



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 7EW5 / pdb_00007ew5
Title : immune complex of HPV6 L1 pentamer and neutralizing antibody 13H5
Authors : Wang, Z.P.; Wang, D.N.; Gu, Y.; Li, S.W.
Deposited on : 2021-05-24
Resolution : 3.61 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

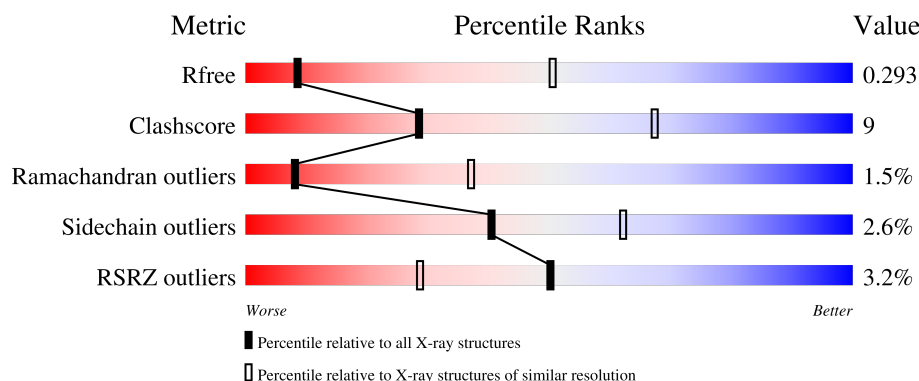
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	496	69% 14% • 16%
1	D	496	68% 15% • 16%
1	G	496	68% 15% • 16%
1	J	496	68% 15% • 16%
1	M	496	67% 16% • 16%

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Mol	Chain	Length	Quality of chain
1	P	496	
1	S	496	
1	V	496	
1	Y	496	
1	b	496	
2	B	221	
2	E	221	
2	H	221	
2	K	221	
2	N	221	
2	Q	221	
2	T	221	
2	W	221	
2	Z	221	
2	g	221	
3	C	214	
3	F	214	
3	I	214	
3	L	214	
3	O	214	
3	R	214	
3	U	214	
3	X	214	
3	a	214	
3	j	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 65550 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	D	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	G	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	J	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	M	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	P	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	S	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	V	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	Y	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	b	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q9W9C6
A	376	VAL	MET	conflict	UNP Q9W9C6
D	-2	MET	-	initiating methionine	UNP Q9W9C6
D	376	VAL	MET	conflict	UNP Q9W9C6
G	-2	MET	-	initiating methionine	UNP Q9W9C6
G	376	VAL	MET	conflict	UNP Q9W9C6
J	-2	MET	-	initiating methionine	UNP Q9W9C6
J	376	VAL	MET	conflict	UNP Q9W9C6
M	-2	MET	-	initiating methionine	UNP Q9W9C6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	376	VAL	MET	conflict	UNP Q9W9C6
P	-2	MET	-	initiating methionine	UNP Q9W9C6
P	376	VAL	MET	conflict	UNP Q9W9C6
S	-2	MET	-	initiating methionine	UNP Q9W9C6
S	376	VAL	MET	conflict	UNP Q9W9C6
V	-2	MET	-	initiating methionine	UNP Q9W9C6
V	376	VAL	MET	conflict	UNP Q9W9C6
Y	-2	MET	-	initiating methionine	UNP Q9W9C6
Y	376	VAL	MET	conflict	UNP Q9W9C6
b	-2	MET	-	initiating methionine	UNP Q9W9C6
b	376	VAL	MET	conflict	UNP Q9W9C6

- Molecule 2 is a protein called Heavy chain of 13H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	E	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	H	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	K	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	N	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	g	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	Q	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	T	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	W	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	Z	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			

- Molecule 3 is a protein called Light chain of 13H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	F	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			

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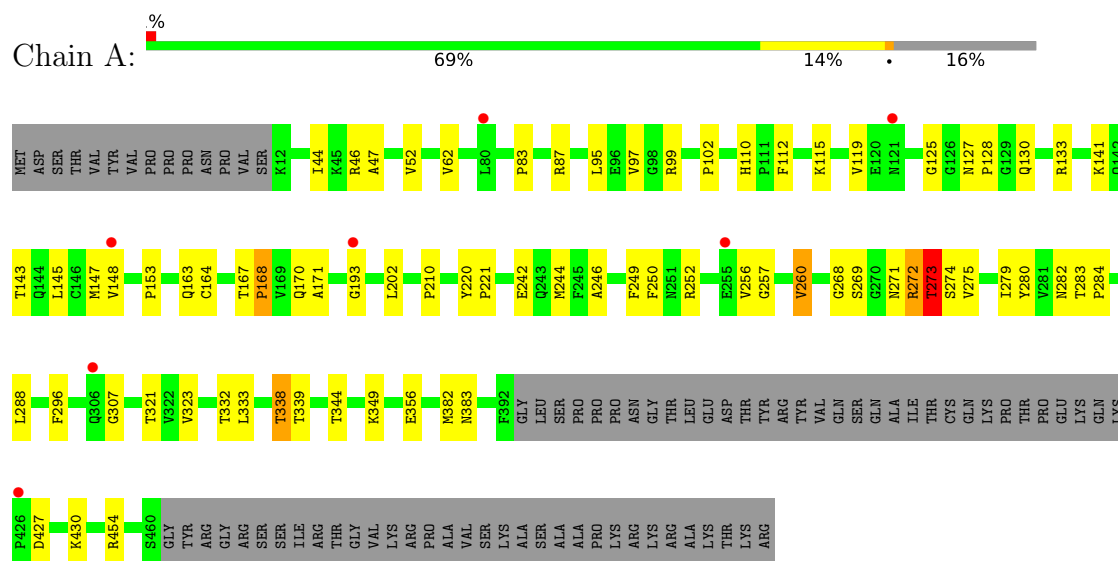
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	L	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	O	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	j	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	R	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	U	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	X	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	a	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			

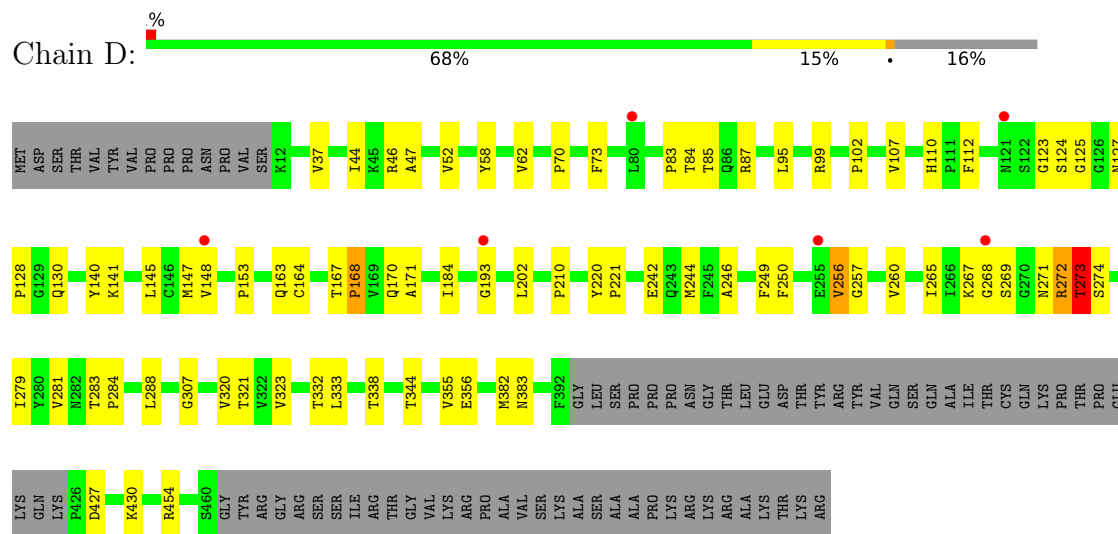
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Major capsid protein L1

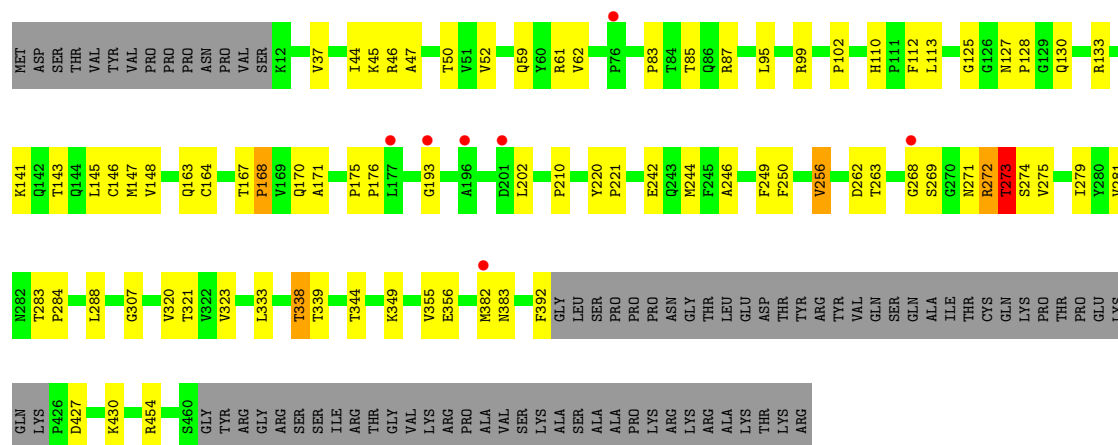


• Molecule 1: Major capsid protein L1

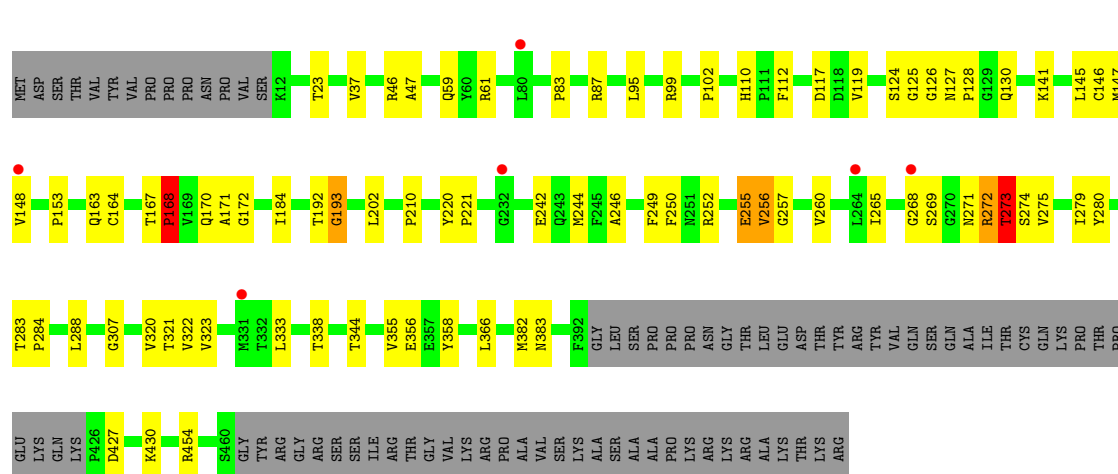


• Molecule 1: Major capsid protein L1

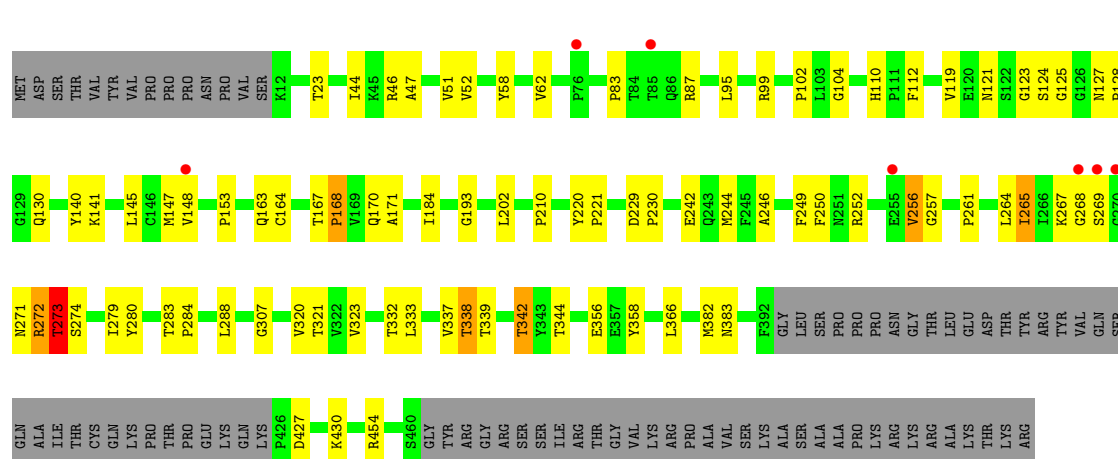




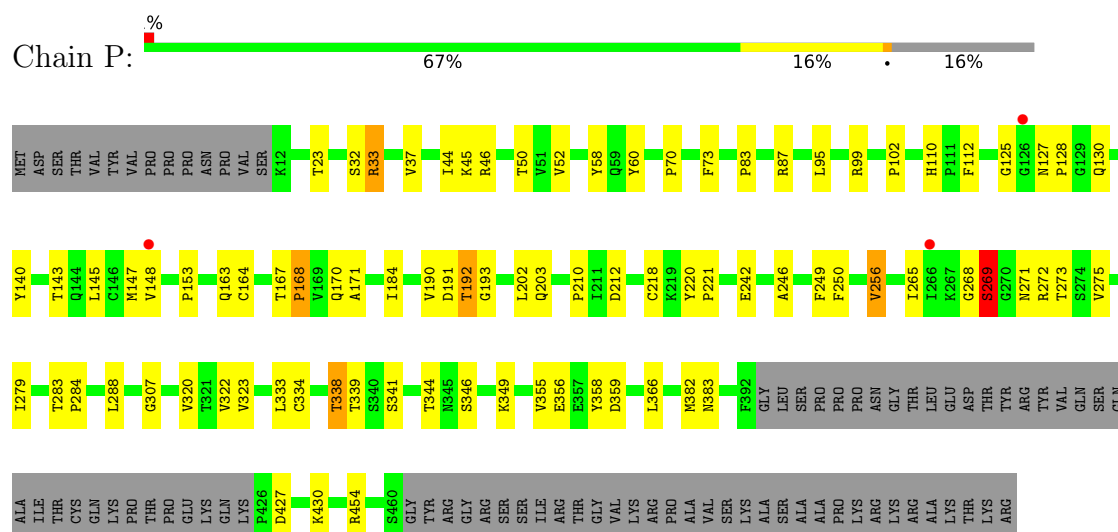
• Molecule 1: Major capsid protein L1



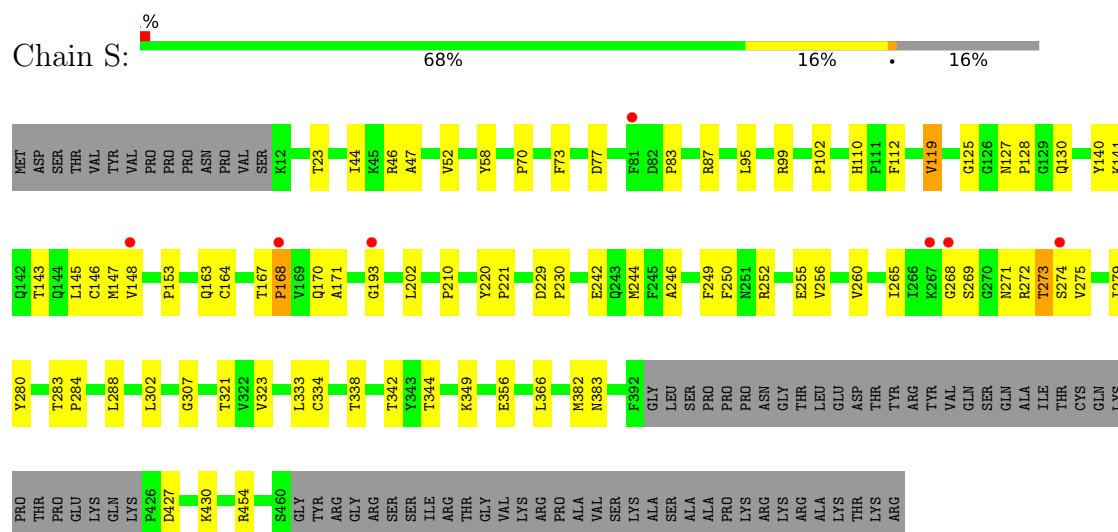
• Molecule 1: Major capsid protein L1



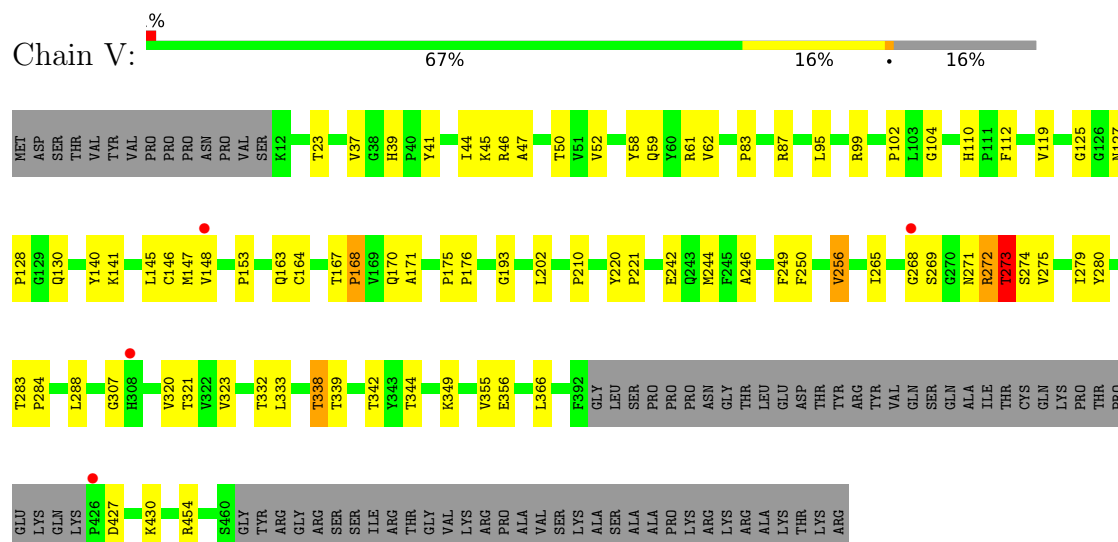
• Molecule 1: Major capsid protein L1



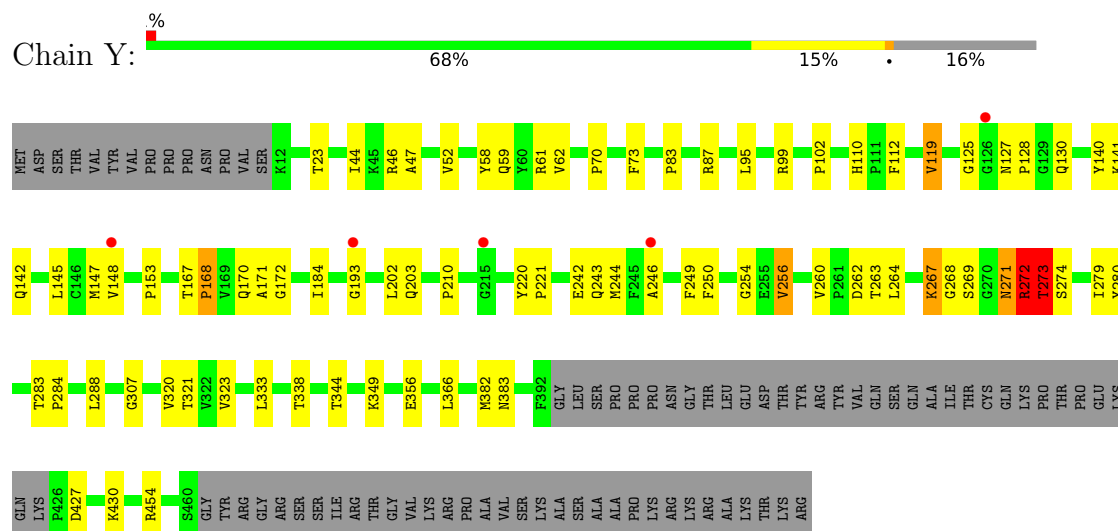
- Molecule 1: Major capsid protein L1



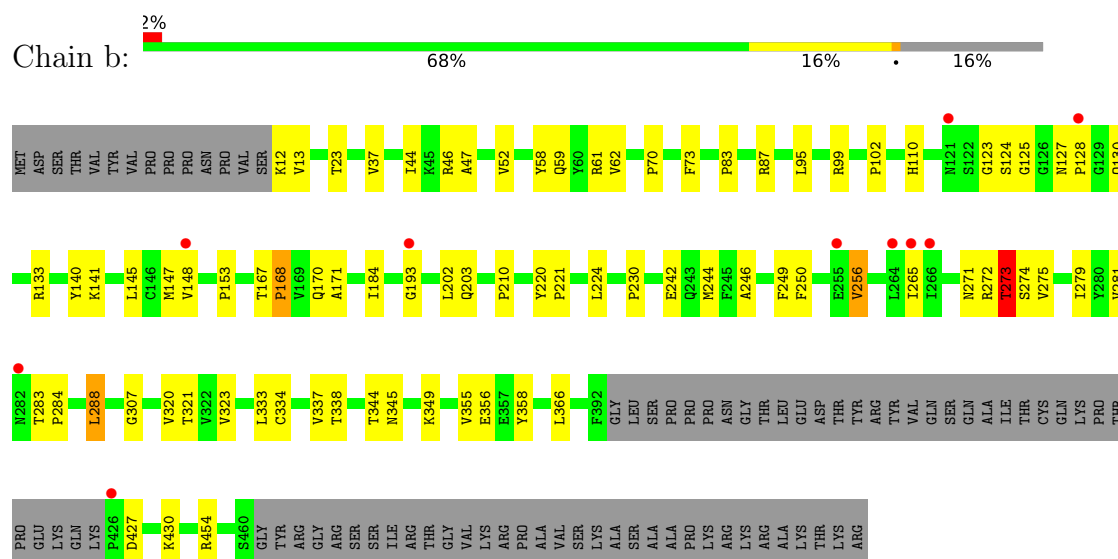
- Molecule 1: Major capsid protein L1



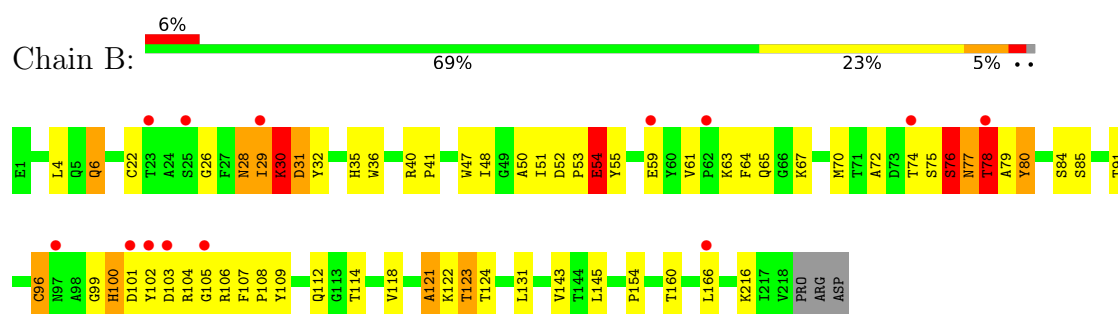
- Molecule 1: Major capsid protein L1



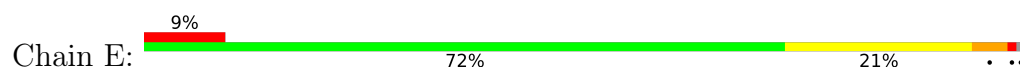
- Molecule 1: Major capsid protein L1

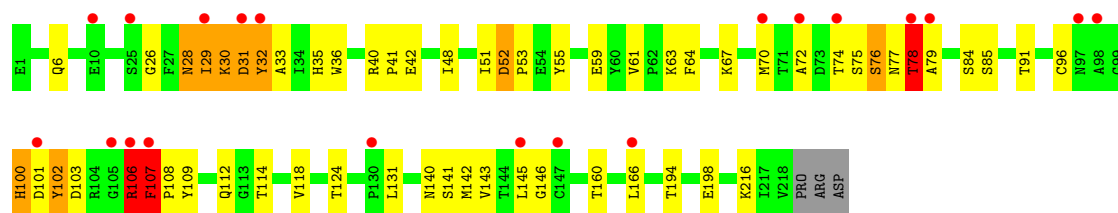


- Molecule 2: Heavy chain of 13H5

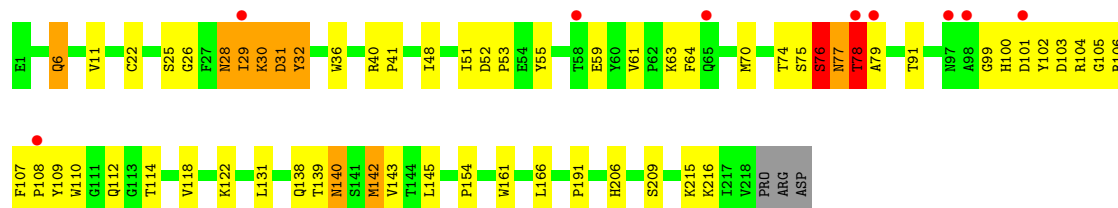


- Molecule 2: Heavy chain of 13H5

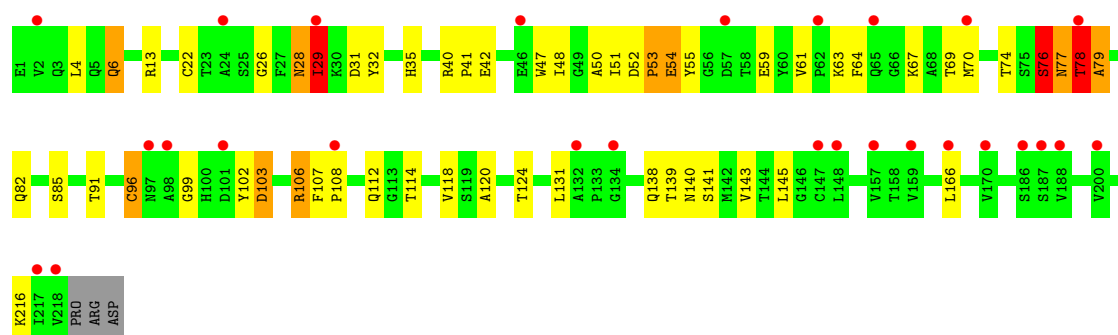
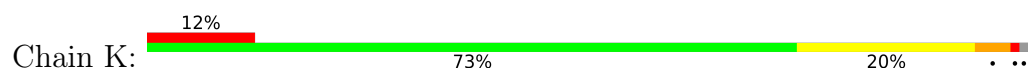




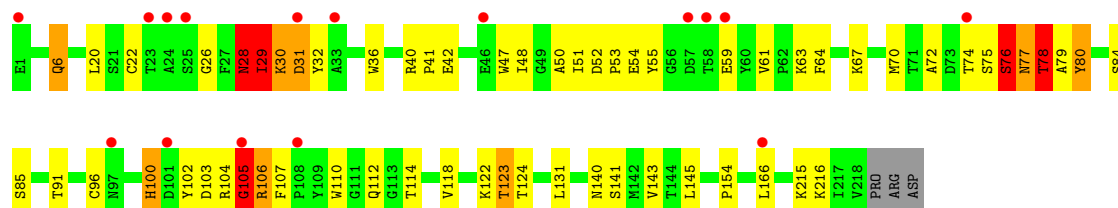
• Molecule 2: Heavy chain of 13H5



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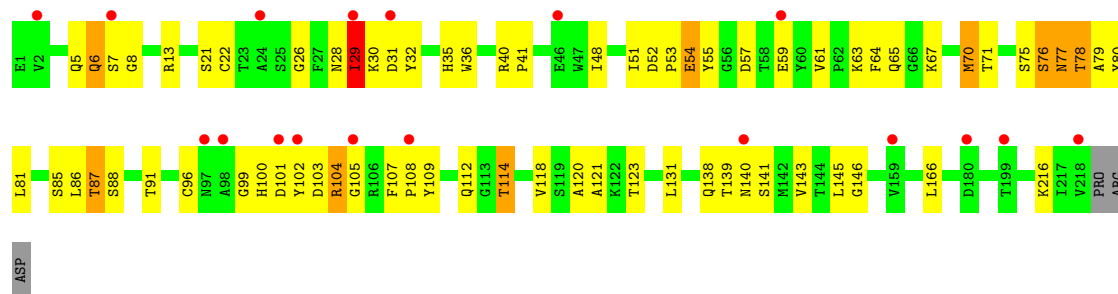


• Molecule 2: Heavy chain of 13H5

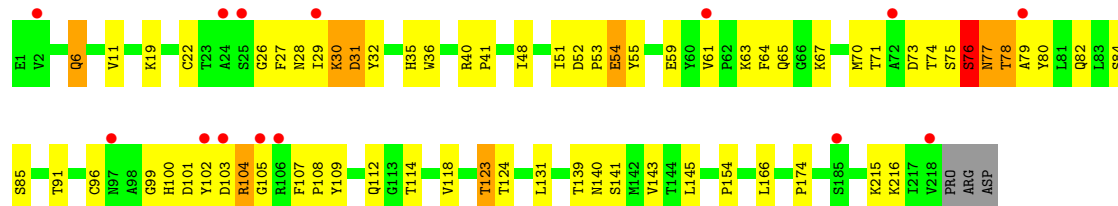




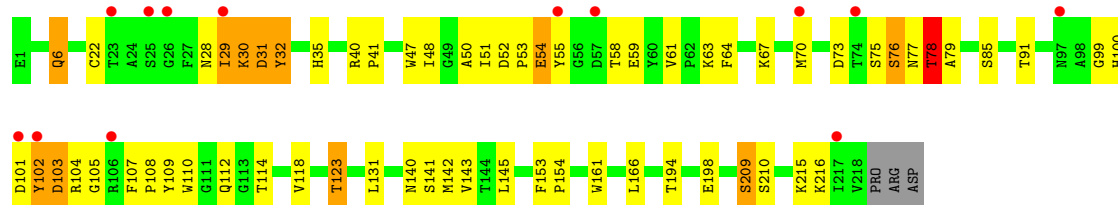
• Molecule 2: Heavy chain of 13H5



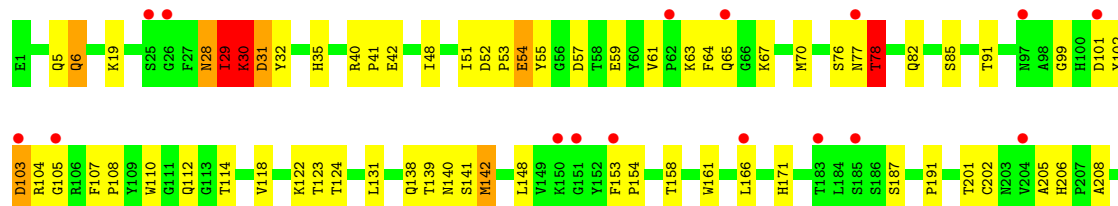
• Molecule 2: Heavy chain of 13H5



• Molecule 2: Heavy chain of 13H5

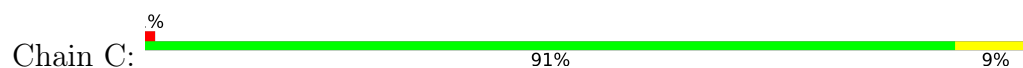


• Molecule 2: Heavy chain of 13H5

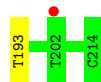
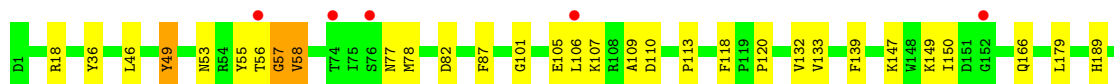
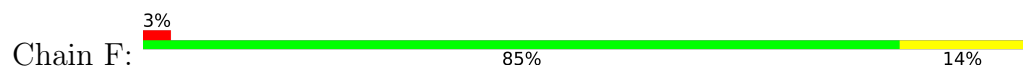




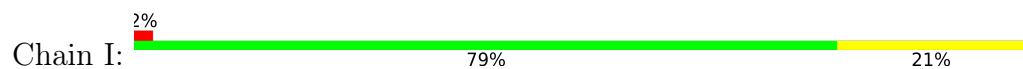
- Molecule 3: Light chain of 13H5



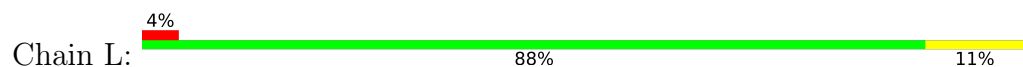
- Molecule 3: Light chain of 13H5



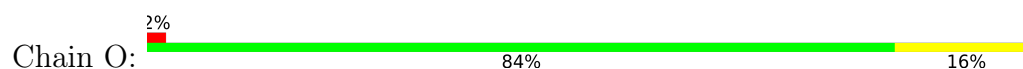
- Molecule 3: Light chain of 13H5



- Molecule 3: Light chain of 13H5

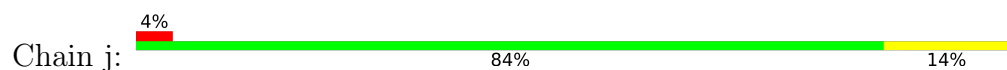


- Molecule 3: Light chain of 13H5

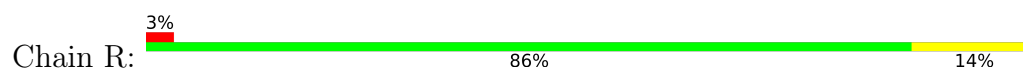




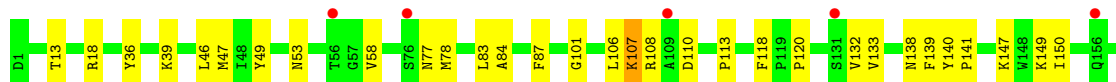
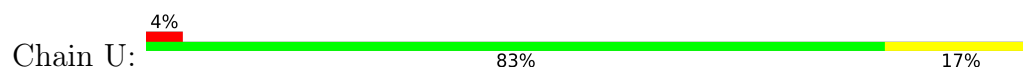
- Molecule 3: Light chain of 13H5



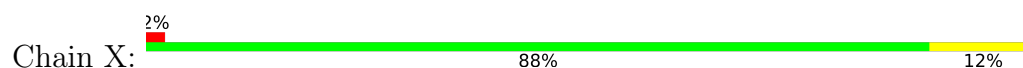
- Molecule 3: Light chain of 13H5



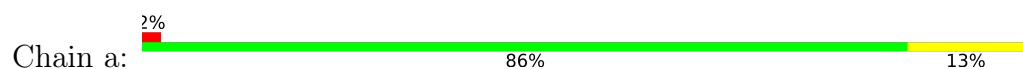
- Molecule 3: Light chain of 13H5



- Molecule 3: Light chain of 13H5



- Molecule 3: Light chain of 13H5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.09Å 208.31Å 205.95Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	49.02 – 3.61 49.02 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.02-3.61) 99.5 (49.02-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.31	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.252 , 0.293 0.251 , 0.293	Depositor DCC
R_{free} test set	6719 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	65550	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/3342	0.35	0/4544
1	D	0.12	0/3342	0.34	0/4544
1	G	0.11	0/3342	0.35	0/4544
1	J	0.12	0/3342	0.35	0/4544
1	M	0.12	0/3342	0.35	0/4544
1	P	0.12	0/3342	0.35	0/4544
1	S	0.12	0/3342	0.35	0/4544
1	V	0.12	0/3342	0.35	0/4544
1	Y	0.11	0/3342	0.34	0/4544
1	b	0.12	0/3342	0.35	0/4544
2	B	0.17	0/1686	0.60	6/2309 (0.3%)
2	E	0.18	0/1686	0.61	7/2309 (0.3%)
2	H	0.17	0/1686	0.58	4/2309 (0.2%)
2	K	0.17	0/1686	0.57	2/2309 (0.1%)
2	N	0.18	0/1686	0.61	6/2309 (0.3%)
2	Q	0.18	0/1686	0.59	2/2309 (0.1%)
2	T	0.17	0/1686	0.57	4/2309 (0.2%)
2	W	0.17	0/1686	0.60	6/2309 (0.3%)
2	Z	0.16	0/1686	0.56	2/2309 (0.1%)
2	g	0.18	0/1686	0.61	4/2309 (0.2%)
3	C	0.11	0/1688	0.35	0/2286
3	F	0.11	0/1688	0.46	4/2286 (0.2%)
3	I	0.10	0/1688	0.33	0/2286
3	L	0.10	0/1688	0.32	0/2286
3	O	0.10	0/1688	0.32	0/2286
3	R	0.12	0/1688	0.35	0/2286
3	U	0.10	0/1688	0.37	0/2286
3	X	0.10	0/1688	0.30	0/2286
3	a	0.11	0/1688	0.32	0/2286
3	j	0.12	0/1688	0.39	0/2286
All	All	0.13	0/67160	0.42	47/91390 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
2	E	0	2
2	H	0	2
2	N	0	2
2	T	0	2
2	W	0	1
2	Z	0	2
2	g	0	2
3	F	0	1
All	All	0	17

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	76	SER	CA-C-N	9.88	139.48	121.70
2	K	76	SER	C-N-CA	9.88	139.48	121.70
2	Q	76	SER	CA-C-N	8.40	136.82	121.70
2	Q	76	SER	C-N-CA	8.40	136.82	121.70
2	T	30	LYS	CA-C-N	8.32	136.67	121.70
2	T	30	LYS	C-N-CA	8.32	136.67	121.70
2	g	30	LYS	CA-C-N	7.82	135.77	121.70
2	g	30	LYS	C-N-CA	7.82	135.77	121.70
2	B	76	SER	CA-C-N	7.61	136.07	121.54
2	B	76	SER	C-N-CA	7.61	136.07	121.54
2	N	105	GLY	CA-C-N	7.51	135.22	121.70
2	N	105	GLY	C-N-CA	7.51	135.22	121.70
2	N	30	LYS	CA-C-N	7.38	134.98	121.70
2	N	30	LYS	C-N-CA	7.38	134.98	121.70
2	T	76	SER	CA-C-N	7.32	135.51	121.54
2	T	76	SER	C-N-CA	7.32	135.51	121.54
2	N	76	SER	CA-C-N	7.29	135.47	121.54
2	N	76	SER	C-N-CA	7.29	135.47	121.54
2	W	76	SER	CA-C-N	7.29	134.82	121.70
2	W	76	SER	C-N-CA	7.29	134.82	121.70
2	E	30	LYS	CA-C-N	7.28	134.80	121.70
2	E	30	LYS	C-N-CA	7.28	134.80	121.70
2	W	30	LYS	CA-C-N	7.25	134.75	121.70
2	W	30	LYS	C-N-CA	7.25	134.75	121.70
3	F	58	VAL	N-CA-C	-7.24	90.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	76	SER	CA-C-N	7.24	135.37	121.54
2	H	76	SER	C-N-CA	7.24	135.37	121.54
2	g	76	SER	CA-C-N	7.23	135.34	121.54
2	g	76	SER	C-N-CA	7.23	135.34	121.54
2	E	107	PHE	CA-C-N	7.15	144.16	127.00
2	E	107	PHE	C-N-CA	7.15	144.16	127.00
2	Z	30	LYS	CA-C-N	7.12	134.51	121.70
2	Z	30	LYS	C-N-CA	7.12	134.51	121.70
2	B	30	LYS	CA-C-N	7.05	134.39	121.70
2	B	30	LYS	C-N-CA	7.05	134.39	121.70
2	H	30	LYS	CA-C-N	6.92	134.16	121.70
2	H	30	LYS	C-N-CA	6.92	134.16	121.70
2	E	107	PHE	C-N-CD	-6.65	105.98	120.60
3	F	57	GLY	N-CA-C	-5.90	99.20	113.18
2	W	102	TYR	CA-C-N	5.58	132.20	121.54
2	W	102	TYR	C-N-CA	5.58	132.20	121.54
2	E	106	ARG	CA-C-N	5.54	131.67	121.70
2	E	106	ARG	C-N-CA	5.54	131.67	121.70
3	F	57	GLY	CA-C-N	5.51	131.61	121.70
3	F	57	GLY	C-N-CA	5.51	131.61	121.70
2	B	121	ALA	CA-C-N	5.24	131.13	121.70
2	B	121	ALA	C-N-CA	5.24	131.13	121.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	30	LYS	Peptide
2	B	76	SER	Peptide
2	B	78	THR	Peptide
2	E	76	SER	Peptide
2	E	78	THR	Peptide
3	F	57	GLY	Peptide
2	H	76	SER	Peptide
2	H	78	THR	Peptide
2	N	76	SER	Peptide
2	N	78	THR	Peptide
2	T	76	SER	Peptide
2	T	78	THR	Peptide
2	W	78	THR	Peptide
2	Z	30	LYS	Peptide
2	Z	78	THR	Peptide

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Mol	Chain	Res	Type	Group
2	g	76	SER	Peptide
2	g	78	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3258	0	3150	55	0
1	D	3258	0	3150	56	0
1	G	3258	0	3150	56	0
1	J	3258	0	3150	58	0
1	M	3258	0	3150	63	0
1	P	3258	0	3150	62	0
1	S	3258	0	3150	57	1
1	V	3258	0	3150	61	0
1	Y	3258	0	3150	60	0
1	b	3258	0	3150	59	0
2	B	1643	0	1590	55	0
2	E	1643	0	1590	50	0
2	H	1643	0	1590	46	0
2	K	1643	0	1590	43	0
2	N	1643	0	1590	59	0
2	Q	1643	0	1590	54	1
2	T	1643	0	1590	55	0
2	W	1643	0	1590	53	0
2	Z	1643	0	1590	50	0
2	g	1643	0	1590	50	0
3	C	1654	0	1582	15	0
3	F	1654	0	1582	22	1
3	I	1654	0	1582	30	1
3	L	1654	0	1582	17	0
3	O	1654	0	1582	25	0
3	R	1654	0	1582	19	0
3	U	1654	0	1582	27	0
3	X	1654	0	1582	20	0
3	a	1654	0	1582	22	0
3	j	1654	0	1582	23	0
All	All	65550	0	63220	1133	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:LYS:HA	2:H:31:ASP:HB2	1.52	0.90
3:U:83:LEU:HD21	3:U:106:LEU:HG	1.53	0.89
1:b:349:LYS:HE2	2:g:101:ASP:OD2	1.75	0.87
2:E:30:LYS:HA	2:E:31:ASP:HB2	1.55	0.86
2:W:30:LYS:HA	2:W:31:ASP:HB2	1.57	0.86
3:U:106:LEU:HB2	3:U:166:GLN:HE22	1.37	0.85
2:W:91:THR:HG22	2:W:118:VAL:H	1.42	0.84
1:S:349:LYS:HE2	2:T:101:ASP:OD2	1.79	0.83
3:I:83:LEU:HD21	3:I:106:LEU:HG	1.60	0.83
2:g:30:LYS:HA	2:g:31:ASP:HB2	1.60	0.83
2:Z:142:MET:HG2	2:Z:191:PRO:HA	1.61	0.83
2:H:76:SER:HB2	2:H:77:ASN:HB2	1.62	0.82
2:B:91:THR:HG22	2:B:118:VAL:H	1.43	0.82
2:Z:91:THR:HG22	2:Z:118:VAL:H	1.45	0.82
2:g:22:CYS:HB3	2:g:79:ALA:H	1.46	0.81
1:Y:349:LYS:HE2	2:Z:101:ASP:OD2	1.80	0.81
2:Q:91:THR:HG22	2:Q:118:VAL:H	1.45	0.81
2:T:91:THR:HG22	2:T:118:VAL:H	1.45	0.80
3:R:105:GLU:OE2	3:R:173:TYR:OH	2.00	0.80
2:H:91:THR:HG22	2:H:118:VAL:H	1.46	0.79
1:G:349:LYS:HE2	2:H:101:ASP:OD2	1.83	0.79
2:N:91:THR:HG22	2:N:118:VAL:H	1.46	0.79
2:T:30:LYS:HA	2:T:31:ASP:HB2	1.63	0.78
2:g:91:THR:HG22	2:g:118:VAL:H	1.49	0.78
2:B:121:ALA:HB1	2:B:122:LYS:HA	1.65	0.78
2:B:28:ASN:OD1	2:B:28:ASN:N	2.17	0.78
2:E:91:THR:HG22	2:E:118:VAL:H	1.48	0.77
2:H:28:ASN:N	2:H:28:ASN:OD1	2.17	0.77
2:B:6:GLN:HG3	2:B:112:GLN:HG2	1.66	0.77
2:K:6:GLN:HG3	2:K:112:GLN:HG2	1.67	0.77
2:T:22:CYS:HB3	2:T:79:ALA:H	1.49	0.77
1:A:349:LYS:HE2	2:B:101:ASP:OD2	1.85	0.77
2:E:108:PRO:HB3	3:F:46:LEU:HB3	1.67	0.76
1:P:349:LYS:HE2	2:Q:101:ASP:OD2	1.86	0.76
1:Y:272:ARG:O	1:Y:274:SER:N	2.18	0.75
3:I:106:LEU:HB2	3:I:166:GLN:HE22	1.50	0.75
2:g:73:ASP:H	2:g:78:THR:HG21	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:91:THR:HG22	2:K:118:VAL:H	1.51	0.75
2:E:6:GLN:HG3	2:E:112:GLN:HG2	1.69	0.74
2:N:30:LYS:HA	2:N:31:ASP:HB2	1.69	0.74
2:N:28:ASN:O	2:N:30:LYS:N	2.20	0.74
1:A:275:VAL:HG22	1:D:112:PHE:HE2	1.53	0.74
2:K:77:ASN:O	2:K:78:THR:OG1	2.04	0.74
2:g:6:GLN:HG3	2:g:112:GLN:HG2	1.70	0.74
1:P:341:SER:O	1:Y:267:LYS:NZ	2.20	0.73
2:W:6:GLN:HG3	2:W:112:GLN:HG2	1.70	0.73
2:E:100:HIS:HB3	2:E:109:TYR:HE2	1.52	0.73
2:Z:6:GLN:HG3	2:Z:112:GLN:HG2	1.71	0.73
2:W:209:SER:OG	2:W:210:SER:N	2.21	0.72
2:B:51:ILE:HG13	2:B:70:MET:HE2	1.69	0.72
2:K:26:GLY:HA3	2:K:78:THR:HG21	1.71	0.72
2:W:76:SER:HB3	2:W:77:ASN:HB2	1.71	0.72
2:Q:70:MET:HE2	2:Q:81:LEU:HD13	1.70	0.72
2:K:28:ASN:OD1	2:K:28:ASN:N	2.20	0.71
2:g:72:ALA:HA	2:g:78:THR:HG21	1.71	0.71
2:T:51:ILE:HG13	2:T:70:MET:HE2	1.72	0.70
1:V:349:LYS:HE2	2:W:101:ASP:OD2	1.90	0.70
2:Q:75:SER:O	2:Q:77:ASN:HB2	1.92	0.70
2:T:30:LYS:HA	2:T:31:ASP:CB	2.20	0.70
1:G:193:GLY:HA3	1:G:284:PRO:HG3	1.74	0.70
1:V:275:VAL:HG22	1:Y:112:PHE:HE2	1.56	0.70
2:g:51:ILE:HG13	2:g:70:MET:HE2	1.73	0.70
1:D:202:LEU:HB3	1:G:333:LEU:HD22	1.73	0.69
2:T:78:THR:HB	2:T:79:ALA:HA	1.73	0.69
1:b:193:GLY:HA3	1:b:284:PRO:HG3	1.73	0.69
2:K:51:ILE:HG13	2:K:70:MET:HE2	1.74	0.69
2:K:131:LEU:HD13	3:L:133:VAL:HG21	1.75	0.69
2:T:6:GLN:HG3	2:T:112:GLN:HG2	1.75	0.69
1:S:255:GLU:OE2	2:W:102:TYR:HB3	1.93	0.69
2:E:51:ILE:HG13	2:E:70:MET:HE2	1.73	0.69
2:N:6:GLN:HG3	2:N:112:GLN:HG2	1.73	0.69
2:N:131:LEU:HD13	3:O:133:VAL:HG21	1.74	0.69
2:g:131:LEU:HD13	3:j:133:VAL:HG21	1.73	0.69
1:J:427:ASP:HB3	1:J:430:LYS:HG3	1.75	0.68
2:T:73:ASP:H	2:T:78:THR:HG21	1.56	0.68
3:C:108:ARG:HH11	3:C:109:ALA:H	1.41	0.68
1:D:272:ARG:O	1:D:274:SER:N	2.23	0.68
1:S:273:THR:HG21	2:W:59:GLU:OE2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:193:GLY:HA3	1:V:284:PRO:HG3	1.75	0.68
2:N:51:ILE:HG13	2:N:70:MET:HE2	1.76	0.68
2:B:131:LEU:HD13	3:C:133:VAL:HG21	1.74	0.68
2:E:131:LEU:HD13	3:F:133:VAL:HG21	1.76	0.68
2:Z:67:LYS:NZ	2:Z:85:SER:O	2.24	0.68
2:Q:6:GLN:HG3	2:Q:112:GLN:HG2	1.75	0.68
1:Y:130:GLN:HG3	1:b:344:THR:HG22	1.76	0.67
1:A:250:PHE:HE1	1:A:283:THR:HG23	1.60	0.67
1:J:275:VAL:HG22	1:M:112:PHE:HE2	1.58	0.67
1:A:193:GLY:HA3	1:A:284:PRO:HG3	1.77	0.67
2:H:6:GLN:HG3	2:H:112:GLN:HG2	1.75	0.67
2:W:131:LEU:HD13	3:X:133:VAL:HG21	1.75	0.67
1:P:112:PHE:HE2	1:b:275:VAL:HG22	1.60	0.67
2:g:52:ASP:HB3	2:g:57:ASP:HB2	1.75	0.67
2:E:108:PRO:HB3	3:F:46:LEU:CB	2.25	0.67
2:Z:131:LEU:HD13	3:a:133:VAL:HG21	1.75	0.67
2:Q:131:LEU:HD13	3:R:133:VAL:HG21	1.76	0.66
3:a:110:ASP:N	3:a:110:ASP:OD1	2.27	0.66
1:G:272:ARG:O	1:G:274:SER:N	2.26	0.66
1:J:272:ARG:O	1:J:274:SER:N	2.22	0.66
2:T:131:LEU:HD13	3:U:133:VAL:HG21	1.76	0.66
2:g:30:LYS:HA	2:g:31:ASP:CB	2.26	0.66
2:E:198:GLU:OE2	2:Z:5:GLN:NE2	2.28	0.65
1:S:99:ARG:NH2	1:S:356:GLU:OE1	2.30	0.65
2:H:131:LEU:HD13	3:I:133:VAL:HG21	1.78	0.65
1:A:272:ARG:O	1:A:274:SER:N	2.28	0.65
2:H:51:ILE:HG13	2:H:70:MET:HE2	1.78	0.65
2:Z:107:PHE:HB2	3:a:36:TYR:HE1	1.61	0.64
3:j:109:ALA:HB1	3:j:110:ASP:HA	1.79	0.64
2:T:77:ASN:HB3	2:T:78:THR:HG23	1.78	0.64
1:Y:272:ARG:NH2	1:b:133:ARG:O	2.29	0.64
2:Q:120:ALA:HB1	2:Q:121:ALA:HB2	1.78	0.64
1:J:202:LEU:HB3	1:M:333:LEU:HD22	1.80	0.64
2:Z:51:ILE:HG13	2:Z:70:MET:HE2	1.78	0.64
1:J:141:LYS:HB3	1:J:192:THR:O	1.97	0.64
2:N:105:GLY:HA3	2:N:106:ARG:HG3	1.79	0.64
1:b:250:PHE:HE1	1:b:283:THR:HG23	1.61	0.64
2:N:22:CYS:HB3	2:N:79:ALA:H	1.62	0.64
1:G:83:PRO:O	1:G:87:ARG:NH1	2.31	0.64
2:K:22:CYS:HB3	2:K:79:ALA:HB3	1.80	0.64
1:V:250:PHE:HE1	1:V:283:THR:HG23	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:193:GLY:HA3	1:Y:284:PRO:HG3	1.78	0.63
1:A:115:LYS:NZ	1:M:121:ASN:O	2.30	0.63
2:Q:40:ARG:HH11	2:Q:41:PRO:HD2	1.63	0.63
1:G:275:VAL:HG22	1:J:112:PHE:HE2	1.63	0.63
2:B:107:PHE:HB2	3:C:36:TYR:HE1	1.63	0.62
1:S:193:GLY:HA3	1:S:284:PRO:HG3	1.81	0.62
1:b:141:LYS:HE3	1:b:242:GLU:HB3	1.81	0.62
3:R:105:GLU:OE2	3:R:142:LYS:HD3	1.99	0.62
1:J:99:ARG:NH2	1:J:356:GLU:OE1	2.33	0.62
1:P:265:ILE:HD11	2:T:55:TYR:CE1	2.34	0.62
2:K:61:VAL:HG12	2:K:63:LYS:H	1.63	0.62
2:Z:104:ARG:HG3	3:a:91:TYR:HB2	1.81	0.62
1:P:269:SER:HB2	1:P:272:ARG:HG3	1.82	0.62
1:P:344:THR:HG22	1:b:130:GLN:HG3	1.82	0.62
1:J:167:THR:HB	1:J:168:PRO:HB3	1.82	0.62
1:S:141:LYS:HE3	1:S:242:GLU:HB3	1.82	0.61
2:N:61:VAL:HG12	2:N:63:LYS:H	1.65	0.61
2:g:104:ARG:HG3	3:j:91:TYR:HB2	1.80	0.61
2:Q:36:TRP:HB2	2:Q:70:MET:HE1	1.81	0.61
2:Z:76:SER:OG	2:Z:77:ASN:N	2.33	0.61
1:J:130:GLN:HG3	1:M:344:THR:HG22	1.82	0.61
1:V:202:LEU:HB3	1:Y:333:LEU:HD22	1.83	0.61
1:V:272:ARG:O	1:V:274:SER:N	2.25	0.61
1:D:250:PHE:HE1	1:D:283:THR:HG23	1.65	0.61
2:T:73:ASP:H	2:T:78:THR:CG2	2.13	0.61
2:W:40:ARG:HH11	2:W:41:PRO:HD2	1.65	0.61
2:g:40:ARG:HH11	2:g:41:PRO:HD2	1.65	0.61
2:T:40:ARG:HH11	2:T:41:PRO:HD2	1.65	0.61
1:D:141:LYS:HE3	1:D:242:GLU:HB3	1.82	0.61
2:B:40:ARG:HH11	2:B:41:PRO:HD2	1.64	0.61
2:H:140:ASN:N	2:H:140:ASN:OD1	2.33	0.61
2:Z:61:VAL:HG12	2:Z:63:LYS:H	1.65	0.61
2:E:30:LYS:HA	2:E:31:ASP:CB	2.31	0.61
3:U:120:PRO:HD3	3:U:132:VAL:HG22	1.82	0.61
2:Z:29:ILE:O	2:Z:30:LYS:HE3	2.01	0.61
3:F:120:PRO:HD3	3:F:132:VAL:HG22	1.83	0.60
2:K:102:TYR:CG	2:K:103:ASP:N	2.68	0.60
1:S:147:MET:HE1	1:S:221:PRO:HB3	1.82	0.60
1:Y:250:PHE:HE1	1:Y:283:THR:HG23	1.64	0.60
1:A:333:LEU:HD22	1:M:202:LEU:HB3	1.82	0.60
2:g:102:TYR:CG	2:g:103:ASP:N	2.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:250:PHE:HE1	1:M:283:THR:HG23	1.66	0.60
1:M:272:ARG:O	1:M:274:SER:N	2.27	0.60
2:Z:40:ARG:HH11	2:Z:41:PRO:HD2	1.65	0.60
2:H:61:VAL:HG12	2:H:63:LYS:H	1.66	0.60
2:T:61:VAL:HG12	2:T:63:LYS:H	1.67	0.60
3:U:46:LEU:HD21	3:U:49:TYR:HD2	1.65	0.60
2:Z:30:LYS:HA	2:Z:31:ASP:CB	2.31	0.60
1:P:333:LEU:HD22	1:b:202:LEU:HB3	1.82	0.60
2:g:61:VAL:HG12	2:g:63:LYS:H	1.67	0.60
2:Q:61:VAL:HG12	2:Q:63:LYS:H	1.66	0.60
2:W:61:VAL:HG12	2:W:63:LYS:H	1.67	0.60
1:P:202:LEU:HB3	1:S:333:LEU:HD22	1.84	0.60
2:E:40:ARG:HH11	2:E:41:PRO:HD2	1.67	0.60
2:T:67:LYS:NZ	2:T:85:SER:O	2.34	0.60
1:M:145:LEU:HD13	1:M:147:MET:HE3	1.83	0.60
1:S:202:LEU:HB3	1:V:333:LEU:HD22	1.83	0.60
2:K:40:ARG:HH11	2:K:41:PRO:HD2	1.67	0.60
1:A:99:ARG:NH2	1:A:356:GLU:OE1	2.35	0.60
1:G:130:GLN:HG3	1:J:344:THR:HG22	1.84	0.60
1:M:83:PRO:O	1:M:87:ARG:NH1	2.33	0.59
1:S:250:PHE:HE1	1:S:283:THR:HG23	1.67	0.59
2:E:78:THR:HG22	2:E:79:ALA:HA	1.82	0.59
2:E:106:ARG:HD2	3:F:49:TYR:HD1	1.68	0.59
3:U:118:PHE:HB2	3:U:133:VAL:HG22	1.84	0.59
2:W:107:PHE:HB2	3:X:36:TYR:HE1	1.67	0.59
2:B:61:VAL:HG12	2:B:63:LYS:H	1.67	0.59
2:E:61:VAL:HG12	2:E:63:LYS:H	1.67	0.59
3:L:118:PHE:HB2	3:L:133:VAL:HG22	1.84	0.59
2:N:105:GLY:HA3	2:N:106:ARG:HB2	1.84	0.59
3:j:120:PRO:HD3	3:j:132:VAL:HG22	1.84	0.59
3:R:120:PRO:HD3	3:R:132:VAL:HG22	1.84	0.59
3:X:120:PRO:HD3	3:X:132:VAL:HG22	1.83	0.59
1:J:250:PHE:HE1	1:J:283:THR:HG23	1.67	0.59
3:I:120:PRO:HD3	3:I:132:VAL:HG22	1.85	0.59
3:O:120:PRO:HD3	3:O:132:VAL:HG22	1.85	0.59
1:D:193:GLY:HA3	1:D:284:PRO:HG3	1.84	0.59
1:S:265:ILE:HD11	2:W:55:TYR:CE1	2.38	0.59
1:b:147:MET:HE1	1:b:221:PRO:HB3	1.84	0.59
2:N:40:ARG:HH11	2:N:41:PRO:HD2	1.68	0.59
2:N:105:GLY:HA3	2:N:106:ARG:CB	2.33	0.59
1:A:141:LYS:HE3	1:A:242:GLU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:99:ARG:NH2	1:P:356:GLU:OE1	2.36	0.59
2:E:106:ARG:HA	2:E:107:PHE:HB2	1.84	0.59
2:N:30:LYS:HA	2:N:31:ASP:CB	2.33	0.59
2:B:76:SER:CB	2:B:77:ASN:HB2	2.33	0.59
1:J:265:ILE:HD11	2:N:55:TYR:CE1	2.38	0.59
1:P:250:PHE:HE1	1:P:283:THR:HG23	1.66	0.59
1:S:275:VAL:HG22	1:V:112:PHE:HE2	1.68	0.59
2:g:140:ASN:OD1	2:g:140:ASN:N	2.32	0.59
3:j:18:ARG:NH2	2:Z:65:GLN:O	2.30	0.59
2:T:107:PHE:HB2	3:U:36:TYR:HE1	1.67	0.59
2:W:99:GLY:HA2	2:W:108:PRO:HD2	1.85	0.59
2:B:30:LYS:HA	2:B:31:ASP:HB2	1.85	0.58
3:F:106:LEU:H	3:F:166:GLN:HE22	1.51	0.58
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.85	0.58
2:T:22:CYS:HB3	2:T:79:ALA:N	2.17	0.58
3:a:120:PRO:HD3	3:a:132:VAL:HG22	1.84	0.58
1:M:141:LYS:HE3	1:M:242:GLU:HB3	1.86	0.58
2:B:22:CYS:HB3	2:B:79:ALA:H	1.68	0.58
2:Q:107:PHE:HB2	3:R:36:TYR:HE1	1.68	0.58
1:V:147:MET:HE1	1:V:221:PRO:HB3	1.85	0.58
3:C:118:PHE:HB2	3:C:133:VAL:HG22	1.85	0.58
3:O:149:LYS:HB2	3:O:193:THR:HB	1.86	0.58
3:j:149:LYS:HB2	3:j:193:THR:HB	1.85	0.58
3:F:109:ALA:HB1	3:F:110:ASP:HB3	1.84	0.58
3:I:106:LEU:HB2	3:I:166:GLN:NE2	2.19	0.58
1:D:147:MET:HE1	1:D:221:PRO:HB3	1.85	0.58
1:G:99:ARG:NH2	1:G:356:GLU:OE1	2.37	0.58
1:Y:427:ASP:HB3	1:Y:430:LYS:HG3	1.84	0.58
1:M:47:ALA:HB1	2:N:28:ASN:HD21	1.67	0.58
2:E:67:LYS:NZ	2:E:85:SER:O	2.36	0.58
1:A:130:GLN:HG3	1:D:344:THR:HG22	1.86	0.58
1:Y:148:VAL:HG22	1:Y:320:VAL:HG22	1.85	0.58
2:E:28:ASN:OD1	2:E:28:ASN:N	2.32	0.58
2:H:22:CYS:HB3	2:H:79:ALA:H	1.69	0.58
1:M:99:ARG:NH2	1:M:356:GLU:OE1	2.37	0.58
2:H:40:ARG:HH11	2:H:41:PRO:HD2	1.67	0.58
2:Z:158:THR:HB	2:Z:205:ALA:HB3	1.85	0.58
1:P:275:VAL:HG22	1:S:112:PHE:HE2	1.69	0.58
1:M:257:GLY:O	2:B:30:LYS:HE2	2.04	0.57
1:V:265:ILE:HD11	2:Z:55:TYR:CE1	2.38	0.57
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:103:ASP:HB3	2:N:106:ARG:NH2	2.19	0.57
1:A:344:THR:HG22	1:M:130:GLN:HG3	1.86	0.57
1:J:193:GLY:HA3	1:J:284:PRO:HG3	1.85	0.57
1:V:62:VAL:HG22	1:V:321:THR:HG23	1.86	0.57
3:I:13:THR:O	3:I:107:LYS:N	2.37	0.57
2:W:76:SER:HB3	2:W:77:ASN:CB	2.33	0.57
1:b:83:PRO:O	1:b:87:ARG:NH1	2.36	0.57
3:a:118:PHE:HB2	3:a:133:VAL:HG22	1.86	0.57
1:G:202:LEU:HB3	1:J:333:LEU:HD22	1.86	0.57
1:D:260:VAL:O	2:H:55:TYR:OH	2.22	0.57
2:B:99:GLY:HA2	2:B:108:PRO:HD2	1.86	0.57
2:N:52:ASP:OD2	2:N:55:TYR:HB2	2.03	0.57
2:Q:48:ILE:HG23	2:Q:64:PHE:HD1	1.69	0.57
2:W:30:LYS:HA	2:W:31:ASP:CB	2.33	0.57
1:V:130:GLN:HG3	1:Y:344:THR:HG22	1.86	0.57
1:V:141:LYS:HE3	1:V:242:GLU:HB3	1.85	0.57
3:j:118:PHE:HB2	3:j:133:VAL:HG22	1.87	0.57
3:X:147:LYS:HD2	3:X:149:LYS:HZ1	1.70	0.57
2:W:48:ILE:HG23	2:W:64:PHE:HD1	1.69	0.57
1:A:145:LEU:HG	1:A:323:VAL:HB	1.87	0.57
1:M:193:GLY:HA3	1:M:284:PRO:HG3	1.86	0.57
3:I:118:PHE:HB2	3:I:133:VAL:HG22	1.87	0.57
3:R:118:PHE:HB2	3:R:133:VAL:HG22	1.86	0.57
2:W:102:TYR:CG	2:W:103:ASP:N	2.73	0.57
3:X:149:LYS:HB2	3:X:193:THR:HB	1.87	0.57
2:Z:102:TYR:CG	2:Z:103:ASP:N	2.72	0.57
1:A:83:PRO:O	1:A:87:ARG:NH1	2.36	0.56
1:D:344:THR:HG21	3:F:53:ASN:ND2	2.20	0.56
1:P:143:THR:HG23	1:P:242:GLU:HG2	1.86	0.56
1:V:110:HIS:HB2	1:V:210:PRO:HA	1.86	0.56
3:U:149:LYS:HB2	3:U:193:THR:HB	1.86	0.56
1:A:202:LEU:HB3	1:D:333:LEU:HD22	1.85	0.56
1:V:99:ARG:NH2	1:V:356:GLU:OE1	2.38	0.56
1:J:83:PRO:O	1:J:87:ARG:NH1	2.38	0.56
1:Y:271:ASN:O	1:Y:273:THR:N	2.38	0.56
1:G:62:VAL:HG22	1:G:321:THR:HG23	1.87	0.56
1:G:141:LYS:HE3	1:G:242:GLU:HB3	1.87	0.56
1:Y:268:GLY:HA3	1:Y:269:SER:HB2	1.87	0.56
2:H:107:PHE:HB2	3:I:36:TYR:HE1	1.70	0.56
1:P:130:GLN:HG3	1:S:344:THR:HG22	1.86	0.56
1:Y:141:LYS:HB2	1:Y:244:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:202:LEU:HB3	1:b:333:LEU:HD22	1.87	0.56
1:G:147:MET:HE1	1:G:221:PRO:HB3	1.86	0.56
1:M:167:THR:HB	1:M:168:PRO:HB3	1.88	0.56
2:B:131:LEU:H	2:B:216:LYS:HZ3	1.53	0.56
2:W:73:ASP:H	2:W:78:THR:HG21	1.71	0.56
1:V:148:VAL:HG22	1:V:320:VAL:HG22	1.88	0.56
1:V:83:PRO:O	1:V:87:ARG:NH1	2.38	0.56
1:Y:273:THR:HG21	2:g:59:GLU:OE2	2.05	0.56
3:j:147:LYS:HD2	3:j:149:LYS:HZ1	1.70	0.56
2:Q:76:SER:HB3	2:Q:77:ASN:CB	2.36	0.56
1:b:148:VAL:HG22	1:b:320:VAL:HG22	1.88	0.55
2:H:145:LEU:HD13	2:H:216:LYS:HD3	1.88	0.55
2:Q:131:LEU:H	2:Q:216:LYS:HZ3	1.52	0.55
3:X:118:PHE:HB2	3:X:133:VAL:HG22	1.87	0.55
1:G:85:THR:H	1:G:392:PHE:HE2	1.53	0.55
2:T:99:GLY:HA2	2:T:108:PRO:HD2	1.88	0.55
1:b:99:ARG:NH2	1:b:356:GLU:OE1	2.40	0.55
3:O:118:PHE:HB2	3:O:133:VAL:HG22	1.87	0.55
2:T:40:ARG:HD2	2:T:41:PRO:HD2	1.89	0.55
3:U:107:LYS:HA	3:U:140:TYR:OH	2.07	0.55
1:b:427:ASP:HB3	1:b:430:LYS:HG3	1.88	0.55
2:K:145:LEU:HD13	2:K:216:LYS:HD3	1.89	0.55
3:L:149:LYS:HB2	3:L:193:THR:HB	1.89	0.55
2:Q:76:SER:HB3	2:Q:77:ASN:HB2	1.89	0.55
2:N:106:ARG:HG2	3:O:49:TYR:HB2	1.87	0.55
1:D:272:ARG:HG2	1:G:112:PHE:HE1	1.72	0.55
1:J:141:LYS:HE3	1:J:242:GLU:HB3	1.88	0.55
3:X:113:PRO:HB3	3:X:139:PHE:HB3	1.88	0.55
1:G:273:THR:HG21	2:K:59:GLU:OE2	2.07	0.55
2:E:52:ASP:OD2	2:E:55:TYR:HB2	2.06	0.55
2:K:40:ARG:HD2	2:K:41:PRO:HD2	1.88	0.55
2:Z:52:ASP:OD2	2:Z:55:TYR:HB2	2.05	0.55
1:P:307:GLY:HA2	1:S:454:ARG:NH1	2.22	0.55
2:N:105:GLY:HA3	2:N:106:ARG:CG	2.36	0.55
3:U:166:GLN:HE21	3:U:171:SER:HB3	1.72	0.55
1:Y:203:GLN:HA	1:b:334:CYS:HB3	1.89	0.55
2:N:131:LEU:H	2:N:216:LYS:HZ3	1.55	0.55
1:P:145:LEU:HG	1:P:323:VAL:HB	1.89	0.54
1:b:265:ILE:HD11	2:Q:55:TYR:CE1	2.42	0.54
2:H:105:GLY:O	3:I:36:TYR:OH	2.25	0.54
3:j:46:LEU:HD21	3:j:49:TYR:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:15:VAL:HG23	3:R:106:LEU:HD21	1.88	0.54
2:Z:40:ARG:HD2	2:Z:41:PRO:HD2	1.88	0.54
1:D:130:GLN:HG3	1:G:344:THR:HG22	1.87	0.54
1:G:427:ASP:HB3	1:G:430:LYS:HG3	1.89	0.54
1:J:145:LEU:HD13	1:J:147:MET:HE3	1.89	0.54
1:D:62:VAL:HG22	1:D:321:THR:HG23	1.88	0.54
1:J:271:ASN:CG	1:J:272:ARG:H	2.15	0.54
2:E:40:ARG:HD2	2:E:41:PRO:HD2	1.89	0.54
3:I:15:VAL:HG22	3:I:106:LEU:HD13	1.89	0.54
2:Q:40:ARG:HD2	2:Q:41:PRO:HD2	1.89	0.54
1:Y:145:LEU:HD13	1:Y:147:MET:HE3	1.89	0.54
1:A:145:LEU:HD13	1:A:147:MET:HE3	1.88	0.54
1:J:147:MET:HE1	1:J:221:PRO:HB3	1.87	0.54
1:M:427:ASP:HB3	1:M:430:LYS:HG3	1.89	0.54
1:S:145:LEU:HD13	1:S:147:MET:HE3	1.89	0.54
1:Y:83:PRO:O	1:Y:87:ARG:NH1	2.41	0.54
2:B:30:LYS:HA	2:B:31:ASP:CB	2.38	0.54
1:S:349:LYS:HZ3	2:T:30:LYS:HE2	1.72	0.54
2:B:105:GLY:O	3:C:36:TYR:OH	2.24	0.54
2:Q:32:TYR:O	2:Q:53:PRO:HD2	2.07	0.54
1:V:275:VAL:HG22	1:Y:112:PHE:CE2	2.41	0.54
1:Y:262:ASP:O	1:Y:264:LEU:N	2.41	0.54
1:b:272:ARG:O	1:b:274:SER:N	2.33	0.54
2:B:40:ARG:HD2	2:B:41:PRO:HD2	1.89	0.54
2:B:102:TYR:CG	2:B:103:ASP:N	2.75	0.54
3:F:118:PHE:HB2	3:F:133:VAL:HG22	1.89	0.54
2:T:52:ASP:OD2	2:T:55:TYR:HB2	2.08	0.54
1:J:307:GLY:HA2	1:M:454:ARG:NH1	2.23	0.54
3:C:149:LYS:HB2	3:C:193:THR:HB	1.90	0.54
3:F:150:ILE:HD11	3:F:179:LEU:HD21	1.89	0.54
3:L:106:LEU:HD22	3:L:107:LYS:H	1.73	0.54
2:N:107:PHE:O	2:N:110:TRP:NE1	2.41	0.54
1:G:141:LYS:HB2	1:G:244:MET:HB3	1.89	0.54
1:M:273:THR:HG21	2:B:59:GLU:OE2	2.07	0.54
3:F:149:LYS:HB2	3:F:193:THR:HB	1.90	0.54
3:O:147:LYS:HD2	3:O:149:LYS:HZ1	1.73	0.54
3:j:75:ILE:HG21	3:j:78:MET:HE3	1.90	0.54
2:W:40:ARG:HD2	2:W:41:PRO:HD2	1.89	0.54
2:g:73:ASP:H	2:g:78:THR:CG2	2.18	0.53
2:T:32:TYR:O	2:T:53:PRO:HD2	2.08	0.53
1:V:427:ASP:HB3	1:V:430:LYS:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:102:TYR:CG	2:Q:103:ASP:N	2.76	0.53
2:Z:99:GLY:HA2	2:Z:108:PRO:HD2	1.91	0.53
1:D:273:THR:HG21	2:H:59:GLU:OE2	2.08	0.53
1:J:170:GLN:HB3	1:J:171:ALA:HA	1.89	0.53
1:V:145:LEU:HG	1:V:323:VAL:HB	1.90	0.53
2:g:32:TYR:O	2:g:53:PRO:HD2	2.08	0.53
1:D:427:ASP:HB3	1:D:430:LYS:HG3	1.91	0.53
1:P:147:MET:HE1	1:P:221:PRO:HB3	1.89	0.53
1:P:265:ILE:HD11	2:T:55:TYR:HE1	1.74	0.53
1:b:145:LEU:HG	1:b:323:VAL:HB	1.90	0.53
2:E:75:SER:O	2:E:77:ASN:HB2	2.09	0.53
1:J:273:THR:HG21	2:N:59:GLU:OE2	2.09	0.53
1:M:145:LEU:HG	1:M:323:VAL:HB	1.91	0.53
1:Y:172:GLY:HA3	1:b:337:VAL:HG22	1.91	0.53
3:U:39:LYS:HG2	3:U:84:ALA:HB2	1.91	0.53
1:V:271:ASN:CG	1:V:272:ARG:H	2.17	0.53
1:b:153:PRO:HG2	1:b:184:ILE:HB	1.91	0.53
3:I:149:LYS:HB2	3:I:193:THR:HB	1.90	0.53
2:g:22:CYS:HB3	2:g:79:ALA:N	2.21	0.53
3:R:149:LYS:HB2	3:R:193:THR:HB	1.90	0.53
1:D:271:ASN:CG	1:D:272:ARG:H	2.17	0.53
1:Y:99:ARG:NH2	1:Y:356:GLU:OE1	2.42	0.53
2:E:131:LEU:H	2:E:216:LYS:HZ3	1.55	0.53
1:D:170:GLN:HB3	1:D:171:ALA:HA	1.91	0.53
1:J:127:ASN:N	1:J:128:PRO:HD3	2.24	0.53
2:B:145:LEU:HD13	2:B:216:LYS:HD3	1.90	0.53
2:H:102:TYR:CG	2:H:103:ASP:N	2.77	0.53
1:D:145:LEU:HD13	1:D:147:MET:HE3	1.90	0.53
1:Y:145:LEU:HG	1:Y:323:VAL:HB	1.91	0.53
1:Y:170:GLN:HB3	1:Y:171:ALA:HA	1.90	0.53
3:a:149:LYS:HB2	3:a:193:THR:HB	1.91	0.53
1:G:59:GLN:OE1	1:G:61:ARG:NH2	2.42	0.53
1:G:145:LEU:HD13	1:G:147:MET:HE3	1.91	0.53
1:J:110:HIS:HB2	1:J:210:PRO:HA	1.90	0.53
1:P:246:ALA:HB1	1:P:249:PHE:HE2	1.74	0.53
2:B:48:ILE:HG23	2:B:64:PHE:HD1	1.74	0.53
2:H:131:LEU:H	2:H:216:LYS:HZ3	1.57	0.53
2:K:31:ASP:OD2	2:K:32:TYR:N	2.42	0.53
2:Q:52:ASP:OD1	2:Q:55:TYR:HB2	2.09	0.53
1:J:252:ARG:HE	1:M:332:THR:HG21	1.74	0.52
2:N:145:LEU:HD13	2:N:216:LYS:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:65:GLN:O	3:X:18:ARG:NH2	2.33	0.52
1:A:147:MET:HE1	1:A:221:PRO:HB3	1.92	0.52
1:J:145:LEU:HG	1:J:323:VAL:HB	1.91	0.52
2:K:107:PHE:HB2	3:L:36:TYR:HE1	1.73	0.52
2:Z:19:LYS:HG3	2:Z:82:GLN:HB3	1.90	0.52
1:D:110:HIS:HB2	1:D:210:PRO:HA	1.92	0.52
1:D:141:LYS:HB2	1:D:244:MET:HB3	1.91	0.52
1:G:170:GLN:HB3	1:G:171:ALA:HA	1.92	0.52
1:P:192:THR:HG22	1:P:193:GLY:H	1.75	0.52
1:S:170:GLN:HB3	1:S:171:ALA:HA	1.92	0.52
1:b:110:HIS:HB2	1:b:210:PRO:HA	1.92	0.52
1:b:167:THR:HB	1:b:168:PRO:HB3	1.91	0.52
2:E:102:TYR:CG	2:E:103:ASP:N	2.76	0.52
2:H:40:ARG:HD2	2:H:41:PRO:HD2	1.90	0.52
2:K:48:ILE:HG23	2:K:64:PHE:HD1	1.75	0.52
2:N:76:SER:CB	2:N:77:ASN:HB2	2.39	0.52
1:P:191:ASP:HA	1:P:218:CYS:HB3	1.90	0.52
2:H:30:LYS:HA	2:H:31:ASP:CB	2.30	0.52
2:H:106:ARG:HD2	3:I:49:TYR:CD1	2.44	0.52
2:Q:7:SER:HB2	2:Q:21:SER:H	1.74	0.52
2:Q:67:LYS:NZ	2:Q:85:SER:O	2.42	0.52
2:T:102:TYR:CG	2:T:103:ASP:N	2.78	0.52
2:W:145:LEU:HD13	2:W:216:LYS:HD3	1.92	0.52
3:a:106:LEU:HB2	3:a:166:GLN:HE22	1.74	0.52
1:S:127:ASN:N	1:S:128:PRO:HD3	2.25	0.52
2:N:40:ARG:HD2	2:N:41:PRO:HD2	1.91	0.52
2:T:76:SER:CB	2:T:77:ASN:HB2	2.40	0.52
1:G:145:LEU:HG	1:G:323:VAL:HB	1.92	0.52
1:M:110:HIS:HB2	1:M:210:PRO:HA	1.91	0.52
1:b:170:GLN:HB3	1:b:171:ALA:HA	1.92	0.52
2:Q:87:THR:OG1	2:Q:88:SER:N	2.42	0.52
2:W:52:ASP:OD2	2:W:55:TYR:HB2	2.09	0.52
1:V:170:GLN:HB3	1:V:171:ALA:HA	1.92	0.52
1:Y:127:ASN:N	1:Y:128:PRO:HD3	2.25	0.52
2:H:78:THR:HG22	2:H:79:ALA:HB2	1.92	0.52
2:K:76:SER:CB	2:K:77:ASN:HB2	2.39	0.52
1:A:260:VAL:HG23	2:E:55:TYR:OH	2.10	0.52
1:S:167:THR:HB	1:S:168:PRO:HB3	1.92	0.52
1:V:167:THR:HB	1:V:168:PRO:HB3	1.92	0.52
1:D:127:ASN:N	1:D:128:PRO:HD3	2.25	0.52
1:M:271:ASN:CG	1:M:272:ARG:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:170:GLN:HB3	1:P:171:ALA:HA	1.92	0.52
2:K:67:LYS:NZ	2:K:85:SER:O	2.43	0.52
2:K:131:LEU:H	2:K:216:LYS:HZ3	1.57	0.52
2:W:51:ILE:HG22	2:W:58:THR:HG22	1.91	0.52
2:W:67:LYS:NZ	2:W:85:SER:O	2.43	0.52
1:D:145:LEU:HG	1:D:323:VAL:HB	1.92	0.51
1:M:141:LYS:HB2	1:M:244:MET:HB3	1.92	0.51
1:V:265:ILE:HD11	2:Z:55:TYR:HE1	1.75	0.51
2:g:40:ARG:HD2	2:g:41:PRO:HD2	1.91	0.51
2:T:105:GLY:O	3:U:36:TYR:OH	2.28	0.51
3:X:46:LEU:HD21	3:X:49:TYR:HD2	1.75	0.51
3:O:47:MET:HA	3:O:58:VAL:HG21	1.92	0.51
1:M:170:GLN:HB3	1:M:171:ALA:HA	1.92	0.51
2:B:32:TYR:O	2:B:53:PRO:HD2	2.10	0.51
2:B:35:HIS:CE1	2:B:104:ARG:HA	2.45	0.51
2:g:28:ASN:O	2:g:29:ILE:HG22	2.10	0.51
2:g:48:ILE:HG23	2:g:64:PHE:HD1	1.76	0.51
2:T:11:VAL:HG21	2:T:154:PRO:HG3	1.93	0.51
1:b:127:ASN:N	1:b:128:PRO:HD3	2.26	0.51
1:A:62:VAL:HG22	1:A:321:THR:HG23	1.92	0.51
2:Q:76:SER:HB3	2:Q:77:ASN:CA	2.40	0.51
2:Q:105:GLY:O	3:R:36:TYR:OH	2.29	0.51
1:D:268:GLY:HA3	1:D:269:SER:HB2	1.92	0.51
1:M:127:ASN:N	1:M:128:PRO:HD3	2.26	0.51
1:b:273:THR:HG21	2:Q:59:GLU:OE2	2.10	0.51
2:Q:145:LEU:HD13	2:Q:216:LYS:HD3	1.92	0.51
1:D:167:THR:HB	1:D:168:PRO:HB3	1.92	0.51
2:T:35:HIS:CE1	2:T:104:ARG:HA	2.45	0.51
2:Z:105:GLY:O	3:a:36:TYR:OH	2.28	0.51
1:G:127:ASN:N	1:G:128:PRO:HD3	2.25	0.51
3:L:147:LYS:HD2	3:L:149:LYS:HZ1	1.75	0.51
1:J:141:LYS:HB2	1:J:244:MET:HB3	1.93	0.51
1:P:268:GLY:HA3	1:P:269:SER:OG	2.11	0.51
1:P:454:ARG:NH1	1:b:307:GLY:HA2	2.26	0.51
1:S:141:LYS:HB2	1:S:244:MET:HB3	1.93	0.51
1:b:246:ALA:HB1	1:b:249:PHE:HE2	1.76	0.51
2:E:72:ALA:HA	2:E:78:THR:HG23	1.93	0.51
3:j:47:MET:HA	3:j:58:VAL:HG21	1.93	0.51
1:A:271:ASN:CG	1:A:272:ARG:H	2.17	0.51
1:M:147:MET:HE1	1:M:221:PRO:HB3	1.93	0.51
1:P:167:THR:HB	1:P:168:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:31:ASP:O	2:K:53:PRO:HG2	2.11	0.51
3:L:14:SER:HA	3:L:106:LEU:HD23	1.93	0.51
3:U:150:ILE:HD11	3:U:179:LEU:HD21	1.93	0.51
1:M:58:TYR:CZ	1:M:140:TYR:HB2	2.46	0.50
1:P:334:CYS:HB3	1:b:203:GLN:HA	1.92	0.50
1:Y:110:HIS:HB2	1:Y:210:PRO:HA	1.94	0.50
1:Y:246:ALA:HB1	1:Y:249:PHE:HE2	1.76	0.50
2:W:76:SER:HB2	2:W:78:THR:OG1	2.12	0.50
1:A:102:PRO:HG3	1:M:220:TYR:CG	2.46	0.50
1:G:167:THR:HB	1:G:168:PRO:HB3	1.93	0.50
1:P:44:ILE:HD12	1:P:52:VAL:HB	1.91	0.50
1:Y:147:MET:HE1	1:Y:221:PRO:HB3	1.93	0.50
1:P:145:LEU:HD13	1:P:147:MET:HE3	1.94	0.50
1:V:127:ASN:N	1:V:128:PRO:HD3	2.26	0.50
2:E:194:THR:HG23	2:E:198:GLU:OE2	2.12	0.50
3:C:87:PHE:HE1	3:C:101:GLY:HA2	1.76	0.50
2:H:75:SER:O	2:H:77:ASN:HB2	2.12	0.50
3:O:46:LEU:HD21	3:O:49:TYR:HD2	1.75	0.50
3:R:147:LYS:HD2	3:R:149:LYS:HZ1	1.75	0.50
1:P:58:TYR:CZ	1:P:140:TYR:HB2	2.46	0.50
1:S:83:PRO:O	1:S:87:ARG:NH1	2.44	0.50
1:S:271:ASN:CG	1:S:272:ARG:H	2.19	0.50
1:S:427:ASP:HB3	1:S:430:LYS:HG3	1.91	0.50
1:V:273:THR:HG21	2:Z:59:GLU:OE2	2.12	0.50
2:g:76:SER:CB	2:g:77:ASN:HB2	2.41	0.50
2:Z:48:ILE:HG23	2:Z:64:PHE:HD1	1.76	0.50
1:G:271:ASN:CG	1:G:272:ARG:H	2.20	0.50
1:Y:141:LYS:HE3	1:Y:242:GLU:HB3	1.92	0.50
2:W:32:TYR:H	2:W:32:TYR:HD2	1.59	0.50
1:M:229:ASP:OD1	1:M:230:PRO:HD2	2.12	0.50
1:P:273:THR:HG21	2:T:59:GLU:OE2	2.11	0.50
1:S:344:THR:HG21	3:U:53:ASN:ND2	2.27	0.50
1:A:127:ASN:N	1:A:128:PRO:HD3	2.26	0.50
1:A:170:GLN:HB3	1:A:171:ALA:HA	1.94	0.50
1:D:246:ALA:HB1	1:D:249:PHE:HE2	1.77	0.50
1:J:172:GLY:HA3	1:M:337:VAL:HG22	1.94	0.50
1:P:44:ILE:HG23	2:Q:29:ILE:HD11	1.94	0.50
1:P:127:ASN:N	1:P:128:PRO:HD3	2.26	0.50
1:S:145:LEU:HG	1:S:323:VAL:HB	1.93	0.50
1:V:246:ALA:HB1	1:V:249:PHE:HE2	1.75	0.50
1:Y:344:THR:HG21	3:a:53:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:THR:HG23	2:B:154:PRO:HD3	1.93	0.50
2:H:76:SER:HB2	2:H:77:ASN:CB	2.40	0.50
1:A:268:GLY:HA3	1:A:269:SER:HB2	1.94	0.50
1:A:273:THR:HG21	2:E:59:GLU:OE2	2.11	0.50
1:G:148:VAL:HG22	1:G:320:VAL:HG22	1.94	0.50
1:G:246:ALA:HB1	1:G:249:PHE:HE2	1.77	0.50
1:S:307:GLY:HA2	1:V:454:ARG:NH1	2.27	0.50
2:H:145:LEU:HB3	2:H:216:LYS:HE2	1.94	0.50
2:W:22:CYS:HB3	2:W:79:ALA:HB3	1.94	0.50
1:A:167:THR:HB	1:A:168:PRO:HB3	1.94	0.49
1:A:427:ASP:HB3	1:A:430:LYS:HG3	1.92	0.49
1:D:256:VAL:HG13	1:D:279:ILE:HD11	1.94	0.49
1:M:46:ARG:CB	2:N:29:ILE:HG12	2.42	0.49
1:V:307:GLY:HA2	1:Y:454:ARG:NH1	2.26	0.49
2:T:73:ASP:N	2:T:78:THR:HG21	2.25	0.49
3:j:17:ASP:O	3:j:77:ASN:HA	2.12	0.49
2:T:145:LEU:HD13	2:T:216:LYS:HD3	1.93	0.49
1:A:307:GLY:HA2	1:D:454:ARG:NH1	2.27	0.49
2:B:100:HIS:HD2	2:B:106:ARG:NH2	2.09	0.49
2:Q:104:ARG:HB3	3:R:96:LEU:HD11	1.94	0.49
2:W:131:LEU:H	2:W:216:LYS:NZ	2.10	0.49
1:D:148:VAL:HG22	1:D:320:VAL:HG22	1.93	0.49
2:E:145:LEU:HB3	2:E:216:LYS:HE2	1.94	0.49
2:K:53:PRO:O	2:K:54:GLU:HB3	2.12	0.49
2:N:67:LYS:NZ	2:N:85:SER:O	2.45	0.49
2:T:22:CYS:CB	2:T:79:ALA:H	2.21	0.49
1:S:229:ASP:OD1	1:S:230:PRO:HD2	2.12	0.49
1:Y:220:TYR:CG	1:b:102:PRO:HG3	2.47	0.49
2:g:36:TRP:CZ2	2:g:96:CYS:HB3	2.48	0.49
2:Q:65:GLN:O	3:U:18:ARG:NH2	2.38	0.49
3:R:47:MET:HA	3:R:58:VAL:HG21	1.95	0.49
2:T:19:LYS:HG3	2:T:82:GLN:HB3	1.95	0.49
1:A:141:LYS:HB2	1:A:244:MET:HB3	1.94	0.49
1:G:275:VAL:HG22	1:J:112:PHE:CE2	2.46	0.49
3:I:39:LYS:HG2	3:I:84:ALA:HB2	1.94	0.49
2:K:145:LEU:HB3	2:K:216:LYS:HE2	1.95	0.49
2:Q:131:LEU:H	2:Q:216:LYS:NZ	2.11	0.49
1:D:272:ARG:NH2	1:G:133:ARG:O	2.46	0.49
1:G:143:THR:HG23	1:G:242:GLU:HG2	1.94	0.49
1:J:47:ALA:HB1	2:K:28:ASN:ND2	2.28	0.49
1:M:246:ALA:HB1	1:M:249:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLN:O	3:F:18:ARG:NH2	2.37	0.49
2:g:36:TRP:CH2	2:g:96:CYS:HB3	2.47	0.49
2:Q:145:LEU:HB3	2:Q:216:LYS:HE2	1.95	0.49
2:W:100:HIS:HB3	2:W:109:TYR:HE2	1.78	0.49
1:A:269:SER:O	1:A:269:SER:OG	2.30	0.49
1:Y:167:THR:HB	1:Y:168:PRO:HB3	1.94	0.49
3:O:142:LYS:HE3	3:O:142:LYS:HB2	1.55	0.49
2:T:53:PRO:O	2:T:54:GLU:HB3	2.13	0.49
1:J:257:GLY:O	2:N:30:LYS:HE2	2.13	0.48
1:S:246:ALA:HB1	1:S:249:PHE:HE2	1.77	0.48
2:H:131:LEU:H	2:H:216:LYS:NZ	2.11	0.48
2:g:131:LEU:H	2:g:216:LYS:HZ3	1.59	0.48
1:D:265:ILE:HD11	2:H:55:TYR:CE1	2.49	0.48
1:P:23:THR:OG1	1:P:366:LEU:O	2.26	0.48
1:S:265:ILE:HD11	2:W:55:TYR:HE1	1.77	0.48
2:E:145:LEU:HD13	2:E:216:LYS:HD3	1.93	0.48
3:U:13:THR:O	3:U:106:LEU:HA	2.13	0.48
2:W:145:LEU:HB3	2:W:216:LYS:HE2	1.95	0.48
1:G:307:GLY:HA2	1:J:454:ARG:NH1	2.28	0.48
1:J:59:GLN:OE1	1:J:61:ARG:NH2	2.47	0.48
1:Y:193:GLY:HA3	1:Y:284:PRO:CG	2.42	0.48
2:H:26:GLY:HA2	2:H:53:PRO:HG3	1.96	0.48
3:I:113:PRO:HB3	3:I:139:PHE:HB3	1.96	0.48
1:A:110:HIS:HB2	1:A:210:PRO:HA	1.95	0.48
1:b:95:LEU:HD22	1:b:148:VAL:HG21	1.95	0.48
1:b:145:LEU:HD13	1:b:147:MET:HE3	1.94	0.48
3:F:87:PHE:HE1	3:F:101:GLY:HA2	1.79	0.48
2:N:28:ASN:OD1	2:N:28:ASN:N	2.34	0.48
2:Q:53:PRO:O	2:Q:54:GLU:HB3	2.14	0.48
2:T:11:VAL:CG2	2:T:154:PRO:HG3	2.44	0.48
3:U:147:LYS:HD2	3:U:149:LYS:HZ1	1.78	0.48
2:W:131:LEU:H	2:W:216:LYS:HZ3	1.61	0.48
1:D:307:GLY:HA2	1:G:454:ARG:NH1	2.29	0.48
1:G:268:GLY:HA2	1:M:342:THR:HG22	1.95	0.48
1:V:220:TYR:CG	1:Y:102:PRO:HG3	2.48	0.48
2:B:72:ALA:HA	2:B:78:THR:OG1	2.13	0.48
2:E:100:HIS:HB3	2:E:109:TYR:CE2	2.42	0.48
2:H:138:GLN:HE22	2:H:143:VAL:HG23	1.79	0.48
2:N:72:ALA:HA	2:N:78:THR:OG1	2.13	0.48
2:N:145:LEU:HB3	2:N:216:LYS:HE2	1.96	0.48
3:O:108:ARG:HH12	3:O:111:ALA:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:147:LYS:HD2	3:j:149:LYS:NZ	2.28	0.48
3:X:46:LEU:HD21	3:X:49:TYR:CD2	2.49	0.48
1:V:272:ARG:HG2	1:Y:112:PHE:HE1	1.78	0.48
2:B:131:LEU:H	2:B:216:LYS:NZ	2.10	0.48
2:H:52:ASP:OD2	2:H:55:TYR:HB2	2.14	0.48
2:B:103:ASP:OD1	2:B:104:ARG:HG2	2.13	0.48
2:H:100:HIS:HB3	2:H:109:TYR:HE2	1.79	0.48
3:L:150:ILE:HD11	3:L:179:LEU:HD21	1.96	0.48
1:J:246:ALA:HB1	1:J:249:PHE:HE2	1.79	0.48
2:E:48:ILE:HG23	2:E:64:PHE:HD1	1.78	0.48
2:H:28:ASN:C	2:H:30:LYS:H	2.22	0.48
2:W:99:GLY:HA2	2:W:108:PRO:CD	2.44	0.48
1:D:153:PRO:HG2	1:D:184:ILE:HB	1.96	0.48
1:G:110:HIS:HB2	1:G:210:PRO:HA	1.96	0.48
2:B:52:ASP:OD2	2:B:55:TYR:HB2	2.14	0.48
3:I:47:MET:HA	3:I:58:VAL:HG21	1.95	0.48
2:Z:28:ASN:C	2:Z:29:ILE:HG23	2.39	0.48
1:A:246:ALA:HB1	1:A:249:PHE:HE2	1.79	0.48
1:P:110:HIS:HB2	1:P:210:PRO:HA	1.96	0.48
2:N:22:CYS:HB3	2:N:79:ALA:N	2.28	0.48
2:g:22:CYS:CB	2:g:79:ALA:H	2.23	0.48
2:B:53:PRO:O	2:B:54:GLU:HB3	2.13	0.47
2:N:36:TRP:CH2	2:N:96:CYS:HB3	2.48	0.47
2:g:99:GLY:HA2	2:g:108:PRO:HD2	1.95	0.47
2:T:131:LEU:H	2:T:216:LYS:HZ3	1.62	0.47
2:Z:206:HIS:CE1	2:Z:208:ALA:HB3	2.49	0.47
1:J:170:GLN:HB3	1:J:171:ALA:CA	2.43	0.47
1:S:95:LEU:HD22	1:S:148:VAL:HG21	1.95	0.47
1:S:130:GLN:HG3	1:V:344:THR:HG22	1.96	0.47
1:V:119:VAL:HG21	1:V:280:TYR:HE1	1.79	0.47
1:V:170:GLN:HB3	1:V:171:ALA:CA	2.45	0.47
2:B:145:LEU:HB3	2:B:216:LYS:HE2	1.96	0.47
3:j:107:LYS:O	3:j:108:ARG:HB2	2.14	0.47
1:A:44:ILE:HD12	1:A:52:VAL:HB	1.96	0.47
1:A:275:VAL:HG22	1:D:112:PHE:CE2	2.41	0.47
1:D:95:LEU:HD22	1:D:148:VAL:HG21	1.96	0.47
1:D:170:GLN:HB3	1:D:171:ALA:CA	2.44	0.47
1:V:44:ILE:HD12	1:V:52:VAL:HB	1.96	0.47
2:N:102:TYR:CG	2:N:103:ASP:N	2.81	0.47
3:j:150:ILE:HD11	3:j:179:LEU:HD21	1.97	0.47
2:K:29:ILE:HD12	2:K:29:ILE:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:99:GLY:HA2	2:Q:108:PRO:HD2	1.97	0.47
2:T:131:LEU:H	2:T:216:LYS:NZ	2.12	0.47
1:J:95:LEU:HD22	1:J:148:VAL:HG21	1.97	0.47
1:M:46:ARG:HA	1:M:47:ALA:HA	1.60	0.47
1:Y:95:LEU:HD22	1:Y:148:VAL:HG21	1.97	0.47
1:Y:170:GLN:HB3	1:Y:171:ALA:CA	2.44	0.47
2:g:36:TRP:HZ2	2:g:79:ALA:O	1.98	0.47
2:T:100:HIS:HB3	2:T:109:TYR:HE2	1.79	0.47
1:V:145:LEU:HD13	1:V:147:MET:HE3	1.96	0.47
2:E:32:TYR:H	2:E:32:TYR:HD2	1.63	0.47
1:J:46:ARG:HA	1:J:47:ALA:HA	1.56	0.47
1:J:256:VAL:HG13	1:J:279:ILE:HD11	1.97	0.47
1:P:95:LEU:HD22	1:P:148:VAL:HG21	1.96	0.47
1:V:256:VAL:HG13	1:V:279:ILE:HD11	1.97	0.47
1:Y:254:GLY:HA2	1:b:345:ASN:HB3	1.97	0.47
1:b:141:LYS:HB2	1:b:244:MET:HB3	1.95	0.47
2:g:131:LEU:H	2:g:216:LYS:NZ	2.12	0.47
3:j:87:PHE:HE1	3:j:101:GLY:HA2	1.80	0.47
2:Q:31:ASP:HB3	2:Q:54:GLU:HB3	1.97	0.47
2:Z:107:PHE:HB2	3:a:36:TYR:CE1	2.47	0.47
2:Z:138:GLN:O	2:Z:139:THR:HG22	2.14	0.47
3:a:151:ASP:HA	3:a:191:SER:HB3	1.95	0.47
1:M:148:VAL:HG22	1:M:320:VAL:HG22	1.95	0.47
1:M:170:GLN:HB3	1:M:171:ALA:CA	2.45	0.47
1:M:261:PRO:HD2	1:M:264:LEU:HD12	1.95	0.47
1:V:95:LEU:HD22	1:V:148:VAL:HG21	1.97	0.47
2:Z:201:THR:HG21	2:Z:213:VAL:HG13	1.97	0.47
1:A:95:LEU:HD22	1:A:148:VAL:HG21	1.97	0.47
1:M:268:GLY:HA3	1:M:269:SER:HB2	1.96	0.47
1:P:102:PRO:HG3	1:b:220:TYR:CG	2.49	0.47
2:B:75:SER:HG	2:W:123:THR:HB	1.80	0.47
2:B:80:TYR:CD2	2:B:80:TYR:N	2.83	0.47
3:C:147:LYS:HD2	3:C:149:LYS:HZ1	1.79	0.47
3:C:150:ILE:HD11	3:C:179:LEU:HD21	1.96	0.47
2:H:22:CYS:HB3	2:H:79:ALA:N	2.29	0.47
3:R:150:ILE:HD11	3:R:179:LEU:HD21	1.96	0.47
1:P:427:ASP:HB3	1:P:430:LYS:HG3	1.96	0.47
2:T:145:LEU:HB3	2:T:216:LYS:HE2	1.97	0.47
3:U:47:MET:HA	3:U:58:VAL:HG21	1.97	0.47
1:M:46:ARG:HB3	2:N:29:ILE:HG12	1.97	0.46
1:b:170:GLN:HB3	1:b:171:ALA:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:ARG:HA	2:E:107:PHE:CB	2.44	0.46
3:I:80:SER:HB3	3:I:168:SER:O	2.14	0.46
2:K:76:SER:HB2	2:K:77:ASN:HB2	1.96	0.46
3:j:110:ASP:HB3	3:j:200:THR:HG22	1.98	0.46
1:P:37:VAL:HG22	1:P:355:VAL:HG12	1.97	0.46
1:S:44:ILE:HD12	1:S:52:VAL:HB	1.98	0.46
1:S:170:GLN:HB3	1:S:171:ALA:CA	2.45	0.46
3:I:150:ILE:HD11	3:I:179:LEU:HD21	1.97	0.46
2:K:99:GLY:HA2	2:K:108:PRO:HD2	1.98	0.46
2:Z:140:ASN:HA	2:Z:141:SER:HA	1.55	0.46
1:A:119:VAL:HG21	1:A:280:TYR:HE1	1.80	0.46
1:A:332:THR:HG21	1:M:252:ARG:HE	1.80	0.46
1:J:268:GLY:HA3	1:J:269:SER:HB2	1.96	0.46
1:M:95:LEU:HD22	1:M:148:VAL:HG21	1.97	0.46
2:B:121:ALA:CB	2:B:122:LYS:HA	2.41	0.46
2:E:140:ASN:HA	2:E:141:SER:HA	1.66	0.46
3:F:55:TYR:O	3:F:58:VAL:HG23	2.15	0.46
2:g:53:PRO:O	2:g:54:GLU:HB3	2.16	0.46
1:J:37:VAL:HG22	1:J:355:VAL:HG12	1.97	0.46
1:Y:307:GLY:HA2	1:b:454:ARG:NH1	2.31	0.46
1:b:13:VAL:HG21	1:b:230:PRO:HB2	1.96	0.46
2:K:131:LEU:H	2:K:216:LYS:NZ	2.14	0.46
2:T:99:GLY:HA2	2:T:108:PRO:CD	2.44	0.46
1:P:170:GLN:HB3	1:P:171:ALA:CA	2.45	0.46
1:Y:46:ARG:HA	1:Y:47:ALA:HA	1.51	0.46
2:H:32:TYR:H	2:H:32:TYR:HD2	1.62	0.46
2:K:106:ARG:HD2	3:L:49:TYR:HB2	1.98	0.46
2:N:123:THR:HG23	2:N:154:PRO:HD3	1.98	0.46
2:Q:138:GLN:O	2:Q:139:THR:HG22	2.16	0.46
2:Q:140:ASN:HA	2:Q:141:SER:HA	1.69	0.46
3:U:106:LEU:HB2	3:U:166:GLN:NE2	2.19	0.46
3:a:150:ILE:HD11	3:a:179:LEU:HD21	1.97	0.46
1:D:44:ILE:HD12	1:D:52:VAL:HB	1.98	0.46
1:D:46:ARG:HA	1:D:47:ALA:HA	1.56	0.46
1:D:220:TYR:CG	1:G:102:PRO:HG3	2.50	0.46
1:G:170:GLN:HB3	1:G:171:ALA:CA	2.45	0.46
1:G:250:PHE:HE1	1:G:283:THR:HG23	1.80	0.46
1:V:338:THR:HG22	1:V:339:THR:H	1.81	0.46
3:O:138:ASN:HA	3:O:172:THR:HB	1.98	0.46
1:V:37:VAL:HG22	1:V:355:VAL:HG12	1.97	0.46
1:b:44:ILE:HD12	1:b:52:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:100:HIS:HE1	3:O:49:TYR:CZ	2.33	0.46
2:g:145:LEU:HD13	2:g:216:LYS:HD3	1.97	0.46
1:J:344:THR:HG21	3:L:53:ASN:ND2	2.31	0.46
1:P:220:TYR:CG	1:S:102:PRO:HG3	2.51	0.46
3:O:46:LEU:HD21	3:O:49:TYR:CD2	2.51	0.46
1:D:83:PRO:O	1:D:87:ARG:NH1	2.48	0.46
1:M:44:ILE:HD12	1:M:52:VAL:HB	1.98	0.46
1:Y:62:VAL:HG22	1:Y:321:THR:HG23	1.98	0.46
2:E:107:PHE:HB3	2:E:108:PRO:HA	1.98	0.46
2:E:131:LEU:H	2:E:216:LYS:NZ	2.14	0.46
2:N:53:PRO:O	2:N:54:GLU:HB3	2.15	0.46
3:U:147:LYS:HD2	3:U:149:LYS:NZ	2.31	0.46
1:P:322:VAL:HG11	1:P:358:TYR:HE1	1.82	0.45
1:S:268:GLY:HA3	1:S:269:SER:HB2	1.98	0.45
1:Y:59:GLN:OE1	1:Y:61:ARG:NH2	2.49	0.45
3:O:147:LYS:HD2	3:O:149:LYS:NZ	2.31	0.45
1:D:163:GLN:HA	1:D:164:CYS:HA	1.72	0.45
1:V:141:LYS:HB2	1:V:244:MET:HB3	1.97	0.45
2:N:26:GLY:HA2	2:N:53:PRO:HG3	1.98	0.45
2:Q:100:HIS:HB3	2:Q:109:TYR:HE2	1.81	0.45
1:A:170:GLN:HB3	1:A:171:ALA:CA	2.46	0.45
1:A:220:TYR:CG	1:D:102:PRO:HG3	2.50	0.45
1:P:203:GLN:HA	1:S:334:CYS:HB3	1.97	0.45
2:Q:146:GLY:O	2:Q:216:LYS:NZ	2.44	0.45
2:T:36:TRP:CZ2	2:T:96:CYS:HB3	2.51	0.45
2:H:48:ILE:HG23	2:H:64:PHE:HD1	1.82	0.45
3:I:123:GLU:O	3:I:126:THR:OG1	2.31	0.45
3:L:147:LYS:HD2	3:L:149:LYS:NZ	2.32	0.45
2:N:36:TRP:HZ2	2:N:79:ALA:O	2.00	0.45
2:N:48:ILE:HG23	2:N:64:PHE:HD1	1.81	0.45
1:J:23:THR:OG1	1:J:366:LEU:O	2.26	0.45
2:K:4:LEU:HD23	2:K:96:CYS:SG	2.56	0.45
2:g:67:LYS:NZ	2:g:85:SER:O	2.50	0.45
3:R:14:SER:HA	3:R:106:LEU:HD23	1.97	0.45
2:W:105:GLY:O	3:X:36:TYR:OH	2.34	0.45
3:X:147:LYS:HD2	3:X:149:LYS:NZ	2.30	0.45
1:P:338:THR:HG22	1:P:339:THR:H	1.82	0.45
1:V:193:GLY:HA3	1:V:284:PRO:CG	2.43	0.45
1:V:268:GLY:HA3	1:V:269:SER:HB2	1.99	0.45
3:j:138:ASN:HA	3:j:172:THR:HB	1.99	0.45
2:Q:78:THR:HB	2:Q:79:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:28:ASN:C	2:W:30:LYS:H	2.25	0.45
2:Z:53:PRO:O	2:Z:54:GLU:HB3	2.16	0.45
1:M:119:VAL:HG21	1:M:280:TYR:HE1	1.82	0.45
1:P:140:TYR:CD1	1:P:192:THR:HG21	2.52	0.45
1:Y:172:GLY:O	1:b:349:LYS:HD2	2.17	0.45
2:B:67:LYS:NZ	2:B:85:SER:O	2.49	0.45
2:B:99:GLY:HA2	2:B:108:PRO:CD	2.46	0.45
3:I:151:ASP:HA	3:I:191:SER:HB3	1.98	0.45
3:X:87:PHE:HE1	3:X:101:GLY:HA2	1.81	0.45
3:a:147:LYS:HD2	3:a:149:LYS:HZ1	1.81	0.45
1:P:140:TYR:CG	1:P:192:THR:HG21	2.51	0.45
1:S:220:TYR:CG	1:V:102:PRO:HG3	2.51	0.45
1:Y:44:ILE:HD12	1:Y:52:VAL:HB	1.99	0.45
1:b:70:PRO:HA	1:b:73:PHE:HB2	1.98	0.45
1:b:272:ARG:C	1:b:274:SER:H	2.24	0.45
2:B:75:SER:OG	2:W:123:THR:HB	2.16	0.45
2:N:32:TYR:O	2:N:53:PRO:HD2	2.17	0.45
2:Q:13:ARG:HH21	2:Q:121:ALA:HB1	1.82	0.45
3:R:147:LYS:HD2	3:R:149:LYS:NZ	2.32	0.45
3:U:87:PHE:HE1	3:U:101:GLY:HA2	1.82	0.45
1:J:119:VAL:HG21	1:J:280:TYR:HE1	1.81	0.45
1:b:62:VAL:HG22	1:b:321:THR:HG23	1.98	0.45
2:g:140:ASN:HA	2:g:141:SER:HA	1.69	0.45
2:g:209:SER:HB3	2:g:210:SER:H	1.63	0.45
2:Q:22:CYS:H	2:Q:79:ALA:H	1.65	0.45
3:U:113:PRO:HB3	3:U:139:PHE:HB3	1.99	0.45
2:E:36:TRP:CH2	2:E:96:CYS:HB3	2.51	0.45
2:K:140:ASN:HA	2:K:141:SER:HA	1.67	0.45
3:R:87:PHE:HE1	3:R:101:GLY:HA2	1.82	0.45
2:Z:30:LYS:HA	2:Z:31:ASP:HB2	1.98	0.45
1:A:112:PHE:HE1	1:M:272:ARG:HG2	1.82	0.44
1:A:272:ARG:HG2	1:D:112:PHE:HE1	1.81	0.44
1:D:58:TYR:CE1	1:D:140:TYR:HB2	2.52	0.44
1:M:153:PRO:HG2	1:M:184:ILE:HB	1.99	0.44
1:V:163:GLN:HA	1:V:164:CYS:HA	1.72	0.44
1:V:349:LYS:CE	2:W:101:ASP:OD2	2.64	0.44
2:K:52:ASP:OD2	2:K:53:PRO:O	2.35	0.44
2:T:174:PRO:O	3:U:162:SER:OG	2.29	0.44
3:X:47:MET:HA	3:X:58:VAL:HG21	1.99	0.44
1:S:143:THR:HG23	1:S:242:GLU:HG2	1.99	0.44
2:B:78:THR:HG23	2:B:79:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:78:THR:HG23	2:N:79:ALA:HB2	1.98	0.44
2:W:53:PRO:O	2:W:54:GLU:HB3	2.16	0.44
2:W:161:TRP:HZ3	2:W:216:LYS:HD2	1.82	0.44
1:A:338:THR:HG22	1:A:339:THR:H	1.82	0.44
1:S:163:GLN:HA	1:S:164:CYS:HA	1.70	0.44
2:B:100:HIS:HB3	2:B:109:TYR:HE2	1.83	0.44
2:H:206:HIS:ND1	2:H:209:SER:HB2	2.33	0.44
3:I:147:LYS:HD2	3:I:149:LYS:NZ	2.33	0.44
2:Q:80:TYR:N	2:Q:80:TYR:CD2	2.84	0.44
2:T:26:GLY:HA2	2:T:53:PRO:HG3	1.99	0.44
1:P:163:GLN:HA	1:P:164:CYS:HA	1.71	0.44
3:C:147:LYS:HD2	3:C:149:LYS:NZ	2.32	0.44
3:I:125:LEU:O	3:I:183:LYS:HD3	2.17	0.44
3:I:138:ASN:HA	3:I:172:THR:HB	1.99	0.44
3:U:46:LEU:HD21	3:U:49:TYR:CD2	2.50	0.44
1:J:163:GLN:HA	1:J:164:CYS:HA	1.70	0.44
1:S:260:VAL:N	2:W:55:TYR:OH	2.51	0.44
1:Y:271:ASN:O	1:Y:273:THR:OG1	2.33	0.44
2:E:107:PHE:HD2	3:F:36:TYR:CE1	2.36	0.44
2:H:161:TRP:HZ3	2:H:216:LYS:HD2	1.83	0.44
2:K:76:SER:HB2	2:K:77:ASN:CB	2.48	0.44
3:O:150:ILE:HD11	3:O:179:LEU:HD21	2.00	0.44
1:G:44:ILE:HD12	1:G:52:VAL:HB	2.00	0.44
1:S:46:ARG:HA	1:S:47:ALA:HA	1.55	0.44
1:V:46:ARG:HA	1:V:47:ALA:HA	1.55	0.44
2:H:25:SER:O	2:H:78:THR:HB	2.16	0.44
2:g:145:LEU:HB3	2:g:216:LYS:HE2	2.00	0.44
1:P:153:PRO:HG2	1:P:184:ILE:HB	2.00	0.44
1:P:256:VAL:HG13	1:P:279:ILE:HD11	2.00	0.44
3:C:47:MET:HA	3:C:58:VAL:HG21	2.00	0.44
3:O:105:GLU:OE1	3:O:173:TYR:OH	2.36	0.44
3:R:151:ASP:HA	3:R:191:SER:HB3	2.00	0.44
3:X:150:ILE:HD11	3:X:179:LEU:HD21	1.99	0.44
1:G:46:ARG:HA	1:G:47:ALA:HA	1.58	0.44
1:G:268:GLY:HA3	1:G:269:SER:HB2	1.99	0.44
1:M:356:GLU:HB3	1:M:358:TYR:HE2	1.83	0.44
2:B:76:SER:HB2	2:B:77:ASN:HB2	1.99	0.44
2:B:107:PHE:HB2	3:C:36:TYR:CE1	2.47	0.44
3:L:87:PHE:HE1	3:L:101:GLY:HA2	1.83	0.44
1:A:97:VAL:O	1:A:296:PHE:HB3	2.18	0.44
1:D:272:ARG:C	1:D:274:SER:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:TYR:CG	1:M:102:PRO:HG3	2.53	0.44
2:K:35:HIS:CD2	2:K:107:PHE:HE1	2.36	0.44
2:N:131:LEU:H	2:N:216:LYS:NZ	2.14	0.44
2:g:75:SER:O	2:g:77:ASN:HB2	2.18	0.44
2:T:29:ILE:HG23	2:T:30:LYS:HG3	2.00	0.44
2:W:48:ILE:HG12	2:W:64:PHE:CE1	2.53	0.44
1:G:220:TYR:CG	1:J:102:PRO:HG3	2.53	0.43
1:M:256:VAL:HG13	1:M:279:ILE:HD11	1.99	0.43
1:P:46:ARG:CZ	2:Q:29:ILE:HG21	2.48	0.43
2:E:35:HIS:HB2	2:E:107:PHE:HE1	1.83	0.43
2:W:47:TRP:HZ2	2:W:50:ALA:HB2	1.82	0.43
1:Y:260:VAL:O	2:g:55:TYR:OH	2.30	0.43
2:B:47:TRP:HZ2	2:B:50:ALA:HB2	1.82	0.43
2:g:106:ARG:HD2	3:j:49:TYR:HB2	2.00	0.43
2:T:36:TRP:HZ2	2:T:79:ALA:O	2.01	0.43
2:Z:29:ILE:HG12	2:Z:30:LYS:HG2	2.00	0.43
2:Z:31:ASP:OD2	2:Z:101:ASP:HB3	2.19	0.43
3:a:108:ARG:HB2	3:a:171:SER:HB2	2.00	0.43
3:a:147:LYS:HD2	3:a:149:LYS:NZ	2.33	0.43
1:G:256:VAL:HG13	1:G:279:ILE:HD11	2.00	0.43
1:P:265:ILE:HG22	1:S:110:HIS:CE1	2.53	0.43
2:E:28:ASN:C	2:E:30:LYS:H	2.26	0.43
2:H:36:TRP:HZ2	2:H:79:ALA:O	2.02	0.43
2:T:48:ILE:HG23	2:T:64:PHE:HD1	1.82	0.43
3:a:39:LYS:HG2	3:a:84:ALA:HB2	2.00	0.43
3:a:138:ASN:HA	3:a:172:THR:HB	2.00	0.43
3:F:113:PRO:HB3	3:F:139:PHE:HB3	2.00	0.43
3:F:147:LYS:HD2	3:F:149:LYS:NZ	2.34	0.43
2:Z:48:ILE:HG12	2:Z:64:PHE:CE1	2.53	0.43
1:M:163:GLN:HA	1:M:164:CYS:HA	1.70	0.43
1:Y:256:VAL:HG13	1:Y:279:ILE:HD11	2.00	0.43
2:B:26:GLY:HA2	2:B:53:PRO:HG3	1.99	0.43
2:N:75:SER:O	2:N:77:ASN:HB2	2.18	0.43
3:j:142:LYS:HB2	3:j:142:LYS:HE3	1.66	0.43
1:A:454:ARG:NH1	1:M:307:GLY:HA2	2.33	0.43
1:D:382:MET:HG2	1:D:383:ASN:H	1.84	0.43
1:P:346:SER:O	2:Q:100:HIS:NE2	2.51	0.43
2:B:36:TRP:HZ2	2:B:79:ALA:O	2.01	0.43
2:K:48:ILE:HG12	2:K:64:PHE:CE1	2.53	0.43
2:g:48:ILE:HG12	2:g:64:PHE:CE1	2.54	0.43
2:E:6:GLN:NE2	2:E:114:THR:OG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:138:GLN:O	2:K:139:THR:HG22	2.18	0.43
3:j:35:TRP:CD2	3:j:73:LEU:HD12	2.53	0.43
2:Z:77:ASN:OD1	2:Z:78:THR:N	2.45	0.43
3:a:87:PHE:HE1	3:a:101:GLY:HA2	1.83	0.43
1:A:193:GLY:HA3	1:A:284:PRO:CG	2.47	0.43
1:G:193:GLY:HA3	1:G:284:PRO:CG	2.46	0.43
1:P:268:GLY:HA2	1:V:342:THR:OG1	2.19	0.43
1:S:119:VAL:HG21	1:S:280:TYR:HE1	1.84	0.43
2:N:78:THR:OG1	2:N:79:ALA:HA	2.19	0.43
2:Q:35:HIS:CE1	2:Q:104:ARG:HA	2.53	0.43
3:U:140:TYR:CG	3:U:141:PRO:HA	2.53	0.43
2:W:32:TYR:O	2:W:53:PRO:HD2	2.18	0.43
1:A:382:MET:HG2	1:A:383:ASN:H	1.84	0.43
1:D:99:ARG:NH2	1:D:356:GLU:OE1	2.50	0.43
1:G:344:THR:HG21	3:I:53:ASN:ND2	2.33	0.43
1:J:322:VAL:HG11	1:J:358:TYR:HE1	1.84	0.43
1:M:46:ARG:HG2	1:M:51:VAL:HG21	2.01	0.43
1:S:70:PRO:HA	1:S:73:PHE:HB2	2.00	0.43
3:O:78:MET:HE2	3:O:78:MET:HB3	1.94	0.43
1:A:257:GLY:O	2:E:30:LYS:HE2	2.18	0.43
1:G:272:ARG:C	1:G:274:SER:H	2.21	0.43
1:G:338:THR:HG22	1:G:339:THR:H	1.84	0.43
1:J:153:PRO:HG2	1:J:184:ILE:HB	2.00	0.43
1:J:255:GLU:OE2	2:N:102:TYR:HB3	2.18	0.43
1:M:338:THR:HG22	1:M:339:THR:H	1.84	0.43
1:b:256:VAL:HG13	1:b:279:ILE:HD11	2.01	0.43
2:E:106:ARG:HD2	3:F:49:TYR:CD1	2.52	0.43
2:H:99:GLY:HA2	2:H:108:PRO:HD2	2.00	0.43
2:K:53:PRO:O	2:K:55:TYR:N	2.52	0.43
2:g:28:ASN:C	2:g:30:LYS:H	2.27	0.43
3:a:105:GLU:HB3	3:a:166:GLN:OE1	2.18	0.43
1:A:252:ARG:HE	1:D:332:THR:HG21	1.84	0.42
1:J:275:VAL:HG22	1:M:112:PHE:CE2	2.46	0.42
2:E:101:ASP:O	2:E:102:TYR:HB2	2.19	0.42
2:K:13:ARG:HE	2:K:120:ALA:HB1	1.83	0.42
2:N:36:TRP:CZ2	2:N:96:CYS:HB3	2.54	0.42
2:Z:131:LEU:H	2:Z:216:LYS:NZ	2.16	0.42
2:Z:131:LEU:H	2:Z:216:LYS:HZ3	1.67	0.42
1:M:123:GLY:HA2	1:M:124:SER:HA	1.76	0.42
1:P:359:ASP:HB2	1:b:224:LEU:HD13	2.01	0.42
1:S:110:HIS:HB2	1:S:210:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:23:THR:OG1	1:V:366:LEU:O	2.31	0.42
3:O:87:PHE:HE1	3:O:101:GLY:HA2	1.84	0.42
3:O:151:ASP:HA	3:O:191:SER:HB3	2.00	0.42
2:Q:26:GLY:HA2	2:Q:53:PRO:HG3	1.99	0.42
1:A:143:THR:HG23	1:A:242:GLU:HG2	2.01	0.42
1:S:193:GLY:HA3	1:S:284:PRO:CG	2.47	0.42
1:S:382:MET:HG2	1:S:383:ASN:H	1.84	0.42
1:V:269:SER:O	1:V:269:SER:OG	2.28	0.42
3:I:87:PHE:HE1	3:I:101:GLY:HA2	1.83	0.42
2:N:106:ARG:HG2	3:O:49:TYR:CB	2.50	0.42
3:O:105:GLU:HB3	3:O:166:GLN:OE1	2.19	0.42
2:g:146:GLY:O	2:g:216:LYS:NZ	2.43	0.42
1:P:193:GLY:HA3	1:P:284:PRO:HG3	2.02	0.42
1:D:123:GLY:HA2	1:D:124:SER:HA	1.79	0.42
1:G:269:SER:O	1:G:269:SER:OG	2.30	0.42
1:b:46:ARG:HA	1:b:47:ALA:HA	1.57	0.42
2:N:103:ASP:OD1	2:N:104:ARG:HG2	2.20	0.42
2:Q:36:TRP:CZ2	2:Q:96:CYS:HB3	2.55	0.42
2:W:32:TYR:HA	2:W:101:ASP:O	2.19	0.42
2:W:140:ASN:HA	2:W:141:SER:HA	1.68	0.42
1:P:83:PRO:O	1:P:87:ARG:NH1	2.50	0.42
2:T:140:ASN:HA	2:T:141:SER:HA	1.69	0.42
2:W:110:TRP:CE3	3:X:44:PRO:HD2	2.55	0.42
1:Y:153:PRO:HG2	1:Y:184:ILE:HB	2.00	0.42
1:b:23:THR:OG1	1:b:366:LEU:O	2.28	0.42
1:b:271:ASN:OD1	1:b:272:ARG:N	2.47	0.42
2:B:76:SER:OG	2:B:77:ASN:HB2	2.19	0.42
3:I:107:LYS:HE2	3:I:107:LYS:HB3	1.83	0.42
2:K:47:TRP:HZ2	2:K:50:ALA:HB2	1.84	0.42
2:W:51:ILE:HG21	2:W:70:MET:HB3	2.01	0.42
1:S:256:VAL:HG12	1:S:279:ILE:HD11	2.01	0.42
1:Y:58:TYR:CE1	1:Y:140:TYR:HB2	2.54	0.42
3:F:105:GLU:HB3	3:F:166:GLN:OE1	2.20	0.42
2:H:11:VAL:HG22	2:H:154:PRO:HG3	2.02	0.42
2:g:73:ASP:N	2:g:78:THR:HG21	2.26	0.42
2:Q:8:GLY:H	2:Q:114:THR:HG22	1.85	0.42
2:Z:110:TRP:CE3	3:a:44:PRO:HD2	2.55	0.42
3:a:47:MET:HA	3:a:58:VAL:HG21	2.01	0.42
1:S:252:ARG:HE	1:V:332:THR:HG21	1.84	0.42
3:I:106:LEU:HD23	3:I:106:LEU:HA	1.85	0.42
3:L:47:MET:HA	3:L:58:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:8:GLY:H	2:Q:114:THR:CG2	2.32	0.42
2:Q:29:ILE:HG23	2:Q:30:LYS:HG2	2.02	0.42
2:Z:161:TRP:CZ3	2:Z:202:CYS:HB3	2.55	0.42
1:D:193:GLY:HA3	1:D:284:PRO:CG	2.49	0.42
1:G:95:LEU:HD22	1:G:148:VAL:HG21	2.01	0.42
1:P:70:PRO:HA	1:P:73:PHE:HB2	2.02	0.42
1:S:265:ILE:HG22	1:V:110:HIS:CE1	2.55	0.42
1:V:39:HIS:CE1	1:V:41:TYR:HB2	2.55	0.42
1:V:58:TYR:CE1	1:V:140:TYR:HB2	2.55	0.42
2:B:36:TRP:CH2	2:B:96:CYS:HB2	2.55	0.42
2:E:33:ALA:HB2	2:E:102:TYR:HD1	1.85	0.42
3:F:109:ALA:HA	3:F:110:ASP:HA	1.86	0.42
1:A:112:PHE:O	1:A:133:ARG:HD2	2.20	0.41
1:J:146:CYS:HA	1:J:321:THR:O	2.20	0.41
1:P:32:SER:OG	1:P:33:ARG:N	2.53	0.41
1:V:273:THR:HG22	2:Z:57:ASP:HB3	2.03	0.41
1:Y:193:GLY:HA3	1:Y:284:PRO:HB3	2.01	0.41
1:Y:267:LYS:H	1:Y:267:LYS:HG3	1.46	0.41
2:B:22:CYS:HB3	2:B:79:ALA:N	2.35	0.41
2:K:31:ASP:O	2:K:32:TYR:HB2	2.19	0.41
3:L:151:ASP:HA	3:L:191:SER:HB3	2.01	0.41
2:N:47:TRP:HZ2	2:N:50:ALA:HB2	1.85	0.41
1:A:256:VAL:HG13	1:A:279:ILE:HD11	2.02	0.41
1:S:272:ARG:C	1:S:274:SER:H	2.26	0.41
1:Y:23:THR:OG1	1:Y:366:LEU:O	2.28	0.41
1:Y:70:PRO:HA	1:Y:73:PHE:HB2	2.02	0.41
2:B:48:ILE:HG12	2:B:64:PHE:CE1	2.54	0.41
2:E:36:TRP:CZ2	2:E:96:CYS:HB3	2.56	0.41
3:j:151:ASP:HA	3:j:191:SER:HB3	2.03	0.41
1:G:163:GLN:HA	1:G:164:CYS:HA	1.69	0.41
1:P:45:LYS:HG2	1:P:50:THR:HG22	2.01	0.41
1:S:153:PRO:HG3	1:S:321:THR:OG1	2.20	0.41
1:V:153:PRO:HG3	1:V:321:THR:OG1	2.20	0.41
1:b:193:GLY:HA3	1:b:284:PRO:CG	2.47	0.41
2:B:4:LEU:HD23	2:B:96:CYS:SG	2.60	0.41
3:I:14:SER:HB3	3:I:17:ASP:OD1	2.20	0.41
2:Z:40:ARG:HG3	2:Z:42:GLU:H	1.85	0.41
1:A:163:GLN:HA	1:A:164:CYS:HA	1.72	0.41
1:D:37:VAL:HG22	1:D:355:VAL:HG12	2.02	0.41
1:G:175:PRO:HA	1:G:176:PRO:HD3	1.97	0.41
1:M:382:MET:HG2	1:M:383:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:271:ASN:O	1:b:273:THR:OG1	2.37	0.41
3:C:87:PHE:CE1	3:C:101:GLY:HA2	2.55	0.41
2:H:110:TRP:CE3	3:I:44:PRO:HD2	2.55	0.41
3:L:138:ASN:HA	3:L:172:THR:HB	2.02	0.41
3:L:142:LYS:HB2	3:L:142:LYS:HE3	1.85	0.41
2:g:100:HIS:HB3	2:g:109:TYR:HE2	1.85	0.41
2:T:71:THR:OG1	2:T:80:TYR:HB2	2.20	0.41
1:M:265:ILE:HD11	2:B:55:TYR:CD1	2.56	0.41
1:M:344:THR:HG21	3:O:53:ASN:ND2	2.35	0.41
1:V:175:PRO:HA	1:V:176:PRO:HD3	1.97	0.41
1:b:271:ASN:CG	1:b:272:ARG:H	2.28	0.41
2:B:28:ASN:C	2:B:30:LYS:H	2.29	0.41
2:E:40:ARG:HG3	2:E:42:GLU:H	1.84	0.41
2:Q:51:ILE:HG13	2:Q:70:MET:HB3	2.02	0.41
1:A:46:ARG:HA	1:A:47:ALA:HA	1.57	0.41
1:V:59:GLN:OE1	1:V:61:ARG:NH2	2.54	0.41
2:H:103:ASP:HB3	2:H:106:ARG:NH1	2.36	0.41
2:N:20:LEU:O	2:N:80:TYR:HA	2.21	0.41
2:N:100:HIS:N	2:N:100:HIS:CD2	2.88	0.41
1:A:272:ARG:C	1:A:274:SER:H	2.23	0.41
1:J:117:ASP:OD2	1:J:124:SER:HB3	2.20	0.41
1:J:272:ARG:HB2	1:J:273:THR:H	1.71	0.41
1:M:46:ARG:CZ	2:N:29:ILE:HG21	2.50	0.41
2:Q:86:LEU:HA	2:Q:86:LEU:HD23	1.87	0.41
2:T:28:ASN:OD1	2:T:28:ASN:N	2.51	0.41
2:T:76:SER:HB2	2:T:77:ASN:CA	2.51	0.41
1:A:282:ASN:HB3	1:D:107:VAL:HG11	2.03	0.41
1:J:244:MET:SD	1:M:104:GLY:HA2	2.60	0.41
1:M:62:VAL:HG22	1:M:321:THR:HG23	2.03	0.41
1:P:148:VAL:HG22	1:P:320:VAL:HG22	2.03	0.41
1:S:58:TYR:CE1	1:S:140:TYR:HB2	2.55	0.41
1:V:45:LYS:HG2	1:V:50:THR:HG22	2.03	0.41
1:V:146:CYS:HA	1:V:321:THR:O	2.21	0.41
1:Y:244:MET:O	1:b:288:LEU:HD23	2.20	0.41
1:b:37:VAL:HG22	1:b:355:VAL:HG12	2.02	0.41
3:C:83:LEU:HD11	3:C:106:LEU:HG	2.01	0.41
3:I:184:ASP:O	3:I:188:ARG:HG3	2.21	0.41
2:N:40:ARG:HG3	2:N:42:GLU:H	1.85	0.41
2:T:78:THR:CB	2:T:79:ALA:HA	2.46	0.41
2:W:107:PHE:HB2	3:X:36:TYR:CE1	2.51	0.41
2:Z:35:HIS:CE1	2:Z:104:ARG:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:153:PHE:HA	2:Z:154:PRO:HA	1.88	0.41
1:A:153:PRO:HG3	1:A:321:THR:OG1	2.20	0.41
1:D:70:PRO:HA	1:D:73:PHE:HB2	2.02	0.41
1:D:84:THR:O	1:D:85:THR:OG1	2.36	0.41
1:D:257:GLY:O	2:H:30:LYS:HE2	2.21	0.41
1:D:268:GLY:O	1:D:273:THR:HA	2.20	0.41
1:G:382:MET:HG2	1:G:383:ASN:H	1.85	0.41
1:S:23:THR:OG1	1:S:366:LEU:O	2.31	0.41
1:S:244:MET:SD	1:V:104:GLY:HA2	2.61	0.41
1:b:59:GLN:OE1	1:b:61:ARG:NH2	2.53	0.41
1:b:356:GLU:HB3	1:b:358:TYR:HE2	1.85	0.41
2:E:108:PRO:HB3	3:F:46:LEU:HB2	2.02	0.41
2:E:146:GLY:O	2:E:216:LYS:NZ	2.47	0.41
2:K:40:ARG:HG3	2:K:42:GLU:H	1.85	0.41
2:N:140:ASN:HA	2:N:141:SER:HA	1.70	0.41
3:O:29:VAL:HG11	3:O:90:GLN:HG3	2.03	0.41
2:g:40:ARG:HG3	2:g:42:GLU:H	1.86	0.41
2:g:47:TRP:HZ2	2:g:50:ALA:HB2	1.86	0.41
2:T:123:THR:HG23	2:T:154:PRO:HD3	2.02	0.41
3:U:138:ASN:HA	3:U:172:THR:HB	2.02	0.41
2:W:104:ARG:HG3	3:X:91:TYR:HB2	2.03	0.41
3:X:120:PRO:HG2	3:X:130:ALA:HB1	2.02	0.41
1:G:146:CYS:HA	1:G:321:THR:O	2.21	0.41
1:G:262:ASP:OD2	1:G:263:THR:N	2.54	0.41
1:M:23:THR:OG1	1:M:366:LEU:O	2.26	0.41
1:S:146:CYS:HA	1:S:321:THR:O	2.21	0.41
1:Y:142:GLN:OE1	1:Y:243:GLN:NE2	2.54	0.41
3:I:147:LYS:HD2	3:I:149:LYS:HZ1	1.85	0.41
3:O:35:TRP:CD2	3:O:73:LEU:HD12	2.56	0.41
3:j:87:PHE:CE1	3:j:101:GLY:HA2	2.56	0.41
3:R:107:LYS:HA	3:R:140:TYR:OH	2.21	0.41
2:W:153:PHE:HA	2:W:154:PRO:HA	1.85	0.41
3:X:138:ASN:HA	3:X:172:THR:HB	2.03	0.41
2:Z:32:TYR:O	2:Z:53:PRO:HD2	2.20	0.41
1:G:37:VAL:HG22	1:G:355:VAL:HG12	2.03	0.40
1:G:45:LYS:HG2	1:G:50:THR:HG22	2.04	0.40
1:P:60:TYR:CE2	1:P:190:VAL:HA	2.57	0.40
1:b:58:TYR:CE1	1:b:140:TYR:HB2	2.56	0.40
1:b:123:GLY:HA2	1:b:124:SER:HA	1.78	0.40
3:O:113:PRO:HB3	3:O:139:PHE:HB3	2.03	0.40
2:g:78:THR:CB	2:g:79:ALA:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:78:MET:HE2	3:U:78:MET:HB3	1.96	0.40
2:W:194:THR:HG23	2:W:198:GLU:OE2	2.21	0.40
1:G:110:HIS:HB3	1:G:113:LEU:HB2	2.03	0.40
1:Y:119:VAL:HG21	1:Y:280:TYR:HE1	1.86	0.40
1:b:273:THR:HG22	2:Q:57:ASP:HB3	2.04	0.40
2:B:100:HIS:N	2:B:106:ARG:HH12	2.18	0.40
2:E:26:GLY:HA2	2:E:53:PRO:HG3	2.02	0.40
2:H:142:MET:HA	2:H:191:PRO:HA	2.03	0.40
2:g:29:ILE:HD12	2:g:29:ILE:HA	1.82	0.40
3:R:39:LYS:HG2	3:R:84:ALA:HB2	2.02	0.40
1:J:126:GLY:C	1:J:128:PRO:HD3	2.47	0.40
1:Y:382:MET:HG2	1:Y:383:ASN:H	1.86	0.40
1:b:46:ARG:HG3	1:b:46:ARG:O	2.21	0.40
3:F:78:MET:HE3	3:F:82:ASP:HB2	2.02	0.40
2:K:69:THR:HB	2:K:82:GLN:HG2	2.04	0.40
2:K:76:SER:HB2	2:K:77:ASN:CA	2.51	0.40
2:Z:171:HIS:HB2	2:Z:187:SER:OG	2.22	0.40
1:J:148:VAL:HG22	1:J:320:VAL:HG22	2.02	0.40
1:P:140:TYR:OH	1:P:212:ASP:OD1	2.39	0.40
2:E:77:ASN:HB3	2:E:78:THR:H	1.63	0.40
2:N:48:ILE:HG12	2:N:64:PHE:CE1	2.55	0.40
2:g:99:GLY:HA2	2:g:108:PRO:CD	2.52	0.40
2:T:75:SER:O	2:T:77:ASN:HB2	2.21	0.40
2:Z:131:LEU:HD11	2:Z:148:LEU:HB2	2.03	0.40
1:J:260:VAL:N	2:N:55:TYR:OH	2.55	0.40
1:J:382:MET:HG2	1:J:383:ASN:H	1.85	0.40
1:M:46:ARG:HB2	2:N:29:ILE:HG12	2.04	0.40
1:P:46:ARG:O	1:P:46:ARG:HG3	2.20	0.40
1:P:382:MET:HG2	1:P:383:ASN:H	1.86	0.40
2:W:35:HIS:CE1	2:W:104:ARG:HA	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:77:ASP:OD2	3:F:189:HIS:NE2[2_545]	2.05	0.15
3:I:127:SER:OG	2:Q:5:GLN:OE1[1_565]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	12	45
1	D	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	12	45
1	G	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	12	45
1	J	412/496 (83%)	383 (93%)	24 (6%)	5 (1%)	10	41
1	M	412/496 (83%)	384 (93%)	24 (6%)	4 (1%)	12	45
1	P	412/496 (83%)	386 (94%)	22 (5%)	4 (1%)	12	45
1	S	412/496 (83%)	382 (93%)	28 (7%)	2 (0%)	24	57
1	V	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	12	45
1	Y	412/496 (83%)	381 (92%)	26 (6%)	5 (1%)	10	41
1	b	412/496 (83%)	382 (93%)	27 (7%)	3 (1%)	18	51
2	B	216/221 (98%)	189 (88%)	20 (9%)	7 (3%)	3	24
2	E	216/221 (98%)	187 (87%)	20 (9%)	9 (4%)	2	19
2	H	216/221 (98%)	187 (87%)	22 (10%)	7 (3%)	3	24
2	K	216/221 (98%)	190 (88%)	18 (8%)	8 (4%)	2	21
2	N	216/221 (98%)	186 (86%)	21 (10%)	9 (4%)	2	19
2	Q	216/221 (98%)	191 (88%)	21 (10%)	4 (2%)	6	33
2	T	216/221 (98%)	191 (88%)	20 (9%)	5 (2%)	5	30
2	W	216/221 (98%)	186 (86%)	21 (10%)	9 (4%)	2	19
2	Z	216/221 (98%)	186 (86%)	23 (11%)	7 (3%)	3	24
2	g	216/221 (98%)	188 (87%)	18 (8%)	10 (5%)	2	17
3	C	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	57
3	F	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	57
3	I	212/214 (99%)	202 (95%)	8 (4%)	2 (1%)	14	46
3	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	57
3	O	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	24	57
3	U	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	14	46
3	X	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	57
3	a	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	57
3	j	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	24	57
All	All	8400/9310 (90%)	7731 (92%)	543 (6%)	126 (2%)	8	37

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	273	THR
1	Y	263	THR
1	Y	273	THR
2	B	31	ASP
2	B	77	ASN
2	E	29	ILE
2	E	31	ASP
2	E	32	TYR
2	E	102	TYR
2	H	29	ILE
2	H	31	ASP
2	H	32	TYR
2	H	77	ASN
2	K	29	ILE
2	K	77	ASN
2	N	77	ASN
2	N	106	ARG
2	g	29	ILE
2	g	32	TYR
2	g	77	ASN
2	Q	29	ILE
2	Q	77	ASN
2	T	31	ASP
2	T	77	ASN
2	W	29	ILE
2	W	32	TYR
2	Z	29	ILE
2	Z	122	LYS
1	A	125	GLY
1	A	273	THR

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Mol	Chain	Res	Type
1	D	125	GLY
1	D	273	THR
1	G	125	GLY
1	J	125	GLY
1	M	125	GLY
1	M	273	THR
1	P	125	GLY
1	S	125	GLY
1	V	125	GLY
1	V	273	THR
1	Y	125	GLY
1	Y	272	ARG
1	b	125	GLY
2	B	29	ILE
2	N	31	ASP
2	N	105	GLY
2	g	31	ASP
3	j	108	ARG
3	U	108	ARG
2	W	31	ASP
2	W	75	SER
2	W	103	ASP
2	W	209	SER
2	Z	31	ASP
3	a	77	ASN
1	G	273	THR
1	b	273	THR
2	H	78	THR
2	K	78	THR
2	K	79	ALA
2	N	28	ASN
2	N	122	LYS
2	g	54	GLU
2	g	103	ASP
1	D	168	PRO
1	D	272	ARG
1	G	168	PRO
1	J	168	PRO
1	J	272	ARG
1	M	168	PRO
1	P	168	PRO
1	P	271	ASN

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Mol	Chain	Res	Type
1	V	168	PRO
1	V	272	ARG
1	b	168	PRO
2	B	54	GLU
2	E	78	THR
2	E	107	PHE
2	E	166	LEU
3	I	108	ARG
2	N	166	LEU
3	O	77	ASN
2	g	78	THR
2	Q	54	GLU
2	Z	142	MET
1	A	272	ARG
1	G	272	ARG
1	M	272	ARG
1	P	269	SER
1	S	168	PRO
1	Y	168	PRO
2	B	78	THR
2	B	166	LEU
3	C	77	ASN
2	H	142	MET
3	I	77	ASN
2	K	54	GLU
2	K	166	LEU
2	g	55	TYR
2	g	84	SER
2	g	166	LEU
2	Q	166	LEU
2	T	54	GLU
2	T	166	LEU
2	W	54	GLU
2	W	166	LEU
3	X	77	ASN
2	Z	54	GLU
2	Z	103	ASP
2	Z	166	LEU
1	A	168	PRO
2	B	84	SER
2	E	84	SER
2	E	142	MET

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Mol	Chain	Res	Type
3	F	77	ASN
2	H	166	LEU
2	K	103	ASP
3	L	77	ASN
2	N	84	SER
3	R	77	ASN
2	T	84	SER
3	U	77	ASN
2	W	142	MET
1	J	193	GLY
2	K	53	PRO
2	N	29	ILE

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	363/432 (84%)	359 (99%)	4 (1%)	65	74
1	D	363/432 (84%)	357 (98%)	6 (2%)	53	69
1	G	363/432 (84%)	358 (99%)	5 (1%)	59	71
1	J	363/432 (84%)	357 (98%)	6 (2%)	53	69
1	M	363/432 (84%)	356 (98%)	7 (2%)	50	67
1	P	363/432 (84%)	357 (98%)	6 (2%)	53	69
1	S	363/432 (84%)	357 (98%)	6 (2%)	53	69
1	V	363/432 (84%)	359 (99%)	4 (1%)	65	74
1	Y	363/432 (84%)	355 (98%)	8 (2%)	45	65
1	b	363/432 (84%)	357 (98%)	6 (2%)	53	69
2	B	184/187 (98%)	169 (92%)	15 (8%)	10	36
2	E	184/187 (98%)	173 (94%)	11 (6%)	17	45
2	H	184/187 (98%)	174 (95%)	10 (5%)	20	47
2	K	184/187 (98%)	173 (94%)	11 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	184/187 (98%)	171 (93%)	13 (7%)	13	40
2	Q	184/187 (98%)	173 (94%)	11 (6%)	17	45
2	T	184/187 (98%)	173 (94%)	11 (6%)	17	45
2	W	184/187 (98%)	177 (96%)	7 (4%)	29	55
2	Z	184/187 (98%)	174 (95%)	10 (5%)	20	47
2	g	184/187 (98%)	170 (92%)	14 (8%)	12	39
3	C	189/189 (100%)	189 (100%)	0	100	100
3	F	189/189 (100%)	186 (98%)	3 (2%)	55	69
3	I	189/189 (100%)	187 (99%)	2 (1%)	65	74
3	L	189/189 (100%)	186 (98%)	3 (2%)	55	69
3	O	189/189 (100%)	189 (100%)	0	100	100
3	R	189/189 (100%)	187 (99%)	2 (1%)	65	74
3	U	189/189 (100%)	187 (99%)	2 (1%)	65	74
3	X	189/189 (100%)	189 (100%)	0	100	100
3	a	189/189 (100%)	187 (99%)	2 (1%)	65	74
3	j	189/189 (100%)	186 (98%)	3 (2%)	55	69
All	All	7360/8080 (91%)	7172 (97%)	188 (3%)	40	62

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	VAL
1	A	273	THR
1	A	288	LEU
1	A	338	THR
1	D	256	VAL
1	D	267	LYS
1	D	273	THR
1	D	281	VAL
1	D	288	LEU
1	D	338	THR
1	G	256	VAL
1	G	273	THR
1	G	281	VAL
1	G	288	LEU
1	G	338	THR

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Mol	Chain	Res	Type
1	J	168	PRO
1	J	255	GLU
1	J	256	VAL
1	J	273	THR
1	J	288	LEU
1	J	338	THR
1	M	256	VAL
1	M	265	ILE
1	M	267	LYS
1	M	273	THR
1	M	288	LEU
1	M	338	THR
1	M	342	THR
1	P	33	ARG
1	P	192	THR
1	P	256	VAL
1	P	269	SER
1	P	288	LEU
1	P	338	THR
1	S	119	VAL
1	S	273	THR
1	S	288	LEU
1	S	302	LEU
1	S	338	THR
1	S	342	THR
1	V	256	VAL
1	V	273	THR
1	V	288	LEU
1	V	338	THR
1	Y	119	VAL
1	Y	256	VAL
1	Y	267	LYS
1	Y	271	ASN
1	Y	272	ARG
1	Y	273	THR
1	Y	288	LEU
1	Y	338	THR
1	b	12	LYS
1	b	256	VAL
1	b	273	THR
1	b	281	VAL
1	b	288	LEU

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Mol	Chain	Res	Type
1	b	338	THR
2	B	6	GLN
2	B	28	ASN
2	B	29	ILE
2	B	54	GLU
2	B	74	THR
2	B	76	SER
2	B	78	THR
2	B	80	TYR
2	B	96	CYS
2	B	100	HIS
2	B	114	THR
2	B	123	THR
2	B	124	THR
2	B	143	VAL
2	B	160	THR
2	E	28	ASN
2	E	29	ILE
2	E	52	ASP
2	E	74	THR
2	E	76	SER
2	E	78	THR
2	E	100	HIS
2	E	106	ARG
2	E	124	THR
2	E	143	VAL
2	E	160	THR
3	F	49	TYR
3	F	56	THR
3	F	107	LYS
2	H	6	GLN
2	H	28	ASN
2	H	29	ILE
2	H	74	THR
2	H	104	ARG
2	H	114	THR
2	H	122	LYS
2	H	139	THR
2	H	140	ASN
2	H	215	LYS
3	I	107	LYS
3	I	110	ASP

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Mol	Chain	Res	Type
2	K	6	GLN
2	K	28	ASN
2	K	29	ILE
2	K	74	THR
2	K	76	SER
2	K	78	THR
2	K	96	CYS
2	K	106	ARG
2	K	114	THR
2	K	124	THR
2	K	143	VAL
3	L	106	LEU
3	L	107	LYS
3	L	110	ASP
2	N	6	GLN
2	N	28	ASN
2	N	29	ILE
2	N	74	THR
2	N	76	SER
2	N	78	THR
2	N	80	TYR
2	N	100	HIS
2	N	114	THR
2	N	123	THR
2	N	124	THR
2	N	143	VAL
2	N	215	LYS
2	g	6	GLN
2	g	74	THR
2	g	76	SER
2	g	78	THR
2	g	103	ASP
2	g	104	ARG
2	g	114	THR
2	g	123	THR
2	g	124	THR
2	g	140	ASN
2	g	141	SER
2	g	160	THR
2	g	209	SER
2	g	215	LYS
3	j	31	THR

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Mol	Chain	Res	Type
3	j	77	ASN
3	j	78	MET
2	Q	6	GLN
2	Q	28	ASN
2	Q	29	ILE
2	Q	70	MET
2	Q	71	THR
2	Q	78	THR
2	Q	87	THR
2	Q	104	ARG
2	Q	114	THR
2	Q	123	THR
2	Q	143	VAL
3	R	108	ARG
3	R	110	ASP
2	T	6	GLN
2	T	27	PHE
2	T	74	THR
2	T	76	SER
2	T	104	ARG
2	T	114	THR
2	T	123	THR
2	T	124	THR
2	T	139	THR
2	T	143	VAL
2	T	215	LYS
3	U	107	LYS
3	U	110	ASP
2	W	6	GLN
2	W	29	ILE
2	W	78	THR
2	W	114	THR
2	W	123	THR
2	W	143	VAL
2	W	215	LYS
2	Z	6	GLN
2	Z	28	ASN
2	Z	29	ILE
2	Z	30	LYS
2	Z	78	THR
2	Z	114	THR
2	Z	123	THR

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Mol	Chain	Res	Type
2	Z	124	THR
2	Z	211	THR
2	Z	215	LYS
3	a	106	LEU
3	a	110	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	330	ASN
1	A	361	GLN
1	D	316	ASN
1	D	330	ASN
1	D	361	GLN
1	G	185	GLN
1	G	330	ASN
1	G	361	GLN
1	J	243	GLN
1	J	330	ASN
1	J	361	GLN
1	M	185	GLN
1	M	330	ASN
1	M	361	GLN
1	P	361	GLN
1	S	101	GLN
1	S	308	HIS
1	S	316	ASN
1	S	330	ASN
1	S	361	GLN
1	V	157	HIS
1	V	316	ASN
1	V	330	ASN
1	V	361	GLN
1	Y	330	ASN
1	Y	361	GLN
1	b	157	HIS
1	b	330	ASN
1	b	361	GLN
2	E	77	ASN
3	F	89	GLN
3	F	161	ASN

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Mol	Chain	Res	Type
3	F	166	GLN
3	I	161	ASN
2	K	140	ASN
3	L	161	ASN
2	N	140	ASN
3	O	156	GLN
2	g	100	HIS
3	j	77	ASN
3	j	161	ASN
2	Q	140	ASN
3	R	161	ASN
2	T	140	ASN
3	U	161	ASN
3	U	166	GLN
3	a	161	ASN
3	a	166	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 ⓘ

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	416/496 (83%)	0.17	7 (1%) 69 41	27, 62, 124, 168	0
1	D	416/496 (83%)	0.24	6 (1%) 73 46	37, 70, 124, 189	0
1	G	416/496 (83%)	0.22	7 (1%) 69 41	41, 70, 132, 183	0
1	J	416/496 (83%)	0.26	6 (1%) 73 46	31, 64, 122, 185	0
1	M	416/496 (83%)	0.22	7 (1%) 69 41	28, 59, 118, 184	0
1	P	416/496 (83%)	0.17	3 (0%) 84 61	34, 64, 123, 186	0
1	S	416/496 (83%)	0.26	7 (1%) 69 41	31, 60, 119, 174	0
1	V	416/496 (83%)	0.15	4 (0%) 79 54	30, 64, 118, 183	0
1	Y	416/496 (83%)	0.23	5 (1%) 76 50	40, 71, 132, 169	0
1	b	416/496 (83%)	0.24	10 (2%) 59 34	43, 69, 124, 163	0
2	B	218/221 (98%)	0.52	13 (5%) 27 17	34, 63, 123, 163	0
2	E	218/221 (98%)	0.82	20 (9%) 14 11	52, 109, 174, 217	0
2	H	218/221 (98%)	0.61	9 (4%) 41 23	52, 91, 133, 172	0
2	K	218/221 (98%)	0.95	27 (12%) 8 7	40, 108, 220, 258	0
2	N	218/221 (98%)	0.63	16 (7%) 21 14	38, 73, 144, 204	0
2	Q	218/221 (98%)	0.73	18 (8%) 17 12	53, 98, 148, 174	0
2	T	218/221 (98%)	0.71	14 (6%) 25 16	47, 109, 171, 191	0
2	W	218/221 (98%)	0.59	13 (5%) 27 17	35, 70, 161, 191	0
2	Z	218/221 (98%)	0.88	17 (7%) 19 13	49, 99, 157, 210	0
2	g	218/221 (98%)	0.70	8 (3%) 45 25	58, 105, 196, 218	0
3	C	214/214 (100%)	0.21	2 (0%) 81 56	10, 58, 102, 125	12 (5%)
3	F	214/214 (100%)	0.46	6 (2%) 55 31	10, 97, 175, 211	12 (5%)
3	I	214/214 (100%)	0.40	4 (1%) 66 39	13, 103, 154, 191	12 (5%)
3	L	214/214 (100%)	0.56	8 (3%) 45 25	12, 118, 223, 275	12 (5%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
3	O	214/214 (100%)	0.24	5 (2%)	61	35	10, 77, 140, 193	12 (5%)
3	R	214/214 (100%)	0.44	6 (2%)	55	31	17, 96, 150, 195	12 (5%)
3	U	214/214 (100%)	0.50	9 (4%)	40	22	14, 109, 202, 229	12 (5%)
3	X	214/214 (100%)	0.25	4 (1%)	66	39	8, 80, 141, 189	12 (5%)
3	a	214/214 (100%)	0.35	5 (2%)	61	35	10, 76, 142, 194	12 (5%)
3	j	214/214 (100%)	0.48	9 (4%)	40	22	16, 113, 183, 218	12 (5%)
All	All	8480/9310 (91%)	0.39	275 (3%)	50	29	8, 75, 167, 275	120 (1%)

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	101	ASP	6.3
3	L	56	THR	5.9
3	a	56	THR	5.9
2	E	97	ASN	5.8
3	R	56	THR	5.6
2	N	97	ASN	5.4
3	U	56	THR	5.3
3	F	56	THR	5.2
2	B	97	ASN	5.1
2	K	147	CYS	5.0
2	Z	97	ASN	5.0
2	H	97	ASN	4.7
2	Q	105	GLY	4.7
3	j	56	THR	4.6
2	g	84	SER	4.4
2	T	97	ASN	4.3
2	W	97	ASN	4.2
3	I	56	THR	4.1
2	B	29	ILE	3.9
2	K	218	VAL	3.8
2	g	101	ASP	3.8
2	H	78	THR	3.8
3	I	76	SER	3.8
3	O	56	THR	3.8
2	N	57	ASP	3.7
1	D	193	GLY	3.7
3	L	119	PRO	3.7
1	S	274	SER	3.6
2	g	65	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
2	g	97	ASN	3.6
1	J	80	LEU	3.6
2	Z	105	GLY	3.6
3	C	56	THR	3.5
3	U	156	GLN	3.5
1	b	255	GLU	3.5
1	M	270	GLY	3.5
1	V	148	VAL	3.5
2	K	29	ILE	3.4
1	S	148	VAL	3.4
2	K	132	ALA	3.3
2	T	79	ALA	3.3
2	g	29	ILE	3.3
3	X	56	THR	3.3
2	N	105	GLY	3.3
2	H	29	ILE	3.3
2	K	186	SER	3.3
1	Y	193	GLY	3.3
2	E	70	MET	3.2
2	N	74	THR	3.2
2	Z	183	THR	3.2
2	E	29	ILE	3.2
2	H	101	ASP	3.1
1	V	268	GLY	3.1
2	H	65	GLN	3.1
2	W	101	ASP	3.1
1	Y	148	VAL	3.0
2	E	166	LEU	3.0
2	Q	59	GLU	3.0
3	R	74	THR	3.0
1	M	148	VAL	3.0
2	K	187	SER	3.0
3	R	148	TRP	3.0
2	K	97	ASN	3.0
2	Q	97	ASN	3.0
1	M	255	GLU	3.0
1	A	148	VAL	3.0
2	N	1	GLU	3.0
2	K	188	VAL	3.0
2	g	25	SER	3.0
2	Z	25	SER	3.0
3	j	178	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	R	157	ASN	2.9
2	B	105	GLY	2.9
3	U	109	ALA	2.9
2	Z	166	LEU	2.9
3	U	178	THR	2.9
2	B	25	SER	2.9
3	j	106	LEU	2.9
1	J	268	GLY	2.8
2	E	78	THR	2.8
2	W	29	ILE	2.8
1	D	268	GLY	2.8
1	D	80	LEU	2.8
2	Z	62	PRO	2.8
1	Y	246	ALA	2.8
1	A	426	PRO	2.8
1	b	426	PRO	2.8
2	H	79	ALA	2.8
1	A	80	LEU	2.7
2	Q	29	ILE	2.7
1	G	382	MET	2.7
1	J	148	VAL	2.7
2	Q	218	VAL	2.7
3	a	131	SER	2.7
2	T	102	TYR	2.7
2	K	217	ILE	2.7
2	E	107	PHE	2.7
2	Z	218	VAL	2.7
1	b	264	LEU	2.7
2	Q	24	ALA	2.7
3	L	131	SER	2.7
1	D	255	GLU	2.7
3	L	76	SER	2.7
3	j	160	LEU	2.7
2	T	29	ILE	2.6
3	U	163	ALA	2.6
2	N	59	GLU	2.6
2	K	159	VAL	2.6
2	Q	2	VAL	2.6
2	E	106	ARG	2.6
2	Q	7	SER	2.6
2	E	98	ALA	2.6
1	J	264	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	K	166	LEU	2.6
2	K	62	PRO	2.6
2	E	74	THR	2.5
2	E	25	SER	2.5
1	V	426	PRO	2.5
3	X	135	PHE	2.5
3	U	76	SER	2.5
2	B	101	ASP	2.5
2	W	57	ASP	2.5
1	M	268	GLY	2.5
3	R	76	SER	2.5
2	N	101	ASP	2.5
1	A	306	GLN	2.5
1	S	268	GLY	2.5
2	T	25	SER	2.5
2	Z	185	SER	2.5
1	b	121	ASN	2.5
2	B	59	GLU	2.5
2	K	98	ALA	2.5
2	Q	108	PRO	2.5
2	B	102	TYR	2.5
2	Z	153	PHE	2.4
2	W	74	THR	2.4
2	T	2	VAL	2.4
2	W	106	ARG	2.4
2	Z	77	ASN	2.4
2	K	108	PRO	2.4
1	G	268	GLY	2.4
2	Q	101	ASP	2.4
3	I	133	VAL	2.4
2	E	147	CYS	2.4
3	X	47	MET	2.4
3	F	152	GLY	2.4
1	b	148	VAL	2.4
2	W	55	TYR	2.4
3	U	131	SER	2.4
1	D	148	VAL	2.4
3	U	180	THR	2.4
3	a	126	THR	2.4
2	K	57	ASP	2.4
2	Q	180	ASP	2.4
2	W	70	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLU	2.4
1	A	121	ASN	2.3
2	K	170	VAL	2.3
2	E	32	TYR	2.3
3	a	47	MET	2.3
2	Q	46	GLU	2.3
3	j	131	SER	2.3
2	K	70	MET	2.3
2	Q	98	ALA	2.3
2	T	24	ALA	2.3
2	B	103	ASP	2.3
2	E	31	ASP	2.3
1	G	76	PRO	2.3
1	b	193	GLY	2.3
2	N	25	SER	2.3
2	K	200	VAL	2.3
2	B	74	THR	2.3
2	H	98	ALA	2.3
3	I	186	TYR	2.3
3	j	150	ILE	2.3
1	S	168	PRO	2.3
1	V	308	HIS	2.3
2	Q	102	TYR	2.3
2	W	102	TYR	2.3
2	W	25	SER	2.3
2	Z	204	VAL	2.3
3	j	80	SER	2.3
1	S	193	GLY	2.3
2	B	62	PRO	2.3
2	W	26	GLY	2.3
3	F	202	THR	2.2
1	b	266	ILE	2.2
2	Z	150	LYS	2.2
2	H	58	THR	2.2
3	X	106	LEU	2.2
2	K	24	ALA	2.2
1	J	232	GLY	2.2
2	K	157	VAL	2.2
2	E	130	PRO	2.2
2	W	23	THR	2.2
2	K	101	ASP	2.2
2	N	31	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	Q	159	VAL	2.2
2	Z	151	GLY	2.2
3	L	164	THR	2.2
2	Q	31	ASP	2.2
2	Q	140	ASN	2.2
1	M	269	SER	2.2
2	E	10	GLU	2.2
2	N	108	PRO	2.2
2	B	78	THR	2.2
3	O	178	THR	2.2
2	E	72	ALA	2.2
1	G	177	LEU	2.2
1	P	148	VAL	2.1
1	A	193	GLY	2.1
1	P	126	GLY	2.1
1	b	128	PRO	2.1
2	N	58	THR	2.1
2	E	145	LEU	2.1
2	g	184	LEU	2.1
1	S	81	PHE	2.1
2	K	78	THR	2.1
1	J	331	MET	2.1
2	N	166	LEU	2.1
2	N	24	ALA	2.1
3	O	150	ILE	2.1
3	L	101	GLY	2.1
2	H	108	PRO	2.1
3	L	160	LEU	2.1
3	a	127	SER	2.1
2	Z	65	GLN	2.1
2	T	61	VAL	2.1
3	L	136	LEU	2.1
3	O	47	MET	2.1
1	S	267	LYS	2.1
2	T	185	SER	2.1
2	K	65	GLN	2.1
3	j	133	VAL	2.1
2	K	148	LEU	2.1
3	F	106	LEU	2.1
1	M	76	PRO	2.1
2	Z	103	ASP	2.1
2	B	23	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	j	13	THR	2.1
2	E	79	ALA	2.1
2	N	33	ALA	2.1
3	F	76	SER	2.1
3	O	131	SER	2.1
1	b	282	ASN	2.1
2	K	2	VAL	2.1
2	g	37	VAL	2.1
1	M	85	THR	2.0
2	Q	199	THR	2.0
2	T	106	ARG	2.0
2	Z	101	ASP	2.0
2	N	46	GLU	2.0
3	R	13	THR	2.0
1	G	196	ALA	2.0
1	Y	126	GLY	2.0
1	Y	215	GLY	2.0
2	K	134	GLY	2.0
2	Z	26	GLY	2.0
1	P	266	ILE	2.0
1	D	121	ASN	2.0
3	U	161	ASN	2.0
1	G	193	GLY	2.0
2	E	105	GLY	2.0
2	T	105	GLY	2.0
1	b	265	ILE	2.0
2	W	217	ILE	2.0
2	N	23	THR	2.0
3	F	74	THR	2.0
2	B	166	LEU	2.0
2	K	46	GLU	2.0
1	G	201	ASP	2.0
2	T	72	ALA	2.0
2	T	103	ASP	2.0
3	C	76	SER	2.0
2	T	218	VAL	2.0

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

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

6.3 Carbohydrates [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.