



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:02 AM UTC

PDB ID : 4YO3 / pdb_00004yo3
Title : Enteroaggregative Escherichia Coli TssA N-terminal fragment
Authors : Durand, E.; Zoued, A.; Spinelli, S.; Douzi, B.; Brunet, Y.R.; Bebeacua, C.;
Legrand, P.; Journet, L.; Mignot, T.; Cambillau, C.; Cascales, E.
Deposited on : 2015-03-11
Resolution : 3.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

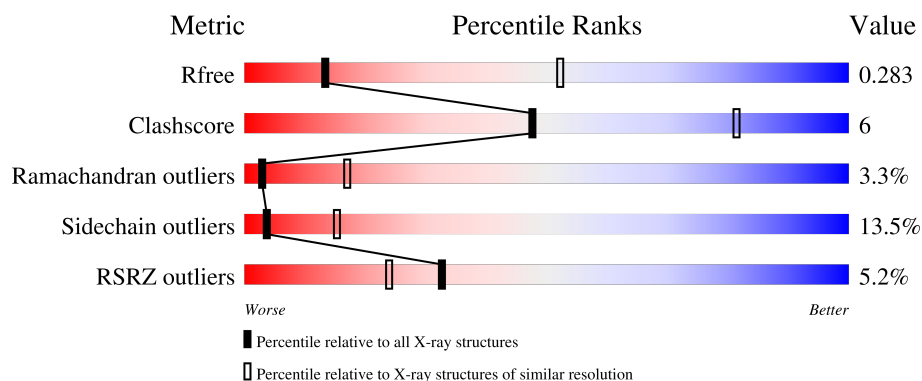
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	157	2% 73% 22% • •
1	B	157	2% 74% 21% • •
1	C	157	4% 72% 22% 5% •
1	D	157	2% 75% 22% • •
1	E	157	3% 75% 22% • •

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Mol	Chain	Length	Quality of chain
1	F	157	2% 76% 19%
1	G	157	2% 75% 21%
1	H	157	3% 75% 23%
1	I	157	4% 76% 20%
1	J	157	3% 78% 18%
1	K	157	4% 76% 22%
1	L	157	30% 70% 25%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14496 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.

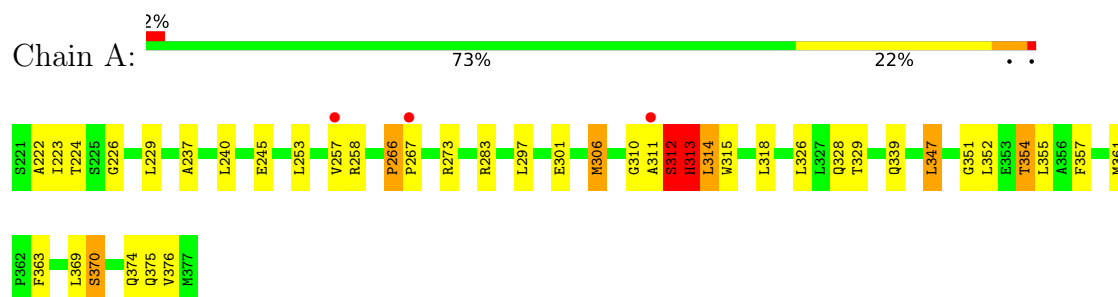
- Molecule 1 is a protein called TssA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	B	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	C	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	D	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	E	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	F	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	G	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	H	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	I	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	J	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	K	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	L	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			

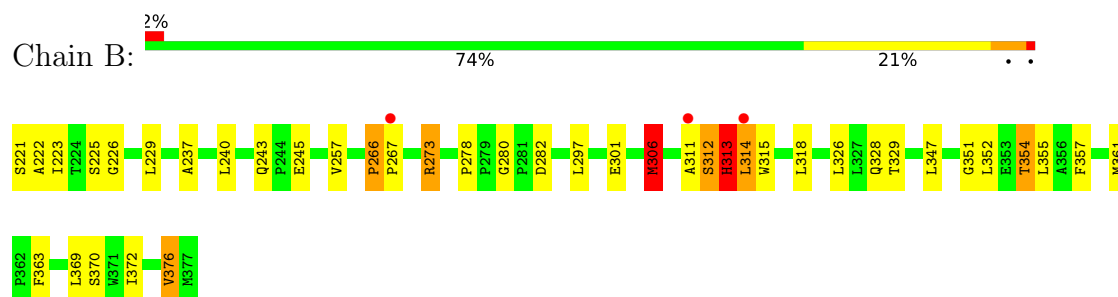
3 Residue-property plots [i](#)

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.

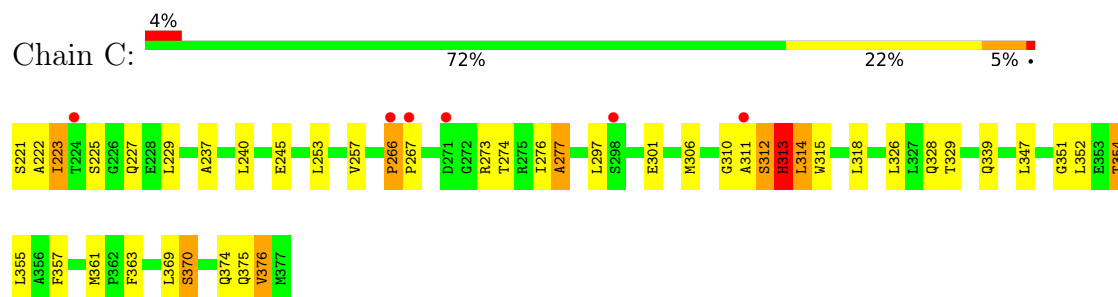
• Molecule 1: TssA



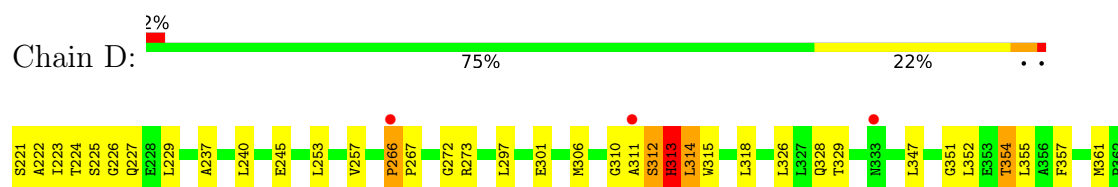
• Molecule 1: TssA



• Molecule 1: TssA

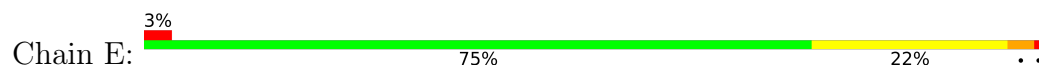


• Molecule 1: TssA

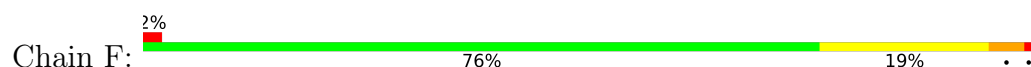




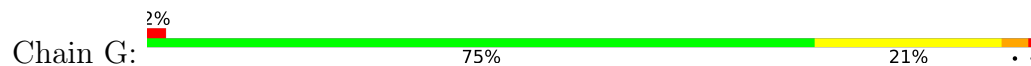
- Molecule 1: TssA



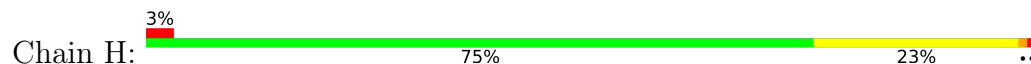
- Molecule 1: TssA



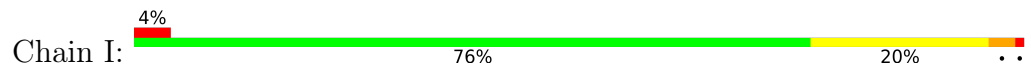
- Molecule 1: TssA

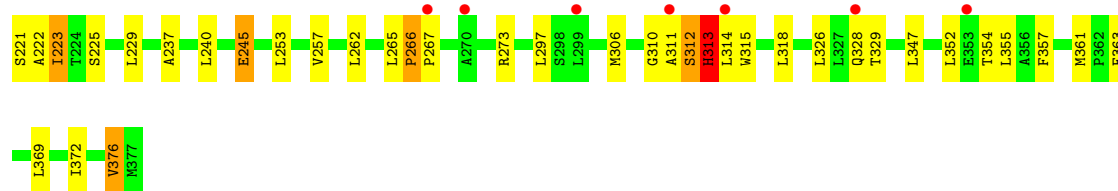


- Molecule 1: TssA

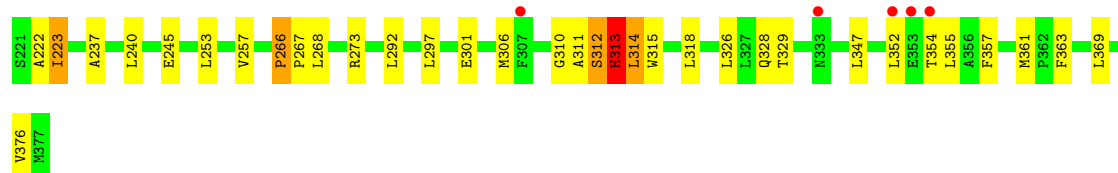
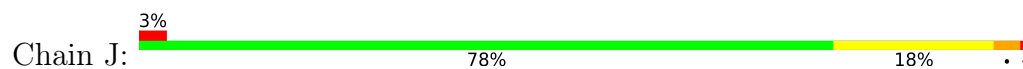


- Molecule 1: TssA

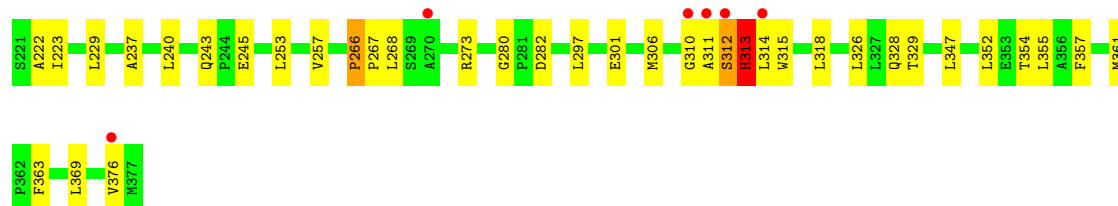
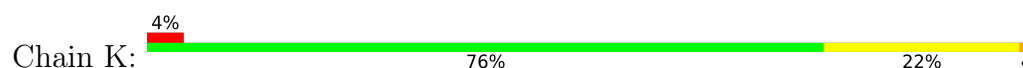




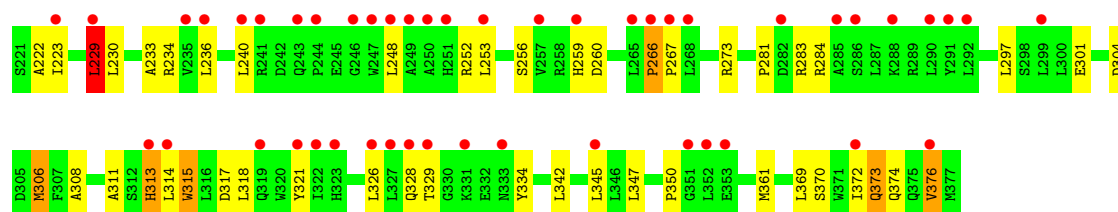
• Molecule 1: TssA



• Molecule 1: TssA



• Molecule 1: TssA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.13Å 178.05Å 106.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.39 – 3.37 28.39 – 3.37	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.39-3.37) 99.8 (28.39-3.37)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 3.39Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.250 , 0.261 0.274 , 0.283	Depositor DCC
R_{free} test set	1839 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14496	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% 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

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	0.88	0/1232	1.54	12/1673 (0.7%)
1	B	0.87	1/1232 (0.1%)	1.49	10/1673 (0.6%)
1	C	0.83	0/1232	1.49	9/1673 (0.5%)
1	D	0.83	0/1232	1.49	11/1673 (0.7%)
1	E	0.83	0/1232	1.48	9/1673 (0.5%)
1	F	0.82	0/1232	1.49	10/1673 (0.6%)
1	G	0.84	0/1232	1.49	10/1673 (0.6%)
1	H	0.82	0/1232	1.48	9/1673 (0.5%)
1	I	0.80	0/1232	1.50	7/1673 (0.4%)
1	J	0.80	0/1232	1.45	8/1673 (0.5%)
1	K	0.80	0/1232	1.48	7/1673 (0.4%)
1	L	0.94	0/1232	1.60	12/1673 (0.7%)
All	All	0.84	1/14784 (0.0%)	1.50	114/20076 (0.6%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	MSE	SE-CE	7.53	2.18	1.95

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	HIS	CA-CB-CG	-8.26	105.55	113.80
1	C	357	PHE	CA-C-N	6.86	129.35	120.44
1	C	357	PHE	C-N-CA	6.86	129.35	120.44
1	A	312	SER	CA-C-N	6.75	134.42	121.54
1	A	312	SER	C-N-CA	6.75	134.42	121.54
1	E	313	HIS	CA-CB-CG	-6.68	107.12	113.80
1	E	312	SER	CA-C-N	6.65	134.24	121.54
1	E	312	SER	C-N-CA	6.65	134.24	121.54
1	G	313	HIS	CA-CB-CG	-6.63	107.17	113.80
1	B	313	HIS	CA-CB-CG	-6.62	107.17	113.80
1	F	313	HIS	CA-CB-CG	-6.57	107.23	113.80
1	H	313	HIS	CA-CB-CG	-6.56	107.24	113.80
1	D	312	SER	CA-C-N	6.51	133.97	121.54
1	D	312	SER	C-N-CA	6.51	133.97	121.54
1	H	312	SER	CA-C-N	6.49	133.93	121.54
1	H	312	SER	C-N-CA	6.49	133.93	121.54
1	K	312	SER	CA-C-N	6.49	133.93	121.54
1	K	312	SER	C-N-CA	6.49	133.93	121.54
1	I	313	HIS	CA-CB-CG	-6.47	107.33	113.80
1	K	313	HIS	CA-CB-CG	-6.46	107.34	113.80
1	F	312	SER	CA-C-N	6.45	133.86	121.54
1	F	312	SER	C-N-CA	6.45	133.86	121.54
1	C	313	HIS	CA-CB-CG	-6.45	107.35	113.80
1	I	312	SER	CA-C-N	6.44	133.84	121.54
1	I	312	SER	C-N-CA	6.44	133.84	121.54
1	B	312	SER	CA-C-N	6.43	133.82	121.54
1	B	312	SER	C-N-CA	6.43	133.82	121.54
1	G	312	SER	CA-C-N	6.40	133.77	121.54
1	G	312	SER	C-N-CA	6.40	133.77	121.54
1	C	312	SER	CA-C-N	6.40	133.76	121.54
1	C	312	SER	C-N-CA	6.40	133.76	121.54
1	J	313	HIS	CA-CB-CG	-6.31	107.49	113.80
1	J	312	SER	CA-C-N	6.27	133.51	121.54
1	J	312	SER	C-N-CA	6.27	133.51	121.54
1	D	313	HIS	CA-CB-CG	-6.17	107.63	113.80
1	G	226	GLY	CA-C-N	6.06	128.40	120.28
1	G	226	GLY	C-N-CA	6.06	128.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	314	LEU	N-CA-C	-5.97	105.58	112.92
1	L	229	LEU	CA-C-N	5.96	130.76	120.58
1	L	229	LEU	C-N-CA	5.96	130.76	120.58
1	D	226	GLY	CA-C-N	5.95	132.13	121.66
1	D	226	GLY	C-N-CA	5.95	132.13	121.66
1	A	226	GLY	N-CA-C	-5.87	107.06	114.16
1	L	252	ARG	CA-C-N	5.72	127.88	120.44
1	L	252	ARG	C-N-CA	5.72	127.88	120.44
1	B	357	PHE	CA-C-N	5.66	128.66	120.79
1	B	357	PHE	C-N-CA	5.66	128.66	120.79
1	H	222	ALA	CA-C-N	5.63	132.11	121.97
1	H	222	ALA	C-N-CA	5.63	132.11	121.97
1	K	222	ALA	CA-C-N	5.60	132.06	121.97
1	K	222	ALA	C-N-CA	5.60	132.06	121.97
1	D	314	LEU	N-CA-C	-5.60	106.03	112.92
1	D	222	ALA	CA-C-N	5.59	132.03	121.97
1	D	222	ALA	C-N-CA	5.59	132.03	121.97
1	C	222	ALA	CA-C-N	5.58	132.01	121.97
1	C	222	ALA	C-N-CA	5.58	132.01	121.97
1	E	222	ALA	CA-C-N	5.56	131.97	121.97
1	E	222	ALA	C-N-CA	5.56	131.97	121.97
1	I	222	ALA	CA-C-N	5.55	131.96	121.97
1	I	222	ALA	C-N-CA	5.55	131.96	121.97
1	F	222	ALA	CA-C-N	5.53	131.93	121.97
1	F	222	ALA	C-N-CA	5.53	131.93	121.97
1	A	314	LEU	N-CA-C	-5.51	106.15	112.92
1	F	357	PHE	CA-C-N	5.47	128.40	120.79
1	F	357	PHE	C-N-CA	5.47	128.40	120.79
1	L	222	ALA	CA-C-N	5.46	131.81	121.97
1	L	222	ALA	C-N-CA	5.46	131.81	121.97
1	J	222	ALA	CA-C-N	5.46	131.80	121.97
1	J	222	ALA	C-N-CA	5.46	131.80	121.97
1	E	352	LEU	CA-C-N	5.45	127.85	120.38
1	E	352	LEU	C-N-CA	5.45	127.85	120.38
1	B	314	LEU	N-CA-C	-5.45	106.22	112.92
1	J	314	LEU	N-CA-C	-5.45	106.22	112.92
1	A	357	PHE	CA-C-N	5.44	128.35	120.79
1	A	357	PHE	C-N-CA	5.44	128.35	120.79
1	K	357	PHE	CA-C-N	5.43	128.33	120.79
1	K	357	PHE	C-N-CA	5.43	128.33	120.79
1	L	304	ASP	CA-C-N	5.43	127.55	120.28
1	L	304	ASP	C-N-CA	5.43	127.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ALA	CA-C-N	5.41	131.71	121.97
1	B	222	ALA	C-N-CA	5.41	131.71	121.97
1	A	222	ALA	CA-C-N	5.41	131.70	121.97
1	A	222	ALA	C-N-CA	5.41	131.70	121.97
1	D	357	PHE	CA-C-N	5.40	128.29	120.79
1	D	357	PHE	C-N-CA	5.40	128.29	120.79
1	J	357	PHE	CA-C-N	5.39	128.28	120.79
1	J	357	PHE	C-N-CA	5.39	128.28	120.79
1	A	226	GLY	CA-C-N	5.39	127.50	120.28
1	A	226	GLY	C-N-CA	5.39	127.50	120.28
1	G	222	ALA	CA-C-N	5.37	131.64	121.97
1	G	222	ALA	C-N-CA	5.37	131.64	121.97
1	F	226	GLY	CA-C-N	5.36	128.45	120.31
1	F	226	GLY	C-N-CA	5.36	128.45	120.31
1	H	357	PHE	CA-C-N	5.34	128.21	120.79
1	H	357	PHE	C-N-CA	5.34	128.21	120.79
1	E	357	PHE	CA-C-N	5.33	128.20	120.79
1	E	357	PHE	C-N-CA	5.33	128.20	120.79
1	B	226	GLY	CA-C-N	5.31	128.38	120.31
1	B	226	GLY	C-N-CA	5.31	128.38	120.31
1	G	357	PHE	CA-C-N	5.27	128.11	120.79
1	G	357	PHE	C-N-CA	5.27	128.11	120.79
1	I	357	PHE	CA-C-N	5.17	127.97	120.79
1	I	357	PHE	C-N-CA	5.17	127.97	120.79
1	C	314	LEU	N-CA-C	-5.16	106.58	112.92
1	D	226	GLY	N-CA-C	-5.13	109.03	114.67
1	L	321	TYR	CA-C-N	5.09	127.44	120.46
1	L	321	TYR	C-N-CA	5.09	127.44	120.46
1	H	226	GLY	CA-C-N	5.08	128.04	120.31
1	H	226	GLY	C-N-CA	5.08	128.04	120.31
1	L	315	TRP	CA-C-N	5.07	128.79	120.63
1	L	315	TRP	C-N-CA	5.07	128.79	120.63
1	F	314	LEU	N-CA-C	-5.03	106.73	112.92
1	C	277	ALA	N-CA-C	5.01	116.15	109.93
1	A	347	LEU	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	PRO	Peptide
1	B	266	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	C	266	PRO	Peptide
1	D	266	PRO	Peptide
1	E	266	PRO	Peptide
1	F	266	PRO	Peptide
1	G	266	PRO	Peptide
1	H	266	PRO	Peptide
1	I	265	LEU	Peptide
1	I	266	PRO	Peptide
1	J	266	PRO	Peptide
1	K	266	PRO	Peptide
1	L	266	PRO	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	1208	0	1151	14	0
1	B	1208	0	1151	18	0
1	C	1208	0	1151	17	0
1	D	1208	0	1151	14	0
1	E	1208	0	1151	16	0
1	F	1208	0	1151	12	0
1	G	1208	0	1151	14	0
1	H	1208	0	1151	14	0
1	I	1208	0	1151	12	0
1	J	1208	0	1151	11	0
1	K	1208	0	1151	11	0
1	L	1208	0	1151	19	0
All	All	14496	0	13812	157	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 (157) 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:B:306:MSE:SE	1:B:306:MSE:CE	2.18	1.41
1:L:236:LEU:HD23	1:L:253:LEU:HD11	1.49	0.95
1:G:311:ALA:C	1:G:313:HIS:H	1.99	0.69
1:L:236:LEU:CD2	1:L:253:LEU:HD11	2.23	0.67
1:C:370:SER:O	1:C:374:GLN:HG2	1.95	0.66
1:L:240:LEU:HD22	1:L:253:LEU:HD12	1.78	0.64
1:D:311:ALA:C	1:D:313:HIS:H	2.05	0.64
1:J:311:ALA:C	1:J:313:HIS:H	2.06	0.64
1:L:259:HIS:HB3	1:L:345:LEU:HD13	1.80	0.62
1:H:311:ALA:C	1:H:313:HIS:H	2.06	0.62
1:D:310:GLY:HA3	1:D:313:HIS:CE1	2.35	0.62
1:I:311:ALA:C	1:I:313:HIS:H	2.07	0.62
1:F:311:ALA:C	1:F:313:HIS:H	2.07	0.61
1:K:311:ALA:C	1:K:313:HIS:H	2.07	0.61
1:E:311:ALA:C	1:E:313:HIS:H	2.09	0.61
1:B:311:ALA:C	1:B:313:HIS:H	2.07	0.60
1:B:282:ASP:HA	1:E:272:GLY:CA	2.32	0.60
1:B:282:ASP:HA	1:E:272:GLY:HA3	1.84	0.58
1:A:311:ALA:C	1:A:313:HIS:H	2.11	0.58
1:C:311:ALA:C	1:C:313:HIS:H	2.09	0.58
1:D:221:SER:N	1:D:225:SER:HG	2.02	0.57
1:G:310:GLY:HA3	1:G:313:HIS:CE1	2.41	0.55
1:A:310:GLY:HA3	1:A:313:HIS:CE1	2.42	0.54
1:F:352:LEU:HA	1:F:355:LEU:HD12	1.91	0.53
1:E:352:LEU:HA	1:E:355:LEU:HD12	1.91	0.52
1:C:277:ALA:HB2	1:L:373:GLN:CD	2.35	0.52
1:J:352:LEU:HA	1:J:355:LEU:HD12	1.92	0.52
1:C:352:LEU:HA	1:C:355:LEU:HD12	1.93	0.51
1:K:352:LEU:HA	1:K:355:LEU:HD12	1.93	0.51
1:L:248:LEU:HB2	1:L:334:TYR:CE1	2.45	0.51
1:L:342:LEU:HD23	1:L:376:VAL:HG21	1.90	0.51
1:G:221:SER:N	1:G:225:SER:HG	2.07	0.51
1:H:352:LEU:HA	1:H:355:LEU:HD12	1.91	0.51
1:K:310:GLY:HA3	1:K:313:HIS:CE1	2.45	0.51
1:L:372:ILE:HA	1:L:376:VAL:HG22	1.92	0.51
1:D:272:GLY:CA	1:K:282:ASP:HA	2.40	0.51
1:A:352:LEU:HA	1:A:355:LEU:HD12	1.93	0.50
1:D:352:LEU:HA	1:D:355:LEU:HD12	1.93	0.50
1:I:352:LEU:HA	1:I:355:LEU:HD12	1.92	0.50
1:H:243:GLN:HE22	1:I:223:ILE:HD12	1.77	0.50
1:L:281:PRO:HA	1:L:284:ARG:HG2	1.94	0.50
1:A:339:GLN:HE22	1:A:375:GLN:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:ARG:HD3	1:L:306:MSE:HG2	1.92	0.50
1:G:352:LEU:HA	1:G:355:LEU:HD12	1.92	0.50
1:J:223:ILE:HD12	1:K:243:GLN:HE22	1.77	0.49
1:I:221:SER:N	1:I:225:SER:HG	2.09	0.49
1:C:310:GLY:HA3	1:C:313:HIS:CE1	2.48	0.49
1:E:221:SER:N	1:E:225:SER:HG	2.10	0.49
1:D:354:THR:HG23	1:K:280:GLY:HA2	1.94	0.49
1:B:352:LEU:HA	1:B:355:LEU:HD12	1.94	0.49
1:L:370:SER:O	1:L:374:GLN:HG2	2.13	0.48
1:A:370:SER:O	1:A:374:GLN:HG2	2.13	0.48
1:B:221:SER:N	1:B:225:SER:HG	2.11	0.47
1:G:354:THR:HG23	1:H:280:GLY:HA2	1.97	0.47
1:D:326:LEU:HA	1:D:329:THR:HG22	1.97	0.47
1:B:326:LEU:HA	1:B:329:THR:HG22	1.96	0.47
1:J:310:GLY:HA3	1:J:313:HIS:CE1	2.48	0.47
1:A:311:ALA:C	1:A:313:HIS:N	2.72	0.47
1:H:221:SER:N	1:H:225:SER:HG	2.13	0.47
1:B:315:TRP:CD1	1:B:318:LEU:HD13	2.50	0.47
1:F:221:SER:N	1:F:225:SER:HG	2.12	0.47
1:L:326:LEU:HA	1:L:329:THR:HG22	1.97	0.46
1:C:326:LEU:HA	1:C:329:THR:HG22	1.97	0.46
1:J:315:TRP:CD1	1:J:318:LEU:HD13	2.51	0.46
1:B:355:LEU:HB2	1:B:363:PHE:CE2	2.50	0.46
1:C:227:GLN:NE2	1:L:350:PRO:HG3	2.31	0.46
1:L:315:TRP:O	1:L:318:LEU:HB2	2.15	0.46
1:C:221:SER:N	1:C:225:SER:HG	2.14	0.46
1:G:326:LEU:HA	1:G:329:THR:HG22	1.98	0.46
1:F:223:ILE:HD12	1:G:243:GLN:HE22	1.81	0.45
1:F:315:TRP:CD1	1:F:318:LEU:HD13	2.51	0.45
1:F:264:GLN:HE22	1:J:310:GLY:N	2.15	0.45
1:F:326:LEU:HA	1:F:329:THR:HG22	1.98	0.45
1:G:315:TRP:CD1	1:G:318:LEU:HD13	2.51	0.45
1:A:326:LEU:HA	1:A:329:THR:HG22	1.99	0.45
1:G:355:LEU:HB2	1:G:363:PHE:CE2	2.52	0.45
1:C:315:TRP:CD1	1:C:318:LEU:HD13	2.52	0.45
1:H:326:LEU:HA	1:H:329:THR:HG22	1.99	0.45
1:A:355:LEU:HB2	1:A:363:PHE:CE2	2.52	0.44
1:H:315:TRP:CD1	1:H:318:LEU:HD13	2.53	0.44
1:K:315:TRP:CD1	1:K:318:LEU:HD13	2.52	0.44
1:B:278:PRO:HG2	1:E:354:THR:HG21	1.99	0.44
1:C:374:GLN:HG3	1:C:375:GLN:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:LEU:HB2	1:D:363:PHE:CE2	2.53	0.44
1:E:315:TRP:CD1	1:E:318:LEU:HD13	2.52	0.44
1:B:355:LEU:HB2	1:B:363:PHE:CD2	2.53	0.44
1:D:315:TRP:CD1	1:D:318:LEU:HD13	2.52	0.44
1:E:326:LEU:HA	1:E:329:THR:HG22	2.00	0.44
1:L:311:ALA:C	1:L:313:HIS:H	2.24	0.44
1:B:280:GLY:HA2	1:E:354:THR:HG23	2.00	0.44
1:F:237:ALA:HA	1:F:240:LEU:HD12	1.99	0.44
1:G:272:GLY:CA	1:H:282:ASP:HA	2.48	0.44
1:B:273:ARG:H	1:B:273:ARG:HG2	1.55	0.43
1:F:273:ARG:H	1:F:273:ARG:HG2	1.61	0.43
1:I:310:GLY:HA3	1:I:313:HIS:CE1	2.53	0.43
1:L:230:LEU:HA	1:L:233:ALA:HB3	2.01	0.43
1:A:315:TRP:CD1	1:A:318:LEU:HD13	2.53	0.43
1:B:243:GLN:HE22	1:C:223:ILE:HD12	1.82	0.43
1:J:326:LEU:HA	1:J:329:THR:HG22	1.99	0.43
1:E:310:GLY:HA3	1:E:313:HIS:CE1	2.54	0.43
1:I:355:LEU:HB2	1:I:363:PHE:CE2	2.54	0.43
1:B:237:ALA:HA	1:B:240:LEU:HD12	2.00	0.43
1:B:351:GLY:O	1:B:354:THR:HG22	2.19	0.43
1:H:237:ALA:HA	1:H:240:LEU:HD12	2.00	0.43
1:I:326:LEU:HA	1:I:329:THR:HG22	1.99	0.43
1:J:355:LEU:HB2	1:J:363:PHE:CE2	2.54	0.43
1:B:372:ILE:HA	1:B:376:VAL:HG22	2.01	0.43
1:E:355:LEU:HB2	1:E:363:PHE:CE2	2.54	0.43
1:I:237:ALA:HA	1:I:240:LEU:HD12	2.01	0.43
1:K:326:LEU:HA	1:K:329:THR:HG22	2.00	0.43
1:L:229:LEU:O	1:L:233:ALA:HB2	2.19	0.43
1:D:224:THR:HG22	1:D:225:SER:H	1.84	0.42
1:D:237:ALA:HA	1:D:240:LEU:HD12	2.00	0.42
1:G:273:ARG:H	1:G:273:ARG:HG2	1.56	0.42
1:K:237:ALA:HA	1:K:240:LEU:HD12	2.01	0.42
1:C:355:LEU:HB2	1:C:363:PHE:CE2	2.54	0.42
1:H:355:LEU:HB2	1:H:363:PHE:CE2	2.55	0.42
1:C:237:ALA:HA	1:C:240:LEU:HD12	2.01	0.42
1:E:237:ALA:HA	1:E:240:LEU:HD12	2.01	0.42
1:E:273:ARG:H	1:E:273:ARG:HG2	1.59	0.42
1:E:351:GLY:O	1:E:354:THR:HG22	2.20	0.42
1:A:237:ALA:HA	1:A:240:LEU:HD12	2.02	0.42
1:I:315:TRP:CD1	1:I:318:LEU:HD13	2.54	0.42
1:K:355:LEU:HB2	1:K:363:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:310:GLY:HA3	1:H:313:HIS:CE1	2.55	0.42
1:K:355:LEU:HB2	1:K:363:PHE:CE2	2.54	0.42
1:F:372:ILE:HA	1:F:376:VAL:HG22	2.02	0.42
1:L:256:SER:HA	1:L:260:ASP:OD2	2.20	0.42
1:E:355:LEU:HB2	1:E:363:PHE:CD2	2.55	0.41
1:G:237:ALA:HA	1:G:240:LEU:HD12	2.02	0.41
1:J:355:LEU:HB2	1:J:363:PHE:CD2	2.55	0.41
1:A:351:GLY:O	1:A:354:THR:HG22	2.20	0.41
1:D:225:SER:C	1:D:227:GLN:H	2.27	0.41
1:G:355:LEU:HB2	1:G:363:PHE:CD2	2.55	0.41
1:H:355:LEU:HB2	1:H:363:PHE:CD2	2.55	0.41
1:C:339:GLN:HE21	1:C:376:VAL:HG12	1.85	0.41
1:G:311:ALA:C	1:G:313:HIS:N	2.71	0.41
1:C:274:THR:C	1:C:276:ILE:H	2.29	0.41
1:B:311:ALA:C	1:B:313:HIS:N	2.78	0.41
1:C:351:GLY:O	1:C:354:THR:HG22	2.21	0.41
1:D:351:GLY:O	1:D:354:THR:HG22	2.21	0.41
1:F:355:LEU:HB2	1:F:363:PHE:CE2	2.56	0.41
1:I:355:LEU:HB2	1:I:363:PHE:CD2	2.56	0.41
1:A:283:ARG:CD	1:A:306:MSE:HE3	2.51	0.40
1:A:355:LEU:HB2	1:A:363:PHE:CD2	2.56	0.40
1:E:281:PRO:HA	1:E:284:ARG:HG2	2.03	0.40
1:F:355:LEU:HB2	1:F:363:PHE:CD2	2.56	0.40
1:L:234:ARG:HD3	1:L:308:ALA:HB1	2.03	0.40
1:A:258:ARG:NH2	1:A:312:SER:H	2.19	0.40
1:C:355:LEU:HB2	1:C:363:PHE:CD2	2.56	0.40
1:D:355:LEU:HB2	1:D:363:PHE:CD2	2.56	0.40
1:H:224:THR:HG22	1:H:225:SER:H	1.87	0.40
1:H:311:ALA:C	1:H:313:HIS:N	2.77	0.40
1:I:372:ILE:HA	1:I:376:VAL:HG22	2.03	0.40
1:J:237:ALA:HA	1:J:240:LEU:HD12	2.02	0.40
1:I:262:LEU:HD13	1:I:262:LEU:HA	1.98	0.40
1:J:311:ALA:C	1:J:313:HIS:N	2.77	0.40

There are no symmetry-related clashes.

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	155/157 (99%)	140 (90%)	10 (6%)	5 (3%)	3	17
1	B	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	3	17
1	C	155/157 (99%)	140 (90%)	10 (6%)	5 (3%)	3	17
1	D	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	3	17
1	E	155/157 (99%)	142 (92%)	8 (5%)	5 (3%)	3	17
1	F	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	3	17
1	G	155/157 (99%)	140 (90%)	9 (6%)	6 (4%)	2	14
1	H	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	3	17
1	I	155/157 (99%)	141 (91%)	8 (5%)	6 (4%)	2	14
1	J	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	3	17
1	K	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	3	17
1	L	155/157 (99%)	138 (89%)	13 (8%)	4 (3%)	4	21
All	All	1860/1884 (99%)	1687 (91%)	112 (6%)	61 (3%)	3	17

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	PRO
1	A	267	PRO
1	B	223	ILE
1	B	266	PRO
1	B	267	PRO
1	C	223	ILE
1	C	266	PRO
1	C	267	PRO
1	D	223	ILE
1	D	266	PRO
1	D	267	PRO
1	E	266	PRO

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Mol	Chain	Res	Type
1	E	267	PRO
1	F	266	PRO
1	F	267	PRO
1	G	266	PRO
1	G	267	PRO
1	H	266	PRO
1	H	267	PRO
1	I	245	GLU
1	I	266	PRO
1	I	267	PRO
1	J	223	ILE
1	J	266	PRO
1	J	267	PRO
1	K	266	PRO
1	K	267	PRO
1	L	266	PRO
1	L	267	PRO
1	A	223	ILE
1	A	313	HIS
1	B	313	HIS
1	C	313	HIS
1	D	313	HIS
1	E	223	ILE
1	E	313	HIS
1	F	223	ILE
1	F	313	HIS
1	G	223	ILE
1	G	312	SER
1	G	313	HIS
1	H	223	ILE
1	H	313	HIS
1	I	223	ILE
1	I	313	HIS
1	J	313	HIS
1	K	223	ILE
1	K	313	HIS
1	L	223	ILE
1	A	312	SER
1	D	312	SER
1	E	312	SER
1	F	312	SER
1	H	312	SER

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Mol	Chain	Res	Type
1	J	312	SER
1	K	312	SER
1	L	313	HIS
1	B	312	SER
1	C	312	SER
1	I	312	SER
1	G	265	LEU

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	118/129 (92%)	100 (85%)	18 (15%)	3	11
1	B	118/129 (92%)	102 (86%)	16 (14%)	3	15
1	C	118/129 (92%)	101 (86%)	17 (14%)	3	13
1	D	118/129 (92%)	102 (86%)	16 (14%)	3	15
1	E	118/129 (92%)	103 (87%)	15 (13%)	4	17
1	F	118/129 (92%)	102 (86%)	16 (14%)	3	15
1	G	118/129 (92%)	102 (86%)	16 (14%)	3	15
1	H	118/129 (92%)	103 (87%)	15 (13%)	4	17
1	I	118/129 (92%)	103 (87%)	15 (13%)	4	17
1	J	118/129 (92%)	101 (86%)	17 (14%)	3	13
1	K	118/129 (92%)	101 (86%)	17 (14%)	3	13
1	L	118/129 (92%)	105 (89%)	13 (11%)	6	22
All	All	1416/1548 (92%)	1225 (86%)	191 (14%)	4	15

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	THR
1	A	229	LEU
1	A	245	GLU

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	257	VAL
1	A	273	ARG
1	A	297	LEU
1	A	301	GLU
1	A	306	MSE
1	A	313	HIS
1	A	314	LEU
1	A	328	GLN
1	A	347	LEU
1	A	354	THR
1	A	361	MSE
1	A	369	LEU
1	A	370	SER
1	A	376	VAL
1	B	229	LEU
1	B	245	GLU
1	B	257	VAL
1	B	273	ARG
1	B	297	LEU
1	B	301	GLU
1	B	306	MSE
1	B	313	HIS
1	B	314	LEU
1	B	328	GLN
1	B	347	LEU
1	B	354	THR
1	B	361	MSE
1	B	369	LEU
1	B	370	SER
1	B	376	VAL
1	C	229	LEU
1	C	245	GLU
1	C	253	LEU
1	C	257	VAL
1	C	273	ARG
1	C	297	LEU
1	C	301	GLU
1	C	306	MSE
1	C	313	HIS
1	C	314	LEU
1	C	328	GLN

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Mol	Chain	Res	Type
1	C	347	LEU
1	C	354	THR
1	C	361	MSE
1	C	369	LEU
1	C	370	SER
1	C	376	VAL
1	D	229	LEU
1	D	245	GLU
1	D	253	LEU
1	D	257	VAL
1	D	273	ARG
1	D	297	LEU
1	D	301	GLU
1	D	306	MSE
1	D	313	HIS
1	D	314	LEU
1	D	328	GLN
1	D	347	LEU
1	D	354	THR
1	D	361	MSE
1	D	369	LEU
1	D	376	VAL
1	E	229	LEU
1	E	245	GLU
1	E	257	VAL
1	E	268	LEU
1	E	273	ARG
1	E	297	LEU
1	E	301	GLU
1	E	306	MSE
1	E	313	HIS
1	E	314	LEU
1	E	328	GLN
1	E	347	LEU
1	E	361	MSE
1	E	369	LEU
1	E	376	VAL
1	F	229	LEU
1	F	245	GLU
1	F	253	LEU
1	F	257	VAL
1	F	273	ARG

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Mol	Chain	Res	Type
1	F	297	LEU
1	F	301	GLU
1	F	306	MSE
1	F	313	HIS
1	F	314	LEU
1	F	328	GLN
1	F	347	LEU
1	F	354	THR
1	F	361	MSE
1	F	369	LEU
1	F	376	VAL
1	G	229	LEU
1	G	245	GLU
1	G	253	LEU
1	G	257	VAL
1	G	273	ARG
1	G	297	LEU
1	G	301	GLU
1	G	306	MSE
1	G	313	HIS
1	G	314	LEU
1	G	328	GLN
1	G	347	LEU
1	G	354	THR
1	G	361	MSE
1	G	369	LEU
1	G	376	VAL
1	H	229	LEU
1	H	253	LEU
1	H	257	VAL
1	H	268	LEU
1	H	273	ARG
1	H	297	LEU
1	H	301	GLU
1	H	306	MSE
1	H	313	HIS
1	H	314	LEU
1	H	328	GLN
1	H	347	LEU
1	H	361	MSE
1	H	369	LEU
1	H	376	VAL

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Mol	Chain	Res	Type
1	I	229	LEU
1	I	245	GLU
1	I	253	LEU
1	I	257	VAL
1	I	273	ARG
1	I	297	LEU
1	I	306	MSE
1	I	313	HIS
1	I	314	LEU
1	I	328	GLN
1	I	347	LEU
1	I	354	THR
1	I	361	MSE
1	I	369	LEU
1	I	376	VAL
1	J	245	GLU
1	J	253	LEU
1	J	257	VAL
1	J	268	LEU
1	J	273	ARG
1	J	292	LEU
1	J	297	LEU
1	J	301	GLU
1	J	306	MSE
1	J	313	HIS
1	J	314	LEU
1	J	328	GLN
1	J	347	LEU
1	J	354	THR
1	J	361	MSE
1	J	369	LEU
1	J	376	VAL
1	K	229	LEU
1	K	245	GLU
1	K	253	LEU
1	K	257	VAL
1	K	268	LEU
1	K	273	ARG
1	K	297	LEU
1	K	301	GLU
1	K	306	MSE
1	K	313	HIS

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Mol	Chain	Res	Type
1	K	314	LEU
1	K	328	GLN
1	K	347	LEU
1	K	354	THR
1	K	361	MSE
1	K	369	LEU
1	K	376	VAL
1	L	229	LEU
1	L	273	ARG
1	L	297	LEU
1	L	301	GLU
1	L	306	MSE
1	L	314	LEU
1	L	317	ASP
1	L	328	GLN
1	L	347	LEU
1	L	361	MSE
1	L	369	LEU
1	L	373	GLN
1	L	376	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	339	GLN
1	A	358	ASN
1	A	374	GLN
1	A	375	GLN
1	B	243	GLN
1	B	339	GLN
1	B	358	ASN
1	B	374	GLN
1	B	375	GLN
1	C	227	GLN
1	C	313	HIS
1	C	339	GLN
1	C	358	ASN
1	D	339	GLN
1	D	358	ASN
1	E	339	GLN
1	E	358	ASN

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Mol	Chain	Res	Type
1	F	264	GLN
1	F	323	HIS
1	F	339	GLN
1	F	358	ASN
1	G	227	GLN
1	G	243	GLN
1	G	313	HIS
1	G	339	GLN
1	G	358	ASN
1	H	243	GLN
1	H	339	GLN
1	H	358	ASN
1	I	243	GLN
1	I	339	GLN
1	I	358	ASN
1	J	243	GLN
1	J	313	HIS
1	J	339	GLN
1	J	358	ASN
1	K	243	GLN
1	K	313	HIS
1	K	339	GLN
1	K	358	ASN
1	L	232	GLN
1	L	302	GLN
1	L	323	HIS
1	L	358	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	153/157 (97%)	0.21	3 (1%) 65 49	54, 76, 109, 162	0
1	B	153/157 (97%)	0.21	3 (1%) 65 49	57, 81, 116, 175	0
1	C	153/157 (97%)	0.40	6 (3%) 43 30	63, 102, 138, 171	0
1	D	153/157 (97%)	0.21	3 (1%) 65 49	65, 98, 130, 168	0
1	E	153/157 (97%)	0.23	4 (2%) 57 42	57, 95, 135, 170	0
1	F	153/157 (97%)	0.26	3 (1%) 65 49	69, 106, 145, 160	0
1	G	153/157 (97%)	0.30	3 (1%) 65 49	66, 89, 119, 176	0
1	H	153/157 (97%)	0.27	5 (3%) 49 36	74, 109, 149, 167	0
1	I	153/157 (97%)	0.51	7 (4%) 37 27	76, 134, 169, 181	0
1	J	153/157 (97%)	0.29	5 (3%) 49 36	93, 125, 159, 178	0
1	K	153/157 (97%)	0.37	6 (3%) 43 30	92, 122, 157, 178	0
1	L	153/157 (97%)	1.58	47 (30%) 1 2	121, 184, 211, 221	0
All	All	1836/1884 (97%)	0.40	95 (5%) 33 24	54, 106, 182, 221	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	311	ALA	8.0
1	B	311	ALA	5.5
1	D	311	ALA	5.3
1	H	311	ALA	5.1
1	I	314	LEU	5.1
1	L	250	ALA	4.5
1	A	267	PRO	4.5
1	L	265	LEU	4.2
1	L	240	LEU	4.1
1	H	257	VAL	4.1
1	L	251	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	311	ALA	3.8
1	B	314	LEU	3.7
1	L	241	ARG	3.7
1	L	223	ILE	3.7
1	L	352	LEU	3.7
1	L	327	LEU	3.7
1	L	259	HIS	3.6
1	I	311	ALA	3.6
1	L	353	GLU	3.5
1	K	312	SER	3.5
1	K	314	LEU	3.5
1	A	311	ALA	3.5
1	L	229	LEU	3.4
1	L	291	TYR	3.4
1	L	247	TRP	3.4
1	F	267	PRO	3.3
1	L	326	LEU	3.3
1	L	333	ASN	3.3
1	F	311	ALA	3.3
1	L	266	PRO	3.2
1	L	319	GLN	3.2
1	L	323	HIS	3.2
1	L	313	HIS	2.9
1	L	236	LEU	2.9
1	I	267	PRO	2.9
1	L	249	ALA	2.8
1	I	353	GLU	2.8
1	L	243	GLN	2.8
1	E	311	ALA	2.8
1	L	292	LEU	2.8
1	H	267	PRO	2.7
1	C	311	ALA	2.7
1	L	288	LYS	2.6
1	L	235	VAL	2.6
1	L	299	LEU	2.6
1	K	310	GLY	2.6
1	J	352	LEU	2.6
1	J	353	GLU	2.6
1	B	267	PRO	2.6
1	L	329	THR	2.6
1	C	298	SER	2.5
1	L	253	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	331	LYS	2.5
1	H	223	ILE	2.5
1	C	271	ASP	2.5
1	E	270	ALA	2.5
1	L	285	ALA	2.5
1	L	282	ASP	2.5
1	G	325	ALA	2.4
1	L	345	LEU	2.4
1	L	246	GLY	2.4
1	K	270	ALA	2.4
1	C	267	PRO	2.4
1	L	267	PRO	2.4
1	L	321	TYR	2.4
1	L	314	LEU	2.3
1	I	270	ALA	2.3
1	L	244	PRO	2.2
1	K	376	VAL	2.2
1	E	353	GLU	2.2
1	L	322	ILE	2.2
1	L	248	LEU	2.2
1	C	224	THR	2.2
1	L	286	SER	2.2
1	L	268	LEU	2.2
1	D	333	ASN	2.2
1	C	266	PRO	2.2
1	L	257	VAL	2.1
1	L	372	ILE	2.1
1	L	328	GLN	2.1
1	L	290	LEU	2.1
1	L	376	VAL	2.1
1	J	333	ASN	2.1
1	I	299	LEU	2.1
1	D	266	PRO	2.1
1	G	266	PRO	2.1
1	J	307	PHE	2.1
1	A	257	VAL	2.0
1	J	354	THR	2.0
1	I	328	GLN	2.0
1	H	244	PRO	2.0
1	F	312	SER	2.0
1	E	282	ASP	2.0
1	L	351	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.