



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 08:50 AM EDT

PDB ID : 3O44
Title : Crystal Structure of the Vibrio cholerae Cytolysin (HlyA) Heptameric Pore
Authors : De, S.; Olson, R.
Deposited on : 2010-07-26
Resolution : 2.88 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:

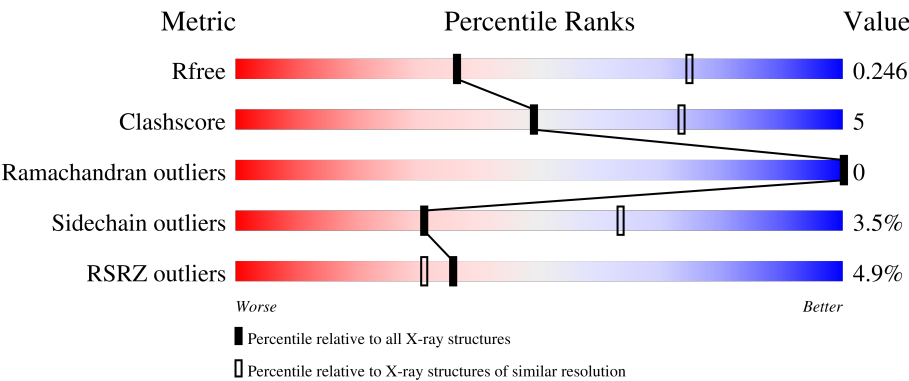
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.88 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}	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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	593	<div><div>2%</div><div><div></div><div>83%</div><div>14%</div><div>..</div></div></div>
1	B	593	<div><div>4%</div><div><div></div><div>85%</div><div>12%</div><div>..</div></div></div>
1	C	593	<div><div>4%</div><div><div></div><div>86%</div><div>11%</div><div>..</div></div></div>
1	D	593	<div><div>8%</div><div><div></div><div>84%</div><div>13%</div><div>..</div></div></div>
1	E	593	<div><div>3%</div><div><div></div><div>85%</div><div>12%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	593	<div><div></div><div>5%</div><div>86%</div><div>11%</div><div>••</div></div>
1	G	593	<div><div></div><div>8%</div><div>84%</div><div>13%</div><div>••</div></div>
1	H	593	<div><div></div><div>2%</div><div>85%</div><div>13%</div><div>•</div></div>
1	I	593	<div><div></div><div>9%</div><div>85%</div><div>13%</div><div>••</div></div>
1	J	593	<div><div></div><div>4%</div><div>85%</div><div>12%</div><div>••</div></div>
1	K	593	<div><div></div><div>7%</div><div>83%</div><div>14%</div><div>••</div></div>
1	L	593	<div><div></div><div>3%</div><div>81%</div><div>16%</div><div>••</div></div>
1	M	593	<div><div></div><div>3%</div><div>83%</div><div>14%</div><div>••</div></div>
1	N	593	<div><div></div><div>4%</div><div>83%</div><div>14%</div><div>••</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 62948 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 Hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4464	2784	779	892	9			
1	B	581	Total	C	N	O	S	0	0	0
			4457	2783	778	887	9			
1	C	581	Total	C	N	O	S	0	0	0
			4431	2759	776	887	9			
1	D	581	Total	C	N	O	S	0	0	0
			4471	2794	778	890	9			
1	E	581	Total	C	N	O	S	0	0	0
			4460	2784	777	890	9			
1	F	581	Total	C	N	O	S	0	0	0
			4412	2746	768	889	9			
1	G	581	Total	C	N	O	S	0	0	0
			4436	2764	777	886	9			
1	H	581	Total	C	N	O	S	0	0	0
			4468	2791	774	894	9			
1	I	581	Total	C	N	O	S	0	0	0
			4479	2797	780	893	9			
1	J	581	Total	C	N	O	S	0	0	0
			4487	2804	782	892	9			
1	K	581	Total	C	N	O	S	0	0	0
			4417	2755	772	881	9			
1	L	581	Total	C	N	O	S	0	0	0
			4449	2773	779	888	9			
1	M	581	Total	C	N	O	S	0	0	0
			4447	2773	777	888	9			
1	N	581	Total	C	N	O	S	0	0	0
			4420	2759	769	883	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	606	ASN	HIS	conflict	UNP C2C744

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Chain	Residue	Modelled	Actual	Comment	Reference
B	606	ASN	HIS	conflict	UNP C2C744
C	606	ASN	HIS	conflict	UNP C2C744
D	606	ASN	HIS	conflict	UNP C2C744
E	606	ASN	HIS	conflict	UNP C2C744
F	606	ASN	HIS	conflict	UNP C2C744
G	606	ASN	HIS	conflict	UNP C2C744
H	606	ASN	HIS	conflict	UNP C2C744
I	606	ASN	HIS	conflict	UNP C2C744
J	606	ASN	HIS	conflict	UNP C2C744
K	606	ASN	HIS	conflict	UNP C2C744
L	606	ASN	HIS	conflict	UNP C2C744
M	606	ASN	HIS	conflict	UNP C2C744
N	606	ASN	HIS	conflict	UNP C2C744

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	B	62	Total O 62 62	0	0
2	C	57	Total O 57 57	0	0
2	D	65	Total O 65 65	0	0
2	E	44	Total O 44 44	0	0
2	F	26	Total O 26 26	0	0
2	G	50	Total O 50 50	0	0
2	H	48	Total O 48 48	0	0
2	I	61	Total O 61 61	0	0
2	J	32	Total O 32 32	0	0
2	K	25	Total O 25 25	0	0
2	L	43	Total O 43 43	0	0
2	M	43	Total O 43 43	0	0

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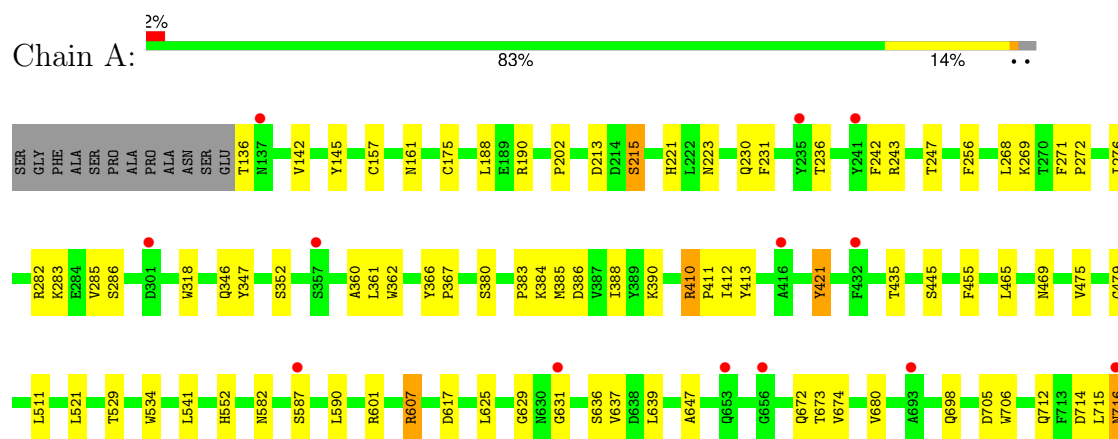
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	36	Total	O	0	0
			36	36		

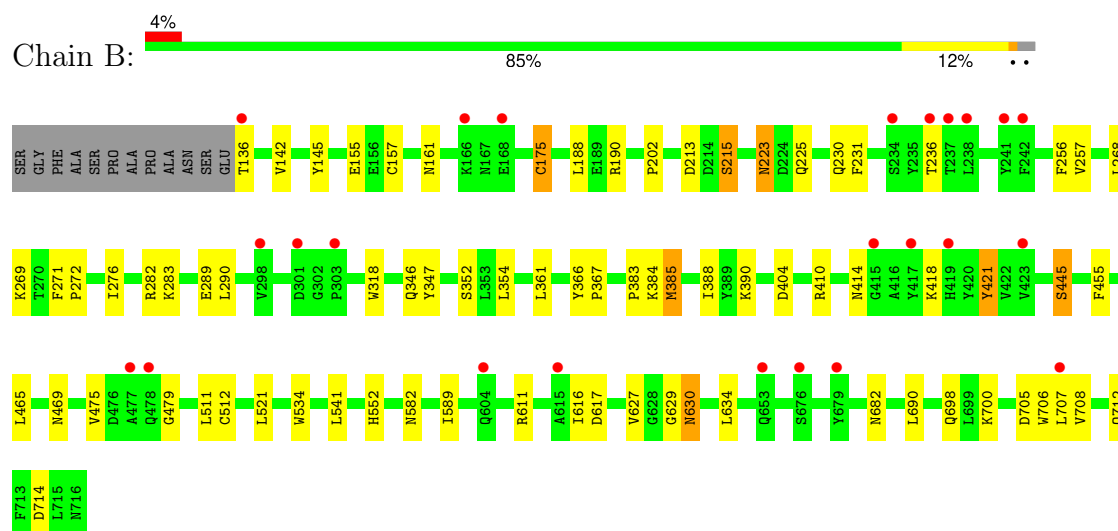
3 Residue-property plots [i](#)

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.

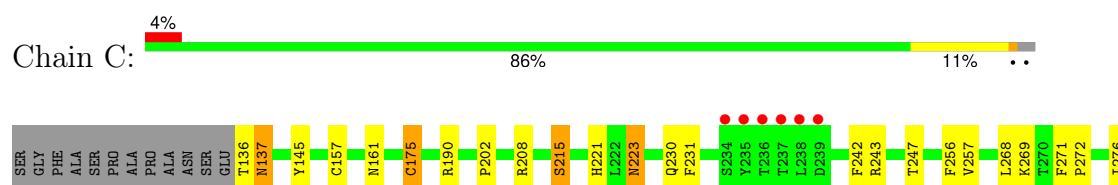
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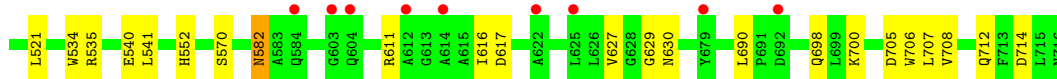


• Molecule 1: Hemolysin

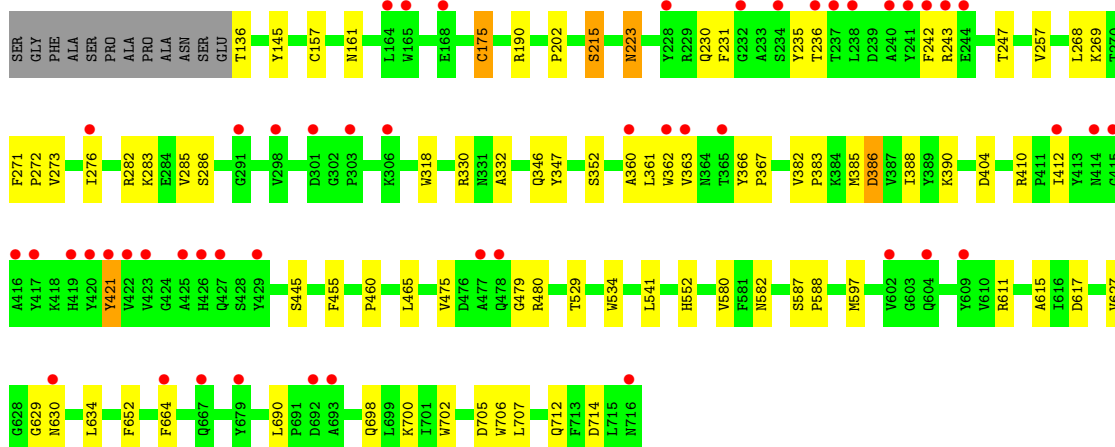
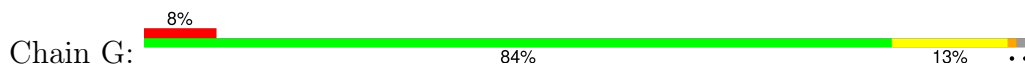


• Molecule 1: Hemolysin

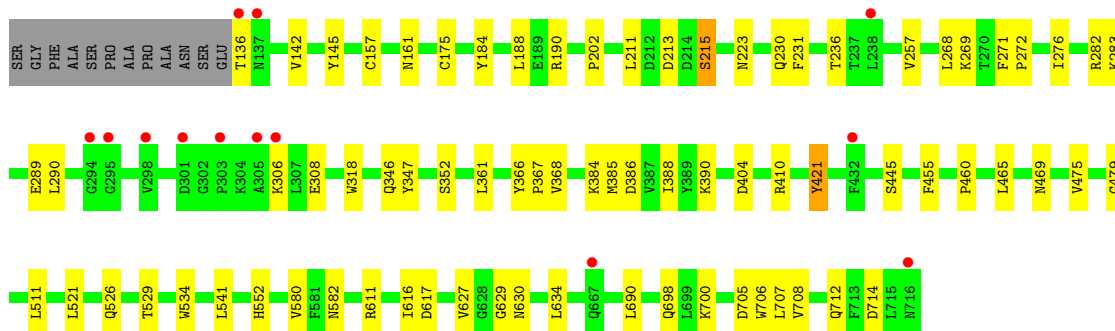
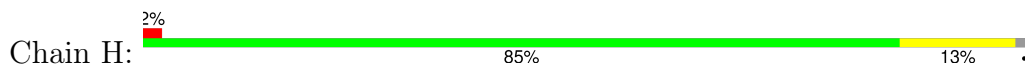




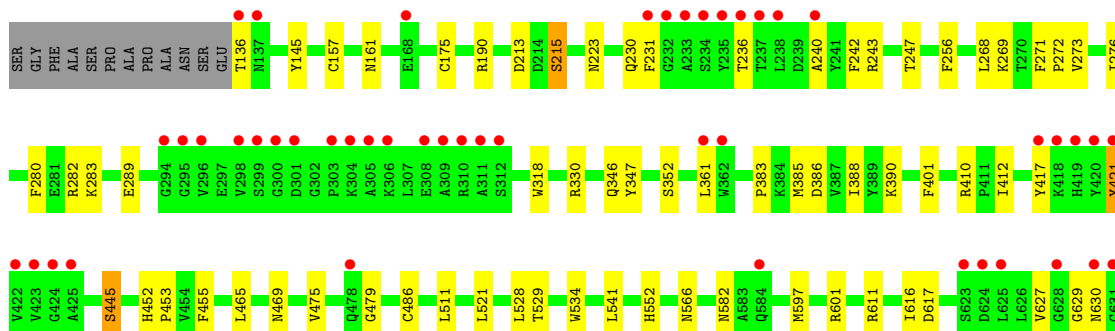
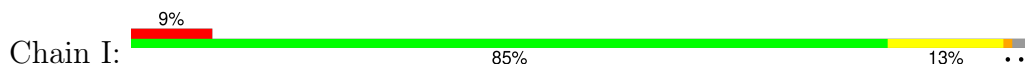
• Molecule 1: Hemolysin

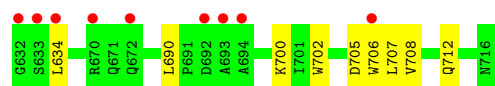


• Molecule 1: Hemolysin

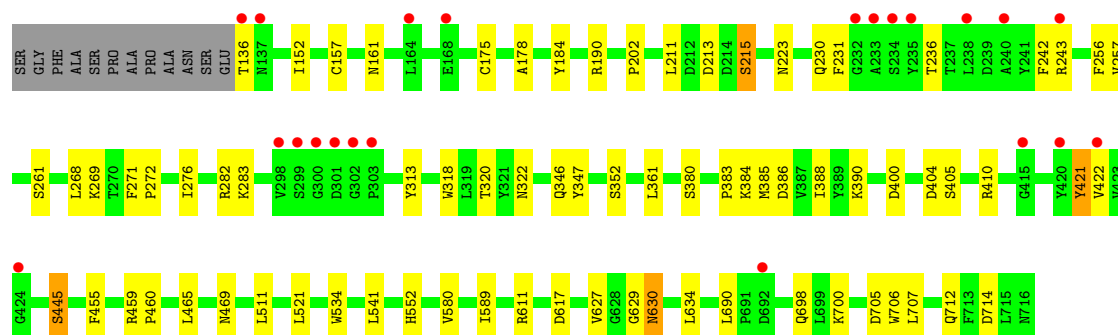
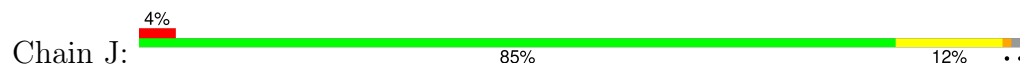


• Molecule 1: Hemolysin

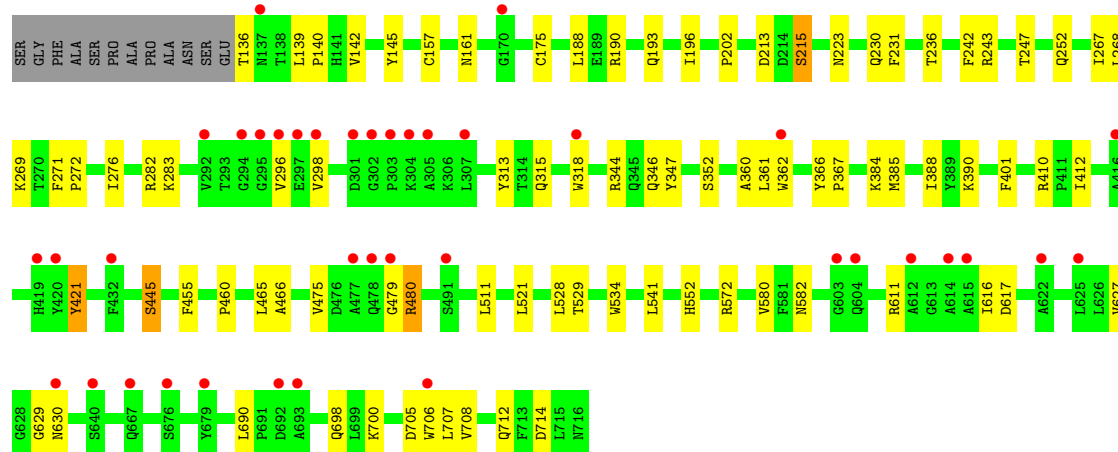
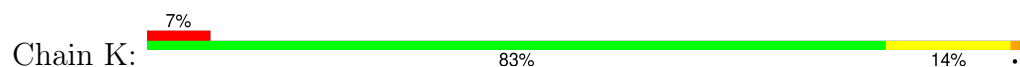




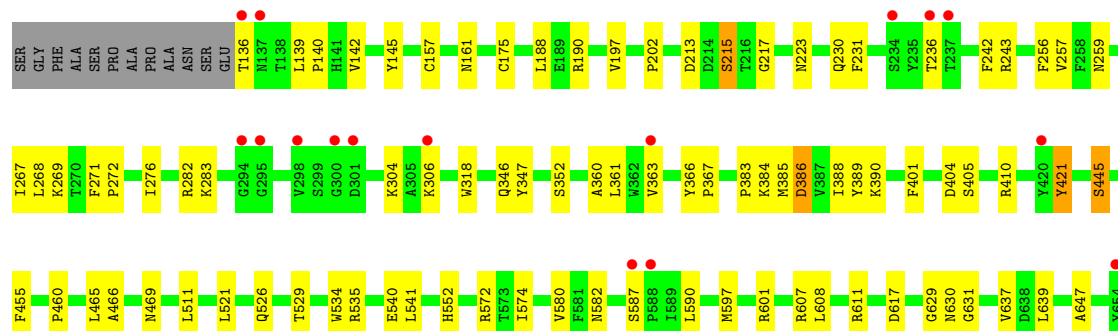
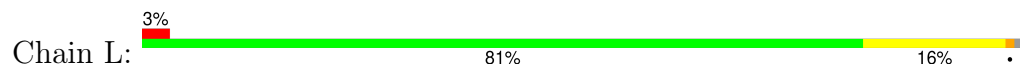
• Molecule 1: Hemolysin



• Molecule 1: Hemolysin

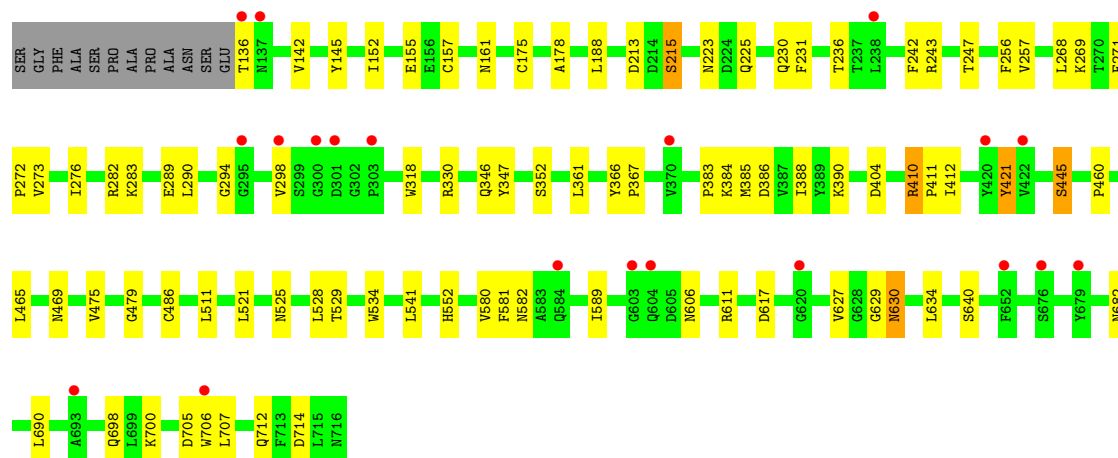
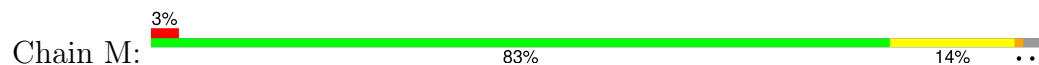


• Molecule 1: Hemolysin

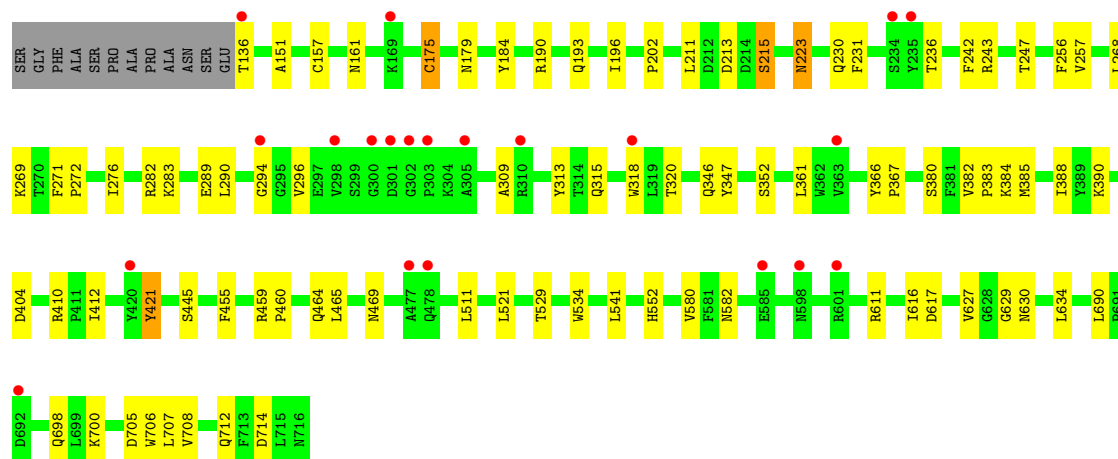
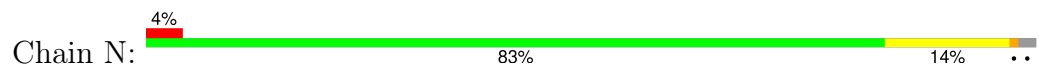




• Molecule 1: Hemolysin



• Molecule 1: Hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	172.35Å 182.86Å 430.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.96 – 2.88 43.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.8 (43.96-2.88) 98.4 (43.96-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.218 , 0.249 0.217 , 0.246	Depositor DCC
R_{free} test set	15098 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	62948	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/4557	0.57	0/6204
1	B	0.43	0/4551	0.56	0/6198
1	C	0.44	0/4523	0.55	0/6164
1	D	0.45	0/4567	0.56	0/6221
1	E	0.43	0/4555	0.55	0/6205
1	F	0.42	0/4503	0.56	0/6139
1	G	0.45	0/4528	0.56	0/6168
1	H	0.40	0/4564	0.55	0/6219
1	I	0.44	0/4575	0.56	0/6233
1	J	0.42	0/4583	0.55	0/6240
1	K	0.43	0/4509	0.56	0/6146
1	L	0.43	0/4541	0.58	0/6183
1	M	0.43	0/4539	0.57	0/6183
1	N	0.42	0/4513	0.56	0/6153
All	All	0.43	0/63608	0.56	0/86656

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4464	0	4169	57	0
1	B	4457	0	4163	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4431	0	4100	50	0
1	D	4471	0	4172	57	1
1	E	4460	0	4146	46	0
1	F	4412	0	4065	47	0
1	G	4436	0	4120	55	1
1	H	4468	0	4156	51	0
1	I	4479	0	4178	55	0
1	J	4487	0	4205	50	0
1	K	4417	0	4093	58	0
1	L	4449	0	4145	67	0
1	M	4447	0	4147	61	0
1	N	4420	0	4094	61	0
2	A	58	0	0	1	0
2	B	62	0	0	1	0
2	C	57	0	0	1	0
2	D	65	0	0	2	0
2	E	44	0	0	0	0
2	F	26	0	0	2	0
2	G	50	0	0	0	0
2	H	48	0	0	0	0
2	I	61	0	0	1	0
2	J	32	0	0	0	0
2	K	25	0	0	0	0
2	L	43	0	0	1	0
2	M	43	0	0	2	0
2	N	36	0	0	1	0
All	All	62948	0	57953	639	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (639) 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:283:LYS:HB2	1:C:318:TRP:HB2	1.36	1.04
1:K:480:ARG:HH11	1:K:480:ARG:HB3	1.22	1.02
1:N:283:LYS:HB2	1:N:318:TRP:HB2	1.41	1.02
1:F:283:LYS:HB2	1:F:318:TRP:HB2	1.43	1.01
1:H:283:LYS:HB2	1:H:318:TRP:HB2	1.38	1.01
1:K:283:LYS:HB2	1:K:318:TRP:HB2	1.42	1.01
1:L:283:LYS:HB2	1:L:318:TRP:HB2	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:GLN:HE22	1:N:282:ARG:HH11	1.03	1.00
1:E:282:ARG:HH11	1:F:346:GLN:HE22	1.08	0.99
1:J:283:LYS:HB2	1:J:318:TRP:HB2	1.44	0.99
1:E:283:LYS:HB2	1:E:318:TRP:HB2	1.45	0.98
1:I:283:LYS:HB2	1:I:318:TRP:HB2	1.43	0.98
1:K:282:ARG:HH11	1:L:346:GLN:HE22	1.10	0.98
1:B:283:LYS:HB2	1:B:318:TRP:HB2	1.44	0.98
1:B:282:ARG:HH11	1:C:346:GLN:HE22	1.10	0.97
1:G:283:LYS:HB2	1:G:318:TRP:HB2	1.44	0.97
1:M:283:LYS:HB2	1:M:318:TRP:HB2	1.45	0.97
1:A:282:ARG:HH11	1:B:346:GLN:HE22	1.11	0.96
1:A:283:LYS:HB2	1:A:318:TRP:HB2	1.45	0.96
1:F:282:ARG:NH1	1:G:346:GLN:HE22	1.64	0.95
1:J:282:ARG:HH11	1:K:346:GLN:HE22	1.00	0.95
1:D:283:LYS:HB2	1:D:318:TRP:HB2	1.45	0.94
1:H:282:ARG:HH11	1:I:346:GLN:HE22	1.09	0.94
1:M:282:ARG:HH11	1:N:346:GLN:HE22	1.14	0.93
1:F:282:ARG:HH11	1:G:346:GLN:NE2	1.67	0.93
1:A:346:GLN:HE22	1:G:282:ARG:HH11	1.16	0.92
1:C:282:ARG:HH11	1:D:346:GLN:HE22	0.98	0.90
1:F:282:ARG:HH11	1:G:346:GLN:HE22	0.90	0.89
1:C:282:ARG:HH11	1:D:346:GLN:NE2	1.70	0.89
1:C:282:ARG:NH1	1:D:346:GLN:HE22	1.72	0.89
1:I:282:ARG:HH11	1:J:346:GLN:HE22	1.20	0.88
1:L:282:ARG:HH11	1:M:346:GLN:HE22	1.14	0.88
1:D:282:ARG:HH11	1:E:346:GLN:HE22	1.21	0.88
1:J:282:ARG:NH1	1:K:346:GLN:HE22	1.73	0.86
1:H:346:GLN:HE22	1:N:282:ARG:NH1	1.73	0.85
1:K:268:LEU:HD11	1:L:215:SER:HB2	1.59	0.85
1:F:282:ARG:NH1	1:G:346:GLN:NE2	2.24	0.84
1:H:282:ARG:HH11	1:I:346:GLN:NE2	1.76	0.83
1:C:282:ARG:NH1	1:D:346:GLN:NE2	2.27	0.81
1:J:282:ARG:HH11	1:K:346:GLN:NE2	1.77	0.81
1:C:137:ASN:HD22	1:C:137:ASN:N	1.80	0.78
1:A:282:ARG:NH1	1:B:346:GLN:HE22	1.81	0.78
1:E:282:ARG:NH1	1:F:346:GLN:HE22	1.82	0.78
1:E:268:LEU:HD11	1:F:215:SER:HB2	1.65	0.78
1:L:587:SER:OG	1:L:714:ASP:HA	1.84	0.77
1:B:282:ARG:NH1	1:C:346:GLN:HE22	1.82	0.77
1:H:346:GLN:NE2	1:N:282:ARG:HH11	1.83	0.77
1:J:282:ARG:NH1	1:K:346:GLN:NE2	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASN:HD22	1:C:137:ASN:H	1.29	0.76
1:K:282:ARG:NH1	1:L:346:GLN:HE22	1.83	0.76
1:E:282:ARG:HH11	1:F:346:GLN:NE2	1.84	0.75
1:K:282:ARG:HH11	1:L:346:GLN:NE2	1.85	0.75
1:L:268:LEU:HD11	1:M:215:SER:HB2	1.68	0.74
1:F:269:LYS:HE3	1:F:388:ILE:HD12	1.70	0.73
1:A:215:SER:HB2	1:G:268:LEU:HD11	1.69	0.73
1:C:269:LYS:HE3	1:C:388:ILE:HD12	1.71	0.73
1:L:282:ARG:HH11	1:M:346:GLN:NE2	1.87	0.73
1:J:269:LYS:HE3	1:J:388:ILE:HD12	1.71	0.72
1:I:269:LYS:HE3	1:I:388:ILE:HD12	1.69	0.72
1:B:269:LYS:HE3	1:B:388:ILE:HD12	1.71	0.72
1:M:282:ARG:NH1	1:N:346:GLN:HE22	1.88	0.72
1:I:268:LEU:HD11	1:J:215:SER:HB2	1.70	0.71
1:A:346:GLN:HE22	1:G:282:ARG:NH1	1.87	0.71
1:B:282:ARG:HH11	1:C:346:GLN:NE2	1.85	0.71
1:H:346:GLN:NE2	1:N:282:ARG:NH1	2.37	0.71
1:L:259:ASN:HB2	2:L:841:HOH:O	1.90	0.71
1:A:268:LEU:HD11	1:B:215:SER:HB2	1.72	0.71
1:H:282:ARG:NH1	1:I:346:GLN:HE22	1.87	0.71
1:N:269:LYS:HE3	1:N:388:ILE:HD12	1.73	0.71
1:H:282:ARG:NH1	1:I:346:GLN:NE2	2.39	0.71
1:H:215:SER:HB2	1:N:268:LEU:HD11	1.71	0.71
1:K:269:LYS:HE3	1:K:388:ILE:HD12	1.73	0.70
1:D:269:LYS:HE3	1:D:388:ILE:HD12	1.73	0.70
1:L:282:ARG:NH1	1:M:346:GLN:HE22	1.88	0.70
1:E:269:LYS:HE3	1:E:388:ILE:HD12	1.73	0.69
1:G:269:LYS:HE3	1:G:388:ILE:HD12	1.74	0.69
1:M:282:ARG:HH11	1:N:346:GLN:NE2	1.90	0.69
1:M:269:LYS:HE3	1:M:388:ILE:HD12	1.75	0.68
1:H:268:LEU:HD11	1:I:215:SER:HB2	1.76	0.68
1:A:282:ARG:HH11	1:B:346:GLN:NE2	1.90	0.68
1:E:282:ARG:NH1	1:F:346:GLN:NE2	2.42	0.68
1:D:361:LEU:HD12	1:D:361:LEU:H	1.57	0.67
1:L:269:LYS:HE3	1:L:388:ILE:HD12	1.75	0.67
1:D:268:LEU:HD11	1:E:215:SER:HB2	1.75	0.67
1:H:269:LYS:HE3	1:H:388:ILE:HD12	1.76	0.67
1:F:582:ASN:HB2	2:F:822:HOH:O	1.95	0.67
1:B:268:LEU:HD11	1:C:215:SER:HB2	1.76	0.67
1:B:282:ARG:NH1	1:C:346:GLN:NE2	2.41	0.66
1:A:282:ARG:NH1	1:B:346:GLN:NE2	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:HE3	1:A:388:ILE:HD12	1.78	0.65
1:J:268:LEU:HD11	1:K:215:SER:HB2	1.78	0.65
1:E:445:SER:HB3	1:E:589:ILE:HD11	1.79	0.65
1:G:361:LEU:HD12	1:G:361:LEU:H	1.61	0.64
1:L:282:ARG:NH1	1:M:346:GLN:NE2	2.45	0.64
1:N:582:ASN:HB2	2:N:826:HOH:O	1.98	0.64
1:I:361:LEU:HD12	1:I:361:LEU:H	1.64	0.63
1:I:282:ARG:NH1	1:J:346:GLN:HE22	1.93	0.63
1:K:282:ARG:NH1	1:L:346:GLN:NE2	2.43	0.63
1:L:637:VAL:HG22	1:L:672:GLN:NE2	2.12	0.63
1:D:282:ARG:NH1	1:E:346:GLN:HE22	1.94	0.63
1:C:268:LEU:HD11	1:D:215:SER:HB2	1.80	0.62
1:C:361:LEU:HD12	1:C:361:LEU:H	1.64	0.62
1:M:282:ARG:NH1	1:N:346:GLN:NE2	2.47	0.62
1:A:637:VAL:HG22	1:A:672:GLN:NE2	2.15	0.61
1:A:625:LEU:HD12	1:I:601:ARG:HG2	1.81	0.61
1:H:161:ASN:HB3	1:H:231:PHE:CZ	2.36	0.61
1:A:346:GLN:NE2	1:G:282:ARG:HH11	1.94	0.61
1:M:361:LEU:H	1:M:361:LEU:HD12	1.63	0.61
1:N:213:ASP:OD1	1:N:384:LYS:NZ	2.31	0.61
1:C:137:ASN:H	1:C:137:ASN:ND2	1.99	0.60
1:D:161:ASN:HB3	1:D:231:PHE:CZ	2.36	0.60
1:F:629:GLY:HA2	1:F:705:ASP:O	2.01	0.60
1:I:161:ASN:HB3	1:I:231:PHE:CZ	2.36	0.60
1:M:268:LEU:HD11	1:N:215:SER:HB2	1.83	0.59
1:F:268:LEU:HD11	1:G:215:SER:HB2	1.82	0.59
1:K:629:GLY:HA2	1:K:705:ASP:O	2.02	0.59
1:A:361:LEU:HD12	1:A:361:LEU:H	1.67	0.59
1:K:361:LEU:HD12	1:K:361:LEU:H	1.66	0.59
1:J:629:GLY:HA2	1:J:705:ASP:O	2.03	0.59
1:E:465:LEU:HB3	1:E:552:HIS:CD2	2.37	0.58
1:A:346:GLN:NE2	1:G:282:ARG:NH1	2.50	0.58
1:M:273:VAL:HG13	2:M:839:HOH:O	2.02	0.58
1:N:629:GLY:HA2	1:N:705:ASP:O	2.02	0.58
1:G:617:ASP:HA	1:G:707:LEU:HD23	1.84	0.58
1:L:361:LEU:HD12	1:L:361:LEU:H	1.67	0.58
1:N:161:ASN:HB3	1:N:231:PHE:CZ	2.39	0.58
1:C:629:GLY:HA2	1:C:705:ASP:O	2.04	0.58
1:K:465:LEU:HB3	1:K:552:HIS:CD2	2.39	0.58
1:I:282:ARG:HH11	1:J:346:GLN:NE2	1.96	0.58
1:G:629:GLY:HA2	1:G:705:ASP:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:629:GLY:HA2	1:H:705:ASP:O	2.04	0.57
1:A:534:TRP:CE2	1:A:541:LEU:HD13	2.40	0.57
1:B:611:ARG:NH2	1:B:630:ASN:O	2.35	0.57
1:D:282:ARG:HH11	1:E:346:GLN:NE2	1.97	0.57
1:C:161:ASN:HB3	1:C:231:PHE:CZ	2.39	0.56
1:E:161:ASN:HB3	1:E:231:PHE:CZ	2.39	0.56
1:E:629:GLY:HA2	1:E:705:ASP:O	2.05	0.56
1:B:361:LEU:HD12	1:B:361:LEU:H	1.70	0.56
1:E:271:PHE:HA	1:E:272:PRO:C	2.26	0.56
1:K:617:ASP:HA	1:K:707:LEU:HD23	1.88	0.56
1:M:465:LEU:HB3	1:M:552:HIS:CD2	2.41	0.56
1:F:617:ASP:HA	1:F:707:LEU:HD23	1.88	0.56
1:N:361:LEU:HD12	1:N:361:LEU:H	1.69	0.56
1:E:190:ARG:HD2	1:E:455:PHE:O	2.06	0.56
1:F:465:LEU:HB3	1:F:552:HIS:CD2	2.41	0.56
1:I:190:ARG:HD2	1:I:455:PHE:O	2.06	0.56
1:J:161:ASN:HB3	1:J:231:PHE:CZ	2.41	0.56
1:J:271:PHE:HA	1:J:272:PRO:C	2.26	0.56
1:C:465:LEU:HB3	1:C:552:HIS:CD2	2.41	0.56
1:D:190:ARG:HD2	1:D:455:PHE:O	2.06	0.56
1:B:161:ASN:HB3	1:B:231:PHE:CZ	2.40	0.56
1:J:361:LEU:HD12	1:J:361:LEU:H	1.70	0.56
1:H:306:LYS:HA	1:N:296:VAL:O	2.06	0.55
1:B:361:LEU:CD2	1:B:418:LYS:HG2	2.36	0.55
1:B:629:GLY:HA2	1:B:705:ASP:O	2.07	0.55
1:F:161:ASN:HB3	1:F:231:PHE:CZ	2.41	0.55
1:B:271:PHE:HA	1:B:272:PRO:C	2.27	0.55
1:A:161:ASN:HB3	1:A:231:PHE:CZ	2.42	0.55
1:K:161:ASN:HB3	1:K:231:PHE:CZ	2.41	0.55
1:M:629:GLY:HA2	1:M:705:ASP:O	2.07	0.55
1:F:361:LEU:HD12	1:F:361:LEU:H	1.71	0.55
1:I:273:VAL:HG11	1:J:384:LYS:HZ1	1.72	0.55
1:I:282:ARG:NH1	1:J:346:GLN:NE2	2.54	0.55
1:N:465:LEU:HB3	1:N:552:HIS:CD2	2.42	0.55
1:D:282:ARG:NH1	1:E:346:GLN:NE2	2.54	0.55
1:M:161:ASN:HB3	1:M:231:PHE:CZ	2.41	0.55
1:C:421:TYR:N	1:C:421:TYR:CD2	2.74	0.54
1:I:629:GLY:HA2	1:I:705:ASP:O	2.08	0.54
1:I:534:TRP:CE2	1:I:541:LEU:HD13	2.42	0.54
1:G:465:LEU:HB3	1:G:552:HIS:CD2	2.42	0.54
1:A:380:SER:HB3	1:G:330:ARG:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:LEU:HB3	1:D:552:HIS:CD2	2.43	0.54
1:D:611:ARG:NH2	1:D:630:ASN:O	2.35	0.54
1:E:361:LEU:HD12	1:E:361:LEU:H	1.71	0.54
1:M:155:GLU:CD	1:M:682:ASN:H	2.11	0.54
1:L:347:TYR:HA	1:L:352:SER:OG	2.08	0.54
1:A:698:GLN:HB2	1:A:714:ASP:HB2	1.89	0.54
1:A:421:TYR:N	1:A:421:TYR:CD2	2.76	0.53
1:H:421:TYR:N	1:H:421:TYR:CD2	2.76	0.53
1:B:230:GLN:HG2	1:B:231:PHE:N	2.23	0.53
1:G:161:ASN:HB3	1:G:231:PHE:CZ	2.44	0.53
1:H:361:LEU:H	1:H:361:LEU:HD12	1.72	0.53
1:H:617:ASP:HA	1:H:707:LEU:HD23	1.90	0.53
1:J:190:ARG:HD2	1:J:455:PHE:O	2.08	0.53
1:B:190:ARG:HD2	1:B:455:PHE:O	2.08	0.53
1:F:421:TYR:N	1:F:421:TYR:CD2	2.76	0.53
1:D:271:PHE:HA	1:D:272:PRO:C	2.29	0.53
1:M:611:ARG:NH2	1:M:630:ASN:O	2.38	0.53
1:B:421:TYR:CD2	1:B:421:TYR:N	2.77	0.53
1:D:629:GLY:HA2	1:D:705:ASP:O	2.08	0.53
1:D:230:GLN:HG2	1:D:231:PHE:N	2.24	0.53
1:B:629:GLY:HA3	1:B:706:TRP:O	2.07	0.52
1:M:142:VAL:HB	1:M:188:LEU:HB2	1.91	0.52
1:N:421:TYR:N	1:N:421:TYR:CD2	2.77	0.52
1:N:617:ASP:HA	1:N:707:LEU:HD23	1.90	0.52
1:J:465:LEU:HB3	1:J:552:HIS:CD2	2.45	0.52
1:M:421:TYR:N	1:M:421:TYR:CD2	2.78	0.52
1:A:213:ASP:OD1	1:A:384:LYS:NZ	2.36	0.52
1:F:271:PHE:HA	1:F:272:PRO:C	2.30	0.52
1:K:421:TYR:N	1:K:421:TYR:CD2	2.77	0.52
1:I:271:PHE:HA	1:I:272:PRO:C	2.29	0.52
1:L:698:GLN:HB2	1:L:714:ASP:HB2	1.91	0.52
1:M:617:ASP:HA	1:M:707:LEU:HD23	1.92	0.52
1:C:525:ASN:HB2	2:D:810:HOH:O	2.07	0.52
1:G:230:GLN:HG2	1:G:231:PHE:N	2.24	0.52
1:H:271:PHE:HA	1:H:272:PRO:C	2.29	0.52
1:A:465:LEU:HB3	1:A:552:HIS:CD2	2.45	0.52
1:A:617:ASP:OD1	1:A:631:GLY:HA3	2.09	0.52
1:B:617:ASP:HA	1:B:707:LEU:HD23	1.91	0.52
1:H:465:LEU:HB3	1:H:552:HIS:CD2	2.44	0.52
1:N:271:PHE:HA	1:N:272:PRO:C	2.30	0.52
1:C:629:GLY:HA3	1:C:706:TRP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:611:ARG:NH2	1:H:630:ASN:O	2.37	0.52
1:L:529:THR:HG23	1:M:469:ASN:OD1	2.10	0.52
1:C:230:GLN:HG2	1:C:231:PHE:N	2.25	0.52
1:J:421:TYR:CD2	1:J:421:TYR:N	2.78	0.52
1:K:534:TRP:CE2	1:K:541:LEU:HD13	2.44	0.52
1:E:617:ASP:HA	1:E:707:LEU:HD23	1.92	0.51
1:L:608:LEU:HB2	1:L:639:LEU:HD11	1.91	0.51
1:M:271:PHE:HA	1:M:272:PRO:C	2.30	0.51
1:L:161:ASN:HB3	1:L:231:PHE:CZ	2.45	0.51
1:A:271:PHE:HA	1:A:272:PRO:C	2.29	0.51
1:K:190:ARG:HD2	1:K:455:PHE:O	2.11	0.51
1:M:230:GLN:HG2	1:M:231:PHE:N	2.26	0.51
1:C:534:TRP:CE2	1:C:541:LEU:HD13	2.45	0.51
1:D:421:TYR:N	1:D:421:TYR:CD2	2.78	0.51
1:C:617:ASP:HA	1:C:707:LEU:HD23	1.93	0.51
1:J:213:ASP:OD1	1:J:384:LYS:NZ	2.36	0.51
1:K:271:PHE:HA	1:K:272:PRO:C	2.30	0.51
1:A:625:LEU:CD1	1:I:601:ARG:HG2	2.41	0.51
1:J:617:ASP:HA	1:J:707:LEU:HD23	1.92	0.51
1:D:617:ASP:HA	1:D:707:LEU:HD23	1.93	0.51
1:J:629:GLY:HA3	1:J:706:TRP:O	2.11	0.51
1:M:700:LYS:HB2	1:M:712:GLN:HB3	1.93	0.51
1:L:421:TYR:CD2	1:L:421:TYR:N	2.78	0.51
1:L:590:LEU:HB3	1:L:647:ALA:CB	2.41	0.51
1:I:511:LEU:HB3	1:I:521:LEU:HB3	1.93	0.50
1:G:190:ARG:HD2	1:G:455:PHE:O	2.12	0.50
1:A:247:THR:HB	1:A:412:ILE:HB	1.94	0.50
1:M:529:THR:HG23	1:N:469:ASN:OD1	2.12	0.50
1:N:256:PHE:CZ	1:N:383:PRO:HG3	2.46	0.50
1:A:230:GLN:HG2	1:A:231:PHE:N	2.26	0.50
1:B:155:GLU:CD	1:B:682:ASN:H	2.14	0.50
1:B:465:LEU:HB3	1:B:552:HIS:CD2	2.47	0.50
1:I:347:TYR:HA	1:I:352:SER:OG	2.10	0.50
1:C:190:ARG:HD2	1:C:455:PHE:O	2.11	0.50
1:I:421:TYR:N	1:I:421:TYR:CD2	2.79	0.50
1:L:465:LEU:HB3	1:L:552:HIS:CD2	2.46	0.50
1:F:611:ARG:O	1:F:617:ASP:HB2	2.11	0.50
1:I:330:ARG:O	1:J:380:SER:HB3	2.11	0.50
1:N:190:ARG:HD2	1:N:455:PHE:O	2.12	0.50
1:D:629:GLY:HA3	1:D:706:TRP:O	2.12	0.50
1:G:347:TYR:HA	1:G:352:SER:OG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:GLN:HG2	1:I:231:PHE:N	2.26	0.50
1:L:190:ARG:HD2	1:L:455:PHE:O	2.12	0.49
1:G:629:GLY:HA3	1:G:706:TRP:O	2.12	0.49
1:C:611:ARG:O	1:C:617:ASP:HB2	2.12	0.49
1:E:700:LYS:HB2	1:E:712:GLN:HB3	1.94	0.49
1:I:629:GLY:HA3	1:I:706:TRP:O	2.12	0.49
1:J:611:ARG:NH2	1:J:630:ASN:O	2.37	0.49
1:E:421:TYR:N	1:E:421:TYR:CD2	2.80	0.49
1:F:700:LYS:HB2	1:F:712:GLN:HB3	1.95	0.49
1:I:617:ASP:HA	1:I:707:LEU:HD23	1.94	0.49
1:J:230:GLN:HG2	1:J:231:PHE:N	2.26	0.49
1:G:421:TYR:CD2	1:G:421:TYR:N	2.80	0.49
1:A:673:THR:HG22	1:A:674:VAL:N	2.27	0.49
1:K:230:GLN:HG2	1:K:231:PHE:N	2.27	0.49
1:K:142:VAL:HB	1:K:188:LEU:HB2	1.95	0.49
1:N:629:GLY:HA3	1:N:706:TRP:O	2.12	0.49
1:D:611:ARG:O	1:D:617:ASP:HB2	2.12	0.49
1:G:271:PHE:HA	1:G:272:PRO:C	2.33	0.49
1:N:230:GLN:HG2	1:N:231:PHE:N	2.27	0.49
1:E:629:GLY:HA3	1:E:706:TRP:O	2.12	0.49
1:H:230:GLN:HG2	1:H:231:PHE:N	2.28	0.49
1:E:611:ARG:NH2	1:E:630:ASN:O	2.37	0.49
1:L:213:ASP:OD1	1:L:384:LYS:NZ	2.41	0.49
1:C:271:PHE:HA	1:C:272:PRO:C	2.32	0.48
1:D:247:THR:HB	1:D:412:ILE:HB	1.94	0.48
1:E:690:LEU:N	1:E:690:LEU:HD12	2.28	0.48
1:L:673:THR:HG22	1:L:674:VAL:N	2.27	0.48
1:N:175:CYS:HA	1:N:223:ASN:OD1	2.13	0.48
1:G:690:LEU:N	1:G:690:LEU:HD12	2.28	0.48
1:K:629:GLY:HA3	1:K:706:TRP:O	2.13	0.48
1:G:360:ALA:O	1:G:363:VAL:HG23	2.13	0.48
1:J:347:TYR:HA	1:J:352:SER:OG	2.13	0.48
1:K:480:ARG:HH11	1:K:480:ARG:CB	2.10	0.48
1:M:525:ASN:HB2	2:M:831:HOH:O	2.13	0.48
1:B:534:TRP:CE2	1:B:541:LEU:HD13	2.47	0.48
1:D:161:ASN:HB3	1:D:231:PHE:CE2	2.49	0.48
1:I:690:LEU:N	1:I:690:LEU:HD12	2.28	0.48
1:L:271:PHE:HA	1:L:272:PRO:C	2.33	0.48
1:F:534:TRP:CE2	1:F:541:LEU:HD13	2.48	0.48
1:L:202:PRO:HB2	1:M:145:TYR:CE1	2.49	0.48
1:L:534:TRP:CE2	1:L:541:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:GLN:HG2	1:F:231:PHE:N	2.28	0.48
1:H:213:ASP:OD1	1:H:384:LYS:NZ	2.36	0.48
1:N:690:LEU:N	1:N:690:LEU:HD12	2.28	0.48
1:J:257:VAL:HB	1:J:404:ASP:HB2	1.95	0.48
1:K:296:VAL:O	1:L:306:LYS:HA	2.14	0.48
1:L:617:ASP:OD1	1:L:631:GLY:HA3	2.13	0.48
1:K:347:TYR:HA	1:K:352:SER:OG	2.14	0.48
1:G:700:LYS:HB2	1:G:712:GLN:HB3	1.95	0.48
1:F:202:PRO:HB2	1:G:145:TYR:CE1	2.49	0.47
1:I:269:LYS:HD3	1:J:213:ASP:O	2.14	0.47
1:M:213:ASP:OD1	1:M:384:LYS:NZ	2.37	0.47
1:C:208:ARG:NH1	2:C:835:HOH:O	2.40	0.47
1:L:230:GLN:HG2	1:L:231:PHE:N	2.28	0.47
1:B:512:CYS:HB3	2:B:823:HOH:O	2.15	0.47
1:F:190:ARG:HD2	1:F:455:PHE:O	2.14	0.47
1:F:629:GLY:HA3	1:F:706:TRP:O	2.14	0.47
1:I:611:ARG:NH2	1:I:630:ASN:O	2.40	0.47
1:L:715:LEU:O	1:L:716:ASN:O	2.32	0.47
1:F:690:LEU:HD12	1:F:690:LEU:N	2.29	0.47
1:B:634:LEU:C	1:B:634:LEU:HD23	2.35	0.47
1:E:142:VAL:HB	1:E:188:LEU:HB2	1.96	0.47
1:K:202:PRO:HB2	1:L:145:TYR:CE1	2.49	0.47
1:K:480:ARG:HB3	1:K:480:ARG:NH1	2.07	0.47
1:A:384:LYS:HZ1	1:G:273:VAL:HG11	1.80	0.47
1:C:529:THR:HG23	1:D:469:ASN:OD1	2.14	0.47
1:H:190:ARG:HD2	1:H:455:PHE:O	2.14	0.47
1:L:590:LEU:HB3	1:L:647:ALA:HB2	1.95	0.47
1:A:213:ASP:O	1:G:269:LYS:HD3	2.15	0.47
1:M:534:TRP:CE2	1:M:541:LEU:HD13	2.50	0.47
1:H:629:GLY:HA3	1:H:706:TRP:O	2.14	0.47
1:I:256:PHE:CZ	1:I:383:PRO:HG3	2.50	0.47
1:K:366:TYR:HA	1:K:367:PRO:HD3	1.77	0.47
1:M:256:PHE:CZ	1:M:383:PRO:HG3	2.50	0.47
1:M:629:GLY:HA3	1:M:706:TRP:O	2.14	0.47
1:G:534:TRP:CE2	1:G:541:LEU:HD13	2.50	0.47
1:L:629:GLY:HA2	1:L:705:ASP:O	2.15	0.47
1:C:202:PRO:HB2	1:D:145:TYR:CE1	2.50	0.46
1:D:534:TRP:CE2	1:D:541:LEU:HD13	2.50	0.46
1:I:161:ASN:HB3	1:I:231:PHE:CE2	2.50	0.46
1:J:611:ARG:O	1:J:617:ASP:HB2	2.15	0.46
1:E:257:VAL:HB	1:E:404:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:534:TRP:CE2	1:J:541:LEU:HD13	2.50	0.46
1:K:269:LYS:HD3	1:L:213:ASP:O	2.16	0.46
1:M:247:THR:HB	1:M:412:ILE:HB	1.97	0.46
1:A:715:LEU:O	1:A:716:ASN:O	2.34	0.46
1:E:230:GLN:HG2	1:E:231:PHE:N	2.30	0.46
1:F:511:LEU:HB3	1:F:521:LEU:HB3	1.96	0.46
1:I:283:LYS:HG3	1:J:320:THR:HG23	1.97	0.46
1:I:465:LEU:HB3	1:I:552:HIS:CD2	2.50	0.46
1:M:528:LEU:HG	1:N:469:ASN:O	2.15	0.46
1:E:221:HIS:CE1	1:E:223:ASN:O	2.69	0.46
1:H:475:VAL:CG2	1:H:479:GLY:HA2	2.46	0.46
1:L:269:LYS:HD3	1:M:213:ASP:O	2.15	0.46
1:M:611:ARG:O	1:M:617:ASP:HB2	2.15	0.46
1:B:202:PRO:HB2	1:C:145:TYR:CE1	2.50	0.46
1:I:289:GLU:HA	1:J:313:TYR:O	2.16	0.46
1:M:634:LEU:C	1:M:634:LEU:HD23	2.36	0.46
1:A:142:VAL:HB	1:A:188:LEU:HB2	1.97	0.46
1:J:690:LEU:N	1:J:690:LEU:HD12	2.31	0.46
1:A:529:THR:HG23	1:B:469:ASN:OD1	2.15	0.46
1:D:269:LYS:HD3	1:E:213:ASP:O	2.15	0.46
1:E:256:PHE:CZ	1:E:383:PRO:HG3	2.50	0.46
1:H:534:TRP:CE2	1:H:541:LEU:HD13	2.51	0.46
1:I:247:THR:HB	1:I:412:ILE:HB	1.98	0.46
1:J:445:SER:HB3	1:J:589:ILE:HD11	1.98	0.46
1:N:347:TYR:HA	1:N:352:SER:OG	2.15	0.46
1:G:242:PHE:CD2	1:G:243:ARG:HG3	2.51	0.46
1:M:445:SER:HB3	1:M:589:ILE:HD11	1.97	0.46
1:M:330:ARG:O	1:N:380:SER:HB3	2.16	0.46
1:B:511:LEU:HB3	1:B:521:LEU:HB3	1.98	0.45
1:C:690:LEU:HD12	1:C:690:LEU:N	2.30	0.45
1:D:511:LEU:HB3	1:D:521:LEU:HB3	1.98	0.45
1:B:445:SER:HB3	1:B:589:ILE:HD11	1.98	0.45
1:C:511:LEU:HB3	1:C:521:LEU:HB3	1.99	0.45
1:H:634:LEU:C	1:H:634:LEU:HD23	2.37	0.45
1:B:690:LEU:N	1:B:690:LEU:HD12	2.31	0.45
1:G:360:ALA:HB1	1:G:362:TRP:CZ3	2.52	0.45
1:I:616:ILE:HG22	1:I:708:VAL:HB	1.99	0.45
1:M:698:GLN:HB2	1:M:714:ASP:HB2	1.99	0.45
1:K:616:ILE:HG22	1:K:708:VAL:HB	1.98	0.45
1:A:590:LEU:HB3	1:A:647:ALA:CB	2.46	0.45
1:B:289:GLU:O	1:B:290:LEU:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:TYR:HA	1:D:352:SER:OG	2.16	0.45
1:I:475:VAL:CG2	1:I:479:GLY:HA2	2.46	0.45
1:N:193:GLN:HB2	1:N:196:ILE:HD12	1.99	0.45
1:F:347:TYR:HA	1:F:352:SER:OG	2.15	0.45
1:J:700:LYS:HB2	1:J:712:GLN:HB3	1.99	0.45
1:E:268:LEU:CD1	1:F:215:SER:HB2	2.43	0.45
1:H:161:ASN:HB3	1:H:231:PHE:CE2	2.52	0.45
1:L:511:LEU:HB3	1:L:521:LEU:HB3	1.99	0.45
1:C:366:TYR:HA	1:C:367:PRO:HD3	1.83	0.45
1:C:221:HIS:CE1	1:C:223:ASN:O	2.69	0.45
1:H:690:LEU:HD12	1:H:690:LEU:N	2.32	0.45
1:H:700:LYS:HB2	1:H:712:GLN:HB3	1.99	0.45
1:L:142:VAL:HB	1:L:188:LEU:HB2	1.99	0.45
1:N:289:GLU:O	1:N:290:LEU:HD12	2.17	0.45
1:A:629:GLY:HA2	1:A:705:ASP:O	2.17	0.45
1:H:616:ILE:HG22	1:H:708:VAL:HB	1.99	0.45
1:K:528:LEU:HD13	1:L:574:ILE:HD12	1.99	0.45
1:K:690:LEU:HD12	1:K:690:LEU:N	2.32	0.45
1:K:700:LYS:HB2	1:K:712:GLN:HB3	1.98	0.45
1:M:690:LEU:HD12	1:M:690:LEU:N	2.32	0.45
1:A:347:TYR:HA	1:A:352:SER:OG	2.17	0.44
1:C:664:PHE:CD1	1:C:664:PHE:N	2.85	0.44
1:D:361:LEU:HD12	1:D:361:LEU:N	2.29	0.44
1:J:511:LEU:HB3	1:J:521:LEU:HB3	1.99	0.44
1:K:230:GLN:NE2	1:K:243:ARG:HD3	2.33	0.44
1:K:611:ARG:O	1:K:617:ASP:HB2	2.17	0.44
1:L:703:ALA:CB	1:L:708:VAL:HA	2.48	0.44
1:M:257:VAL:HB	1:M:404:ASP:HB2	2.00	0.44
1:N:611:ARG:O	1:N:617:ASP:HB2	2.18	0.44
1:A:413:TYR:HD1	1:A:435:THR:HG21	1.82	0.44
1:A:469:ASN:OD1	1:G:529:THR:HG23	2.17	0.44
1:E:346:GLN:HE21	1:E:346:GLN:HB2	1.55	0.44
1:F:447:THR:N	2:F:810:HOH:O	2.39	0.44
1:G:247:THR:HB	1:G:412:ILE:HB	2.00	0.44
1:I:240:ALA:HA	1:I:417:TYR:CE1	2.52	0.44
1:J:242:PHE:CD2	1:J:243:ARG:HG3	2.52	0.44
1:M:460:PRO:HG2	1:M:580:VAL:HG21	2.00	0.44
1:A:511:LEU:HB3	1:A:521:LEU:HB3	1.98	0.44
1:D:202:PRO:HB2	1:E:145:TYR:CE1	2.52	0.44
1:G:285:VAL:HG12	1:G:286:SER:N	2.32	0.44
1:C:242:PHE:CD2	1:C:243:ARG:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:475:VAL:CG2	1:K:479:GLY:HA2	2.47	0.44
1:M:347:TYR:HA	1:M:352:SER:OG	2.18	0.44
1:A:202:PRO:HB2	1:B:145:TYR:CE1	2.52	0.44
1:E:347:TYR:HA	1:E:352:SER:OG	2.17	0.44
1:H:511:LEU:HB3	1:H:521:LEU:HB3	2.00	0.44
1:J:184:TYR:HA	1:J:211:LEU:HD23	2.00	0.44
1:J:698:GLN:HB2	1:J:714:ASP:HB2	2.00	0.44
1:B:213:ASP:OD1	1:B:384:LYS:NZ	2.42	0.44
1:L:703:ALA:HB2	1:L:708:VAL:HA	1.99	0.44
1:A:629:GLY:HA3	1:A:706:TRP:O	2.17	0.44
1:C:347:TYR:HA	1:C:352:SER:OG	2.17	0.44
1:F:552:HIS:CE1	1:F:570:SER:HB3	2.53	0.44
1:I:242:PHE:CD2	1:I:243:ARG:HG3	2.53	0.44
1:N:700:LYS:HB2	1:N:712:GLN:HB3	1.98	0.44
1:B:256:PHE:CZ	1:B:383:PRO:HG3	2.53	0.44
1:D:184:TYR:HA	1:D:211:LEU:HD23	2.00	0.44
1:D:242:PHE:CD2	1:D:243:ARG:HG3	2.53	0.44
1:H:460:PRO:HG2	1:H:580:VAL:HG21	2.00	0.44
1:H:698:GLN:HB2	1:H:714:ASP:HB2	2.00	0.44
1:A:190:ARG:HD2	1:A:455:PHE:O	2.18	0.43
1:A:221:HIS:HB2	1:G:332:ALA:O	2.18	0.43
1:B:611:ARG:O	1:B:617:ASP:HB2	2.17	0.43
1:L:256:PHE:CZ	1:L:383:PRO:HG3	2.53	0.43
1:N:247:THR:HB	1:N:412:ILE:HB	1.98	0.43
1:N:459:ARG:HA	1:N:460:PRO:HD3	1.87	0.43
1:B:700:LYS:HB2	1:B:712:GLN:HB3	1.99	0.43
1:C:296:VAL:O	1:D:306:LYS:HA	2.18	0.43
1:H:184:TYR:HA	1:H:211:LEU:HD23	2.00	0.43
1:M:289:GLU:HA	1:N:313:TYR:O	2.17	0.43
1:A:256:PHE:CZ	1:A:383:PRO:HG3	2.53	0.43
1:F:698:GLN:HB2	1:F:714:ASP:HB2	2.00	0.43
1:K:511:LEU:HB3	1:K:521:LEU:HB3	2.01	0.43
1:K:528:LEU:CD1	1:L:574:ILE:HD12	2.49	0.43
1:M:366:TYR:HA	1:M:367:PRO:HD3	1.78	0.43
1:M:528:LEU:HD21	1:N:464:GLN:NE2	2.33	0.43
1:L:629:GLY:HA3	1:L:706:TRP:O	2.18	0.43
1:B:698:GLN:HB2	1:B:714:ASP:HB2	2.01	0.43
1:G:611:ARG:O	1:G:617:ASP:HB2	2.18	0.43
1:B:257:VAL:HB	1:B:404:ASP:HB2	2.01	0.43
1:G:366:TYR:HA	1:G:367:PRO:HD3	1.80	0.43
1:K:460:PRO:HG2	1:K:580:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:HB	1:B:188:LEU:HB2	2.00	0.43
1:F:242:PHE:CD2	1:F:243:ARG:HG3	2.54	0.43
1:L:366:TYR:HA	1:L:367:PRO:HD3	1.77	0.43
1:A:190:ARG:NE	2:A:838:HOH:O	2.52	0.43
1:C:256:PHE:CZ	1:C:383:PRO:HG3	2.54	0.43
1:D:466:ALA:HB3	1:D:572:ARG:HG2	2.01	0.43
1:D:512:CYS:HB3	2:D:830:HOH:O	2.18	0.43
1:E:247:THR:HB	1:E:412:ILE:HB	2.01	0.43
1:F:616:ILE:HG22	1:F:708:VAL:HB	2.01	0.43
1:M:294:GLY:N	1:N:309:ALA:O	2.46	0.43
1:M:361:LEU:HD12	1:M:361:LEU:N	2.33	0.43
1:N:534:TRP:CE2	1:N:541:LEU:HD13	2.53	0.43
1:A:366:TYR:HA	1:A:367:PRO:HD3	1.81	0.43
1:G:698:GLN:HB2	1:G:714:ASP:HB2	2.00	0.43
1:I:597:MET:HG3	1:I:702:TRP:CE2	2.54	0.43
1:I:700:LYS:HB2	1:I:712:GLN:HB3	2.00	0.43
1:D:330:ARG:O	1:E:380:SER:HB3	2.19	0.43
1:N:313:TYR:OH	1:N:315:GLN:NE2	2.52	0.43
1:C:698:GLN:HB2	1:C:714:ASP:HB2	2.01	0.42
1:C:700:LYS:HB2	1:C:712:GLN:HB3	2.00	0.42
1:D:152:ILE:HB	1:D:178:ALA:HB3	2.01	0.42
1:F:385:MET:HE3	1:F:385:MET:HB3	1.91	0.42
1:L:271:PHE:HB3	1:L:386:ASP:HB2	2.01	0.42
1:L:460:PRO:HG2	1:L:580:VAL:HG21	2.01	0.42
1:D:271:PHE:HB3	1:D:386:ASP:HB2	2.00	0.42
1:D:452:HIS:ND1	1:D:453:PRO:HD2	2.34	0.42
1:F:139:LEU:HA	1:F:140:PRO:HD3	1.85	0.42
1:G:257:VAL:HB	1:G:404:ASP:HB2	2.01	0.42
1:I:566:ASN:HB3	2:I:816:HOH:O	2.18	0.42
1:L:257:VAL:HB	1:L:404:ASP:HB2	2.01	0.42
1:H:347:TYR:HA	1:H:352:SER:OG	2.20	0.42
1:J:256:PHE:CZ	1:J:383:PRO:HG3	2.54	0.42
1:K:298:VAL:O	1:L:304:LYS:HA	2.19	0.42
1:N:698:GLN:HB2	1:N:714:ASP:HB2	2.02	0.42
1:G:634:LEU:C	1:G:634:LEU:HD23	2.40	0.42
1:H:526:GLN:HB2	1:I:486:CYS:HB2	2.00	0.42
1:I:452:HIS:ND1	1:I:453:PRO:HD2	2.34	0.42
1:J:634:LEU:C	1:J:634:LEU:HD23	2.40	0.42
1:M:290:LEU:O	1:N:313:TYR:N	2.45	0.42
1:C:247:THR:HB	1:C:412:ILE:HB	2.01	0.42
1:D:142:VAL:HB	1:D:188:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:PHE:CZ	1:F:383:PRO:HG3	2.54	0.42
1:G:597:MET:HG3	1:G:702:TRP:CE2	2.54	0.42
1:H:257:VAL:HB	1:H:404:ASP:HB2	2.00	0.42
1:J:202:PRO:HB2	1:K:145:TYR:CE1	2.54	0.42
1:D:230:GLN:NE2	1:D:243:ARG:HD3	2.35	0.42
1:D:360:ALA:HB1	1:D:362:TRP:CZ3	2.55	0.42
1:E:698:GLN:HB2	1:E:714:ASP:HB2	2.02	0.42
1:G:161:ASN:HB3	1:G:231:PHE:CE2	2.55	0.42
1:I:401:PHE:O	1:I:445:SER:HA	2.19	0.42
1:N:230:GLN:NE2	1:N:243:ARG:HD3	2.34	0.42
1:N:242:PHE:CD2	1:N:243:ARG:HG3	2.54	0.42
1:A:145:TYR:CE1	1:G:202:PRO:HB2	2.54	0.42
1:H:142:VAL:HB	1:H:188:LEU:HB2	2.02	0.42
1:J:152:ILE:HB	1:J:178:ALA:HB3	2.02	0.42
1:J:459:ARG:HA	1:J:460:PRO:HD3	1.82	0.42
1:K:360:ALA:HB1	1:K:362:TRP:CZ3	2.55	0.42
1:K:698:GLN:HB2	1:K:714:ASP:HB2	2.00	0.42
1:E:511:LEU:HB3	1:E:521:LEU:HB3	2.02	0.42
1:F:142:VAL:HB	1:F:188:LEU:HB2	2.01	0.42
1:K:193:GLN:HB2	1:K:196:ILE:HD12	2.02	0.42
1:L:197:VAL:HG13	1:M:581:PHE:HD2	1.84	0.42
1:A:587:SER:HB2	1:A:712:GLN:HG2	2.01	0.42
1:G:271:PHE:HB3	1:G:386:ASP:HB2	2.02	0.42
1:H:308:GLU:HA	1:N:294:GLY:O	2.20	0.42
1:H:469:ASN:OD1	1:N:529:THR:HG23	2.20	0.42
1:K:401:PHE:O	1:K:445:SER:HA	2.20	0.42
1:B:161:ASN:HB3	1:B:231:PHE:CE2	2.54	0.42
1:B:385:MET:HE3	1:B:385:MET:HB3	1.90	0.42
1:E:366:TYR:HA	1:E:367:PRO:HD3	1.78	0.42
1:L:611:ARG:NH1	1:L:630:ASN:HA	2.35	0.42
1:M:298:VAL:O	1:M:298:VAL:HG13	2.19	0.42
1:B:354:LEU:HD21	1:B:414:ASN:HD22	1.84	0.41
1:G:475:VAL:CG2	1:G:479:GLY:HA2	2.50	0.41
1:L:597:MET:HB2	1:L:702:TRP:CD1	2.54	0.41
1:B:346:GLN:HE21	1:B:346:GLN:HB2	1.65	0.41
1:C:257:VAL:HB	1:C:404:ASP:HB2	2.01	0.41
1:C:360:ALA:HB1	1:C:362:TRP:CZ3	2.54	0.41
1:D:366:TYR:HA	1:D:367:PRO:HD3	1.77	0.41
1:F:247:THR:HB	1:F:412:ILE:HB	2.02	0.41
1:F:475:VAL:CG2	1:F:479:GLY:HA2	2.49	0.41
1:H:202:PRO:HB2	1:I:145:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:269:LYS:HD3	1:I:213:ASP:O	2.20	0.41
1:I:529:THR:HG23	1:J:469:ASN:OD1	2.21	0.41
1:K:213:ASP:OD1	1:K:384:LYS:NZ	2.37	0.41
1:L:242:PHE:CD2	1:L:243:ARG:HG3	2.55	0.41
1:L:267:ILE:HG13	1:L:389:TYR:CE1	2.55	0.41
1:A:680:VAL:O	1:A:680:VAL:HG13	2.20	0.41
1:J:460:PRO:HG2	1:J:580:VAL:HG21	2.03	0.41
1:M:511:LEU:HB3	1:M:521:LEU:HB3	2.01	0.41
1:N:366:TYR:HA	1:N:367:PRO:HD3	1.80	0.41
1:C:161:ASN:HB3	1:C:231:PHE:CE2	2.55	0.41
1:D:475:VAL:CG2	1:D:479:GLY:HA2	2.50	0.41
1:D:597:MET:HG3	1:D:702:TRP:CE2	2.56	0.41
1:D:616:ILE:HG22	1:D:708:VAL:HB	2.02	0.41
1:D:690:LEU:HD12	1:D:690:LEU:N	2.35	0.41
1:E:242:PHE:CD2	1:E:243:ARG:HG3	2.56	0.41
1:E:562:TYR:CE2	1:E:569:VAL:HG21	2.55	0.41
1:K:247:THR:HB	1:K:412:ILE:HB	2.02	0.41
1:K:313:TYR:OH	1:K:315:GLN:NE2	2.53	0.41
1:A:607:ARG:NE	1:A:636:SER:OG	2.51	0.41
1:K:267:ILE:O	1:L:217:GLY:HA2	2.20	0.41
1:L:401:PHE:O	1:L:445:SER:HA	2.19	0.41
1:M:410:ARG:HA	1:M:411:PRO:HD2	1.97	0.41
1:D:175:CYS:HA	1:D:223:ASN:OD1	2.19	0.41
1:D:475:VAL:HG23	1:D:479:GLY:HA2	2.02	0.41
1:E:534:TRP:CE2	1:E:541:LEU:HD13	2.55	0.41
1:G:175:CYS:HA	1:G:223:ASN:OD1	2.20	0.41
1:G:230:GLN:NE2	1:G:243:ARG:HD3	2.34	0.41
1:G:361:LEU:HD12	1:G:361:LEU:N	2.34	0.41
1:H:475:VAL:HG23	1:H:479:GLY:HA2	2.03	0.41
1:M:152:ILE:HB	1:M:178:ALA:HB3	2.03	0.41
1:C:361:LEU:HD12	1:C:361:LEU:N	2.34	0.41
1:D:256:PHE:CZ	1:D:383:PRO:HG3	2.56	0.41
1:G:382:VAL:HA	1:G:383:PRO:HD3	1.88	0.41
1:I:475:VAL:HG23	1:I:479:GLY:HA2	2.03	0.41
1:K:466:ALA:HB3	1:K:572:ARG:HG2	2.02	0.41
1:M:475:VAL:CG2	1:M:479:GLY:HA2	2.50	0.41
1:A:410:ARG:HA	1:A:411:PRO:HD2	1.99	0.41
1:A:673:THR:CG2	1:A:674:VAL:N	2.84	0.41
1:B:475:VAL:CG2	1:B:479:GLY:HA2	2.51	0.41
1:E:634:LEU:C	1:E:634:LEU:HD23	2.40	0.41
1:G:587:SER:HA	1:G:588:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:528:LEU:HG	1:J:469:ASN:O	2.21	0.41
1:K:252:GLN:O	1:K:344:ARG:HG3	2.21	0.41
1:A:242:PHE:CD2	1:A:243:ARG:HG3	2.56	0.41
1:B:347:TYR:HA	1:B:352:SER:OG	2.20	0.41
1:C:175:CYS:HA	1:C:223:ASN:OD1	2.21	0.41
1:D:401:PHE:O	1:D:445:SER:HA	2.21	0.41
1:D:698:GLN:HB2	1:D:714:ASP:HB2	2.03	0.41
1:F:161:ASN:HB3	1:F:231:PHE:CE2	2.56	0.41
1:G:460:PRO:HG2	1:G:580:VAL:HG21	2.02	0.41
1:H:289:GLU:O	1:H:290:LEU:HD12	2.21	0.41
1:H:529:THR:HG23	1:I:469:ASN:OD1	2.21	0.41
1:I:280:PHE:O	1:J:322:ASN:HA	2.20	0.41
1:K:242:PHE:CD2	1:K:243:ARG:HG3	2.56	0.41
1:K:346:GLN:HE21	1:K:346:GLN:HB2	1.54	0.41
1:L:360:ALA:O	1:L:363:VAL:HG23	2.21	0.41
1:M:242:PHE:CD2	1:M:243:ARG:HG3	2.55	0.41
1:B:175:CYS:HA	1:B:223:ASN:OD1	2.21	0.41
1:B:616:ILE:HG22	1:B:708:VAL:HB	2.03	0.41
1:E:606:ASN:ND2	1:E:640:SER:HB3	2.36	0.41
1:G:664:PHE:CD1	1:G:664:PHE:N	2.89	0.41
1:H:366:TYR:HA	1:H:367:PRO:HD3	1.80	0.41
1:M:606:ASN:ND2	1:M:640:SER:HB3	2.36	0.41
1:N:346:GLN:HE21	1:N:346:GLN:HB2	1.57	0.41
1:N:616:ILE:HG22	1:N:708:VAL:HB	2.03	0.41
1:N:634:LEU:HD23	1:N:634:LEU:C	2.42	0.41
1:A:285:VAL:HG12	1:A:286:SER:N	2.37	0.40
1:A:360:ALA:HB1	1:A:362:TRP:CZ3	2.56	0.40
1:F:230:GLN:NE2	1:F:243:ARG:HD3	2.36	0.40
1:H:145:TYR:CE1	1:N:202:PRO:HB2	2.56	0.40
1:I:634:LEU:C	1:I:634:LEU:HD23	2.41	0.40
1:L:673:THR:CG2	1:L:674:VAL:N	2.84	0.40
1:A:475:VAL:CG2	1:A:479:GLY:HA2	2.50	0.40
1:D:257:VAL:HB	1:D:404:ASP:HB2	2.02	0.40
1:H:366:TYR:CZ	1:H:368:VAL:HB	2.56	0.40
1:J:261:SER:HB3	1:J:400:ASP:HB2	2.04	0.40
1:K:529:THR:HG23	1:L:469:ASN:OD1	2.21	0.40
1:N:382:VAL:HA	1:N:383:PRO:HD3	1.89	0.40
1:N:460:PRO:HG2	1:N:580:VAL:HG21	2.03	0.40
1:N:511:LEU:HB3	1:N:521:LEU:HB3	2.03	0.40
1:F:346:GLN:HE21	1:F:346:GLN:HB2	1.50	0.40
1:L:466:ALA:HB3	1:L:572:ARG:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:535:ARG:NH1	1:L:540:GLU:OE1	2.55	0.40
1:M:283:LYS:HG3	1:N:320:THR:HG23	2.02	0.40
1:C:466:ALA:HB3	1:C:572:ARG:HG2	2.03	0.40
1:E:360:ALA:HB1	1:E:362:TRP:CZ3	2.56	0.40
1:F:535:ARG:NH1	1:F:540:GLU:OE1	2.54	0.40
1:H:271:PHE:HB3	1:H:386:ASP:HB2	2.03	0.40
1:K:139:LEU:HA	1:K:140:PRO:HD3	1.87	0.40
1:L:139:LEU:HA	1:L:140:PRO:HD3	1.82	0.40
1:L:657:GLN:C	1:L:658:GLN:HG2	2.41	0.40
1:A:590:LEU:HB3	1:A:647:ALA:HB2	2.03	0.40
1:B:366:TYR:HA	1:B:367:PRO:HD3	1.77	0.40
1:F:271:PHE:HB3	1:F:386:ASP:HB2	2.04	0.40
1:G:615:ALA:HB2	1:G:652:PHE:CE1	2.56	0.40
1:L:526:GLN:HB2	1:M:486:CYS:HB2	2.02	0.40
1:N:151:ALA:HA	1:N:179:ASN:HD22	1.86	0.40
1:N:184:TYR:HA	1:N:211:LEU:HD23	2.03	0.40
1:N:257:VAL:HB	1:N:404:ASP:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:THR:OG1	1:G:235:TYR:CE2[4_456]	1.90	0.30

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	579/593 (98%)	557 (96%)	22 (4%)	0	100	100
1	B	579/593 (98%)	556 (96%)	23 (4%)	0	100	100
1	C	579/593 (98%)	554 (96%)	25 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	579/593 (98%)	556 (96%)	23 (4%)	0	100	100
1	E	579/593 (98%)	553 (96%)	26 (4%)	0	100	100
1	F	579/593 (98%)	555 (96%)	24 (4%)	0	100	100
1	G	579/593 (98%)	556 (96%)	23 (4%)	0	100	100
1	H	579/593 (98%)	555 (96%)	24 (4%)	0	100	100
1	I	579/593 (98%)	552 (95%)	27 (5%)	0	100	100
1	J	579/593 (98%)	554 (96%)	25 (4%)	0	100	100
1	K	579/593 (98%)	553 (96%)	26 (4%)	0	100	100
1	L	579/593 (98%)	555 (96%)	24 (4%)	0	100	100
1	M	579/593 (98%)	554 (96%)	25 (4%)	0	100	100
1	N	579/593 (98%)	559 (96%)	20 (4%)	0	100	100
All	All	8106/8302 (98%)	7769 (96%)	337 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	464/495 (94%)	446 (96%)	18 (4%)	27	59
1	B	462/495 (93%)	446 (96%)	16 (4%)	31	63
1	C	456/495 (92%)	440 (96%)	16 (4%)	31	63
1	D	464/495 (94%)	448 (97%)	16 (3%)	32	64
1	E	461/495 (93%)	445 (96%)	16 (4%)	31	63
1	F	453/495 (92%)	436 (96%)	17 (4%)	28	60
1	G	457/495 (92%)	440 (96%)	17 (4%)	29	61
1	H	464/495 (94%)	450 (97%)	14 (3%)	36	68
1	I	466/495 (94%)	451 (97%)	15 (3%)	34	66
1	J	468/495 (94%)	451 (96%)	17 (4%)	30	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	453/495 (92%)	437 (96%)	16 (4%)	31	63
1	L	460/495 (93%)	442 (96%)	18 (4%)	27	59
1	M	461/495 (93%)	444 (96%)	17 (4%)	29	61
1	N	454/495 (92%)	440 (97%)	14 (3%)	35	67
All	All	6443/6930 (93%)	6216 (96%)	227 (4%)	31	63

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	THR
1	A	157	CYS
1	A	175	CYS
1	A	215	SER
1	A	223	ASN
1	A	236	THR
1	A	276	ILE
1	A	385	MET
1	A	386	ASP
1	A	390	LYS
1	A	410	ARG
1	A	421	TYR
1	A	445	SER
1	A	582	ASN
1	A	601	ARG
1	A	607	ARG
1	A	639	LEU
1	A	716	ASN
1	B	136	THR
1	B	157	CYS
1	B	175	CYS
1	B	215	SER
1	B	223	ASN
1	B	225	GLN
1	B	236	THR
1	B	276	ILE
1	B	385	MET
1	B	390	LYS
1	B	410	ARG
1	B	421	TYR
1	B	445	SER
1	B	582	ASN

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Mol	Chain	Res	Type
1	B	627	VAL
1	B	630	ASN
1	C	136	THR
1	C	137	ASN
1	C	157	CYS
1	C	175	CYS
1	C	215	SER
1	C	223	ASN
1	C	276	ILE
1	C	385	MET
1	C	386	ASP
1	C	390	LYS
1	C	410	ARG
1	C	421	TYR
1	C	445	SER
1	C	582	ASN
1	C	627	VAL
1	C	630	ASN
1	D	136	THR
1	D	157	CYS
1	D	175	CYS
1	D	215	SER
1	D	223	ASN
1	D	236	THR
1	D	276	ILE
1	D	385	MET
1	D	386	ASP
1	D	390	LYS
1	D	410	ARG
1	D	421	TYR
1	D	445	SER
1	D	582	ASN
1	D	627	VAL
1	D	630	ASN
1	E	136	THR
1	E	157	CYS
1	E	175	CYS
1	E	215	SER
1	E	223	ASN
1	E	236	THR
1	E	276	ILE
1	E	385	MET

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Mol	Chain	Res	Type
1	E	386	ASP
1	E	390	LYS
1	E	410	ARG
1	E	421	TYR
1	E	445	SER
1	E	582	ASN
1	E	627	VAL
1	E	630	ASN
1	F	136	THR
1	F	157	CYS
1	F	175	CYS
1	F	215	SER
1	F	223	ASN
1	F	236	THR
1	F	276	ILE
1	F	385	MET
1	F	386	ASP
1	F	390	LYS
1	F	405	SER
1	F	410	ARG
1	F	421	TYR
1	F	445	SER
1	F	582	ASN
1	F	627	VAL
1	F	630	ASN
1	G	136	THR
1	G	157	CYS
1	G	175	CYS
1	G	215	SER
1	G	223	ASN
1	G	236	THR
1	G	276	ILE
1	G	385	MET
1	G	386	ASP
1	G	390	LYS
1	G	410	ARG
1	G	421	TYR
1	G	445	SER
1	G	480	ARG
1	G	582	ASN
1	G	627	VAL
1	G	630	ASN

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Mol	Chain	Res	Type
1	H	136	THR
1	H	157	CYS
1	H	175	CYS
1	H	215	SER
1	H	223	ASN
1	H	236	THR
1	H	276	ILE
1	H	385	MET
1	H	390	LYS
1	H	410	ARG
1	H	421	TYR
1	H	445	SER
1	H	582	ASN
1	H	627	VAL
1	I	136	THR
1	I	157	CYS
1	I	175	CYS
1	I	215	SER
1	I	223	ASN
1	I	236	THR
1	I	276	ILE
1	I	385	MET
1	I	386	ASP
1	I	390	LYS
1	I	410	ARG
1	I	421	TYR
1	I	445	SER
1	I	582	ASN
1	I	627	VAL
1	J	136	THR
1	J	157	CYS
1	J	175	CYS
1	J	215	SER
1	J	223	ASN
1	J	236	THR
1	J	276	ILE
1	J	385	MET
1	J	386	ASP
1	J	390	LYS
1	J	405	SER
1	J	410	ARG
1	J	421	TYR

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Mol	Chain	Res	Type
1	J	422	VAL
1	J	445	SER
1	J	627	VAL
1	J	630	ASN
1	K	136	THR
1	K	157	CYS
1	K	175	CYS
1	K	215	SER
1	K	223	ASN
1	K	236	THR
1	K	276	ILE
1	K	385	MET
1	K	390	LYS
1	K	410	ARG
1	K	421	TYR
1	K	445	SER
1	K	480	ARG
1	K	582	ASN
1	K	627	VAL
1	K	630	ASN
1	L	136	THR
1	L	157	CYS
1	L	175	CYS
1	L	215	SER
1	L	223	ASN
1	L	236	THR
1	L	276	ILE
1	L	385	MET
1	L	386	ASP
1	L	390	LYS
1	L	405	SER
1	L	410	ARG
1	L	421	TYR
1	L	445	SER
1	L	582	ASN
1	L	601	ARG
1	L	607	ARG
1	L	716	ASN
1	M	136	THR
1	M	157	CYS
1	M	175	CYS
1	M	215	SER

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Mol	Chain	Res	Type
1	M	223	ASN
1	M	225	GLN
1	M	236	THR
1	M	276	ILE
1	M	385	MET
1	M	386	ASP
1	M	390	LYS
1	M	410	ARG
1	M	421	TYR
1	M	445	SER
1	M	582	ASN
1	M	627	VAL
1	M	630	ASN
1	N	136	THR
1	N	157	CYS
1	N	175	CYS
1	N	215	SER
1	N	223	ASN
1	N	236	THR
1	N	276	ILE
1	N	385	MET
1	N	390	LYS
1	N	410	ARG
1	N	421	TYR
1	N	445	SER
1	N	627	VAL
1	N	630	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	315	GLN
1	A	346	GLN
1	A	427	GLN
1	A	478	GLN
1	A	672	GLN
1	B	179	ASN
1	B	315	GLN
1	B	346	GLN
1	B	427	GLN
1	C	137	ASN

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Mol	Chain	Res	Type
1	C	179	ASN
1	C	315	GLN
1	C	346	GLN
1	C	427	GLN
1	D	179	ASN
1	D	315	GLN
1	D	346	GLN
1	D	426	HIS
1	D	427	GLN
1	E	179	ASN
1	E	315	GLN
1	E	346	GLN
1	E	427	GLN
1	F	179	ASN
1	F	315	GLN
1	F	346	GLN
1	F	427	GLN
1	G	179	ASN
1	G	315	GLN
1	G	346	GLN
1	G	426	HIS
1	G	427	GLN
1	H	179	ASN
1	H	315	GLN
1	H	346	GLN
1	H	427	GLN
1	I	179	ASN
1	I	315	GLN
1	I	346	GLN
1	I	427	GLN
1	I	672	GLN
1	J	179	ASN
1	J	315	GLN
1	J	346	GLN
1	J	427	GLN
1	K	179	ASN
1	K	315	GLN
1	K	346	GLN
1	K	427	GLN
1	L	179	ASN
1	L	315	GLN
1	L	346	GLN

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Mol	Chain	Res	Type
1	L	426	HIS
1	L	427	GLN
1	M	179	ASN
1	M	315	GLN
1	M	346	GLN
1	M	427	GLN
1	N	179	ASN
1	N	315	GLN
1	N	346	GLN
1	N	427	GLN

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 [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	581/593 (97%)	-0.03	13 (2%)	62	56	29, 48, 92, 128	0
1	B	581/593 (97%)	0.07	24 (4%)	42	36	29, 50, 93, 132	0
1	C	581/593 (97%)	0.11	23 (3%)	43	37	28, 51, 94, 129	0
1	D	581/593 (97%)	0.35	49 (8%)	18	16	29, 49, 93, 128	0
1	E	581/593 (97%)	0.09	17 (2%)	54	49	31, 50, 94, 131	0
1	F	581/593 (97%)	0.25	30 (5%)	34	29	31, 53, 96, 130	0
1	G	581/593 (97%)	0.38	50 (8%)	18	15	31, 53, 96, 127	0
1	H	581/593 (97%)	0.04	13 (2%)	62	56	29, 51, 94, 132	0
1	I	581/593 (97%)	0.34	56 (9%)	15	13	29, 49, 89, 129	0
1	J	581/593 (97%)	0.17	22 (3%)	44	39	31, 51, 94, 128	0
1	K	581/593 (97%)	0.36	39 (6%)	25	21	33, 53, 96, 130	0
1	L	581/593 (97%)	0.11	19 (3%)	49	44	31, 51, 93, 128	0
1	M	581/593 (97%)	0.12	20 (3%)	48	42	31, 52, 92, 127	0
1	N	581/593 (97%)	0.18	21 (3%)	46	41	31, 52, 96, 132	0
All	All	8134/8302 (97%)	0.18	396 (4%)	36	31	28, 51, 94, 132	0

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	THR	6.0
1	K	297	GLU	5.8
1	D	238	LEU	5.3
1	B	478	GLN	5.3
1	F	301	ASP	5.3
1	D	236	THR	5.0
1	E	301	ASP	4.8
1	I	420	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	I	422	VAL	4.7
1	G	234	SER	4.7
1	N	478	GLN	4.7
1	C	654	TYR	4.6
1	D	420	TYR	4.6
1	C	236	THR	4.5
1	L	237	THR	4.5
1	I	421	TYR	4.5
1	C	239	ASP	4.5
1	J	233	ALA	4.4
1	G	237	THR	4.4
1	J	422	VAL	4.4
1	F	236	THR	4.4
1	C	234	SER	4.4
1	C	420	TYR	4.3
1	B	676	SER	4.3
1	D	301	ASP	4.3
1	C	235	TYR	4.3
1	D	240	ALA	4.3
1	I	234	SER	4.3
1	N	301	ASP	4.2
1	D	419	HIS	4.1
1	K	305	ALA	4.1
1	H	303	PRO	4.1
1	G	421	TYR	4.1
1	M	679	TYR	4.1
1	I	423	VAL	4.1
1	D	418	LYS	4.1
1	J	303	PRO	4.0
1	K	301	ASP	4.0
1	D	425	ALA	4.0
1	N	303	PRO	3.9
1	D	421	TYR	3.9
1	K	478	GLN	3.9
1	L	301	ASP	3.8
1	E	300	GLY	3.8
1	D	417	TYR	3.8
1	J	415	GLY	3.8
1	F	240	ALA	3.8
1	F	234	SER	3.8
1	I	236	THR	3.7
1	E	567	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	298	VAL	3.7
1	A	587	SER	3.7
1	G	165	TRP	3.7
1	E	415	GLY	3.7
1	N	300	GLY	3.7
1	F	416	ALA	3.7
1	H	137	ASN	3.7
1	I	631	GLY	3.7
1	H	238	LEU	3.6
1	D	632	GLY	3.6
1	E	631	GLY	3.6
1	C	301	ASP	3.6
1	B	477	ALA	3.6
1	G	478	GLN	3.6
1	I	672	GLN	3.6
1	K	706	TRP	3.6
1	C	238	LEU	3.6
1	I	235	TYR	3.5
1	H	306	LYS	3.5
1	I	238	LEU	3.5
1	D	422	VAL	3.5
1	G	236	THR	3.5
1	I	311	ALA	3.4
1	H	301	ASP	3.4
1	G	679	TYR	3.4
1	I	237	THR	3.4
1	A	416	ALA	3.3
1	L	656	GLY	3.3
1	I	312	SER	3.3
1	I	633	SER	3.3
1	B	301	ASP	3.3
1	B	679	TYR	3.3
1	C	652	PHE	3.3
1	B	415	GLY	3.3
1	D	429	TYR	3.2
1	K	679	TYR	3.2
1	G	693	ALA	3.2
1	H	294	GLY	3.2
1	F	241	TYR	3.2
1	G	240	ALA	3.2
1	I	418	LYS	3.2
1	K	477	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	N	477	ALA	3.2
1	K	692	ASP	3.2
1	M	301	ASP	3.2
1	J	300	GLY	3.2
1	I	309	ALA	3.2
1	M	137	ASN	3.2
1	D	423	VAL	3.2
1	G	363	VAL	3.2
1	C	416	ALA	3.2
1	D	360	ALA	3.2
1	J	238	LEU	3.2
1	G	429	TYR	3.1
1	G	422	VAL	3.1
1	C	237	THR	3.1
1	E	237	THR	3.1
1	I	624	ASP	3.1
1	D	362	TRP	3.1
1	J	298	VAL	3.1
1	G	419	HIS	3.1
1	K	604	GLN	3.1
1	M	676	SER	3.1
1	I	628	GLY	3.1
1	J	137	ASN	3.1
1	J	234	SER	3.1
1	L	587	SER	3.1
1	I	630	ASN	3.1
1	C	303	PRO	3.1
1	B	298	VAL	3.0
1	G	276	ILE	3.0
1	I	240	ALA	3.0
1	I	424	GLY	3.0
1	K	303	PRO	3.0
1	I	632	GLY	3.0
1	F	235	TYR	3.0
1	G	303	PRO	3.0
1	F	622	ALA	3.0
1	G	360	ALA	3.0
1	G	423	VAL	3.0
1	D	239	ASP	2.9
1	J	301	ASP	2.9
1	G	420	TYR	2.9
1	G	238	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	670	ARG	2.9
1	L	588	PRO	2.9
1	J	235	TYR	2.9
1	G	164	LEU	2.9
1	M	238	LEU	2.9
1	D	233	ALA	2.9
1	A	716	ASN	2.9
1	D	242	PHE	2.8
1	G	301	ASP	2.8
1	I	233	ALA	2.8
1	D	241	TYR	2.8
1	G	242	PHE	2.8
1	H	305	ALA	2.8
1	D	363	VAL	2.8
1	E	420	TYR	2.8
1	I	306	LYS	2.8
1	G	417	TYR	2.8
1	N	235	TYR	2.8
1	G	244	GLU	2.8
1	B	653	GLN	2.8
1	N	298	VAL	2.8
1	N	420	TYR	2.8
1	B	236	THR	2.8
1	I	295	GLY	2.8
1	I	478	GLN	2.7
1	I	584	GLN	2.7
1	N	692	ASP	2.7
1	C	630	ASN	2.7
1	I	693	ALA	2.7
1	I	299	SER	2.7
1	B	707	LEU	2.7
1	E	692	ASP	2.7
1	D	235	TYR	2.7
1	L	654	TYR	2.7
1	F	692	ASP	2.7
1	I	692	ASP	2.7
1	I	305	ALA	2.7
1	C	653	GLN	2.7
1	F	584	GLN	2.7
1	G	426	HIS	2.7
1	K	302	GLY	2.7
1	K	676	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	136	THR	2.6
1	K	667	GLN	2.6
1	D	286	SER	2.6
1	D	313	TYR	2.6
1	M	604	GLN	2.6
1	M	652	PHE	2.6
1	I	168	GLU	2.6
1	G	415	GLY	2.6
1	D	366	TYR	2.6
1	K	296	VAL	2.6
1	L	363	VAL	2.6
1	M	422	VAL	2.6
1	D	630	ASN	2.6
1	I	303	PRO	2.6
1	B	238	LEU	2.6
1	D	604	GLN	2.5
1	B	303	PRO	2.5
1	D	232	GLY	2.5
1	J	302	GLY	2.5
1	G	232	GLY	2.5
1	H	716	ASN	2.5
1	J	168	GLU	2.5
1	K	603	GLY	2.5
1	L	295	GLY	2.5
1	L	300	GLY	2.5
1	F	233	ALA	2.5
1	K	615	ALA	2.5
1	K	640	SER	2.5
1	F	614	ALA	2.5
1	G	241	TYR	2.5
1	K	420	TYR	2.5
1	J	299	SER	2.5
1	I	301	ASP	2.5
1	G	427	GLN	2.5
1	H	667	GLN	2.5
1	H	295	GLY	2.5
1	K	295	GLY	2.5
1	N	294	GLY	2.5
1	I	137	ASN	2.5
1	L	298	VAL	2.5
1	L	716	ASN	2.5
1	G	609	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	631	GLY	2.4
1	N	302	GLY	2.4
1	G	630	ASN	2.4
1	G	477	ALA	2.4
1	M	693	ALA	2.4
1	N	169	LYS	2.4
1	M	420	TYR	2.4
1	L	692	ASP	2.4
1	F	298	VAL	2.4
1	K	416	ALA	2.4
1	K	622	ALA	2.4
1	K	630	ASN	2.4
1	L	137	ASN	2.4
1	F	604	GLN	2.4
1	A	301	ASP	2.4
1	M	300	GLY	2.4
1	B	168	GLU	2.4
1	D	298	VAL	2.4
1	K	614	ALA	2.4
1	K	432	PHE	2.4
1	K	137	ASN	2.4
1	L	136	THR	2.4
1	D	234	SER	2.4
1	J	692	ASP	2.4
1	B	615	ALA	2.4
1	D	416	ALA	2.4
1	J	240	ALA	2.4
1	G	414	ASN	2.4
1	F	420	TYR	2.3
1	A	656	GLY	2.3
1	D	426	HIS	2.3
1	K	419	HIS	2.3
1	G	362	TRP	2.3
1	G	602	VAL	2.3
1	I	362	TRP	2.3
1	I	706	TRP	2.3
1	G	168	GLU	2.3
1	I	308	GLU	2.3
1	G	243	ARG	2.3
1	C	679	TYR	2.3
1	F	679	TYR	2.3
1	J	420	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	298	VAL	2.3
1	B	242	PHE	2.3
1	F	432	PHE	2.3
1	K	693	ALA	2.3
1	N	305	ALA	2.3
1	I	310	ARG	2.3
1	F	303	PRO	2.3
1	B	241	TYR	2.3
1	I	417	TYR	2.3
1	G	291	GLY	2.3
1	K	294	GLY	2.3
1	M	603	GLY	2.3
1	D	428	SER	2.3
1	K	307	LEU	2.3
1	G	365	THR	2.3
1	D	355	ASN	2.3
1	L	306	LYS	2.3
1	B	417	TYR	2.3
1	B	419	HIS	2.3
1	C	424	GLY	2.3
1	I	294	GLY	2.3
1	K	292	VAL	2.3
1	K	479	GLY	2.3
1	K	362	TRP	2.3
1	D	693	ALA	2.3
1	D	299	SER	2.3
1	I	625	LEU	2.3
1	B	423	VAL	2.2
1	G	664	PHE	2.2
1	D	165	TRP	2.2
1	E	240	ALA	2.2
1	E	243	ARG	2.2
1	F	612	ALA	2.2
1	N	585	GLU	2.2
1	A	357	SER	2.2
1	E	676	SER	2.2
1	F	625	LEU	2.2
1	K	625	LEU	2.2
1	N	234	SER	2.2
1	A	631	GLY	2.2
1	C	642	VAL	2.2
1	G	228	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	604	GLN	2.2
1	I	232	GLY	2.2
1	I	296	VAL	2.2
1	L	294	GLY	2.2
1	N	310	ARG	2.2
1	C	351	GLU	2.2
1	K	612	ALA	2.2
1	C	304	LYS	2.2
1	I	136	THR	2.2
1	F	603	GLY	2.2
1	J	232	GLY	2.2
1	K	170	GLY	2.2
1	A	653	GLN	2.2
1	G	416	ALA	2.2
1	G	425	ALA	2.2
1	L	234	SER	2.2
1	E	236	THR	2.2
1	F	237	THR	2.2
1	H	298	VAL	2.2
1	C	641	GLY	2.2
1	J	424	GLY	2.2
1	M	620	GLY	2.2
1	D	137	ASN	2.2
1	N	601	ARG	2.2
1	D	434	ASP	2.2
1	F	239	ASP	2.2
1	G	412	ILE	2.2
1	C	298	VAL	2.2
1	D	368	VAL	2.2
1	J	136	THR	2.1
1	I	419	HIS	2.1
1	A	432	PHE	2.1
1	H	432	PHE	2.1
1	M	584	GLN	2.1
1	F	238	LEU	2.1
1	F	360	ALA	2.1
1	G	306	LYS	2.1
1	I	634	LEU	2.1
1	G	298	VAL	2.1
1	K	298	VAL	2.1
1	E	234	SER	2.1
1	I	300	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	304	LYS	2.1
1	A	693	ALA	2.1
1	L	420	TYR	2.1
1	J	243	ARG	2.1
1	I	231	PHE	2.1
1	B	166	LYS	2.1
1	E	425	ALA	2.1
1	I	694	ALA	2.1
1	D	168	GLU	2.1
1	E	168	GLU	2.1
1	M	303	PRO	2.1
1	K	318	TRP	2.1
1	M	370	VAL	2.1
1	F	415	GLY	2.1
1	F	419	HIS	2.1
1	K	304	LYS	2.1
1	A	241	TYR	2.1
1	G	716	ASN	2.1
1	N	598	ASN	2.1
1	M	706	TRP	2.1
1	F	422	VAL	2.1
1	D	294	GLY	2.1
1	E	242	PHE	2.1
1	J	164	LEU	2.0
1	B	604	GLN	2.0
1	D	314	THR	2.0
1	D	427	GLN	2.0
1	D	692	ASP	2.0
1	G	692	ASP	2.0
1	H	136	THR	2.0
1	I	425	ALA	2.0
1	I	623	SER	2.0
1	A	137	ASN	2.0
1	N	363	VAL	2.0
1	F	232	GLY	2.0
1	M	295	GLY	2.0
1	I	361	LEU	2.0
1	B	237	THR	2.0
1	C	365	THR	2.0
1	C	604	GLN	2.0
1	D	672	GLN	2.0
1	G	667	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	236	THR	2.0
1	M	136	THR	2.0
1	N	136	THR	2.0
1	B	234	SER	2.0
1	K	491	SER	2.0
1	A	235	TYR	2.0
1	E	303	PRO	2.0
1	N	318	TRP	2.0
1	D	300	GLY	2.0
1	F	431	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.