 (5%)	29	25	7, 16, 40, 46	0
1	C	501/503 (99%)	0.30	28 (5%)	30	27	8, 16, 39, 44	0
1	D	501/503 (99%)	0.37	35 (6%)	22	19	11, 17, 39, 45	0
1	E	501/503 (99%)	0.18	21 (4%)	40	37	8, 16, 38, 44	0
1	F	501/503 (99%)	0.36	18 (3%)	46	43	9, 16, 39, 44	0
1	G	501/503 (99%)	0.21	23 (4%)	37	34	10, 16, 38, 45	0
1	H	501/503 (99%)	0.18	23 (4%)	37	34	8, 16, 38, 45	0
All	All	4008/4024 (99%)	0.26	201 (5%)	34	31	7, 16, 40, 46	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	405	SER	5.9
1	F	404	VAL	5.7
1	A	404	VAL	5.2
1	E	405	SER	5.2
1	F	405	SER	5.1
1	D	2	GLY	5.1
1	B	404	VAL	5.0
1	H	2	GLY	4.8
1	D	405	SER	4.7
1	D	459	ALA	4.7
1	H	404	VAL	4.6
1	B	465	HIS	4.6
1	G	462	GLY	4.6
1	B	271	HIS	4.5
1	G	404	VAL	4.4
1	A	405	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	406	GLU	4.3
1	A	465	HIS	4.3
1	C	2	GLY	4.3
1	E	461	ASP	4.2
1	G	2	GLY	4.2
1	E	458	ARG	4.1
1	D	404	VAL	4.1
1	D	460	THR	4.1
1	F	465	HIS	4.1
1	A	2	GLY	4.0
1	E	460	THR	4.0
1	D	463	VAL	3.9
1	A	461	ASP	3.9
1	G	465	HIS	3.9
1	C	403	PRO	3.9
1	B	405	SER	3.9
1	B	3	VAL	3.8
1	C	459	ALA	3.8
1	E	11	ARG	3.8
1	C	462	GLY	3.8
1	C	460	THR	3.8
1	E	465	HIS	3.8
1	D	465	HIS	3.7
1	F	3	VAL	3.7
1	D	406	GLU	3.6
1	C	213	HIS	3.6
1	C	404	VAL	3.6
1	E	459	ALA	3.6
1	F	393	GLY	3.5
1	A	70	ASP	3.5
1	F	213	HIS	3.5
1	G	459	ALA	3.5
1	B	213	HIS	3.5
1	D	213	HIS	3.5
1	C	463	VAL	3.4
1	H	463	VAL	3.4
1	B	2	GLY	3.4
1	C	395	THR	3.4
1	H	393	GLY	3.4
1	B	460	THR	3.4
1	A	460	THR	3.3
1	B	406	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	393	GLY	3.3
1	B	70	ASP	3.3
1	C	465	HIS	3.3
1	E	2	GLY	3.3
1	H	462	GLY	3.3
1	H	11	ARG	3.3
1	E	8	SER	3.3
1	F	2	GLY	3.3
1	H	213	HIS	3.2
1	A	462	GLY	3.2
1	C	47	GLY	3.2
1	D	461	ASP	3.2
1	B	459	ALA	3.2
1	G	461	ASP	3.1
1	H	394	LEU	3.1
1	H	407	SER	3.1
1	C	461	ASP	3.1
1	A	403	PRO	3.1
1	B	395	THR	3.1
1	F	395	THR	3.0
1	D	464	ILE	3.0
1	E	213	HIS	3.0
1	G	460	THR	3.0
1	A	394	LEU	2.9
1	B	463	VAL	2.9
1	G	463	VAL	2.9
1	D	70	ASP	2.9
1	G	3	VAL	2.9
1	C	393	GLY	2.9
1	H	70	ASP	2.9
1	D	462	GLY	2.8
1	B	6	VAL	2.8
1	E	404	VAL	2.8
1	B	407	SER	2.8
1	F	394	LEU	2.8
1	C	271	HIS	2.8
1	H	460	THR	2.8
1	C	458	ARG	2.8
1	B	236	HIS	2.7
1	H	465	HIS	2.7
1	B	403	PRO	2.7
1	F	460	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	392	GLU	2.7
1	C	406	GLU	2.7
1	B	461	ASP	2.7
1	A	393	GLY	2.7
1	F	401	VAL	2.6
1	H	3	VAL	2.6
1	H	405	SER	2.6
1	D	9	ASN	2.6
1	D	47	GLY	2.6
1	G	405	SER	2.6
1	H	406	GLU	2.6
1	B	458	ARG	2.6
1	D	402	ILE	2.6
1	C	38	HIS	2.6
1	G	394	LEU	2.6
1	C	217	GLU	2.6
1	G	458	ARG	2.6
1	D	419	GLN	2.5
1	A	236	HIS	2.5
1	A	458	ARG	2.5
1	D	8	SER	2.5
1	G	407	SER	2.5
1	B	219	ARG	2.5
1	D	458	ARG	2.5
1	E	406	GLU	2.5
1	F	402	ILE	2.5
1	F	236	HIS	2.5
1	D	6	VAL	2.4
1	D	396	LYS	2.4
1	A	459	ALA	2.4
1	D	395	THR	2.4
1	D	394	LEU	2.4
1	F	403	PRO	2.4
1	G	403	PRO	2.4
1	G	395	THR	2.4
1	D	11	ARG	2.4
1	H	461	ASP	2.4
1	A	71	GLY	2.4
1	E	393	GLY	2.4
1	E	395	THR	2.4
1	G	402	ILE	2.4
1	H	67	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	400	LEU	2.4
1	H	403	PRO	2.3
1	A	407	SER	2.3
1	D	401	VAL	2.3
1	E	67	VAL	2.3
1	G	213	HIS	2.3
1	C	392	GLU	2.3
1	G	406	GLU	2.3
1	E	3	VAL	2.3
1	E	401	VAL	2.3
1	G	70	ASP	2.3
1	D	271	HIS	2.3
1	A	463	VAL	2.3
1	B	466	LEU	2.3
1	C	394	LEU	2.3
1	C	360	ASP	2.3
1	F	458	ARG	2.3
1	B	246	GLU	2.3
1	B	394	LEU	2.2
1	H	459	ALA	2.2
1	D	407	SER	2.2
1	B	402	ILE	2.2
1	E	463	VAL	2.2
1	G	398	VAL	2.2
1	B	12	GLU	2.2
1	E	251	GLU	2.2
1	G	397	GLU	2.2
1	A	69	ILE	2.2
1	A	67	VAL	2.2
1	D	238	LYS	2.2
1	A	3	VAL	2.1
1	C	4	VAL	2.1
1	G	67	VAL	2.1
1	C	7	PRO	2.1
1	D	468	ILE	2.1
1	H	402	ILE	2.1
1	H	392	GLU	2.1
1	B	398	VAL	2.1
1	F	459	ALA	2.1
1	G	464	ILE	2.1
1	F	271	HIS	2.1
1	D	222	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	462	GLY	2.1
1	D	391	GLY	2.1
1	B	11	ARG	2.1
1	D	15	LYS	2.1
1	A	290	HIS	2.1
1	E	394	LEU	2.1
1	C	243	TYR	2.1
1	D	3	VAL	2.1
1	H	458	ARG	2.1
1	E	467	SER	2.0
1	A	408	ALA	2.0
1	C	408	ALA	2.0
1	C	399	GLN	2.0
1	B	401	VAL	2.0
1	C	11	ARG	2.0
1	F	222	VAL	2.0
1	D	397	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	F	1503	1/1	0.96	0.07	29,29,29,29	0
2	CA	E	1503	1/1	0.98	0.06	24,24,24,24	0
2	CA	D	1503	1/1	0.99	0.07	24,24,24,24	0
2	CA	A	1503	1/1	0.99	0.03	23,23,23,23	0
2	CA	C	1503	1/1	0.99	0.04	24,24,24,24	0
2	CA	H	1503	1/1	0.99	0.04	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	G	1503	1/1	1.00	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.