



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:00 PM UTC

PDB ID : 5GQC / pdb_00005gqc
Title : Crystal structure of lacto-N-biosidase LnbX from Bifidobacterium longum subsp. longum, ligand-free form
Authors : Yamada, C.; Arakawa, T.; Katayama, T.; Fushinobu, S.
Deposited on : 2016-08-07
Resolution : 2.36 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

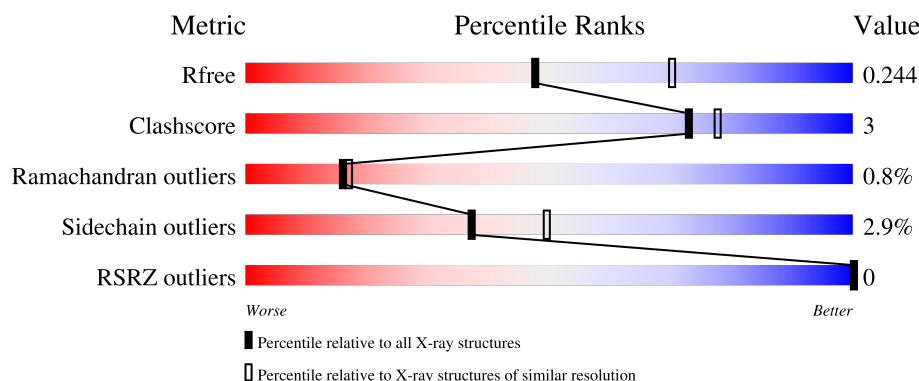
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

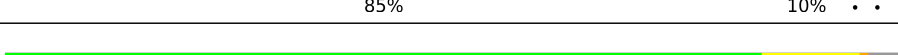
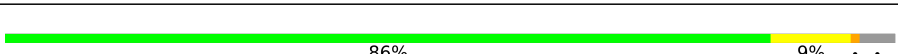
The reported resolution of this entry is 2.36 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	606	 82% 14% .
1	B	606	 85% 10% .
1	C	606	 85% 10% . .
1	D	606	 85% 11% . .
1	E	606	 86% 9% . .

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Mol	Chain	Length	Quality of chain
1	F	606	 86% 9% . .
1	G	606	 83% 12% . .
1	H	606	 86% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36887 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 Lacto-N-biosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4468	2760	772	924	12			
1	B	582	Total	C	N	O	S	0	0	0
			4468	2760	772	924	12			
1	C	582	Total	C	N	O	S	0	0	0
			4468	2760	772	924	12			
1	D	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	E	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	F	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	G	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	H	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP A0A024QYS6
A	626	ALA	-	expression tag	UNP A0A024QYS6
A	627	ALA	-	expression tag	UNP A0A024QYS6
A	628	LEU	-	expression tag	UNP A0A024QYS6
A	629	GLU	-	expression tag	UNP A0A024QYS6
A	630	HIS	-	expression tag	UNP A0A024QYS6
A	631	HIS	-	expression tag	UNP A0A024QYS6
A	632	HIS	-	expression tag	UNP A0A024QYS6
A	633	HIS	-	expression tag	UNP A0A024QYS6
A	634	HIS	-	expression tag	UNP A0A024QYS6
A	635	HIS	-	expression tag	UNP A0A024QYS6
B	30	MET	-	expression tag	UNP A0A024QYS6
B	626	ALA	-	expression tag	UNP A0A024QYS6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	627	ALA	-	expression tag	UNP A0A024QYS6
B	628	LEU	-	expression tag	UNP A0A024QYS6
B	629	GLU	-	expression tag	UNP A0A024QYS6
B	630	HIS	-	expression tag	UNP A0A024QYS6
B	631	HIS	-	expression tag	UNP A0A024QYS6
B	632	HIS	-	expression tag	UNP A0A024QYS6
B	633	HIS	-	expression tag	UNP A0A024QYS6
B	634	HIS	-	expression tag	UNP A0A024QYS6
B	635	HIS	-	expression tag	UNP A0A024QYS6
C	30	MET	-	expression tag	UNP A0A024QYS6
C	626	ALA	-	expression tag	UNP A0A024QYS6
C	627	ALA	-	expression tag	UNP A0A024QYS6
C	628	LEU	-	expression tag	UNP A0A024QYS6
C	629	GLU	-	expression tag	UNP A0A024QYS6
C	630	HIS	-	expression tag	UNP A0A024QYS6
C	631	HIS	-	expression tag	UNP A0A024QYS6
C	632	HIS	-	expression tag	UNP A0A024QYS6
C	633	HIS	-	expression tag	UNP A0A024QYS6
C	634	HIS	-	expression tag	UNP A0A024QYS6
C	635	HIS	-	expression tag	UNP A0A024QYS6
D	30	MET	-	expression tag	UNP A0A024QYS6
D	626	ALA	-	expression tag	UNP A0A024QYS6
D	627	ALA	-	expression tag	UNP A0A024QYS6
D	628	LEU	-	expression tag	UNP A0A024QYS6
D	629	GLU	-	expression tag	UNP A0A024QYS6
D	630	HIS	-	expression tag	UNP A0A024QYS6
D	631	HIS	-	expression tag	UNP A0A024QYS6
D	632	HIS	-	expression tag	UNP A0A024QYS6
D	633	HIS	-	expression tag	UNP A0A024QYS6
D	634	HIS	-	expression tag	UNP A0A024QYS6
D	635	HIS	-	expression tag	UNP A0A024QYS6
E	30	MET	-	expression tag	UNP A0A024QYS6
E	626	ALA	-	expression tag	UNP A0A024QYS6
E	627	ALA	-	expression tag	UNP A0A024QYS6
E	628	LEU	-	expression tag	UNP A0A024QYS6
E	629	GLU	-	expression tag	UNP A0A024QYS6
E	630	HIS	-	expression tag	UNP A0A024QYS6
E	631	HIS	-	expression tag	UNP A0A024QYS6
E	632	HIS	-	expression tag	UNP A0A024QYS6
E	633	HIS	-	expression tag	UNP A0A024QYS6
E	634	HIS	-	expression tag	UNP A0A024QYS6
E	635	HIS	-	expression tag	UNP A0A024QYS6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	MET	-	expression tag	UNP A0A024QYS6
F	626	ALA	-	expression tag	UNP A0A024QYS6
F	627	ALA	-	expression tag	UNP A0A024QYS6
F	628	LEU	-	expression tag	UNP A0A024QYS6
F	629	GLU	-	expression tag	UNP A0A024QYS6
F	630	HIS	-	expression tag	UNP A0A024QYS6
F	631	HIS	-	expression tag	UNP A0A024QYS6
F	632	HIS	-	expression tag	UNP A0A024QYS6
F	633	HIS	-	expression tag	UNP A0A024QYS6
F	634	HIS	-	expression tag	UNP A0A024QYS6
F	635	HIS	-	expression tag	UNP A0A024QYS6
G	30	MET	-	expression tag	UNP A0A024QYS6
G	626	ALA	-	expression tag	UNP A0A024QYS6
G	627	ALA	-	expression tag	UNP A0A024QYS6
G	628	LEU	-	expression tag	UNP A0A024QYS6
G	629	GLU	-	expression tag	UNP A0A024QYS6
G	630	HIS	-	expression tag	UNP A0A024QYS6
G	631	HIS	-	expression tag	UNP A0A024QYS6
G	632	HIS	-	expression tag	UNP A0A024QYS6
G	633	HIS	-	expression tag	UNP A0A024QYS6
G	634	HIS	-	expression tag	UNP A0A024QYS6
G	635	HIS	-	expression tag	UNP A0A024QYS6
H	30	MET	-	expression tag	UNP A0A024QYS6
H	626	ALA	-	expression tag	UNP A0A024QYS6
H	627	ALA	-	expression tag	UNP A0A024QYS6
H	628	LEU	-	expression tag	UNP A0A024QYS6
H	629	GLU	-	expression tag	UNP A0A024QYS6
H	630	HIS	-	expression tag	UNP A0A024QYS6
H	631	HIS	-	expression tag	UNP A0A024QYS6
H	632	HIS	-	expression tag	UNP A0A024QYS6
H	633	HIS	-	expression tag	UNP A0A024QYS6
H	634	HIS	-	expression tag	UNP A0A024QYS6
H	635	HIS	-	expression tag	UNP A0A024QYS6

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0
3	G	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0

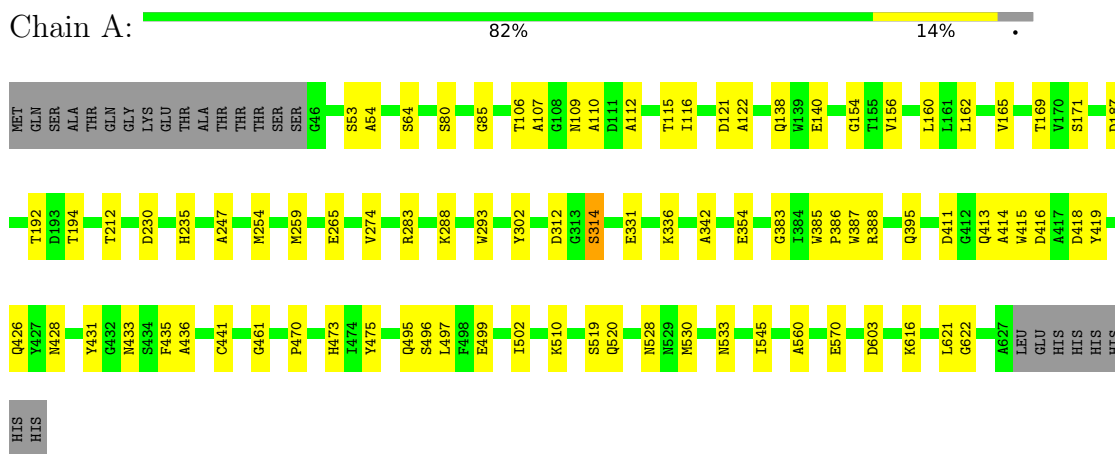
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	118	Total O 118 118	0	0
4	B	138	Total O 138 138	0	0
4	C	126	Total O 126 126	0	0
4	D	144	Total O 144 144	0	0
4	E	159	Total O 159 159	0	0
4	F	150	Total O 150 150	0	0
4	G	121	Total O 121 121	0	0
4	H	142	Total O 142 142	0	0

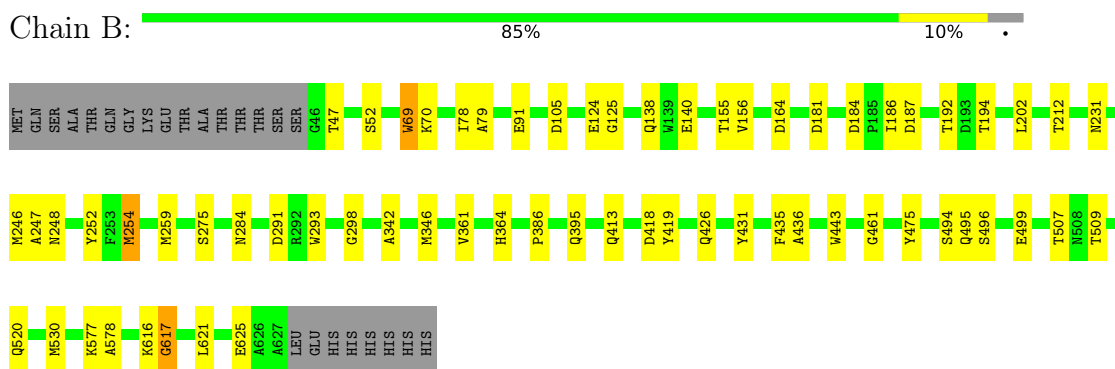
3 Residue-property plots [i](#)

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.

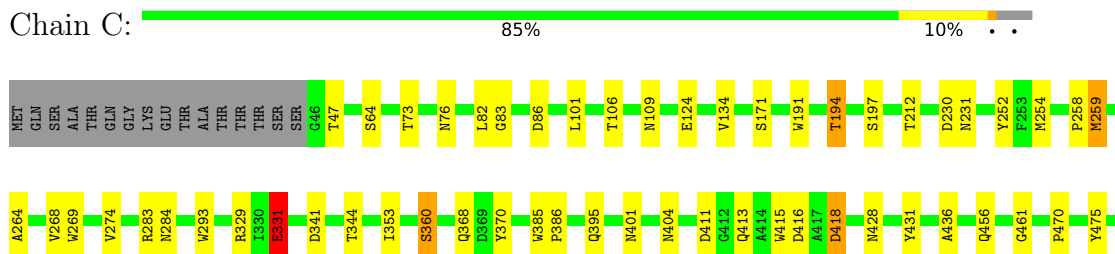
- Molecule 1: Lacto-N-biosidase



- Molecule 1: Lacto-N-biosidase



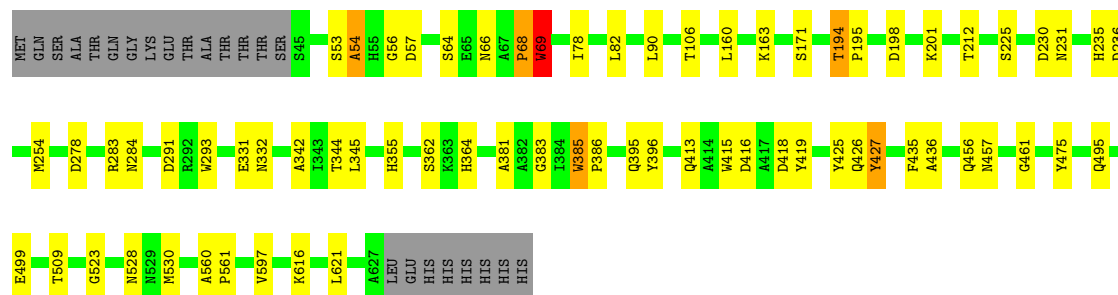
- Molecule 1: Lacto-N-biosidase





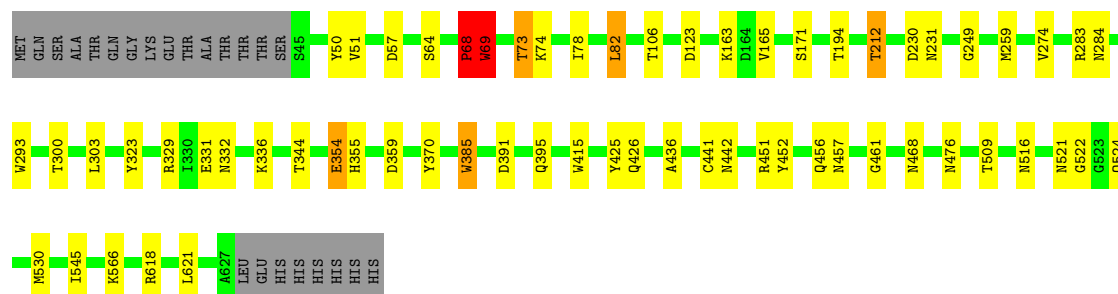
- Molecule 1: Lacto-N-biosidase

Chain D: 85% 11% . .



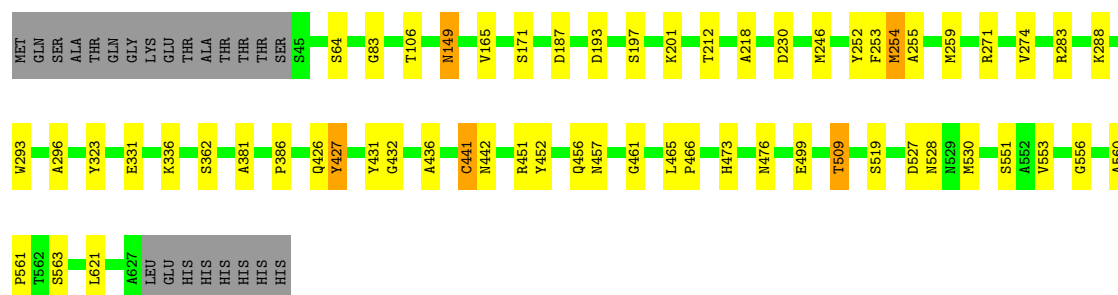
- Molecule 1: Lacto-N-biosidase

Chain E: 86% 9% . .



- Molecule 1: Lacto-N-biosidase

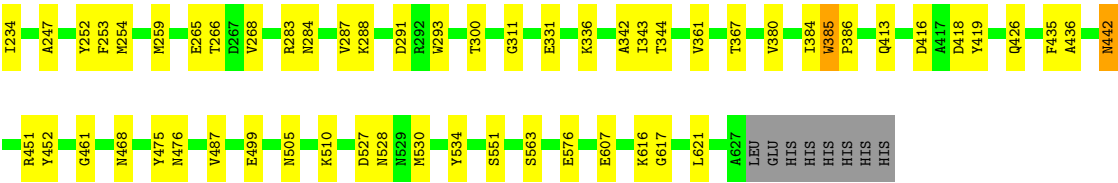
Chain F: 86% 9% . .



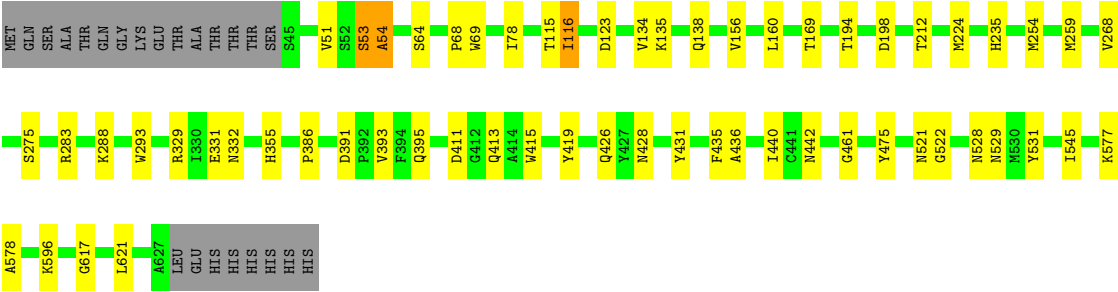
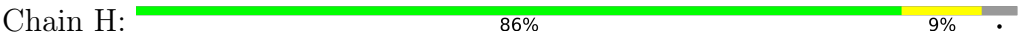
- Molecule 1: Lacto-N-biosidase

Chain G: 83% 12% . .





• Molecule 1: Lacto-N-biosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.32Å 142.72Å 157.01Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	143.39 – 2.36 143.39 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (143.39-2.36) 99.6 (143.39-2.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.182 , 0.240 0.189 , 0.244	Depositor DCC
R_{free} test set	10451 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.337 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36887	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 65.93 % 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 6.5566e-06. 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, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	1/4567 (0.0%)	1.02	6/6224 (0.1%)
1	B	0.95	0/4567	1.01	6/6224 (0.1%)
1	C	1.02	1/4567 (0.0%)	1.06	12/6224 (0.2%)
1	D	1.01	1/4573 (0.0%)	1.03	3/6232 (0.0%)
1	E	1.02	3/4573 (0.1%)	1.03	7/6232 (0.1%)
1	F	0.97	0/4573	1.01	6/6232 (0.1%)
1	G	0.94	0/4573	1.01	6/6232 (0.1%)
1	H	0.97	2/4573 (0.0%)	1.00	3/6232 (0.0%)
All	All	0.98	8/36566 (0.0%)	1.02	49/49832 (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	F	0	1
1	G	0	1
1	H	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	391	ASP	C-O	-8.01	1.20	1.23
1	E	69	TRP	N-CA	6.09	1.54	1.46
1	E	391	ASP	C-O	-6.02	1.20	1.23
1	H	329	ARG	C-O	-5.22	1.18	1.23
1	A	140	GLU	CA-C	5.22	1.59	1.52
1	E	370	TYR	CA-C	5.19	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	TRP	N-CA	5.17	1.52	1.46
1	C	370	TYR	CA-C	5.02	1.59	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	385	TRP	N-CA-C	11.52	118.50	108.13
1	C	385	TRP	N-CA-C	8.94	116.18	108.13
1	G	385	TRP	N-CA-C	7.94	115.28	108.13
1	E	385	TRP	N-CA-C	7.40	114.79	108.13
1	A	107	ALA	N-CA-C	6.87	118.58	108.14
1	C	494	SER	N-CA-C	6.52	116.61	108.19
1	G	68	PRO	N-CA-C	6.27	122.89	114.18
1	H	475	TYR	N-CA-C	6.21	118.85	109.23
1	B	124	GLU	N-CA-C	-6.20	99.90	109.76
1	B	69	TRP	N-CA-C	6.08	120.69	113.16
1	B	186	ILE	N-CA-C	6.06	116.80	110.62
1	E	441	CYS	N-CA-C	6.03	119.59	107.41
1	C	134	VAL	CB-CA-C	-6.02	104.71	111.45
1	G	487	VAL	N-CA-C	6.00	116.18	110.42
1	A	560	ALA	CA-C-N	-5.95	113.84	119.85
1	A	560	ALA	C-N-CA	-5.95	113.84	119.85
1	C	478	THR	N-CA-C	-5.93	98.85	108.52
1	C	124	GLU	N-CA-C	-5.89	103.17	110.41
1	B	79	ALA	N-CA-C	5.83	118.38	111.33
1	A	154	GLY	N-CA-C	5.75	118.54	110.38
1	H	522	GLY	N-CA-C	5.73	126.76	113.18
1	C	331	GLU	N-CA-C	5.69	118.73	109.06
1	F	149	ASN	CB-CA-C	5.66	120.86	112.03
1	D	597	VAL	N-CA-C	-5.61	102.29	109.30
1	F	441	CYS	N-CA-C	5.61	118.18	107.75
1	E	73	THR	CB-CA-C	5.58	121.39	110.67
1	C	274	VAL	N-CA-C	5.58	115.63	107.37
1	C	475	TYR	N-CA-C	5.55	117.62	109.24
1	F	271	ARG	N-CA-C	5.52	119.11	112.38
1	E	395	GLN	N-CA-C	5.30	118.08	109.06
1	A	603	ASP	N-CA-C	5.28	118.99	112.24
1	C	395	GLN	N-CA-C	5.22	117.32	109.23
1	G	154	GLY	N-CA-C	5.19	117.88	110.46
1	F	83	GLY	CA-C-N	-5.19	113.96	119.98
1	F	83	GLY	C-N-CA	-5.19	113.96	119.98
1	B	105	ASP	N-CA-C	5.14	118.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	404	ASN	N-CA-C	5.14	119.50	113.23
1	C	584	ARG	CA-C-N	5.14	125.43	119.93
1	C	584	ARG	C-N-CA	5.14	125.43	119.93
1	B	164	ASP	N-CA-C	5.11	118.67	111.52
1	E	82	LEU	N-CA-C	-5.11	103.66	110.55
1	G	97	ASN	N-CA-C	5.11	117.84	110.28
1	E	68	PRO	N-CA-C	5.10	122.97	112.47
1	G	475	TYR	N-CA-C	5.09	116.98	108.99
1	F	553	VAL	CB-CA-C	-5.05	106.64	111.44
1	A	441	CYS	N-CA-C	5.03	117.11	107.75
1	H	224	MET	N-CA-C	-5.02	100.33	108.52
1	E	354	GLU	N-CA-C	5.01	116.99	109.23
1	D	345	LEU	N-CA-C	-5.01	101.53	109.59

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	521	ASN	Peptide
1	F	197	SER	Peptide
1	G	442	ASN	Peptide
1	H	521	ASN	Peptide

5.2 Too-close contacts [i](#)

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	4468	0	4135	35	0
1	B	4468	0	4135	26	0
1	C	4468	0	4135	32	0
1	D	4474	0	4140	30	0
1	E	4474	0	4140	29	1
1	F	4474	0	4140	28	1
1	G	4474	0	4140	27	0
1	H	4474	0	4140	21	0
2	A	1	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	118	0	0	1	0
4	B	138	0	0	0	0
4	C	126	0	0	1	0
4	D	144	0	0	1	0
4	E	159	0	0	0	0
4	F	150	0	0	1	0
4	G	121	0	0	0	0
4	H	142	0	0	0	0
All	All	36887	0	33105	221	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 3.

All (221) 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:A:115:THR:O	1:A:169:THR:O	2.06	0.73
1:F:253:PHE:C	1:F:254:MET:HG3	2.14	0.72
1:G:252:TYR:HB3	1:G:254:MET:HE1	1.69	0.72
1:C:252:TYR:HB3	1:C:254:MET:HE1	1.74	0.67
1:B:291:ASP:OD1	1:B:364:HIS:ND1	2.25	0.66
1:G:54:ALA:O	1:G:55:HIS:ND1	2.29	0.64
1:E:82:LEU:O	1:E:106:THR:OG1	2.11	0.64
1:A:520:GLN:NE2	4:A:801:HOH:O	2.30	0.64
1:B:52:SER:OG	1:B:91:GLU:OE1	2.16	0.63
1:D:68:PRO:O	1:D:69:TRP:O	2.16	0.63
1:E:436:ALA:HA	1:E:461:GLY:O	1.98	0.63
1:F:442:ASN:ND2	1:F:466:PRO:O	2.32	0.62
1:C:293:TRP:CZ3	1:C:344:THR:HB	2.36	0.60
1:D:291:ASP:OD1	1:D:364:HIS:ND1	2.30	0.60
1:G:288:LYS:HA	1:G:336:LYS:O	2.02	0.60
1:A:187:ASP:HB3	1:E:509:THR:HG23	1.84	0.59
1:B:509:THR:HG22	1:F:187:ASP:HB3	1.84	0.59
1:B:52:SER:O	1:B:70:LYS:HA	2.03	0.59
1:G:342:ALA:HB2	1:G:361:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:HB3	1:F:509:THR:HG23	1.85	0.59
1:D:53:SER:OG	1:D:53:SER:O	2.19	0.59
1:H:115:THR:O	1:H:169:THR:O	2.21	0.58
1:A:106:THR:O	1:A:165:VAL:HA	2.03	0.58
1:A:413:GLN:HG3	1:A:435:PHE:O	2.04	0.58
1:F:441:CYS:SG	4:F:813:HOH:O	2.57	0.58
1:B:342:ALA:HB2	1:B:361:VAL:HG11	1.86	0.57
1:A:312:ASP:OD1	1:A:314:SER:OG	2.21	0.57
1:C:231:ASN:HA	1:C:284:ASN:O	2.05	0.56
1:C:470:PRO:HA	1:C:495:GLN:HG2	1.87	0.56
1:A:470:PRO:HA	1:A:495:GLN:HG2	1.88	0.56
1:E:171:SER:HA	1:E:230:ASP:O	2.06	0.56
1:B:443:TRP:CG	1:C:73:THR:HG23	2.41	0.55
1:G:51:VAL:HA	1:G:68:PRO:O	2.06	0.55
1:E:283:ARG:HA	1:E:331:GLU:O	2.06	0.55
1:F:252:TYR:HA	1:F:296:ALA:O	2.06	0.55
1:C:283:ARG:HA	1:C:331:GLU:O	2.06	0.55
1:C:191:TRP:CH2	1:C:368:GLN:HG3	2.43	0.55
1:E:545:ILE:HD13	1:E:621:LEU:HD11	1.88	0.55
1:F:436:ALA:HA	1:F:461:GLY:O	2.07	0.54
1:G:82:LEU:O	1:G:106:THR:OG1	2.21	0.54
1:G:413:GLN:HG3	1:G:435:PHE:O	2.07	0.54
1:D:530:MET:HB2	1:D:621:LEU:HD13	1.90	0.54
1:G:231:ASN:HA	1:G:284:ASN:O	2.07	0.54
1:E:106:THR:O	1:E:165:VAL:HA	2.07	0.54
1:G:436:ALA:HA	1:G:461:GLY:O	2.07	0.54
1:B:509:THR:CG2	1:F:187:ASP:HB3	2.37	0.53
1:D:283:ARG:HA	1:D:331:GLU:O	2.08	0.53
1:E:329:ARG:NH2	1:E:354:GLU:OE2	2.40	0.53
1:G:216:GLY:O	1:G:253:PHE:HA	2.08	0.53
1:E:331:GLU:HA	1:E:354:GLU:O	2.09	0.53
1:B:252:TYR:CE1	1:B:254:MET:HE3	2.43	0.53
1:H:411:ASP:HB3	1:H:413:GLN:OE1	2.09	0.53
1:E:212:THR:HA	1:E:249:GLY:O	2.10	0.52
1:F:106:THR:O	1:F:165:VAL:HA	2.09	0.52
1:E:530:MET:HB2	1:E:621:LEU:HD13	1.92	0.52
1:F:274:VAL:HG11	1:F:323:TYR:HA	1.91	0.52
1:H:235:HIS:HA	1:H:288:LYS:O	2.09	0.52
1:A:411:ASP:HB3	1:A:413:GLN:OE1	2.10	0.52
1:B:413:GLN:HG3	1:B:435:PHE:O	2.10	0.52
1:H:53:SER:O	1:H:54:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:332:ASN:HA	1:H:355:HIS:O	2.09	0.52
1:D:194:THR:HG22	1:D:195:PRO:HD2	1.91	0.51
1:E:336:LYS:HA	1:E:359:ASP:O	2.10	0.51
1:D:436:ALA:HA	1:D:461:GLY:O	2.10	0.51
1:C:109:ASN:HB2	4:C:855:HOH:O	2.10	0.51
1:H:419:TYR:HE1	1:H:442:ASN:HB2	1.76	0.50
1:A:283:ARG:HA	1:A:331:GLU:O	2.11	0.50
1:G:283:ARG:HA	1:G:331:GLU:O	2.12	0.50
1:A:473:HIS:CD2	1:A:497:LEU:HD23	2.46	0.50
1:A:171:SER:HA	1:A:230:ASP:O	2.12	0.50
1:D:396:TYR:HA	1:D:427:TYR:O	2.12	0.50
1:C:416:ASP:OD2	1:C:418:ASP:OD2	2.29	0.50
1:D:284:ASN:HA	1:D:332:ASN:O	2.12	0.49
1:B:443:TRP:HH2	1:C:76:ASN:HD22	1.59	0.49
1:C:545:ILE:HD13	1:C:621:LEU:HD11	1.94	0.49
1:E:68:PRO:O	1:E:69:TRP:O	2.29	0.49
1:A:530:MET:HB2	1:A:621:LEU:HD13	1.94	0.49
1:C:360:SER:HA	1:C:401:ASN:O	2.13	0.49
1:B:298:GLY:HA3	1:B:346:MET:O	2.12	0.49
1:G:505:ASN:HB2	1:G:534:TYR:CE1	2.48	0.49
1:F:283:ARG:HA	1:F:331:GLU:O	2.12	0.49
1:G:418:ASP:O	1:G:419:TYR:C	2.55	0.49
1:A:395:GLN:HA	1:A:426:GLN:O	2.13	0.48
1:F:530:MET:HB2	1:F:621:LEU:HD13	1.94	0.48
1:B:246:MET:O	1:B:248:ASN:N	2.47	0.48
1:D:225:SER:HA	1:D:278:ASP:O	2.13	0.48
1:A:53:SER:O	1:A:54:ALA:HB3	2.12	0.48
1:C:293:TRP:CZ3	1:C:344:THR:CB	2.96	0.48
1:G:499:GLU:HA	1:G:527:ASP:O	2.13	0.48
1:B:138:GLN:HA	1:B:156:VAL:O	2.13	0.48
1:C:436:ALA:HA	1:C:461:GLY:O	2.13	0.48
1:H:413:GLN:HG3	1:H:435:PHE:O	2.13	0.48
1:A:85:GLY:CA	1:A:112:ALA:HB1	2.43	0.48
1:H:528:ASN:HD22	1:H:596:LYS:HB3	1.79	0.48
1:E:332:ASN:HA	1:E:355:HIS:O	2.14	0.47
1:H:395:GLN:HA	1:H:426:GLN:O	2.14	0.47
1:A:387:TRP:O	1:A:388:ARG:C	2.57	0.47
1:B:436:ALA:HA	1:B:461:GLY:O	2.14	0.47
1:C:411:ASP:HB3	1:C:413:GLN:OE1	2.15	0.47
1:F:432:GLY:HA2	1:F:457:ASN:O	2.15	0.47
1:H:529:ASN:HB2	1:H:531:TYR:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:HB2	1:B:202:LEU:HD21	1.96	0.47
1:C:293:TRP:CZ3	1:C:341:ASP:HB2	2.50	0.47
1:D:386:PRO:HD2	1:D:416:ASP:O	2.15	0.47
1:A:235:HIS:HA	1:A:288:LYS:O	2.15	0.46
1:A:475:TYR:HA	1:A:499:GLU:O	2.15	0.46
1:A:502:ILE:HD12	1:A:622:GLY:HA3	1.97	0.46
1:D:231:ASN:HA	1:D:284:ASN:O	2.15	0.46
1:A:160:LEU:HD11	1:A:162:LEU:HD21	1.97	0.46
1:G:234:ILE:O	1:G:287:VAL:HA	2.14	0.46
1:E:51:VAL:HA	1:E:68:PRO:O	2.16	0.46
1:B:530:MET:HB2	1:B:621:LEU:HD13	1.97	0.46
1:F:452:TYR:HA	1:F:476:ASN:O	2.16	0.46
1:H:436:ALA:HA	1:H:461:GLY:O	2.16	0.46
1:B:231:ASN:HA	1:B:284:ASN:O	2.16	0.46
1:A:274:VAL:HA	1:A:302:TYR:CZ	2.52	0.45
1:E:303:LEU:C	1:E:303:LEU:HD12	2.41	0.45
1:H:283:ARG:HA	1:H:331:GLU:O	2.16	0.45
1:A:342:ALA:HB3	1:A:383:GLY:O	2.17	0.45
1:C:504:ILE:HD13	1:C:550:VAL:HG21	1.97	0.45
1:F:499:GLU:HA	1:F:527:ASP:O	2.17	0.45
1:B:431:TYR:CD1	1:B:431:TYR:C	2.95	0.45
1:C:329:ARG:HD3	1:C:331:GLU:OE2	2.17	0.45
1:A:533:ASN:OD1	1:E:566:LYS:NZ	2.45	0.45
1:A:288:LYS:HA	1:A:336:LYS:O	2.17	0.45
1:A:436:ALA:HA	1:A:461:GLY:O	2.17	0.45
1:C:615:VAL:HG22	1:C:625:GLU:OE1	2.17	0.45
1:E:452:TYR:HA	1:E:476:ASN:O	2.16	0.45
1:D:495:GLN:HA	1:D:523:GLY:O	2.17	0.44
1:E:57:ASP:O	1:E:69:TRP:HA	2.17	0.44
1:E:231:ASN:HA	1:E:284:ASN:O	2.17	0.44
1:G:47:THR:O	1:G:86:ASP:HA	2.17	0.44
1:A:138:GLN:HA	1:A:156:VAL:O	2.18	0.44
1:C:259:MET:HE1	1:C:269:TRP:CZ3	2.52	0.44
1:A:418:ASP:O	1:A:419:TYR:C	2.59	0.44
1:A:545:ILE:HD13	1:A:621:LEU:HD11	2.00	0.44
1:C:258:PRO:HG2	1:C:259:MET:CE	2.48	0.44
1:F:246:MET:C	1:F:254:MET:HE1	2.43	0.44
1:H:78:ILE:HG22	1:H:78:ILE:O	2.17	0.44
1:D:362:SER:OG	1:D:381:ALA:HB3	2.18	0.44
1:D:395:GLN:HA	1:D:426:GLN:O	2.18	0.44
1:G:138:GLN:HA	1:G:156:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:LYS:O	1:B:617:GLY:O	2.36	0.44
1:D:332:ASN:HA	1:D:355:HIS:O	2.17	0.44
1:D:418:ASP:O	1:D:419:TYR:C	2.60	0.44
1:C:194:THR:HG23	1:C:197:SER:HB3	2.00	0.44
1:F:252:TYR:CD1	1:F:254:MET:HE3	2.53	0.44
1:H:138:GLN:HA	1:H:156:VAL:O	2.18	0.44
1:C:431:TYR:CD1	1:C:431:TYR:C	2.96	0.43
1:C:82:LEU:O	1:C:106:THR:OG1	2.25	0.43
1:C:573:ARG:CZ	1:C:610:PHE:CZ	3.02	0.43
1:D:457:ASN:HA	4:D:903:HOH:O	2.18	0.43
1:G:259:MET:HE2	1:G:266:THR:HG22	1.99	0.43
1:H:545:ILE:HD13	1:H:621:LEU:HD11	2.00	0.43
1:F:427:TYR:HA	1:F:452:TYR:O	2.18	0.43
1:G:344:THR:HA	1:G:385:TRP:O	2.19	0.43
1:H:431:TYR:CD1	1:H:431:TYR:C	2.96	0.43
1:B:577:LYS:O	1:B:578:ALA:C	2.61	0.43
1:G:426:GLN:HA	1:G:451:ARG:O	2.18	0.43
1:G:133:GLY:HA2	1:G:157:SER:OG	2.19	0.43
1:F:426:GLN:HA	1:F:451:ARG:O	2.19	0.43
1:F:288:LYS:HA	1:F:336:LYS:O	2.18	0.43
1:G:343:ILE:HD12	1:G:384:ILE:HD12	2.01	0.43
1:H:415:TRP:CZ2	1:H:428:ASN:HB3	2.53	0.43
1:B:395:GLN:HA	1:B:426:GLN:O	2.19	0.43
1:C:415:TRP:CZ2	1:C:428:ASN:HB3	2.54	0.43
1:F:473:HIS:NE2	1:F:499:GLU:OE1	2.43	0.43
1:B:475:TYR:HA	1:B:499:GLU:O	2.19	0.42
1:B:494:SER:OG	1:B:495:GLN:N	2.51	0.42
1:C:293:TRP:HZ3	1:C:344:THR:HG1	1.63	0.42
1:G:343:ILE:HB	1:G:384:ILE:HD12	2.00	0.42
1:C:83:GLY:HA3	1:C:86:ASP:CG	2.44	0.42
1:D:82:LEU:O	1:D:106:THR:OG1	2.22	0.42
1:A:385:TRP:HB2	1:A:416:ASP:O	2.19	0.42
1:C:431:TYR:HA	1:C:456:GLN:O	2.19	0.42
1:E:442:ASN:O	1:E:468:ASN:HA	2.20	0.42
1:G:452:TYR:HA	1:G:476:ASN:O	2.19	0.42
1:A:415:TRP:CZ2	1:A:428:ASN:HB3	2.55	0.42
1:E:50:TYR:O	1:E:68:PRO:O	2.38	0.42
1:E:344:THR:HA	1:E:385:TRP:O	2.19	0.42
1:A:156:VAL:HG11	1:A:247:ALA:HB3	2.01	0.42
1:E:456:GLN:HG2	1:E:457:ASN:OD1	2.19	0.42
1:F:171:SER:HA	1:F:230:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:SER:O	1:H:54:ALA:CB	2.67	0.42
1:C:353:ILE:HD12	1:C:353:ILE:N	2.35	0.42
1:F:218:ALA:O	1:F:255:ALA:HA	2.20	0.42
1:A:414:ALA:HB2	1:A:433:ASN:ND2	2.35	0.41
1:D:415:TRP:HB3	1:D:425:TYR:CZ	2.55	0.41
1:F:465:LEU:N	1:F:466:PRO:CD	2.83	0.41
1:G:442:ASN:O	1:G:468:ASN:HA	2.20	0.41
1:C:264:ALA:O	1:C:268:VAL:HG23	2.20	0.41
1:D:344:THR:HA	1:D:385:TRP:O	2.20	0.41
1:G:530:MET:HB2	1:G:621:LEU:HD13	2.01	0.41
1:E:415:TRP:HB3	1:E:425:TYR:CZ	2.55	0.41
1:E:516:ASN:ND2	1:E:524:GLN:O	2.51	0.41
1:H:115:THR:O	1:H:116:ILE:HG12	2.20	0.41
1:F:362:SER:OG	1:F:381:ALA:HB3	2.20	0.41
1:E:274:VAL:HG11	1:E:323:TYR:HA	2.03	0.41
1:F:253:PHE:O	1:F:254:MET:HG3	2.21	0.41
1:H:577:LYS:O	1:H:578:ALA:C	2.63	0.41
1:A:121:ASP:O	1:A:122:ALA:C	2.64	0.41
1:A:354:GLU:HA	1:A:395:GLN:O	2.21	0.41
1:B:418:ASP:O	1:B:419:TYR:C	2.61	0.41
1:D:475:TYR:HA	1:D:499:GLU:O	2.21	0.41
1:G:385:TRP:HB2	1:G:416:ASP:O	2.20	0.41
1:D:456:GLN:HG2	1:D:457:ASN:OD1	2.21	0.41
1:E:426:GLN:HA	1:E:451:ARG:O	2.21	0.41
1:F:560:ALA:HB1	1:F:561:PRO:CD	2.51	0.41
1:A:431:TYR:CD1	1:A:431:TYR:C	2.99	0.40
1:D:56:GLY:HA2	1:D:68:PRO:O	2.21	0.40
1:D:413:GLN:HG3	1:D:435:PHE:O	2.21	0.40
1:H:134:VAL:O	1:H:135:LYS:C	2.63	0.40
1:C:171:SER:HA	1:C:230:ASP:O	2.21	0.40
1:D:53:SER:O	1:D:54:ALA:HB2	2.21	0.40
1:D:171:SER:HA	1:D:230:ASP:O	2.21	0.40
1:F:431:TYR:HA	1:F:456:GLN:O	2.20	0.40
1:B:140:GLU:OE2	1:B:155:THR:OG1	2.37	0.40
1:D:560:ALA:HB1	1:D:561:PRO:CD	2.52	0.40
1:E:284:ASN:HA	1:E:332:ASN:O	2.22	0.40
1:D:342:ALA:HB3	1:D:383:GLY:O	2.21	0.40
1:D:235:HIS:ND1	1:D:236:ASP:OD2	2.53	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:E:123:ASP:OD2	1:F:519:SER:OG[1_655]	1.98	0.22

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	580/606 (96%)	525 (90%)	50 (9%)	5 (1%)	14	14
1	B	580/606 (96%)	533 (92%)	43 (7%)	4 (1%)	18	20
1	C	580/606 (96%)	545 (94%)	32 (6%)	3 (0%)	24	27
1	D	581/606 (96%)	535 (92%)	41 (7%)	5 (1%)	14	14
1	E	581/606 (96%)	542 (93%)	35 (6%)	4 (1%)	18	20
1	F	581/606 (96%)	542 (93%)	37 (6%)	2 (0%)	36	43
1	G	581/606 (96%)	520 (90%)	53 (9%)	8 (1%)	9	7
1	H	581/606 (96%)	532 (92%)	41 (7%)	8 (1%)	9	7
All	All	4645/4848 (96%)	4274 (92%)	332 (7%)	39 (1%)	16	17

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	617	GLY
1	D	57	ASP
1	D	68	PRO
1	D	69	TRP
1	E	69	TRP
1	G	616	LYS
1	H	68	PRO
1	H	69	TRP
1	A	64	SER
1	A	110	ALA
1	A	616	LYS
1	B	125	GLY

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Mol	Chain	Res	Type
1	B	247	ALA
1	C	64	SER
1	D	54	ALA
1	G	617	GLY
1	H	64	SER
1	H	116	ILE
1	H	386	PRO
1	H	617	GLY
1	A	386	PRO
1	B	386	PRO
1	C	616	LYS
1	D	64	SER
1	E	64	SER
1	G	510	LYS
1	H	54	ALA
1	E	68	PRO
1	G	64	SER
1	G	69	TRP
1	G	247	ALA
1	E	522	GLY
1	H	53	SER
1	A	116	ILE
1	C	386	PRO
1	G	386	PRO
1	F	386	PRO
1	G	311	GLY
1	F	556	GLY

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	470/491 (96%)	455 (97%)	15 (3%)	34	46
1	B	470/491 (96%)	455 (97%)	15 (3%)	34	46
1	C	470/491 (96%)	460 (98%)	10 (2%)	47	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	471/491 (96%)	456 (97%)	15 (3%)	34	46
1	E	471/491 (96%)	461 (98%)	10 (2%)	47	61
1	F	471/491 (96%)	458 (97%)	13 (3%)	38	51
1	G	471/491 (96%)	452 (96%)	19 (4%)	28	37
1	H	471/491 (96%)	458 (97%)	13 (3%)	38	51
All	All	3765/3928 (96%)	3655 (97%)	110 (3%)	37	49

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	109	ASN
1	A	192	THR
1	A	194	THR
1	A	212	THR
1	A	254	MET
1	A	259	MET
1	A	265	GLU
1	A	293	TRP
1	A	314	SER
1	A	496	SER
1	A	510	LYS
1	A	519	SER
1	A	528	ASN
1	A	570	GLU
1	B	47	THR
1	B	69	TRP
1	B	78	ILE
1	B	181	ASP
1	B	192	THR
1	B	194	THR
1	B	212	THR
1	B	254	MET
1	B	259	MET
1	B	275	SER
1	B	293	TRP
1	B	496	SER
1	B	507	THR
1	B	520	GLN
1	B	625	GLU

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Mol	Chain	Res	Type
1	C	47	THR
1	C	101	LEU
1	C	194	THR
1	C	212	THR
1	C	259	MET
1	C	331	GLU
1	C	360	SER
1	C	418	ASP
1	C	590	LYS
1	C	625	GLU
1	D	66	ASN
1	D	78	ILE
1	D	90	LEU
1	D	160	LEU
1	D	163	LYS
1	D	194	THR
1	D	198	ASP
1	D	201	LYS
1	D	212	THR
1	D	254	MET
1	D	293	TRP
1	D	427	TYR
1	D	509	THR
1	D	528	ASN
1	D	616	LYS
1	E	73	THR
1	E	74	LYS
1	E	78	ILE
1	E	163	LYS
1	E	194	THR
1	E	212	THR
1	E	259	MET
1	E	293	TRP
1	E	300	THR
1	E	618	ARG
1	F	64	SER
1	F	149	ASN
1	F	193	ASP
1	F	201	LYS
1	F	212	THR
1	F	254	MET
1	F	259	MET

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Mol	Chain	Res	Type
1	F	293	TRP
1	F	427	TYR
1	F	509	THR
1	F	528	ASN
1	F	551	SER
1	F	563	SER
1	G	64	SER
1	G	90	LEU
1	G	106	THR
1	G	163	LYS
1	G	192	THR
1	G	198	ASP
1	G	212	THR
1	G	265	GLU
1	G	268	VAL
1	G	291	ASP
1	G	293	TRP
1	G	300	THR
1	G	367	THR
1	G	380	VAL
1	G	528	ASN
1	G	551	SER
1	G	563	SER
1	G	576	GLU
1	G	607	GLU
1	H	51	VAL
1	H	123	ASP
1	H	160	LEU
1	H	194	THR
1	H	198	ASP
1	H	212	THR
1	H	254	MET
1	H	259	MET
1	H	268	VAL
1	H	275	SER
1	H	293	TRP
1	H	393	VAL
1	H	440	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	231	ASN
1	A	273	HIS
1	A	327	ASN
1	A	332	ASN
1	A	407	HIS
1	A	447	ASN
1	A	508	ASN
1	B	97	ASN
1	B	226	ASN
1	B	368	GLN
1	B	442	ASN
1	B	460	GLN
1	B	508	ASN
1	B	528	ASN
1	C	327	ASN
1	C	520	GLN
1	C	528	ASN
1	C	608	ASN
1	D	442	ASN
1	D	520	GLN
1	D	608	ASN
1	E	66	ASN
1	E	132	ASN
1	E	226	ASN
1	E	368	GLN
1	E	407	HIS
1	E	460	GLN
1	E	486	GLN
1	E	528	ASN
1	E	608	ASN
1	F	226	ASN
1	F	273	HIS
1	F	332	ASN
1	F	593	ASN
1	G	97	ASN
1	G	226	ASN
1	G	231	ASN
1	G	284	ASN
1	G	332	ASN
1	G	368	GLN
1	G	407	HIS
1	G	593	ASN

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Mol	Chain	Res	Type
1	H	172	ASN
1	H	460	GLN
1	H	505	ASN
1	H	593	ASN

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 15 ligands modelled in this entry, 15 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	582/606 (96%)	-1.42	0 100 100	26, 40, 66, 95	0
1	B	582/606 (96%)	-1.43	0 100 100	26, 39, 65, 94	0
1	C	582/606 (96%)	-1.45	0 100 100	24, 38, 57, 80	0
1	D	583/606 (96%)	-1.46	0 100 100	23, 35, 60, 91	0
1	E	583/606 (96%)	-1.47	0 100 100	23, 36, 55, 84	0
1	F	583/606 (96%)	-1.47	0 100 100	25, 36, 56, 81	0
1	G	583/606 (96%)	-1.39	0 100 100	26, 42, 69, 99	0
1	H	583/606 (96%)	-1.44	0 100 100	22, 37, 65, 96	0
All	All	4661/4848 (96%)	-1.44	0 100 100	22, 38, 63, 99	0

There are no RSRZ outliers to report.

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
3	CA	C	701	1/1	0.97	0.08	76,76,76,76	0
3	CA	D	701	1/1	0.98	0.04	78,78,78,78	0
3	CA	G	701	1/1	0.98	0.04	67,67,67,67	0
3	CA	H	702	1/1	0.98	0.05	64,64,64,64	0
3	CA	B	702	1/1	0.99	0.04	68,68,68,68	0
3	CA	E	701	1/1	0.99	0.03	79,79,79,79	0
3	CA	E	702	1/1	0.99	0.03	58,58,58,58	0
3	CA	F	701	1/1	0.99	0.05	65,65,65,65	0
3	CA	F	702	1/1	0.99	0.03	61,61,61,61	0
2	NA	A	701	1/1	0.99	0.03	38,38,38,38	0
3	CA	G	702	1/1	0.99	0.04	72,72,72,72	0
3	CA	H	701	1/1	0.99	0.04	66,66,66,66	0
3	CA	C	702	1/1	0.99	0.06	61,61,61,61	0
3	CA	B	701	1/1	1.00	0.03	57,57,57,57	0
3	CA	D	702	1/1	1.00	0.03	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.