



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:07 PM UTC

PDB ID : 4EP0 / pdb_00004ep0
Title : Structure of the bacteriophage C1 tail knob protein, gp12
Authors : Aksyuk, A.A.; Rossmann, M.G.
Deposited on : 2012-04-16
Resolution : 4.00 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:

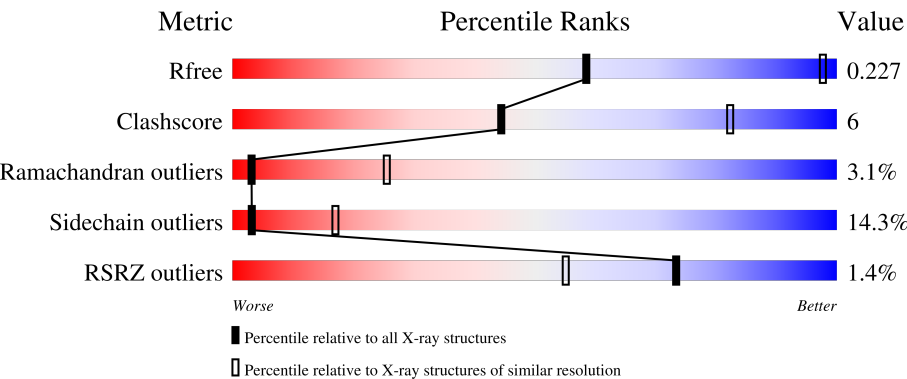
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	583	% 62%18% • • 16%
1	B	583	% 62%18% • • 16%
1	C	583	2% 60%20% • • 16%
1	D	583	2% 59%21% • • 16%
1	E	583	% 61%20% • • 16%

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Mol	Chain	Length	Quality of chain
1	F	583	% 61% 19% 16%
1	G	583	% 61% 20% 16%
1	H	583	% 62% 18% 16%
1	I	583	% 61% 19% 16%
1	J	583	% 62% 18% 16%
1	K	583	% 62% 18% 16%
1	L	583	2% 62% 18% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 47376 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 Major tail protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	B	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	C	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	D	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	E	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	F	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	G	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	H	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	I	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	J	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	K	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	L	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP Q7Y3F0
A	576	LEU	-	expression tag	UNP Q7Y3F0
A	577	GLU	-	expression tag	UNP Q7Y3F0
A	578	HIS	-	expression tag	UNP Q7Y3F0
A	579	HIS	-	expression tag	UNP Q7Y3F0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	HIS	-	expression tag	UNP Q7Y3F0
A	581	HIS	-	expression tag	UNP Q7Y3F0
A	582	HIS	-	expression tag	UNP Q7Y3F0
A	583	HIS	-	expression tag	UNP Q7Y3F0
B	575	SER	-	expression tag	UNP Q7Y3F0
B	576	LEU	-	expression tag	UNP Q7Y3F0
B	577	GLU	-	expression tag	UNP Q7Y3F0
B	578	HIS	-	expression tag	UNP Q7Y3F0
B	579	HIS	-	expression tag	UNP Q7Y3F0
B	580	HIS	-	expression tag	UNP Q7Y3F0
B	581	HIS	-	expression tag	UNP Q7Y3F0
B	582	HIS	-	expression tag	UNP Q7Y3F0
B	583	HIS	-	expression tag	UNP Q7Y3F0
C	575	SER	-	expression tag	UNP Q7Y3F0
C	576	LEU	-	expression tag	UNP Q7Y3F0
C	577	GLU	-	expression tag	UNP Q7Y3F0
C	578	HIS	-	expression tag	UNP Q7Y3F0
C	579	HIS	-	expression tag	UNP Q7Y3F0
C	580	HIS	-	expression tag	UNP Q7Y3F0
C	581	HIS	-	expression tag	UNP Q7Y3F0
C	582	HIS	-	expression tag	UNP Q7Y3F0
C	583	HIS	-	expression tag	UNP Q7Y3F0
D	575	SER	-	expression tag	UNP Q7Y3F0
D	576	LEU	-	expression tag	UNP Q7Y3F0
D	577	GLU	-	expression tag	UNP Q7Y3F0
D	578	HIS	-	expression tag	UNP Q7Y3F0
D	579	HIS	-	expression tag	UNP Q7Y3F0
D	580	HIS	-	expression tag	UNP Q7Y3F0
D	581	HIS	-	expression tag	UNP Q7Y3F0
D	582	HIS	-	expression tag	UNP Q7Y3F0
D	583	HIS	-	expression tag	UNP Q7Y3F0
E	575	SER	-	expression tag	UNP Q7Y3F0
E	576	LEU	-	expression tag	UNP Q7Y3F0
E	577	GLU	-	expression tag	UNP Q7Y3F0
E	578	HIS	-	expression tag	UNP Q7Y3F0
E	579	HIS	-	expression tag	UNP Q7Y3F0
E	580	HIS	-	expression tag	UNP Q7Y3F0
E	581	HIS	-	expression tag	UNP Q7Y3F0
E	582	HIS	-	expression tag	UNP Q7Y3F0
E	583	HIS	-	expression tag	UNP Q7Y3F0
F	575	SER	-	expression tag	UNP Q7Y3F0
F	576	LEU	-	expression tag	UNP Q7Y3F0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	577	GLU	-	expression tag	UNP Q7Y3F0
F	578	HIS	-	expression tag	UNP Q7Y3F0
F	579	HIS	-	expression tag	UNP Q7Y3F0
F	580	HIS	-	expression tag	UNP Q7Y3F0
F	581	HIS	-	expression tag	UNP Q7Y3F0
F	582	HIS	-	expression tag	UNP Q7Y3F0
F	583	HIS	-	expression tag	UNP Q7Y3F0
G	575	SER	-	expression tag	UNP Q7Y3F0
G	576	LEU	-	expression tag	UNP Q7Y3F0
G	577	GLU	-	expression tag	UNP Q7Y3F0
G	578	HIS	-	expression tag	UNP Q7Y3F0
G	579	HIS	-	expression tag	UNP Q7Y3F0
G	580	HIS	-	expression tag	UNP Q7Y3F0
G	581	HIS	-	expression tag	UNP Q7Y3F0
G	582	HIS	-	expression tag	UNP Q7Y3F0
G	583	HIS	-	expression tag	UNP Q7Y3F0
H	575	SER	-	expression tag	UNP Q7Y3F0
H	576	LEU	-	expression tag	UNP Q7Y3F0
H	577	GLU	-	expression tag	UNP Q7Y3F0
H	578	HIS	-	expression tag	UNP Q7Y3F0
H	579	HIS	-	expression tag	UNP Q7Y3F0
H	580	HIS	-	expression tag	UNP Q7Y3F0
H	581	HIS	-	expression tag	UNP Q7Y3F0
H	582	HIS	-	expression tag	UNP Q7Y3F0
H	583	HIS	-	expression tag	UNP Q7Y3F0
I	575	SER	-	expression tag	UNP Q7Y3F0
I	576	LEU	-	expression tag	UNP Q7Y3F0
I	577	GLU	-	expression tag	UNP Q7Y3F0
I	578	HIS	-	expression tag	UNP Q7Y3F0
I	579	HIS	-	expression tag	UNP Q7Y3F0
I	580	HIS	-	expression tag	UNP Q7Y3F0
I	581	HIS	-	expression tag	UNP Q7Y3F0
I	582	HIS	-	expression tag	UNP Q7Y3F0
I	583	HIS	-	expression tag	UNP Q7Y3F0
J	575	SER	-	expression tag	UNP Q7Y3F0
J	576	LEU	-	expression tag	UNP Q7Y3F0
J	577	GLU	-	expression tag	UNP Q7Y3F0
J	578	HIS	-	expression tag	UNP Q7Y3F0
J	579	HIS	-	expression tag	UNP Q7Y3F0
J	580	HIS	-	expression tag	UNP Q7Y3F0
J	581	HIS	-	expression tag	UNP Q7Y3F0
J	582	HIS	-	expression tag	UNP Q7Y3F0

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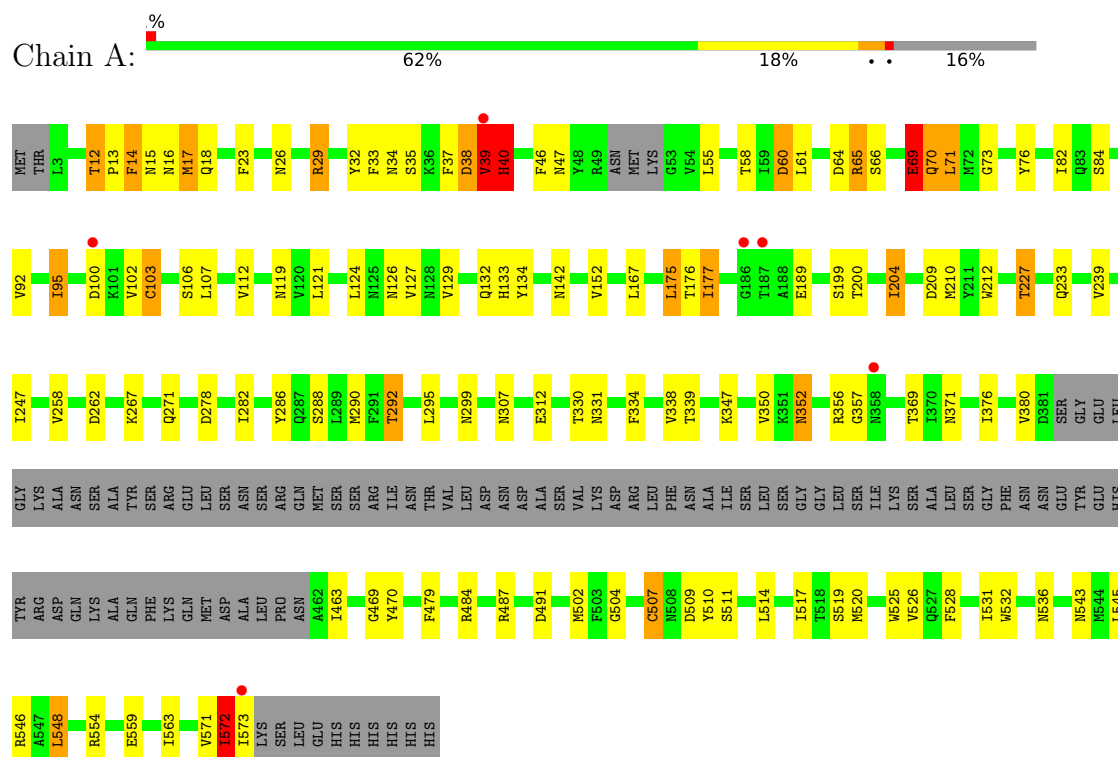
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Chain	Residue	Modelled	Actual	Comment	Reference
J	583	HIS	-	expression tag	UNP Q7Y3F0
K	575	SER	-	expression tag	UNP Q7Y3F0
K	576	LEU	-	expression tag	UNP Q7Y3F0
K	577	GLU	-	expression tag	UNP Q7Y3F0
K	578	HIS	-	expression tag	UNP Q7Y3F0
K	579	HIS	-	expression tag	UNP Q7Y3F0
K	580	HIS	-	expression tag	UNP Q7Y3F0
K	581	HIS	-	expression tag	UNP Q7Y3F0
K	582	HIS	-	expression tag	UNP Q7Y3F0
K	583	HIS	-	expression tag	UNP Q7Y3F0
L	575	SER	-	expression tag	UNP Q7Y3F0
L	576	LEU	-	expression tag	UNP Q7Y3F0
L	577	GLU	-	expression tag	UNP Q7Y3F0
L	578	HIS	-	expression tag	UNP Q7Y3F0
L	579	HIS	-	expression tag	UNP Q7Y3F0
L	580	HIS	-	expression tag	UNP Q7Y3F0
L	581	HIS	-	expression tag	UNP Q7Y3F0
L	582	HIS	-	expression tag	UNP Q7Y3F0
L	583	HIS	-	expression tag	UNP Q7Y3F0

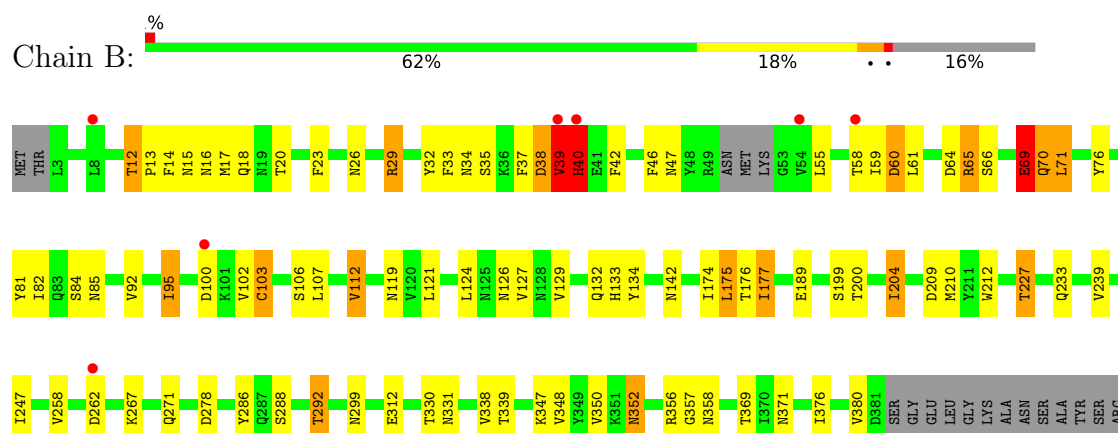
3 Residue-property plots [i](#)

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.

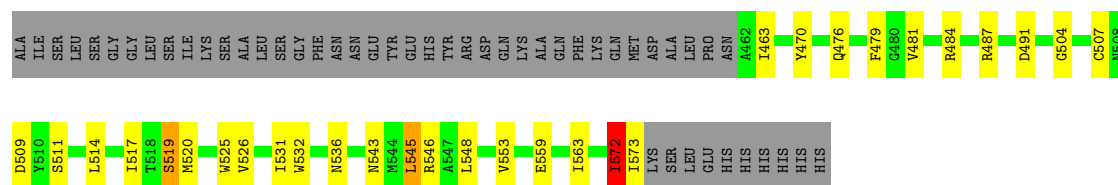
• Molecule 1: Major tail protein



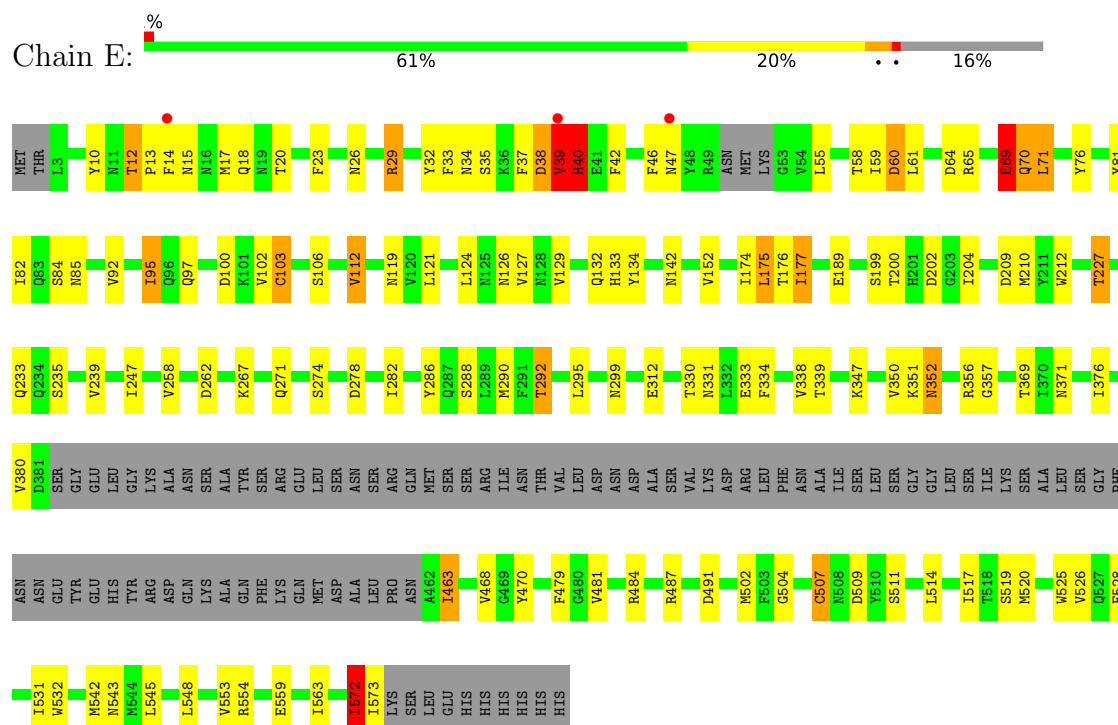
• Molecule 1: Major tail protein



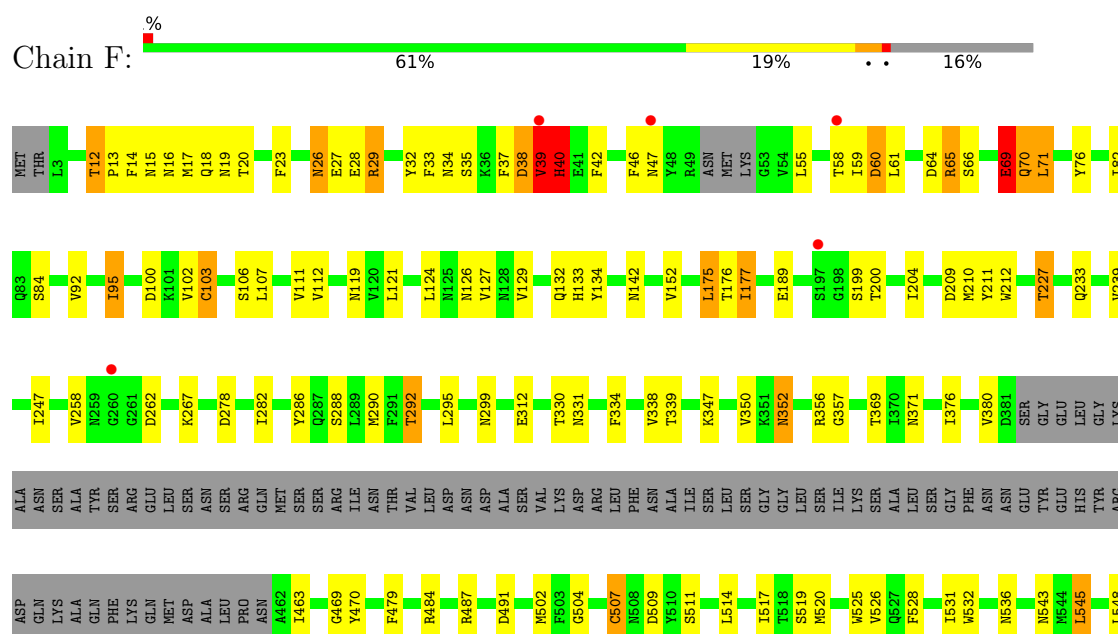


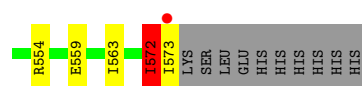


• Molecule 1: Major tail protein

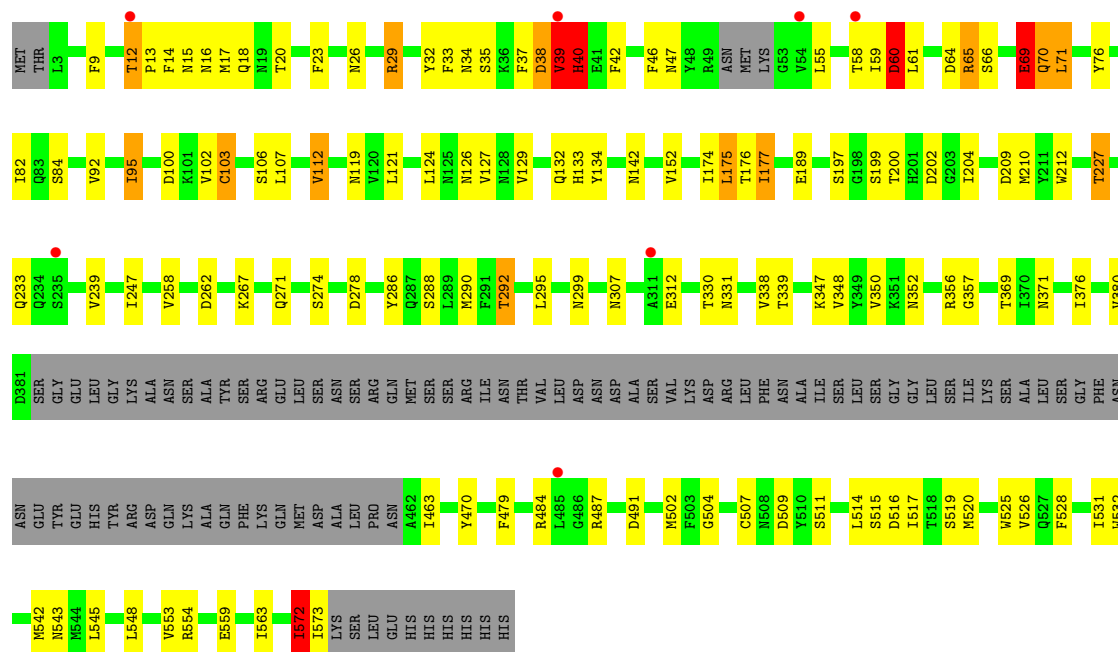


• Molecule 1: Major tail protein

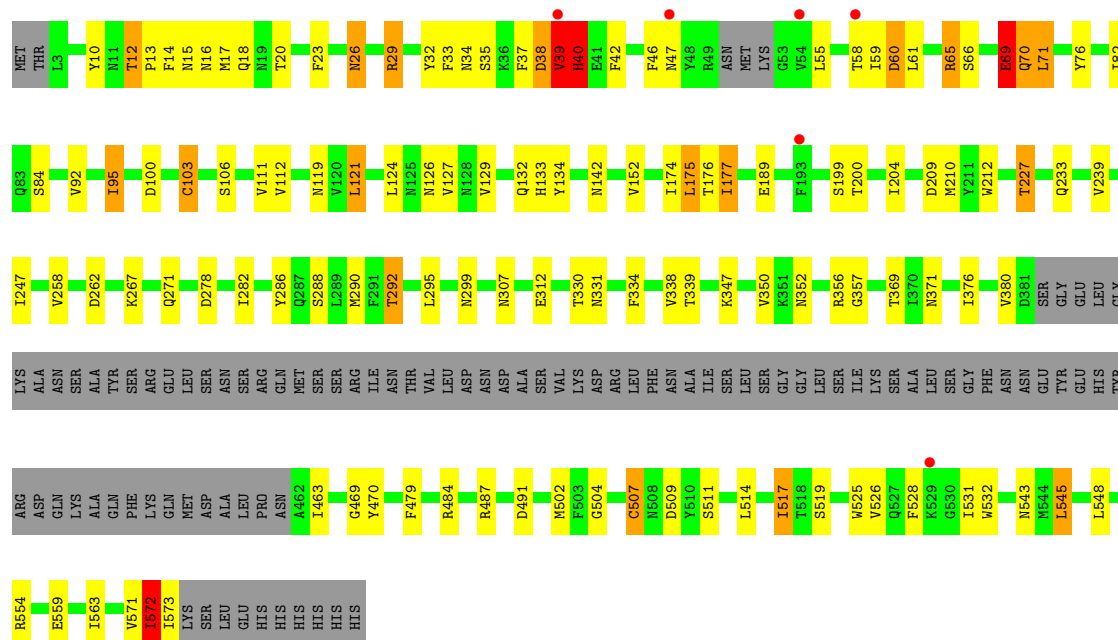




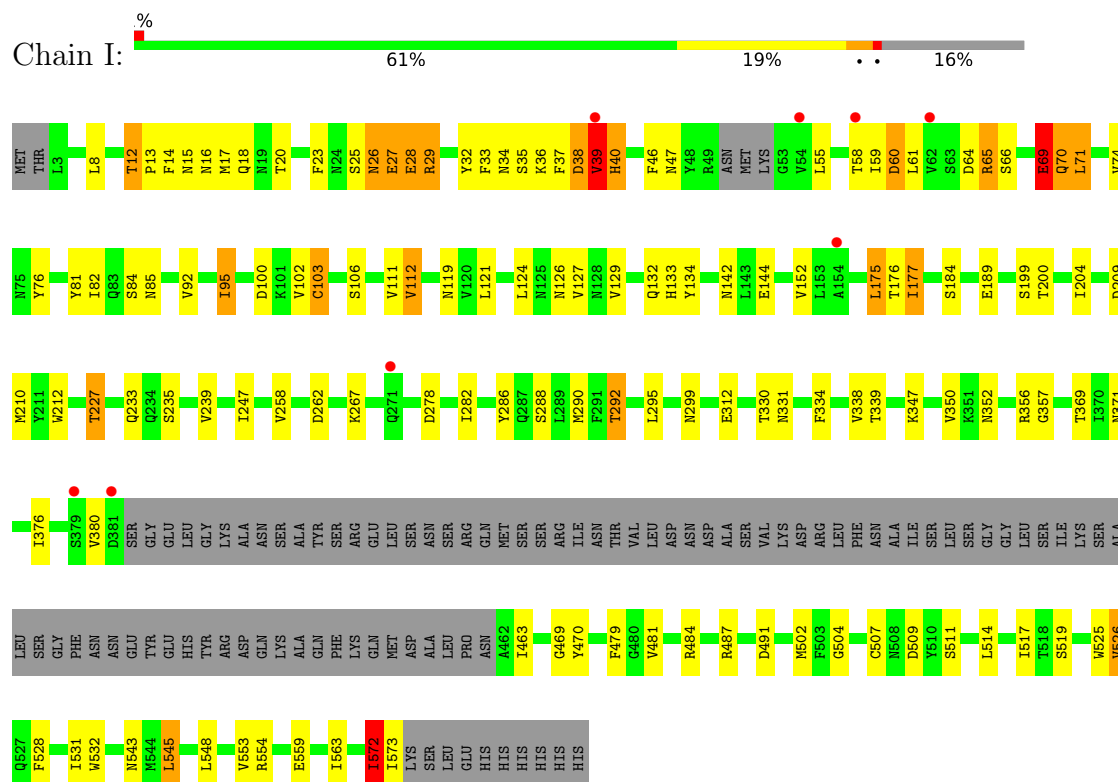
• Molecule 1: Major tail protein



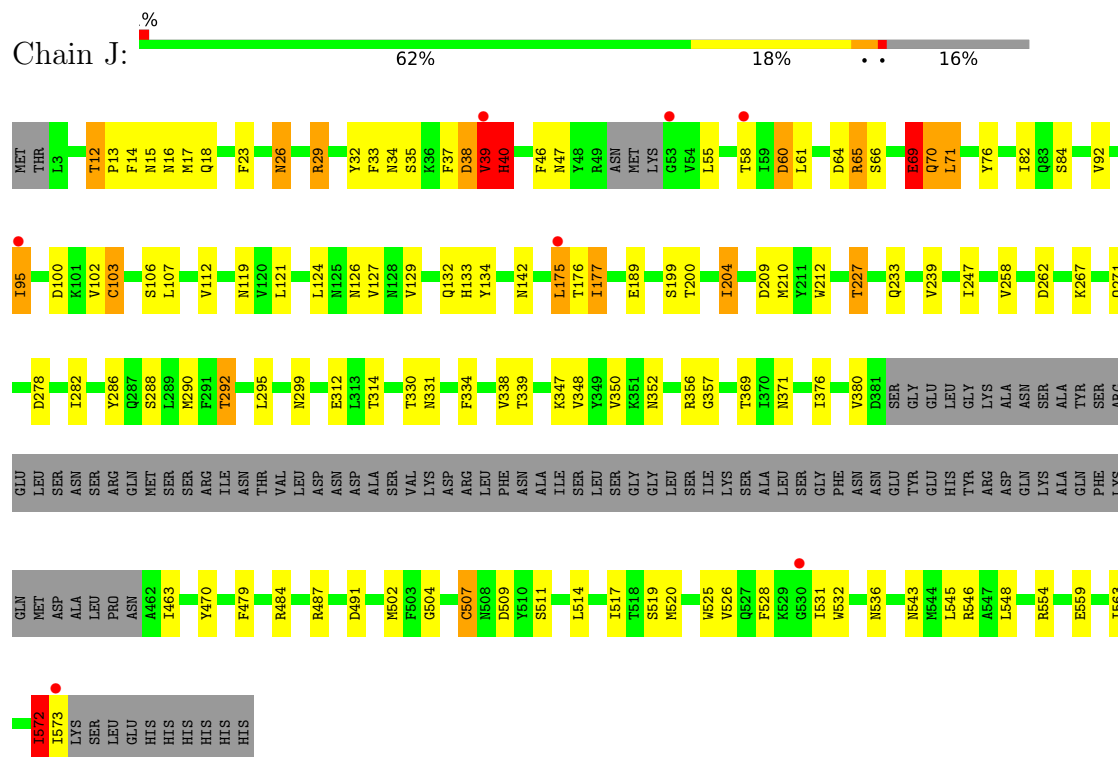
• Molecule 1: Major tail protein



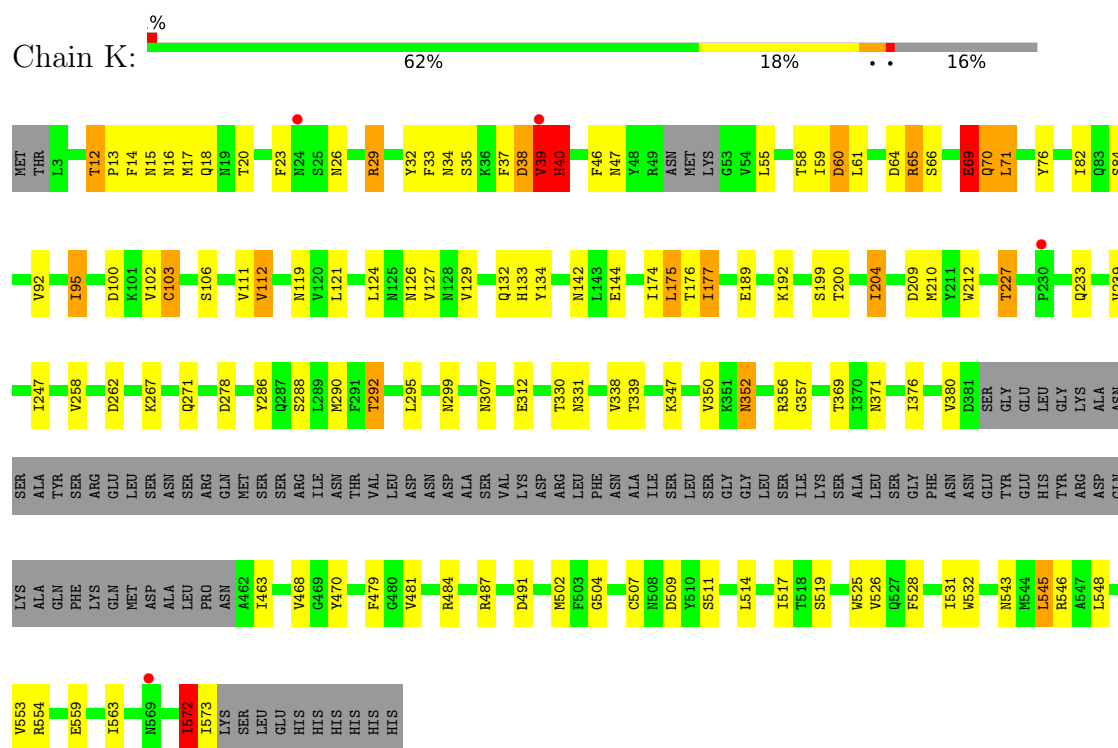
- Molecule 1: Major tail protein



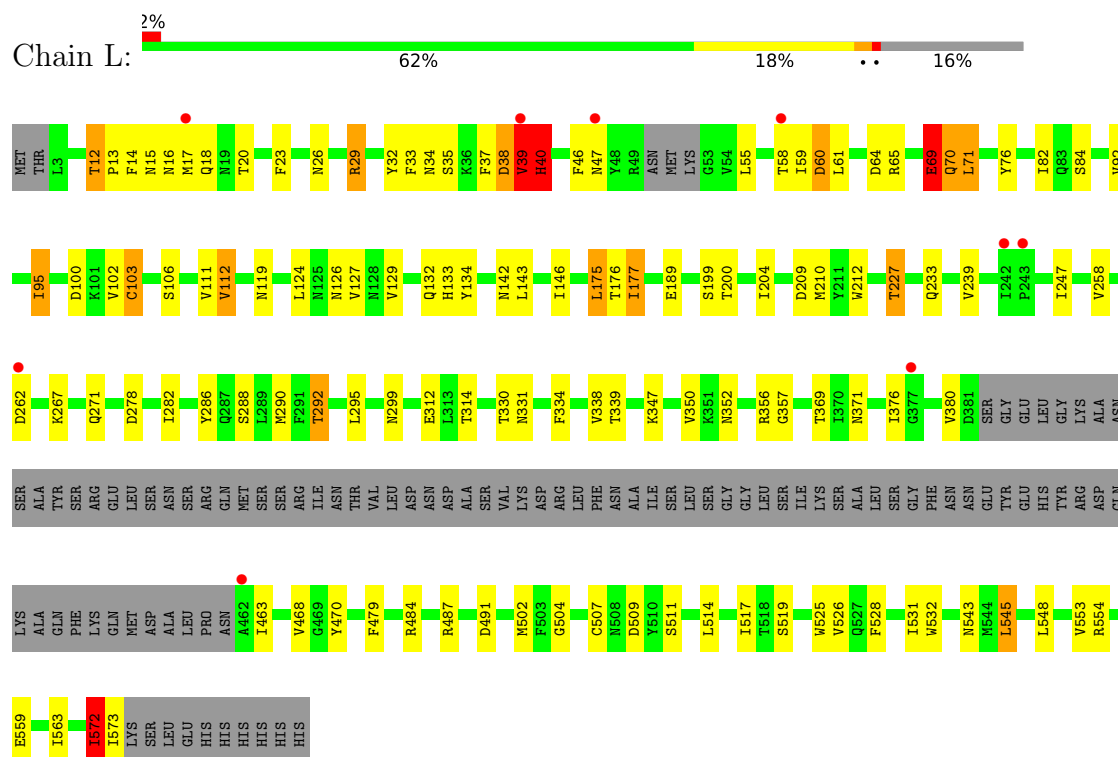
- Molecule 1: Major tail protein



- Molecule 1: Major tail protein



• Molecule 1: Major tail protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	316.87Å 211.38Å 178.60Å 90.00° 116.53° 90.00°	Depositor
Resolution (Å)	49.73 – 4.00 49.73 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.73-4.00) 99.3 (49.73-4.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.233 0.186 , 0.227	Depositor DCC
R_{free} test set	4429 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 119.3	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	0.88	EDS
Total number of atoms	47376	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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	0.63	1/4030 (0.0%)	0.90	8/5464 (0.1%)
1	B	0.63	1/4030 (0.0%)	0.90	6/5464 (0.1%)
1	C	0.68	1/4030 (0.0%)	0.91	11/5464 (0.2%)
1	D	0.65	0/4030	0.92	9/5464 (0.2%)
1	E	0.64	1/4030 (0.0%)	0.89	6/5464 (0.1%)
1	F	0.67	0/4030	0.92	7/5464 (0.1%)
1	G	0.61	1/4030 (0.0%)	0.89	8/5464 (0.1%)
1	H	0.62	0/4030	0.89	5/5464 (0.1%)
1	I	0.66	0/4030	0.93	8/5464 (0.1%)
1	J	0.62	0/4030	0.89	6/5464 (0.1%)
1	K	0.62	1/4030 (0.0%)	0.90	6/5464 (0.1%)
1	L	0.62	0/4030	0.88	6/5464 (0.1%)
All	All	0.64	6/48360 (0.0%)	0.90	86/65568 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	174	ILE	CA-CB	6.01	1.61	1.54
1	C	291	PHE	CE1-CZ	-5.66	1.21	1.38
1	A	39	VAL	CA-C	5.14	1.59	1.52
1	B	39	VAL	CA-C	5.14	1.59	1.52
1	E	39	VAL	CA-C	5.04	1.59	1.52
1	G	39	VAL	CA-C	5.01	1.59	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	28	GLU	N-CA-C	-8.71	102.78	113.41
1	I	28	GLU	N-CA-C	-7.87	103.81	113.41
1	I	525	TRP	N-CA-C	-7.51	98.79	110.42
1	J	525	TRP	N-CA-C	-7.19	99.28	110.42
1	E	525	TRP	N-CA-C	-7.15	99.33	110.42
1	A	525	TRP	N-CA-C	-6.96	98.96	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	525	TRP	N-CA-C	-6.96	99.63	110.42
1	G	525	TRP	N-CA-C	-6.95	98.98	110.17
1	D	525	TRP	N-CA-C	-6.88	99.10	110.17
1	F	71	LEU	N-CA-C	-6.86	103.58	112.23
1	K	525	TRP	N-CA-C	-6.61	100.18	110.42
1	G	71	LEU	N-CA-C	-6.56	103.96	112.23
1	D	71	LEU	N-CA-C	-6.55	103.97	112.23
1	E	39	VAL	N-CA-C	6.51	122.87	109.34
1	G	39	VAL	N-CA-C	6.50	122.85	109.34
1	D	39	VAL	N-CA-C	6.49	122.84	109.34
1	C	39	VAL	N-CA-C	6.48	122.81	109.34
1	I	39	VAL	N-CA-C	6.47	122.79	109.34
1	L	39	VAL	N-CA-C	6.46	122.77	109.34
1	F	39	VAL	N-CA-C	6.44	122.74	109.34
1	K	71	LEU	N-CA-C	-6.43	104.12	112.23
1	H	39	VAL	N-CA-C	6.42	122.69	109.34
1	A	39	VAL	N-CA-C	6.40	122.66	109.34
1	B	39	VAL	N-CA-C	6.36	122.56	109.34
1	I	71	LEU	N-CA-C	-6.35	104.23	112.23
1	K	39	VAL	N-CA-C	6.35	122.55	109.34
1	B	525	TRP	N-CA-C	-6.34	100.59	110.42
1	J	39	VAL	N-CA-C	6.34	122.52	109.34
1	B	71	LEU	N-CA-C	-6.27	104.32	112.23
1	L	71	LEU	N-CA-C	-6.26	104.34	112.23
1	C	71	LEU	N-CA-C	-6.26	104.34	112.23
1	J	71	LEU	N-CA-C	-6.22	104.39	112.23
1	H	71	LEU	N-CA-C	-6.16	104.47	112.23
1	A	71	LEU	N-CA-C	-6.12	104.52	112.23
1	J	528	PHE	N-CA-C	6.12	119.21	108.75
1	C	525	TRP	N-CA-C	-6.08	100.39	110.17
1	C	184	SER	N-CA-C	6.05	119.11	110.10
1	K	528	PHE	N-CA-C	5.98	118.98	108.75
1	F	40	HIS	N-CA-C	5.95	123.48	110.80
1	A	528	PHE	N-CA-C	5.89	118.82	108.75
1	C	528	PHE	N-CA-C	5.86	118.77	108.75
1	E	71	LEU	N-CA-C	-5.85	104.85	112.23
1	H	525	TRP	N-CA-C	-5.85	100.75	110.17
1	H	528	PHE	N-CA-C	5.84	118.73	108.75
1	I	528	PHE	N-CA-C	5.82	118.70	108.75
1	I	40	HIS	N-CA-C	5.81	123.17	110.80
1	L	528	PHE	N-CA-C	5.75	118.58	108.75
1	D	40	HIS	N-CA-C	5.73	123.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	525	TRP	N-CA-C	-5.71	100.98	110.17
1	A	40	HIS	N-CA-C	5.69	122.92	110.80
1	D	229	TYR	CA-C-N	5.68	125.39	119.82
1	D	229	TYR	C-N-CA	5.68	125.39	119.82
1	E	40	HIS	N-CA-C	5.68	122.89	110.80
1	H	40	HIS	N-CA-C	5.64	122.82	110.80
1	G	40	HIS	N-CA-C	5.64	122.82	110.80
1	B	528	PHE	N-CA-C	5.60	118.33	108.75
1	B	40	HIS	N-CA-C	5.59	122.70	110.80
1	J	40	HIS	N-CA-C	5.54	122.60	110.80
1	F	528	PHE	N-CA-C	5.53	118.21	108.75
1	L	40	HIS	N-CA-C	5.53	122.58	110.80
1	E	528	PHE	N-CA-C	5.48	118.13	108.75
1	C	40	HIS	N-CA-C	5.39	122.28	110.80
1	D	64	ASP	N-CA-C	5.39	117.26	109.07
1	G	528	PHE	N-CA-C	5.38	117.95	108.75
1	K	64	ASP	N-CA-C	5.30	117.13	109.07
1	J	64	ASP	N-CA-C	5.30	117.13	109.07
1	A	64	ASP	N-CA-C	5.24	117.04	109.07
1	G	9	PHE	N-CA-C	5.22	117.60	110.24
1	B	64	ASP	N-CA-C	5.21	116.99	109.07
1	F	64	ASP	N-CA-C	5.20	116.98	109.07
1	A	548	LEU	N-CA-C	-5.17	105.72	112.23
1	C	17	MET	N-CA-C	-5.14	105.73	112.72
1	K	40	HIS	N-CA-C	5.12	121.71	110.80
1	E	64	ASP	N-CA-C	5.12	116.85	109.07
1	I	64	ASP	N-CA-C	5.11	116.83	109.07
1	C	510	TYR	N-CA-C	-5.10	103.66	110.55
1	L	64	ASP	N-CA-C	5.10	116.83	109.07
1	D	519	SER	N-CA-C	-5.08	105.63	111.07
1	D	8	LEU	N-CA-C	5.06	116.84	108.49
1	G	60	ASP	N-CA-C	5.06	116.68	109.14
1	G	64	ASP	N-CA-C	5.05	116.74	109.07
1	C	64	ASP	N-CA-C	5.03	116.71	109.07
1	I	184	SER	N-CA-C	5.02	117.58	110.10
1	C	181	LEU	N-CA-C	5.02	118.86	112.34
1	C	60	ASP	N-CA-C	5.01	116.80	109.24
1	A	17	MET	N-CA-C	-5.00	105.91	112.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3832	48	0
1	B	3948	0	3832	53	0
1	C	3948	0	3832	70	2
1	D	3948	0	3832	57	1
1	E	3948	0	3832	52	0
1	F	3948	0	3832	47	0
1	G	3948	0	3832	46	0
1	H	3948	0	3832	47	0
1	I	3948	0	3832	72	0
1	J	3948	0	3832	45	0
1	K	3948	0	3832	47	1
1	L	3948	0	3832	47	0
All	All	47376	0	45984	556	2

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 (556) 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:C:291:PHE:HZ	1:I:26:ASN:N	1.74	0.85
1:C:291:PHE:CZ	1:I:25:SER:HB2	2.22	0.74
1:C:291:PHE:CZ	1:I:25:SER:C	2.67	0.73
1:L:312:GLU:OE2	1:L:484:ARG:NH1	2.23	0.72
1:F:286:TYR:N	1:F:331:ASN:OD1	2.24	0.71
1:F:32:TYR:OH	1:F:559:GLU:OE2	2.09	0.70
1:D:312:GLU:OE2	1:D:484:ARG:NH1	2.24	0.70
1:E:312:GLU:OE2	1:E:484:ARG:NH1	2.25	0.70
1:A:286:TYR:N	1:A:331:ASN:OD1	2.26	0.69
1:C:286:TYR:N	1:C:331:ASN:OD1	2.26	0.68
1:B:358:ASN:HB2	1:I:36:LYS:CA	2.23	0.68
1:E:286:TYR:N	1:E:331:ASN:OD1	2.28	0.67
1:K:286:TYR:N	1:K:331:ASN:OD1	2.27	0.67
1:B:358:ASN:HB2	1:I:36:LYS:N	2.10	0.67
1:H:312:GLU:OE2	1:H:484:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:286:TYR:N	1:H:331:ASN:OD1	2.28	0.66
1:C:291:PHE:CZ	1:I:26:ASN:N	2.61	0.65
1:L:286:TYR:N	1:L:331:ASN:OD1	2.29	0.65
1:C:291:PHE:CE1	1:I:25:SER:HB2	2.31	0.65
1:J:286:TYR:N	1:J:331:ASN:OD1	2.30	0.64
1:G:286:TYR:N	1:G:331:ASN:OD1	2.31	0.64
1:F:312:GLU:OE2	1:F:484:ARG:NH1	2.31	0.64
1:D:233:GLN:NE2	1:D:380:VAL:HG22	2.13	0.63
1:I:286:TYR:N	1:I:331:ASN:OD1	2.30	0.63
1:D:286:TYR:N	1:D:331:ASN:OD1	2.31	0.63
1:A:491:ASP:OD2	1:F:142:ASN:ND2	2.32	0.63
1:F:69:GLU:HA	1:F:103:CYS:SG	2.38	0.63
1:A:312:GLU:OE2	1:A:484:ARG:NH1	2.32	0.63
1:F:233:GLN:NE2	1:F:380:VAL:HG22	2.13	0.62
1:B:286:TYR:N	1:B:331:ASN:OD1	2.32	0.62
1:D:356:ARG:NH2	1:E:487:ARG:O	2.32	0.62
1:A:69:GLU:HA	1:A:103:CYS:SG	2.40	0.62
1:A:142:ASN:ND2	1:B:491:ASP:OD2	2.31	0.62
1:G:233:GLN:NE2	1:G:380:VAL:HG22	2.14	0.62
1:I:312:GLU:OE2	1:I:484:ARG:NH1	2.33	0.62
1:H:69:GLU:O	1:H:71:LEU:N	2.32	0.62
1:B:312:GLU:OE2	1:B:484:ARG:NH1	2.32	0.62
1:C:291:PHE:CD1	1:I:27:GLU:CD	2.78	0.62
1:C:291:PHE:CZ	1:I:25:SER:CB	2.82	0.62
1:D:142:ASN:ND2	1:E:491:ASP:OD2	2.33	0.62
1:H:233:GLN:NE2	1:H:380:VAL:HG22	2.15	0.62
1:C:291:PHE:CE2	1:I:25:SER:OG	2.48	0.61
1:K:312:GLU:OE2	1:K:484:ARG:NH1	2.32	0.61
1:C:291:PHE:CD2	1:I:27:GLU:HG2	2.34	0.61
1:B:26:ASN:OD1	1:B:29:ARG:NH1	2.33	0.61
1:C:312:GLU:OE2	1:C:484:ARG:NH1	2.34	0.61
1:J:233:GLN:NE2	1:J:380:VAL:HG22	2.15	0.61
1:E:26:ASN:OD1	1:E:29:ARG:NH1	2.34	0.61
1:I:233:GLN:NE2	1:I:380:VAL:HG22	2.16	0.61
1:I:356:ARG:NH2	1:J:487:ARG:O	2.34	0.61
1:E:69:GLU:HA	1:E:103:CYS:SG	2.41	0.61
1:A:69:GLU:O	1:A:71:LEU:N	2.34	0.61
1:D:204:ILE:HD13	1:E:468:VAL:HG21	1.83	0.61
1:K:69:GLU:O	1:K:71:LEU:N	2.34	0.60
1:E:233:GLN:NE2	1:E:380:VAL:HG22	2.15	0.60
1:A:233:GLN:NE2	1:A:380:VAL:HG22	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:GLU:O	1:G:71:LEU:N	2.35	0.60
1:J:69:GLU:O	1:J:71:LEU:N	2.33	0.60
1:J:312:GLU:OE2	1:J:484:ARG:NH1	2.35	0.60
1:B:358:ASN:HB2	1:I:36:LYS:HA	1.82	0.59
1:J:26:ASN:OD1	1:J:29:ARG:NH1	2.35	0.59
1:F:26:ASN:OD1	1:F:29:ARG:NH1	2.35	0.59
1:L:32:TYR:OH	1:L:559:GLU:OE2	2.21	0.59
1:D:69:GLU:O	1:D:71:LEU:N	2.35	0.59
1:G:312:GLU:OE2	1:G:484:ARG:NH1	2.36	0.59
1:J:142:ASN:ND2	1:K:491:ASP:OD2	2.35	0.59
1:C:291:PHE:HZ	1:I:26:ASN:CA	2.15	0.59
1:E:69:GLU:O	1:E:71:LEU:N	2.35	0.59
1:A:26:ASN:OD1	1:A:29:ARG:NH1	2.36	0.59
1:L:69:GLU:O	1:L:71:LEU:N	2.35	0.59
1:L:233:GLN:NE2	1:L:380:VAL:HG22	2.17	0.59
1:C:69:GLU:HA	1:C:103:CYS:SG	2.44	0.58
1:A:16:ASN:HB2	1:F:531:ILE:HD13	1.85	0.58
1:G:142:ASN:ND2	1:H:491:ASP:OD2	2.36	0.58
1:D:133:HIS:CE1	1:D:504:GLY:HA2	2.39	0.58
1:K:233:GLN:NE2	1:K:380:VAL:HG22	2.19	0.57
1:C:291:PHE:CE2	1:I:25:SER:CB	2.88	0.57
1:H:142:ASN:ND2	1:I:491:ASP:OD2	2.38	0.57
1:A:32:TYR:OH	1:A:559:GLU:OE2	2.22	0.57
1:C:209:ASP:OD2	1:C:267:LYS:NZ	2.37	0.57
1:G:491:ASP:OD2	1:L:142:ASN:ND2	2.38	0.57
1:A:288:SER:O	1:A:292:THR:OG1	2.22	0.57
1:K:32:TYR:OH	1:K:559:GLU:OE2	2.22	0.57
1:B:69:GLU:O	1:B:71:LEU:N	2.38	0.56
1:G:69:GLU:HA	1:G:103:CYS:SG	2.45	0.56
1:C:32:TYR:OH	1:C:559:GLU:OE2	2.22	0.56
1:G:26:ASN:OD1	1:G:29:ARG:NH1	2.37	0.56
1:I:32:TYR:OH	1:I:559:GLU:OE2	2.23	0.56
1:K:69:GLU:HA	1:K:103:CYS:SG	2.45	0.56
1:C:291:PHE:CZ	1:I:27:GLU:N	2.73	0.56
1:F:69:GLU:O	1:F:71:LEU:N	2.39	0.56
1:C:69:GLU:O	1:C:71:LEU:N	2.37	0.56
1:D:26:ASN:OD1	1:D:29:ARG:NH1	2.39	0.56
1:K:209:ASP:OD2	1:K:267:LYS:NZ	2.38	0.56
1:C:142:ASN:ND2	1:D:491:ASP:OD2	2.39	0.56
1:D:69:GLU:HA	1:D:103:CYS:SG	2.45	0.55
1:C:288:SER:HA	1:I:27:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:PHE:CD2	1:I:29:ARG:HB2	2.41	0.55
1:I:26:ASN:OD1	1:I:29:ARG:NH1	2.39	0.55
1:C:13:PRO:O	1:C:15:ASN:ND2	2.40	0.55
1:D:227:THR:HA	1:D:233:GLN:HE22	1.71	0.55
1:C:352:ASN:N	1:C:352:ASN:OD1	2.39	0.55
1:J:209:ASP:OD2	1:J:267:LYS:NZ	2.40	0.55
1:B:288:SER:O	1:B:292:THR:OG1	2.25	0.55
1:E:32:TYR:OH	1:E:559:GLU:OE2	2.23	0.55
1:I:133:HIS:CE1	1:I:504:GLY:HA2	2.42	0.55
1:K:26:ASN:OD1	1:K:29:ARG:NH1	2.39	0.55
1:C:119:ASN:ND2	1:C:119:ASN:O	2.40	0.55
1:B:209:ASP:OD2	1:B:267:LYS:NZ	2.39	0.54
1:B:233:GLN:NE2	1:B:380:VAL:HG22	2.21	0.54
1:I:288:SER:O	1:I:292:THR:OG1	2.24	0.54
1:L:69:GLU:HA	1:L:103:CYS:SG	2.48	0.54
1:L:209:ASP:OD2	1:L:267:LYS:NZ	2.41	0.54
1:F:502:MET:O	1:F:554:ARG:NH1	2.41	0.54
1:A:227:THR:HA	1:A:233:GLN:HE22	1.73	0.54
1:J:69:GLU:HA	1:J:103:CYS:SG	2.48	0.54
1:H:37:PHE:CZ	1:H:40:HIS:O	2.61	0.54
1:B:37:PHE:CZ	1:B:40:HIS:O	2.61	0.54
1:B:69:GLU:HA	1:B:103:CYS:SG	2.48	0.54
1:I:119:ASN:O	1:I:119:ASN:ND2	2.41	0.54
1:C:37:PHE:CZ	1:C:40:HIS:O	2.61	0.54
1:H:209:ASP:OD2	1:H:267:LYS:NZ	2.41	0.54
1:K:175:LEU:HD13	1:K:177:ILE:HG23	1.90	0.53
1:B:227:THR:HA	1:B:233:GLN:HE22	1.73	0.53
1:E:119:ASN:O	1:E:119:ASN:ND2	2.41	0.53
1:I:69:GLU:HA	1:I:103:CYS:SG	2.48	0.53
1:L:37:PHE:CZ	1:L:40:HIS:O	2.62	0.53
1:C:233:GLN:NE2	1:C:380:VAL:HG22	2.23	0.53
1:C:291:PHE:CD2	1:I:25:SER:OG	2.60	0.53
1:D:288:SER:O	1:D:292:THR:OG1	2.27	0.53
1:H:69:GLU:HA	1:H:103:CYS:SG	2.48	0.53
1:K:37:PHE:CZ	1:K:40:HIS:O	2.61	0.53
1:K:288:SER:O	1:K:292:THR:OG1	2.27	0.53
1:B:119:ASN:O	1:B:119:ASN:ND2	2.42	0.53
1:H:32:TYR:OH	1:H:559:GLU:OE2	2.24	0.53
1:H:23:PHE:CD2	1:H:29:ARG:HB2	2.44	0.53
1:H:26:ASN:OD1	1:H:29:ARG:NH1	2.41	0.53
1:E:209:ASP:OD2	1:E:267:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:PHE:C	1:I:35:SER:H	2.17	0.53
1:A:209:ASP:OD2	1:A:267:LYS:NZ	2.42	0.52
1:J:32:TYR:OH	1:J:559:GLU:OE2	2.26	0.52
1:C:26:ASN:OD1	1:C:29:ARG:NH1	2.42	0.52
1:A:13:PRO:O	1:A:15:ASN:ND2	2.42	0.52
1:L:26:ASN:OD1	1:L:29:ARG:NH1	2.42	0.52
1:J:133:HIS:CE1	1:J:504:GLY:HA2	2.44	0.52
1:G:209:ASP:OD2	1:G:267:LYS:NZ	2.42	0.52
1:I:69:GLU:O	1:I:71:LEU:N	2.42	0.52
1:I:142:ASN:ND2	1:J:491:ASP:OD2	2.42	0.52
1:J:288:SER:O	1:J:292:THR:OG1	2.27	0.52
1:L:134:TYR:CE2	1:L:142:ASN:HB2	2.45	0.52
1:G:37:PHE:CZ	1:G:40:HIS:O	2.62	0.52
1:H:119:ASN:ND2	1:H:119:ASN:O	2.43	0.52
1:G:288:SER:O	1:G:292:THR:OG1	2.28	0.51
1:H:133:HIS:CE1	1:H:504:GLY:HA2	2.45	0.51
1:D:32:TYR:OH	1:D:559:GLU:OE2	2.24	0.51
1:H:531:ILE:HD13	1:I:16:ASN:HB2	1.92	0.51
1:C:291:PHE:CE2	1:I:25:SER:C	2.88	0.51
1:E:288:SER:O	1:E:292:THR:OG1	2.28	0.51
1:H:12:THR:HG21	1:H:76:TYR:HB2	1.93	0.51
1:J:531:ILE:HD13	1:K:16:ASN:HB2	1.91	0.51
1:C:133:HIS:CE1	1:C:504:GLY:HA2	2.45	0.51
1:J:356:ARG:NH2	1:K:487:ARG:O	2.43	0.51
1:L:119:ASN:O	1:L:119:ASN:ND2	2.44	0.51
1:D:134:TYR:CE2	1:D:142:ASN:HB2	2.46	0.51
1:F:119:ASN:ND2	1:F:119:ASN:O	2.44	0.51
1:F:133:HIS:CE1	1:F:504:GLY:HA2	2.45	0.51
1:H:288:SER:O	1:H:292:THR:OG1	2.28	0.51
1:B:133:HIS:CE1	1:B:504:GLY:HA2	2.46	0.51
1:F:38:ASP:N	1:F:38:ASP:OD1	2.44	0.51
1:G:16:ASN:HB2	1:L:531:ILE:HD13	1.91	0.51
1:G:227:THR:HA	1:G:233:GLN:HE22	1.76	0.51
1:G:119:ASN:O	1:G:119:ASN:ND2	2.43	0.51
1:I:37:PHE:CZ	1:I:40:HIS:O	2.64	0.51
1:E:23:PHE:CD2	1:E:29:ARG:HB2	2.45	0.51
1:E:142:ASN:ND2	1:F:491:ASP:OD2	2.44	0.51
1:E:133:HIS:CE1	1:E:504:GLY:HA2	2.46	0.51
1:I:209:ASP:OD2	1:I:267:LYS:NZ	2.44	0.50
1:K:142:ASN:ND2	1:L:491:ASP:OD2	2.44	0.50
1:L:288:SER:O	1:L:292:THR:OG1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:TYR:HB3	1:C:479:PHE:CD1	2.46	0.50
1:D:60:ASP:HB3	1:D:102:VAL:HG22	1.93	0.50
1:F:288:SER:O	1:F:292:THR:OG1	2.29	0.50
1:G:32:TYR:OH	1:G:559:GLU:OE2	2.26	0.50
1:H:227:THR:HA	1:H:233:GLN:HE22	1.76	0.50
1:K:352:ASN:OD1	1:K:352:ASN:N	2.44	0.50
1:F:23:PHE:CD2	1:F:29:ARG:HB2	2.46	0.50
1:J:227:THR:HA	1:J:233:GLN:HE22	1.77	0.50
1:D:209:ASP:OD2	1:D:267:LYS:NZ	2.45	0.50
1:D:37:PHE:CZ	1:D:40:HIS:O	2.64	0.50
1:F:209:ASP:OD2	1:F:267:LYS:NZ	2.44	0.50
1:B:32:TYR:OH	1:B:559:GLU:OE2	2.28	0.50
1:F:37:PHE:CZ	1:F:40:HIS:O	2.65	0.50
1:C:291:PHE:CE1	1:I:27:GLU:OE1	2.65	0.50
1:E:227:THR:HA	1:E:233:GLN:HE22	1.76	0.50
1:I:531:ILE:HD13	1:J:16:ASN:HB2	1.94	0.50
1:J:23:PHE:CD2	1:J:29:ARG:HB2	2.47	0.50
1:H:134:TYR:HH	1:H:507:CYS:HG	1.58	0.50
1:A:487:ARG:O	1:F:356:ARG:NH2	2.45	0.49
1:K:23:PHE:CD2	1:K:29:ARG:HB2	2.47	0.49
1:A:119:ASN:ND2	1:A:119:ASN:O	2.45	0.49
1:D:13:PRO:O	1:D:15:ASN:ND2	2.45	0.49
1:J:119:ASN:O	1:J:119:ASN:ND2	2.45	0.49
1:C:531:ILE:HD13	1:D:16:ASN:HB2	1.94	0.49
1:H:13:PRO:O	1:H:15:ASN:ND2	2.46	0.49
1:J:13:PRO:O	1:J:15:ASN:ND2	2.46	0.49
1:F:12:THR:HG21	1:F:76:TYR:HB2	1.93	0.49
1:F:33:PHE:C	1:F:35:SER:H	2.21	0.49
1:G:23:PHE:CD2	1:G:29:ARG:HB2	2.46	0.49
1:K:134:TYR:CE2	1:K:142:ASN:HB2	2.47	0.49
1:D:23:PHE:CD2	1:D:29:ARG:HB2	2.47	0.49
1:L:23:PHE:CD2	1:L:29:ARG:HB2	2.47	0.49
1:L:133:HIS:CE1	1:L:504:GLY:HA2	2.47	0.49
1:K:12:THR:HG21	1:K:76:TYR:HB2	1.94	0.49
1:A:37:PHE:CZ	1:A:40:HIS:O	2.66	0.49
1:B:358:ASN:C	1:I:35:SER:HA	2.38	0.49
1:B:470:TYR:HB3	1:B:479:PHE:CD1	2.48	0.49
1:C:291:PHE:CE2	1:I:27:GLU:N	2.81	0.49
1:B:124:LEU:HD22	1:B:532:TRP:HB2	1.94	0.49
1:E:134:TYR:CE2	1:E:142:ASN:HB2	2.48	0.49
1:G:124:LEU:HD22	1:G:532:TRP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:THR:HG21	1:J:76:TYR:HB2	1.95	0.49
1:K:119:ASN:ND2	1:K:119:ASN:O	2.46	0.49
1:K:227:THR:HA	1:K:233:GLN:HE22	1.78	0.48
1:D:290:MET:HE3	1:D:295:LEU:HB3	1.96	0.48
1:L:38:ASP:OD1	1:L:38:ASP:N	2.46	0.48
1:I:13:PRO:O	1:I:15:ASN:ND2	2.46	0.48
1:A:133:HIS:CE1	1:A:504:GLY:HA2	2.48	0.48
1:B:352:ASN:OD1	1:B:352:ASN:N	2.43	0.48
1:A:212:TRP:CZ3	1:A:247:ILE:HG13	2.48	0.48
1:C:337:PHE:CE2	1:D:476:GLN:HG3	2.49	0.48
1:D:33:PHE:C	1:D:35:SER:H	2.21	0.48
1:E:12:THR:HG21	1:E:76:TYR:HB2	1.96	0.48
1:E:124:LEU:HD22	1:E:532:TRP:HB2	1.96	0.48
1:F:59:ILE:HG12	1:F:60:ASP:N	2.29	0.48
1:A:502:MET:O	1:A:554:ARG:NH1	2.47	0.48
1:B:12:THR:HG21	1:B:76:TYR:HB2	1.96	0.48
1:J:314:THR:HG21	1:J:484:ARG:NH2	2.28	0.48
1:K:356:ARG:NH2	1:L:487:ARG:O	2.47	0.48
1:F:227:THR:HA	1:F:233:GLN:HE22	1.78	0.48
1:G:133:HIS:CE1	1:G:504:GLY:HA2	2.49	0.48
1:H:502:MET:O	1:H:554:ARG:NH1	2.45	0.48
1:A:204:ILE:HD13	1:B:468:VAL:HG21	1.95	0.48
1:E:37:PHE:CZ	1:E:40:HIS:O	2.66	0.48
1:I:227:THR:HA	1:I:233:GLN:HE22	1.78	0.48
1:D:352:ASN:OD1	1:D:352:ASN:N	2.46	0.47
1:G:356:ARG:NH2	1:H:487:ARG:O	2.47	0.47
1:K:133:HIS:CE1	1:K:504:GLY:HA2	2.49	0.47
1:D:212:TRP:CZ3	1:D:247:ILE:HG13	2.49	0.47
1:F:212:TRP:CZ3	1:F:247:ILE:HG13	2.49	0.47
1:I:12:THR:HG21	1:I:76:TYR:HB2	1.97	0.47
1:L:12:THR:HG21	1:L:76:TYR:HB2	1.96	0.47
1:B:212:TRP:CZ3	1:B:247:ILE:HG13	2.50	0.47
1:J:38:ASP:OD1	1:J:38:ASP:N	2.48	0.47
1:E:38:ASP:OD1	1:E:38:ASP:N	2.48	0.47
1:E:352:ASN:N	1:E:352:ASN:OD1	2.46	0.47
1:L:227:THR:HA	1:L:233:GLN:HE22	1.78	0.47
1:C:212:TRP:CZ3	1:C:247:ILE:HG13	2.49	0.47
1:D:119:ASN:O	1:D:119:ASN:ND2	2.47	0.47
1:E:202:ASP:OD2	1:E:274:SER:OG	2.31	0.47
1:G:13:PRO:O	1:G:15:ASN:ND2	2.48	0.47
1:K:470:TYR:HB3	1:K:479:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PHE:CD2	1:B:29:ARG:HB2	2.49	0.47
1:B:38:ASP:OD1	1:B:38:ASP:N	2.48	0.47
1:E:282:ILE:HG23	1:E:334:PHE:CD2	2.50	0.47
1:E:356:ARG:NH2	1:F:487:ARG:O	2.47	0.47
1:F:175:LEU:HD13	1:F:177:ILE:HG23	1.96	0.47
1:F:282:ILE:HG23	1:F:334:PHE:CD2	2.50	0.47
1:G:531:ILE:HD13	1:H:16:ASN:HB2	1.97	0.47
1:F:134:TYR:CE2	1:F:142:ASN:HB2	2.50	0.47
1:A:23:PHE:CD2	1:A:29:ARG:HB2	2.49	0.47
1:I:38:ASP:OD1	1:I:38:ASP:N	2.48	0.47
1:I:134:TYR:CE2	1:I:142:ASN:HB2	2.49	0.47
1:K:13:PRO:O	1:K:15:ASN:ND2	2.47	0.47
1:C:502:MET:O	1:C:554:ARG:NH1	2.46	0.47
1:J:572:ILE:C	1:J:573:ILE:HG13	2.40	0.47
1:A:60:ASP:HB3	1:A:102:VAL:HG22	1.97	0.46
1:H:356:ARG:NH2	1:I:487:ARG:O	2.47	0.46
1:I:23:PHE:CG	1:I:29:ARG:HB2	2.49	0.46
1:I:212:TRP:CZ3	1:I:247:ILE:HG13	2.50	0.46
1:A:134:TYR:HH	1:A:507:CYS:HG	1.63	0.46
1:A:531:ILE:HD11	1:B:15:ASN:OD1	2.15	0.46
1:C:12:THR:HG21	1:C:76:TYR:HB2	1.98	0.46
1:H:38:ASP:N	1:H:38:ASP:OD1	2.48	0.46
1:A:12:THR:HG21	1:A:76:TYR:HB2	1.97	0.46
1:E:112:VAL:HG11	1:E:553:VAL:HG11	1.98	0.46
1:G:290:MET:HE3	1:G:295:LEU:HB3	1.97	0.46
1:J:60:ASP:HB3	1:J:102:VAL:HG22	1.96	0.46
1:L:572:ILE:C	1:L:573:ILE:HG13	2.41	0.46
1:E:502:MET:O	1:E:554:ARG:NH1	2.48	0.46
1:G:134:TYR:CE2	1:G:142:ASN:HB2	2.51	0.46
1:H:134:TYR:OH	1:H:507:CYS:SG	2.73	0.46
1:I:282:ILE:HG23	1:I:334:PHE:CD2	2.51	0.46
1:J:352:ASN:OD1	1:J:352:ASN:N	2.48	0.46
1:L:33:PHE:C	1:L:35:SER:H	2.23	0.46
1:A:352:ASN:N	1:A:352:ASN:OD1	2.46	0.46
1:F:290:MET:HE3	1:F:295:LEU:HB3	1.98	0.46
1:K:71:LEU:HD21	1:K:95:ILE:HG21	1.97	0.46
1:K:502:MET:O	1:K:554:ARG:NH1	2.47	0.46
1:C:175:LEU:HD13	1:C:177:ILE:HG23	1.97	0.46
1:D:572:ILE:C	1:D:573:ILE:HG13	2.41	0.46
1:E:174:ILE:O	1:E:174:ILE:HG13	2.15	0.46
1:K:33:PHE:C	1:K:35:SER:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:PRO:O	1:L:15:ASN:ND2	2.49	0.46
1:C:71:LEU:HD21	1:C:95:ILE:HG21	1.97	0.46
1:C:134:TYR:CE2	1:C:142:ASN:HB2	2.50	0.46
1:C:333:GLU:OE1	1:C:351:LYS:NZ	2.47	0.46
1:G:212:TRP:CZ3	1:G:247:ILE:HG13	2.51	0.46
1:L:124:LEU:HD22	1:L:532:TRP:HB2	1.97	0.46
1:G:174:ILE:O	1:G:174:ILE:HG13	2.16	0.46
1:B:13:PRO:O	1:B:15:ASN:ND2	2.48	0.45
1:C:291:PHE:HE2	1:I:28:GLU:H	1.64	0.45
1:L:71:LEU:HD21	1:L:95:ILE:HG21	1.98	0.45
1:C:356:ARG:NH2	1:D:487:ARG:O	2.48	0.45
1:E:60:ASP:HB3	1:E:102:VAL:HG22	1.98	0.45
1:F:352:ASN:OD1	1:F:352:ASN:N	2.46	0.45
1:H:124:LEU:HD22	1:H:532:TRP:HB2	1.99	0.45
1:I:352:ASN:OD1	1:I:352:ASN:N	2.48	0.45
1:A:282:ILE:HG23	1:A:334:PHE:CD2	2.51	0.45
1:E:134:TYR:HH	1:E:507:CYS:HG	1.58	0.45
1:F:13:PRO:O	1:F:15:ASN:ND2	2.49	0.45
1:B:134:TYR:CE2	1:B:142:ASN:HB2	2.52	0.45
1:C:38:ASP:OD1	1:C:38:ASP:N	2.49	0.45
1:D:38:ASP:OD1	1:D:38:ASP:N	2.50	0.45
1:H:134:TYR:CE2	1:H:142:ASN:HB2	2.52	0.45
1:F:124:LEU:HD22	1:F:532:TRP:HB2	1.98	0.45
1:G:33:PHE:C	1:G:35:SER:H	2.25	0.45
1:K:60:ASP:HB3	1:K:102:VAL:HG22	1.98	0.45
1:C:111:VAL:CG2	1:C:545:LEU:HD13	2.47	0.45
1:D:531:ILE:HD11	1:E:15:ASN:OD1	2.17	0.45
1:F:470:TYR:HB3	1:F:479:PHE:CD1	2.51	0.45
1:H:290:MET:HE3	1:H:295:LEU:HB3	1.97	0.45
1:J:212:TRP:CZ3	1:J:247:ILE:HG13	2.52	0.45
1:K:124:LEU:HD22	1:K:532:TRP:HB2	1.99	0.45
1:H:352:ASN:N	1:H:352:ASN:OD1	2.48	0.45
1:K:212:TRP:CZ3	1:K:247:ILE:HG13	2.52	0.45
1:A:290:MET:HE3	1:A:295:LEU:HB3	1.98	0.45
1:A:572:ILE:C	1:A:573:ILE:HG13	2.41	0.45
1:F:60:ASP:HB3	1:F:102:VAL:HG22	1.99	0.45
1:H:33:PHE:C	1:H:35:SER:H	2.24	0.45
1:K:531:ILE:HD13	1:L:16:ASN:HB2	1.99	0.45
1:L:352:ASN:OD1	1:L:352:ASN:N	2.49	0.45
1:E:212:TRP:CZ3	1:E:247:ILE:HG13	2.51	0.45
1:G:352:ASN:OD1	1:G:352:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:PHE:CD2	1:C:29:ARG:HB2	2.52	0.45
1:D:572:ILE:O	1:D:573:ILE:CG1	2.65	0.45
1:G:112:VAL:HG11	1:G:553:VAL:HG11	1.99	0.45
1:A:124:LEU:HD22	1:A:532:TRP:HB2	1.99	0.44
1:C:470:TYR:CG	1:C:479:PHE:CE1	3.05	0.44
1:D:12:THR:HG21	1:D:76:TYR:HB2	1.99	0.44
1:D:81:TYR:O	1:D:85:ASN:N	2.50	0.44
1:D:175:LEU:HD13	1:D:177:ILE:HG23	1.98	0.44
1:E:13:PRO:O	1:E:15:ASN:ND2	2.50	0.44
1:H:470:TYR:HB3	1:H:479:PHE:CD1	2.52	0.44
1:L:60:ASP:HB3	1:L:102:VAL:HG22	1.98	0.44
1:C:60:ASP:HB3	1:C:102:VAL:HG22	2.00	0.44
1:C:572:ILE:C	1:C:573:ILE:HG13	2.41	0.44
1:D:33:PHE:O	1:D:35:SER:N	2.50	0.44
1:G:12:THR:HG21	1:G:76:TYR:HB2	1.99	0.44
1:H:212:TRP:CZ3	1:H:247:ILE:HG13	2.52	0.44
1:L:175:LEU:HD13	1:L:177:ILE:HG23	1.99	0.44
1:A:356:ARG:NH2	1:B:487:ARG:O	2.48	0.44
1:B:60:ASP:HB3	1:B:102:VAL:HG22	2.00	0.44
1:I:59:ILE:HG12	1:I:60:ASP:N	2.32	0.44
1:I:470:TYR:HB3	1:I:479:PHE:CD1	2.52	0.44
1:K:572:ILE:C	1:K:573:ILE:HG13	2.42	0.44
1:B:71:LEU:HD21	1:B:95:ILE:HG21	1.99	0.44
1:C:33:PHE:C	1:C:35:SER:H	2.25	0.44
1:I:290:MET:HE3	1:I:295:LEU:HB3	2.00	0.44
1:J:134:TYR:CE2	1:J:142:ASN:HB2	2.52	0.44
1:D:124:LEU:HD22	1:D:532:TRP:HB2	1.99	0.44
1:E:572:ILE:C	1:E:573:ILE:HG13	2.42	0.44
1:G:38:ASP:OD1	1:G:38:ASP:N	2.50	0.44
1:H:572:ILE:C	1:H:573:ILE:HG13	2.43	0.44
1:I:112:VAL:HG11	1:I:553:VAL:HG11	1.99	0.44
1:J:124:LEU:HD22	1:J:532:TRP:HB2	1.99	0.44
1:B:358:ASN:H	1:I:35:SER:C	2.25	0.44
1:C:124:LEU:HD22	1:C:532:TRP:HB2	1.99	0.44
1:C:572:ILE:O	1:C:573:ILE:CG1	2.66	0.44
1:E:42:PHE:CE1	1:E:59:ILE:HD12	2.53	0.44
1:F:23:PHE:CG	1:F:29:ARG:HB2	2.53	0.44
1:F:71:LEU:HD21	1:F:95:ILE:HG21	1.99	0.44
1:I:71:LEU:HD21	1:I:95:ILE:HG21	1.98	0.44
1:J:33:PHE:C	1:J:35:SER:H	2.26	0.44
1:B:33:PHE:C	1:B:35:SER:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:OD1	1:A:38:ASP:N	2.51	0.44
1:C:174:ILE:HG13	1:C:174:ILE:O	2.17	0.44
1:E:470:TYR:HB3	1:E:479:PHE:CD1	2.53	0.44
1:B:356:ARG:NH2	1:C:487:ARG:O	2.51	0.43
1:I:124:LEU:HD22	1:I:532:TRP:HB2	2.00	0.43
1:J:502:MET:O	1:J:554:ARG:NH1	2.51	0.43
1:K:23:PHE:CG	1:K:29:ARG:HB2	2.53	0.43
1:L:572:ILE:O	1:L:573:ILE:CG1	2.66	0.43
1:H:174:ILE:O	1:H:174:ILE:HG13	2.19	0.43
1:A:546:ARG:CZ	1:B:15:ASN:OD1	2.66	0.43
1:E:33:PHE:C	1:E:35:SER:H	2.25	0.43
1:F:572:ILE:C	1:F:573:ILE:HG13	2.43	0.43
1:G:42:PHE:CE1	1:G:59:ILE:HD12	2.53	0.43
1:L:212:TRP:CZ3	1:L:247:ILE:HG13	2.53	0.43
1:I:572:ILE:C	1:I:573:ILE:HG13	2.44	0.43
1:K:38:ASP:OD1	1:K:38:ASP:N	2.51	0.43
1:A:134:TYR:CE2	1:A:142:ASN:HB2	2.54	0.43
1:F:572:ILE:O	1:F:573:ILE:CG1	2.67	0.43
1:A:531:ILE:HD13	1:B:16:ASN:HB2	2.00	0.43
1:B:23:PHE:CG	1:B:29:ARG:HB2	2.54	0.43
1:E:290:MET:HE3	1:E:295:LEU:HB3	2.01	0.43
1:J:23:PHE:CG	1:J:29:ARG:HB2	2.54	0.43
1:L:111:VAL:CG2	1:L:545:LEU:HD13	2.49	0.43
1:A:33:PHE:C	1:A:35:SER:H	2.25	0.43
1:G:572:ILE:C	1:G:573:ILE:HG13	2.43	0.43
1:J:175:LEU:HD13	1:J:177:ILE:HG23	2.00	0.43
1:B:142:ASN:ND2	1:C:491:ASP:OD2	2.51	0.43
1:D:174:ILE:O	1:D:174:ILE:HG13	2.17	0.43
1:H:23:PHE:CG	1:H:29:ARG:HB2	2.53	0.43
1:I:175:LEU:HD13	1:I:177:ILE:HG23	2.01	0.43
1:J:71:LEU:HD21	1:J:95:ILE:HG21	1.99	0.43
1:L:314:THR:HG21	1:L:484:ARG:NH2	2.34	0.43
1:E:175:LEU:HD13	1:E:177:ILE:HG23	2.01	0.43
1:G:197:SER:OG	1:G:267:LYS:NZ	2.39	0.43
1:L:59:ILE:HG12	1:L:60:ASP:N	2.34	0.43
1:C:290:MET:HE3	1:C:295:LEU:HB3	2.01	0.43
1:C:313:LEU:HB3	1:C:368:LEU:HD22	2.01	0.43
1:G:175:LEU:HD13	1:G:177:ILE:HG23	2.01	0.43
1:G:502:MET:O	1:G:554:ARG:NH1	2.50	0.43
1:J:572:ILE:O	1:J:573:ILE:CG1	2.67	0.43
1:J:572:ILE:O	1:J:573:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:290:MET:HE3	1:L:295:LEU:HB3	2.00	0.43
1:B:227:THR:HA	1:B:233:GLN:NE2	2.34	0.42
1:D:282:ILE:HG23	1:D:334:PHE:CD2	2.54	0.42
1:H:59:ILE:HG12	1:H:60:ASP:N	2.34	0.42
1:I:572:ILE:O	1:I:573:ILE:CG1	2.67	0.42
1:C:227:THR:HA	1:C:233:GLN:HE22	1.84	0.42
1:E:71:LEU:HD21	1:E:95:ILE:HG21	2.01	0.42
1:G:531:ILE:HD11	1:H:15:ASN:OD1	2.19	0.42
1:H:42:PHE:CE1	1:H:59:ILE:HD12	2.54	0.42
1:H:282:ILE:HG23	1:H:334:PHE:CD2	2.55	0.42
1:J:282:ILE:HG23	1:J:334:PHE:CD2	2.53	0.42
1:D:42:PHE:CE1	1:D:59:ILE:HD12	2.55	0.42
1:E:59:ILE:HG12	1:E:60:ASP:N	2.34	0.42
1:I:33:PHE:O	1:I:35:SER:N	2.52	0.42
1:I:502:MET:O	1:I:554:ARG:NH1	2.51	0.42
1:L:502:MET:O	1:L:554:ARG:NH1	2.50	0.42
1:A:65:ARG:HG2	1:A:66:SER:N	2.33	0.42
1:A:175:LEU:HD13	1:A:177:ILE:HG23	2.02	0.42
1:E:23:PHE:CG	1:E:29:ARG:HB2	2.55	0.42
1:J:470:TYR:HB3	1:J:479:PHE:CD1	2.54	0.42
1:A:470:TYR:HB3	1:A:479:PHE:CD1	2.54	0.42
1:B:572:ILE:C	1:B:573:ILE:HG13	2.45	0.42
1:D:531:ILE:HD12	1:D:531:ILE:HA	1.93	0.42
1:F:16:ASN:OD1	1:F:19:ASN:N	2.52	0.42
1:G:60:ASP:HB3	1:G:102:VAL:HG22	2.01	0.42
1:A:71:LEU:HD21	1:A:95:ILE:HG21	2.01	0.42
1:C:291:PHE:CD1	1:I:27:GLU:OE2	2.73	0.42
1:F:111:VAL:CG2	1:F:545:LEU:HD13	2.49	0.42
1:I:60:ASP:HB3	1:I:102:VAL:HG22	2.00	0.42
1:J:204:ILE:HD13	1:K:468:VAL:HG21	2.01	0.42
1:A:510:TYR:HB3	1:B:502:MET:CE	2.50	0.42
1:C:112:VAL:HG11	1:C:553:VAL:HG11	2.01	0.42
1:D:112:VAL:HG11	1:D:553:VAL:HG11	2.01	0.42
1:F:33:PHE:O	1:F:35:SER:N	2.53	0.42
1:G:65:ARG:HG2	1:G:66:SER:N	2.35	0.42
1:G:71:LEU:HD21	1:G:95:ILE:HG21	2.02	0.42
1:G:202:ASP:OD2	1:G:274:SER:OG	2.37	0.42
1:K:204:ILE:HD13	1:L:468:VAL:HG21	2.01	0.42
1:B:175:LEU:HD13	1:B:177:ILE:HG23	2.02	0.42
1:G:572:ILE:O	1:G:573:ILE:CG1	2.68	0.42
1:D:173:TYR:CD2	1:D:173:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:TYR:O	1:E:85:ASN:N	2.53	0.42
1:G:487:ARG:O	1:L:356:ARG:NH2	2.52	0.42
1:J:134:TYR:OH	1:J:507:CYS:SG	2.76	0.42
1:J:290:MET:HE3	1:J:295:LEU:HB3	2.01	0.42
1:L:572:ILE:O	1:L:573:ILE:HG13	2.20	0.42
1:A:23:PHE:CG	1:A:29:ARG:HB2	2.55	0.41
1:B:59:ILE:HG12	1:B:60:ASP:N	2.35	0.41
1:C:539:THR:HG23	1:D:94:ASP:HA	2.01	0.41
1:D:16:ASN:OD1	1:D:19:ASN:N	2.53	0.41
1:D:65:ARG:HG2	1:D:66:SER:N	2.34	0.41
1:D:470:TYR:HB3	1:D:479:PHE:CD1	2.54	0.41
1:I:111:VAL:CG2	1:I:545:LEU:HD13	2.50	0.41
1:J:134:TYR:HH	1:J:507:CYS:HG	1.62	0.41
1:K:33:PHE:O	1:K:35:SER:N	2.53	0.41
1:K:59:ILE:HG12	1:K:60:ASP:N	2.35	0.41
1:B:112:VAL:HG11	1:B:553:VAL:HG11	2.02	0.41
1:C:59:ILE:HG12	1:C:60:ASP:N	2.35	0.41
1:H:71:LEU:HD21	1:H:95:ILE:HG21	2.02	0.41
1:H:572:ILE:O	1:H:573:ILE:CG1	2.68	0.41
1:I:144:GLU:OE1	1:I:356:ARG:NH1	2.53	0.41
1:K:531:ILE:HD11	1:L:15:ASN:OD1	2.19	0.41
1:A:73:GLY:HA3	1:F:536:ASN:HA	2.02	0.41
1:J:37:PHE:CZ	1:J:40:HIS:O	2.73	0.41
1:K:290:MET:HE3	1:K:295:LEU:HB3	2.01	0.41
1:L:33:PHE:O	1:L:35:SER:N	2.54	0.41
1:A:12:THR:HG23	1:A:14:PHE:N	2.35	0.41
1:D:143:LEU:HA	1:D:146:ILE:HG22	2.03	0.41
1:E:531:ILE:HD13	1:F:16:ASN:HB2	2.01	0.41
1:I:8:LEU:HD22	1:I:74:VAL:HG21	2.03	0.41
1:L:23:PHE:CG	1:L:29:ARG:HB2	2.55	0.41
1:L:112:VAL:HG11	1:L:553:VAL:HG11	2.02	0.41
1:B:65:ARG:HG2	1:B:66:SER:N	2.35	0.41
1:D:71:LEU:HD21	1:D:95:ILE:HG21	2.02	0.41
1:G:572:ILE:O	1:G:573:ILE:HG13	2.21	0.41
1:I:65:ARG:HG2	1:I:66:SER:N	2.35	0.41
1:H:121:LEU:HD13	1:H:517:ILE:HG12	2.02	0.41
1:H:175:LEU:HD13	1:H:177:ILE:HG23	2.01	0.41
1:I:81:TYR:O	1:I:85:ASN:N	2.53	0.41
1:J:65:ARG:HG2	1:J:66:SER:N	2.34	0.41
1:L:143:LEU:HA	1:L:146:ILE:HG22	2.03	0.41
1:L:282:ILE:HG23	1:L:334:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:CG2	1:D:545:LEU:HD13	2.51	0.41
1:D:204:ILE:HD13	1:E:468:VAL:CG2	2.50	0.41
1:F:209:ASP:HB3	1:F:211:TYR:CE2	2.56	0.41
1:L:470:TYR:HB3	1:L:479:PHE:CD1	2.55	0.41
1:C:134:TYR:OH	1:C:507:CYS:SG	2.76	0.41
1:F:65:ARG:HG2	1:F:66:SER:N	2.36	0.41
1:G:515:SER:OG	1:G:516:ASP:N	2.54	0.41
1:K:111:VAL:CG2	1:K:545:LEU:HD13	2.51	0.41
1:K:112:VAL:HG11	1:K:553:VAL:HG11	2.02	0.41
1:A:572:ILE:O	1:A:573:ILE:CG1	2.68	0.41
1:B:42:PHE:CE1	1:B:59:ILE:HD12	2.56	0.41
1:C:282:ILE:HG23	1:C:334:PHE:CD2	2.56	0.41
1:C:291:PHE:CG	1:I:27:GLU:CD	2.99	0.41
1:E:33:PHE:O	1:E:35:SER:N	2.54	0.41
1:K:144:GLU:OE1	1:K:356:ARG:NH1	2.52	0.41
1:A:38:ASP:C	1:A:39:VAL:HG22	2.46	0.41
1:B:174:ILE:O	1:B:174:ILE:HG13	2.21	0.41
1:B:204:ILE:HD13	1:C:468:VAL:HG21	2.02	0.41
1:E:572:ILE:O	1:E:573:ILE:CG1	2.69	0.41
1:H:65:ARG:HG2	1:H:66:SER:N	2.35	0.41
1:J:532:TRP:CZ2	1:J:546:ARG:HA	2.56	0.41
1:K:65:ARG:HG2	1:K:66:SER:N	2.36	0.41
1:K:532:TRP:CZ2	1:K:546:ARG:HA	2.56	0.41
1:K:572:ILE:O	1:K:573:ILE:CG1	2.69	0.41
1:D:197:SER:OG	1:D:267:LYS:NZ	2.42	0.40
1:D:208:TYR:HE2	1:E:463:ILE:HB	1.86	0.40
1:F:134:TYR:HH	1:F:507:CYS:HG	1.59	0.40
1:G:470:TYR:HB3	1:G:479:PHE:CD1	2.55	0.40
1:B:81:TYR:O	1:B:85:ASN:N	2.54	0.40
1:C:185:PHE:CE2	1:C:259:ASN:HB2	2.56	0.40
1:D:144:GLU:OE1	1:D:356:ARG:NH1	2.54	0.40
1:H:572:ILE:O	1:H:573:ILE:HG13	2.22	0.40
1:D:59:ILE:HG12	1:D:60:ASP:N	2.36	0.40
1:E:333:GLU:OE1	1:E:351:LYS:NZ	2.51	0.40
1:F:42:PHE:CE1	1:F:59:ILE:HD12	2.57	0.40
1:A:286:TYR:CD2	1:A:286:TYR:C	3.00	0.40
1:B:470:TYR:CG	1:B:479:PHE:CE1	3.08	0.40
1:C:202:ASP:OD2	1:C:274:SER:OG	2.36	0.40
1:D:324:ASP:OD1	1:D:324:ASP:C	2.64	0.40
1:G:59:ILE:HG12	1:G:60:ASP:N	2.36	0.40
1:H:111:VAL:CG2	1:H:545:LEU:HD13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PHE:CD2	1:B:23:PHE:N	2.89	0.40
1:B:33:PHE:O	1:B:35:SER:N	2.54	0.40
1:C:16:ASN:OD1	1:C:19:ASN:N	2.55	0.40
1:C:23:PHE:CD2	1:C:23:PHE:N	2.89	0.40
1:D:532:TRP:CZ2	1:D:546:ARG:HA	2.57	0.40
1:E:69:GLU:HB2	1:E:97:GLN:CD	2.47	0.40
1:E:177:ILE:HB	1:E:235:SER:O	2.22	0.40
1:I:177:ILE:HB	1:I:235:SER:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ASP:O	1:K:192:LYS:NZ[4_547]	2.08	0.12
1:C:260:GLY:O	1:D:187:THR:OG1[2_556]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/583 (83%)	408 (85%)	58 (12%)	16 (3%)	3	24
1	B	482/583 (83%)	408 (85%)	60 (12%)	14 (3%)	3	26
1	C	482/583 (83%)	407 (84%)	59 (12%)	16 (3%)	3	24
1	D	482/583 (83%)	410 (85%)	57 (12%)	15 (3%)	3	25
1	E	482/583 (83%)	412 (86%)	56 (12%)	14 (3%)	3	26
1	F	482/583 (83%)	408 (85%)	58 (12%)	16 (3%)	3	24
1	G	482/583 (83%)	409 (85%)	59 (12%)	14 (3%)	3	26
1	H	482/583 (83%)	410 (85%)	56 (12%)	16 (3%)	3	24
1	I	482/583 (83%)	406 (84%)	60 (12%)	16 (3%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	482/583 (83%)	410 (85%)	56 (12%)	16 (3%)	3	24
1	K	482/583 (83%)	411 (85%)	57 (12%)	14 (3%)	3	26
1	L	482/583 (83%)	410 (85%)	58 (12%)	14 (3%)	3	26
All	All	5784/6996 (83%)	4909 (85%)	694 (12%)	181 (3%)	3	25

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	70	GLN
1	A	84	SER
1	A	258	VAL
1	B	18	GLN
1	B	70	GLN
1	B	84	SER
1	B	258	VAL
1	C	18	GLN
1	C	70	GLN
1	C	84	SER
1	C	258	VAL
1	D	18	GLN
1	D	70	GLN
1	D	84	SER
1	D	258	VAL
1	E	18	GLN
1	E	70	GLN
1	E	84	SER
1	E	258	VAL
1	F	18	GLN
1	F	26	ASN
1	F	70	GLN
1	F	84	SER
1	F	258	VAL
1	G	18	GLN
1	G	70	GLN
1	G	84	SER
1	G	258	VAL
1	H	18	GLN
1	H	70	GLN
1	H	84	SER
1	H	258	VAL

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Mol	Chain	Res	Type
1	I	18	GLN
1	I	26	ASN
1	I	70	GLN
1	I	84	SER
1	I	258	VAL
1	J	18	GLN
1	J	70	GLN
1	J	84	SER
1	J	258	VAL
1	K	18	GLN
1	K	70	GLN
1	K	84	SER
1	K	258	VAL
1	L	18	GLN
1	L	70	GLN
1	L	84	SER
1	L	258	VAL
1	A	34	ASN
1	A	357	GLY
1	A	572	ILE
1	B	34	ASN
1	B	357	GLY
1	B	572	ILE
1	C	34	ASN
1	C	357	GLY
1	C	572	ILE
1	D	34	ASN
1	D	69	GLU
1	D	100	ASP
1	D	357	GLY
1	D	572	ILE
1	E	34	ASN
1	E	100	ASP
1	E	357	GLY
1	E	572	ILE
1	F	27	GLU
1	F	34	ASN
1	F	100	ASP
1	F	357	GLY
1	F	572	ILE
1	G	34	ASN
1	G	100	ASP

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Mol	Chain	Res	Type
1	G	357	GLY
1	G	572	ILE
1	H	34	ASN
1	H	357	GLY
1	H	572	ILE
1	I	27	GLU
1	I	34	ASN
1	I	100	ASP
1	I	357	GLY
1	I	572	ILE
1	J	34	ASN
1	J	357	GLY
1	J	572	ILE
1	K	34	ASN
1	K	357	GLY
1	K	572	ILE
1	L	34	ASN
1	L	357	GLY
1	L	572	ILE
1	A	14	PHE
1	A	69	GLU
1	A	100	ASP
1	A	536	ASN
1	B	14	PHE
1	B	69	GLU
1	B	100	ASP
1	C	69	GLU
1	C	100	ASP
1	C	371	ASN
1	D	14	PHE
1	E	69	GLU
1	F	14	PHE
1	G	69	GLU
1	H	69	GLU
1	H	100	ASP
1	I	14	PHE
1	I	69	GLU
1	J	69	GLU
1	J	100	ASP
1	K	69	GLU
1	K	100	ASP
1	L	69	GLU

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Mol	Chain	Res	Type
1	L	100	ASP
1	B	371	ASN
1	C	14	PHE
1	D	371	ASN
1	E	14	PHE
1	F	69	GLU
1	G	371	ASN
1	H	14	PHE
1	I	371	ASN
1	J	14	PHE
1	J	371	ASN
1	K	371	ASN
1	L	14	PHE
1	L	371	ASN
1	A	271	GLN
1	A	371	ASN
1	B	271	GLN
1	C	271	GLN
1	D	40	HIS
1	D	271	GLN
1	D	536	ASN
1	E	271	GLN
1	E	371	ASN
1	F	40	HIS
1	F	371	ASN
1	G	14	PHE
1	G	40	HIS
1	G	271	GLN
1	H	40	HIS
1	H	271	GLN
1	H	371	ASN
1	J	40	HIS
1	J	271	GLN
1	J	536	ASN
1	K	40	HIS
1	K	271	GLN
1	L	40	HIS
1	L	271	GLN
1	A	40	HIS
1	B	40	HIS
1	C	40	HIS
1	C	101	LYS

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Mol	Chain	Res	Type
1	E	40	HIS
1	H	26	ASN
1	J	26	ASN
1	K	14	PHE
1	A	39	VAL
1	B	39	VAL
1	C	39	VAL
1	D	39	VAL
1	E	39	VAL
1	F	39	VAL
1	G	39	VAL
1	H	39	VAL
1	I	39	VAL
1	J	39	VAL
1	K	39	VAL
1	L	39	VAL
1	F	469	GLY
1	I	469	GLY
1	I	526	VAL
1	A	469	GLY
1	C	469	GLY
1	H	469	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/529 (84%)	380 (85%)	66 (15%)	3	16
1	B	446/529 (84%)	382 (86%)	64 (14%)	3	17
1	C	446/529 (84%)	385 (86%)	61 (14%)	3	17
1	D	446/529 (84%)	380 (85%)	66 (15%)	3	16
1	E	446/529 (84%)	380 (85%)	66 (15%)	3	16
1	F	446/529 (84%)	382 (86%)	64 (14%)	3	17
1	G	446/529 (84%)	380 (85%)	66 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	446/529 (84%)	382 (86%)	64 (14%)	3	17
1	I	446/529 (84%)	384 (86%)	62 (14%)	3	17
1	J	446/529 (84%)	384 (86%)	62 (14%)	3	17
1	K	446/529 (84%)	383 (86%)	63 (14%)	3	17
1	L	446/529 (84%)	387 (87%)	59 (13%)	4	18
All	All	5352/6348 (84%)	4589 (86%)	763 (14%)	3	17

All (763) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	17	MET
1	A	29	ARG
1	A	38	ASP
1	A	39	VAL
1	A	46	PHE
1	A	47	ASN
1	A	55	LEU
1	A	58	THR
1	A	60	ASP
1	A	61	LEU
1	A	65	ARG
1	A	69	GLU
1	A	70	GLN
1	A	82	ILE
1	A	92	VAL
1	A	95	ILE
1	A	103	CYS
1	A	106	SER
1	A	107	LEU
1	A	112	VAL
1	A	121	LEU
1	A	126	ASN
1	A	127	VAL
1	A	129	VAL
1	A	132	GLN
1	A	152	VAL
1	A	167	LEU
1	A	175	LEU
1	A	176	THR

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Mol	Chain	Res	Type
1	A	177	ILE
1	A	189	GLU
1	A	199	SER
1	A	200	THR
1	A	204	ILE
1	A	210	MET
1	A	227	THR
1	A	239	VAL
1	A	262	ASP
1	A	278	ASP
1	A	292	THR
1	A	299	ASN
1	A	307	ASN
1	A	330	THR
1	A	338	VAL
1	A	339	THR
1	A	347	LYS
1	A	350	VAL
1	A	352	ASN
1	A	369	THR
1	A	376	ILE
1	A	463	ILE
1	A	507	CYS
1	A	509	ASP
1	A	511	SER
1	A	514	LEU
1	A	517	ILE
1	A	519	SER
1	A	520	MET
1	A	526	VAL
1	A	543	ASN
1	A	545	LEU
1	A	548	LEU
1	A	563	ILE
1	A	571	VAL
1	A	572	ILE
1	B	12	THR
1	B	17	MET
1	B	20	THR
1	B	29	ARG
1	B	38	ASP
1	B	39	VAL

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Mol	Chain	Res	Type
1	B	46	PHE
1	B	47	ASN
1	B	55	LEU
1	B	58	THR
1	B	60	ASP
1	B	61	LEU
1	B	65	ARG
1	B	69	GLU
1	B	70	GLN
1	B	82	ILE
1	B	92	VAL
1	B	95	ILE
1	B	103	CYS
1	B	106	SER
1	B	107	LEU
1	B	112	VAL
1	B	121	LEU
1	B	126	ASN
1	B	127	VAL
1	B	129	VAL
1	B	132	GLN
1	B	175	LEU
1	B	176	THR
1	B	177	ILE
1	B	189	GLU
1	B	199	SER
1	B	200	THR
1	B	204	ILE
1	B	210	MET
1	B	227	THR
1	B	239	VAL
1	B	262	ASP
1	B	278	ASP
1	B	292	THR
1	B	299	ASN
1	B	330	THR
1	B	338	VAL
1	B	339	THR
1	B	347	LYS
1	B	348	VAL
1	B	350	VAL
1	B	352	ASN

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Mol	Chain	Res	Type
1	B	369	THR
1	B	376	ILE
1	B	463	ILE
1	B	507	CYS
1	B	509	ASP
1	B	511	SER
1	B	514	LEU
1	B	517	ILE
1	B	519	SER
1	B	526	VAL
1	B	543	ASN
1	B	545	LEU
1	B	548	LEU
1	B	563	ILE
1	B	571	VAL
1	B	572	ILE
1	C	12	THR
1	C	17	MET
1	C	29	ARG
1	C	38	ASP
1	C	39	VAL
1	C	46	PHE
1	C	47	ASN
1	C	55	LEU
1	C	58	THR
1	C	60	ASP
1	C	61	LEU
1	C	65	ARG
1	C	69	GLU
1	C	70	GLN
1	C	82	ILE
1	C	92	VAL
1	C	95	ILE
1	C	103	CYS
1	C	106	SER
1	C	112	VAL
1	C	126	ASN
1	C	127	VAL
1	C	129	VAL
1	C	132	GLN
1	C	175	LEU
1	C	176	THR

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Mol	Chain	Res	Type
1	C	177	ILE
1	C	189	GLU
1	C	199	SER
1	C	200	THR
1	C	204	ILE
1	C	210	MET
1	C	227	THR
1	C	239	VAL
1	C	262	ASP
1	C	278	ASP
1	C	292	THR
1	C	299	ASN
1	C	330	THR
1	C	338	VAL
1	C	339	THR
1	C	347	LYS
1	C	350	VAL
1	C	352	ASN
1	C	369	THR
1	C	376	ILE
1	C	463	ILE
1	C	507	CYS
1	C	509	ASP
1	C	511	SER
1	C	514	LEU
1	C	517	ILE
1	C	519	SER
1	C	520	MET
1	C	526	VAL
1	C	543	ASN
1	C	545	LEU
1	C	548	LEU
1	C	563	ILE
1	C	571	VAL
1	C	572	ILE
1	D	10	TYR
1	D	12	THR
1	D	17	MET
1	D	20	THR
1	D	29	ARG
1	D	38	ASP
1	D	39	VAL

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Mol	Chain	Res	Type
1	D	46	PHE
1	D	47	ASN
1	D	55	LEU
1	D	58	THR
1	D	60	ASP
1	D	61	LEU
1	D	65	ARG
1	D	69	GLU
1	D	70	GLN
1	D	82	ILE
1	D	92	VAL
1	D	95	ILE
1	D	103	CYS
1	D	106	SER
1	D	107	LEU
1	D	112	VAL
1	D	121	LEU
1	D	126	ASN
1	D	127	VAL
1	D	129	VAL
1	D	132	GLN
1	D	152	VAL
1	D	175	LEU
1	D	176	THR
1	D	177	ILE
1	D	189	GLU
1	D	199	SER
1	D	200	THR
1	D	204	ILE
1	D	210	MET
1	D	227	THR
1	D	239	VAL
1	D	262	ASP
1	D	278	ASP
1	D	292	THR
1	D	299	ASN
1	D	330	THR
1	D	338	VAL
1	D	339	THR
1	D	347	LYS
1	D	350	VAL
1	D	352	ASN

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Mol	Chain	Res	Type
1	D	369	THR
1	D	376	ILE
1	D	463	ILE
1	D	481	VAL
1	D	507	CYS
1	D	509	ASP
1	D	511	SER
1	D	514	LEU
1	D	517	ILE
1	D	519	SER
1	D	520	MET
1	D	526	VAL
1	D	543	ASN
1	D	545	LEU
1	D	548	LEU
1	D	563	ILE
1	D	572	ILE
1	E	10	TYR
1	E	12	THR
1	E	17	MET
1	E	20	THR
1	E	29	ARG
1	E	38	ASP
1	E	39	VAL
1	E	46	PHE
1	E	47	ASN
1	E	55	LEU
1	E	58	THR
1	E	60	ASP
1	E	61	LEU
1	E	65	ARG
1	E	69	GLU
1	E	70	GLN
1	E	82	ILE
1	E	92	VAL
1	E	95	ILE
1	E	103	CYS
1	E	106	SER
1	E	112	VAL
1	E	121	LEU
1	E	126	ASN
1	E	127	VAL

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Mol	Chain	Res	Type
1	E	129	VAL
1	E	132	GLN
1	E	152	VAL
1	E	175	LEU
1	E	176	THR
1	E	177	ILE
1	E	189	GLU
1	E	199	SER
1	E	200	THR
1	E	204	ILE
1	E	210	MET
1	E	227	THR
1	E	239	VAL
1	E	262	ASP
1	E	278	ASP
1	E	292	THR
1	E	299	ASN
1	E	330	THR
1	E	338	VAL
1	E	339	THR
1	E	347	LYS
1	E	350	VAL
1	E	352	ASN
1	E	369	THR
1	E	376	ILE
1	E	463	ILE
1	E	481	VAL
1	E	507	CYS
1	E	509	ASP
1	E	511	SER
1	E	514	LEU
1	E	517	ILE
1	E	519	SER
1	E	520	MET
1	E	526	VAL
1	E	542	MET
1	E	543	ASN
1	E	545	LEU
1	E	548	LEU
1	E	563	ILE
1	E	572	ILE
1	F	12	THR

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Mol	Chain	Res	Type
1	F	17	MET
1	F	20	THR
1	F	29	ARG
1	F	38	ASP
1	F	39	VAL
1	F	46	PHE
1	F	47	ASN
1	F	55	LEU
1	F	58	THR
1	F	60	ASP
1	F	61	LEU
1	F	65	ARG
1	F	69	GLU
1	F	70	GLN
1	F	82	ILE
1	F	92	VAL
1	F	95	ILE
1	F	103	CYS
1	F	106	SER
1	F	107	LEU
1	F	112	VAL
1	F	121	LEU
1	F	126	ASN
1	F	127	VAL
1	F	129	VAL
1	F	132	GLN
1	F	152	VAL
1	F	175	LEU
1	F	176	THR
1	F	177	ILE
1	F	189	GLU
1	F	199	SER
1	F	200	THR
1	F	204	ILE
1	F	210	MET
1	F	227	THR
1	F	239	VAL
1	F	262	ASP
1	F	278	ASP
1	F	292	THR
1	F	299	ASN
1	F	330	THR

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Mol	Chain	Res	Type
1	F	338	VAL
1	F	339	THR
1	F	347	LYS
1	F	350	VAL
1	F	352	ASN
1	F	369	THR
1	F	376	ILE
1	F	463	ILE
1	F	507	CYS
1	F	509	ASP
1	F	511	SER
1	F	514	LEU
1	F	517	ILE
1	F	519	SER
1	F	520	MET
1	F	526	VAL
1	F	543	ASN
1	F	545	LEU
1	F	548	LEU
1	F	563	ILE
1	F	572	ILE
1	G	12	THR
1	G	17	MET
1	G	20	THR
1	G	29	ARG
1	G	38	ASP
1	G	39	VAL
1	G	46	PHE
1	G	47	ASN
1	G	55	LEU
1	G	58	THR
1	G	60	ASP
1	G	61	LEU
1	G	65	ARG
1	G	69	GLU
1	G	70	GLN
1	G	82	ILE
1	G	92	VAL
1	G	95	ILE
1	G	103	CYS
1	G	106	SER
1	G	107	LEU

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Mol	Chain	Res	Type
1	G	112	VAL
1	G	121	LEU
1	G	126	ASN
1	G	127	VAL
1	G	129	VAL
1	G	132	GLN
1	G	152	VAL
1	G	175	LEU
1	G	176	THR
1	G	177	ILE
1	G	189	GLU
1	G	199	SER
1	G	200	THR
1	G	204	ILE
1	G	210	MET
1	G	227	THR
1	G	239	VAL
1	G	262	ASP
1	G	278	ASP
1	G	292	THR
1	G	299	ASN
1	G	307	ASN
1	G	330	THR
1	G	338	VAL
1	G	339	THR
1	G	347	LYS
1	G	348	VAL
1	G	350	VAL
1	G	369	THR
1	G	376	ILE
1	G	463	ILE
1	G	507	CYS
1	G	509	ASP
1	G	511	SER
1	G	514	LEU
1	G	517	ILE
1	G	519	SER
1	G	520	MET
1	G	526	VAL
1	G	542	MET
1	G	543	ASN
1	G	545	LEU

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Mol	Chain	Res	Type
1	G	548	LEU
1	G	563	ILE
1	G	572	ILE
1	H	10	TYR
1	H	12	THR
1	H	17	MET
1	H	20	THR
1	H	29	ARG
1	H	38	ASP
1	H	39	VAL
1	H	46	PHE
1	H	47	ASN
1	H	55	LEU
1	H	58	THR
1	H	60	ASP
1	H	61	LEU
1	H	65	ARG
1	H	69	GLU
1	H	70	GLN
1	H	82	ILE
1	H	92	VAL
1	H	95	ILE
1	H	103	CYS
1	H	106	SER
1	H	112	VAL
1	H	121	LEU
1	H	126	ASN
1	H	127	VAL
1	H	129	VAL
1	H	132	GLN
1	H	152	VAL
1	H	175	LEU
1	H	176	THR
1	H	177	ILE
1	H	189	GLU
1	H	199	SER
1	H	200	THR
1	H	204	ILE
1	H	210	MET
1	H	227	THR
1	H	239	VAL
1	H	262	ASP

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Mol	Chain	Res	Type
1	H	278	ASP
1	H	292	THR
1	H	299	ASN
1	H	307	ASN
1	H	330	THR
1	H	338	VAL
1	H	339	THR
1	H	347	LYS
1	H	350	VAL
1	H	369	THR
1	H	376	ILE
1	H	463	ILE
1	H	507	CYS
1	H	509	ASP
1	H	511	SER
1	H	514	LEU
1	H	517	ILE
1	H	519	SER
1	H	526	VAL
1	H	543	ASN
1	H	545	LEU
1	H	548	LEU
1	H	563	ILE
1	H	571	VAL
1	H	572	ILE
1	I	12	THR
1	I	17	MET
1	I	20	THR
1	I	29	ARG
1	I	38	ASP
1	I	39	VAL
1	I	46	PHE
1	I	47	ASN
1	I	55	LEU
1	I	58	THR
1	I	60	ASP
1	I	61	LEU
1	I	65	ARG
1	I	69	GLU
1	I	70	GLN
1	I	82	ILE
1	I	92	VAL

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Mol	Chain	Res	Type
1	I	95	ILE
1	I	103	CYS
1	I	106	SER
1	I	112	VAL
1	I	121	LEU
1	I	126	ASN
1	I	127	VAL
1	I	129	VAL
1	I	132	GLN
1	I	152	VAL
1	I	175	LEU
1	I	176	THR
1	I	177	ILE
1	I	189	GLU
1	I	199	SER
1	I	200	THR
1	I	204	ILE
1	I	210	MET
1	I	227	THR
1	I	239	VAL
1	I	262	ASP
1	I	278	ASP
1	I	292	THR
1	I	299	ASN
1	I	330	THR
1	I	338	VAL
1	I	339	THR
1	I	347	LYS
1	I	350	VAL
1	I	369	THR
1	I	376	ILE
1	I	463	ILE
1	I	481	VAL
1	I	507	CYS
1	I	509	ASP
1	I	511	SER
1	I	514	LEU
1	I	517	ILE
1	I	519	SER
1	I	526	VAL
1	I	543	ASN
1	I	545	LEU

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Mol	Chain	Res	Type
1	I	548	LEU
1	I	563	ILE
1	I	572	ILE
1	J	12	THR
1	J	17	MET
1	J	29	ARG
1	J	38	ASP
1	J	39	VAL
1	J	46	PHE
1	J	47	ASN
1	J	55	LEU
1	J	58	THR
1	J	60	ASP
1	J	61	LEU
1	J	65	ARG
1	J	69	GLU
1	J	70	GLN
1	J	82	ILE
1	J	92	VAL
1	J	95	ILE
1	J	103	CYS
1	J	106	SER
1	J	107	LEU
1	J	112	VAL
1	J	121	LEU
1	J	126	ASN
1	J	127	VAL
1	J	129	VAL
1	J	132	GLN
1	J	175	LEU
1	J	176	THR
1	J	177	ILE
1	J	189	GLU
1	J	199	SER
1	J	200	THR
1	J	204	ILE
1	J	210	MET
1	J	227	THR
1	J	239	VAL
1	J	262	ASP
1	J	278	ASP
1	J	292	THR

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Mol	Chain	Res	Type
1	J	299	ASN
1	J	330	THR
1	J	338	VAL
1	J	339	THR
1	J	347	LYS
1	J	348	VAL
1	J	350	VAL
1	J	369	THR
1	J	376	ILE
1	J	463	ILE
1	J	507	CYS
1	J	509	ASP
1	J	511	SER
1	J	514	LEU
1	J	517	ILE
1	J	519	SER
1	J	520	MET
1	J	526	VAL
1	J	543	ASN
1	J	545	LEU
1	J	548	LEU
1	J	563	ILE
1	J	572	ILE
1	K	12	THR
1	K	17	MET
1	K	20	THR
1	K	29	ARG
1	K	38	ASP
1	K	39	VAL
1	K	46	PHE
1	K	47	ASN
1	K	55	LEU
1	K	58	THR
1	K	60	ASP
1	K	61	LEU
1	K	65	ARG
1	K	69	GLU
1	K	70	GLN
1	K	82	ILE
1	K	92	VAL
1	K	95	ILE
1	K	103	CYS

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Mol	Chain	Res	Type
1	K	106	SER
1	K	112	VAL
1	K	121	LEU
1	K	126	ASN
1	K	127	VAL
1	K	129	VAL
1	K	132	GLN
1	K	175	LEU
1	K	176	THR
1	K	177	ILE
1	K	189	GLU
1	K	199	SER
1	K	200	THR
1	K	204	ILE
1	K	210	MET
1	K	227	THR
1	K	239	VAL
1	K	262	ASP
1	K	278	ASP
1	K	292	THR
1	K	299	ASN
1	K	307	ASN
1	K	330	THR
1	K	338	VAL
1	K	339	THR
1	K	347	LYS
1	K	350	VAL
1	K	352	ASN
1	K	369	THR
1	K	376	ILE
1	K	463	ILE
1	K	481	VAL
1	K	507	CYS
1	K	509	ASP
1	K	511	SER
1	K	514	LEU
1	K	517	ILE
1	K	519	SER
1	K	526	VAL
1	K	543	ASN
1	K	545	LEU
1	K	548	LEU

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Mol	Chain	Res	Type
1	K	563	ILE
1	K	572	ILE
1	L	12	THR
1	L	17	MET
1	L	20	THR
1	L	29	ARG
1	L	38	ASP
1	L	39	VAL
1	L	46	PHE
1	L	47	ASN
1	L	55	LEU
1	L	58	THR
1	L	60	ASP
1	L	61	LEU
1	L	65	ARG
1	L	69	GLU
1	L	70	GLN
1	L	82	ILE
1	L	92	VAL
1	L	95	ILE
1	L	103	CYS
1	L	106	SER
1	L	112	VAL
1	L	126	ASN
1	L	127	VAL
1	L	129	VAL
1	L	132	GLN
1	L	175	LEU
1	L	176	THR
1	L	177	ILE
1	L	189	GLU
1	L	199	SER
1	L	200	THR
1	L	204	ILE
1	L	210	MET
1	L	227	THR
1	L	239	VAL
1	L	262	ASP
1	L	278	ASP
1	L	292	THR
1	L	299	ASN
1	L	330	THR

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Mol	Chain	Res	Type
1	L	338	VAL
1	L	339	THR
1	L	347	LYS
1	L	350	VAL
1	L	369	THR
1	L	376	ILE
1	L	463	ILE
1	L	507	CYS
1	L	509	ASP
1	L	511	SER
1	L	514	LEU
1	L	517	ILE
1	L	519	SER
1	L	526	VAL
1	L	543	ASN
1	L	545	LEU
1	L	548	LEU
1	L	563	ILE
1	L	572	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	122	ASN
1	A	233	GLN
1	A	366	ASN
1	B	119	ASN
1	B	122	ASN
1	B	233	GLN
1	B	366	ASN
1	C	22	HIS
1	C	119	ASN
1	C	122	ASN
1	C	233	GLN
1	C	362	GLN
1	C	366	ASN
1	D	119	ASN
1	D	122	ASN
1	D	233	GLN
1	D	366	ASN
1	E	119	ASN

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Mol	Chain	Res	Type
1	E	122	ASN
1	E	233	GLN
1	E	362	GLN
1	E	366	ASN
1	F	119	ASN
1	F	122	ASN
1	F	233	GLN
1	F	362	GLN
1	F	366	ASN
1	G	22	HIS
1	G	119	ASN
1	G	122	ASN
1	G	233	GLN
1	G	366	ASN
1	H	233	GLN
1	H	366	ASN
1	I	119	ASN
1	I	122	ASN
1	I	233	GLN
1	I	366	ASN
1	J	24	ASN
1	J	119	ASN
1	J	122	ASN
1	J	132	GLN
1	J	233	GLN
1	J	366	ASN
1	K	119	ASN
1	K	122	ASN
1	K	233	GLN
1	K	362	GLN
1	K	366	ASN
1	L	24	ASN
1	L	233	GLN
1	L	366	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	488/583 (83%)	0.08	6 (1%) 76 59	25, 83, 153, 207	0
1	B	488/583 (83%)	0.12	8 (1%) 70 52	28, 81, 148, 232	0
1	C	488/583 (83%)	0.16	10 (2%) 65 48	16, 72, 151, 222	0
1	D	488/583 (83%)	0.13	9 (1%) 67 50	18, 72, 140, 212	0
1	E	488/583 (83%)	0.10	3 (0%) 85 71	27, 82, 146, 215	0
1	F	488/583 (83%)	0.15	6 (1%) 76 59	17, 79, 158, 247	0
1	G	488/583 (83%)	0.18	7 (1%) 73 55	41, 97, 171, 227	0
1	H	488/583 (83%)	0.09	6 (1%) 76 59	35, 91, 170, 258	0
1	I	488/583 (83%)	0.12	8 (1%) 70 52	20, 84, 160, 222	0
1	J	488/583 (83%)	0.05	7 (1%) 73 55	35, 93, 162, 211	0
1	K	488/583 (83%)	0.16	4 (0%) 82 65	36, 94, 159, 226	0
1	L	488/583 (83%)	0.09	9 (1%) 67 50	37, 90, 174, 247	0
All	All	5856/6996 (83%)	0.12	83 (1%) 73 55	16, 85, 161, 258	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	39	VAL	5.0
1	H	39	VAL	4.4
1	B	39	VAL	4.3
1	E	39	VAL	4.2
1	D	58	THR	3.7
1	L	47	ASN	3.6
1	I	62	VAL	3.6
1	K	230	PRO	3.5
1	C	54	VAL	3.3
1	J	39	VAL	3.3
1	C	188	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	39	VAL	3.2
1	B	40	HIS	3.2
1	H	193	PHE	3.1
1	C	263	LEU	3.1
1	F	39	VAL	3.1
1	C	8	LEU	3.1
1	D	39	VAL	3.0
1	A	358	ASN	2.9
1	F	47	ASN	2.9
1	D	186	GLY	2.9
1	B	262	ASP	2.8
1	B	100	ASP	2.8
1	K	39	VAL	2.8
1	H	54	VAL	2.8
1	A	100	ASP	2.8
1	L	243	PRO	2.7
1	A	187	THR	2.6
1	G	58	THR	2.6
1	D	262	ASP	2.5
1	G	12	THR	2.5
1	A	39	VAL	2.5
1	A	186	GLY	2.5
1	G	54	VAL	2.5
1	I	271	GLN	2.5
1	C	40	HIS	2.5
1	E	47	ASN	2.5
1	L	58	THR	2.4
1	I	379	SER	2.4
1	D	187	THR	2.4
1	F	197	SER	2.4
1	I	154	ALA	2.4
1	L	377	GLY	2.4
1	D	171	LEU	2.4
1	E	14	PHE	2.3
1	K	24	ASN	2.3
1	F	58	THR	2.3
1	H	58	THR	2.3
1	B	54	VAL	2.3
1	C	58	THR	2.3
1	D	293	LEU	2.3
1	B	8	LEU	2.3
1	D	56	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	39	VAL	2.3
1	L	242	ILE	2.2
1	C	191	PRO	2.2
1	F	573	ILE	2.2
1	G	485	LEU	2.2
1	C	100	ASP	2.2
1	H	529	LYS	2.2
1	L	17	MET	2.2
1	J	573	ILE	2.2
1	L	462	ALA	2.2
1	J	58	THR	2.2
1	J	53	GLY	2.1
1	J	530	GLY	2.1
1	A	573	ILE	2.1
1	I	58	THR	2.1
1	I	54	VAL	2.1
1	G	235	SER	2.1
1	L	39	VAL	2.1
1	G	311	ALA	2.1
1	I	381	ASP	2.1
1	K	569	ASN	2.1
1	J	95	ILE	2.1
1	F	260	GLY	2.1
1	J	175	LEU	2.1
1	B	573	ILE	2.1
1	B	58	THR	2.1
1	C	509	ASP	2.0
1	L	262	ASP	2.0
1	H	47	ASN	2.0
1	D	246	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.