



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:26 PM UTC

PDB ID : 4P5H / pdb_00004p5h
Title : Structure of Clostridium perfringens Enterotoxin with a peptide derived from a modified version of ECL-2 of Claudin 2
Authors : Naylor, C.E.; Yelland, T.S.; Basak, A.K.
Deposited on : 2014-03-17
Resolution : 3.38 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

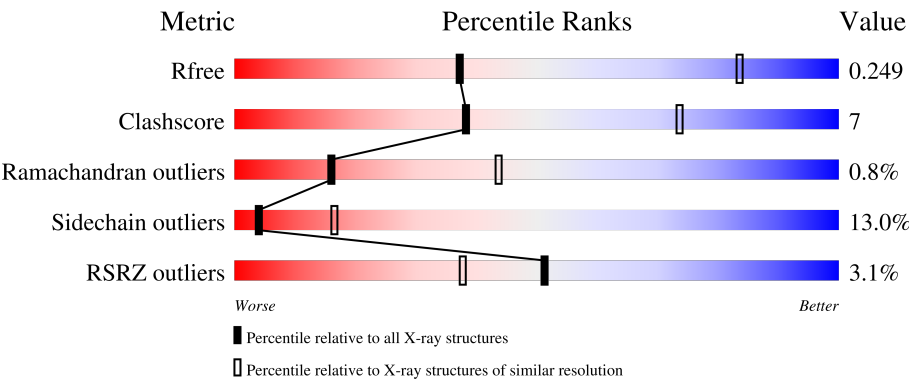
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1	20	15% 15%10%20%55%
1	2	20	5% 15%15%10%5%55%
1	3	20	10% 20%15%10%55%
1	4	20	5% 15%20%10%55%
1	P	20	5% 15%15%15%55%

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Mol	Chain	Length	Quality of chain
1	Q	20	
1	R	20	
1	S	20	
1	T	20	
1	U	20	
1	V	20	
1	W	20	
1	X	20	
1	Y	20	
1	Z	20	
2	A	286	
2	B	286	
2	C	286	
2	D	286	
2	E	286	
2	F	286	
2	G	286	
2	H	286	
2	I	286	
2	J	286	
2	K	286	
2	L	286	
2	M	286	
2	N	286	
2	O	286	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34251 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 Claudin-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	1	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	2	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	3	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	4	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	P	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	Q	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	R	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	S	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	T	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	U	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	V	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	W	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	X	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	Y	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	Z	9	Total	C	N	O	0	0	0
			60	38	10	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	149	ASN	SER	engineered mutation	UNP O88552
1	155	ALA	SER	engineered mutation	UNP O88552
2	149	ASN	SER	engineered mutation	UNP O88552
2	155	ALA	SER	engineered mutation	UNP O88552
3	149	ASN	SER	engineered mutation	UNP O88552
3	155	ALA	SER	engineered mutation	UNP O88552
4	149	ASN	SER	engineered mutation	UNP O88552
4	155	ALA	SER	engineered mutation	UNP O88552
P	149	ASN	SER	engineered mutation	UNP O88552
P	155	ALA	SER	engineered mutation	UNP O88552
Q	149	ASN	SER	engineered mutation	UNP O88552
Q	155	ALA	SER	engineered mutation	UNP O88552
R	149	ASN	SER	engineered mutation	UNP O88552
R	155	ALA	SER	engineered mutation	UNP O88552
S	149	ASN	SER	engineered mutation	UNP O88552
S	155	ALA	SER	engineered mutation	UNP O88552
T	149	ASN	SER	engineered mutation	UNP O88552
T	155	ALA	SER	engineered mutation	UNP O88552
U	149	ASN	SER	engineered mutation	UNP O88552
U	155	ALA	SER	engineered mutation	UNP O88552
V	149	ASN	SER	engineered mutation	UNP O88552
V	155	ALA	SER	engineered mutation	UNP O88552
W	149	ASN	SER	engineered mutation	UNP O88552
W	155	ALA	SER	engineered mutation	UNP O88552
X	149	ASN	SER	engineered mutation	UNP O88552
X	155	ALA	SER	engineered mutation	UNP O88552
Y	149	ASN	SER	engineered mutation	UNP O88552
Y	155	ALA	SER	engineered mutation	UNP O88552
Z	149	ASN	SER	engineered mutation	UNP O88552
Z	155	ALA	SER	engineered mutation	UNP O88552

- Molecule 2 is a protein called Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	B	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	C	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	D	286	Total	C	N	O	S	0	4	0
			2229	1413	360	452	4			
2	E	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	G	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	H	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	I	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	J	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	K	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	L	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	M	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	N	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	O	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP P01558
A	35	ALA	-	expression tag	UNP P01558
A	36	MET	-	expression tag	UNP P01558
A	37	GLY	-	expression tag	UNP P01558
B	34	GLY	-	expression tag	UNP P01558
B	35	ALA	-	expression tag	UNP P01558
B	36	MET	-	expression tag	UNP P01558
B	37	GLY	-	expression tag	UNP P01558
C	34	GLY	-	expression tag	UNP P01558
C	35	ALA	-	expression tag	UNP P01558
C	36	MET	-	expression tag	UNP P01558
C	37	GLY	-	expression tag	UNP P01558
D	34	GLY	-	expression tag	UNP P01558
D	35	ALA	-	expression tag	UNP P01558
D	36	MET	-	expression tag	UNP P01558
D	37	GLY	-	expression tag	UNP P01558
E	34	GLY	-	expression tag	UNP P01558
E	35	ALA	-	expression tag	UNP P01558
E	36	MET	-	expression tag	UNP P01558

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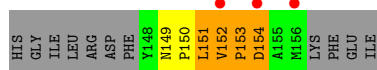
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Chain	Residue	Modelled	Actual	Comment	Reference
E	37	GLY	-	expression tag	UNP P01558
F	34	GLY	-	expression tag	UNP P01558
F	35	ALA	-	expression tag	UNP P01558
F	36	MET	-	expression tag	UNP P01558
F	37	GLY	-	expression tag	UNP P01558
G	34	GLY	-	expression tag	UNP P01558
G	35	ALA	-	expression tag	UNP P01558
G	36	MET	-	expression tag	UNP P01558
G	37	GLY	-	expression tag	UNP P01558
H	34	GLY	-	expression tag	UNP P01558
H	35	ALA	-	expression tag	UNP P01558
H	36	MET	-	expression tag	UNP P01558
H	37	GLY	-	expression tag	UNP P01558
I	34	GLY	-	expression tag	UNP P01558
I	35	ALA	-	expression tag	UNP P01558
I	36	MET	-	expression tag	UNP P01558
I	37	GLY	-	expression tag	UNP P01558
J	34	GLY	-	expression tag	UNP P01558
J	35	ALA	-	expression tag	UNP P01558
J	36	MET	-	expression tag	UNP P01558
J	37	GLY	-	expression tag	UNP P01558
K	34	GLY	-	expression tag	UNP P01558
K	35	ALA	-	expression tag	UNP P01558
K	36	MET	-	expression tag	UNP P01558
K	37	GLY	-	expression tag	UNP P01558
L	34	GLY	-	expression tag	UNP P01558
L	35	ALA	-	expression tag	UNP P01558
L	36	MET	-	expression tag	UNP P01558
L	37	GLY	-	expression tag	UNP P01558
M	34	GLY	-	expression tag	UNP P01558
M	35	ALA	-	expression tag	UNP P01558
M	36	MET	-	expression tag	UNP P01558
M	37	GLY	-	expression tag	UNP P01558
N	34	GLY	-	expression tag	UNP P01558
N	35	ALA	-	expression tag	UNP P01558
N	36	MET	-	expression tag	UNP P01558
N	37	GLY	-	expression tag	UNP P01558
O	34	GLY	-	expression tag	UNP P01558
O	35	ALA	-	expression tag	UNP P01558
O	36	MET	-	expression tag	UNP P01558
O	37	GLY	-	expression tag	UNP P01558

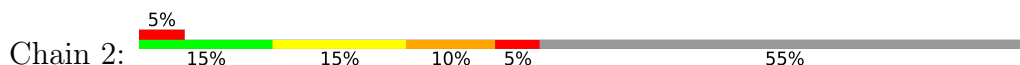
3 Residue-property plots [i](#)

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.

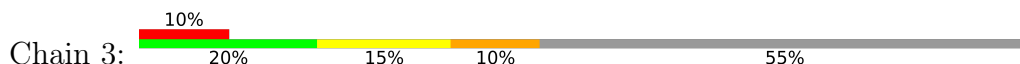
- Molecule 1: Claudin-2



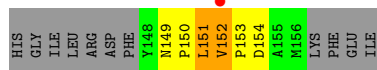
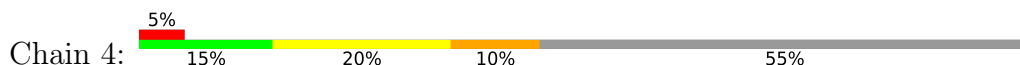
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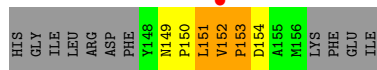
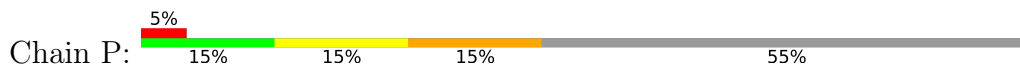
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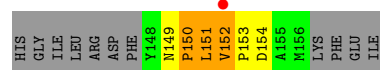
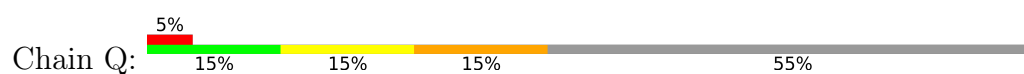
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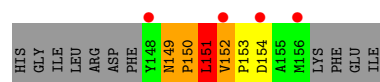
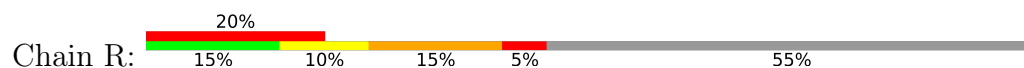
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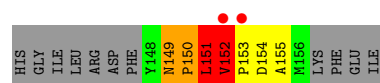
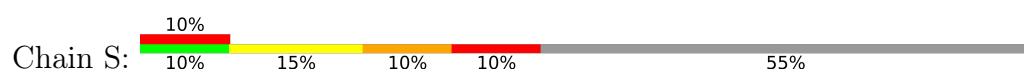
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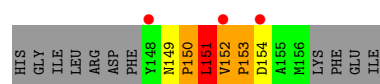
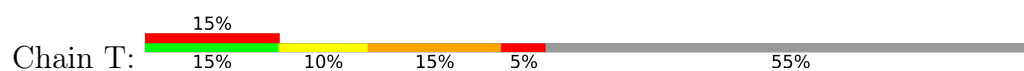
• Molecule 1: Claudin-2



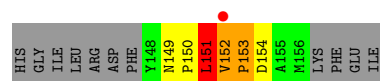
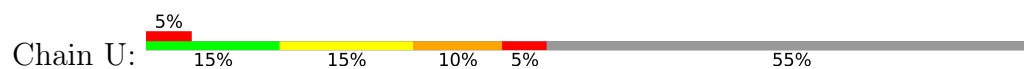
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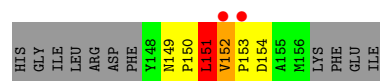
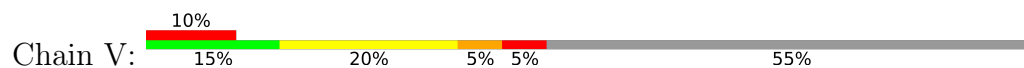
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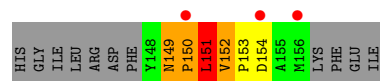
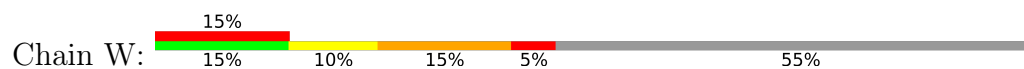
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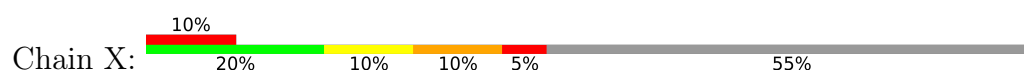
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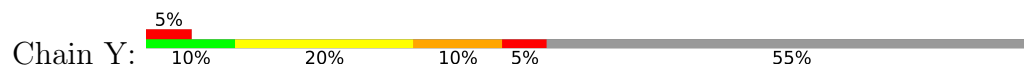
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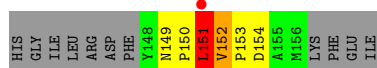
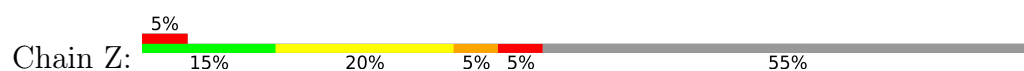
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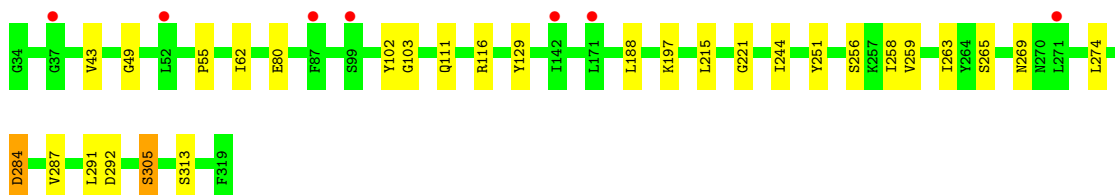
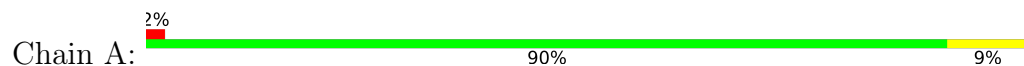
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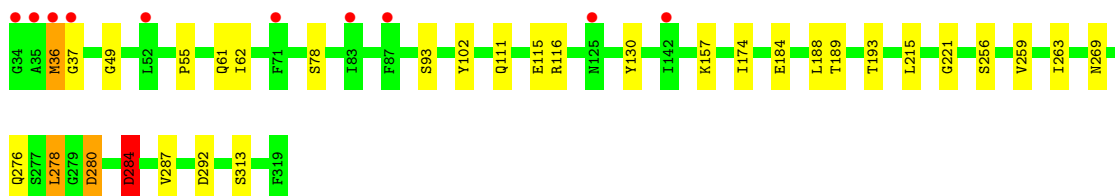
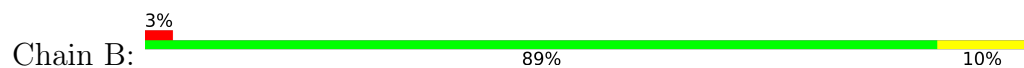
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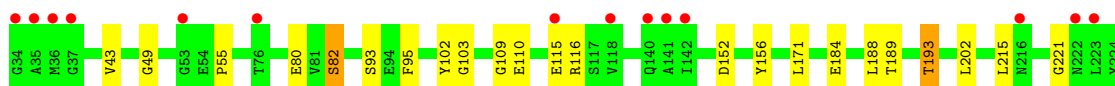
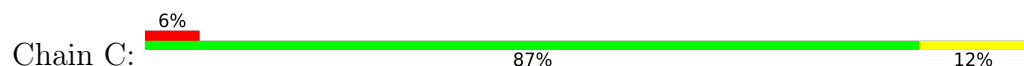
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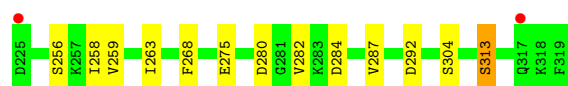


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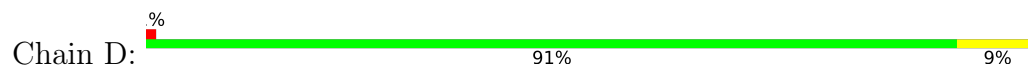


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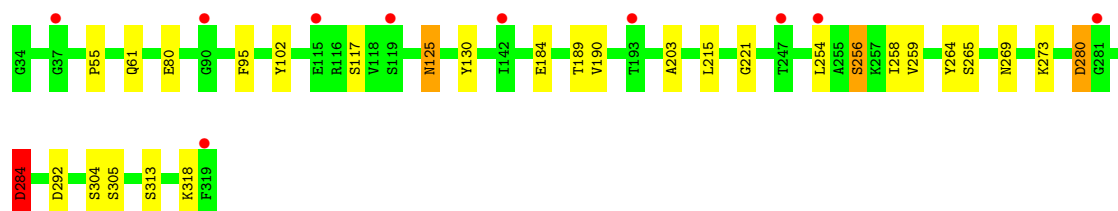




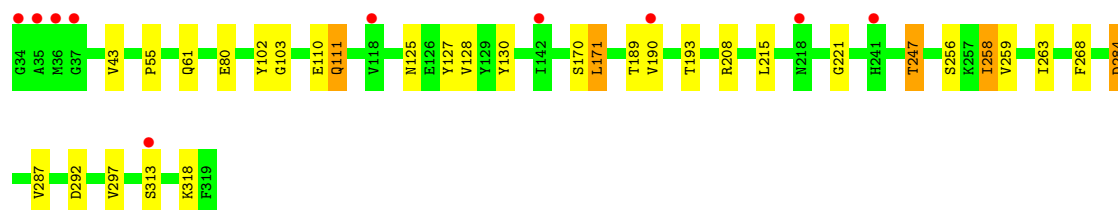
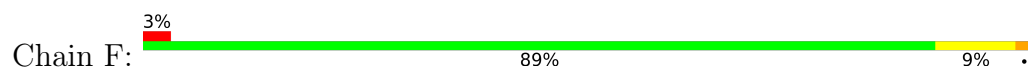
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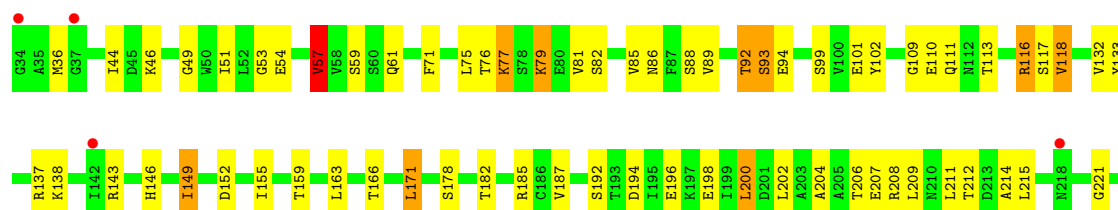
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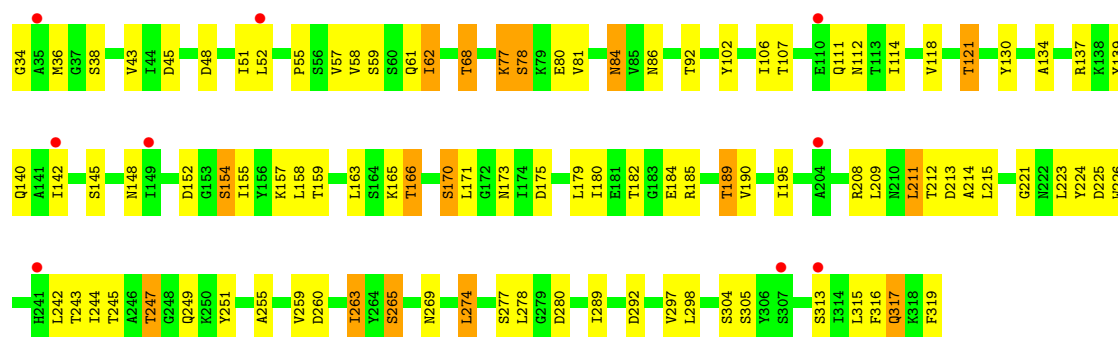


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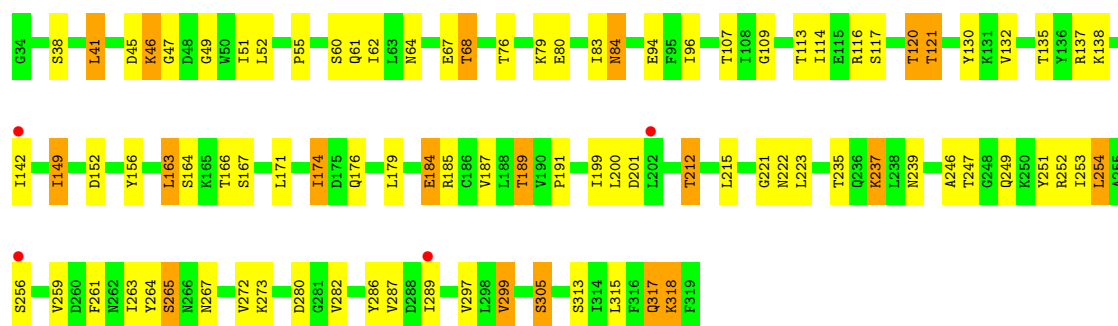


- Molecule 2: Heat-labile enterotoxin B chain

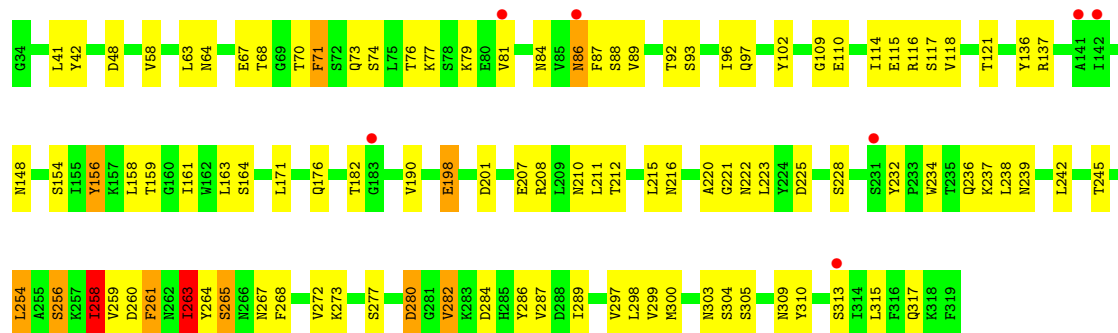




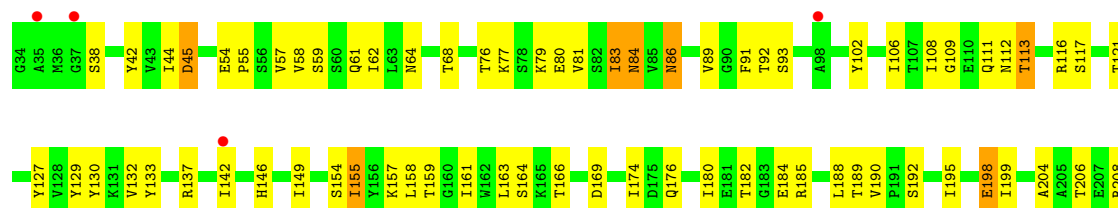
• Molecule 2: Heat-labile enterotoxin B chain

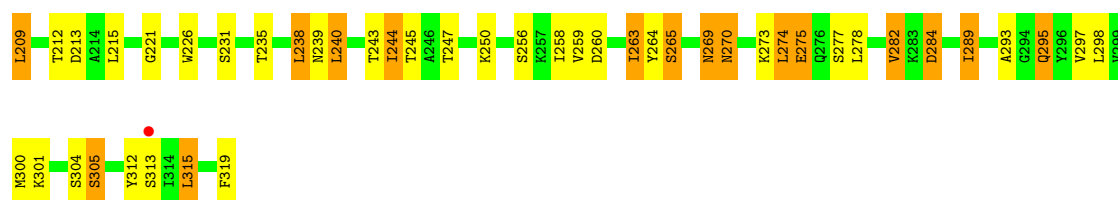


• Molecule 2: Heat-labile enterotoxin B chain

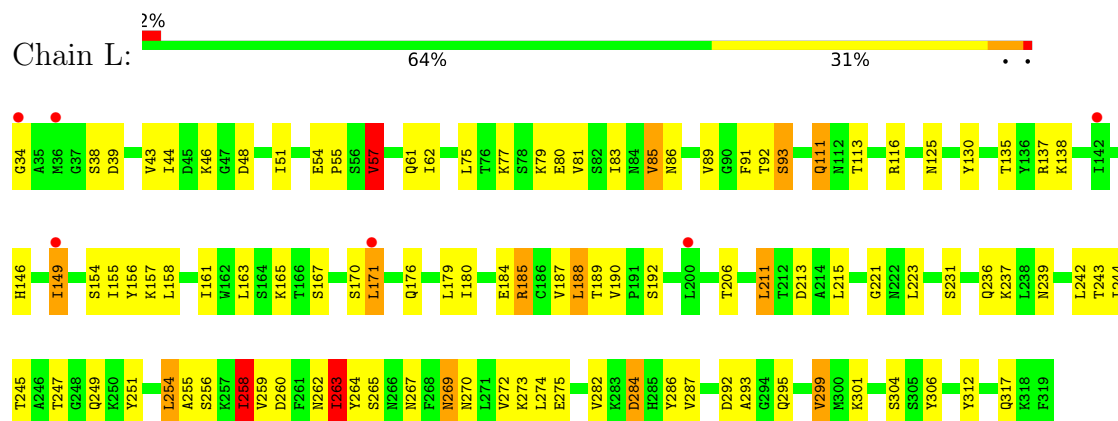


• Molecule 2: Heat-labile enterotoxin B chain

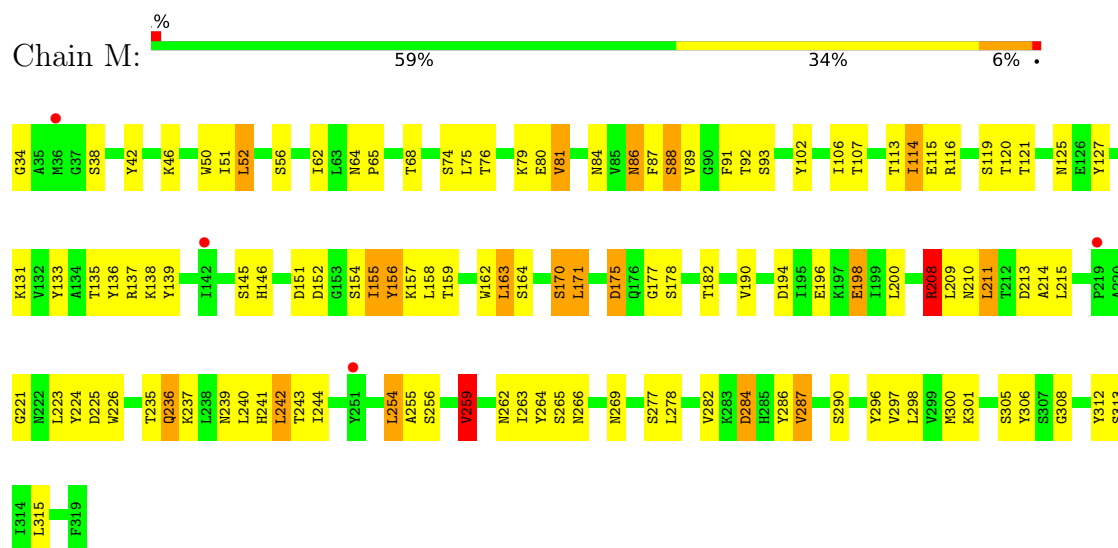




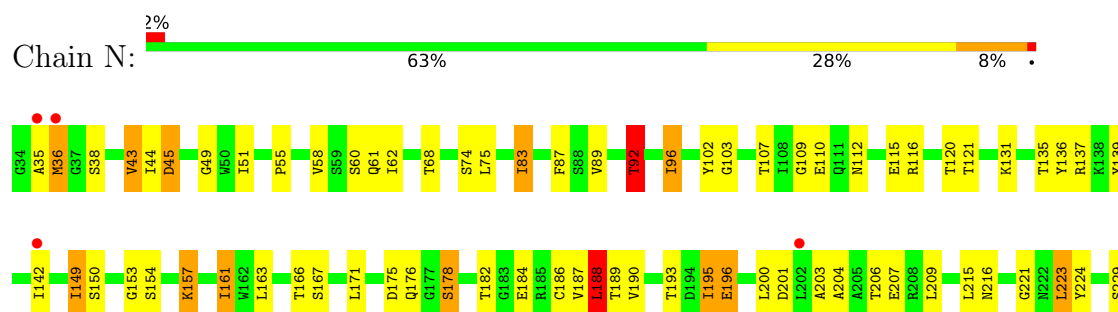
• Molecule 2: Heat-labile enterotoxin B chain



• Molecule 2: Heat-labile enterotoxin B chain

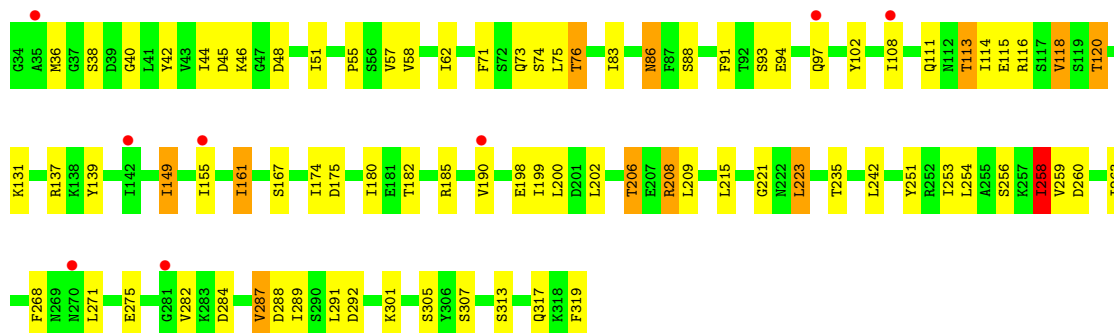


• Molecule 2: Heat-labile enterotoxin B chain





● Molecule 2: Heat-labile enterotoxin B chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	369.60Å 100.26Å 265.36Å 90.00° 119.74° 90.00°	Depositor
Resolution (Å)	48.98 – 3.38 48.98 – 3.38	Depositor EDS
% Data completeness (in resolution range)	80.8 (48.98-3.38) 81.4 (48.98-3.38)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.204 , 0.240 (Not available) , 0.249	Depositor DCC
R_{free} test set	4849 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	1.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 137.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	34251	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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	1	1.70	1/61 (1.6%)	2.42	10/85 (11.8%)
1	2	1.93	3/61 (4.9%)	2.47	8/85 (9.4%)
1	3	1.76	1/61 (1.6%)	2.41	6/85 (7.1%)
1	4	1.89	1/61 (1.6%)	2.43	8/85 (9.4%)
1	P	1.53	1/61 (1.6%)	2.29	8/85 (9.4%)
1	Q	1.89	2/61 (3.3%)	2.61	8/85 (9.4%)
1	R	1.95	3/61 (4.9%)	2.40	6/85 (7.1%)
1	S	2.20	4/61 (6.6%)	2.58	8/85 (9.4%)
1	T	1.78	2/61 (3.3%)	2.15	8/85 (9.4%)
1	U	1.79	1/61 (1.6%)	2.35	4/85 (4.7%)
1	V	1.65	1/61 (1.6%)	2.53	8/85 (9.4%)
1	W	2.07	4/61 (6.6%)	2.30	8/85 (9.4%)
1	X	1.85	2/61 (3.3%)	2.93	7/85 (8.2%)
1	Y	1.92	2/61 (3.3%)	2.37	8/85 (9.4%)
1	Z	1.74	1/61 (1.6%)	2.29	6/85 (7.1%)
2	A	0.73	0/2276	1.14	3/3094 (0.1%)
2	B	0.74	0/2276	1.15	4/3094 (0.1%)
2	C	0.76	0/2276	1.18	8/3094 (0.3%)
2	D	0.79	0/2282	1.16	3/3101 (0.1%)
2	E	0.72	0/2276	1.15	8/3094 (0.3%)
2	F	0.73	0/2276	1.15	5/3094 (0.2%)
2	G	0.82	0/2276	1.34	17/3094 (0.5%)
2	H	0.86	0/2276	1.36	22/3094 (0.7%)
2	I	0.81	1/2276 (0.0%)	1.30	14/3094 (0.5%)
2	J	0.82	0/2276	1.29	16/3094 (0.5%)
2	K	0.84	1/2276 (0.0%)	1.33	15/3094 (0.5%)
2	L	0.81	0/2276	1.32	19/3094 (0.6%)
2	M	0.84	0/2276	1.35	17/3094 (0.5%)
2	N	0.85	1/2276 (0.0%)	1.36	22/3094 (0.7%)
2	O	0.87	1/2276 (0.0%)	1.33	17/3094 (0.5%)
All	All	0.85	33/35061 (0.1%)	1.31	301/47692 (0.6%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	151	LEU	C-N	8.10	1.42	1.33
1	W	152	VAL	CA-C	7.17	1.60	1.52
1	W	150	PRO	C-N	7.00	1.43	1.33
1	2	152	VAL	CA-C	6.90	1.60	1.52
1	W	151	LEU	CA-C	6.86	1.61	1.52
1	U	152	VAL	CA-C	6.28	1.59	1.52
1	S	152	VAL	CA-C	6.23	1.59	1.52
1	R	151	LEU	C-N	6.10	1.40	1.33
1	T	152	VAL	CA-C	6.10	1.59	1.52
2	N	35	ALA	C-N	6.09	1.38	1.33
1	Z	152	VAL	CA-C	5.97	1.59	1.52
1	V	152	VAL	CA-C	5.95	1.59	1.52
1	R	152	VAL	CA-C	5.80	1.58	1.52
1	Q	150	PRO	C-N	5.73	1.41	1.33
1	X	151	LEU	CA-C	5.66	1.60	1.52
1	Y	150	PRO	C-N	5.61	1.41	1.33
1	3	149	ASN	CA-C	5.54	1.59	1.53
2	O	258	ILE	CA-CB	5.53	1.61	1.54
1	S	151	LEU	CA-C	5.49	1.60	1.52
1	1	151	LEU	CA-C	5.39	1.59	1.52
1	X	152	VAL	CA-C	5.36	1.58	1.52
1	Y	151	LEU	CA-C	5.34	1.59	1.52
1	W	151	LEU	C-N	5.33	1.39	1.33
1	S	152	VAL	N-CA	5.32	1.53	1.46
1	P	152	VAL	CA-C	5.24	1.58	1.52
1	2	151	LEU	C-N	5.22	1.39	1.33
1	2	150	PRO	C-N	5.21	1.41	1.33
1	Q	151	LEU	C-N	5.13	1.39	1.33
1	T	150	PRO	C-N	5.13	1.40	1.33
2	K	149	ILE	CG1-CD1	5.13	1.71	1.51
1	4	152	VAL	CA-C	5.10	1.58	1.52
2	I	149	ILE	CG1-CD1	5.05	1.71	1.51
1	R	150	PRO	C-N	5.01	1.40	1.33

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	190	VAL	N-CA-CB	14.86	126.66	111.36
2	E	190	VAL	N-CA-CB	10.34	122.01	111.36
1	X	150	PRO	CA-C-N	9.98	140.60	121.54
1	X	150	PRO	C-N-CA	9.98	140.60	121.54
2	B	284	ASP	CA-CB-CG	9.65	122.25	112.60
2	A	284	ASP	CA-CB-CG	9.37	121.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	151	LEU	N-CA-C	9.20	130.40	110.80
1	Q	154	ASP	N-CA-C	8.84	123.32	108.20
2	O	319	PHE	CA-CB-CG	8.78	122.58	113.80
1	S	154	ASP	N-CA-C	8.69	122.41	108.41
2	H	280	ASP	CA-CB-CG	8.48	121.08	112.60
1	Q	151	LEU	N-CA-C	8.42	128.74	110.80
2	F	284	ASP	CA-CB-CG	8.38	120.98	112.60
1	U	154	ASP	N-CA-C	8.36	122.49	108.20
1	S	149	ASN	N-CA-C	8.29	124.05	108.97
1	3	151	LEU	N-CA-C	8.23	128.32	110.80
1	1	152	VAL	N-CA-C	8.18	126.54	108.88
1	V	152	VAL	N-CA-C	8.15	126.48	108.88
1	2	154	ASP	N-CA-C	8.10	121.93	108.73
1	U	152	VAL	N-CA-C	8.08	126.34	108.88
2	K	83	ILE	N-CA-CB	8.02	121.69	111.83
2	A	80	GLU	CB-CG-CD	7.99	126.18	112.60
1	3	152	VAL	N-CA-C	7.98	126.12	108.88
1	P	152	VAL	N-CA-C	7.98	126.12	108.88
2	N	83	ILE	N-CA-CB	7.97	121.64	111.83
1	V	154	ASP	N-CA-C	7.97	121.73	108.73
2	O	83	ILE	N-CA-CB	7.92	121.58	111.83
1	W	154	ASP	N-CA-C	7.88	121.67	108.20
2	G	260	ASP	CA-CB-CG	7.83	120.43	112.60
1	U	151	LEU	N-CA-C	7.81	127.44	110.80
1	Y	152	VAL	N-CA-C	7.78	125.69	108.88
2	D	86	ASN	CA-CB-CG	7.78	120.38	112.60
2	K	269	ASN	CA-CB-CG	7.76	120.36	112.60
2	H	190	VAL	CB-CA-C	7.74	118.44	111.08
1	Z	154	ASP	N-CA-C	7.72	121.40	108.20
2	N	239	ASN	CA-CB-CG	7.67	120.28	112.60
2	I	45	ASP	CA-CB-CG	7.67	120.27	112.60
2	I	261	PHE	CA-CB-CG	7.67	121.47	113.80
2	G	92	THR	CB-CA-C	-7.67	96.02	110.51
2	O	287	VAL	N-CA-CB	7.66	124.01	111.45
1	4	152	VAL	N-CA-C	7.65	125.41	108.88
1	X	154	ASP	N-CA-C	7.62	121.23	108.20
2	M	152	ASP	CA-CB-CG	7.61	120.21	112.60
1	Q	149	ASN	N-CA-C	7.61	123.57	110.02
1	4	154	ASP	N-CA-C	7.56	120.58	108.41
1	T	154	ASP	N-CA-C	7.55	121.10	108.20
1	Q	152	VAL	N-CA-C	7.52	125.12	108.88
1	P	151	LEU	N-CA-C	7.49	126.74	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	216	ASN	CA-CB-CG	7.48	120.08	112.60
1	R	154	ASP	N-CA-C	7.48	120.99	108.20
2	H	319	PHE	CA-CB-CG	7.41	121.21	113.80
1	R	152	VAL	N-CA-C	7.41	124.87	108.88
1	4	151	LEU	N-CA-C	7.35	126.45	110.80
2	G	259	VAL	N-CA-CB	7.31	121.50	111.41
2	O	57	VAL	N-CA-CB	7.30	119.29	110.31
2	I	64	ASN	CB-CA-C	7.29	120.96	109.37
2	J	303	ASN	CA-CB-CG	7.28	119.88	112.60
2	O	190	VAL	N-CA-CB	7.27	118.85	111.36
1	R	149	ASN	N-CA-C	7.24	122.91	110.02
1	T	152	VAL	N-CA-C	7.24	124.52	108.88
2	N	190	VAL	CB-CA-C	7.22	117.94	111.08
1	V	151	LEU	N-CA-C	7.19	126.11	110.80
2	H	57	VAL	N-CA-CB	7.14	119.10	110.31
1	Z	152	VAL	N-CA-C	7.11	124.24	108.88
1	1	151	LEU	N-CA-C	7.11	125.93	110.80
1	Y	154	ASP	N-CA-C	7.10	120.35	108.20
1	S	151	LEU	CA-C-N	7.09	135.25	122.13
1	S	151	LEU	C-N-CA	7.09	135.25	122.13
2	O	260	ASP	CA-CB-CG	7.07	119.67	112.60
2	K	284	ASP	CA-CB-CG	7.06	119.66	112.60
2	N	230	ASN	CA-CB-CG	7.05	119.65	112.60
1	U	149	ASN	N-CA-C	7.04	121.79	108.97
2	J	212	THR	CB-CA-C	7.03	122.46	110.79
2	M	284	ASP	CA-CB-CG	7.01	119.61	112.60
2	H	212	THR	CB-CA-C	7.00	122.41	110.79
2	N	87	PHE	CA-CB-CG	6.94	120.74	113.80
2	L	57	VAL	N-CA-CB	6.94	118.85	110.31
1	Z	151	LEU	N-CA-C	6.92	125.53	110.80
2	G	110	GLU	CB-CG-CD	6.91	124.35	112.60
1	X	152	VAL	N-CA-C	6.89	123.76	108.88
1	2	152	VAL	N-CA-C	6.88	123.74	108.88
1	S	152	VAL	N-CA-C	6.85	123.67	108.88
1	3	154	ASP	N-CA-C	6.82	119.86	108.20
1	R	151	LEU	N-CA-C	6.81	125.31	110.80
2	O	45	ASP	CA-CB-CG	6.79	119.39	112.60
2	N	247	THR	CB-CA-C	6.77	120.94	109.50
2	H	190	VAL	N-CA-CB	6.76	118.33	111.36
2	O	190	VAL	CB-CA-C	6.76	117.50	111.08
2	K	45	ASP	CA-CB-CG	6.73	119.33	112.60
2	M	239	ASN	CA-CB-CG	6.73	119.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	154	ASP	N-CA-C	6.71	119.67	108.20
2	C	80	GLU	CB-CG-CD	6.70	123.98	112.60
1	1	149	ASN	N-CA-C	6.68	121.13	108.97
2	H	189	THR	CB-CA-C	6.67	121.86	110.79
2	G	212	THR	CB-CA-C	6.66	121.33	110.88
1	2	151	LEU	CA-C-N	6.65	134.43	122.13
1	2	151	LEU	C-N-CA	6.65	134.43	122.13
1	T	151	LEU	N-CA-C	6.64	124.94	110.80
1	V	149	ASN	N-CA-C	6.63	121.03	108.97
1	S	151	LEU	N-CA-C	6.62	124.91	110.80
1	4	149	ASN	N-CA-C	6.62	121.80	110.02
2	O	94	GLU	CB-CG-CD	6.62	123.85	112.60
2	E	284	ASP	CA-CB-CG	6.61	119.21	112.60
2	J	261	PHE	CA-CB-CG	6.60	120.40	113.80
2	M	87	PHE	CA-CB-CG	-6.59	107.21	113.80
2	O	206	THR	CB-CA-C	6.58	122.38	109.35
2	I	280	ASP	CA-CB-CG	6.57	119.17	112.60
1	R	151	LEU	CA-C-N	6.56	134.26	122.13
1	R	151	LEU	C-N-CA	6.56	134.26	122.13
2	J	225	ASP	CA-CB-CG	6.55	119.16	112.60
2	K	260	ASP	CA-CB-CG	6.55	119.15	112.60
2	E	80	GLU	CB-CG-CD	6.53	123.69	112.60
1	X	150	PRO	CB-CA-C	6.52	128.31	112.00
1	Y	151	LEU	N-CA-C	6.51	124.67	110.80
2	O	86	ASN	CA-CB-CG	6.51	119.11	112.60
2	J	216	ASN	CA-CB-CG	-6.50	106.10	112.60
1	2	149	ASN	N-CA-C	6.49	120.79	108.97
1	2	151	LEU	N-CA-C	6.46	124.56	110.80
2	K	282	VAL	CB-CA-C	6.44	117.22	110.91
2	K	86	ASN	CA-CB-CG	6.41	119.01	112.60
2	L	239	ASN	CA-CB-CG	6.39	118.99	112.60
2	N	262	ASN	CA-CB-CG	6.38	118.98	112.60
2	G	303	ASN	CA-CB-CG	6.38	118.98	112.60
1	W	152	VAL	N-CA-C	6.37	122.64	108.88
2	M	86	ASN	CA-CB-CG	6.33	118.93	112.60
1	W	150	PRO	CA-C-N	6.32	133.61	121.54
1	W	150	PRO	C-N-CA	6.32	133.61	121.54
2	K	270	ASN	CA-CB-CG	6.31	118.91	112.60
2	C	152	ASP	CA-CB-CG	6.31	118.91	112.60
2	N	188	LEU	CA-C-N	6.30	128.64	120.44
2	N	188	LEU	C-N-CA	6.30	128.64	120.44
1	P	149	ASN	N-CA-C	6.30	121.24	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	152	ASP	CA-CB-CG	6.28	118.88	112.60
1	W	151	LEU	CA-C-N	6.28	133.75	122.13
1	W	151	LEU	C-N-CA	6.28	133.75	122.13
1	Z	150	PRO	CA-C-N	6.28	133.53	121.54
1	Z	150	PRO	C-N-CA	6.28	133.53	121.54
2	L	284	ASP	CA-CB-CG	6.27	118.87	112.60
2	N	92	THR	CB-CA-C	-6.27	99.06	111.60
2	M	259	VAL	N-CA-CB	6.26	120.06	111.41
2	I	189	THR	CB-CA-C	6.26	121.50	110.85
2	M	196	GLU	CB-CG-CD	6.23	123.19	112.60
2	O	120	THR	CB-CA-C	6.23	122.03	109.38
2	N	107	THR	CB-CA-C	6.21	120.53	109.65
2	D	152	ASP	CA-CB-CG	6.21	118.81	112.60
1	W	149	ASN	N-CA-C	6.19	120.24	108.97
1	2	150	PRO	CA-C-N	6.19	133.36	121.54
1	2	150	PRO	C-N-CA	6.19	133.36	121.54
1	Y	151	LEU	CA-C-N	6.16	133.53	122.13
1	Y	151	LEU	C-N-CA	6.16	133.53	122.13
2	L	80	GLU	CB-CG-CD	6.16	123.07	112.60
2	L	188	LEU	CA-C-N	6.16	128.44	120.44
2	L	188	LEU	C-N-CA	6.16	128.44	120.44
2	K	84	ASN	CA-CB-CG	6.15	118.75	112.60
2	J	86	ASN	CA-CB-CG	6.12	118.72	112.60
2	J	280	ASP	CA-CB-CG	6.11	118.71	112.60
2	F	189	THR	CB-CA-C	6.09	121.21	110.85
2	M	80	GLU	CB-CG-CD	6.08	122.93	112.60
1	Y	149	ASN	N-CA-C	6.06	120.00	108.97
2	I	239	ASN	CA-CB-CG	6.02	118.62	112.60
2	E	190	VAL	CB-CA-C	5.99	116.77	111.08
2	C	189	THR	CB-CA-C	5.99	121.03	110.85
2	J	239	ASN	CA-CB-CG	5.98	118.58	112.60
1	1	154	ASP	CA-C-N	5.98	129.70	121.33
1	1	154	ASP	C-N-CA	5.98	129.70	121.33
2	L	85	VAL	CB-CA-C	5.97	119.71	110.28
1	W	151	LEU	N-CA-C	5.96	123.49	110.80
2	G	314	ILE	N-CA-CB	5.95	120.21	111.52
2	I	191	PRO	CB-CA-C	5.89	119.06	111.46
2	I	152	ASP	CA-CB-CG	5.88	118.48	112.60
2	G	272	VAL	CB-CA-C	5.88	118.36	110.42
1	V	151	LEU	CA-C-N	5.88	133.00	122.13
1	V	151	LEU	C-N-CA	5.88	133.00	122.13
1	T	149	ASN	N-CA-C	5.87	119.65	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	247	THR	CB-CA-C	5.86	119.41	109.50
2	G	253	ILE	N-CA-CB	5.85	119.04	111.67
2	O	42	TYR	CA-CB-CG	5.84	124.42	113.90
2	I	84	ASN	CA-CB-CG	5.82	118.42	112.60
1	Y	150	PRO	CA-C-N	5.82	132.66	121.54
1	Y	150	PRO	C-N-CA	5.82	132.66	121.54
1	S	150	PRO	CA-C-N	5.80	132.62	121.54
1	S	150	PRO	C-N-CA	5.80	132.62	121.54
2	H	80	GLU	CB-CG-CD	5.78	122.43	112.60
1	P	151	LEU	CA-C-N	5.77	132.81	122.13
1	P	151	LEU	C-N-CA	5.77	132.81	122.13
2	K	212	THR	CB-CA-C	5.76	119.92	110.88
1	Z	149	ASN	N-CA-C	5.76	119.45	108.97
2	L	213	ASP	CA-CB-CG	5.75	118.35	112.60
2	C	110	GLU	CB-CG-CD	5.72	122.32	112.60
2	G	132	VAL	CB-CA-C	5.71	119.29	110.96
2	O	288	ASP	CA-CB-CG	5.71	118.31	112.60
1	Q	151	LEU	CA-C-N	5.70	132.67	122.13
1	Q	151	LEU	C-N-CA	5.70	132.67	122.13
1	1	151	LEU	CA-C-N	5.66	132.59	122.13
1	1	151	LEU	C-N-CA	5.66	132.59	122.13
2	H	247	THR	CB-CA-C	5.65	119.05	109.50
2	D	80	GLU	CB-CG-CD	5.64	122.19	112.60
2	L	247	THR	CB-CA-C	5.64	119.03	109.50
1	1	154	ASP	N-CA-C	5.63	118.22	107.75
2	M	135	THR	CB-CA-C	5.63	119.68	109.37
1	Q	154	ASP	CA-CB-CG	-5.63	106.97	112.60
2	L	34	GLY	CA-C-N	5.63	127.75	120.44
2	L	34	GLY	C-N-CA	5.63	127.75	120.44
2	H	81	VAL	N-CA-CB	5.62	119.16	111.41
2	B	189	THR	CB-CA-C	5.61	120.09	110.79
2	I	212	THR	CB-CA-C	5.60	120.08	110.79
2	H	175	ASP	CA-CB-CG	5.59	118.19	112.60
2	M	208	ARG	CB-CA-C	5.59	121.06	109.38
2	I	120	THR	CB-CA-C	5.59	120.72	109.38
2	M	225	ASP	CA-CB-CG	5.58	118.18	112.60
2	M	242	LEU	N-CA-C	5.57	118.04	109.07
2	L	263	ILE	N-CA-CB	5.57	118.82	111.25
2	E	280	ASP	CA-CB-CG	5.56	118.16	112.60
2	J	245	THR	CB-CA-C	5.55	118.96	109.24
1	V	154	ASP	CA-C-N	5.55	129.10	121.33
1	V	154	ASP	C-N-CA	5.55	129.10	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	149	ASN	N-CA-C	5.55	119.90	110.02
2	G	266	ASN	CA-CB-CG	5.55	118.15	112.60
2	L	83	ILE	N-CA-CB	5.55	118.66	111.83
2	G	319	PHE	CA-CB-CG	5.53	119.33	113.80
2	H	152	ASP	CA-CB-CG	5.52	118.12	112.60
2	H	84	ASN	CA-CB-CG	5.51	118.11	112.60
1	T	151	LEU	CA-C-N	5.50	132.31	122.13
1	T	151	LEU	C-N-CA	5.50	132.31	122.13
2	M	175	ASP	CA-CB-CG	5.49	118.09	112.60
2	K	80	GLU	CB-CG-CD	5.49	121.93	112.60
2	G	265	SER	N-CA-C	-5.43	101.68	110.32
1	P	150	PRO	CA-C-N	5.41	131.88	121.54
1	P	150	PRO	C-N-CA	5.41	131.88	121.54
2	K	265	SER	N-CA-C	-5.41	101.72	110.32
2	K	188	LEU	CA-C-N	5.40	127.46	120.44
2	K	188	LEU	C-N-CA	5.40	127.46	120.44
2	O	242	LEU	N-CA-C	5.38	117.73	109.07
2	G	309	ASN	CA-CB-CG	5.38	117.97	112.60
2	O	175	ASP	CA-CB-CG	5.37	117.97	112.60
2	L	258	ILE	CB-CA-C	-5.37	104.52	111.88
2	I	265	SER	N-CA-C	-5.36	101.80	110.32
2	F	297	VAL	N-CA-CB	5.36	120.26	111.58
2	N	36[A]	MET	CA-C-O	5.33	121.03	117.94
2	N	36[B]	MET	CA-C-O	5.33	121.03	117.94
2	B	269	ASN	CA-CB-CG	5.32	117.92	112.60
2	J	258	ILE	CB-CA-C	5.31	119.16	111.88
2	J	210	ASN	N-CA-CB	5.31	118.26	110.35
2	G	149	ILE	CB-CA-C	-5.31	105.56	111.35
1	4	151	LEU	CA-C-N	5.31	131.95	122.13
1	4	151	LEU	C-N-CA	5.31	131.95	122.13
2	H	225	ASP	CA-CB-CG	5.31	117.91	112.60
2	L	189	THR	CA-C-N	5.30	131.94	122.13
2	L	189	THR	C-N-CA	5.30	131.94	122.13
2	N	45	ASP	CA-CB-CG	5.30	117.90	112.60
1	1	150	PRO	CA-C-N	5.30	131.66	121.54
1	1	150	PRO	C-N-CA	5.30	131.66	121.54
1	T	150	PRO	CA-C-N	5.30	131.66	121.54
1	T	150	PRO	C-N-CA	5.30	131.66	121.54
2	H	265	SER	N-CA-C	-5.27	101.93	110.32
2	H	213	ASP	CA-CB-CG	5.27	117.87	112.60
2	K	289	ILE	N-CA-C	5.26	115.29	108.35
2	M	266	ASN	CA-CB-CG	5.25	117.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	151	LEU	CA-C-N	5.24	131.82	122.13
1	3	151	LEU	C-N-CA	5.24	131.82	122.13
2	N	284	ASP	N-CA-CB	5.24	117.85	110.36
2	C	280	ASP	CA-CB-CG	5.22	117.82	112.60
2	H	58	VAL	CB-CA-C	5.22	116.57	110.88
2	J	260	ASP	CA-CB-CG	5.22	117.82	112.60
1	X	150	PRO	CA-N-CD	-5.21	104.21	111.50
2	E	125	ASN	CA-CB-CG	-5.21	107.39	112.60
2	H	289	ILE	N-CA-C	5.18	115.19	108.35
2	N	43	VAL	CB-CA-C	5.17	118.29	110.63
2	H	43	VAL	N-CA-CB	5.17	118.54	111.41
2	I	94	GLU	CB-CG-CD	5.16	121.37	112.60
2	J	87	PHE	CA-CB-CG	-5.15	108.65	113.80
2	L	260	ASP	CA-CB-CG	5.15	117.75	112.60
2	M	34	GLY	CA-C-N	5.15	127.13	120.44
2	M	34	GLY	C-N-CA	5.15	127.13	120.44
2	F	80	GLU	CB-CG-CD	5.12	121.31	112.60
2	A	265	SER	N-CA-C	-5.12	102.19	110.32
2	J	263	ILE	N-CA-CB	5.11	120.67	111.21
2	C	282	VAL	N-CA-CB	5.11	115.83	111.64
2	C	193[A]	THR	CB-CA-C	5.08	118.02	109.89
2	C	193[B]	THR	CB-CA-C	5.08	118.02	109.89
2	I	289	ILE	N-CA-C	5.07	115.04	108.35
2	L	89	VAL	CB-CA-C	5.07	118.88	111.33
2	B	280	ASP	CA-CB-CG	5.06	117.66	112.60
2	N	201	ASP	CA-CB-CG	5.06	117.66	112.60
1	4	150	PRO	CA-C-N	5.06	131.20	121.54
1	4	150	PRO	C-N-CA	5.06	131.20	121.54
2	E	265	SER	N-CA-C	-5.06	102.28	110.32
2	N	244	ILE	N-CA-CB	5.05	118.20	111.64
2	M	265	SER	N-CA-C	-5.05	102.29	110.32
2	J	265	SER	N-CA-C	-5.04	102.30	110.32
2	H	148	ASN	CA-CB-CG	5.04	117.64	112.60
2	J	110	GLU	CB-CG-CD	5.04	121.17	112.60
2	L	236	GLN	N-CA-C	5.04	116.94	108.73
2	N	284	ASP	CA-CB-CG	5.03	117.63	112.60
2	G	57	VAL	N-CA-CB	5.02	116.48	110.31
2	H	34	GLY	CA-C-N	5.02	126.97	120.44
2	H	34	GLY	C-N-CA	5.02	126.97	120.44
1	Q	149	ASN	CA-CB-CG	-5.02	107.58	112.60
2	N	236	GLN	N-CA-C	5.01	116.90	108.73
2	E	189	THR	CB-CA-C	5.00	119.35	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	282	VAL	CB-CA-C	5.00	115.50	111.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	60	0	52	5	0
1	2	60	0	52	6	0
1	3	60	0	52	1	0
1	4	60	0	52	3	0
1	P	60	0	52	4	0
1	Q	60	0	52	3	0
1	R	60	0	52	4	0
1	S	60	0	52	5	0
1	T	60	0	52	7	0
1	U	60	0	52	5	0
1	V	60	0	52	4	0
1	W	60	0	52	5	0
1	X	60	0	52	2	0
1	Y	60	0	52	2	0
1	Z	60	0	52	4	0
2	A	2223	0	2147	21	0
2	B	2223	0	2147	19	0
2	C	2223	0	2147	21	0
2	D	2229	0	2158	15	0
2	E	2223	0	2147	16	0
2	F	2223	0	2147	16	0
2	G	2223	0	2147	49	0
2	H	2223	0	2147	37	0
2	I	2223	0	2147	34	0
2	J	2223	0	2147	46	0
2	K	2223	0	2147	53	0
2	L	2223	0	2147	46	0
2	M	2223	0	2147	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	2223	0	2147	50	0
2	O	2223	0	2147	33	0
All	All	34251	0	32996	461	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 7.

All (461) 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)
2:G:111:GLN:HE22	2:I:109:GLY:HA2	1.19	1.07
2:A:259:VAL:HG21	1:P:152:VAL:HG21	1.46	0.97
2:M:254:LEU:HG	2:M:286:TYR:HB3	1.50	0.94
2:B:259:VAL:HG21	1:Q:152:VAL:HG21	1.51	0.93
2:E:259:VAL:HG21	1:T:152:VAL:HG21	1.52	0.91
2:L:54:GLU:O	2:L:57:VAL:HG22	1.78	0.84
2:B:263:ILE:HD11	2:B:287:VAL:HG21	1.60	0.83
2:K:81:VAL:HG21	2:K:93:SER:HB3	1.62	0.81
2:G:46:LYS:HD2	2:G:194:ASP:OD2	1.83	0.80
2:G:111:GLN:NE2	2:I:109:GLY:HA2	1.98	0.79
2:D:254:LEU:HD12	2:D:286:TYR:HB3	1.65	0.78
2:D:259:VAL:HG21	1:S:152:VAL:HG21	1.66	0.77
2:G:54:GLU:O	2:G:57:VAL:HG23	1.84	0.77
2:L:86:ASN:ND2	2:L:91:PHE:HB3	1.99	0.77
2:G:57:VAL:HG22	2:G:133:TYR:CE2	2.19	0.77
2:K:263:ILE:HD12	2:K:274:LEU:HB2	1.67	0.77
2:H:259:VAL:HG21	1:W:152:VAL:HG21	1.67	0.76
2:L:171:LEU:HD12	2:L:171:LEU:H	1.52	0.74
2:N:276:GLN:HE21	2:N:278:LEU:HD11	1.53	0.73
2:M:262:ASN:HB3	2:M:264:TYR:HE1	1.52	0.73
1:4:152:VAL:HG21	2:O:259:VAL:HG21	1.69	0.73
2:F:263:ILE:HD11	2:F:287:VAL:HG21	1.71	0.72
1:4:152:VAL:H	2:O:256:SER:HB3	1.54	0.72
2:A:258:ILE:HD11	1:P:153:PRO:HG3	1.72	0.72
2:F:259:VAL:HG21	1:U:152:VAL:HG21	1.72	0.72
2:F:313:SER:H	1:U:152:VAL:HG22	1.53	0.72
1:S:150:PRO:O	1:S:151:LEU:HD12	1.90	0.72
2:K:68:THR:OG1	2:K:121:THR:HG23	1.88	0.71
2:E:61:GLN:HB3	2:E:130:TYR:CE2	2.25	0.71
2:K:259:VAL:HG21	1:Z:152:VAL:HG21	1.72	0.71
2:C:259:VAL:HG21	1:R:152:VAL:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:212:THR:HG21	2:I:246:ALA:H	1.56	0.71
2:G:71:PHE:HB3	2:G:118:VAL:HG23	1.74	0.70
2:I:130:TYR:HB2	2:I:163:LEU:HD21	1.73	0.70
2:L:264:TYR:CE2	2:L:273:LYS:HG3	2.27	0.70
1:I:152:VAL:HG21	2:L:259:VAL:HG21	1.73	0.70
2:C:313:SER:H	1:R:152:VAL:HG22	1.56	0.70
2:E:258:ILE:HD11	1:T:153:PRO:HG3	1.73	0.70
2:D:304:SER:HB3	2:L:116:ARG:HD3	1.74	0.69
2:D:61:GLN:HB3	2:D:130:TYR:CE2	2.28	0.69
2:H:265:SER:HB3	2:H:274:LEU:HD21	1.76	0.67
2:A:111:GLN:HE22	2:C:109:GLY:HA2	1.60	0.67
2:C:304:SER:HB3	2:I:116:ARG:HD3	1.75	0.67
2:I:166:THR:HG23	2:I:174:ILE:HD12	1.76	0.67
2:K:137:ARG:HB2	2:K:159:THR:HG21	1.75	0.67
2:N:137:ARG:HG3	2:N:139:TYR:CE2	2.29	0.67
2:K:116:ARG:HG3	2:K:161:ILE:HG12	1.77	0.67
2:N:109:GLY:HA2	2:O:111:GLN:HE22	1.59	0.67
2:G:79:LYS:HD2	2:G:155:ILE:HD11	1.77	0.66
2:H:134:ALA:HB1	2:H:158:LEU:HD11	1.77	0.66
2:B:313:SER:H	1:Q:152:VAL:HG22	1.60	0.66
1:I:153:PRO:HD3	2:L:258:ILE:HD11	1.78	0.66
2:J:267:ASN:HA	2:K:176:GLN:HE22	1.61	0.66
2:B:116:ARG:HD3	2:J:304:SER:HB3	1.78	0.65
2:K:265:SER:HB3	2:K:274:LEU:HD21	1.78	0.65
2:M:102:TYR:CE1	2:N:55:PRO:HA	2.32	0.65
2:K:130:TYR:HB2	2:K:163:LEU:HD11	1.78	0.65
2:B:61:GLN:HB3	2:B:130:TYR:CE2	2.32	0.64
1:2:151:LEU:HD12	2:M:255:ALA:HA	1.80	0.64
2:J:263:ILE:HD11	2:J:287:VAL:HG21	1.80	0.64
1:2:152:VAL:HG21	2:M:259:VAL:HG21	1.80	0.63
2:I:130:TYR:HB2	2:I:163:LEU:CD2	2.27	0.63
2:I:200:LEU:HD21	2:I:297:VAL:HG11	1.81	0.63
2:O:258:ILE:HD13	2:O:258:ILE:H	1.64	0.63
2:M:50:TRP:CD1	2:M:138:LYS:HB3	2.34	0.62
2:N:186:CYS:SG	2:N:188:LEU:HB2	2.39	0.62
1:2:150:PRO:O	1:2:151:LEU:HG	1.99	0.62
2:L:254:LEU:HD12	2:L:286:TYR:HB3	1.80	0.62
2:C:263:ILE:HD11	2:C:287:VAL:HG21	1.81	0.62
2:N:92:THR:O	2:N:96:ILE:HG13	1.99	0.62
2:A:129:TYR:CZ	2:C:268:PHE:HD1	2.17	0.62
2:H:77:LYS:HB2	2:H:158:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:TYR:HB2	2:H:155:ILE:HG23	1.82	0.62
2:N:149:ILE:H	2:N:149:ILE:HD12	1.64	0.62
2:G:204:ALA:HB2	2:G:237:LYS:HD2	1.81	0.62
2:H:211:LEU:HD22	2:H:244:ILE:HG12	1.81	0.62
2:K:42:TYR:CE2	2:K:198:GLU:HB2	2.35	0.61
2:D:55:PRO:HA	2:F:102:TYR:CE1	2.35	0.61
2:H:130:TYR:HB2	2:H:163:LEU:HD21	1.83	0.61
2:C:256:SER:HB2	1:R:152:VAL:H	1.66	0.61
2:H:223:LEU:HD12	2:H:317:GLN:HG3	1.83	0.60
2:L:258:ILE:HD13	2:L:258:ILE:H	1.66	0.60
2:H:137:ARG:HB2	2:H:159:THR:HG21	1.83	0.60
2:N:109:GLY:HA2	2:O:111:GLN:NE2	2.17	0.60
2:M:236:GLN:HA	2:M:236:GLN:HE21	1.67	0.60
2:N:102:TYR:CE1	2:O:55:PRO:HA	2.36	0.60
2:I:46:LYS:HG3	2:I:138:LYS:HE2	1.83	0.60
2:N:252:ARG:HG3	2:N:288:ASP:OD1	2.01	0.60
2:E:95:PHE:HE2	2:E:203:ALA:HB2	1.67	0.59
2:N:112:ASN:HB2	2:N:157:LYS:HE2	1.84	0.59
2:J:261:PHE:HD2	2:J:298:LEU:HD11	1.66	0.59
2:L:86:ASN:HD22	2:L:91:PHE:HB3	1.68	0.59
2:N:149:ILE:H	2:N:149:ILE:CD1	2.15	0.59
2:E:284:ASP:OD2	1:T:150:PRO:HA	2.02	0.59
2:G:109:GLY:HA2	2:H:111:GLN:HE22	1.67	0.59
2:H:62:ILE:H	2:H:62:ILE:HD12	1.67	0.59
2:A:116:ARG:HD3	2:L:304:SER:HB3	1.84	0.59
2:N:171:LEU:HD12	2:N:171:LEU:H	1.67	0.59
2:N:200:LEU:HG	2:N:271:LEU:HD13	1.85	0.59
2:F:61:GLN:HB3	2:F:130:TYR:CE2	2.38	0.59
1:3:152:VAL:HG23	2:N:256:SER:HB2	1.85	0.59
2:G:300:MET:HE1	2:G:314:ILE:HD11	1.84	0.59
2:B:263:ILE:CD1	2:B:287:VAL:HG21	2.30	0.59
2:N:44:ILE:HG13	2:N:196:GLU:HB2	1.85	0.59
2:N:276:GLN:NE2	2:N:278:LEU:HD11	2.18	0.59
2:I:138:LYS:HG3	2:I:156:TYR:CE2	2.38	0.58
2:K:256:SER:HB2	1:Z:152:VAL:H	1.68	0.58
2:H:305:SER:O	2:O:116:ARG:NH2	2.36	0.58
2:H:304:SER:HB3	2:O:116:ARG:HD3	1.85	0.58
2:F:171:LEU:H	2:F:171:LEU:HD23	1.68	0.58
2:K:313:SER:H	1:Z:152:VAL:HG22	1.68	0.57
2:H:170:SER:HB3	2:H:173:ASN:HD22	1.69	0.57
2:H:51:ILE:HD11	2:H:185:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:209:LEU:HD11	2:M:214:ALA:HB2	1.86	0.57
2:E:102:TYR:CE1	2:F:55:PRO:HA	2.39	0.57
2:N:68:THR:OG1	2:N:121:THR:HG23	2.04	0.57
2:D:254:LEU:HD23	1:S:151:LEU:HD11	1.87	0.57
2:J:81:VAL:HG11	2:J:93:SER:HA	1.87	0.57
2:I:259:VAL:HG21	1:X:152:VAL:HG21	1.87	0.57
2:G:256:SER:HB3	1:V:152:VAL:H	1.69	0.56
2:M:50:TRP:CE2	2:M:138:LYS:HD3	2.40	0.56
2:G:209:LEU:HD11	2:G:214:ALA:HB2	1.87	0.56
2:I:164:SER:OG	2:I:179:LEU:HD22	2.02	0.56
2:J:71:PHE:CD1	2:J:71:PHE:C	2.85	0.55
2:N:116:ARG:HB3	2:N:161:ILE:HD11	1.88	0.55
2:H:313:SER:H	1:W:152:VAL:HG22	1.71	0.55
2:L:237:LYS:HE2	2:L:299:VAL:HG13	1.88	0.55
2:O:235:THR:HA	2:O:301:LYS:NZ	2.21	0.55
2:I:237:LYS:HD3	2:I:299:VAL:HG13	1.88	0.55
2:D:62:ILE:HD11	2:F:268:PHE:CD2	2.42	0.55
2:G:102:TYR:CE1	2:H:55:PRO:HA	2.42	0.55
2:M:162:TRP:CZ3	2:M:164:SER:HB2	2.41	0.55
2:M:208:ARG:HB2	2:M:241:HIS:HB2	1.88	0.55
2:N:262:ASN:ND2	2:N:276:GLN:OE1	2.39	0.55
2:B:102:TYR:CE1	2:C:55:PRO:HA	2.43	0.54
2:K:81:VAL:CG1	2:K:155:ILE:HD12	2.37	0.54
2:K:244:ILE:HG22	2:K:293:ALA:HA	1.89	0.54
2:M:114:ILE:HD13	2:M:116:ARG:HG3	1.88	0.54
2:O:114:ILE:HD12	2:O:116:ARG:HG2	1.89	0.54
2:G:46:LYS:HG3	2:G:138:LYS:HG2	1.89	0.54
2:B:284:ASP:OD2	1:Q:150:PRO:HA	2.07	0.54
2:O:149:ILE:HD12	2:O:149:ILE:H	1.72	0.54
2:O:223:LEU:HD11	2:O:317:GLN:HG2	1.90	0.54
2:C:115:GLU:H	2:K:305:SER:HB3	1.72	0.54
2:K:226:TRP:HH2	2:K:238:LEU:HD21	1.71	0.54
2:K:295:GLN:CG	2:L:176:GLN:HB2	2.37	0.54
2:G:51:ILE:HD12	2:G:53:GLY:H	1.74	0.53
2:H:140:GLN:HG3	2:H:154:SER:OG	2.08	0.53
2:M:262:ASN:HB3	2:M:264:TYR:CE1	2.40	0.53
2:N:96:ILE:HD13	2:N:153:GLY:HA3	1.91	0.53
2:F:263:ILE:CD1	2:F:287:VAL:HG21	2.37	0.53
2:H:45:ASP:HB3	2:H:195:ILE:HB	1.90	0.53
2:K:102:TYR:HE2	2:K:199:ILE:HB	1.72	0.53
2:M:156:TYR:N	2:M:156:TYR:CD1	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:223:LEU:CD1	2:O:317:GLN:HG2	2.38	0.53
1:U:150:PRO:O	1:U:151:LEU:HG	2.09	0.53
1:W:150:PRO:O	1:W:151:LEU:HD12	2.09	0.53
2:I:41:LEU:HD23	2:I:201:ASP:HA	1.91	0.53
2:M:286:TYR:C	2:M:286:TYR:CD2	2.87	0.53
2:L:46:LYS:HG3	2:L:138:LYS:HE3	1.90	0.53
1:2:151:LEU:HB2	2:M:256:SER:HB2	1.90	0.52
2:J:298:LEU:HD23	2:J:300:MET:CE	2.39	0.52
2:G:208:ARG:NH1	2:H:180:ILE:O	2.43	0.52
2:M:131:LYS:HD3	2:M:133:TYR:OH	2.10	0.52
2:A:102:TYR:CE1	2:B:55:PRO:HA	2.45	0.52
2:H:112:ASN:HB2	2:H:157:LYS:HE2	1.92	0.52
2:K:263:ILE:HD11	2:K:275:GLU:HB2	1.90	0.52
1:V:150:PRO:O	1:V:151:LEU:HD12	2.10	0.52
2:J:136:TYR:HB3	2:J:156:TYR:HB3	1.91	0.52
2:M:46:LYS:HG3	2:M:138:LYS:HE2	1.92	0.52
2:A:313:SER:H	1:P:152:VAL:HG22	1.75	0.52
2:D:55:PRO:HA	2:F:102:TYR:HE1	1.75	0.51
2:M:244:ILE:HD12	2:M:296:TYR:CD2	2.45	0.51
2:N:280:ASP:OD2	2:N:282:VAL:HG23	2.09	0.51
2:J:92:THR:O	2:J:96:ILE:HG13	2.09	0.51
2:J:109:GLY:HA2	2:K:111:GLN:HE22	1.75	0.51
2:O:71:PHE:HB3	2:O:118:VAL:HG23	1.93	0.51
2:I:249:GLN:HB3	2:I:318:LYS:NZ	2.26	0.51
2:I:247:THR:O	2:I:249:GLN:NE2	2.36	0.51
2:G:200:LEU:HD23	2:G:239:ASN:ND2	2.24	0.51
2:I:68:THR:OG1	2:I:121:THR:HG23	2.11	0.51
2:J:298:LEU:HD23	2:J:300:MET:HE2	1.93	0.51
2:L:48:ASP:OD2	2:L:137:ARG:HD3	2.10	0.51
2:H:166:THR:HB	2:H:179:LEU:HD21	1.92	0.51
2:I:249:GLN:HB2	2:I:251:TYR:CZ	2.46	0.51
2:K:240:LEU:HD23	2:K:298:LEU:HB3	1.92	0.51
2:L:211:LEU:HD12	2:L:242:LEU:HD22	1.92	0.51
2:M:211:LEU:HB2	2:M:242:LEU:HD22	1.92	0.51
2:E:256:SER:HB3	1:T:152:VAL:H	1.76	0.51
2:J:71:PHE:CE1	2:J:73:GLN:HG2	2.46	0.50
2:K:300:MET:HG3	2:K:312:TYR:CD2	2.46	0.50
2:J:261:PHE:CE1	2:J:277:SER:HB3	2.46	0.50
2:N:252:ARG:HB3	2:N:317:GLN:HB2	1.93	0.50
2:B:276:GLN:NE2	2:B:278:LEU:HD21	2.27	0.50
2:I:256:SER:HB3	1:X:152:VAL:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:263:ILE:HG22	2:M:298:LEU:HD13	1.93	0.50
2:J:42:TYR:CE2	2:J:198:GLU:HB2	2.47	0.50
2:M:300:MET:HG3	2:M:312:TYR:CD1	2.47	0.50
2:N:223:LEU:HG	2:N:317:GLN:HG2	1.93	0.50
1:I:152:VAL:H	2:L:256:SER:HB2	1.77	0.49
2:D:61:GLN:HB3	2:D:130:TYR:HE2	1.72	0.49
2:G:259:VAL:HG21	1:V:152:VAL:HG21	1.94	0.49
2:N:206:THR:HG22	2:O:182:THR:HG22	1.93	0.49
2:B:102:TYR:HE1	2:C:55:PRO:HA	1.77	0.49
2:G:101:GLU:OE1	2:H:78:SER:HB2	2.12	0.49
2:G:226:TRP:CZ3	2:G:314:ILE:HD11	2.47	0.49
2:M:224:TYR:CE1	2:M:226:TRP:HB2	2.47	0.49
2:G:49:GLY:O	2:G:187:VAL:HG22	2.13	0.49
2:I:264:TYR:CE2	2:I:273:LYS:HG3	2.47	0.49
2:K:45:ASP:HB3	2:K:195:ILE:HB	1.93	0.49
2:M:306:TYR:HE1	2:M:308:GLY:O	1.95	0.49
1:I:153:PRO:CD	2:L:258:ILE:HD11	2.41	0.49
2:L:263:ILE:HD11	2:L:287:VAL:HG21	1.93	0.49
2:H:214:ALA:HB1	2:H:224:TYR:CD2	2.48	0.49
2:J:71:PHE:C	2:J:71:PHE:HD1	2.21	0.49
2:K:102:TYR:CE1	2:L:55:PRO:HA	2.48	0.49
2:M:210:ASN:HA	2:M:243:THR:HB	1.94	0.49
2:A:256:SER:HB2	1:P:152:VAL:H	1.77	0.49
2:C:49:GLY:HA3	2:C:188:LEU:HG	1.94	0.49
2:D:313:SER:H	1:S:152:VAL:HG22	1.78	0.48
2:I:41:LEU:HG	2:I:199:ILE:HG13	1.94	0.48
2:J:64:ASN:O	2:J:67:GLU:HB2	2.13	0.48
2:J:77:LYS:HB2	2:J:158:LEU:HD22	1.95	0.48
2:M:52:LEU:HG	2:M:56:SER:OG	2.12	0.48
2:B:78:SER:HA	2:B:111:GLN:HG3	1.95	0.48
2:C:116:ARG:HD3	2:K:304:SER:HB3	1.95	0.48
2:G:99:SER:HA	2:G:202:LEU:HD11	1.95	0.48
2:M:127:TYR:HD2	2:M:170:SER:HA	1.79	0.48
2:N:175:ASP:O	2:N:178:SER:OG	2.31	0.48
2:J:309:ASN:O	2:J:310:TYR:HD2	1.96	0.48
2:M:64:ASN:HA	2:M:127:TYR:CD1	2.49	0.48
2:M:81:VAL:HG11	2:M:93:SER:HB2	1.94	0.48
2:G:262:ASN:HB3	2:G:264:TYR:CE1	2.48	0.48
2:I:249:GLN:HB3	2:I:318:LYS:HZ3	1.77	0.48
2:K:295:GLN:HG3	2:L:176:GLN:HB2	1.95	0.48
1:T:150:PRO:O	1:T:151:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:152:VAL:HG21	2:M:259:VAL:CG2	2.43	0.48
2:G:211:LEU:HB2	2:G:242:LEU:HD22	1.96	0.48
2:I:252:ARG:HB3	2:I:317:GLN:HB2	1.96	0.48
2:J:77:LYS:HD3	2:J:77:LYS:HA	1.71	0.47
2:L:265:SER:OG	2:L:272:VAL:HB	2.14	0.47
2:G:259:VAL:CG2	1:V:152:VAL:HG21	2.45	0.47
2:K:264:TYR:CE2	2:K:273:LYS:HE2	2.49	0.47
2:N:112:ASN:HB2	2:N:157:LYS:CE	2.43	0.47
2:O:139:TYR:HB2	2:O:155:ILE:HG23	1.96	0.47
2:B:115:GLU:HB2	2:J:305:SER:HB3	1.96	0.47
2:L:149:ILE:HD12	2:L:149:ILE:O	2.14	0.47
2:G:146:HIS:HA	2:G:278:LEU:HD22	1.95	0.47
2:J:234:TRP:CD2	2:J:305:SER:HA	2.49	0.47
2:O:251:TYR:CD1	2:O:291:LEU:HD12	2.49	0.47
2:A:49:GLY:HA3	2:A:188:LEU:HG	1.96	0.47
2:B:36[A]:MET:HB2	2:B:37:GLY:H	1.53	0.47
2:B:280:ASP:O	2:H:118:VAL:HA	2.15	0.47
2:J:211:LEU:HB2	2:J:242:LEU:HD22	1.97	0.47
1:W:150:PRO:C	1:W:151:LEU:HD12	2.40	0.47
2:C:263:ILE:CD1	2:C:287:VAL:HG21	2.44	0.47
2:G:86:ASN:ND2	2:G:88:SER:O	2.48	0.47
2:G:262:ASN:O	2:G:298:LEU:HD12	2.14	0.47
2:J:256:SER:HB3	1:Y:152:VAL:HG23	1.96	0.47
2:K:81:VAL:HG13	2:K:155:ILE:HD12	1.96	0.47
2:M:42:TYR:CE2	2:M:198:GLU:HB2	2.50	0.47
2:N:43:VAL:HG21	2:N:103:GLY:HA3	1.95	0.47
1:R:150:PRO:O	1:R:151:LEU:HB2	2.14	0.47
2:J:264:TYR:CD1	2:J:273:LYS:HA	2.50	0.47
1:U:150:PRO:C	1:U:151:LEU:HG	2.40	0.47
2:E:61:GLN:HB3	2:E:130:TYR:HE2	1.74	0.46
2:I:282:VAL:HG11	2:M:163:LEU:HD23	1.96	0.46
2:D:315:LEU:HB2	1:S:151:LEU:HD21	1.97	0.46
2:I:254:LEU:HG	2:I:286:TYR:HB3	1.96	0.46
2:K:77:LYS:HB2	2:K:158:LEU:HD22	1.98	0.46
2:J:63:LEU:HD22	2:J:67:GLU:HB3	1.96	0.46
2:O:102:TYR:HD2	2:O:202:LEU:HD11	1.81	0.46
2:F:110:GLU:HG3	2:F:111:GLN:HG3	1.96	0.46
2:G:77:LYS:HD2	2:G:77:LYS:HA	1.67	0.46
2:M:139:TYR:HB2	2:M:155:ILE:HG23	1.98	0.46
2:J:41:LEU:HD22	2:J:201:ASP:HA	1.97	0.46
2:K:146:HIS:HA	2:K:278:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:62:ILE:HD11	2:C:268:PHE:CD1	2.51	0.46
2:G:263:ILE:HD11	2:G:287:VAL:HG21	1.98	0.46
2:G:81:VAL:HG11	2:G:93:SER:HA	1.98	0.45
2:H:260:ASP:HB3	2:H:278:LEU:HD23	1.97	0.45
2:M:137:ARG:HB2	2:M:159:THR:HG21	1.97	0.45
2:A:244:ILE:HD13	2:A:251:TYR:HE1	1.81	0.45
2:K:86:ASN:HD22	2:K:91:PHE:HB3	1.81	0.45
2:H:249:GLN:HB2	2:H:251:TYR:CZ	2.51	0.45
2:J:137:ARG:HB2	2:J:159:THR:HG21	1.97	0.45
2:L:263:ILE:CD1	2:L:275:GLU:HB3	2.47	0.45
2:M:102:TYR:HE1	2:N:55:PRO:HA	1.80	0.45
2:B:49:GLY:HA3	2:B:188:LEU:HG	1.99	0.45
2:G:71:PHE:HB3	2:G:118:VAL:CG2	2.42	0.45
2:G:276:GLN:NE2	2:G:278:LEU:HD11	2.32	0.45
2:H:255:ALA:HA	1:W:151:LEU:HD22	1.98	0.45
2:I:47:GLY:C	2:I:137:ARG:HD2	2.42	0.45
2:N:171:LEU:HD12	2:N:171:LEU:N	2.31	0.45
2:N:315:LEU:HD21	2:N:317:GLN:HE21	1.81	0.45
2:D:215:LEU:O	2:D:221:GLY:HA2	2.17	0.45
2:I:49:GLY:O	2:I:187:VAL:HG22	2.17	0.45
2:N:207:GLU:OE2	2:N:229:SER:N	2.49	0.45
2:E:304:SER:HB3	2:J:116:ARG:HD2	1.99	0.44
2:H:263:ILE:HG23	2:H:298:LEU:CD1	2.47	0.44
2:K:76:THR:OG1	2:K:113:THR:HG23	2.17	0.44
2:N:171:LEU:H	2:N:171:LEU:CD1	2.30	0.44
2:H:112:ASN:HD22	2:H:157:LYS:HD3	1.82	0.44
2:M:127:TYR:CD2	2:M:170:SER:HA	2.53	0.44
2:N:204:ALA:HB3	2:N:239:ASN:ND2	2.31	0.44
2:G:137:ARG:HB2	2:G:159:THR:HG21	1.99	0.44
2:G:207:GLU:OE2	2:G:228:SER:HB2	2.17	0.44
2:H:68:THR:OG1	2:H:121:THR:HG23	2.17	0.44
2:K:315:LEU:HB2	1:Z:151:LEU:HD21	1.98	0.44
2:L:306:TYR:CD1	2:L:306:TYR:C	2.94	0.44
2:M:88:SER:HB2	2:M:151:ASP:OD1	2.18	0.44
2:L:263:ILE:HD12	2:L:275:GLU:HB3	1.98	0.44
2:N:49:GLY:O	2:N:187:VAL:HG22	2.17	0.44
2:L:75:LEU:HD23	2:L:158:LEU:HD21	1.98	0.44
2:L:185:ARG:NH2	2:L:187:VAL:HG12	2.33	0.44
2:A:263:ILE:HD11	2:A:287:VAL:HG21	2.00	0.44
2:A:305:SER:O	2:G:116:ARG:NH2	2.51	0.44
2:E:254:LEU:HD23	1:T:151:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:280:ASP:O	2:J:118:VAL:HA	2.17	0.44
2:G:215:LEU:O	2:G:221:GLY:HA2	2.18	0.44
2:H:215:LEU:O	2:H:221:GLY:HA2	2.18	0.44
1:2:152:VAL:HG22	2:M:313:SER:H	1.82	0.44
2:G:252:ARG:HB3	2:G:317:GLN:HB2	2.00	0.44
2:O:200:LEU:HG	2:O:271:LEU:HD22	1.99	0.44
2:B:215:LEU:O	2:B:221:GLY:HA2	2.18	0.43
2:I:83:ILE:HG12	2:I:96:ILE:HD11	2.00	0.43
2:J:68:THR:OG1	2:J:121:THR:HG23	2.18	0.43
2:N:230:ASN:HB3	2:N:232:TYR:CZ	2.53	0.43
2:O:131:LYS:NZ	2:O:180:ILE:HD13	2.34	0.43
2:K:54:GLU:O	2:K:57:VAL:HG23	2.18	0.43
2:M:38:SER:O	2:M:42:TYR:OH	2.34	0.43
2:J:220:ALA:HB1	2:J:222:ASN:OD1	2.19	0.43
2:J:254:LEU:HG	2:J:286:TYR:HB3	2.01	0.43
2:K:235:THR:O	2:K:301:LYS:HE2	2.18	0.43
2:M:200:LEU:HD21	2:M:297:VAL:HG11	2.00	0.43
2:O:48:ASP:OD2	2:O:137:ARG:HD3	2.18	0.43
2:K:64:ASN:HD22	2:K:127:TYR:HE1	1.66	0.43
2:L:81:VAL:HG22	2:L:155:ILE:HD12	1.99	0.43
2:M:75:LEU:HD23	2:M:158:LEU:HD21	2.00	0.43
2:M:240:LEU:HD23	2:M:298:LEU:HD23	2.00	0.43
2:A:215:LEU:O	2:A:221:GLY:HA2	2.18	0.43
2:G:304:SER:HB3	2:N:116:ARG:HD3	2.00	0.43
2:J:268:PHE:HB3	2:K:129:TYR:CE1	2.53	0.43
2:I:52:LEU:HD23	2:I:184[B]:GLU:HG3	2.01	0.43
2:J:280:ASP:OD2	2:J:282:VAL:HG22	2.18	0.43
2:D:49:GLY:HA3	2:D:188:LEU:HG	1.99	0.43
2:K:209:LEU:HD13	2:K:226:TRP:CD1	2.54	0.43
2:L:43:VAL:C	2:L:44:ILE:HD12	2.44	0.43
2:L:81:VAL:HG11	2:L:93:SER:HA	2.01	0.43
2:M:175:ASP:OD2	2:M:178:SER:HB3	2.19	0.43
2:N:223:LEU:HD23	2:N:224:TYR:N	2.33	0.43
1:4:152:VAL:HG22	2:O:313:SER:H	1.83	0.43
2:E:95:PHE:CD1	2:E:95:PHE:C	2.96	0.43
2:M:146:HIS:HA	2:M:278:LEU:HD13	2.01	0.43
2:A:43:VAL:HG21	2:A:103:GLY:HA3	2.01	0.43
2:A:102:TYR:HE1	2:B:55:PRO:HA	1.83	0.43
2:A:251:TYR:HD1	2:A:291:LEU:HD12	1.83	0.43
2:G:171:LEU:H	2:G:171:LEU:HG	1.37	0.43
2:J:215:LEU:O	2:J:221:GLY:HA2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:61:GLN:HB3	2:L:130:TYR:CE2	2.53	0.43
2:N:307:SER:O	2:N:310:TYR:HE1	2.02	0.43
2:O:76:THR:OG1	2:O:113:THR:HG23	2.19	0.43
2:O:215:LEU:O	2:O:221:GLY:HA2	2.19	0.43
2:B:263:ILE:HD11	2:B:287:VAL:CG2	2.40	0.42
2:E:215:LEU:O	2:E:221:GLY:HA2	2.19	0.42
2:G:276:GLN:HE21	2:G:278:LEU:HD11	1.84	0.42
2:I:215:LEU:O	2:I:221:GLY:HA2	2.19	0.42
2:K:215:LEU:O	2:K:221:GLY:HA2	2.18	0.42
2:C:215:LEU:O	2:C:221:GLY:HA2	2.18	0.42
2:D:102:TYR:CE1	2:E:55:PRO:HA	2.54	0.42
2:I:253:ILE:HD12	2:I:287:VAL:HG23	2.00	0.42
2:K:58:VAL:HG22	2:K:132:VAL:O	2.20	0.42
2:M:277:SER:OG	2:M:287:VAL:HG13	2.19	0.42
2:F:258:ILE:HD11	1:U:153:PRO:HG3	2.01	0.42
2:I:174:ILE:HD13	2:I:174:ILE:HA	1.96	0.42
2:J:261:PHE:CD2	2:J:298:LEU:HD11	2.52	0.42
2:M:209:LEU:HD23	2:M:242:LEU:HD21	2.00	0.42
2:J:232:TYR:HE2	2:J:238:LEU:HD22	1.85	0.42
2:M:171:LEU:H	2:M:171:LEU:HG	1.46	0.42
2:N:239:ASN:OD1	2:N:299:VAL:HG22	2.19	0.42
2:G:265:SER:HB3	2:G:274:LEU:HD21	2.02	0.42
2:J:182:THR:HG22	2:L:206:THR:HG22	2.02	0.42
2:J:268:PHE:HA	2:K:129:TYR:OH	2.19	0.42
2:K:57:VAL:HG22	2:K:133:TYR:CE2	2.55	0.42
2:K:112:ASN:HB2	2:K:157:LYS:HD3	2.02	0.42
2:K:112:ASN:CB	2:K:157:LYS:HD3	2.50	0.42
2:M:215:LEU:O	2:M:221:GLY:HA2	2.19	0.42
2:N:209:LEU:HB2	2:N:240:LEU:HD11	2.01	0.42
2:F:215:LEU:O	2:F:221:GLY:HA2	2.19	0.42
2:G:253:ILE:HG12	2:G:316:PHE:HD1	1.85	0.42
2:J:102:TYR:CE1	2:K:55:PRO:HA	2.55	0.42
2:L:215:LEU:O	2:L:221:GLY:HA2	2.19	0.42
2:N:102:TYR:HE1	2:O:55:PRO:HA	1.82	0.42
1:1:153:PRO:HB2	1:1:154:ASP:H	1.75	0.42
2:A:305:SER:O	2:G:116:ARG:CZ	2.67	0.42
2:H:226:TRP:HB3	2:H:316:PHE:HE2	1.85	0.42
2:L:265:SER:HB3	2:L:274:LEU:HD21	2.02	0.42
2:M:86:ASN:HD22	2:M:91:PHE:HB3	1.85	0.42
2:E:313:SER:H	1:T:152:VAL:HG22	1.85	0.42
2:N:45:ASP:HB3	2:N:195:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:203:ALA:O	2:N:236:GLN:NE2	2.52	0.42
2:D:177:GLY:O	2:F:208:ARG:NH1	2.53	0.41
2:F:127:TYR:CD1	2:F:170:SER:HA	2.55	0.41
2:K:250:LYS:HB3	2:K:319:PHE:HD2	1.84	0.41
2:K:264:TYR:HA	2:K:274:LEU:HG	2.02	0.41
2:G:300:MET:HE1	2:G:314:ILE:CD1	2.50	0.41
2:J:86:ASN:ND2	2:J:88:SER:O	2.54	0.41
2:K:102:TYR:CE2	2:K:199:ILE:HB	2.55	0.41
2:K:109:GLY:HA2	2:L:111:GLN:HE22	1.84	0.41
2:L:130:TYR:HB2	2:L:163:LEU:HD21	2.01	0.41
2:N:58:VAL:HG11	2:N:75:LEU:HD21	2.01	0.41
2:A:129:TYR:CE1	2:C:268:PHE:CD1	3.09	0.41
2:H:102:TYR:CE1	2:I:55:PRO:HA	2.55	0.41
2:J:208:ARG:NH1	2:K:180:ILE:O	2.53	0.41
2:M:235:THR:HA	2:M:301:LYS:NZ	2.35	0.41
2:N:215:LEU:O	2:N:221:GLY:HA2	2.19	0.41
2:E:264:TYR:CD2	2:E:273:LYS:HA	2.55	0.41
2:L:262:ASN:HB2	2:L:264:TYR:CE1	2.55	0.41
2:O:40:GLY:HA3	2:O:198:GLU:OE2	2.21	0.41
2:C:95:PHE:CE2	2:C:202:LEU:HB2	2.56	0.41
2:I:305:SER:HB3	2:M:115:GLU:H	1.86	0.41
2:C:82:SER:OG	2:C:156:TYR:HE2	2.03	0.41
2:G:282:VAL:HG11	2:N:163:LEU:HD23	2.01	0.41
2:H:112:ASN:ND2	2:H:157:LYS:HD3	2.35	0.41
2:L:86:ASN:HD21	2:L:91:PHE:HB3	1.80	0.41
2:L:301:LYS:HA	2:L:312:TYR:OH	2.21	0.41
2:M:306:TYR:CD1	2:M:306:TYR:C	2.98	0.41
2:G:86:ASN:O	2:G:86:ASN:CG	2.63	0.41
2:G:305:SER:HB3	2:N:115:GLU:HB2	2.01	0.41
2:L:254:LEU:HG	2:L:255:ALA:N	2.36	0.41
2:M:81:VAL:HG11	2:M:93:SER:CB	2.50	0.41
2:F:43:VAL:HG21	2:F:103:GLY:HA3	2.01	0.41
2:L:237:LYS:HG3	2:L:301:LYS:HB2	2.02	0.41
2:M:65:PRO:HD3	2:M:127:TYR:CD1	2.56	0.41
2:J:207:GLU:OE2	2:J:228:SER:HB2	2.20	0.41
2:K:263:ILE:HG23	2:K:298:LEU:CD1	2.50	0.41
2:L:244:ILE:HG22	2:L:293:ALA:HA	2.02	0.41
2:G:254:LEU:HD11	2:G:284:ASP:HB2	2.02	0.40
2:H:134:ALA:HB1	2:H:158:LEU:CD1	2.49	0.40
2:H:263:ILE:HG23	2:H:298:LEU:HD13	2.01	0.40
2:N:51:ILE:HG12	2:N:187:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:116:ARG:HB3	2:O:161:ILE:HD11	2.03	0.40
2:A:129:TYR:CE1	2:C:268:PHE:HD1	2.39	0.40
2:K:204:ALA:HB3	2:K:239:ASN:ND2	2.36	0.40
2:M:136:TYR:HB3	2:M:156:TYR:HB3	2.03	0.40
2:M:237:LYS:HA	2:M:301:LYS:HB2	2.04	0.40
2:O:86:ASN:ND2	2:O:88:SER:O	2.54	0.40
2:J:258:ILE:HG13	2:J:304:SER:HB2	2.03	0.40
2:K:238:LEU:HD12	2:K:239:ASN:N	2.37	0.40
2:N:75:LEU:HD12	2:N:75:LEU:HA	1.98	0.40
2:O:86:ASN:HD22	2:O:91:PHE:HB3	1.86	0.40
2:A:55:PRO:HA	2:C:102:TYR:CE1	2.56	0.40
2:C:43:VAL:HG21	2:C:103:GLY:HA3	2.02	0.40
2:J:176:GLN:HB2	2:L:295:GLN:HB2	2.04	0.40
2:J:259:VAL:HG21	1:Y:152:VAL:HG21	2.04	0.40
2:L:269:ASN:HD22	2:L:269:ASN:HA	1.78	0.40
2:O:86:ASN:ND2	2:O:91:PHE:HB3	2.37	0.40
2:O:268:PHE:CD1	2:O:268:PHE:N	2.89	0.40
2:L:116:ARG:HG3	2:L:161:ILE:HG12	2.02	0.40
2:M:177:GLY:O	2:O:208:ARG:NH1	2.55	0.40
2:O:58:VAL:HG11	2:O:75:LEU:HD21	2.02	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	1	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	2	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	3	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	4	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	Q	7/20 (35%)	1 (14%)	4 (57%)	2 (29%)	0	0
1	R	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	S	7/20 (35%)	2 (29%)	1 (14%)	4 (57%)	0	0
1	T	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	U	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	V	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	W	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	X	7/20 (35%)	1 (14%)	3 (43%)	3 (43%)	0	0
1	Y	7/20 (35%)	2 (29%)	1 (14%)	4 (57%)	0	0
1	Z	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
2	A	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	B	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	C	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	D	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	E	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	F	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	G	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	H	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	I	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	J	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	K	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	L	287/286 (100%)	282 (98%)	5 (2%)	0	100	100
2	M	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	N	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	O	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
All	All	4410/4590 (96%)	4272 (97%)	103 (2%)	35 (1%)	16	44

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	151	LEU
1	1	153	PRO

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Mol	Chain	Res	Type
1	2	151	LEU
1	2	153	PRO
1	3	151	LEU
1	3	153	PRO
1	4	151	LEU
1	4	153	PRO
1	P	151	LEU
1	P	153	PRO
1	Q	151	LEU
1	Q	153	PRO
1	R	151	LEU
1	R	153	PRO
1	S	151	LEU
1	S	153	PRO
1	T	151	LEU
1	T	153	PRO
1	U	151	LEU
1	U	153	PRO
1	V	151	LEU
1	V	153	PRO
1	W	151	LEU
1	W	153	PRO
1	X	150	PRO
1	X	151	LEU
1	X	153	PRO
1	Y	151	LEU
1	Y	153	PRO
1	Z	151	LEU
1	Z	153	PRO
1	S	152	VAL
1	S	155	ALA
1	Y	155	ALA
1	Y	152	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	3/18 (17%)	3 (100%)	0	100	100
1	P	6/18 (33%)	6 (100%)	0	100	100
1	Q	6/18 (33%)	6 (100%)	0	100	100
1	R	6/18 (33%)	5 (83%)	1 (17%)	2	10
1	S	6/18 (33%)	5 (83%)	1 (17%)	2	10
1	T	6/18 (33%)	5 (83%)	1 (17%)	2	10
1	U	6/18 (33%)	6 (100%)	0	100	100
1	V	6/18 (33%)	6 (100%)	0	100	100
1	W	6/18 (33%)	5 (83%)	1 (17%)	2	10
1	X	6/18 (33%)	5 (83%)	1 (17%)	2	10
1	Y	6/18 (33%)	5 (83%)	1 (17%)	2	10
1	Z	6/18 (33%)	6 (100%)	0	100	100
2	A	134/247 (54%)	128 (96%)	6 (4%)	24	50
2	B	245/247 (99%)	231 (94%)	14 (6%)	18	45
2	C	245/247 (99%)	233 (95%)	12 (5%)	22	49
2	D	246/247 (100%)	235 (96%)	11 (4%)	24	50
2	E	245/247 (99%)	235 (96%)	10 (4%)	27	52
2	F	245/247 (99%)	232 (95%)	13 (5%)	20	47
2	G	245/247 (99%)	200 (82%)	45 (18%)	1	7
2	H	245/247 (99%)	201 (82%)	44 (18%)	2	7
2	I	245/247 (99%)	198 (81%)	47 (19%)	1	5
2	J	245/247 (99%)	206 (84%)	39 (16%)	2	10
2	K	245/247 (99%)	191 (78%)	54 (22%)	1	3
2	L	245/247 (99%)	196 (80%)	49 (20%)	1	4
2	M	245/247 (99%)	199 (81%)	46 (19%)	1	6
2	N	245/247 (99%)	192 (78%)	53 (22%)	1	3
2	O	245/247 (99%)	207 (84%)	38 (16%)	2	10
All	All	3634/3921 (93%)	3147 (87%)	487 (13%)	4	15

All (487) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	197	LYS

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Mol	Chain	Res	Type
2	A	269	ASN
2	A	274	LEU
2	A	284	ASP
2	A	292	ASP
2	A	305	SER
2	B	36[A]	MET
2	B	36[B]	MET
2	B	62	ILE
2	B	93	SER
2	B	157	LYS
2	B	174	ILE
2	B	184[A]	GLU
2	B	184[B]	GLU
2	B	193[A]	THR
2	B	193[B]	THR
2	B	256	SER
2	B	278	LEU
2	B	284	ASP
2	B	292	ASP
2	C	82	SER
2	C	93	SER
2	C	171	LEU
2	C	184[A]	GLU
2	C	184[B]	GLU
2	C	193[A]	THR
2	C	193[B]	THR
2	C	258	ILE
2	C	275	GLU
2	C	284	ASP
2	C	292	ASP
2	C	313	SER
2	D	74	SER
2	D	115	GLU
2	D	184[A]	GLU
2	D	184[B]	GLU
2	D	190	VAL
2	D	193[A]	THR
2	D	193[B]	THR
2	D	254	LEU
2	D	258	ILE
2	D	269	ASN
2	D	292	ASP

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Mol	Chain	Res	Type
2	E	117	SER
2	E	125	ASN
2	E	184[A]	GLU
2	E	184[B]	GLU
2	E	256	SER
2	E	269	ASN
2	E	284	ASP
2	E	292	ASP
2	E	305	SER
2	E	318	LYS
2	F	111	GLN
2	F	125	ASN
2	F	128	VAL
2	F	171	LEU
2	F	190	VAL
2	F	193[A]	THR
2	F	193[B]	THR
2	F	247	THR
2	F	256	SER
2	F	258	ILE
2	F	284	ASP
2	F	292	ASP
2	F	318	LYS
2	G	36[A]	MET
2	G	36[B]	MET
2	G	44	ILE
2	G	57	VAL
2	G	59	SER
2	G	61	GLN
2	G	75	LEU
2	G	76	THR
2	G	77	LYS
2	G	79	LYS
2	G	82	SER
2	G	85	VAL
2	G	89	VAL
2	G	92	THR
2	G	93	SER
2	G	94	GLU
2	G	113	THR
2	G	116	ARG
2	G	117	SER

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Mol	Chain	Res	Type
2	G	118	VAL
2	G	143	ARG
2	G	149	ILE
2	G	163	LEU
2	G	166	THR
2	G	171	LEU
2	G	178	SER
2	G	182	THR
2	G	185	ARG
2	G	192	SER
2	G	196	GLU
2	G	198	GLU
2	G	200	LEU
2	G	206	THR
2	G	235	THR
2	G	237	LYS
2	G	254	LEU
2	G	256	SER
2	G	258	ILE
2	G	259	VAL
2	G	263	ILE
2	G	272	VAL
2	G	284	ASP
2	G	309	ASN
2	G	313	SER
2	G	314	ILE
2	H	36[A]	MET
2	H	36[B]	MET
2	H	38	SER
2	H	48	ASP
2	H	52	LEU
2	H	59	SER
2	H	61	GLN
2	H	62	ILE
2	H	68	THR
2	H	77	LYS
2	H	78	SER
2	H	84	ASN
2	H	86	ASN
2	H	92	THR
2	H	106	ILE
2	H	107	THR

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Mol	Chain	Res	Type
2	H	114	ILE
2	H	121	THR
2	H	142[A]	ILE
2	H	145	SER
2	H	154	SER
2	H	165	LYS
2	H	166	THR
2	H	170	SER
2	H	171	LEU
2	H	182	THR
2	H	184[A]	GLU
2	H	184[B]	GLU
2	H	189	THR
2	H	208	ARG
2	H	209	LEU
2	H	211	LEU
2	H	242	LEU
2	H	243	THR
2	H	245	THR
2	H	247	THR
2	H	263	ILE
2	H	269	ASN
2	H	274	LEU
2	H	277	SER
2	H	292	ASP
2	H	297	VAL
2	H	315	LEU
2	H	317	GLN
2	I	38	SER
2	I	41	LEU
2	I	46	LYS
2	I	51	ILE
2	I	60	SER
2	I	61	GLN
2	I	62	ILE
2	I	67	GLU
2	I	68	THR
2	I	76	THR
2	I	79	LYS
2	I	80	GLU
2	I	84	ASN
2	I	107	THR

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Mol	Chain	Res	Type
2	I	113	THR
2	I	114	ILE
2	I	117	SER
2	I	120	THR
2	I	121	THR
2	I	132	VAL
2	I	135	THR
2	I	142[A]	ILE
2	I	149	ILE
2	I	163	LEU
2	I	167	SER
2	I	171	LEU
2	I	174	ILE
2	I	176	GLN
2	I	184[A]	GLU
2	I	184[B]	GLU
2	I	185	ARG
2	I	189	THR
2	I	222	ASN
2	I	223	LEU
2	I	235	THR
2	I	237	LYS
2	I	254	LEU
2	I	263	ILE
2	I	265	SER
2	I	267	ASN
2	I	272	VAL
2	I	299	VAL
2	I	305	SER
2	I	313	SER
2	I	315	LEU
2	I	317	GLN
2	I	318	LYS
2	J	48	ASP
2	J	58	VAL
2	J	70	THR
2	J	71	PHE
2	J	74	SER
2	J	76	THR
2	J	79	LYS
2	J	84	ASN
2	J	89	VAL

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Mol	Chain	Res	Type
2	J	97	GLN
2	J	114	ILE
2	J	115	GLU
2	J	117	SER
2	J	148	ASN
2	J	154	SER
2	J	156	TYR
2	J	161	ILE
2	J	163	LEU
2	J	164	SER
2	J	171	LEU
2	J	190	VAL
2	J	198	GLU
2	J	223	LEU
2	J	236	GLN
2	J	237	LYS
2	J	254	LEU
2	J	256	SER
2	J	258	ILE
2	J	263	ILE
2	J	265	SER
2	J	272	VAL
2	J	282	VAL
2	J	284	ASP
2	J	289	ILE
2	J	297	VAL
2	J	299	VAL
2	J	313	SER
2	J	315	LEU
2	J	317	GLN
2	K	38	SER
2	K	44	ILE
2	K	59	SER
2	K	61	GLN
2	K	62	ILE
2	K	79	LYS
2	K	83	ILE
2	K	84	ASN
2	K	89	VAL
2	K	92	THR
2	K	106	ILE
2	K	108	ILE

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Mol	Chain	Res	Type
2	K	113	THR
2	K	117	SER
2	K	142[A]	ILE
2	K	154	SER
2	K	155	ILE
2	K	164	SER
2	K	166	THR
2	K	169	ASP
2	K	174	ILE
2	K	182	THR
2	K	184[A]	GLU
2	K	184[B]	GLU
2	K	185	ARG
2	K	189	THR
2	K	190	VAL
2	K	192	SER
2	K	198	GLU
2	K	206	THR
2	K	208	ARG
2	K	209	LEU
2	K	213	ASP
2	K	231	SER
2	K	238	LEU
2	K	240	LEU
2	K	243	THR
2	K	244	ILE
2	K	245	THR
2	K	247	THR
2	K	258	ILE
2	K	263	ILE
2	K	269	ASN
2	K	270	ASN
2	K	274	LEU
2	K	275	GLU
2	K	277	SER
2	K	282	VAL
2	K	284	ASP
2	K	289	ILE
2	K	295	GLN
2	K	297	VAL
2	K	305	SER
2	K	315	LEU

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Mol	Chain	Res	Type
2	L	38	SER
2	L	39	ASP
2	L	51	ILE
2	L	57	VAL
2	L	62	ILE
2	L	77	LYS
2	L	79	LYS
2	L	85	VAL
2	L	92	THR
2	L	93	SER
2	L	111	GLN
2	L	113	THR
2	L	125	ASN
2	L	135	THR
2	L	146	HIS
2	L	149	ILE
2	L	154	SER
2	L	156	TYR
2	L	157	LYS
2	L	165	LYS
2	L	167	SER
2	L	170	SER
2	L	171	LEU
2	L	179	LEU
2	L	180	ILE
2	L	184[A]	GLU
2	L	184[B]	GLU
2	L	185	ARG
2	L	188	LEU
2	L	190	VAL
2	L	192	SER
2	L	211	LEU
2	L	223	LEU
2	L	231	SER
2	L	243	THR
2	L	245	THR
2	L	249	GLN
2	L	251	TYR
2	L	254	LEU
2	L	258	ILE
2	L	263	ILE
2	L	267	ASN

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Mol	Chain	Res	Type
2	L	269	ASN
2	L	270	ASN
2	L	282	VAL
2	L	284	ASP
2	L	292	ASP
2	L	299	VAL
2	L	317	GLN
2	M	51	ILE
2	M	52	LEU
2	M	62	ILE
2	M	68	THR
2	M	74	SER
2	M	76	THR
2	M	79	LYS
2	M	81	VAL
2	M	84	ASN
2	M	88	SER
2	M	89	VAL
2	M	92	THR
2	M	106	ILE
2	M	107	THR
2	M	113	THR
2	M	114	ILE
2	M	119	SER
2	M	120	THR
2	M	121	THR
2	M	125	ASN
2	M	145	SER
2	M	154	SER
2	M	155	ILE
2	M	156	TYR
2	M	157	LYS
2	M	163	LEU
2	M	170	SER
2	M	171	LEU
2	M	182	THR
2	M	190	VAL
2	M	194	ASP
2	M	198	GLU
2	M	208	ARG
2	M	211	LEU
2	M	213	ASP

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Mol	Chain	Res	Type
2	M	223	LEU
2	M	236	GLN
2	M	254	LEU
2	M	259	VAL
2	M	269	ASN
2	M	282	VAL
2	M	284	ASP
2	M	287	VAL
2	M	290	SER
2	M	305	SER
2	M	315	LEU
2	N	36[A]	MET
2	N	36[B]	MET
2	N	38	SER
2	N	60	SER
2	N	61	GLN
2	N	62	ILE
2	N	74	SER
2	N	83	ILE
2	N	89	VAL
2	N	92	THR
2	N	96	ILE
2	N	110	GLU
2	N	120	THR
2	N	131	LYS
2	N	135	THR
2	N	136	TYR
2	N	142[A]	ILE
2	N	149	ILE
2	N	150	SER
2	N	154	SER
2	N	157	LYS
2	N	161	ILE
2	N	166	THR
2	N	167	SER
2	N	176	GLN
2	N	178	SER
2	N	182	THR
2	N	184[A]	GLU
2	N	184[B]	GLU
2	N	188	LEU
2	N	189	THR

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Mol	Chain	Res	Type
2	N	193[A]	THR
2	N	193[B]	THR
2	N	195	ILE
2	N	196	GLU
2	N	223	LEU
2	N	244	ILE
2	N	247	THR
2	N	256	SER
2	N	258	ILE
2	N	259	VAL
2	N	263	ILE
2	N	269	ASN
2	N	270	ASN
2	N	271	LEU
2	N	272	VAL
2	N	273	LYS
2	N	280	ASP
2	N	282	VAL
2	N	284	ASP
2	N	292	ASP
2	N	297	VAL
2	N	309	ASN
2	O	36[A]	MET
2	O	36[B]	MET
2	O	38	SER
2	O	44	ILE
2	O	46	LYS
2	O	51	ILE
2	O	62	ILE
2	O	73	GLN
2	O	74	SER
2	O	76	THR
2	O	93	SER
2	O	97	GLN
2	O	108	ILE
2	O	113	THR
2	O	115	GLU
2	O	118	VAL
2	O	120	THR
2	O	149	ILE
2	O	161	ILE
2	O	167	SER

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Mol	Chain	Res	Type
2	O	174	ILE
2	O	185	ARG
2	O	199	ILE
2	O	206	THR
2	O	208	ARG
2	O	209	LEU
2	O	223	LEU
2	O	253	ILE
2	O	254	LEU
2	O	258	ILE
2	O	263	ILE
2	O	275	GLU
2	O	284	ASP
2	O	287	VAL
2	O	289	ILE
2	O	292	ASP
2	O	305	SER
2	O	307	SER
1	R	149	ASN
1	S	149	ASN
1	T	151	LEU
1	W	149	ASN
1	X	150	PRO
1	Y	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	241	HIS
2	A	295	GLN
2	A	309	ASN
2	B	241	HIS
2	B	295	GLN
2	C	241	HIS
2	C	309	ASN
2	D	61	GLN
2	D	66	ASN
2	D	84	ASN
2	D	86	ASN
2	D	173	ASN
2	D	269	ASN
2	D	295	GLN

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Mol	Chain	Res	Type
2	D	309	ASN
2	E	309	ASN
2	F	140	GLN
2	F	295	GLN
2	G	66	ASN
2	G	86	ASN
2	G	111	GLN
2	G	125	ASN
2	G	173	ASN
2	G	230	ASN
2	G	239	ASN
2	G	269	ASN
2	G	309	ASN
2	H	66	ASN
2	H	111	GLN
2	H	148	ASN
2	H	173	ASN
2	H	210	ASN
2	H	241	HIS
2	H	269	ASN
2	I	61	GLN
2	I	64	ASN
2	I	210	ASN
2	I	317	GLN
2	J	61	GLN
2	J	66	ASN
2	J	73	GLN
2	J	86	ASN
2	J	173	ASN
2	J	266	ASN
2	K	64	ASN
2	K	86	ASN
2	K	111	GLN
2	K	266	ASN
2	L	61	GLN
2	L	66	ASN
2	L	111	GLN
2	L	140	GLN
2	L	269	ASN
2	M	61	GLN
2	M	66	ASN
2	M	73	GLN

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Mol	Chain	Res	Type
2	M	86	ASN
2	M	111	GLN
2	M	112	ASN
2	M	236	GLN
2	M	295	GLN
2	N	61	GLN
2	N	262	ASN
2	N	269	ASN
2	N	276	GLN
2	N	317	GLN
2	O	61	GLN
2	O	86	ASN
2	O	97	GLN
2	O	111	GLN
2	O	125	ASN
2	O	140	GLN
2	O	173	ASN
2	O	269	ASN
1	R	149	ASN
1	S	149	ASN
1	W	149	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](#)

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	1	9/20 (45%)	1.32	3 (33%)	1 1	133, 141, 145, 158	0
1	2	9/20 (45%)	0.97	1 (11%)	10 11	120, 130, 150, 156	0
1	3	9/20 (45%)	1.44	2 (22%)	2 4	123, 129, 138, 144	0
1	4	9/20 (45%)	1.09	1 (11%)	10 11	108, 117, 143, 145	0
1	P	9/20 (45%)	1.10	1 (11%)	10 11	125, 137, 144, 155	0
1	Q	9/20 (45%)	1.15	1 (11%)	10 11	103, 113, 129, 169	0
1	R	9/20 (45%)	1.47	4 (44%)	0 0	103, 111, 128, 147	0
1	S	9/20 (45%)	1.41	2 (22%)	2 4	84, 93, 127, 141	0
1	T	9/20 (45%)	1.50	3 (33%)	1 1	140, 148, 156, 157	0
1	U	9/20 (45%)	1.17	1 (11%)	10 11	114, 128, 150, 168	0
1	V	9/20 (45%)	1.34	2 (22%)	2 4	117, 123, 150, 176	0
1	W	9/20 (45%)	1.80	3 (33%)	1 1	116, 127, 138, 142	0
1	X	9/20 (45%)	1.43	2 (22%)	2 4	126, 138, 147, 152	0
1	Y	9/20 (45%)	1.12	1 (11%)	10 11	115, 123, 137, 137	0
1	Z	9/20 (45%)	0.90	1 (11%)	10 11	111, 121, 144, 145	0
2	A	286/286 (100%)	0.48	7 (2%)	59 44	64, 119, 162, 203	4 (1%)
2	B	286/286 (100%)	0.56	10 (3%)	47 34	65, 113, 184, 198	4 (1%)
2	C	286/286 (100%)	0.58	16 (5%)	30 22	58, 104, 159, 207	4 (1%)
2	D	286/286 (100%)	0.37	2 (0%)	84 72	58, 102, 144, 187	4 (1%)
2	E	286/286 (100%)	0.53	10 (3%)	47 34	66, 123, 164, 195	4 (1%)
2	F	286/286 (100%)	0.50	10 (3%)	47 34	68, 117, 165, 206	4 (1%)
2	G	286/286 (100%)	0.36	5 (1%)	69 53	64, 113, 160, 210	4 (1%)
2	H	286/286 (100%)	0.41	9 (3%)	51 38	54, 111, 153, 190	4 (1%)
2	I	286/286 (100%)	0.43	4 (1%)	73 59	58, 117, 160, 184	4 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	J	286/286 (100%)	0.40	7 (2%)	59	44	76, 123, 166, 222	4 (1%)
2	K	286/286 (100%)	0.41	5 (1%)	69	53	63, 112, 155, 199	4 (1%)
2	L	286/286 (100%)	0.34	6 (2%)	63	47	62, 120, 159, 180	4 (1%)
2	M	286/286 (100%)	0.41	4 (1%)	73	59	69, 113, 149, 189	4 (1%)
2	N	286/286 (100%)	0.42	5 (1%)	69	53	64, 110, 152, 186	4 (1%)
2	O	286/286 (100%)	0.48	8 (2%)	55	40	64, 111, 152, 184	4 (1%)
All	All	4425/4590 (96%)	0.47	136 (3%)	51	38	54, 114, 160, 222	60 (1%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	36[A]	MET	5.9
2	J	142[A]	ILE	4.6
2	E	142[A]	ILE	4.5
2	I	142[A]	ILE	4.5
2	M	142[A]	ILE	4.3
2	G	313	SER	4.3
2	L	36[A]	MET	4.2
2	F	142[A]	ILE	4.0
2	O	142[A]	ILE	3.9
2	E	319	PHE	3.8
2	F	35	ALA	3.8
1	1	152	VAL	3.8
2	G	142[A]	ILE	3.8
2	O	190	VAL	3.7
2	C	142[A]	ILE	3.6
2	L	142[A]	ILE	3.6
2	H	142[A]	ILE	3.5
2	A	142[A]	ILE	3.5
2	D	142[A]	ILE	3.5
2	C	37	GLY	3.4
2	B	35	ALA	3.3
2	J	81	VAL	3.2
1	4	152	VAL	3.2
1	R	154	ASP	3.2
2	B	87	PHE	3.2
2	B	142[A]	ILE	3.1
1	U	152	VAL	3.1
2	N	142[A]	ILE	3.0
2	K	142[A]	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	R	152	VAL	3.0
2	H	35	ALA	2.9
2	A	171	LEU	2.9
2	H	52	LEU	2.9
1	S	152	VAL	2.9
2	C	223	LEU	2.9
2	E	281	GLY	2.8
1	V	152	VAL	2.8
2	E	115	GLU	2.8
2	C	35	ALA	2.8
2	E	37	GLY	2.8
2	D	37	GLY	2.7
2	E	193[A]	THR	2.7
2	J	313	SER	2.7
2	N	36[A]	MET	2.7
2	E	254	LEU	2.7
2	B	125	ASN	2.7
2	J	183	GLY	2.6
2	B	37	GLY	2.6
2	M	36[A]	MET	2.6
2	A	271	LEU	2.6
2	F	118	VAL	2.6
2	I	289	ILE	2.6
2	O	155	ILE	2.6
1	Q	152	VAL	2.6
2	F	313	SER	2.5
2	B	34	GLY	2.5
2	B	52	LEU	2.5
2	L	171	LEU	2.5
1	1	154	ASP	2.5
1	3	151	LEU	2.5
2	C	53	GLY	2.5
2	L	34	GLY	2.5
1	Y	152	VAL	2.5
1	R	156	MET	2.5
2	F	36[A]	MET	2.5
2	K	313	SER	2.5
2	C	222	ASN	2.5
2	H	149	ILE	2.4
2	N	202	LEU	2.4
2	A	87	PHE	2.4
2	C	225	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	37	GLY	2.4
2	O	270	ASN	2.4
2	C	141	ALA	2.4
2	N	312	TYR	2.4
2	O	35	ALA	2.4
2	B	71	PHE	2.3
2	L	200	LEU	2.3
2	O	97	GLN	2.3
1	2	152	VAL	2.3
2	A	37	GLY	2.3
2	N	35	ALA	2.3
2	G	218	ASN	2.3
2	M	251	TYR	2.3
1	T	154	ASP	2.3
2	G	37	GLY	2.3
2	C	317	GLN	2.3
2	J	231	SER	2.3
2	C	216	ASN	2.3
2	L	149	ILE	2.2
2	K	98	ALA	2.2
2	O	108	ILE	2.2
2	O	281	GLY	2.2
2	C	76	THR	2.2
2	C	140	GLN	2.2
1	1	156	MET	2.2
1	W	156	MET	2.2
1	Z	151	LEU	2.2
2	F	34	GLY	2.2
2	G	34	GLY	2.2
2	H	204	ALA	2.2
2	K	37	GLY	2.2
2	M	219	PRO	2.2
1	P	152	VAL	2.2
2	F	190	VAL	2.2
2	E	119	SER	2.2
1	S	153	PRO	2.2
2	E	247	THR	2.2
1	X	152	VAL	2.2
2	H	110	GLU	2.2
2	J	141	ALA	2.2
1	T	148	TYR	2.1
1	X	151	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	307	SER	2.1
1	V	153	PRO	2.1
1	T	152	VAL	2.1
2	K	35	ALA	2.1
2	A	99	SER	2.1
2	C	115	GLU	2.1
1	R	148	TYR	2.1
1	W	150	PRO	2.1
2	J	86	ASN	2.1
1	W	154	ASP	2.1
2	F	241	HIS	2.1
2	H	241	HIS	2.1
2	H	313	SER	2.1
2	C	118	VAL	2.1
2	F	218	ASN	2.1
2	A	52	LEU	2.1
2	B	83	ILE	2.1
2	C	36[A]	MET	2.1
2	C	34	GLY	2.1
2	I	256	SER	2.0
2	E	90	GLY	2.0
1	3	152	VAL	2.0
2	I	202	LEU	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.