



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 02:47 PM UTC

PDB ID : 5Y9F / pdb_00005y9f
Title : Crystal structure of HPV59 pentamer in complex with the Fab fragment of antibody 28F10
Authors : Li, S.W.; Li, Z.H.
Deposited on : 2017-08-24
Resolution : 3.35 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

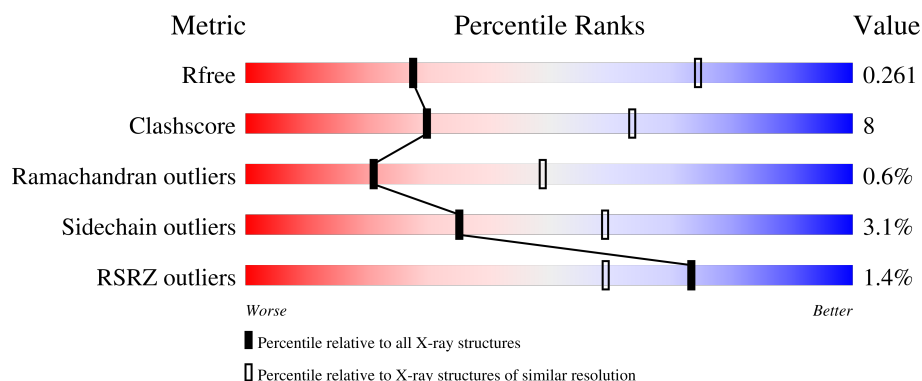
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	500	
1	B	500	
1	C	500	
1	D	500	
1	E	500	

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Mol	Chain	Length	Quality of chain
1	F	500	
1	G	500	
1	H	500	
1	I	500	
1	J	500	
2	K	219	
2	M	219	
2	O	219	
2	Q	219	
2	S	219	
2	U	219	
2	W	219	
2	Y	219	
2	a	219	
2	c	219	
3	L	223	
3	N	223	
3	P	223	
3	R	223	
3	T	223	
3	V	223	
3	X	223	
3	Z	223	
3	b	223	
3	d	223	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 66832 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	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	B	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	C	421	Total	C	N	O	S	0	0	0
			3345	2128	562	638	17			
1	D	421	Total	C	N	O	S	0	0	0
			3345	2128	562	638	17			
1	E	427	Total	C	N	O	S	0	0	0
			3384	2154	568	645	17			
1	F	421	Total	C	N	O	S	0	0	0
			3345	2128	562	638	17			
1	G	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	H	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	I	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	J	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q81971
A	175	SER	CYS	engineered mutation	UNP Q81971
B	9	MET	-	initiating methionine	UNP Q81971
B	175	SER	CYS	engineered mutation	UNP Q81971
C	9	MET	-	initiating methionine	UNP Q81971
C	175	SER	CYS	engineered mutation	UNP Q81971
D	9	MET	-	initiating methionine	UNP Q81971
D	175	SER	CYS	engineered mutation	UNP Q81971
E	9	MET	-	initiating methionine	UNP Q81971

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Chain	Residue	Modelled	Actual	Comment	Reference
E	175	SER	CYS	engineered mutation	UNP Q81971
F	9	MET	-	initiating methionine	UNP Q81971
F	175	SER	CYS	engineered mutation	UNP Q81971
G	9	MET	-	initiating methionine	UNP Q81971
G	175	SER	CYS	engineered mutation	UNP Q81971
H	9	MET	-	initiating methionine	UNP Q81971
H	175	SER	CYS	engineered mutation	UNP Q81971
I	9	MET	-	initiating methionine	UNP Q81971
I	175	SER	CYS	engineered mutation	UNP Q81971
J	9	MET	-	initiating methionine	UNP Q81971
J	175	SER	CYS	engineered mutation	UNP Q81971

- Molecule 2 is a protein called light chains of Fab fragment of antibody 28F10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	O	218	Total	C	N	O	S	0	0	0
			1689	1054	288	341	6			
2	Q	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	S	218	Total	C	N	O	S	0	0	0
			1689	1054	288	341	6			
2	M	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	c	218	Total	C	N	O	S	0	0	0
			1689	1054	288	341	6			
2	W	219	Total	C	N	O	S	0	0	0
			1695	1057	289	342	7			
2	Y	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	a	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	U	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			

- Molecule 3 is a protein called heavy chain of Fab fragment of antibody 28F10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	222	Total	C	N	O	S	0	0	0
			1671	1062	268	332	9			
3	P	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			

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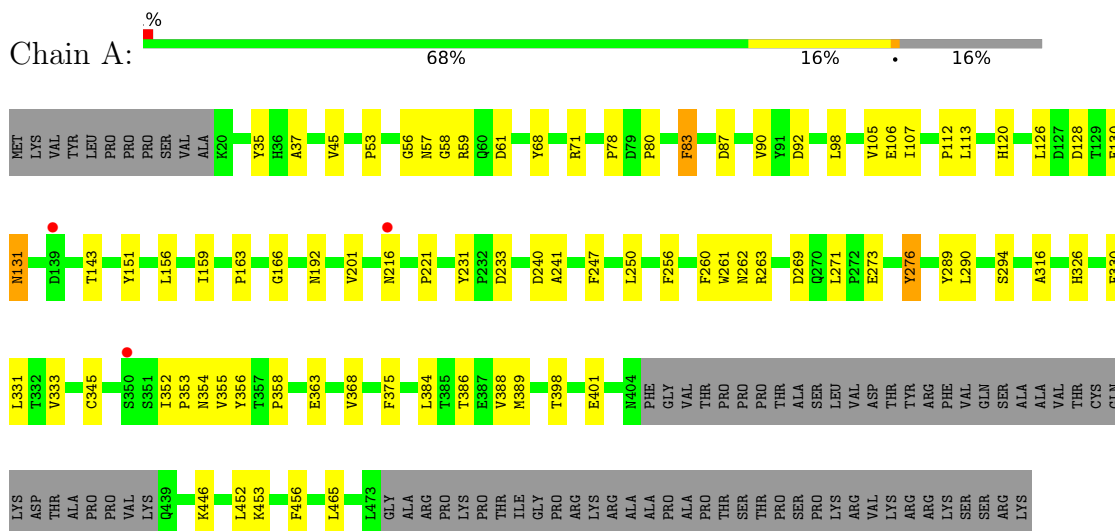
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	221	Total	C	N	O	S	0	0	0
			1666	1059	267	331	9			
3	T	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	N	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	d	221	Total	C	N	O	S	0	0	0
			1666	1059	267	331	9			
3	V	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	X	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	Z	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	b	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			

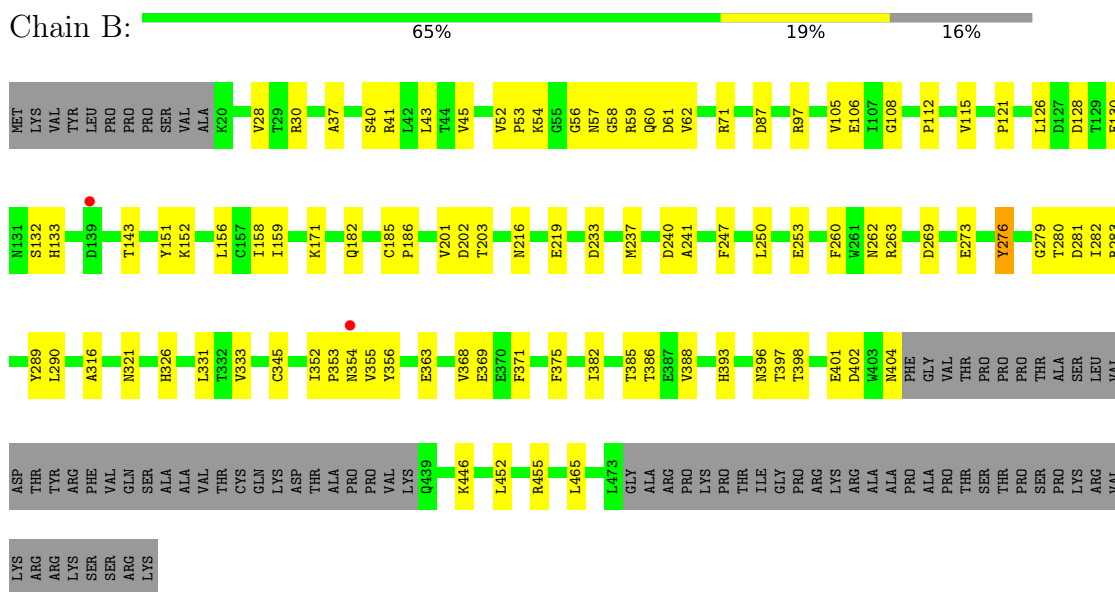
3 Residue-property plots [i](#)

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



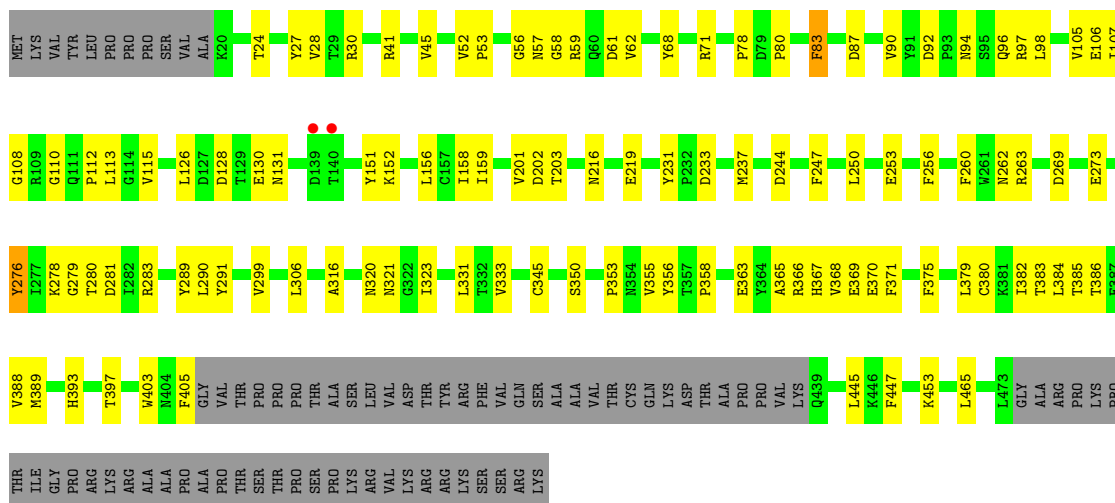
• Molecule 1: Major capsid protein L1



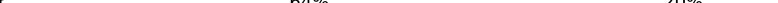
• Molecule 1: Major capsid protein L1

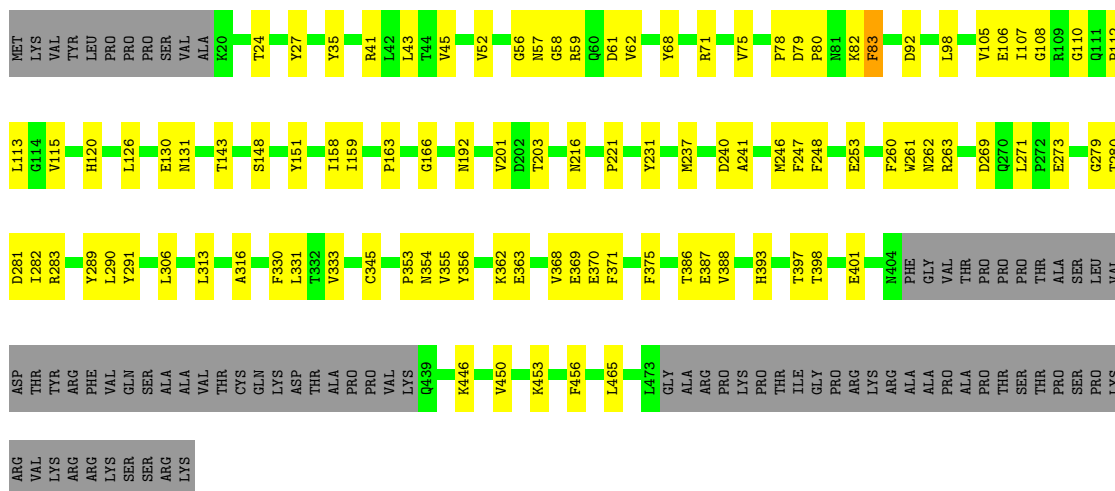
- Molecule 1: Major capsid protein L1

Chain F: 62% 22% 16%

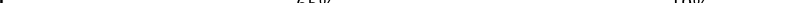


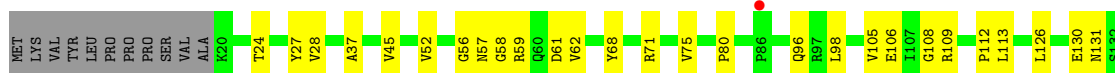
- Molecule 1: Major capsid protein L1

Chain G:  64% 20% 16%

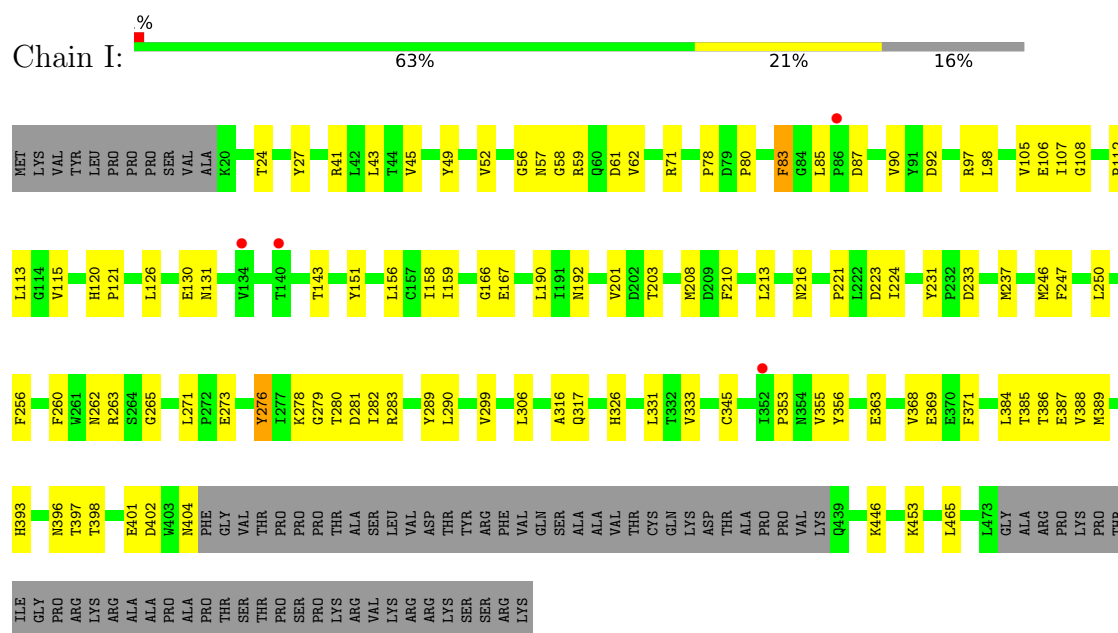


- Molecule 1: Major capsid protein L1

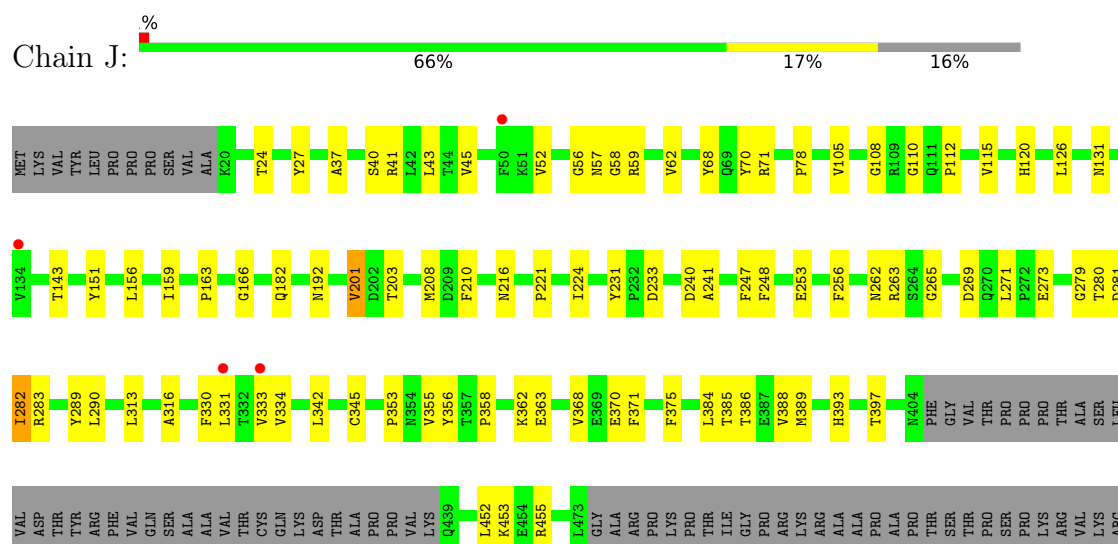
Chain H:  %



- Molecule 1: Major capsid protein L1

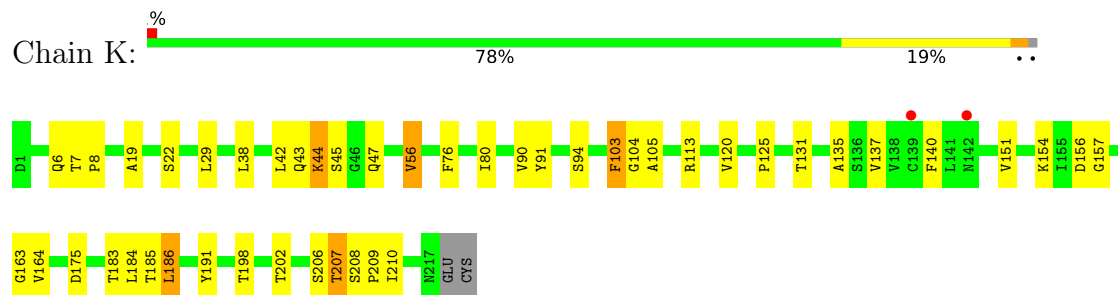


- Molecule 1: Major capsid protein L1

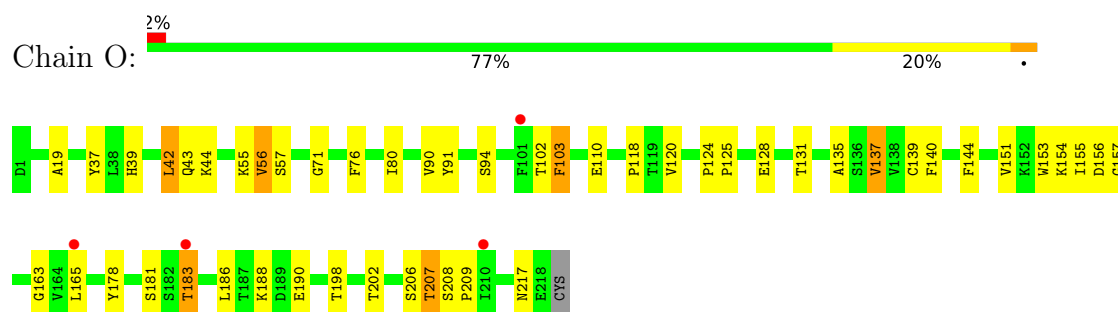


ARG
LYS
SER
SER
ARG
LYS

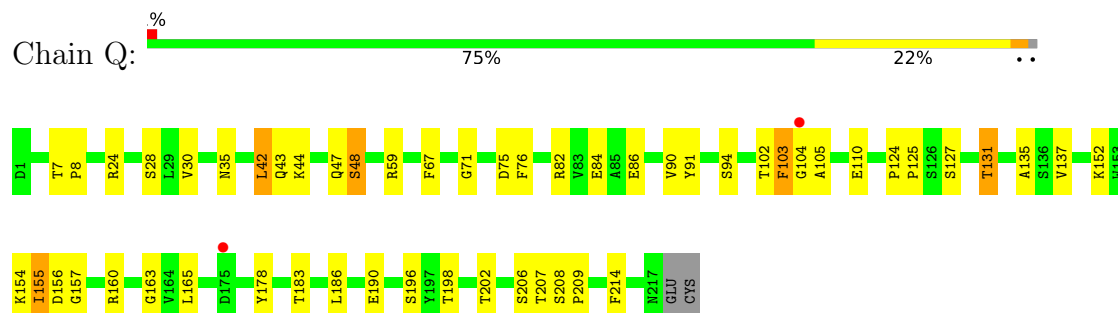
- Molecule 2: light chains of Fab fragment of antibody 28F10



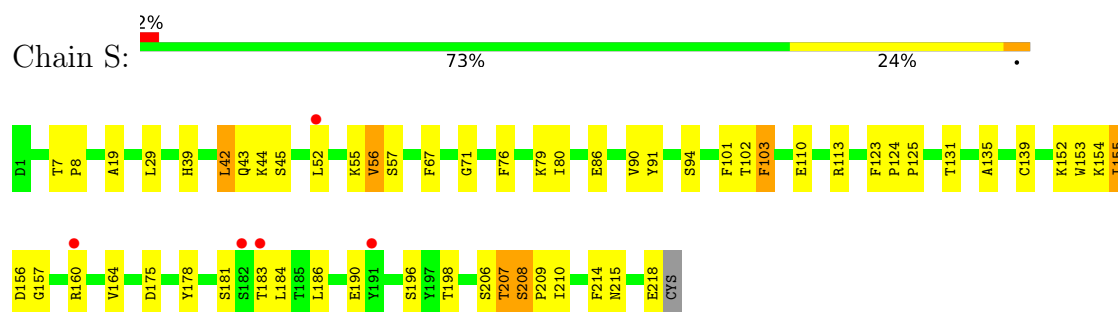
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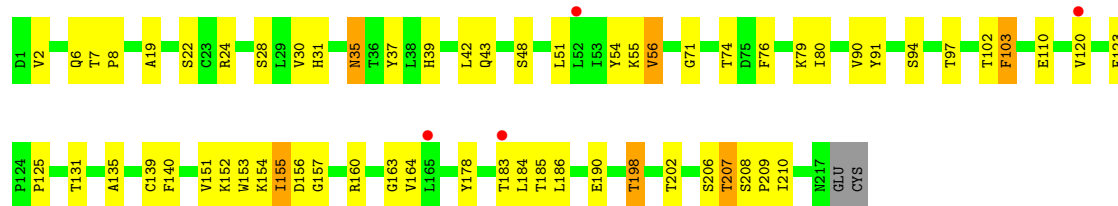


- Molecule 2: light chains of Fab fragment of antibody 28F10

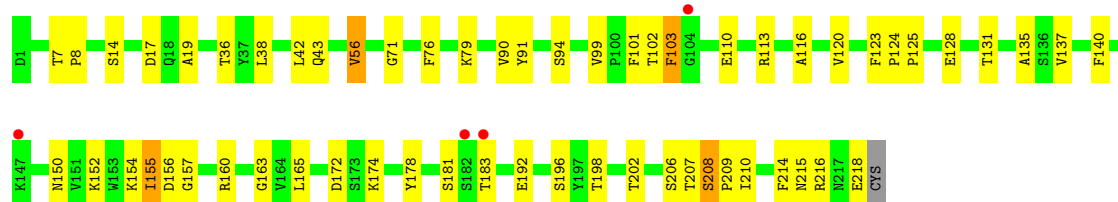
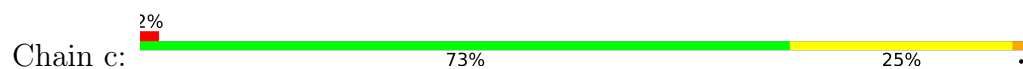


- Molecule 2: light chains of Fab fragment of antibody 28F10

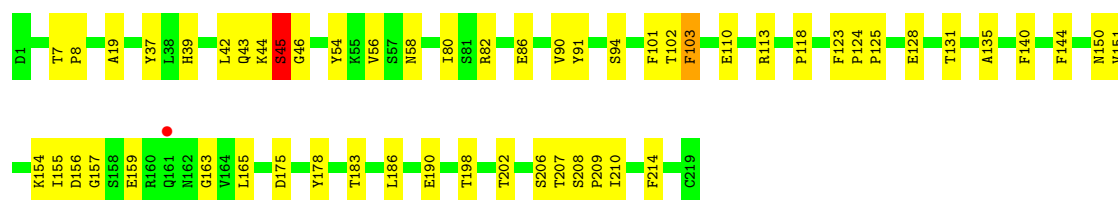
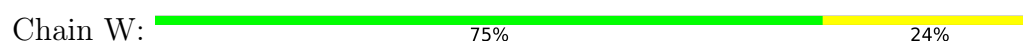




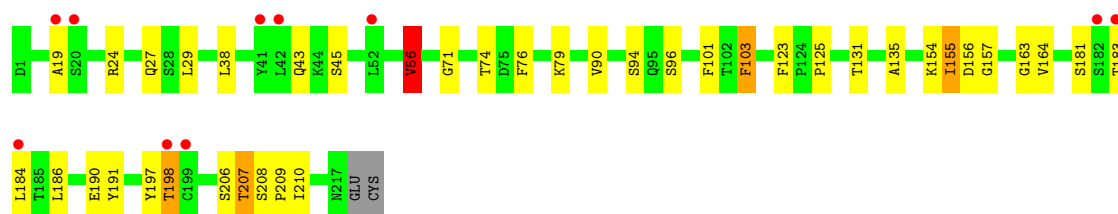
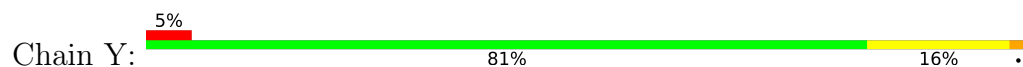
- Molecule 2: light chains of Fab fragment of antibody 28F10



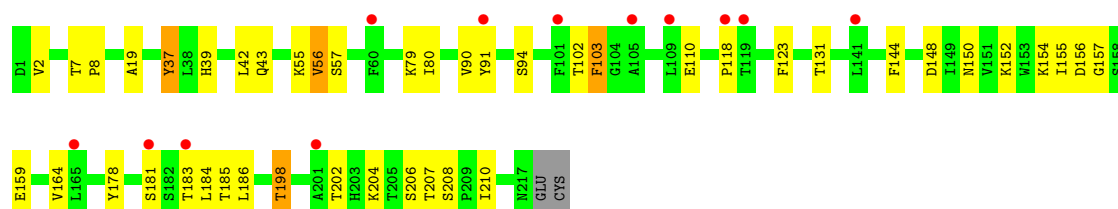
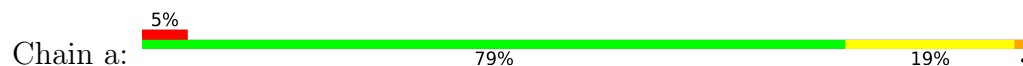
- Molecule 2: light chains of Fab fragment of antibody 28F10



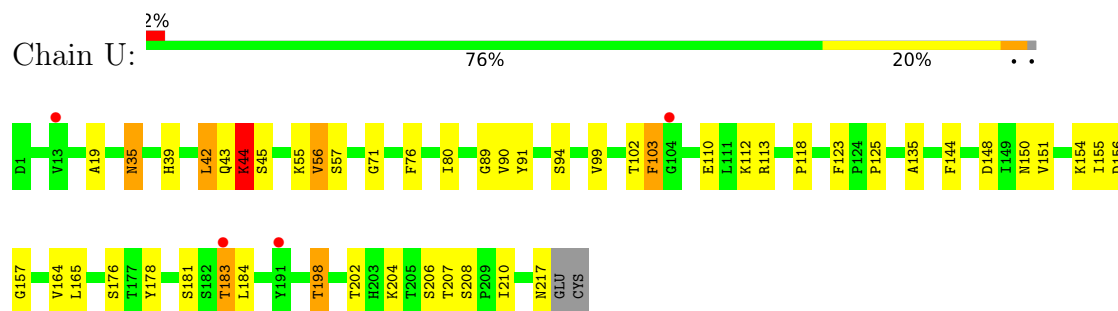
- Molecule 2: light chains of Fab fragment of antibody 28F10



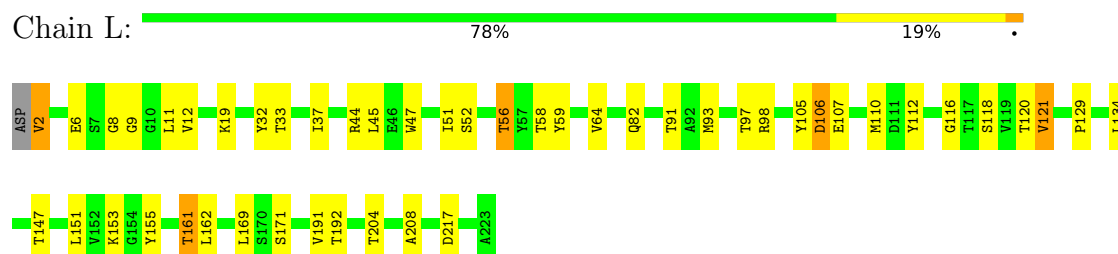
- Molecule 2: light chains of Fab fragment of antibody 28F10



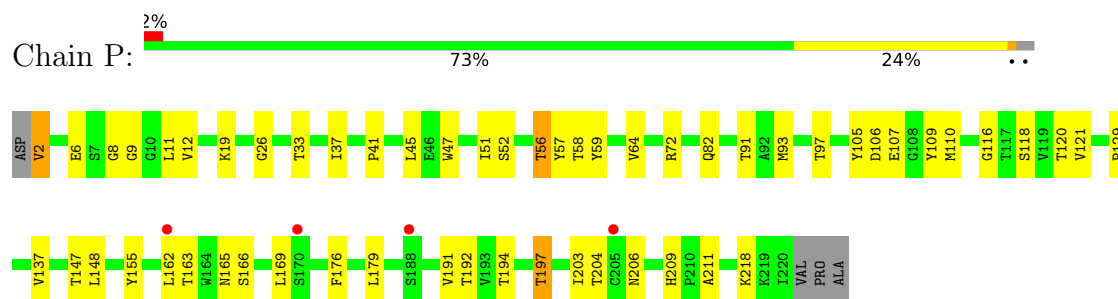
- Molecule 2: light chains of Fab fragment of antibody 28F10



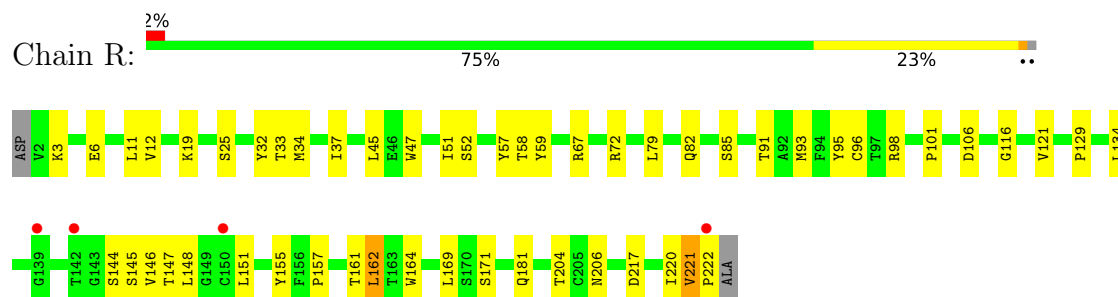
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



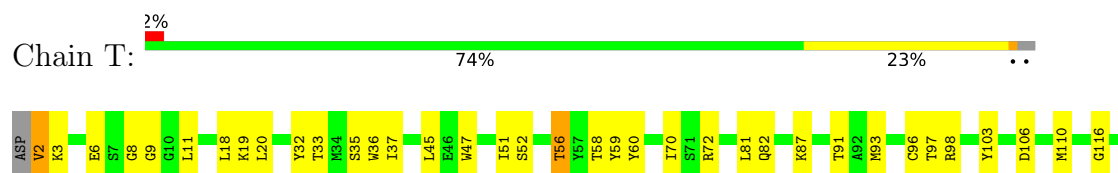
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



- Molecule 3: heavy chain of Fab fragment of antibody 28F10

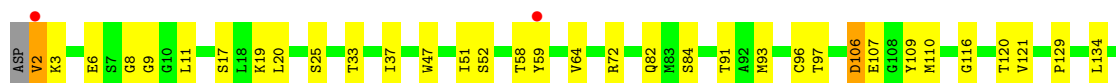
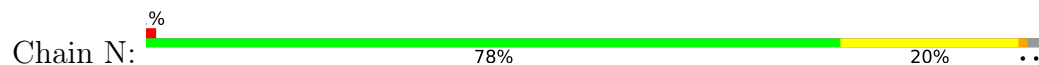


- Molecule 3: heavy chain of Fab fragment of antibody 28F10

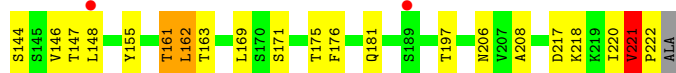
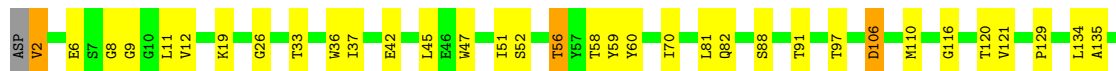
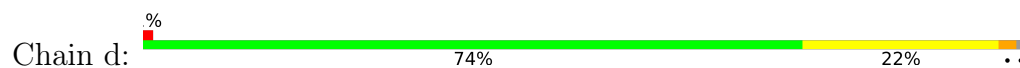




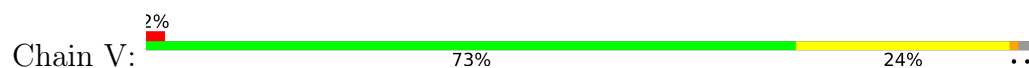
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



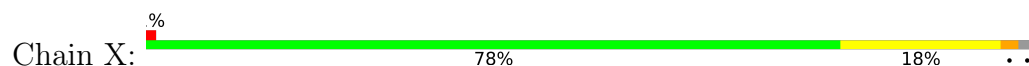
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



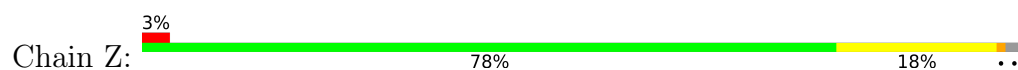
- Molecule 3: heavy chain of Fab fragment of antibody 28F10

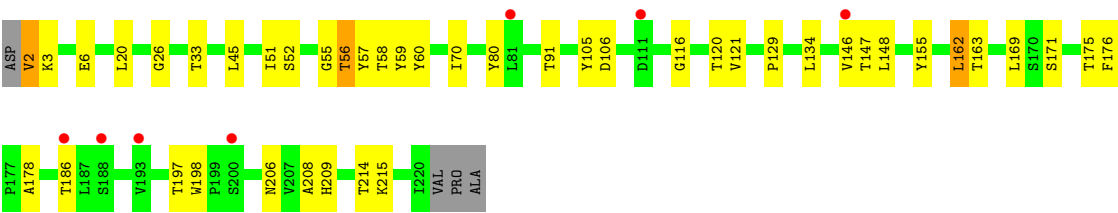


- Molecule 3: heavy chain of Fab fragment of antibody 28F10

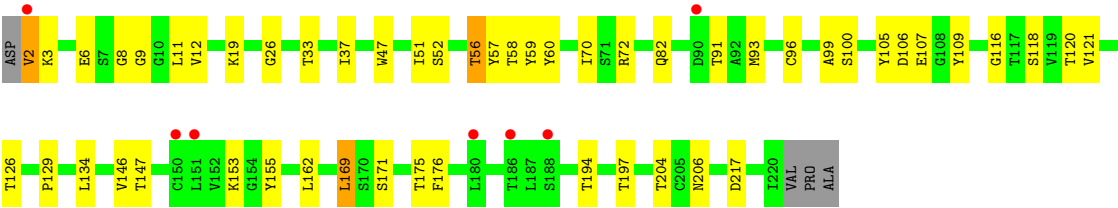


- Molecule 3: heavy chain of Fab fragment of antibody 28F10





● Molecule 3: heavy chain of Fab fragment of antibody 28F10



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.27Å 417.23Å 134.94Å 90.00° 111.02° 90.00°	Depositor
Resolution (Å)	36.53 – 3.35 36.53 – 3.35	Depositor EDS
% Data completeness (in resolution range)	94.0 (36.53-3.35) 94.0 (36.53-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.230 , 0.261 0.230 , 0.261	Depositor DCC
R_{free} test set	8049 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	66832	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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	0.11	0/3421	0.34	0/4656
1	B	0.11	0/3421	0.33	0/4656
1	C	0.12	0/3433	0.34	0/4672
1	D	0.12	0/3433	0.34	0/4672
1	E	0.12	0/3475	0.36	0/4733
1	F	0.11	0/3433	0.32	0/4672
1	G	0.11	0/3421	0.32	0/4656
1	H	0.11	0/3421	0.33	0/4656
1	I	0.11	0/3421	0.32	0/4656
1	J	0.11	0/3421	0.32	0/4656
2	K	0.25	0/1718	0.44	0/2331
2	M	0.14	0/1718	0.42	0/2331
2	O	0.13	0/1727	0.43	0/2343
2	Q	0.13	0/1718	0.41	0/2331
2	S	0.13	0/1727	0.42	0/2343
2	U	0.13	0/1718	0.43	0/2331
2	W	0.12	0/1733	0.41	0/2351
2	Y	0.12	0/1718	0.40	0/2331
2	a	0.13	0/1718	0.40	0/2331
2	c	0.14	0/1727	0.44	0/2343
3	L	0.13	0/1716	0.42	0/2344
3	N	0.12	0/1696	0.37	0/2315
3	P	0.13	0/1696	0.41	0/2315
3	R	0.13	0/1711	0.39	0/2337
3	T	0.12	0/1696	0.39	0/2315
3	V	0.11	0/1696	0.35	0/2315
3	X	0.12	0/1696	0.37	0/2315
3	Z	0.12	0/1696	0.39	0/2315
3	b	0.12	0/1696	0.39	0/2315
3	d	0.13	0/1711	0.41	0/2337
All	All	0.12	0/68532	0.37	0/93274

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3334	0	3234	57	1
1	B	3334	0	3234	65	1
1	C	3345	0	3243	64	2
1	D	3345	0	3243	67	1
1	E	3384	0	3283	59	1
1	F	3345	0	3243	73	1
1	G	3334	0	3234	68	1
1	H	3334	0	3234	65	1
1	I	3334	0	3234	69	2
1	J	3334	0	3234	64	1
2	K	1680	0	1624	27	0
2	M	1680	0	1624	34	0
2	O	1689	0	1630	29	1
2	Q	1680	0	1624	34	1
2	S	1689	0	1630	39	0
2	U	1680	0	1624	29	1
2	W	1695	0	1634	31	1
2	Y	1680	0	1624	22	0
2	a	1680	0	1624	28	0
2	c	1689	0	1630	35	0
3	L	1671	0	1628	28	0
3	N	1652	0	1607	28	0
3	P	1652	0	1607	39	0
3	R	1666	0	1623	30	0
3	T	1652	0	1607	37	0
3	V	1652	0	1607	36	0
3	X	1652	0	1606	29	0
3	Z	1652	0	1607	28	0
3	b	1652	0	1607	31	1
3	d	1666	0	1623	36	1
All	All	66832	0	64806	1114	9

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 8.

All (1114) 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:F:97:ARG:NH1	1:F:403:TRP:O	1.96	0.97
2:c:94:SER:HA	2:c:103:PHE:HB3	1.50	0.92
1:C:283:ARG:HG3	3:P:106:ASP:HB3	1.50	0.91
2:U:94:SER:HA	2:U:103:PHE:HB3	1.52	0.90
2:Q:94:SER:HA	2:Q:103:PHE:HB3	1.50	0.89
3:Z:6:GLU:HG3	3:Z:116:GLY:H	1.39	0.88
2:c:110:GLU:OE2	2:c:178:TYR:OH	1.93	0.87
3:N:6:GLU:HG3	3:N:116:GLY:H	1.39	0.86
3:V:6:GLU:HG3	3:V:116:GLY:H	1.38	0.86
2:S:110:GLU:OE2	2:S:178:TYR:OH	1.94	0.86
3:N:59:TYR:OH	3:N:106:ASP:OD2	1.93	0.85
2:U:110:GLU:OE2	2:U:178:TYR:OH	1.95	0.84
1:F:41:ARG:NH1	1:J:233:ASP:OD2	2.11	0.83
2:O:110:GLU:OE2	2:O:178:TYR:OH	1.97	0.83
3:R:6:GLU:HG3	3:R:116:GLY:H	1.42	0.83
2:O:94:SER:HA	2:O:103:PHE:HB3	1.58	0.83
2:Y:94:SER:HA	2:Y:103:PHE:HB3	1.60	0.83
3:d:91:THR:HG22	3:d:121:VAL:H	1.44	0.83
2:M:94:SER:HA	2:M:103:PHE:HB3	1.60	0.82
2:W:206:SER:HB2	2:W:207:THR:HG22	1.60	0.81
2:S:94:SER:HA	2:S:103:PHE:HB3	1.62	0.81
2:W:94:SER:HA	2:W:103:PHE:HB3	1.62	0.80
2:K:94:SER:HA	2:K:103:PHE:HB3	1.64	0.80
2:K:104:GLY:HA3	3:L:44:ARG:HH11	1.47	0.79
3:T:6:GLU:HG3	3:T:116:GLY:H	1.48	0.79
2:a:94:SER:HA	2:a:103:PHE:HB3	1.65	0.77
2:W:202:THR:HG22	2:W:209:PRO:HB3	1.68	0.76
2:W:110:GLU:OE2	2:W:178:TYR:OH	2.03	0.75
3:R:59:TYR:OH	3:R:106:ASP:OD2	2.04	0.75
3:b:6:GLU:HG3	3:b:116:GLY:H	1.52	0.75
1:I:59:ARG:NH1	1:I:61:ASP:OD2	2.20	0.74
2:K:154:LYS:HG3	2:K:198:THR:HB	1.69	0.74
2:c:154:LYS:HG3	2:c:198:THR:HB	1.68	0.74
2:Q:154:LYS:HG3	2:Q:198:THR:HB	1.69	0.73
3:V:91:THR:HG22	3:V:120:THR:HA	1.70	0.73
3:Z:91:THR:HG22	3:Z:120:THR:HA	1.70	0.73
2:O:42:LEU:HD21	2:O:44:LYS:HE3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:59:TYR:OH	3:T:106:ASP:OD2	2.07	0.73
2:K:43:GLN:HB3	2:K:90:VAL:HG23	1.69	0.72
3:P:2:VAL:HB	3:P:26:GLY:HA3	1.70	0.72
2:W:207:THR:OG1	2:W:208:SER:N	2.19	0.71
1:B:97:ARG:HH12	1:B:404:ASN:HB2	1.54	0.71
3:R:91:THR:HG22	3:R:121:VAL:H	1.55	0.70
2:M:110:GLU:OE1	2:M:178:TYR:OH	2.08	0.70
1:G:356:TYR:H	1:J:279:GLY:HA2	1.57	0.70
3:d:59:TYR:OH	3:d:106:ASP:OD2	2.10	0.69
3:N:129:PRO:HB3	3:N:155:TYR:HB3	1.73	0.69
2:M:154:LYS:HG3	2:M:198:THR:HG23	1.73	0.69
1:F:273:GLU:OE1	3:V:56:THR:OG1	2.11	0.69
3:P:129:PRO:HB3	3:P:155:TYR:HB3	1.74	0.69
3:V:129:PRO:HB3	3:V:155:TYR:HB3	1.74	0.69
3:L:91:THR:HG22	3:L:120:THR:HA	1.76	0.68
3:L:129:PRO:HB3	3:L:155:TYR:HB3	1.75	0.68
3:T:91:THR:HG22	3:T:120:THR:HA	1.74	0.68
2:S:43:GLN:HB3	2:S:90:VAL:HG23	1.74	0.68
1:C:273:GLU:OE1	3:P:56:THR:OG1	2.10	0.68
1:I:233:ASP:OD2	1:J:41:ARG:NH1	2.25	0.68
3:X:91:THR:HG22	3:X:120:THR:HA	1.76	0.68
3:d:162:LEU:HD22	3:d:175:THR:HG21	1.76	0.68
3:Z:129:PRO:HB3	3:Z:155:TYR:HB3	1.75	0.68
2:a:110:GLU:OE2	2:a:178:TYR:OH	2.11	0.68
2:S:154:LYS:HG3	2:S:198:THR:HB	1.75	0.67
2:O:154:LYS:HG3	2:O:198:THR:HB	1.76	0.67
3:b:129:PRO:HB3	3:b:155:TYR:HB3	1.75	0.66
3:N:6:GLU:OE2	3:N:96:CYS:N	2.25	0.66
3:R:129:PRO:HB3	3:R:155:TYR:HB3	1.78	0.66
2:M:43:GLN:HB3	2:M:90:VAL:HG23	1.77	0.66
1:D:41:ARG:NH1	1:E:233:ASP:OD2	2.28	0.65
2:S:215:ASN:HB2	2:S:218:GLU:HB3	1.78	0.65
2:M:37:TYR:HE1	3:N:107:GLU:HG2	1.61	0.65
2:O:19:ALA:HB3	2:O:80:ILE:HB	1.78	0.65
1:J:273:GLU:OE1	3:d:56:THR:OG1	2.14	0.64
2:W:42:LEU:HD21	2:W:44:LYS:HD2	1.77	0.64
3:b:91:THR:HG22	3:b:120:THR:HA	1.78	0.64
1:F:98:LEU:HD13	1:F:379:LEU:HD11	1.80	0.64
3:V:59:TYR:OH	3:V:106:ASP:OD2	2.15	0.64
2:U:154:LYS:HG3	2:U:198:THR:HG23	1.78	0.64
3:L:59:TYR:OH	3:L:106:ASP:OD2	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:43:GLN:HB3	2:O:90:VAL:HG23	1.78	0.64
1:H:283:ARG:NH1	3:Z:105:TYR:HE2	1.96	0.64
2:O:124:PRO:HA	2:O:137:VAL:HG23	1.78	0.64
2:S:160:ARG:HE	2:S:186:LEU:HD21	1.63	0.64
3:b:33:THR:HG23	3:b:99:ALA:HB3	1.80	0.63
3:d:129:PRO:HB3	3:d:155:TYR:HB3	1.80	0.63
3:Z:163:THR:OG1	3:Z:206:ASN:OD1	2.15	0.63
2:Q:160:ARG:HE	2:Q:186:LEU:HD21	1.63	0.63
1:B:45:VAL:HG12	1:B:368:VAL:HG22	1.81	0.63
2:W:154:LYS:HG3	2:W:198:THR:HB	1.80	0.62
3:X:129:PRO:HB3	3:X:155:TYR:HB3	1.81	0.62
3:Z:2:VAL:HB	3:Z:26:GLY:HA3	1.79	0.62
1:B:152:LYS:NZ	1:B:202:ASP:OD2	2.25	0.62
1:C:45:VAL:HG12	1:C:368:VAL:HG22	1.80	0.62
1:G:45:VAL:HG12	1:G:368:VAL:HG22	1.81	0.62
2:W:43:GLN:HB3	2:W:90:VAL:HG23	1.80	0.62
3:N:6:GLU:HG3	3:N:116:GLY:N	2.13	0.62
1:D:45:VAL:HG12	1:D:368:VAL:HG22	1.82	0.62
2:Q:165:LEU:HD21	3:R:181:GLN:HB2	1.81	0.62
1:E:273:GLU:OE1	3:T:56:THR:OG1	2.17	0.62
3:T:162:LEU:HD22	3:T:175:THR:HG21	1.82	0.62
1:F:384:LEU:HB3	1:F:389:MET:HE3	1.82	0.61
1:I:105:VAL:HG21	1:I:159:ILE:HD13	1.82	0.61
1:A:105:VAL:HG21	1:A:159:ILE:HD13	1.83	0.61
2:K:104:GLY:HA3	3:L:44:ARG:NH1	2.13	0.61
1:G:105:VAL:HG21	1:G:159:ILE:HD13	1.82	0.61
1:E:283:ARG:NH1	2:S:101:PHE:HE1	1.98	0.61
3:P:163:THR:OG1	3:P:206:ASN:OD1	2.15	0.61
1:D:393:HIS:CD2	1:D:397:THR:HG22	2.36	0.61
1:J:45:VAL:HG12	1:J:368:VAL:HG22	1.83	0.61
1:A:45:VAL:HG12	1:A:368:VAL:HG22	1.81	0.61
1:G:71:ARG:HB2	1:G:333:VAL:HG13	1.83	0.61
3:b:59:TYR:OH	3:b:106:ASP:OD2	2.19	0.61
1:H:71:ARG:HB2	1:H:333:VAL:HG13	1.83	0.61
3:d:2:VAL:HB	3:d:26:GLY:HA3	1.83	0.60
2:Y:43:GLN:HB3	2:Y:90:VAL:HG23	1.83	0.60
1:F:279:GLY:HA2	1:H:356:TYR:H	1.66	0.60
1:H:45:VAL:HG12	1:H:368:VAL:HG22	1.82	0.60
1:G:386:THR:O	1:G:388:VAL:N	2.33	0.60
2:K:185:THR:HG21	3:L:153:LYS:HE2	1.84	0.60
2:U:35:ASN:OD1	2:U:35:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:221:VAL:HG12	3:d:222:PRO:HD2	1.84	0.60
1:G:126:LEU:HB3	1:G:262:ASN:HB3	1.82	0.60
1:H:105:VAL:HG21	1:H:159:ILE:HD13	1.83	0.60
1:C:71:ARG:HB2	1:C:333:VAL:HG13	1.84	0.60
3:X:2:VAL:HB	3:X:26:GLY:HA3	1.84	0.60
1:B:105:VAL:HG21	1:B:159:ILE:HD13	1.84	0.60
1:A:356:TYR:H	1:D:279:GLY:HA2	1.66	0.59
3:P:91:THR:HG22	3:P:120:THR:HA	1.82	0.59
1:A:59:ARG:HD3	1:A:61:ASP:OD2	2.02	0.59
1:E:393:HIS:CD2	1:E:397:THR:HG22	2.37	0.59
1:J:384:LEU:HB3	1:J:389:MET:HE3	1.85	0.59
1:A:128:ASP:OD2	1:C:131:ASN:ND2	2.27	0.59
1:J:71:ARG:HB2	1:J:333:VAL:HG13	1.84	0.59
2:U:44:LYS:HB3	2:U:89:GLY:HA3	1.83	0.59
1:F:128:ASP:OD2	1:J:131:ASN:ND2	2.35	0.59
2:M:164:VAL:HG22	2:M:184:LEU:HD12	1.84	0.59
1:B:182:GLN:HG2	1:E:350:SER:HA	1.85	0.59
1:A:233:ASP:OD2	1:B:41:ARG:NH1	2.34	0.58
1:C:386:THR:O	1:C:388:VAL:N	2.36	0.58
1:I:384:LEU:HB3	1:I:389:MET:HE3	1.86	0.58
2:M:35:ASN:OD1	2:M:35:ASN:N	2.35	0.58
3:V:2:VAL:HB	3:V:26:GLY:HA3	1.84	0.58
2:W:44:LYS:HE3	2:W:86:GLU:HG2	1.85	0.58
1:D:59:ARG:HD3	1:D:61:ASP:OD2	2.02	0.58
2:S:94:SER:CA	2:S:103:PHE:HB3	2.33	0.58
1:C:105:VAL:HG21	1:C:159:ILE:HD13	1.85	0.58
1:F:263:ARG:HG3	1:F:290:LEU:HD22	1.85	0.58
1:H:384:LEU:HB3	1:H:389:MET:HE3	1.85	0.58
1:I:273:GLU:OE1	3:b:56:THR:OG1	2.22	0.58
3:Z:162:LEU:HD22	3:Z:175:THR:HG21	1.84	0.58
2:Y:186:LEU:HD22	2:Y:190:GLU:HG2	1.84	0.58
1:I:326:HIS:HD2	1:I:402:ASP:OD2	1.87	0.58
3:V:20:LEU:HD12	3:V:81:LEU:HD23	1.84	0.58
1:F:59:ARG:HD3	1:F:61:ASP:OD2	2.04	0.58
2:S:125:PRO:HG3	2:S:135:ALA:HB1	1.85	0.58
1:E:283:ARG:HH12	2:S:101:PHE:HE1	1.50	0.58
1:I:246:MET:O	1:I:317:GLN:NE2	2.29	0.58
2:a:150:ASN:HB2	2:a:202:THR:HG23	1.86	0.58
1:H:393:HIS:CD2	1:H:397:THR:HG22	2.38	0.57
3:b:2:VAL:HB	3:b:26:GLY:HA3	1.86	0.57
1:A:273:GLU:HA	1:A:276:TYR:HE2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:HIS:CD2	1:B:397:THR:HG22	2.39	0.57
1:I:386:THR:O	1:I:388:VAL:N	2.36	0.57
2:a:43:GLN:HB3	2:a:90:VAL:HG23	1.87	0.57
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.84	0.57
1:G:263:ARG:HG3	1:G:290:LEU:HD22	1.86	0.57
1:F:363:GLU:HB3	1:J:290:LEU:HD13	1.85	0.57
2:S:113:ARG:NH1	2:S:175:ASP:HA	2.20	0.57
1:C:78:PRO:HD3	1:C:453:LYS:HA	1.86	0.57
2:U:156:ASP:N	2:U:157:GLY:HA3	2.19	0.57
1:F:105:VAL:HG21	1:F:159:ILE:HD13	1.87	0.57
2:a:156:ASP:N	2:a:157:GLY:HA3	2.20	0.57
2:a:154:LYS:HG3	2:a:198:THR:HG23	1.87	0.57
1:C:393:HIS:CD2	1:C:397:THR:HG22	2.40	0.57
2:Q:186:LEU:HD22	2:Q:190:GLU:HG2	1.87	0.57
1:A:56:GLY:HA3	1:A:57:ASN:C	2.30	0.56
1:D:384:LEU:HB3	1:D:389:MET:HE3	1.87	0.56
3:b:91:THR:HG22	3:b:121:VAL:H	1.70	0.56
1:F:273:GLU:HA	1:F:276:TYR:HE2	1.70	0.56
2:Y:156:ASP:N	2:Y:157:GLY:HA3	2.20	0.56
1:I:247:PHE:HB2	1:I:316:ALA:HB1	1.86	0.56
3:d:19:LYS:HG2	3:d:82:GLN:HG2	1.87	0.56
3:R:221:VAL:HB	3:R:222:PRO:HD3	1.87	0.56
1:J:151:TYR:CG	1:J:203:THR:HB	2.40	0.56
1:J:247:PHE:HB2	1:J:316:ALA:HB1	1.87	0.56
3:R:52:SER:O	3:R:72:ARG:NH2	2.38	0.56
2:c:156:ASP:N	2:c:157:GLY:HA3	2.21	0.56
1:B:290:LEU:HD13	1:E:363:GLU:HB3	1.87	0.56
1:C:283:ARG:NH1	3:P:106:ASP:O	2.39	0.56
1:D:97:ARG:HH12	1:D:404:ASN:H	1.54	0.56
2:O:156:ASP:N	2:O:157:GLY:HA3	2.19	0.56
1:H:56:GLY:HA3	1:H:57:ASN:C	2.31	0.56
1:H:326:HIS:HD2	1:H:402:ASP:OD2	1.89	0.56
3:L:2:VAL:HG11	3:L:112:TYR:CD2	2.40	0.56
2:U:42:LEU:HD21	2:U:44:LYS:HE3	1.86	0.56
1:C:56:GLY:HA3	1:C:57:ASN:C	2.31	0.56
1:F:45:VAL:HG12	1:F:368:VAL:HG22	1.87	0.56
1:I:290:LEU:HD13	1:J:363:GLU:HB3	1.86	0.56
1:I:353:PRO:O	1:I:355:VAL:N	2.35	0.56
2:M:186:LEU:HD22	2:M:190:GLU:HG2	1.88	0.56
2:Y:154:LYS:HG3	2:Y:198:THR:HG23	1.87	0.56
1:E:96:GLN:HG2	1:E:383:THR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:169:LEU:HD21	3:T:191:VAL:HG21	1.87	0.56
1:A:273:GLU:HA	1:A:276:TYR:CE2	2.40	0.56
1:E:71:ARG:HB2	1:E:333:VAL:HG13	1.87	0.56
1:I:393:HIS:CD2	1:I:397:THR:HG22	2.41	0.55
1:J:281:ASP:C	1:J:283:ARG:H	2.14	0.55
1:B:386:THR:O	1:B:388:VAL:N	2.40	0.55
3:R:6:GLU:HG3	3:R:116:GLY:N	2.16	0.55
2:S:156:ASP:N	2:S:157:GLY:HA3	2.22	0.55
3:b:162:LEU:HG	3:b:175:THR:HG21	1.87	0.55
1:B:279:GLY:HA2	1:D:356:TYR:H	1.71	0.55
1:H:283:ARG:HG2	3:Z:106:ASP:HB3	1.89	0.55
1:D:56:GLY:HA3	1:D:57:ASN:C	2.32	0.55
1:D:263:ARG:HG3	1:D:290:LEU:HD22	1.88	0.55
2:Q:110:GLU:OE1	2:Q:178:TYR:OH	2.23	0.55
2:S:103:PHE:HE1	3:T:45:LEU:HB3	1.72	0.55
2:M:156:ASP:N	2:M:157:GLY:HA3	2.21	0.55
3:d:60:TYR:HE1	3:d:70:ILE:HG22	1.72	0.55
1:B:353:PRO:O	1:B:355:VAL:N	2.32	0.55
1:D:78:PRO:HD3	1:D:453:LYS:HA	1.89	0.55
2:S:208:SER:HB3	2:S:209:PRO:HD2	1.88	0.55
3:d:51:ILE:HG13	3:d:58:THR:HG22	1.88	0.55
2:a:181:SER:HB2	3:b:176:PHE:CD2	2.42	0.55
1:A:384:LEU:HB3	1:A:389:MET:HE3	1.89	0.55
1:H:59:ARG:HD3	1:H:61:ASP:OD2	2.07	0.55
2:c:208:SER:HB3	2:c:209:PRO:HD2	1.89	0.55
1:E:56:GLY:HA3	1:E:57:ASN:C	2.31	0.54
1:H:216:ASN:HB2	1:I:345:CYS:SG	2.47	0.54
2:Q:59:ARG:NH1	2:Q:67:PHE:O	2.34	0.54
3:T:35:SER:HG	3:T:97:THR:HG1	1.54	0.54
3:V:6:GLU:HG3	3:V:116:GLY:N	2.16	0.54
2:W:156:ASP:N	2:W:157:GLY:HA3	2.21	0.54
1:G:56:GLY:HA3	1:G:57:ASN:C	2.33	0.54
1:G:163:PRO:HD3	1:G:330:PHE:CE2	2.43	0.54
2:S:19:ALA:HB3	2:S:80:ILE:HB	1.89	0.54
2:Y:125:PRO:HG3	2:Y:135:ALA:HB1	1.90	0.54
1:A:386:THR:O	1:A:388:VAL:N	2.41	0.54
1:D:97:ARG:NH1	1:D:403:TRP:HB3	2.23	0.54
1:G:78:PRO:HD3	1:G:453:LYS:HA	1.89	0.54
1:J:56:GLY:HA3	1:J:57:ASN:C	2.33	0.54
1:J:393:HIS:CD2	1:J:397:THR:HG22	2.42	0.54
3:T:129:PRO:HB3	3:T:155:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PRO:HD3	1:C:330:PHE:CE2	2.42	0.54
1:F:56:GLY:HA3	1:F:57:ASN:C	2.32	0.54
1:F:386:THR:O	1:F:388:VAL:N	2.41	0.54
1:C:451:ASP:OD2	1:C:453:LYS:HE2	2.08	0.54
2:K:156:ASP:N	2:K:157:GLY:HA3	2.21	0.54
3:T:9:GLY:HA3	3:T:18:LEU:HD11	1.89	0.54
2:M:19:ALA:HB3	2:M:80:ILE:HB	1.89	0.54
2:M:19:ALA:O	2:M:79:LYS:HA	2.07	0.54
3:Z:6:GLU:HG3	3:Z:116:GLY:N	2.17	0.54
1:B:151:TYR:CG	1:B:203:THR:HB	2.43	0.54
1:B:263:ARG:HG3	1:B:290:LEU:HD22	1.90	0.54
1:C:263:ARG:HG3	1:C:290:LEU:HD22	1.90	0.54
3:V:97:THR:HB	3:V:110:MET:HB3	1.90	0.54
2:M:208:SER:HB3	2:M:209:PRO:HD2	1.90	0.54
2:c:103:PHE:HE1	3:d:45:LEU:HB3	1.72	0.54
2:U:150:ASN:HB2	2:U:202:THR:HG23	1.89	0.54
1:A:163:PRO:HD3	1:A:330:PHE:CE2	2.43	0.53
1:B:56:GLY:HA3	1:B:57:ASN:C	2.34	0.53
1:C:151:TYR:CG	1:C:203:THR:HB	2.43	0.53
2:Y:164:VAL:HG22	2:Y:184:LEU:HD12	1.90	0.53
1:C:345:CYS:SG	1:D:216:ASN:HB2	2.48	0.53
3:R:51:ILE:HG13	3:R:58:THR:HG22	1.89	0.53
3:b:52:SER:O	3:b:72:ARG:NH2	2.40	0.53
1:D:386:THR:O	1:D:388:VAL:N	2.42	0.53
1:E:105:VAL:HG21	1:E:159:ILE:HD13	1.89	0.53
3:T:6:GLU:HG3	3:T:116:GLY:N	2.20	0.53
3:P:19:LYS:HG2	3:P:82:GLN:HG2	1.91	0.53
2:U:125:PRO:HG3	2:U:135:ALA:HB1	1.90	0.53
1:A:71:ARG:HB2	1:A:333:VAL:HG13	1.90	0.53
1:A:363:GLU:HB3	1:C:290:LEU:HD13	1.91	0.53
1:C:356:TYR:H	1:E:279:GLY:HA2	1.73	0.53
1:G:281:ASP:C	1:G:283:ARG:H	2.16	0.53
2:Q:156:ASP:N	2:Q:157:GLY:HA3	2.23	0.53
1:E:45:VAL:HG12	1:E:368:VAL:HG22	1.90	0.53
1:E:386:THR:O	1:E:388:VAL:N	2.41	0.53
1:D:105:VAL:HG21	1:D:159:ILE:HD13	1.89	0.53
1:F:156:LEU:HA	1:F:250:LEU:O	2.09	0.53
3:N:51:ILE:HG13	3:N:58:THR:HG22	1.91	0.53
1:H:163:PRO:HD3	1:H:330:PHE:CE2	2.44	0.53
3:d:161:THR:OG1	3:d:208:ALA:HB3	2.09	0.53
1:C:363:GLU:HB3	1:D:290:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:163:THR:OG1	3:T:206:ASN:HB2	2.09	0.53
3:X:6:GLU:OE1	3:X:6:GLU:N	2.41	0.53
3:X:148:LEU:HD21	3:X:198:TRP:CE2	2.44	0.53
1:D:97:ARG:HH12	1:D:404:ASN:N	2.07	0.52
1:I:56:GLY:HA3	1:I:57:ASN:C	2.33	0.52
1:I:398:THR:HA	1:I:401:GLU:HB3	1.91	0.52
1:I:45:VAL:HG12	1:I:368:VAL:HG22	1.90	0.52
3:L:11:LEU:HD23	3:L:120:THR:OG1	2.10	0.52
2:O:128:GLU:HG2	3:P:218:LYS:NZ	2.24	0.52
3:V:162:LEU:HD22	3:V:175:THR:HG21	1.89	0.52
1:B:326:HIS:HD2	1:B:402:ASP:OD2	1.92	0.52
1:J:163:PRO:HD3	1:J:330:PHE:CE2	2.45	0.52
3:N:52:SER:O	3:N:72:ARG:NH2	2.41	0.52
1:F:152:LYS:NZ	1:F:202:ASP:OD2	2.30	0.52
3:P:6:GLU:N	3:P:6:GLU:OE1	2.41	0.52
2:c:165:LEU:HD21	3:d:181:GLN:HB3	1.92	0.52
3:L:217:ASP:OD1	3:L:217:ASP:N	2.43	0.52
1:D:163:PRO:HD3	1:D:330:PHE:CE2	2.45	0.52
1:H:386:THR:O	1:H:388:VAL:N	2.43	0.52
1:J:271:LEU:HB2	1:J:289:TYR:CE2	2.44	0.52
3:P:91:THR:HG22	3:P:121:VAL:H	1.75	0.52
3:R:19:LYS:HG2	3:R:82:GLN:HG2	1.91	0.52
3:R:217:ASP:OD1	3:R:217:ASP:N	2.44	0.51
1:B:53:PRO:HA	1:B:61:ASP:OD2	2.11	0.51
1:A:345:CYS:SG	1:C:216:ASN:HB2	2.49	0.51
1:B:71:ARG:HB2	1:B:333:VAL:HG13	1.92	0.51
1:G:130:GLU:HB2	1:G:260:PHE:HB2	1.92	0.51
1:J:386:THR:O	1:J:388:VAL:N	2.42	0.51
3:P:33:THR:HG22	3:P:52:SER:HA	1.92	0.51
3:T:2:VAL:HG12	3:T:3:LYS:HG3	1.92	0.51
1:C:52:VAL:HB	1:C:62:VAL:HG22	1.93	0.51
1:J:263:ARG:HG3	1:J:290:LEU:HD22	1.91	0.51
3:N:2:VAL:HG12	3:N:3:LYS:HG3	1.93	0.51
2:M:35:ASN:HD22	2:M:55:LYS:HD2	1.74	0.51
2:c:192:GLU:CD	2:c:216:ARG:HH12	2.19	0.51
2:U:113:ARG:HG3	2:U:176:SER:HB2	1.92	0.51
1:H:273:GLU:OE1	3:Z:56:THR:OG1	2.26	0.51
1:J:269:ASP:O	1:J:289:TYR:OH	2.26	0.51
3:P:11:LEU:HD23	3:P:120:THR:OG1	2.10	0.51
3:P:59:TYR:OH	3:P:106:ASP:OD2	2.28	0.51
3:V:161:THR:HB	3:V:208:ALA:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:37:ILE:HD13	3:X:47:TRP:HA	1.93	0.51
2:Y:71:GLY:HA3	2:Y:76:PHE:HA	1.92	0.51
2:a:118:PRO:HB3	2:a:144:PHE:HB3	1.93	0.51
1:D:52:VAL:HB	1:D:62:VAL:HG22	1.92	0.51
1:H:289:TYR:HB3	1:I:121:PRO:HG3	1.92	0.51
1:J:68:TYR:CZ	1:J:151:TYR:HB2	2.46	0.51
2:S:186:LEU:HD22	2:S:190:GLU:HG2	1.93	0.51
2:c:42:LEU:HD12	2:c:91:TYR:CZ	2.46	0.51
3:V:51:ILE:HG13	3:V:58:THR:HG22	1.92	0.51
2:Y:27:GLN:O	2:Y:74:THR:HG22	2.11	0.51
1:F:393:HIS:CD2	1:F:397:THR:HG22	2.46	0.51
1:G:353:PRO:O	1:G:355:VAL:N	2.36	0.51
1:I:263:ARG:HG3	1:I:290:LEU:HD22	1.93	0.51
1:F:353:PRO:O	1:F:355:VAL:N	2.38	0.51
3:V:6:GLU:OE2	3:V:96:CYS:N	2.41	0.51
1:B:356:TYR:H	1:C:279:GLY:HA2	1.76	0.50
1:E:269:ASP:O	1:E:289:TYR:OH	2.26	0.50
1:F:244:ASP:OD1	1:F:320:ASN:ND2	2.33	0.50
2:O:103:PHE:HE1	3:P:45:LEU:HB3	1.76	0.50
2:c:71:GLY:HA3	2:c:76:PHE:HA	1.93	0.50
1:A:78:PRO:HD3	1:A:453:LYS:HA	1.93	0.50
1:D:244:ASP:OD1	1:D:320:ASN:ND2	2.32	0.50
1:E:59:ARG:HD3	1:E:61:ASP:OD2	2.11	0.50
1:H:283:ARG:HH21	2:Y:101:PHE:HE1	1.59	0.50
1:I:130:GLU:HB2	1:I:260:PHE:HB2	1.94	0.50
1:A:37:ALA:HB1	1:A:452:LEU:HD13	1.94	0.50
1:H:108:GLY:O	1:H:371:PHE:HA	2.11	0.50
1:H:283:ARG:NH1	3:Z:105:TYR:CE2	2.77	0.50
2:O:208:SER:HB3	2:O:209:PRO:HD2	1.94	0.50
1:D:71:ARG:HB2	1:D:333:VAL:HG13	1.94	0.50
1:F:290:LEU:HD13	1:G:363:GLU:HB3	1.94	0.50
1:J:52:VAL:HB	1:J:62:VAL:HG22	1.94	0.50
3:P:51:ILE:HG13	3:P:58:THR:HG22	1.93	0.50
2:c:125:PRO:HG3	2:c:135:ALA:HB1	1.93	0.50
1:C:384:LEU:HB3	1:C:389:MET:HE3	1.93	0.50
1:H:68:TYR:CZ	1:H:151:TYR:HB2	2.46	0.50
2:O:42:LEU:HD12	2:O:91:TYR:CZ	2.47	0.50
2:a:19:ALA:O	2:a:79:LYS:HA	2.11	0.50
1:B:171:LYS:HG3	1:B:186:PRO:HB2	1.94	0.50
1:B:281:ASP:C	1:B:283:ARG:H	2.20	0.50
1:C:398:THR:O	1:C:402:ASP:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:TYR:CG	1:D:203:THR:HB	2.46	0.50
1:D:363:GLU:HB3	1:E:290:LEU:HD13	1.93	0.50
1:F:151:TYR:CG	1:F:203:THR:HB	2.47	0.50
2:K:208:SER:HB3	2:K:209:PRO:HD2	1.92	0.50
2:M:125:PRO:HG3	2:M:135:ALA:HB1	1.93	0.50
3:V:33:THR:HG22	3:V:52:SER:HA	1.93	0.50
1:A:80:PRO:HB2	1:A:98:LEU:HB3	1.93	0.50
1:C:108:GLY:O	1:C:371:PHE:HA	2.11	0.50
1:D:108:GLY:O	1:D:371:PHE:HA	2.12	0.50
1:D:152:LYS:NZ	1:D:253:GLU:OE1	2.41	0.50
1:G:283:ARG:NH1	2:W:101:PHE:CZ	2.79	0.50
1:I:151:TYR:CG	1:I:203:THR:HB	2.47	0.50
3:V:3:LYS:HB2	3:V:25:SER:HB2	1.93	0.50
3:X:217:ASP:OD1	3:X:217:ASP:N	2.44	0.50
1:D:451:ASP:OD2	1:D:453:LYS:HE2	2.12	0.49
1:J:353:PRO:O	1:J:355:VAL:N	2.38	0.49
2:K:120:VAL:HA	2:K:140:PHE:O	2.12	0.49
3:d:37:ILE:HD13	3:d:47:TRP:HA	1.93	0.49
1:F:68:TYR:CZ	1:F:151:TYR:HB2	2.46	0.49
1:F:350:SER:HA	1:J:182:GLN:HG2	1.93	0.49
3:Z:208:ALA:HB2	3:Z:215:LYS:HD3	1.93	0.49
1:D:345:CYS:SG	1:E:216:ASN:HB2	2.53	0.49
1:F:345:CYS:SG	1:J:216:ASN:HB2	2.52	0.49
1:I:52:VAL:HB	1:I:62:VAL:HG22	1.95	0.49
3:L:134:LEU:HD11	3:L:151:LEU:HB2	1.93	0.49
1:B:247:PHE:HB2	1:B:316:ALA:HB1	1.93	0.49
2:K:125:PRO:HD3	2:K:137:VAL:HG22	1.95	0.49
3:T:19:LYS:HG2	3:T:82:GLN:HG2	1.93	0.49
3:d:163:THR:OG1	3:d:206:ASN:HB2	2.12	0.49
2:Y:38:LEU:HB3	2:Y:56:VAL:HG12	1.95	0.49
3:b:6:GLU:HG3	3:b:116:GLY:N	2.24	0.49
3:T:51:ILE:HG13	3:T:58:THR:HG22	1.95	0.49
2:a:164:VAL:HG22	2:a:184:LEU:HD12	1.95	0.49
1:F:273:GLU:HA	1:F:276:TYR:CE2	2.47	0.49
1:F:366:ARG:NH2	1:J:269:ASP:OD2	2.45	0.49
1:I:281:ASP:C	1:I:283:ARG:H	2.19	0.49
2:Q:44:LYS:NZ	2:Q:86:GLU:HG2	2.28	0.49
3:R:32:TYR:HA	3:R:101:PRO:HA	1.94	0.49
3:N:93:MET:HE3	3:N:116:GLY:HA3	1.95	0.49
1:C:269:ASP:O	1:C:289:TYR:OH	2.28	0.49
1:E:108:GLY:O	1:E:371:PHE:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:GLY:HA2	1:J:59:ARG:HA	1.59	0.49
2:Q:24:ARG:HG2	2:Q:75:ASP:HA	1.95	0.49
2:M:71:GLY:HA3	2:M:76:PHE:HA	1.95	0.49
1:A:231:TYR:CD1	1:B:112:PRO:HB3	2.48	0.49
1:H:353:PRO:O	1:H:355:VAL:N	2.37	0.48
1:J:126:LEU:HB3	1:J:262:ASN:HB3	1.95	0.48
2:S:42:LEU:HD12	2:S:91:TYR:CZ	2.47	0.48
3:V:45:LEU:HB3	2:U:103:PHE:HE1	1.78	0.48
1:E:80:PRO:HA	1:E:83:PHE:HB2	1.94	0.48
1:F:233:ASP:OD2	1:G:41:ARG:NH1	2.41	0.48
1:I:78:PRO:HD3	1:I:453:LYS:HA	1.94	0.48
2:Q:35:ASN:OD1	2:Q:35:ASN:N	2.45	0.48
1:E:52:VAL:HB	1:E:62:VAL:HG22	1.94	0.48
1:H:210:PHE:CE2	1:H:224:ILE:HD12	2.48	0.48
1:I:120:HIS:HB2	1:I:221:PRO:HA	1.94	0.48
3:P:52:SER:O	3:P:72:ARG:NH2	2.45	0.48
3:R:134:LEU:HD11	3:R:151:LEU:HB2	1.96	0.48
3:V:109:TYR:HB3	2:U:39:HIS:CE1	2.48	0.48
2:Y:181:SER:HB2	3:Z:176:PHE:CD2	2.48	0.48
1:A:263:ARG:HG3	1:A:290:LEU:HD22	1.95	0.48
1:F:78:PRO:HD3	1:F:453:LYS:HA	1.95	0.48
1:G:283:ARG:NH1	2:W:101:PHE:HZ	2.11	0.48
2:S:44:LYS:NZ	2:S:86:GLU:HG2	2.28	0.48
1:A:68:TYR:CZ	1:A:151:TYR:HB2	2.48	0.48
1:F:158:ILE:HD13	1:F:237:MET:HE1	1.94	0.48
1:F:216:ASN:HB2	1:G:345:CYS:SG	2.54	0.48
2:Q:103:PHE:HE1	3:R:45:LEU:HB3	1.77	0.48
3:T:93:MET:HE3	3:T:116:GLY:HA3	1.95	0.48
3:b:194:THR:O	3:b:197:THR:OG1	2.31	0.48
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.94	0.48
1:G:216:ASN:HB2	1:H:345:CYS:SG	2.53	0.48
1:G:393:HIS:NE2	1:G:397:THR:HG22	2.28	0.48
1:I:80:PRO:HA	1:I:83:PHE:HB2	1.96	0.48
3:N:2:VAL:N	3:N:25:SER:O	2.47	0.48
3:N:19:LYS:HG2	3:N:82:GLN:HG2	1.96	0.48
1:B:59:ARG:HD3	1:B:61:ASP:OD2	2.14	0.48
1:B:233:ASP:OD2	1:E:41:ARG:NH1	2.37	0.48
1:C:112:PRO:HB3	1:D:231:TYR:CD1	2.49	0.48
1:F:110:GLY:HA3	1:F:370:GLU:CD	2.39	0.48
1:H:109:ARG:NH2	1:H:369:GLU:OE1	2.47	0.48
2:K:103:PHE:HE1	3:L:45:LEU:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:209:HIS:HB3	3:Z:214:THR:HG22	1.95	0.48
1:A:130:GLU:HB2	1:A:260:PHE:HB2	1.96	0.48
1:D:247:PHE:HB2	1:D:316:ALA:HB1	1.94	0.48
2:a:123:PHE:HB2	3:b:134:LEU:HD23	1.96	0.48
1:C:58:GLY:HA2	1:C:59:ARG:HA	1.64	0.48
1:D:68:TYR:CZ	1:D:151:TYR:HB2	2.49	0.48
1:I:158:ILE:HD13	1:I:237:MET:HE1	1.95	0.48
3:P:6:GLU:CD	3:P:116:GLY:H	2.22	0.48
2:Q:127:SER:O	2:Q:131:THR:OG1	2.32	0.48
2:Q:206:SER:HA	2:Q:207:THR:HA	1.62	0.48
2:S:155:ILE:HG22	2:S:196:SER:O	2.14	0.48
3:N:6:GLU:CG	3:N:116:GLY:H	2.21	0.48
2:W:125:PRO:HG3	2:W:135:ALA:HB1	1.94	0.48
3:X:19:LYS:HG2	3:X:82:GLN:HG2	1.96	0.48
1:F:71:ARG:HB2	1:F:333:VAL:HG13	1.96	0.47
1:H:80:PRO:HB2	1:H:98:LEU:HB3	1.96	0.47
1:J:105:VAL:HG21	1:J:159:ILE:HD13	1.96	0.47
2:O:71:GLY:HA3	2:O:76:PHE:HA	1.96	0.47
3:P:194:THR:O	3:P:197:THR:OG1	2.31	0.47
3:X:51:ILE:HG13	3:X:58:THR:HG22	1.94	0.47
1:I:167:GLU:OE2	1:I:190:LEU:HD21	2.14	0.47
2:W:113:ARG:NH1	2:W:175:ASP:HA	2.29	0.47
1:E:91:TYR:HB3	1:E:381:LYS:HZ2	1.79	0.47
1:E:109:ARG:NE	1:E:335:ASP:OD2	2.47	0.47
1:H:130:GLU:HB2	1:H:260:PHE:HB2	1.95	0.47
3:Z:33:THR:HG22	3:Z:52:SER:HA	1.96	0.47
3:b:91:THR:CG2	3:b:121:VAL:H	2.27	0.47
1:C:80:PRO:HA	1:C:83:PHE:HB2	1.96	0.47
1:F:53:PRO:HA	1:F:61:ASP:OD2	2.15	0.47
1:J:108:GLY:O	1:J:371:PHE:HA	2.14	0.47
2:O:118:PRO:HB3	2:O:144:PHE:HB3	1.97	0.47
2:c:19:ALA:O	2:c:79:LYS:HA	2.15	0.47
3:d:97:THR:HB	3:d:110:MET:HB3	1.96	0.47
3:V:2:VAL:HG12	3:V:3:LYS:HG3	1.97	0.47
1:A:261:TRP:HE1	1:C:131:ASN:CG	2.20	0.47
1:B:128:ASP:HB3	1:B:132:SER:HB2	1.96	0.47
1:C:43:LEU:HA	1:C:369:GLU:O	2.14	0.47
3:L:51:ILE:HG13	3:L:58:THR:HG22	1.96	0.47
3:R:3:LYS:HB3	3:R:25:SER:HB2	1.95	0.47
2:c:120:VAL:HA	2:c:140:PHE:O	2.15	0.47
2:c:206:SER:HB3	2:c:207:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:217:ASP:OD1	3:d:217:ASP:N	2.43	0.47
3:V:93:MET:HE3	3:V:116:GLY:HA3	1.96	0.47
1:E:285:ASN:ND2	3:T:103:TYR:O	2.46	0.47
1:F:281:ASP:C	1:F:283:ARG:H	2.23	0.47
1:H:156:LEU:HA	1:H:250:LEU:O	2.15	0.47
1:J:283:ARG:NH1	2:c:101:PHE:CZ	2.82	0.47
2:M:206:SER:HA	2:M:207:THR:HA	1.71	0.47
2:a:39:HIS:CE1	3:b:109:TYR:HB3	2.50	0.47
1:C:273:GLU:HA	1:C:276:TYR:CE2	2.49	0.47
1:C:345:CYS:HA	1:C:362:LYS:O	2.15	0.47
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.96	0.47
1:I:256:PHE:HA	1:J:115:VAL:HG21	1.96	0.47
2:K:42:LEU:HD21	2:K:44:LYS:HG3	1.96	0.47
2:K:125:PRO:HG3	2:K:135:ALA:HB1	1.95	0.47
3:L:6:GLU:CD	3:L:116:GLY:H	2.23	0.47
2:M:39:HIS:CE1	3:N:109:TYR:HB3	2.49	0.47
3:Z:60:TYR:HE1	3:Z:70:ILE:HG22	1.79	0.47
2:U:44:LYS:HD2	2:U:44:LYS:O	2.15	0.47
1:B:273:GLU:HA	1:B:276:TYR:HE2	1.80	0.47
1:D:58:GLY:HA2	1:D:59:ARG:HA	1.60	0.47
1:F:393:HIS:NE2	1:F:397:THR:HG22	2.30	0.47
3:R:32:TYR:CG	3:R:98:ARG:HD2	2.49	0.47
2:a:185:THR:HG21	3:b:153:LYS:HE2	1.96	0.47
3:b:19:LYS:HG2	3:b:82:GLN:HG2	1.97	0.47
1:D:106:GLU:HB2	1:D:465:LEU:HD13	1.97	0.47
1:G:58:GLY:HA2	1:G:59:ARG:HA	1.62	0.47
1:I:59:ARG:HD3	1:I:61:ASP:OD2	2.14	0.47
1:I:108:GLY:O	1:I:371:PHE:HA	2.15	0.47
3:L:32:TYR:CE1	3:L:98:ARG:NH1	2.83	0.47
2:c:150:ASN:HB2	2:c:202:THR:HG23	1.97	0.47
2:W:19:ALA:HB3	2:W:80:ILE:HB	1.96	0.47
3:X:59:TYR:OH	3:X:106:ASP:OD2	2.32	0.47
1:A:289:TYR:HB3	1:B:121:PRO:HG3	1.97	0.47
1:C:28:VAL:HG22	1:C:382:ILE:HG12	1.97	0.47
1:C:247:PHE:HB2	1:C:316:ALA:HB1	1.98	0.47
1:E:283:ARG:NH1	2:S:101:PHE:CE1	2.82	0.47
1:H:231:TYR:CD1	1:I:112:PRO:HB3	2.50	0.47
1:J:41:ARG:HG2	1:J:43:LEU:HD11	1.97	0.47
2:Q:42:LEU:HD12	2:Q:91:TYR:CZ	2.50	0.47
3:T:8:GLY:HA2	3:T:9:GLY:HA2	1.59	0.47
2:M:120:VAL:HA	2:M:140:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:125:PRO:HD3	2:c:137:VAL:HG22	1.97	0.47
1:G:59:ARG:HD3	1:G:61:ASP:OD2	2.15	0.46
1:G:393:HIS:CD2	1:G:397:THR:HG22	2.50	0.46
3:V:11:LEU:HD23	3:V:120:THR:OG1	2.15	0.46
3:V:32:TYR:CE1	3:V:98:ARG:NH1	2.83	0.46
3:Z:148:LEU:HD21	3:Z:198:TRP:CD1	2.50	0.46
2:a:206:SER:HB2	2:a:207:THR:OG1	2.15	0.46
1:D:112:PRO:HB3	1:E:231:TYR:CD1	2.51	0.46
1:D:281:ASP:C	1:D:283:ARG:H	2.23	0.46
1:F:231:TYR:CD1	1:G:112:PRO:HB3	2.50	0.46
1:H:37:ALA:HB1	1:H:452:LEU:HD13	1.97	0.46
1:H:233:ASP:OD2	1:I:41:ARG:NH1	2.46	0.46
1:H:454:GLU:HG3	1:H:455:ARG:HD3	1.98	0.46
2:S:71:GLY:HA3	2:S:76:PHE:HA	1.97	0.46
3:N:97:THR:HB	3:N:110:MET:HB3	1.95	0.46
1:A:398:THR:HA	1:A:401:GLU:HB3	1.96	0.46
1:C:331:LEU:HD12	1:C:375:PHE:HZ	1.80	0.46
1:E:78:PRO:HD3	1:E:453:LYS:HA	1.97	0.46
1:H:282:ILE:CG2	3:Z:57:TYR:HB3	2.44	0.46
2:U:118:PRO:HB3	2:U:144:PHE:HB3	1.97	0.46
1:F:256:PHE:HA	1:G:115:VAL:HG21	1.97	0.46
1:H:263:ARG:HG3	1:H:290:LEU:HD22	1.97	0.46
3:d:162:LEU:HD12	3:d:162:LEU:O	2.15	0.46
3:X:93:MET:HE3	3:X:116:GLY:HA3	1.96	0.46
1:D:389:MET:HE1	1:D:405:PHE:CD2	2.50	0.46
1:G:110:GLY:HA3	1:G:370:GLU:CD	2.41	0.46
3:L:6:GLU:OE1	3:L:6:GLU:N	2.42	0.46
3:L:97:THR:HB	3:L:110:MET:HB3	1.97	0.46
2:Q:125:PRO:HG3	2:Q:135:ALA:HB1	1.97	0.46
2:M:42:LEU:HD12	2:M:91:TYR:CZ	2.50	0.46
2:W:186:LEU:HD22	2:W:190:GLU:HG2	1.98	0.46
3:b:11:LEU:HD23	3:b:120:THR:OG1	2.15	0.46
1:A:166:GLY:O	1:A:192:ASN:HA	2.15	0.46
1:D:110:GLY:HA3	1:D:370:GLU:CD	2.40	0.46
1:J:120:HIS:HB2	1:J:221:PRO:HA	1.98	0.46
2:W:150:ASN:HB3	2:W:202:THR:OG1	2.16	0.46
1:F:356:TYR:H	1:I:279:GLY:HA2	1.80	0.46
3:L:8:GLY:HA2	3:L:9:GLY:HA2	1.51	0.46
3:T:60:TYR:HE1	3:T:70:ILE:HG22	1.79	0.46
2:M:2:VAL:HB	2:M:102:THR:HG21	1.98	0.46
2:U:44:LYS:HA	2:U:45:SER:HA	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:HA2	1:A:59:ARG:HA	1.63	0.46
3:P:166:SER:H	3:P:206:ASN:ND2	2.14	0.46
2:Q:125:PRO:HD3	2:Q:137:VAL:HG22	1.97	0.46
1:B:40:SER:HB2	1:B:455:ARG:HH12	1.81	0.46
1:B:133:HIS:HD2	1:E:134:VAL:HB	1.81	0.46
1:E:240:ASP:OD1	1:E:241:ALA:N	2.49	0.46
1:F:253:GLU:HG3	1:G:113:LEU:HD12	1.98	0.46
2:S:123:PHE:HB2	3:T:134:LEU:HD23	1.97	0.46
3:T:32:TYR:CG	3:T:98:ARG:HD2	2.51	0.46
3:d:11:LEU:HD23	3:d:120:THR:OG1	2.16	0.46
3:Z:59:TYR:OH	3:Z:106:ASP:OD2	2.31	0.46
1:A:290:LEU:HD13	1:B:363:GLU:HB3	1.97	0.46
1:E:263:ARG:HG3	1:E:290:LEU:HD22	1.98	0.46
1:G:80:PRO:HB2	1:G:98:LEU:HB3	1.97	0.46
2:K:6:GLN:HA	2:K:22:SER:O	2.16	0.46
2:Q:155:ILE:HG22	2:Q:196:SER:O	2.16	0.46
3:X:32:TYR:CG	3:X:98:ARG:HD2	2.50	0.46
1:D:398:THR:HA	1:D:401:GLU:HB2	1.97	0.45
1:E:384:LEU:HB3	1:E:389:MET:HE3	1.98	0.45
2:O:94:SER:CA	2:O:103:PHE:HB3	2.40	0.45
1:E:37:ALA:HB1	1:E:452:LEU:HD13	1.97	0.45
1:G:108:GLY:O	1:G:371:PHE:HA	2.16	0.45
1:H:247:PHE:HB2	1:H:316:ALA:HB1	1.98	0.45
1:I:107:ILE:HD11	1:I:331:LEU:HD21	1.98	0.45
2:Q:155:ILE:HD11	2:Q:160:ARG:HD3	1.99	0.45
2:Y:103:PHE:HE1	3:Z:45:LEU:HB3	1.80	0.45
2:a:42:LEU:HD12	2:a:91:TYR:CZ	2.51	0.45
2:U:71:GLY:HA3	2:U:76:PHE:HA	1.98	0.45
1:A:247:PHE:HB2	1:A:316:ALA:HB1	1.98	0.45
1:G:43:LEU:HA	1:G:369:GLU:O	2.16	0.45
1:G:331:LEU:HD12	1:G:375:PHE:HZ	1.82	0.45
1:J:281:ASP:O	1:J:283:ARG:N	2.46	0.45
2:Q:44:LYS:HZ3	2:Q:86:GLU:HG2	1.82	0.45
2:Y:208:SER:HB2	2:Y:209:PRO:HD2	1.99	0.45
3:b:33:THR:HG22	3:b:100:SER:O	2.16	0.45
3:b:60:TYR:HE1	3:b:70:ILE:HG22	1.82	0.45
1:D:113:LEU:HD12	1:E:253:GLU:HG3	1.99	0.45
1:I:231:TYR:CD1	1:J:112:PRO:HB3	2.51	0.45
1:J:240:ASP:OD1	1:J:241:ALA:N	2.49	0.45
2:K:113:ARG:NH1	2:K:175:ASP:O	2.46	0.45
2:Q:206:SER:HB3	2:Q:207:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:39:HIS:HD2	2:S:55:LYS:H	1.64	0.45
1:B:283:ARG:HG2	3:N:106:ASP:HB3	1.98	0.45
1:C:120:HIS:HB2	1:C:221:PRO:HA	1.98	0.45
1:F:96:GLN:HG2	1:F:383:THR:HA	1.97	0.45
1:G:80:PRO:HA	1:G:83:PHE:HB2	1.99	0.45
1:H:126:LEU:HB3	1:H:262:ASN:HB3	1.98	0.45
1:H:290:LEU:HD13	1:I:363:GLU:HB3	1.99	0.45
1:I:166:GLY:O	1:I:192:ASN:HA	2.17	0.45
1:J:37:ALA:HB1	1:J:452:LEU:HD13	1.98	0.45
3:R:6:GLU:OE2	3:R:96:CYS:N	2.42	0.45
3:d:6:GLU:OE1	3:d:6:GLU:N	2.44	0.45
3:V:60:TYR:HE1	3:V:70:ILE:HG22	1.81	0.45
2:Y:206:SER:HB2	2:Y:207:THR:OG1	2.16	0.45
2:U:19:ALA:HB3	2:U:80:ILE:HB	1.97	0.45
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.97	0.45
1:B:253:GLU:HG3	1:E:113:LEU:HD12	1.99	0.45
1:C:273:GLU:HA	1:C:276:TYR:HE2	1.81	0.45
1:E:271:LEU:HB2	1:E:289:TYR:CE2	2.52	0.45
1:G:248:PHE:HB2	1:G:313:LEU:HD12	1.97	0.45
2:S:181:SER:HB2	3:T:176:PHE:CE2	2.52	0.45
3:T:6:GLU:OE2	3:T:96:CYS:N	2.45	0.45
3:V:32:TYR:CZ	3:V:98:ARG:NH1	2.84	0.45
2:W:128:GLU:O	2:W:131:THR:OG1	2.31	0.45
2:U:94:SER:CA	2:U:103:PHE:HB3	2.37	0.45
1:A:53:PRO:HA	1:A:61:ASP:OD2	2.17	0.45
1:H:158:ILE:HG23	1:H:246:MET:HG3	1.99	0.45
1:B:398:THR:HA	1:B:401:GLU:HB3	1.99	0.45
1:C:261:TRP:HZ2	1:D:131:ASN:HB2	1.82	0.45
1:D:80:PRO:HA	1:D:83:PHE:HB2	1.99	0.45
1:F:108:GLY:O	1:F:371:PHE:HA	2.17	0.45
1:I:273:GLU:HA	1:I:276:TYR:CE2	2.51	0.45
3:T:36:TRP:CE2	3:T:81:LEU:HB2	2.52	0.45
2:W:123:PHE:HB2	3:X:134:LEU:HD23	1.99	0.45
1:B:59:ARG:NH1	1:B:61:ASP:OD2	2.49	0.45
1:C:106:GLU:HB2	1:C:465:LEU:HD13	1.99	0.45
1:D:158:ILE:HD13	1:D:237:MET:HE1	1.99	0.45
1:G:247:PHE:HB2	1:G:316:ALA:HB1	1.99	0.45
3:L:19:LYS:HG2	3:L:82:GLN:HG2	1.97	0.45
3:L:91:THR:HG22	3:L:121:VAL:H	1.81	0.45
2:M:139:CYS:HB2	2:M:153:TRP:CZ2	2.52	0.45
2:M:206:SER:HB2	2:M:207:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PRO:HB3	1:C:231:TYR:CD1	2.51	0.44
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.99	0.44
1:C:403:TRP:O	1:C:404:ASN:ND2	2.50	0.44
1:F:247:PHE:HB2	1:F:316:ALA:HB1	1.98	0.44
1:G:290:LEU:HD13	1:H:363:GLU:HB3	1.99	0.44
3:R:67:ARG:HD2	3:R:85:SER:O	2.17	0.44
2:S:164:VAL:HG22	2:S:184:LEU:HD12	1.99	0.44
1:A:269:ASP:O	1:A:289:TYR:OH	2.32	0.44
1:B:28:VAL:HG22	1:B:382:ILE:HG12	1.98	0.44
1:C:278:LYS:HB2	3:P:57:TYR:CE1	2.53	0.44
1:G:283:ARG:HG2	3:X:106:ASP:HB3	1.99	0.44
2:Q:124:PRO:HB3	2:Q:214:PHE:CE1	2.52	0.44
3:X:6:GLU:CD	3:X:116:GLY:H	2.25	0.44
1:A:352:ILE:HD12	1:A:353:PRO:HD2	1.97	0.44
1:G:158:ILE:HD13	1:G:237:MET:HE1	1.99	0.44
2:K:19:ALA:HB3	2:K:80:ILE:HB	2.00	0.44
2:S:206:SER:HB2	2:S:207:THR:OG1	2.17	0.44
3:T:97:THR:HB	3:T:110:MET:HB3	1.99	0.44
2:c:113:ARG:HH22	2:c:116:ALA:HB2	1.82	0.44
3:Z:20:LEU:O	3:Z:80:TYR:HA	2.16	0.44
2:U:164:VAL:HG22	2:U:184:LEU:HD12	1.99	0.44
1:A:256:PHE:HA	1:B:115:VAL:HG21	2.00	0.44
1:B:97:ARG:HH22	1:B:404:ASN:HB2	1.82	0.44
1:C:68:TYR:CE1	1:C:151:TYR:HB2	2.53	0.44
1:D:43:LEU:HA	1:D:369:GLU:O	2.17	0.44
1:G:398:THR:HA	1:G:401:GLU:HB3	1.99	0.44
1:H:253:GLU:HG3	1:I:113:LEU:HD12	1.99	0.44
1:J:110:GLY:HA3	1:J:370:GLU:CD	2.43	0.44
2:c:14:SER:HB2	2:c:17:ASP:OD2	2.17	0.44
2:a:210:ILE:HD12	2:a:210:ILE:HA	1.89	0.44
1:A:271:LEU:HB2	1:A:289:TYR:CE2	2.53	0.44
1:B:269:ASP:O	1:B:289:TYR:OH	2.22	0.44
1:C:37:ALA:HB1	1:C:452:LEU:HD13	2.00	0.44
1:D:262:ASN:ND2	1:D:288:SER:HB3	2.33	0.44
1:F:58:GLY:HA2	1:F:59:ARG:HA	1.62	0.44
2:Q:156:ASP:CG	2:Q:196:SER:HB3	2.42	0.44
3:X:91:THR:HG22	3:X:121:VAL:H	1.82	0.44
1:F:299:VAL:HA	1:J:256:PHE:HB3	1.98	0.44
1:G:231:TYR:OH	1:G:253:GLU:OE2	2.24	0.44
1:G:279:GLY:HA2	1:I:356:TYR:H	1.83	0.44
1:H:52:VAL:HB	1:H:62:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:105:TYR:O	3:P:107:GLU:HG3	2.18	0.44
3:R:206:ASN:HD22	3:R:217:ASP:HB3	1.83	0.44
2:W:165:LEU:HB3	3:X:179:LEU:HD23	2.00	0.44
1:G:271:LEU:HB2	1:G:289:TYR:CE2	2.53	0.44
1:G:446:LYS:HA	1:G:446:LYS:HD2	1.83	0.44
1:I:24:THR:HA	1:I:27:TYR:CE1	2.52	0.44
2:K:94:SER:CA	2:K:103:PHE:HB3	2.42	0.44
3:R:33:THR:HG22	3:R:52:SER:HA	1.99	0.44
2:S:181:SER:HB2	3:T:176:PHE:CD2	2.53	0.44
3:N:144:SER:N	3:N:145:SER:HA	2.32	0.44
3:d:6:GLU:CD	3:d:116:GLY:H	2.26	0.44
2:W:39:HIS:CE1	3:X:109:TYR:HB3	2.52	0.44
2:W:45:SER:HB2	2:W:46:GLY:H	1.67	0.44
1:A:273:GLU:OE1	3:L:56:THR:OG1	2.33	0.44
1:B:97:ARG:NH1	1:B:404:ASN:HB2	2.28	0.44
1:B:216:ASN:HB2	1:E:345:CYS:SG	2.57	0.44
2:K:42:LEU:HD12	2:K:91:TYR:CZ	2.53	0.44
2:S:7:THR:HA	2:S:8:PRO:HA	1.79	0.44
1:B:43:LEU:HA	1:B:369:GLU:O	2.18	0.44
1:C:240:ASP:OD1	1:C:241:ALA:N	2.51	0.44
1:D:24:THR:HA	1:D:27:TYR:CE1	2.53	0.44
1:F:106:GLU:HB2	1:F:465:LEU:HD13	1.99	0.44
1:G:269:ASP:O	1:G:289:TYR:OH	2.34	0.44
1:I:210:PHE:CE2	1:I:224:ILE:HD12	2.53	0.44
1:I:353:PRO:C	1:I:355:VAL:H	2.23	0.44
1:J:210:PHE:CE2	1:J:224:ILE:HD12	2.52	0.44
2:Q:7:THR:HA	2:Q:8:PRO:HA	1.82	0.44
2:M:123:PHE:HB2	3:N:134:LEU:HD23	2.00	0.44
2:c:38:LEU:HD13	2:c:76:PHE:CD2	2.53	0.44
3:V:134:LEU:HD23	2:U:123:PHE:HB2	2.00	0.44
3:Z:2:VAL:HG12	3:Z:3:LYS:HG3	2.00	0.44
1:A:216:ASN:HB2	1:B:345:CYS:SG	2.58	0.43
1:C:281:ASP:O	1:C:283:ARG:N	2.51	0.43
1:D:130:GLU:HB2	1:D:260:PHE:HB2	1.99	0.43
1:D:446:LYS:HA	1:D:446:LYS:HD2	1.89	0.43
1:F:367:HIS:NE2	1:F:369:GLU:OE2	2.49	0.43
1:H:166:GLY:O	1:H:192:ASN:HA	2.18	0.43
1:I:87:ASP:OD1	1:I:87:ASP:N	2.51	0.43
1:I:208:MET:SD	1:J:342:LEU:HD22	2.58	0.43
3:L:37:ILE:HD13	3:L:47:TRP:HA	1.99	0.43
2:O:120:VAL:HA	2:O:140:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:6:GLN:HA	2:M:22:SER:O	2.17	0.43
3:d:221:VAL:HG12	3:d:222:PRO:CD	2.47	0.43
2:a:154:LYS:HA	2:a:159:GLU:HA	2.00	0.43
1:A:107:ILE:HD11	1:A:331:LEU:HD21	1.98	0.43
1:F:24:THR:HA	1:F:27:TYR:CE1	2.53	0.43
1:F:80:PRO:HA	1:F:83:PHE:HB2	1.99	0.43
1:H:24:THR:HA	1:H:27:TYR:CE1	2.53	0.43
3:R:34:MET:HB3	3:R:79:LEU:HD22	1.99	0.43
3:R:144:SER:N	3:R:145:SER:HA	2.32	0.43
3:T:37:ILE:HD13	3:T:47:TRP:HA	1.98	0.43
3:b:8:GLY:HA2	3:b:9:GLY:HA2	1.70	0.43
2:U:55:LYS:O	2:U:57:SER:N	2.46	0.43
1:E:158:ILE:HG23	1:E:246:MET:HG3	1.99	0.43
1:J:283:ARG:NH1	2:c:101:PHE:HZ	2.16	0.43
3:P:97:THR:HB	3:P:110:MET:HB3	1.99	0.43
3:P:209:HIS:CE1	3:P:211:ALA:HB3	2.53	0.43
2:c:155:ILE:HG22	2:c:196:SER:O	2.18	0.43
3:d:135:ALA:HB2	3:d:220:ILE:CG2	2.49	0.43
1:A:35:TYR:HD1	1:A:456:PHE:HB3	1.83	0.43
1:C:148:SER:HB3	1:D:291:TYR:CD1	2.53	0.43
1:E:130:GLU:HB2	1:E:260:PHE:HB2	1.99	0.43
1:G:75:VAL:HA	1:G:450:VAL:O	2.19	0.43
1:I:58:GLY:HA2	1:I:59:ARG:HA	1.57	0.43
1:A:131:ASN:ND2	1:B:128:ASP:OD2	2.33	0.43
1:A:446:LYS:HA	1:A:446:LYS:HD2	1.77	0.43
1:F:105:VAL:HG22	1:F:375:PHE:CD1	2.53	0.43
1:G:68:TYR:CE1	1:G:151:TYR:HB2	2.52	0.43
1:I:271:LEU:HB2	1:I:289:TYR:CE2	2.53	0.43
1:J:393:HIS:NE2	1:J:397:THR:HG22	2.33	0.43
3:T:87:LYS:HB3	3:T:87:LYS:HE3	1.86	0.43
2:M:185:THR:HG21	3:N:153:LYS:HE2	2.00	0.43
2:c:7:THR:HA	2:c:8:PRO:HA	1.73	0.43
3:b:51:ILE:HG13	3:b:58:THR:HG22	2.00	0.43
1:B:87:ASP:OD1	1:B:87:ASP:N	2.51	0.43
1:B:331:LEU:HD12	1:B:375:PHE:HZ	1.83	0.43
1:H:306:LEU:O	1:H:311:TYR:OH	2.29	0.43
2:M:7:THR:HA	2:M:8:PRO:HA	1.77	0.43
1:B:108:GLY:O	1:B:371:PHE:HA	2.17	0.43
1:B:216:ASN:ND2	1:B:219:GLU:OE2	2.41	0.43
1:E:68:TYR:CZ	1:E:151:TYR:HB2	2.52	0.43
1:G:253:GLU:HG3	1:H:113:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:GLY:O	1:I:355:VAL:HG12	2.18	0.43
2:K:44:LYS:O	2:K:47:GLN:HB2	2.18	0.43
2:O:181:SER:HB2	3:P:176:PHE:CE2	2.53	0.43
2:O:206:SER:HA	2:O:207:THR:HA	1.74	0.43
2:Q:43:GLN:HG3	2:Q:47:GLN:O	2.18	0.43
2:S:152:LYS:HB2	2:S:152:LYS:HE2	1.89	0.43
3:T:169:LEU:C	3:T:171:SER:H	2.27	0.43
3:N:37:ILE:HD13	3:N:47:TRP:HA	2.00	0.43
2:c:150:ASN:HB2	2:c:202:THR:CG2	2.49	0.43
3:V:176:PHE:CD2	2:U:181:SER:HB2	2.54	0.43
1:A:331:LEU:HD12	1:A:375:PHE:HZ	1.84	0.43
3:P:8:GLY:HA2	3:P:9:GLY:HA2	1.51	0.43
2:Q:48:SER:HB3	3:R:95:TYR:CE1	2.53	0.43
3:T:52:SER:O	3:T:72:ARG:NH2	2.48	0.43
2:M:51:LEU:HD21	2:M:54:TYR:HB3	2.00	0.43
3:N:33:THR:HG22	3:N:52:SER:HA	2.00	0.43
2:W:124:PRO:HB3	2:W:214:PHE:CE1	2.54	0.43
3:b:93:MET:HA	3:b:118:SER:HA	2.01	0.43
1:A:240:ASP:OD1	1:A:241:ALA:N	2.52	0.43
1:C:152:LYS:NZ	1:C:253:GLU:OE1	2.48	0.43
1:G:166:GLY:O	1:G:192:ASN:HA	2.18	0.43
1:I:326:HIS:CE1	1:I:398:THR:HG23	2.54	0.43
3:P:91:THR:CG2	3:P:121:VAL:H	2.32	0.43
3:R:37:ILE:HD13	3:R:47:TRP:HA	2.01	0.43
2:S:52:LEU:HD21	2:S:67:PHE:CD1	2.54	0.43
2:S:139:CYS:HB2	2:S:153:TRP:CZ2	2.54	0.43
2:M:24:ARG:HA	2:M:74:THR:O	2.19	0.43
3:V:156:PHE:HA	3:V:157:PRO:HA	1.86	0.43
2:W:208:SER:HB2	2:W:209:PRO:HD2	1.99	0.43
3:X:133:PRO:HD3	3:X:218:LYS:HE2	2.01	0.43
1:A:83:PHE:HD1	1:A:83:PHE:HA	1.77	0.43
1:B:106:GLU:HB2	1:B:465:LEU:HD13	1.99	0.43
1:E:58:GLY:HA2	1:E:59:ARG:HA	1.63	0.43
1:F:28:VAL:HG22	1:F:382:ILE:HG12	2.01	0.43
1:I:49:TYR:HA	1:I:223:ASP:OD1	2.19	0.43
1:I:83:PHE:CE2	1:I:85:LEU:HD23	2.53	0.43
1:I:126:LEU:HB3	1:I:262:ASN:HB3	2.01	0.43
1:J:24:THR:HA	1:J:27:TYR:CE1	2.54	0.43
3:L:33:THR:HG22	3:L:52:SER:HA	2.00	0.43
2:O:165:LEU:HD23	3:P:179:LEU:HD23	2.00	0.43
3:T:20:LEU:HD12	3:T:81:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:206:ASN:HD22	3:N:217:ASP:CG	2.26	0.43
3:X:91:THR:CG2	3:X:121:VAL:H	2.32	0.43
2:Y:19:ALA:O	2:Y:79:LYS:HA	2.19	0.43
2:a:150:ASN:HB2	2:a:202:THR:CG2	2.49	0.43
2:U:43:GLN:HB3	2:U:90:VAL:HG23	2.01	0.43
1:C:342:LEU:HD22	1:D:208:MET:SD	2.59	0.42
1:C:353:PRO:O	1:C:355:VAL:N	2.41	0.42
1:F:126:LEU:HB3	1:F:262:ASN:HB3	2.01	0.42
1:G:291:TYR:CD1	1:H:148:SER:HB3	2.53	0.42
1:H:217:LYS:HG2	1:H:226:GLN:NE2	2.34	0.42
2:K:43:GLN:HB3	2:K:90:VAL:CG2	2.44	0.42
2:S:206:SER:HA	2:S:207:THR:HA	1.71	0.42
2:c:124:PRO:HB3	2:c:214:PHE:CE1	2.54	0.42
2:U:148:ASP:HB3	2:U:204:LYS:HE3	2.01	0.42
1:A:87:ASP:O	1:A:90:VAL:HG22	2.19	0.42
1:D:299:VAL:HA	1:E:256:PHE:HB3	2.02	0.42
1:F:24:THR:HB	1:F:323:ILE:HD12	2.01	0.42
1:G:231:TYR:CD1	1:H:112:PRO:HB3	2.54	0.42
1:G:273:GLU:OE2	3:X:54:GLY:N	2.50	0.42
1:H:208:MET:HE2	1:H:210:PHE:CD1	2.54	0.42
1:H:256:PHE:HA	1:I:115:VAL:HG21	2.00	0.42
3:T:156:PHE:HA	3:T:157:PRO:HA	1.79	0.42
3:d:148:LEU:HD23	3:d:220:ILE:HD13	2.01	0.42
3:V:22:CYS:HB3	3:V:79:LEU:HB3	2.01	0.42
1:E:24:THR:HA	1:E:27:TYR:CE1	2.54	0.42
1:E:97:ARG:NH1	1:E:405:PHE:CZ	2.87	0.42
1:E:403:TRP:O	1:E:404:ASN:HB2	2.20	0.42
1:G:35:TYR:HD1	1:G:456:PHE:HB3	1.83	0.42
1:H:279:GLY:HA2	1:J:356:TYR:H	1.84	0.42
1:I:71:ARG:HB2	1:I:333:VAL:HG13	2.02	0.42
3:L:169:LEU:HD21	3:L:191:VAL:HG21	2.02	0.42
2:S:124:PRO:HB3	2:S:214:PHE:CE1	2.54	0.42
2:c:123:PHE:CG	3:d:134:LEU:HB3	2.54	0.42
2:c:128:GLU:HG2	3:d:218:LYS:NZ	2.35	0.42
2:W:42:LEU:HD12	2:W:91:TYR:CZ	2.54	0.42
2:a:7:THR:HA	2:a:8:PRO:HA	1.77	0.42
3:b:206:ASN:HD22	3:b:217:ASP:CG	2.27	0.42
1:A:113:LEU:HD12	1:C:253:GLU:HG3	2.01	0.42
1:F:87:ASP:O	1:F:90:VAL:HG22	2.19	0.42
1:G:281:ASP:C	1:G:283:ARG:N	2.77	0.42
1:H:105:VAL:HG22	1:H:375:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:87:ASP:O	1:I:90:VAL:HG22	2.19	0.42
1:I:208:MET:HE3	1:I:213:LEU:HD12	2.02	0.42
2:K:164:VAL:HG22	2:K:184:LEU:HD12	2.02	0.42
2:O:55:LYS:O	2:O:57:SER:N	2.43	0.42
3:P:93:MET:HA	3:P:118:SER:HA	2.02	0.42
3:d:37:ILE:HG13	3:d:110:MET:HE3	2.00	0.42
3:d:91:THR:HG22	3:d:121:VAL:N	2.23	0.42
3:Z:162:LEU:HD12	3:Z:162:LEU:O	2.20	0.42
3:Z:169:LEU:C	3:Z:171:SER:H	2.27	0.42
1:G:61:ASP:OD1	1:G:61:ASP:N	2.53	0.42
1:J:40:SER:HB2	1:J:455:ARG:HH12	1.84	0.42
2:O:103:PHE:CE1	3:P:45:LEU:HB3	2.55	0.42
3:T:11:LEU:HD23	3:T:120:THR:OG1	2.19	0.42
2:M:94:SER:CA	2:M:103:PHE:HB3	2.41	0.42
2:c:215:ASN:HB2	2:c:218:GLU:HB3	2.01	0.42
1:B:37:ALA:HB1	1:B:452:LEU:HD13	2.00	0.42
1:D:278:LYS:HB2	3:R:57:TYR:CE1	2.55	0.42
1:F:445:LEU:HB2	1:F:447:PHE:CE2	2.55	0.42
1:H:210:PHE:HE2	1:H:224:ILE:HD12	1.84	0.42
1:J:70:TYR:CZ	1:J:201:VAL:HG13	2.55	0.42
1:J:353:PRO:C	1:J:355:VAL:H	2.27	0.42
2:K:186:LEU:HD13	2:K:191:TYR:HB2	2.01	0.42
2:S:29:LEU:HD23	2:S:29:LEU:HA	1.84	0.42
1:A:80:PRO:HA	1:A:83:PHE:HB2	2.02	0.42
1:B:156:LEU:HA	1:B:250:LEU:O	2.19	0.42
1:C:158:ILE:HG23	1:C:246:MET:HG3	2.00	0.42
1:E:120:HIS:HB2	1:E:221:PRO:HA	2.01	0.42
1:F:130:GLU:HB2	1:F:260:PHE:HB2	2.01	0.42
1:F:131:ASN:CG	1:G:261:TRP:HE1	2.26	0.42
1:G:52:VAL:HB	1:G:62:VAL:HG22	2.00	0.42
1:G:75:VAL:HG22	1:G:450:VAL:HB	2.01	0.42
1:J:248:PHE:HB2	1:J:313:LEU:HD12	2.02	0.42
3:d:8:GLY:HA2	3:d:9:GLY:HA2	1.57	0.42
3:d:36:TRP:NE1	3:d:81:LEU:HB2	2.34	0.42
3:V:37:ILE:HD13	3:V:47:TRP:HA	2.01	0.42
2:a:206:SER:HA	2:a:207:THR:HA	1.72	0.42
1:B:130:GLU:HG3	1:B:260:PHE:CD2	2.54	0.42
1:B:273:GLU:HA	1:B:276:TYR:CE2	2.55	0.42
1:F:30:ARG:HG2	1:F:380:CYS:SG	2.60	0.42
1:F:52:VAL:HB	1:F:62:VAL:HG22	2.01	0.42
3:L:93:MET:HE3	3:L:116:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:161:THR:OG1	3:L:208:ALA:HB3	2.19	0.42
2:O:124:PRO:HG3	3:P:137:VAL:HG23	2.02	0.42
2:O:206:SER:HB2	2:O:207:THR:OG1	2.19	0.42
3:R:164:TRP:HB3	3:R:169:LEU:HD12	2.01	0.42
3:d:88:SER:O	3:d:91:THR:HG23	2.20	0.42
2:Y:123:PHE:HB2	3:Z:134:LEU:HD23	2.02	0.42
1:G:120:HIS:HB2	1:G:221:PRO:HA	2.00	0.42
1:J:166:GLY:O	1:J:192:ASN:HA	2.20	0.42
2:O:39:HIS:CE1	3:P:109:TYR:HB3	2.55	0.42
2:Q:43:GLN:HB3	2:Q:90:VAL:HG23	2.01	0.42
3:N:91:THR:HG23	3:N:120:THR:HG22	2.02	0.42
2:c:152:LYS:HB2	2:c:152:LYS:HE2	1.89	0.42
2:a:37:TYR:CD2	2:a:37:TYR:N	2.88	0.42
1:D:342:LEU:HD22	1:E:208:MET:SD	2.60	0.42
1:F:269:ASP:O	1:F:289:TYR:OH	2.33	0.42
1:F:278:LYS:HB2	3:V:57:TYR:CE1	2.55	0.42
1:F:365:ALA:HB2	1:J:290:LEU:HG	2.01	0.42
1:G:151:TYR:CG	1:G:203:THR:HB	2.54	0.42
1:G:158:ILE:HG23	1:G:246:MET:HG3	2.01	0.42
1:I:61:ASP:OD1	1:I:61:ASP:N	2.52	0.42
1:I:393:HIS:NE2	1:I:397:THR:HG22	2.35	0.42
2:O:165:LEU:HB2	2:O:183:THR:HG23	2.01	0.42
3:P:169:LEU:HD21	3:P:191:VAL:HG21	2.01	0.42
2:Q:71:GLY:HA3	2:Q:76:PHE:HA	2.02	0.42
2:S:42:LEU:HD21	2:S:44:LYS:HG3	2.02	0.42
2:S:44:LYS:NZ	2:S:86:GLU:OE2	2.53	0.42
2:c:172:ASP:OD2	2:c:174:LYS:HB2	2.20	0.42
2:Y:24:ARG:HA	2:Y:74:THR:O	2.20	0.42
2:a:94:SER:CA	2:a:103:PHE:HB3	2.44	0.42
1:H:171:LYS:HG3	1:H:186:PRO:HB2	2.01	0.41
1:I:446:LYS:HA	1:I:446:LYS:HD2	1.86	0.41
1:J:78:PRO:HD3	1:J:453:LYS:HA	2.02	0.41
2:K:104:GLY:HA2	2:K:105:ALA:HA	1.94	0.41
3:L:93:MET:HA	3:L:118:SER:HA	2.02	0.41
2:S:103:PHE:CE1	3:T:45:LEU:HB3	2.52	0.41
2:c:38:LEU:HD22	2:c:76:PHE:CD1	2.55	0.41
3:X:33:THR:HG22	3:X:52:SER:HA	2.01	0.41
3:X:51:ILE:HD11	3:X:55:GLY:HA2	2.02	0.41
2:U:42:LEU:HD12	2:U:91:TYR:CZ	2.55	0.41
1:A:120:HIS:HB2	1:A:221:PRO:HA	2.03	0.41
1:B:54:LYS:HE3	1:B:60:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASP:OD1	1:B:241:ALA:N	2.53	0.41
1:C:41:ARG:NH1	1:D:233:ASP:OD2	2.48	0.41
1:C:116:GLY:HA3	1:C:339:SER:O	2.20	0.41
1:E:68:TYR:CE1	1:E:151:TYR:HB2	2.55	0.41
1:E:466:GLY:O	1:E:470:LEU:HG	2.20	0.41
1:F:68:TYR:CE1	1:F:151:TYR:HB2	2.55	0.41
1:G:79:ASP:HB3	1:G:82:LYS:HB3	2.01	0.41
1:H:96:GLN:HG2	1:H:383:THR:HA	2.03	0.41
1:H:106:GLU:HB2	1:H:465:LEU:HD13	2.00	0.41
1:H:208:MET:HE3	1:H:213:LEU:HD12	2.02	0.41
1:H:256:PHE:HB3	1:I:299:VAL:HA	2.02	0.41
1:H:283:ARG:NH2	2:Y:96:SER:O	2.53	0.41
1:I:156:LEU:HA	1:I:250:LEU:O	2.20	0.41
3:X:209:HIS:HB3	3:X:214:THR:HG22	2.01	0.41
3:b:6:GLU:OE2	3:b:96:CYS:HB3	2.20	0.41
1:E:110:GLY:HA3	1:E:370:GLU:CD	2.45	0.41
1:E:254:GLN:NE2	1:E:297:GLY:O	2.40	0.41
2:K:29:LEU:HD23	2:K:29:LEU:HA	1.83	0.41
2:Q:28:SER:C	2:Q:30:VAL:H	2.28	0.41
3:N:8:GLY:HA2	3:N:9:GLY:HA2	1.74	0.41
3:V:8:GLY:HA2	3:V:9:GLY:HA2	1.71	0.41
3:V:35:SER:OG	3:V:97:THR:OG1	2.34	0.41
2:a:152:LYS:HB2	2:a:152:LYS:HE2	1.89	0.41
3:b:105:TYR:O	3:b:107:GLU:HG3	2.19	0.41
1:A:68:TYR:CE1	1:A:151:TYR:HB2	2.55	0.41
1:A:358:PRO:HG3	1:C:139:ASP:O	2.21	0.41
1:B:97:ARG:HH12	1:B:404:ASN:CB	2.29	0.41
1:C:115:VAL:HG21	1:D:256:PHE:HA	2.01	0.41
1:F:358:PRO:O	1:J:265:GLY:HA2	2.20	0.41
2:c:181:SER:HB2	3:d:176:PHE:CD2	2.55	0.41
3:V:34:MET:HB3	3:V:79:LEU:HD22	2.03	0.41
2:W:7:THR:HA	2:W:8:PRO:HA	1.78	0.41
2:W:103:PHE:HE1	3:X:45:LEU:HB3	1.86	0.41
2:Y:155:ILE:HA	2:Y:156:ASP:HA	1.87	0.41
3:Z:178:ALA:HA	3:Z:186:THR:O	2.21	0.41
2:a:19:ALA:HB3	2:a:80:ILE:HB	2.02	0.41
2:a:37:TYR:N	2:a:37:TYR:HD2	2.18	0.41
1:A:261:TRP:CZ3	1:A:294:SER:HB3	2.55	0.41
1:B:30:ARG:HH21	1:B:321:ASN:HD22	1.68	0.41
1:C:68:TYR:CZ	1:C:151:TYR:HB2	2.55	0.41
1:E:97:ARG:HG3	1:E:97:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:ILE:HA	1:H:248:PHE:O	2.20	0.41
1:I:106:GLU:HB2	1:I:465:LEU:HD13	2.03	0.41
3:R:148:LEU:CD1	3:R:220:ILE:HG13	2.51	0.41
3:T:33:THR:HG23	3:T:51:ILE:O	2.20	0.41
2:M:28:SER:C	2:M:30:VAL:H	2.28	0.41
2:c:43:GLN:HB3	2:c:90:VAL:HG23	2.02	0.41
2:U:165:LEU:HB2	2:U:183:THR:HG23	2.03	0.41
1:C:148:SER:OG	1:D:129:THR:OG1	2.35	0.41
1:H:240:ASP:OD1	1:H:241:ALA:N	2.54	0.41
1:J:208:MET:HE2	1:J:210:PHE:CD1	2.55	0.41
2:S:55:LYS:O	2:S:57:SER:N	2.45	0.41
3:T:162:LEU:O	3:T:162:LEU:HD12	2.20	0.41
2:M:155:ILE:HA	2:M:156:ASP:HA	1.88	0.41
3:X:143:GLY:HA2	3:X:195:SER:HB3	2.02	0.41
1:A:106:GLU:HB2	1:A:465:LEU:HD13	2.02	0.41
1:A:353:PRO:O	1:A:355:VAL:N	2.40	0.41
1:B:58:GLY:HA2	1:B:59:ARG:HA	1.64	0.41
1:C:24:THR:HB	1:C:323:ILE:HD12	2.03	0.41
1:F:61:ASP:OD1	1:F:61:ASP:N	2.53	0.41
1:F:92:ASP:C	1:F:94:ASN:H	2.29	0.41
1:G:355:VAL:HG12	1:J:279:GLY:O	2.21	0.41
2:Q:208:SER:HB2	2:Q:209:PRO:HD2	2.03	0.41
3:N:156:PHE:HA	3:N:157:PRO:HA	1.85	0.41
2:c:155:ILE:HD11	2:c:160:ARG:HD3	2.02	0.41
3:d:12:VAL:O	3:d:121:VAL:HA	2.21	0.41
3:V:51:ILE:HD11	3:V:55:GLY:HA2	2.03	0.41
2:W:123:PHE:HE2	2:W:140:PHE:HD2	1.68	0.41
2:W:154:LYS:HA	2:W:159:GLU:HA	2.01	0.41
2:a:55:LYS:O	2:a:57:SER:N	2.46	0.41
1:B:40:SER:N	1:B:455:ARG:NH1	2.69	0.41
1:B:61:ASP:N	1:B:61:ASP:OD1	2.54	0.41
1:C:79:ASP:HB3	1:C:82:LYS:HB3	2.01	0.41
1:D:156:LEU:HA	1:D:250:LEU:O	2.21	0.41
1:F:291:TYR:CD1	1:G:148:SER:HB3	2.56	0.41
1:H:58:GLY:HA2	1:H:59:ARG:HA	1.62	0.41
1:J:156:LEU:HG	1:J:334:VAL:HB	2.03	0.41
2:K:7:THR:HA	2:K:8:PRO:HA	1.79	0.41
2:O:125:PRO:HG3	2:O:135:ALA:HB1	2.02	0.41
3:P:37:ILE:HD13	3:P:47:TRP:HA	2.02	0.41
3:d:33:THR:HG22	3:d:52:SER:HA	2.03	0.41
3:d:169:LEU:C	3:d:171:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:206:SER:HA	2:U:207:THR:HA	1.66	0.41
1:B:52:VAL:HB	1:B:62:VAL:HG22	2.03	0.41
1:B:54:LYS:HG2	1:B:60:GLN:HE21	1.85	0.41
1:D:130:GLU:O	1:D:131:ASN:HB3	2.20	0.41
1:D:152:LYS:HE3	1:D:253:GLU:HB2	2.02	0.41
1:E:83:PHE:HD1	1:E:83:PHE:HA	1.79	0.41
1:F:113:LEU:HD12	1:J:253:GLU:HG3	2.02	0.41
1:G:24:THR:HA	1:G:27:TYR:CE1	2.55	0.41
1:I:80:PRO:HB2	1:I:98:LEU:HB3	2.03	0.41
2:K:206:SER:HB2	2:K:207:THR:OG1	2.21	0.41
3:P:165:ASN:HD21	3:P:203:ILE:HA	1.86	0.41
3:R:93:MET:HE3	3:R:116:GLY:HA3	2.03	0.41
3:R:162:LEU:O	3:R:162:LEU:HD12	2.20	0.41
2:M:31:HIS:HB2	2:M:97:THR:HG23	2.02	0.41
2:M:160:ARG:HE	2:M:186:LEU:HD21	1.85	0.41
3:d:220:ILE:C	3:d:221:VAL:HG23	2.46	0.41
3:Z:51:ILE:HD11	3:Z:55:GLY:HA2	2.03	0.41
1:D:388:VAL:O	1:D:390:SER:N	2.53	0.41
1:F:115:VAL:HG21	1:J:256:PHE:HA	2.02	0.41
3:L:169:LEU:C	3:L:171:SER:H	2.29	0.41
3:P:41:PRO:HD3	3:P:91:THR:O	2.20	0.41
3:R:11:LEU:HD12	3:R:157:PRO:HG3	2.03	0.41
3:V:162:LEU:O	3:V:162:LEU:HD12	2.21	0.41
2:W:54:TYR:O	2:W:58:ASN:HB2	2.21	0.41
2:W:118:PRO:HB3	2:W:144:PHE:HB3	2.02	0.41
2:a:148:ASP:HB3	2:a:204:LYS:HE3	2.04	0.41
2:U:112:LYS:O	2:U:113:ARG:HD3	2.21	0.41
1:A:326:HIS:CE1	1:A:398:THR:HG23	2.56	0.40
1:B:446:LYS:HD2	1:B:446:LYS:HA	1.76	0.40
1:D:61:ASP:OD1	1:D:61:ASP:N	2.54	0.40
1:E:122:LEU:HD13	1:E:144:ARG:NH2	2.37	0.40
1:H:68:TYR:CE1	1:H:151:TYR:HB2	2.56	0.40
1:H:75:VAL:HA	1:H:450:VAL:O	2.21	0.40
1:H:326:HIS:CD2	1:H:402:ASP:OD2	2.70	0.40
1:I:97:ARG:NH1	1:I:404:ASN:H	2.19	0.40
1:I:216:ASN:HB2	1:J:345:CYS:SG	2.60	0.40
1:J:345:CYS:HA	1:J:362:LYS:O	2.21	0.40
2:O:181:SER:HB2	3:P:176:PHE:CD2	2.56	0.40
3:P:147:THR:HA	3:P:192:THR:HA	2.02	0.40
2:M:152:LYS:HB2	2:M:152:LYS:HE2	1.88	0.40
3:N:17:SER:HA	3:N:84:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:169:LEU:C	3:X:171:SER:H	2.29	0.40
3:Z:51:ILE:HG13	3:Z:58:THR:HG22	2.03	0.40
2:a:2:VAL:HB	2:a:102:THR:HG21	2.02	0.40
3:b:37:ILE:HD13	3:b:47:TRP:HA	2.03	0.40
1:A:156:LEU:HA	1:A:250:LEU:O	2.20	0.40
1:B:158:ILE:HD13	1:B:237:MET:HE1	2.03	0.40
1:D:83:PHE:HD1	1:D:83:PHE:HA	1.76	0.40
1:F:30:ARG:HH21	1:F:321:ASN:HD22	1.70	0.40
1:G:240:ASP:OD1	1:G:241:ALA:N	2.54	0.40
1:H:28:VAL:HG22	1:H:382:ILE:HG12	2.03	0.40
1:I:278:LYS:HB2	3:b:57:TYR:CE1	2.56	0.40
3:P:105:TYR:O	3:P:107:GLU:N	2.54	0.40
2:Q:155:ILE:HA	2:Q:156:ASP:HA	1.89	0.40
3:N:8:GLY:O	3:N:20:LEU:HD22	2.21	0.40
3:N:11:LEU:HD23	3:N:120:THR:OG1	2.21	0.40
3:V:176:PHE:CE2	2:U:181:SER:HB2	2.56	0.40
1:B:185:CYS:HB2	1:E:364:TYR:CD2	2.56	0.40
1:C:358:PRO:O	1:D:265:GLY:HA2	2.21	0.40
1:D:353:PRO:O	1:D:355:VAL:N	2.44	0.40
1:F:216:ASN:ND2	1:F:219:GLU:OE2	2.41	0.40
1:G:107:ILE:HD11	1:G:331:LEU:HD21	2.04	0.40
2:K:38:LEU:HD13	2:K:76:PHE:CD2	2.56	0.40
2:O:186:LEU:HD22	2:O:190:GLU:HG2	2.03	0.40
3:T:91:THR:HG22	3:T:121:VAL:H	1.85	0.40
3:X:162:LEU:HD12	3:X:162:LEU:O	2.21	0.40
2:Y:191:TYR:HA	2:Y:197:TYR:OH	2.22	0.40
3:b:169:LEU:C	3:b:171:SER:H	2.30	0.40
1:C:113:LEU:HD12	1:D:253:GLU:HG3	2.04	0.40
1:D:97:ARG:HH11	1:D:403:TRP:HB3	1.85	0.40
1:D:261:TRP:HE1	1:E:131:ASN:CG	2.28	0.40
1:F:112:PRO:HB3	1:J:231:TYR:CD1	2.57	0.40
1:G:106:GLU:HB2	1:G:465:LEU:HD13	2.03	0.40
1:I:43:LEU:HA	1:I:369:GLU:O	2.21	0.40
2:Q:82:ARG:HB2	2:Q:82:ARG:NH1	2.37	0.40
2:Q:104:GLY:HA2	2:Q:105:ALA:HA	1.98	0.40
2:Y:29:LEU:HD23	2:Y:29:LEU:HA	1.91	0.40
1:A:61:ASP:N	1:A:61:ASP:OD1	2.54	0.40
1:D:261:TRP:HZ2	1:E:131:ASN:HB2	1.87	0.40
1:E:409:PRO:HA	1:E:410:PRO:HD3	1.97	0.40
1:F:107:ILE:HD11	1:F:331:LEU:HD21	2.04	0.40
1:G:345:CYS:HA	1:G:362:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:GLY:HA2	1:J:358:PRO:O	2.21	0.40
1:I:273:GLU:HA	1:I:276:TYR:HE2	1.86	0.40
1:J:331:LEU:HD12	1:J:375:PHE:HZ	1.86	0.40
3:L:105:TYR:O	3:L:107:GLU:HG3	2.22	0.40
2:O:139:CYS:HB2	2:O:153:TRP:CH2	2.56	0.40
2:Q:152:LYS:HB2	2:Q:152:LYS:HE2	1.89	0.40
2:S:19:ALA:O	2:S:79:LYS:HA	2.21	0.40
2:c:94:SER:CA	2:c:103:PHE:HB3	2.35	0.40
3:V:144:SER:N	3:V:145:SER:HA	2.35	0.40
3:X:54:GLY:C	3:X:56:THR:H	2.29	0.40
3:b:2:VAL:HG12	3:b:3:LYS:HG3	2.03	0.40

All (9) 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:A:92:ASP:OD2	1:H:386:THR:OG1[2_756]	1.89	0.31
1:B:386:THR:OG1	1:G:92:ASP:OD2[2_756]	1.90	0.30
1:C:92:ASP:OD2	1:I:386:THR:OG1[2_756]	1.90	0.30
1:D:92:ASP:OD2	1:J:386:THR:OG1[2_756]	1.96	0.24
2:O:188:LYS:NZ	2:Q:84:GLU:OE2[1_655]	2.01	0.19
3:d:144:SER:OG	2:W:82:ARG:NH1[1_655]	2.01	0.19
1:E:386:THR:OG1	1:F:92:ASP:OD2[2_756]	2.03	0.17
3:b:9:GLY:O	2:U:217:ASN:ND2[1_656]	2.12	0.08
1:C:386:THR:OG1	1:I:92:ASP:OD2[2_756]	2.19	0.01

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	416/500 (83%)	386 (93%)	28 (7%)	2 (0%)	24 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	416/500 (83%)	388 (93%)	26 (6%)	2 (0%)	24	52
1	C	417/500 (83%)	386 (93%)	29 (7%)	2 (0%)	24	52
1	D	417/500 (83%)	389 (93%)	27 (6%)	1 (0%)	43	70
1	E	423/500 (85%)	390 (92%)	31 (7%)	2 (0%)	24	52
1	F	417/500 (83%)	390 (94%)	27 (6%)	0	100	100
1	G	416/500 (83%)	387 (93%)	25 (6%)	4 (1%)	12	38
1	H	416/500 (83%)	387 (93%)	27 (6%)	2 (0%)	24	52
1	I	416/500 (83%)	386 (93%)	27 (6%)	3 (1%)	18	46
1	J	416/500 (83%)	388 (93%)	27 (6%)	1 (0%)	43	70
2	K	215/219 (98%)	199 (93%)	13 (6%)	3 (1%)	9	30
2	M	215/219 (98%)	199 (93%)	14 (6%)	2 (1%)	14	41
2	O	216/219 (99%)	201 (93%)	12 (6%)	3 (1%)	9	30
2	Q	215/219 (98%)	200 (93%)	14 (6%)	1 (0%)	24	52
2	S	216/219 (99%)	201 (93%)	13 (6%)	2 (1%)	14	41
2	U	215/219 (98%)	200 (93%)	12 (6%)	3 (1%)	9	30
2	W	217/219 (99%)	202 (93%)	13 (6%)	2 (1%)	14	41
2	Y	215/219 (98%)	201 (94%)	11 (5%)	3 (1%)	9	30
2	a	215/219 (98%)	201 (94%)	12 (6%)	2 (1%)	14	41
2	c	216/219 (99%)	201 (93%)	12 (6%)	3 (1%)	9	30
3	L	220/223 (99%)	207 (94%)	12 (6%)	1 (0%)	24	52
3	N	217/223 (97%)	203 (94%)	12 (6%)	2 (1%)	14	41
3	P	217/223 (97%)	204 (94%)	13 (6%)	0	100	100
3	R	219/223 (98%)	205 (94%)	13 (6%)	1 (0%)	24	52
3	T	217/223 (97%)	203 (94%)	14 (6%)	0	100	100
3	V	217/223 (97%)	203 (94%)	13 (6%)	1 (0%)	24	52
3	X	217/223 (97%)	202 (93%)	14 (6%)	1 (0%)	24	52
3	Z	217/223 (97%)	203 (94%)	14 (6%)	0	100	100
3	b	217/223 (97%)	202 (93%)	14 (6%)	1 (0%)	24	52
3	d	219/223 (98%)	204 (93%)	13 (6%)	2 (1%)	14	41
All	All	8502/9420 (90%)	7918 (93%)	532 (6%)	52 (1%)	21	49

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	283	ARG
1	J	282	ILE
2	O	217	ASN
1	D	131	ASN
1	E	131	ASN
1	E	405	PHE
3	R	221	VAL
3	d	221	VAL
2	W	45	SER
3	X	137	VAL
1	A	131	ASN
1	B	354	ASN
1	C	131	ASN
1	B	282	ILE
1	G	387	GLU
1	H	131	ASN
1	H	403	TRP
1	I	131	ASN
3	N	106	ASP
1	A	354	ASN
1	G	131	ASN
1	G	354	ASN
1	I	387	GLU
2	K	45	SER
3	L	106	ASP
3	d	106	ASP
3	V	169	LEU
2	Y	45	SER
3	b	169	LEU
2	U	44	LYS
2	c	208	SER
2	a	208	SER
2	O	163	GLY
2	Q	163	GLY
2	c	163	GLY
1	I	282	ILE
2	K	163	GLY
2	O	56	VAL
2	S	56	VAL
2	M	163	GLY
3	N	64	VAL
2	c	56	VAL
2	Y	56	VAL

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Mol	Chain	Res	Type
2	Y	163	GLY
2	a	56	VAL
2	U	56	VAL
1	G	282	ILE
2	K	56	VAL
2	S	208	SER
2	M	56	VAL
2	W	163	GLY
2	U	208	SER

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	376/444 (85%)	372 (99%)	4 (1%)	65	73
1	B	376/444 (85%)	369 (98%)	7 (2%)	50	66
1	C	377/444 (85%)	371 (98%)	6 (2%)	55	67
1	D	377/444 (85%)	370 (98%)	7 (2%)	50	66
1	E	382/444 (86%)	375 (98%)	7 (2%)	51	66
1	F	377/444 (85%)	370 (98%)	7 (2%)	50	66
1	G	376/444 (85%)	371 (99%)	5 (1%)	61	70
1	H	376/444 (85%)	373 (99%)	3 (1%)	73	76
1	I	376/444 (85%)	368 (98%)	8 (2%)	47	64
1	J	376/444 (85%)	371 (99%)	5 (1%)	61	70
2	K	195/197 (99%)	185 (95%)	10 (5%)	21	48
2	M	195/197 (99%)	183 (94%)	12 (6%)	16	43
2	O	196/197 (100%)	184 (94%)	12 (6%)	17	44
2	Q	195/197 (99%)	187 (96%)	8 (4%)	27	53
2	S	196/197 (100%)	186 (95%)	10 (5%)	21	48
2	U	195/197 (99%)	183 (94%)	12 (6%)	16	43
2	W	197/197 (100%)	188 (95%)	9 (5%)	24	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	195/197 (99%)	187 (96%)	8 (4%)	27	53
2	a	195/197 (99%)	187 (96%)	8 (4%)	27	53
2	c	196/197 (100%)	187 (95%)	9 (5%)	24	50
3	L	189/190 (100%)	179 (95%)	10 (5%)	20	48
3	N	187/190 (98%)	181 (97%)	6 (3%)	34	58
3	P	187/190 (98%)	179 (96%)	8 (4%)	26	52
3	R	189/190 (100%)	182 (96%)	7 (4%)	30	55
3	T	187/190 (98%)	181 (97%)	6 (3%)	34	58
3	V	187/190 (98%)	179 (96%)	8 (4%)	26	52
3	X	187/190 (98%)	179 (96%)	8 (4%)	26	52
3	Z	187/190 (98%)	180 (96%)	7 (4%)	30	55
3	b	187/190 (98%)	180 (96%)	7 (4%)	30	55
3	d	189/190 (100%)	180 (95%)	9 (5%)	23	49
All	All	7600/8310 (92%)	7367 (97%)	233 (3%)	35	59

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	PHE
1	A	143	THR
1	A	201	VAL
1	A	276	TYR
1	B	143	THR
1	B	201	VAL
1	B	276	TYR
1	B	280	THR
1	B	352	ILE
1	B	385	THR
1	B	396	ASN
1	C	83	PHE
1	C	201	VAL
1	C	276	TYR
1	C	283	ARG
1	C	306	LEU
1	C	385	THR
1	D	83	PHE
1	D	201	VAL

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Mol	Chain	Res	Type
1	D	276	TYR
1	D	280	THR
1	D	282	ILE
1	D	385	THR
1	D	405	PHE
1	E	83	PHE
1	E	201	VAL
1	E	280	THR
1	E	306	LEU
1	E	385	THR
1	E	407	VAL
1	E	471	LEU
1	F	83	PHE
1	F	201	VAL
1	F	276	TYR
1	F	280	THR
1	F	306	LEU
1	F	385	THR
1	F	405	PHE
1	G	83	PHE
1	G	143	THR
1	G	201	VAL
1	G	280	THR
1	G	306	LEU
1	H	201	VAL
1	H	283	ARG
1	H	385	THR
1	I	83	PHE
1	I	143	THR
1	I	201	VAL
1	I	276	TYR
1	I	280	THR
1	I	306	LEU
1	I	385	THR
1	I	396	ASN
1	J	143	THR
1	J	201	VAL
1	J	280	THR
1	J	282	ILE
1	J	385	THR
2	K	44	LYS
2	K	56	VAL

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Mol	Chain	Res	Type
2	K	103	PHE
2	K	131	THR
2	K	151	VAL
2	K	183	THR
2	K	186	LEU
2	K	202	THR
2	K	207	THR
2	K	210	ILE
3	L	2	VAL
3	L	12	VAL
3	L	56	THR
3	L	64	VAL
3	L	121	VAL
3	L	147	THR
3	L	161	THR
3	L	162	LEU
3	L	192	THR
3	L	204	THR
2	O	37	TYR
2	O	42	LEU
2	O	56	VAL
2	O	102	THR
2	O	103	PHE
2	O	131	THR
2	O	137	VAL
2	O	151	VAL
2	O	155	ILE
2	O	183	THR
2	O	202	THR
2	O	207	THR
3	P	2	VAL
3	P	12	VAL
3	P	56	THR
3	P	64	VAL
3	P	148	LEU
3	P	162	LEU
3	P	197	THR
3	P	204	THR
2	Q	42	LEU
2	Q	48	SER
2	Q	102	THR
2	Q	103	PHE

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Mol	Chain	Res	Type
2	Q	131	THR
2	Q	155	ILE
2	Q	183	THR
2	Q	202	THR
3	R	12	VAL
3	R	146	VAL
3	R	147	THR
3	R	161	THR
3	R	162	LEU
3	R	171	SER
3	R	204	THR
2	S	42	LEU
2	S	45	SER
2	S	56	VAL
2	S	102	THR
2	S	103	PHE
2	S	131	THR
2	S	155	ILE
2	S	183	THR
2	S	207	THR
2	S	210	ILE
3	T	2	VAL
3	T	56	THR
3	T	146	VAL
3	T	147	THR
3	T	162	LEU
3	T	204	THR
2	M	35	ASN
2	M	48	SER
2	M	56	VAL
2	M	103	PHE
2	M	131	THR
2	M	151	VAL
2	M	155	ILE
2	M	183	THR
2	M	198	THR
2	M	202	THR
2	M	207	THR
2	M	210	ILE
3	N	2	VAL
3	N	121	VAL
3	N	146	VAL

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Mol	Chain	Res	Type
3	N	147	THR
3	N	161	THR
3	N	204	THR
2	c	36	THR
2	c	56	VAL
2	c	99	VAL
2	c	102	THR
2	c	103	PHE
2	c	131	THR
2	c	155	ILE
2	c	183	THR
2	c	210	ILE
3	d	2	VAL
3	d	42	GLU
3	d	56	THR
3	d	146	VAL
3	d	147	THR
3	d	161	THR
3	d	162	LEU
3	d	197	THR
3	d	221	VAL
3	V	2	VAL
3	V	56	THR
3	V	121	VAL
3	V	146	VAL
3	V	147	THR
3	V	162	LEU
3	V	192	THR
3	V	204	THR
2	W	37	TYR
2	W	45	SER
2	W	56	VAL
2	W	102	THR
2	W	103	PHE
2	W	151	VAL
2	W	155	ILE
2	W	183	THR
2	W	210	ILE
3	X	2	VAL
3	X	56	THR
3	X	91	THR
3	X	121	VAL

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Mol	Chain	Res	Type
3	X	147	THR
3	X	162	LEU
3	X	197	THR
3	X	204	THR
2	Y	56	VAL
2	Y	103	PHE
2	Y	131	THR
2	Y	155	ILE
2	Y	183	THR
2	Y	198	THR
2	Y	207	THR
2	Y	210	ILE
3	Z	2	VAL
3	Z	56	THR
3	Z	121	VAL
3	Z	146	VAL
3	Z	147	THR
3	Z	162	LEU
3	Z	197	THR
2	a	37	TYR
2	a	56	VAL
2	a	103	PHE
2	a	131	THR
2	a	155	ILE
2	a	183	THR
2	a	186	LEU
2	a	198	THR
3	b	2	VAL
3	b	12	VAL
3	b	56	THR
3	b	126	THR
3	b	146	VAL
3	b	147	THR
3	b	204	THR
2	U	35	ASN
2	U	42	LEU
2	U	44	LYS
2	U	56	VAL
2	U	99	VAL
2	U	102	THR
2	U	103	PHE
2	U	151	VAL

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Mol	Chain	Res	Type
2	U	155	ILE
2	U	183	THR
2	U	198	THR
2	U	210	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	96	GLN
1	A	270	GLN
1	A	327	ASN
1	B	96	GLN
1	B	133	HIS
1	B	153	GLN
1	B	326	HIS
1	B	327	ASN
1	B	341	ASN
1	C	96	GLN
1	C	259	HIS
1	C	270	GLN
1	C	341	ASN
1	C	374	GLN
1	C	404	ASN
1	D	270	GLN
1	D	327	ASN
1	E	326	HIS
1	F	96	GLN
1	F	153	GLN
1	F	354	ASN
1	F	374	GLN
1	F	404	ASN
1	G	96	GLN
1	G	327	ASN
1	G	341	ASN
1	G	354	ASN
1	H	60	GLN
1	H	326	HIS
1	H	374	GLN
1	I	96	GLN
1	I	259	HIS
1	I	270	GLN

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Mol	Chain	Res	Type
1	J	60	GLN
1	J	153	GLN
1	J	155	GLN
1	J	326	HIS
1	J	327	ASN
1	J	374	GLN
2	K	33	ASN
2	K	195	ASN
3	L	174	HIS
3	L	181	GLN
2	O	143	ASN
2	O	195	ASN
3	P	181	GLN
2	Q	143	ASN
3	R	181	GLN
2	S	33	ASN
2	S	195	ASN
2	M	43	GLN
2	M	98	HIS
2	M	166	ASN
2	M	195	ASN
3	N	39	GLN
3	N	181	GLN
3	N	201	GLN
2	c	43	GLN
2	c	47	GLN
2	c	143	ASN
3	d	39	GLN
3	V	39	GLN
3	V	201	GLN
2	W	43	GLN
2	W	195	ASN
2	W	203	HIS
3	X	39	GLN
2	Y	31	HIS
2	Y	143	ASN
2	Y	166	ASN
2	Y	215	ASN
2	a	27	GLN
2	a	43	GLN
2	a	129	GLN
2	a	166	ASN

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Mol	Chain	Res	Type
3	b	39	GLN
3	b	201	GLN
2	U	43	GLN
2	U	47	GLN
2	U	143	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	420/500 (84%)	-0.13	3 (0%) 84 73	43, 63, 117, 149	0
1	B	420/500 (84%)	-0.12	2 (0%) 87 78	39, 64, 123, 155	0
1	C	421/500 (84%)	-0.16	4 (0%) 79 66	39, 56, 113, 177	0
1	D	421/500 (84%)	-0.15	6 (1%) 73 59	35, 52, 117, 171	0
1	E	427/500 (85%)	-0.16	1 (0%) 91 87	38, 54, 115, 154	0
1	F	421/500 (84%)	-0.09	2 (0%) 87 78	44, 65, 124, 165	0
1	G	420/500 (84%)	-0.10	0 100 100	49, 71, 126, 157	0
1	H	420/500 (84%)	-0.03	5 (1%) 76 63	51, 73, 136, 166	0
1	I	420/500 (84%)	-0.04	4 (0%) 79 66	51, 71, 132, 182	0
1	J	420/500 (84%)	-0.06	4 (0%) 79 66	46, 69, 126, 159	0
2	K	217/219 (99%)	-0.05	2 (0%) 81 69	51, 81, 127, 138	0
2	M	217/219 (99%)	0.22	4 (1%) 67 51	77, 141, 191, 202	0
2	O	218/219 (99%)	0.17	4 (1%) 67 51	69, 133, 179, 196	0
2	Q	217/219 (99%)	-0.04	2 (0%) 81 69	57, 105, 138, 165	0
2	S	218/219 (99%)	0.23	5 (2%) 61 45	69, 128, 219, 236	0
2	U	217/219 (99%)	0.14	4 (1%) 67 51	75, 137, 195, 209	0
2	W	219/219 (100%)	-0.06	1 (0%) 87 78	65, 87, 114, 152	0
2	Y	217/219 (99%)	0.52	10 (4%) 37 27	113, 179, 223, 233	0
2	a	217/219 (99%)	0.36	12 (5%) 30 22	95, 158, 223, 232	0
2	c	218/219 (99%)	0.10	4 (1%) 67 51	62, 90, 140, 149	0
3	L	222/223 (99%)	-0.08	0 100 100	56, 90, 118, 183	0
3	N	219/223 (98%)	0.09	3 (1%) 73 59	57, 104, 176, 194	0
3	P	219/223 (98%)	0.10	4 (1%) 67 51	62, 111, 183, 222	0
3	R	221/223 (99%)	-0.04	4 (1%) 67 51	47, 73, 145, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	T	219/223 (98%)	0.18	5 (2%) 61 45	50, 110, 214, 229	0
3	V	219/223 (98%)	0.23	5 (2%) 61 45	72, 117, 206, 216	0
3	X	219/223 (98%)	-0.01	2 (0%) 81 69	67, 91, 144, 198	0
3	Z	219/223 (98%)	0.45	7 (3%) 50 36	91, 157, 237, 259	0
3	b	219/223 (98%)	0.25	7 (3%) 50 36	73, 130, 224, 232	0
3	d	221/223 (99%)	0.07	2 (0%) 81 69	54, 84, 134, 179	0
All	All	8582/9420 (91%)	0.02	118 (1%) 73 59	35, 82, 200, 259	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	183	THR	5.0
2	a	183	THR	4.9
2	S	183	THR	4.7
3	b	188	SER	4.2
1	C	139	ASP	4.2
2	M	120	VAL	3.8
3	T	150	CYS	3.8
2	Y	184	LEU	3.7
3	Z	111	ASP	3.6
1	D	133	HIS	3.5
1	F	139	ASP	3.5
1	A	139	ASP	3.4
3	V	169	LEU	3.3
2	a	118	PRO	3.2
3	Z	186	THR	3.2
3	b	151	LEU	3.1
2	S	191	TYR	3.1
2	Y	198	THR	3.1
2	M	165	LEU	3.0
3	Z	193	VAL	3.0
3	T	151	LEU	3.0
3	Z	188	SER	3.0
2	U	191	TYR	3.0
3	R	150	CYS	2.9
1	E	381	LYS	2.9
1	D	372	ASP	2.9
2	K	142	ASN	2.9
2	a	181	SER	2.9
3	b	180	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	O	183	THR	2.9
1	I	134	VAL	2.8
3	N	2	VAL	2.8
1	J	331	LEU	2.8
2	Y	182	SER	2.8
1	B	139	ASP	2.8
1	I	140	THR	2.8
3	N	188	SER	2.8
3	d	148	LEU	2.8
1	C	352	ILE	2.8
2	c	104	GLY	2.8
2	Y	42	LEU	2.8
2	c	183	THR	2.8
3	b	90	ASP	2.7
2	Y	19	ALA	2.7
3	T	186	THR	2.6
2	M	52	LEU	2.6
3	Z	200	SER	2.6
1	H	139	ASP	2.6
2	a	141	LEU	2.6
2	Y	52	LEU	2.6
3	V	188	SER	2.6
1	D	216	ASN	2.6
2	a	201	ALA	2.6
1	J	134	VAL	2.5
2	U	13	VAL	2.5
2	Y	41	TYR	2.5
3	V	108	GLY	2.5
3	d	189	SER	2.5
3	R	139	GLY	2.5
3	T	188	SER	2.5
2	c	182	SER	2.4
2	a	119	THR	2.4
2	Y	20	SER	2.4
2	S	182	SER	2.4
3	b	150	CYS	2.4
1	F	140	THR	2.4
1	B	354	ASN	2.4
3	V	37	ILE	2.4
3	P	205	CYS	2.4
2	Q	104	GLY	2.3
2	S	52	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	a	101	PHE	2.3
2	a	165	LEU	2.3
3	b	2	VAL	2.3
2	M	183	THR	2.3
1	D	131	ASN	2.3
2	a	109	LEU	2.3
2	Y	199	CYS	2.3
1	H	381	LYS	2.3
1	I	86	PRO	2.3
3	X	108	GLY	2.3
2	S	160	ARG	2.3
3	Z	146	VAL	2.3
1	A	216	ASN	2.3
3	V	150	CYS	2.3
1	J	50	PHE	2.2
1	D	352	ILE	2.2
2	O	165	LEU	2.2
2	K	139	CYS	2.2
1	C	405	PHE	2.2
1	C	351	SER	2.2
2	U	104	GLY	2.2
1	A	350	SER	2.2
1	J	333	VAL	2.1
2	a	105	ALA	2.1
3	P	188	SER	2.1
3	b	186	THR	2.1
2	a	91	TYR	2.1
2	a	60	PHE	2.1
2	Q	175	ASP	2.1
1	H	133	HIS	2.1
3	N	59	TYR	2.1
3	Z	81	LEU	2.1
1	I	352	ILE	2.1
2	W	161	GLN	2.1
1	H	86	PRO	2.1
3	P	162	LEU	2.1
2	O	101	PHE	2.1
3	P	170	SER	2.0
1	H	216	ASN	2.0
2	O	210	ILE	2.0
3	T	148	LEU	2.0
3	R	142	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	353	PRO	2.0
3	R	222	PRO	2.0
2	c	147	LYS	2.0
3	X	162	LEU	2.0
2	U	183	THR	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.