



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:37 AM UTC

PDB ID : 3O44 / pdb_00003o44
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:

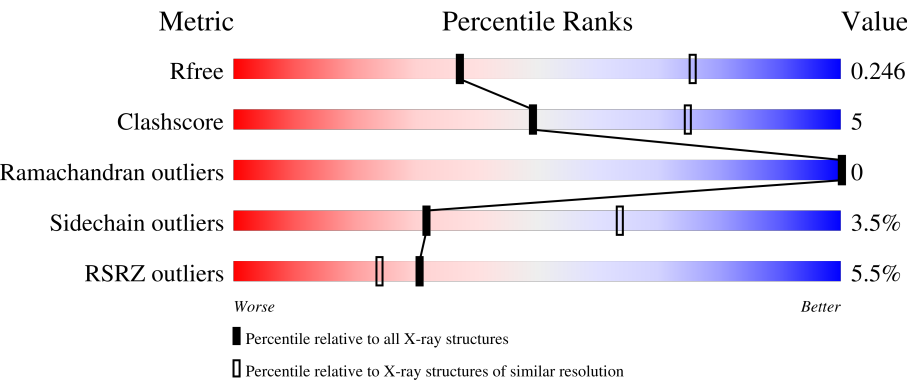
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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



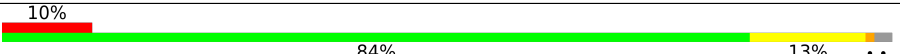
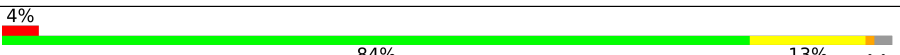
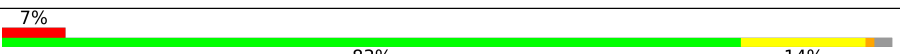
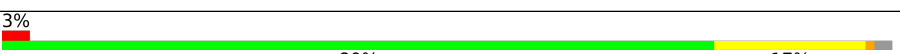
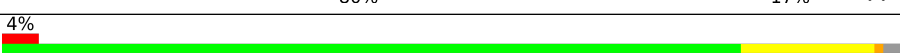
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	3% 82% 16% ..
1	B	593	5% 84% 12% ..
1	C	593	4% 86% 11% ..
1	D	593	9% 82% 15% ..
1	E	593	4% 85% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	593	 5% 85% 13% ..
1	G	593	 9% 84% 13% ..
1	H	593	 3% 85% 13% .
1	I	593	 10% 84% 13% ..
1	J	593	 4% 84% 13% ..
1	K	593	 7% 83% 14% ..
1	L	593	 3% 80% 17% ..
1	M	593	 4% 83% 15% ..
1	N	593	 5% 83% 15% ..

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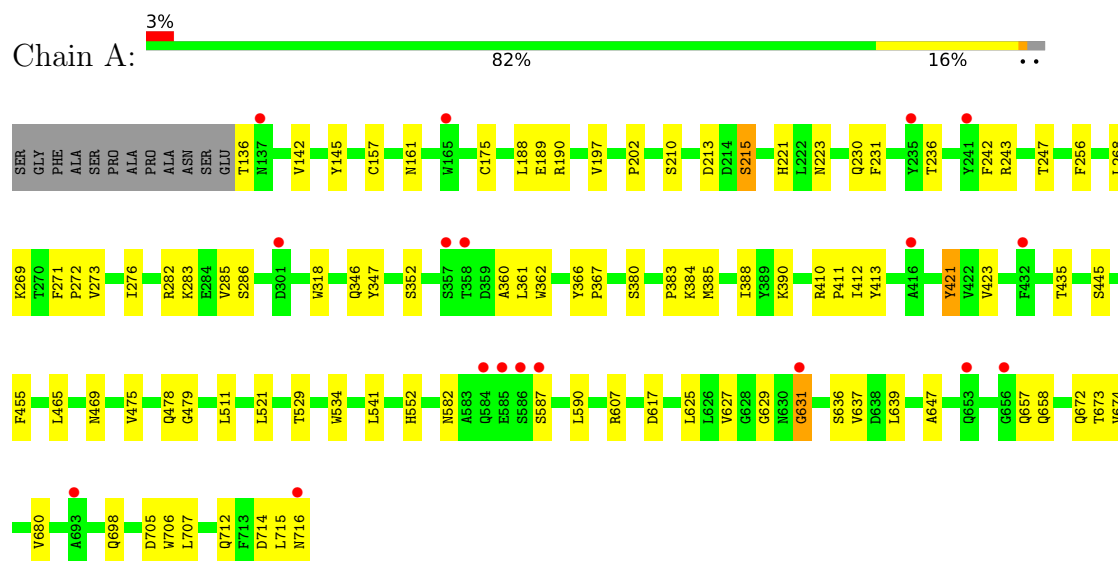
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	36	Total	O	0	0
			36	36		

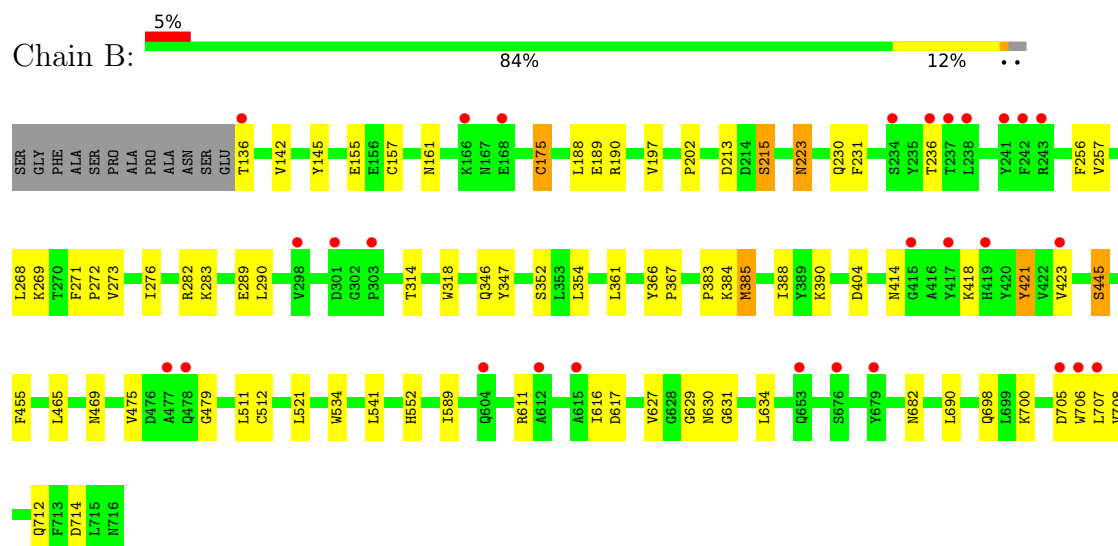
3 Residue-property plots [i](#)

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.

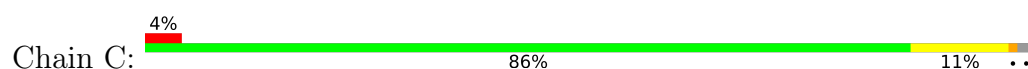
• Molecule 1: Hemolysin

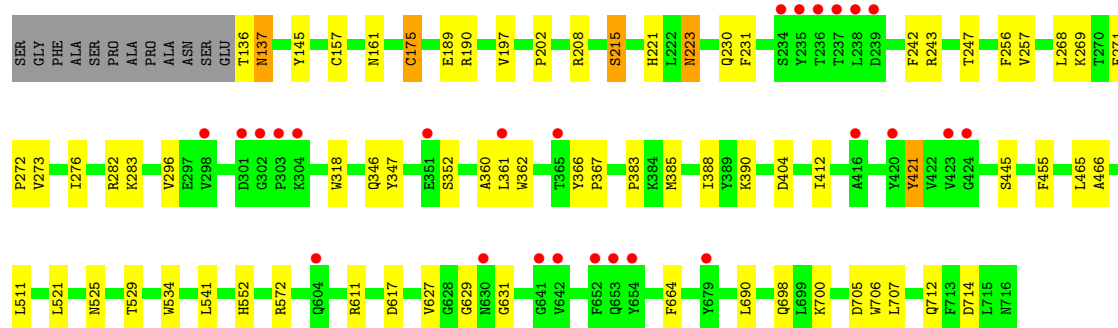


• Molecule 1: Hemolysin

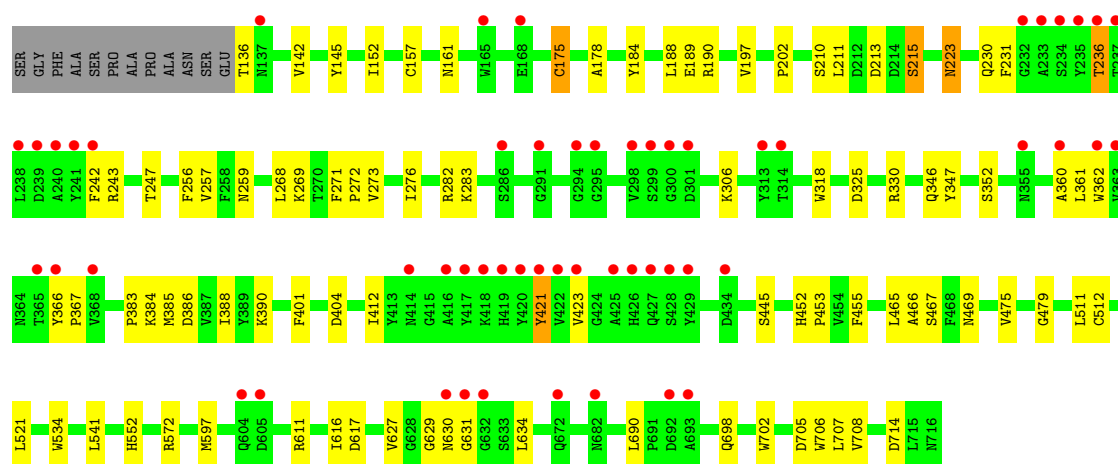
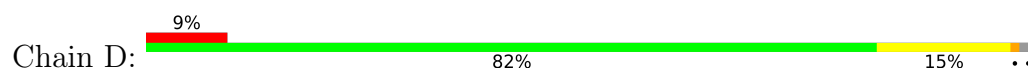


• Molecule 1: Hemolysin

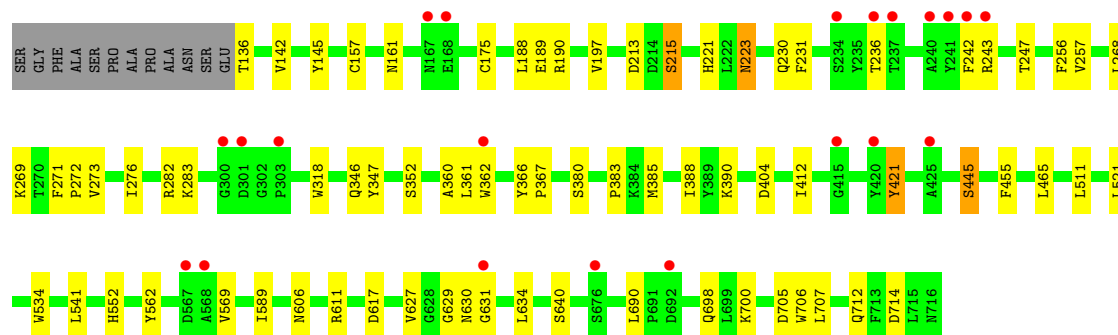
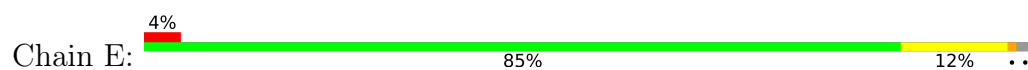




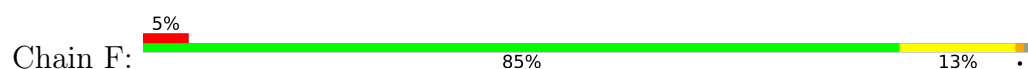
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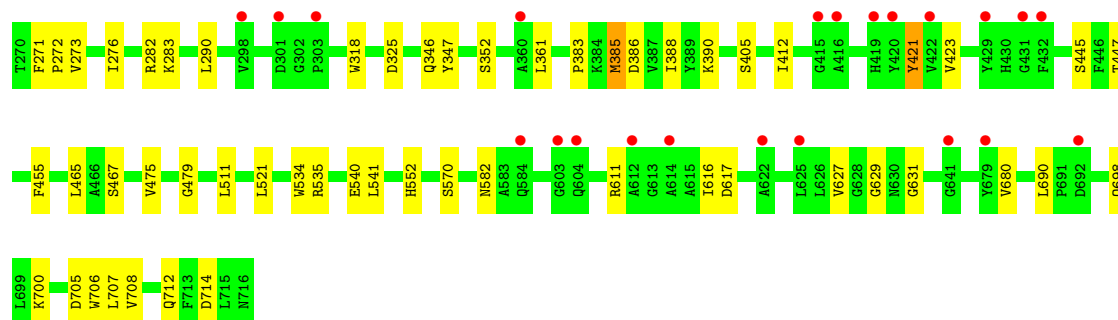


• Molecule 1: Hemolysin

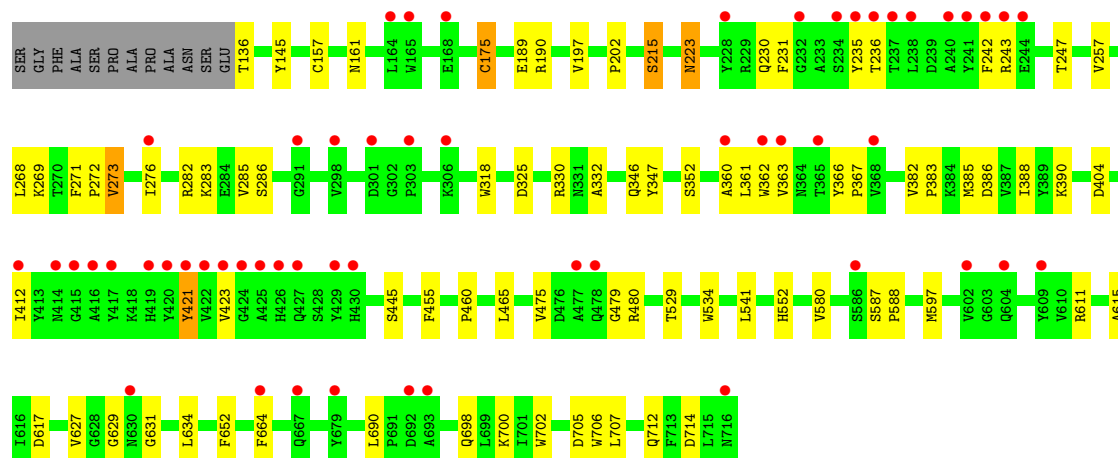
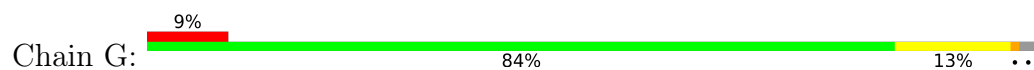


• Molecule 1: Hemolysin

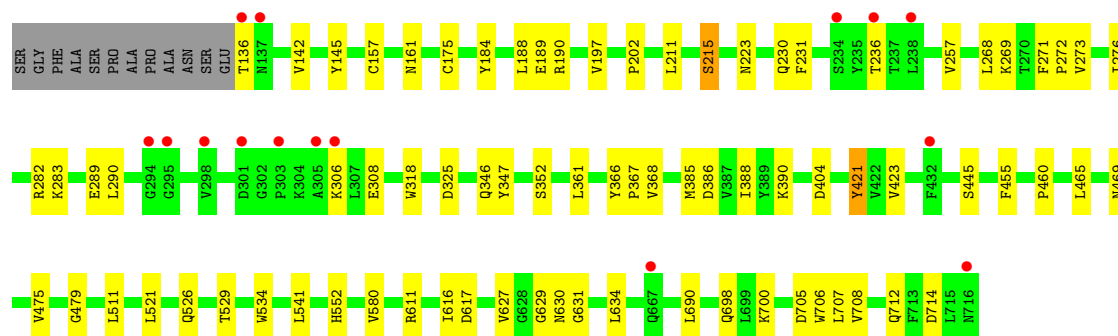
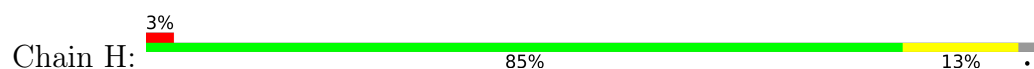




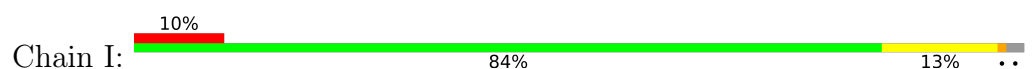
• Molecule 1: Hemolysin

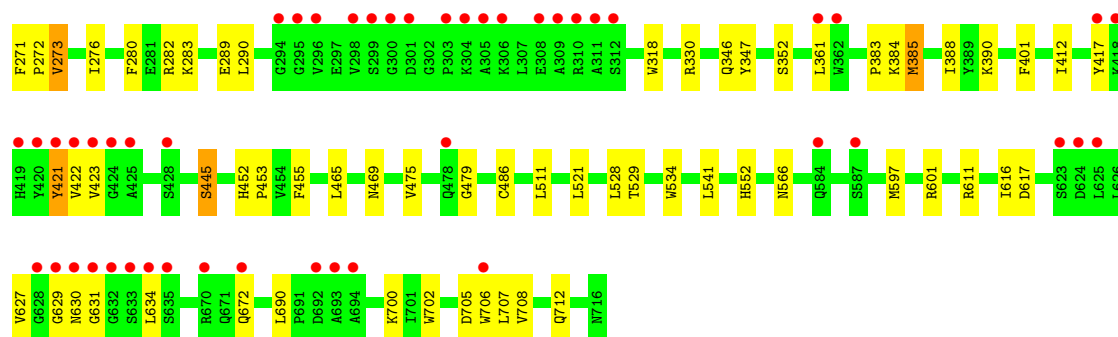


• Molecule 1: Hemolysin

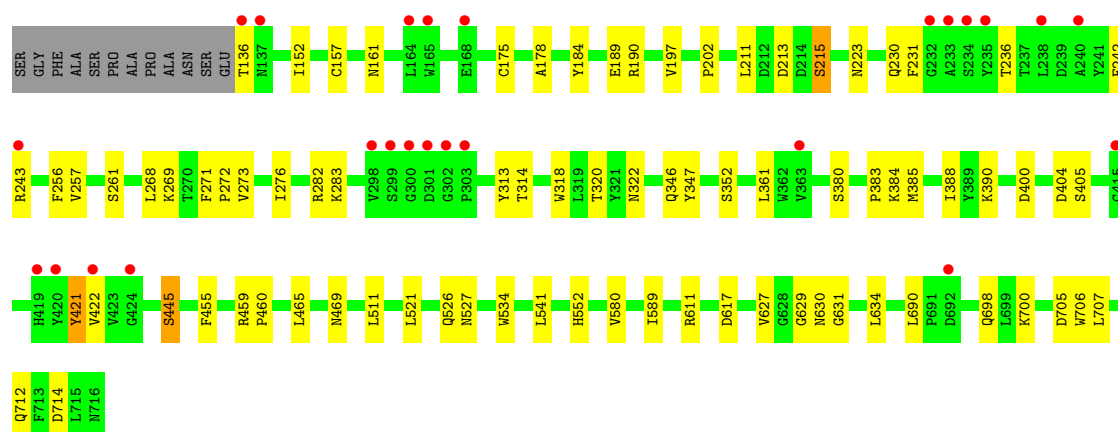
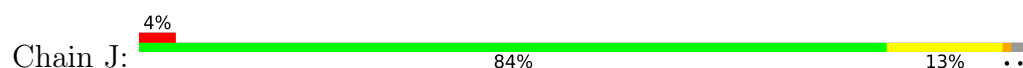


• Molecule 1: Hemolysin

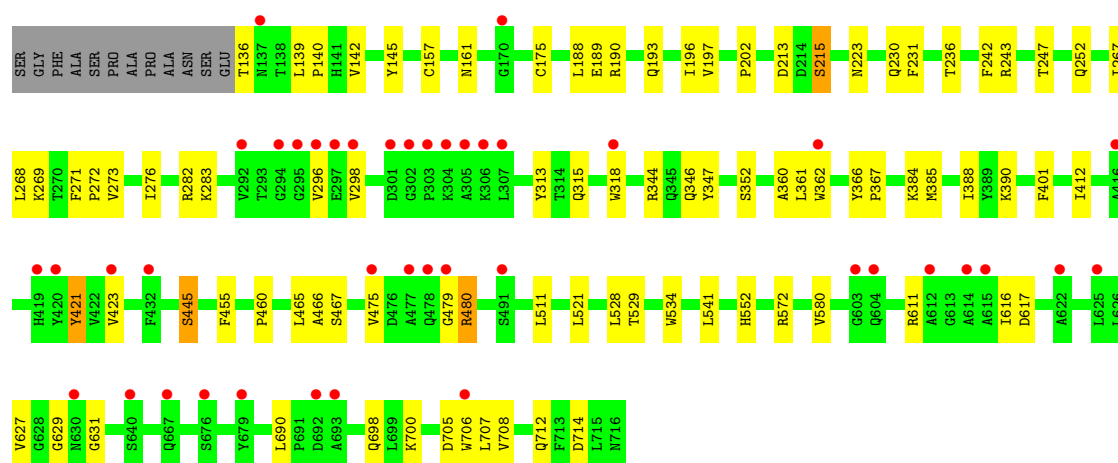
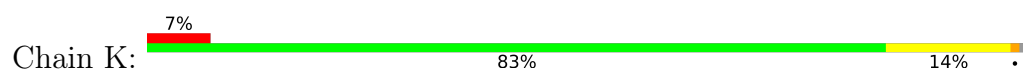




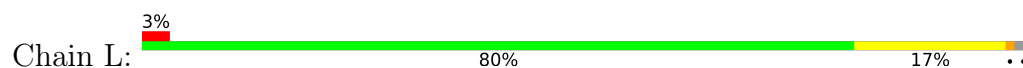
• Molecule 1: Hemolysin

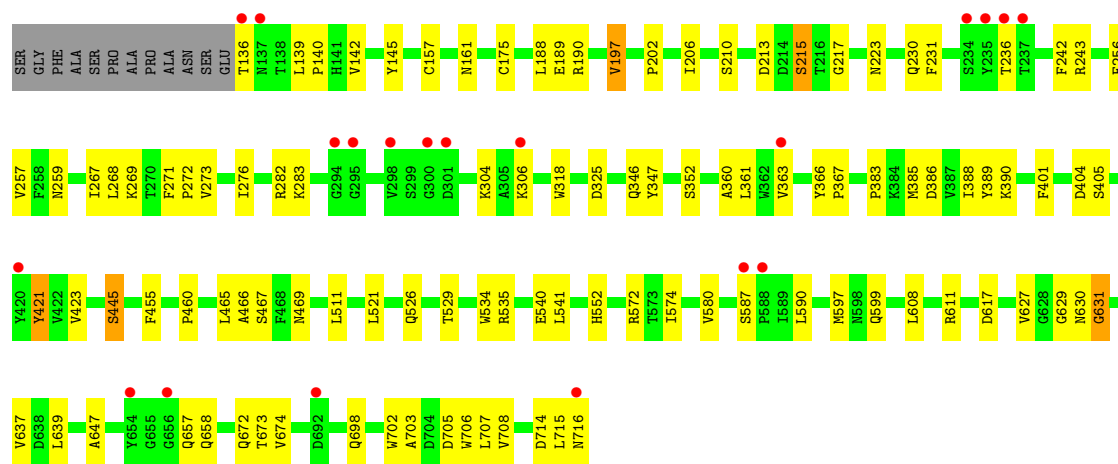


• Molecule 1: Hemolysin

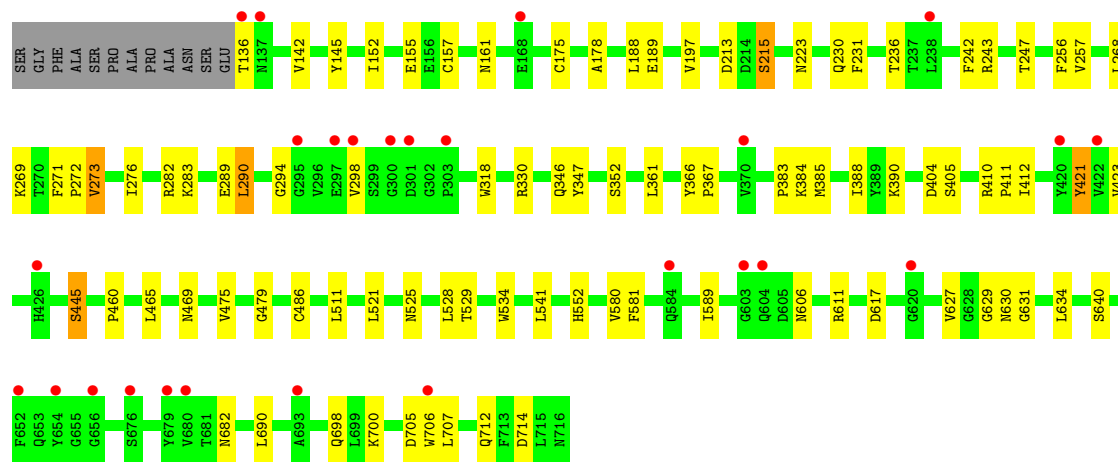
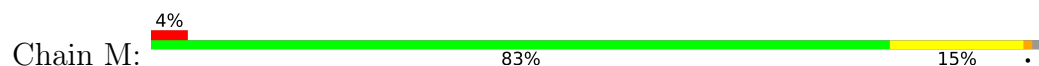


• Molecule 1: Hemolysin

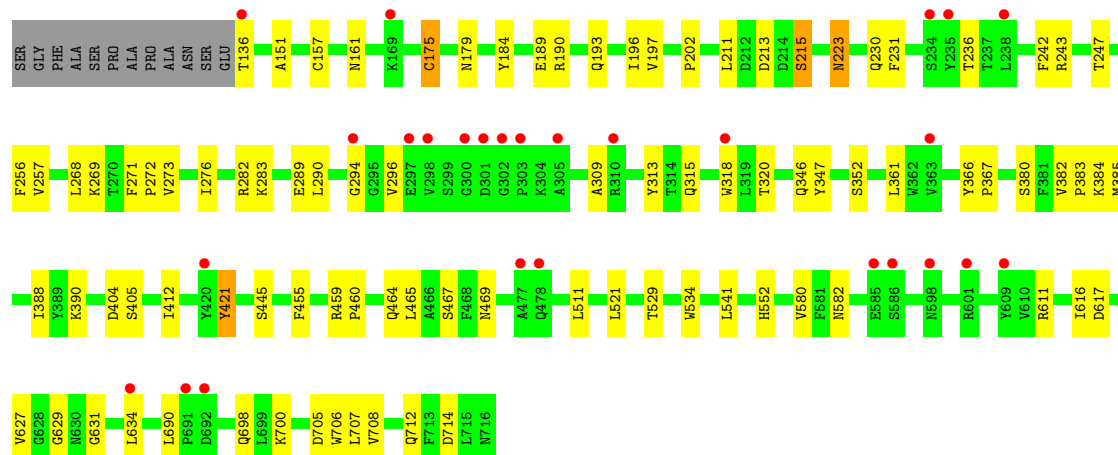
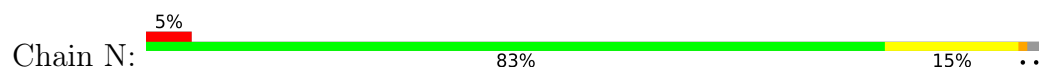




• Molecule 1: Hemolysin



• 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	0.56	0/4557	0.83	4/6204 (0.1%)
1	B	0.56	0/4551	0.81	2/6198 (0.0%)
1	C	0.55	0/4523	0.81	1/6164 (0.0%)
1	D	0.57	0/4567	0.83	5/6221 (0.1%)
1	E	0.55	0/4555	0.81	1/6205 (0.0%)
1	F	0.51	0/4503	0.83	6/6139 (0.1%)
1	G	0.55	0/4528	0.82	3/6168 (0.0%)
1	H	0.49	0/4564	0.81	3/6219 (0.0%)
1	I	0.57	0/4575	0.82	2/6233 (0.0%)
1	J	0.52	0/4583	0.81	1/6240 (0.0%)
1	K	0.50	0/4509	0.82	3/6146 (0.0%)
1	L	0.53	0/4541	0.85	7/6183 (0.1%)
1	M	0.52	0/4539	0.82	2/6183 (0.0%)
1	N	0.52	0/4513	0.82	2/6153 (0.0%)
All	All	0.54	0/63608	0.82	42/86656 (0.0%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	631	GLY	N-CA-C	7.50	122.73	114.40
1	B	631	GLY	N-CA-C	7.40	122.61	114.40
1	D	631	GLY	N-CA-C	7.23	122.42	114.40
1	I	631	GLY	N-CA-C	7.20	122.40	114.40
1	G	423	VAL	N-CA-C	6.85	116.99	110.42
1	N	631	GLY	N-CA-C	6.77	121.92	114.40
1	G	631	GLY	N-CA-C	6.75	121.89	114.40
1	M	631	GLY	N-CA-C	6.73	121.87	114.40
1	C	631	GLY	N-CA-C	6.63	121.76	114.40
1	F	631	GLY	N-CA-C	6.39	121.49	114.40
1	D	423	VAL	N-CA-C	6.32	116.49	110.42
1	H	631	GLY	N-CA-C	6.28	122.03	113.99
1	J	631	GLY	N-CA-C	6.23	121.97	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	631	GLY	N-CA-C	6.01	121.07	114.40
1	D	467	SER	N-CA-C	-5.83	104.88	112.23
1	A	423	VAL	N-CA-C	5.82	116.01	110.42
1	H	325	ASP	N-CA-C	-5.74	104.72	110.97
1	L	325	ASP	N-CA-C	-5.72	104.74	110.97
1	H	423	VAL	N-CA-C	5.69	115.88	110.42
1	L	423	VAL	N-CA-C	5.63	115.82	110.42
1	I	423	VAL	N-CA-C	5.59	115.78	110.42
1	N	467	SER	N-CA-C	-5.57	105.21	112.23
1	F	467	SER	N-CA-C	-5.54	105.24	112.23
1	F	423	VAL	N-CA-C	5.53	115.73	110.42
1	A	707	LEU	N-CA-C	5.45	116.54	108.86
1	K	467	SER	N-CA-C	-5.36	105.48	112.23
1	B	423	VAL	N-CA-C	5.28	115.48	110.42
1	L	206	ILE	N-CA-C	5.25	115.47	108.11
1	A	631	GLY	N-CA-C	5.24	125.59	113.18
1	L	707	LEU	N-CA-C	5.23	116.93	109.14
1	M	423	VAL	N-CA-C	5.23	115.44	110.42
1	L	467	SER	N-CA-C	-5.22	105.65	112.23
1	A	210	SER	N-CA-C	5.21	117.17	108.99
1	G	325	ASP	N-CA-C	-5.20	105.30	110.97
1	F	680	VAL	N-CA-C	5.18	115.73	108.17
1	K	423	VAL	N-CA-C	5.15	115.36	110.42
1	L	631	GLY	N-CA-C	5.14	125.35	113.18
1	D	325	ASP	N-CA-C	-5.11	105.40	110.97
1	D	210	SER	N-CA-C	5.09	116.97	108.99
1	F	325	ASP	N-CA-C	-5.08	105.44	110.97
1	F	210	SER	N-CA-C	5.03	116.89	108.99
1	L	210	SER	N-CA-C	5.01	116.85	108.99

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	4464	0	4169	59	0
1	B	4457	0	4163	51	0
1	C	4431	0	4100	50	0
1	D	4471	0	4172	59	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	50	0
1	I	4479	0	4178	59	0
1	J	4487	0	4205	51	0
1	K	4417	0	4093	58	0
1	L	4449	0	4145	68	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	647	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 (647) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:LYS:HB2	1:L:318:TRP:HB2	1.44	1.00
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:282:ARG:NH1	1:K:346:GLN:NE2	2.32	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:NH1	1:B:346:GLN:NE2	2.44	0.66
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:E:271:PHE:HA	1:E:272:PRO:C	2.26	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:J:271:PHE:HA	1:J:272:PRO:C	2.26	0.60
1:B:271:PHE:HA	1:B:272:PRO:C	2.27	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:M:155:GLU:CD	1:M:682:ASN:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:271:PHE:HA	1:D:272:PRO:C	2.29	0.57
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:I:271:PHE:HA	1:I:272:PRO:C	2.29	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:H:271:PHE:HA	1:H:272:PRO:C	2.29	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:K:617:ASP:HA	1:K:707:LEU:HD23	1.88	0.56
1:N:271:PHE:HA	1:N:272:PRO:C	2.30	0.56
1:F:271:PHE:HA	1:F:272:PRO:C	2.30	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:A:271:PHE:HA	1:A:272:PRO:C	2.29	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:M:271:PHE:HA	1:M:272:PRO:C	2.30	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:K:271:PHE:HA	1:K:272:PRO:C	2.30	0.55
1:A:213:ASP:OD1	1:A:384:LYS:NZ	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:LEU:HD12	1:F:361:LEU:H	1.71	0.55
1:B:155:GLU:CD	1:B:682:ASN:H	2.14	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:273:VAL:HG11	1:J:384:LYS:HZ1	1.72	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
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: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:C:271:PHE:HA	1:C:272:PRO:C	2.32	0.53
1:F:421:TYR:N	1:F:421:TYR:CD2	2.76	0.53
1:G:271:PHE:HA	1:G:272:PRO:C	2.33	0.53
1:L:271:PHE:HA	1:L:272:PRO:C	2.33	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: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:K:421:TYR:N	1:K:421:TYR:CD2	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:634:LEU:C	1:B:634:LEU:HD23	2.35	0.52
1:D:230:GLN:HG2	1:D:231:PHE:N	2.24	0.52
1:C:629:GLY:HA3	1:C:706:TRP:O	2.09	0.52
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:L:161:ASN:HB3	1:L:231:PHE:CZ	2.45	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: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:M:634:LEU:C	1:M:634:LEU:HD23	2.36	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:H:634:LEU:C	1:H:634:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:611:ARG:NH2	1:E:630:ASN:O	2.37	0.49
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:F:534:TRP:CE2	1:F:541:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:GLN:HG2	1:H:231:PHE:N	2.28	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
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: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:F:230:GLN:HG2	1:F:231:PHE:N	2.28	0.47
1:J:634:LEU:C	1:J:634:LEU:HD23	2.40	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:G:634:LEU:C	1:G:634:LEU:HD23	2.40	0.47
1:L:587:SER:HG	1:L:714:ASP:HA	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:634:LEU:C	1:E:634:LEU:HD23	2.40	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: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:L:657:GLN:C	1:L:658:GLN:HG2	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:634:LEU:HD23	1:N:634:LEU:C	2.42	0.45
1:I:634:LEU:HD23	1:I:634:LEU:C	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:385:MET:HE3	1:F:385:MET:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:213:ASP:OD1	1:I:384:LYS:NZ	2.43	0.43
1:K:460:PRO:HG2	1:K:580:VAL:HG21	2.00	0.43
1:A:478:GLN:CD	1:I:672:GLN:NE2	2.76	0.43
1:A:657:GLN:C	1:A:658:GLN:HG2	2.43	0.43
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:B:385:MET:HE3	1:B:385:MET:HB3	1.90	0.42
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: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:D:213:ASP:OD1	1:D:384:LYS:NZ	2.38	0.42
1:H:347:TYR:HA	1:H:352:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:I:421:TYR:O	1:I:422:VAL:C	2.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:269:LYS:HD3	1:I:213:ASP:O	2.20	0.41
1:I:385:MET:HE3	1:I:385:MET:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:587:SER:HA	1:G:588:PRO:HD3	1.93	0.41
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: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:J:526:GLN:O	1:J:527:ASN:C	2.64	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:D:634:LEU:C	1:D:634:LEU:HD23	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:599:GLN:HE21	1:L:698:GLN:CD	2.30	0.40
1:A:384:LYS:HZ1	1:G:273:VAL:HG11	1.86	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
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%)	447 (96%)	17 (4%)	30	62
1	B	462/495 (93%)	446 (96%)	16 (4%)	32	63
1	C	456/495 (92%)	441 (97%)	15 (3%)	33	65
1	D	464/495 (94%)	449 (97%)	15 (3%)	34	65
1	E	461/495 (93%)	446 (97%)	15 (3%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	453/495 (92%)	436 (96%)	17 (4%)	29	61
1	G	457/495 (92%)	441 (96%)	16 (4%)	32	63
1	H	464/495 (94%)	449 (97%)	15 (3%)	34	65
1	I	466/495 (94%)	450 (97%)	16 (3%)	32	64
1	J	468/495 (94%)	450 (96%)	18 (4%)	29	61
1	K	453/495 (92%)	437 (96%)	16 (4%)	32	63
1	L	460/495 (93%)	444 (96%)	16 (4%)	32	63
1	M	461/495 (93%)	444 (96%)	17 (4%)	30	62
1	N	454/495 (92%)	438 (96%)	16 (4%)	32	63
All	All	6443/6930 (93%)	6218 (96%)	225 (4%)	32	63

All (225) 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	189	GLU
1	A	197	VAL
1	A	215	SER
1	A	223	ASN
1	A	236	THR
1	A	273	VAL
1	A	276	ILE
1	A	385	MET
1	A	390	LYS
1	A	421	TYR
1	A	445	SER
1	A	582	ASN
1	A	627	VAL
1	A	639	LEU
1	B	136	THR
1	B	157	CYS
1	B	175	CYS
1	B	189	GLU
1	B	197	VAL
1	B	215	SER
1	B	223	ASN
1	B	236	THR

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	276	ILE
1	B	314	THR
1	B	385	MET
1	B	390	LYS
1	B	421	TYR
1	B	445	SER
1	B	627	VAL
1	C	136	THR
1	C	137	ASN
1	C	157	CYS
1	C	175	CYS
1	C	189	GLU
1	C	197	VAL
1	C	215	SER
1	C	223	ASN
1	C	273	VAL
1	C	276	ILE
1	C	385	MET
1	C	390	LYS
1	C	421	TYR
1	C	445	SER
1	C	627	VAL
1	D	136	THR
1	D	157	CYS
1	D	175	CYS
1	D	189	GLU
1	D	197	VAL
1	D	215	SER
1	D	223	ASN
1	D	236	THR
1	D	259	ASN
1	D	273	VAL
1	D	276	ILE
1	D	385	MET
1	D	390	LYS
1	D	421	TYR
1	D	627	VAL
1	E	136	THR
1	E	157	CYS
1	E	175	CYS
1	E	189	GLU

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Mol	Chain	Res	Type
1	E	197	VAL
1	E	215	SER
1	E	223	ASN
1	E	236	THR
1	E	273	VAL
1	E	276	ILE
1	E	385	MET
1	E	390	LYS
1	E	421	TYR
1	E	445	SER
1	E	627	VAL
1	F	136	THR
1	F	157	CYS
1	F	175	CYS
1	F	189	GLU
1	F	197	VAL
1	F	215	SER
1	F	223	ASN
1	F	236	THR
1	F	273	VAL
1	F	276	ILE
1	F	290	LEU
1	F	385	MET
1	F	390	LYS
1	F	405	SER
1	F	421	TYR
1	F	445	SER
1	F	627	VAL
1	G	136	THR
1	G	157	CYS
1	G	175	CYS
1	G	189	GLU
1	G	197	VAL
1	G	215	SER
1	G	223	ASN
1	G	236	THR
1	G	273	VAL
1	G	276	ILE
1	G	385	MET
1	G	390	LYS
1	G	421	TYR
1	G	445	SER

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Mol	Chain	Res	Type
1	G	480	ARG
1	G	627	VAL
1	H	136	THR
1	H	157	CYS
1	H	175	CYS
1	H	189	GLU
1	H	197	VAL
1	H	215	SER
1	H	223	ASN
1	H	236	THR
1	H	273	VAL
1	H	276	ILE
1	H	385	MET
1	H	390	LYS
1	H	421	TYR
1	H	445	SER
1	H	627	VAL
1	I	136	THR
1	I	157	CYS
1	I	175	CYS
1	I	189	GLU
1	I	197	VAL
1	I	215	SER
1	I	223	ASN
1	I	236	THR
1	I	273	VAL
1	I	276	ILE
1	I	290	LEU
1	I	385	MET
1	I	390	LYS
1	I	421	TYR
1	I	445	SER
1	I	627	VAL
1	J	136	THR
1	J	157	CYS
1	J	175	CYS
1	J	189	GLU
1	J	197	VAL
1	J	215	SER
1	J	223	ASN
1	J	236	THR
1	J	273	VAL

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Mol	Chain	Res	Type
1	J	276	ILE
1	J	314	THR
1	J	385	MET
1	J	390	LYS
1	J	405	SER
1	J	421	TYR
1	J	422	VAL
1	J	445	SER
1	J	627	VAL
1	K	136	THR
1	K	157	CYS
1	K	175	CYS
1	K	189	GLU
1	K	197	VAL
1	K	215	SER
1	K	223	ASN
1	K	236	THR
1	K	273	VAL
1	K	276	ILE
1	K	385	MET
1	K	390	LYS
1	K	421	TYR
1	K	445	SER
1	K	480	ARG
1	K	627	VAL
1	L	136	THR
1	L	157	CYS
1	L	175	CYS
1	L	189	GLU
1	L	197	VAL
1	L	215	SER
1	L	223	ASN
1	L	236	THR
1	L	273	VAL
1	L	276	ILE
1	L	385	MET
1	L	390	LYS
1	L	405	SER
1	L	421	TYR
1	L	445	SER
1	L	627	VAL
1	M	136	THR

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Mol	Chain	Res	Type
1	M	157	CYS
1	M	175	CYS
1	M	189	GLU
1	M	197	VAL
1	M	215	SER
1	M	223	ASN
1	M	236	THR
1	M	273	VAL
1	M	276	ILE
1	M	290	LEU
1	M	385	MET
1	M	390	LYS
1	M	405	SER
1	M	421	TYR
1	M	445	SER
1	M	627	VAL
1	N	136	THR
1	N	157	CYS
1	N	175	CYS
1	N	189	GLU
1	N	197	VAL
1	N	215	SER
1	N	223	ASN
1	N	236	THR
1	N	273	VAL
1	N	276	ILE
1	N	385	MET
1	N	390	LYS
1	N	405	SER
1	N	421	TYR
1	N	445	SER
1	N	627	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	225	GLN
1	A	315	GLN
1	A	322	ASN
1	A	346	GLN
1	A	427	GLN

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Mol	Chain	Res	Type
1	A	526	GLN
1	A	599	GLN
1	A	658	GLN
1	A	672	GLN
1	A	684	HIS
1	B	179	ASN
1	B	225	GLN
1	B	315	GLN
1	B	322	ASN
1	B	346	GLN
1	B	427	GLN
1	B	478	GLN
1	B	526	GLN
1	B	716	ASN
1	C	137	ASN
1	C	179	ASN
1	C	225	GLN
1	C	315	GLN
1	C	322	ASN
1	C	346	GLN
1	C	427	GLN
1	C	478	GLN
1	C	526	GLN
1	C	684	HIS
1	C	716	ASN
1	D	179	ASN
1	D	225	GLN
1	D	315	GLN
1	D	346	GLN
1	D	427	GLN
1	D	478	GLN
1	D	526	GLN
1	D	716	ASN
1	E	149	ASN
1	E	179	ASN
1	E	225	GLN
1	E	315	GLN
1	E	322	ASN
1	E	346	GLN
1	E	427	GLN
1	E	478	GLN
1	E	526	GLN

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Mol	Chain	Res	Type
1	E	716	ASN
1	F	179	ASN
1	F	225	GLN
1	F	315	GLN
1	F	322	ASN
1	F	346	GLN
1	F	427	GLN
1	F	478	GLN
1	F	598	ASN
1	F	684	HIS
1	F	716	ASN
1	G	179	ASN
1	G	315	GLN
1	G	346	GLN
1	G	427	GLN
1	G	489	GLN
1	G	526	GLN
1	G	684	HIS
1	G	716	ASN
1	H	179	ASN
1	H	225	GLN
1	H	315	GLN
1	H	322	ASN
1	H	346	GLN
1	H	427	GLN
1	H	478	GLN
1	H	526	GLN
1	H	684	HIS
1	H	716	ASN
1	I	179	ASN
1	I	225	GLN
1	I	315	GLN
1	I	324	GLN
1	I	346	GLN
1	I	427	GLN
1	I	526	GLN
1	I	672	GLN
1	I	716	ASN
1	J	179	ASN
1	J	315	GLN
1	J	322	ASN
1	J	346	GLN

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Mol	Chain	Res	Type
1	J	427	GLN
1	J	526	GLN
1	J	594	GLN
1	J	716	ASN
1	K	179	ASN
1	K	225	GLN
1	K	315	GLN
1	K	322	ASN
1	K	324	GLN
1	K	346	GLN
1	K	427	GLN
1	K	526	GLN
1	K	598	ASN
1	K	684	HIS
1	K	716	ASN
1	L	179	ASN
1	L	315	GLN
1	L	346	GLN
1	L	427	GLN
1	L	478	GLN
1	L	526	GLN
1	L	599	GLN
1	L	658	GLN
1	L	682	ASN
1	L	684	HIS
1	M	179	ASN
1	M	225	GLN
1	M	315	GLN
1	M	322	ASN
1	M	346	GLN
1	M	427	GLN
1	M	478	GLN
1	M	526	GLN
1	M	684	HIS
1	M	716	ASN
1	N	179	ASN
1	N	315	GLN
1	N	322	ASN
1	N	346	GLN
1	N	427	GLN
1	N	526	GLN
1	N	684	HIS

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Mol	Chain	Res	Type
1	N	716	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [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%)	0.11	18 (3%)	51	42	29, 48, 92, 128	0
1	B	581/593 (97%)	0.22	28 (4%)	35	28	29, 50, 93, 132	0
1	C	581/593 (97%)	0.26	26 (4%)	38	30	28, 51, 94, 129	0
1	D	581/593 (97%)	0.49	55 (9%)	14	12	29, 49, 93, 128	0
1	E	581/593 (97%)	0.23	21 (3%)	46	38	31, 50, 94, 131	0
1	F	581/593 (97%)	0.40	32 (5%)	30	24	31, 53, 96, 130	0
1	G	581/593 (97%)	0.52	55 (9%)	14	12	31, 53, 96, 127	0
1	H	581/593 (97%)	0.19	15 (2%)	57	48	29, 51, 94, 132	0
1	I	581/593 (97%)	0.48	61 (10%)	11	10	29, 49, 89, 129	0
1	J	581/593 (97%)	0.32	25 (4%)	40	32	31, 51, 94, 128	0
1	K	581/593 (97%)	0.50	42 (7%)	21	17	33, 53, 96, 130	0
1	L	581/593 (97%)	0.26	20 (3%)	48	39	31, 51, 93, 128	0
1	M	581/593 (97%)	0.27	26 (4%)	38	30	31, 52, 92, 127	0
1	N	581/593 (97%)	0.32	27 (4%)	37	29	31, 52, 96, 132	0
All	All	8134/8302 (97%)	0.33	451 (5%)	30	24	28, 51, 94, 132	0

All (451) 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	5.4
1	F	301	ASP	5.3
1	B	478	GLN	5.3
1	D	236	THR	5.0
1	I	420	TYR	4.9
1	E	301	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	422	VAL	4.8
1	C	654	TYR	4.8
1	D	420	TYR	4.8
1	G	234	SER	4.7
1	N	478	GLN	4.7
1	I	421	TYR	4.6
1	C	236	THR	4.6
1	L	237	THR	4.6
1	J	233	ALA	4.5
1	C	239	ASP	4.5
1	G	237	THR	4.5
1	J	422	VAL	4.5
1	F	236	THR	4.5
1	C	420	TYR	4.5
1	C	234	SER	4.4
1	C	235	TYR	4.4
1	B	676	SER	4.4
1	D	301	ASP	4.4
1	D	240	ALA	4.3
1	I	234	SER	4.3
1	N	301	ASP	4.3
1	G	421	TYR	4.2
1	H	303	PRO	4.2
1	M	679	TYR	4.2
1	D	419	HIS	4.2
1	K	305	ALA	4.2
1	I	423	VAL	4.1
1	J	303	PRO	4.1
1	D	418	LYS	4.1
1	K	301	ASP	4.1
1	D	425	ALA	4.1
1	N	303	PRO	4.0
1	D	421	TYR	4.0
1	E	300	GLY	3.9
1	D	417	TYR	3.9
1	L	301	ASP	3.9
1	K	478	GLN	3.9
1	J	415	GLY	3.9
1	F	240	ALA	3.9
1	G	165	TRP	3.8
1	F	234	SER	3.8
1	I	236	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	567	ASP	3.8
1	E	415	GLY	3.8
1	N	300	GLY	3.8
1	I	298	VAL	3.8
1	I	631	GLY	3.8
1	A	587	SER	3.8
1	F	416	ALA	3.8
1	H	238	LEU	3.8
1	D	632	GLY	3.8
1	E	631	GLY	3.8
1	H	137	ASN	3.7
1	C	301	ASP	3.7
1	B	477	ALA	3.7
1	K	706	TRP	3.7
1	C	238	LEU	3.7
1	G	478	GLN	3.7
1	I	235	TYR	3.7
1	I	672	GLN	3.6
1	I	238	LEU	3.6
1	D	422	VAL	3.6
1	G	236	THR	3.6
1	H	306	LYS	3.5
1	I	311	ALA	3.5
1	G	679	TYR	3.5
1	H	301	ASP	3.5
1	I	237	THR	3.5
1	L	656	GLY	3.4
1	A	416	ALA	3.4
1	C	652	PHE	3.4
1	B	679	TYR	3.4
1	I	312	SER	3.4
1	I	633	SER	3.4
1	B	301	ASP	3.4
1	D	429	TYR	3.4
1	K	679	TYR	3.4
1	B	415	GLY	3.4
1	F	241	TYR	3.4
1	H	294	GLY	3.3
1	G	693	ALA	3.3
1	J	300	GLY	3.3
1	G	240	ALA	3.3
1	K	477	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	N	477	ALA	3.3
1	K	692	ASP	3.3
1	M	301	ASP	3.3
1	I	309	ALA	3.3
1	J	238	LEU	3.3
1	D	423	VAL	3.3
1	G	363	VAL	3.3
1	D	362	TRP	3.3
1	G	429	TYR	3.3
1	M	137	ASN	3.3
1	I	418	LYS	3.3
1	C	416	ALA	3.3
1	D	360	ALA	3.3
1	G	422	VAL	3.2
1	C	237	THR	3.2
1	E	237	THR	3.2
1	I	628	GLY	3.2
1	I	624	ASP	3.2
1	G	419	HIS	3.2
1	J	298	VAL	3.2
1	M	676	SER	3.2
1	K	604	GLN	3.2
1	C	303	PRO	3.2
1	J	234	SER	3.2
1	L	587	SER	3.2
1	J	137	ASN	3.2
1	I	630	ASN	3.1
1	B	298	VAL	3.1
1	I	424	GLY	3.1
1	G	276	ILE	3.1
1	K	303	PRO	3.1
1	I	240	ALA	3.1
1	I	632	GLY	3.1
1	F	235	TYR	3.1
1	G	303	PRO	3.1
1	F	622	ALA	3.1
1	G	420	TYR	3.1
1	G	238	LEU	3.1
1	G	360	ALA	3.0
1	G	423	VAL	3.0
1	J	235	TYR	3.0
1	D	239	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	301	ASP	3.0
1	L	588	PRO	3.0
1	G	164	LEU	3.0
1	M	238	LEU	3.0
1	D	242	PHE	3.0
1	D	233	ALA	3.0
1	G	242	PHE	3.0
1	D	241	TYR	3.0
1	I	670	ARG	3.0
1	E	420	TYR	2.9
1	A	716	ASN	2.9
1	G	301	ASP	2.9
1	I	233	ALA	2.9
1	G	417	TYR	2.9
1	N	235	TYR	2.9
1	D	363	VAL	2.9
1	H	305	ALA	2.9
1	N	420	TYR	2.9
1	I	295	GLY	2.9
1	I	306	LYS	2.9
1	N	298	VAL	2.9
1	B	236	THR	2.9
1	B	653	GLN	2.8
1	D	235	TYR	2.8
1	G	244	GLU	2.8
1	L	654	TYR	2.8
1	N	692	ASP	2.8
1	B	707	LEU	2.8
1	I	478	GLN	2.8
1	I	584	GLN	2.8
1	I	693	ALA	2.8
1	C	630	ASN	2.8
1	E	692	ASP	2.8
1	I	299	SER	2.8
1	F	692	ASP	2.8
1	I	692	ASP	2.8
1	K	302	GLY	2.8
1	I	305	ALA	2.8
1	G	426	HIS	2.8
1	C	653	GLN	2.7
1	F	584	GLN	2.7
1	M	652	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	313	TYR	2.7
1	D	366	TYR	2.7
1	B	136	THR	2.7
1	K	676	SER	2.7
1	G	415	GLY	2.7
1	D	286	SER	2.7
1	K	667	GLN	2.7
1	I	303	PRO	2.7
1	M	604	GLN	2.7
1	K	296	VAL	2.7
1	L	363	VAL	2.7
1	M	422	VAL	2.7
1	B	238	LEU	2.7
1	B	303	PRO	2.7
1	D	232	GLY	2.7
1	D	630	ASN	2.7
1	J	302	GLY	2.7
1	I	168	GLU	2.7
1	G	232	GLY	2.6
1	K	603	GLY	2.6
1	L	295	GLY	2.6
1	L	300	GLY	2.6
1	D	604	GLN	2.6
1	G	241	TYR	2.6
1	K	420	TYR	2.6
1	H	716	ASN	2.6
1	F	233	ALA	2.6
1	K	615	ALA	2.6
1	K	640	SER	2.6
1	G	609	TYR	2.6
1	H	295	GLY	2.6
1	K	295	GLY	2.6
1	N	294	GLY	2.6
1	J	168	GLU	2.6
1	F	614	ALA	2.6
1	I	301	ASP	2.6
1	J	299	SER	2.6
1	D	631	GLY	2.6
1	M	420	TYR	2.6
1	N	302	GLY	2.6
1	L	298	VAL	2.6
1	G	427	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	667	GLN	2.6
1	I	137	ASN	2.6
1	L	716	ASN	2.6
1	G	477	ALA	2.5
1	K	432	PHE	2.5
1	M	693	ALA	2.5
1	G	630	ASN	2.5
1	L	692	ASP	2.5
1	M	300	GLY	2.5
1	F	298	VAL	2.5
1	K	416	ALA	2.5
1	K	622	ALA	2.5
1	K	630	ASN	2.5
1	L	137	ASN	2.5
1	A	301	ASP	2.5
1	N	169	LYS	2.5
1	D	298	VAL	2.5
1	G	362	TRP	2.5
1	I	362	TRP	2.5
1	I	706	TRP	2.5
1	F	420	TYR	2.5
1	F	604	GLN	2.5
1	K	614	ALA	2.5
1	L	136	THR	2.5
1	K	137	ASN	2.5
1	J	692	ASP	2.5
1	A	656	GLY	2.5
1	D	234	SER	2.5
1	B	168	GLU	2.5
1	B	242	PHE	2.5
1	C	679	TYR	2.5
1	F	432	PHE	2.5
1	F	679	TYR	2.5
1	J	420	TYR	2.5
1	B	615	ALA	2.5
1	D	416	ALA	2.5
1	J	240	ALA	2.5
1	D	426	HIS	2.5
1	K	419	HIS	2.5
1	G	414	ASN	2.5
1	G	602	VAL	2.4
1	B	241	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	417	TYR	2.4
1	F	303	PRO	2.4
1	G	291	GLY	2.4
1	K	294	GLY	2.4
1	M	298	VAL	2.4
1	M	603	GLY	2.4
1	G	168	GLU	2.4
1	I	308	GLU	2.4
1	K	362	TRP	2.4
1	K	693	ALA	2.4
1	N	305	ALA	2.4
1	B	417	TYR	2.4
1	B	419	HIS	2.4
1	K	307	LEU	2.4
1	C	424	GLY	2.4
1	I	294	GLY	2.4
1	K	479	GLY	2.4
1	G	243	ARG	2.4
1	D	428	SER	2.4
1	G	664	PHE	2.4
1	D	165	TRP	2.4
1	G	365	THR	2.4
1	I	625	LEU	2.4
1	D	355	ASN	2.4
1	K	292	VAL	2.4
1	I	310	ARG	2.4
1	D	693	ALA	2.4
1	D	299	SER	2.4
1	G	228	TYR	2.4
1	F	625	LEU	2.4
1	K	625	LEU	2.4
1	B	423	VAL	2.3
1	L	306	LYS	2.3
1	A	631	GLY	2.3
1	I	232	GLY	2.3
1	L	294	GLY	2.3
1	E	240	ALA	2.3
1	F	612	ALA	2.3
1	A	357	SER	2.3
1	E	676	SER	2.3
1	N	234	SER	2.3
1	C	642	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	296	VAL	2.3
1	F	603	GLY	2.3
1	J	232	GLY	2.3
1	K	170	GLY	2.3
1	K	612	ALA	2.3
1	N	585	GLU	2.3
1	G	604	GLN	2.3
1	I	136	THR	2.3
1	E	243	ARG	2.3
1	C	641	GLY	2.3
1	J	424	GLY	2.3
1	M	620	GLY	2.3
1	A	432	PHE	2.3
1	H	432	PHE	2.3
1	C	351	GLU	2.3
1	G	416	ALA	2.3
1	G	425	ALA	2.3
1	A	653	GLN	2.3
1	C	304	LYS	2.3
1	L	234	SER	2.3
1	E	236	THR	2.3
1	F	237	THR	2.3
1	N	310	ARG	2.3
1	H	298	VAL	2.3
1	D	137	ASN	2.3
1	D	434	ASP	2.3
1	F	238	LEU	2.3
1	F	239	ASP	2.3
1	I	634	LEU	2.3
1	G	412	ILE	2.3
1	I	419	HIS	2.3
1	J	136	THR	2.3
1	L	420	TYR	2.3
1	C	298	VAL	2.3
1	D	368	VAL	2.3
1	I	300	GLY	2.3
1	I	231	PHE	2.2
1	F	360	ALA	2.2
1	M	584	GLN	2.2
1	N	601	ARG	2.2
1	K	318	TRP	2.2
1	E	234	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	298	VAL	2.2
1	K	298	VAL	2.2
1	A	693	ALA	2.2
1	G	306	LYS	2.2
1	M	303	PRO	2.2
1	M	706	TRP	2.2
1	A	241	TYR	2.2
1	F	415	GLY	2.2
1	E	242	PHE	2.2
1	E	425	ALA	2.2
1	I	304	LYS	2.2
1	I	694	ALA	2.2
1	F	419	HIS	2.2
1	M	370	VAL	2.2
1	D	294	GLY	2.2
1	B	166	LYS	2.2
1	J	164	LEU	2.2
1	D	168	GLU	2.2
1	E	168	GLU	2.2
1	J	243	ARG	2.2
1	G	716	ASN	2.2
1	N	598	ASN	2.2
1	D	692	ASP	2.2
1	F	422	VAL	2.2
1	G	692	ASP	2.2
1	D	314	THR	2.2
1	H	136	THR	2.2
1	F	232	GLY	2.2
1	M	295	GLY	2.2
1	N	318	TRP	2.2
1	K	304	LYS	2.2
1	A	235	TYR	2.2
1	I	361	LEU	2.2
1	I	623	SER	2.2
1	I	425	ALA	2.2
1	B	604	GLN	2.1
1	D	427	GLN	2.1
1	A	137	ASN	2.1
1	E	303	PRO	2.1
1	N	363	VAL	2.1
1	B	237	THR	2.1
1	C	365	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	300	GLY	2.1
1	F	431	GLY	2.1
1	L	236	THR	2.1
1	M	136	THR	2.1
1	N	136	THR	2.1
1	A	165	TRP	2.1
1	L	235	TYR	2.1
1	B	234	SER	2.1
1	K	491	SER	2.1
1	C	604	GLN	2.1
1	D	672	GLN	2.1
1	G	667	GLN	2.1
1	D	605	ASP	2.1
1	D	295	GLY	2.1
1	F	641	GLY	2.1
1	G	424	GLY	2.1
1	I	629	GLY	2.1
1	N	238	LEU	2.1
1	B	706	TRP	2.1
1	B	612	ALA	2.1
1	M	654	TYR	2.1
1	I	635	SER	2.1
1	N	586	SER	2.1
1	G	430	HIS	2.1
1	B	705	ASP	2.1
1	C	302	GLY	2.1
1	J	165	TRP	2.1
1	G	586	SER	2.1
1	I	428	SER	2.1
1	C	423	VAL	2.1
1	K	306	LYS	2.1
1	K	423	VAL	2.1
1	D	414	ASN	2.1
1	B	243	ARG	2.1
1	N	297	GLU	2.1
1	E	241	TYR	2.1
1	N	609	TYR	2.1
1	I	587	SER	2.0
1	A	584	GLN	2.0
1	J	363	VAL	2.0
1	K	475	VAL	2.0
1	M	680	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	691	PRO	2.0
1	C	361	LEU	2.0
1	D	682	ASN	2.0
1	E	167	ASN	2.0
1	M	656	GLY	2.0
1	D	365	THR	2.0
1	H	236	THR	2.0
1	E	568	ALA	2.0
1	E	362	TRP	2.0
1	M	168	GLU	2.0
1	F	429	TYR	2.0
1	G	235	TYR	2.0
1	A	586	SER	2.0
1	G	368	VAL	2.0
1	H	234	SER	2.0
1	J	419	HIS	2.0
1	M	426	HIS	2.0
1	N	634	LEU	2.0
1	D	291	GLY	2.0
1	A	358	THR	2.0
1	A	585	GLU	2.0
1	M	297	GLU	2.0
1	I	165	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.