



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:21 PM UTC

PDB ID : 3NCY / pdb_00003ncy
Title : X-ray crystal structure of an arginine agmatine antiporter (AdiC) in complex with a Fab fragment
Authors : Fang, Y.; Jayaram, H.; Shane, T.; Komalkova-Partensky, L.; Wu, F.; Williams, C.; Xiong, Y.; Miller, C.
Deposited on : 2010-06-06
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

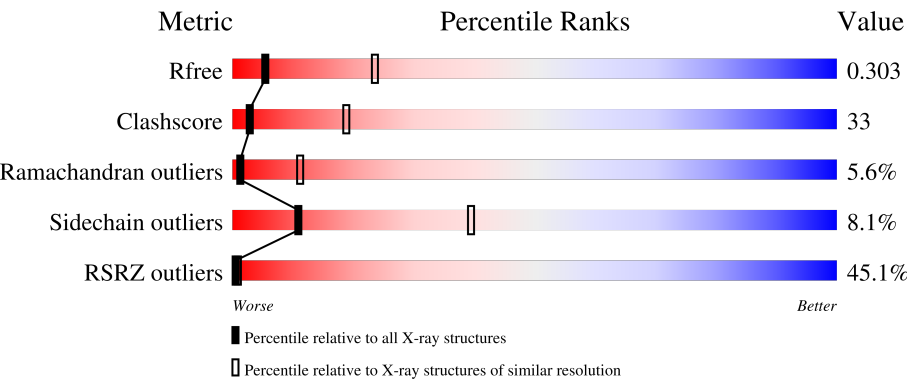
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	445	46% 45% 41% 8% • 5%
1	B	445	45% 45% 40% 7% • 6%
1	C	445	46% 44% 43% 8% 6%
1	D	445	42% 44% 42% 8% 6%
2	P	219	47% 46% 46% 9%

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Mol	Chain	Length	Quality of chain
2	Q	219	38%46%45%9%
3	S	211	45%56%36%7%
3	W	211	31%55%36%8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18693 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 AdiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3052	2018	489	524	21			
1	B	420	Total	C	N	O	S	5	0	0
			3039	2009	489	520	21			
1	C	420	Total	C	N	O	S	0	0	0
			3034	2006	487	520	21			
1	D	419	Total	C	N	O	S	17	0	0
			3031	2005	486	519	21			

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	218	Total	C	N	O	S	16	0	0
			1640	1044	264	325	7			
2	P	219	Total	C	N	O	S	15	0	0
			1647	1049	265	326	7			

- Molecule 3 is a protein called Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	211	Total	C	N	O	S	40	0	0
			1625	1011	271	333	10			
3	S	211	Total	C	N	O	S	20	0	0
			1625	1011	271	333	10			

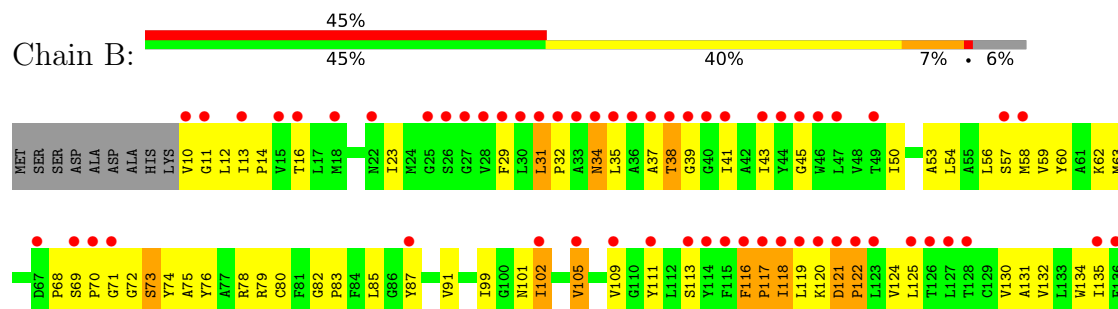
3 Residue-property plots

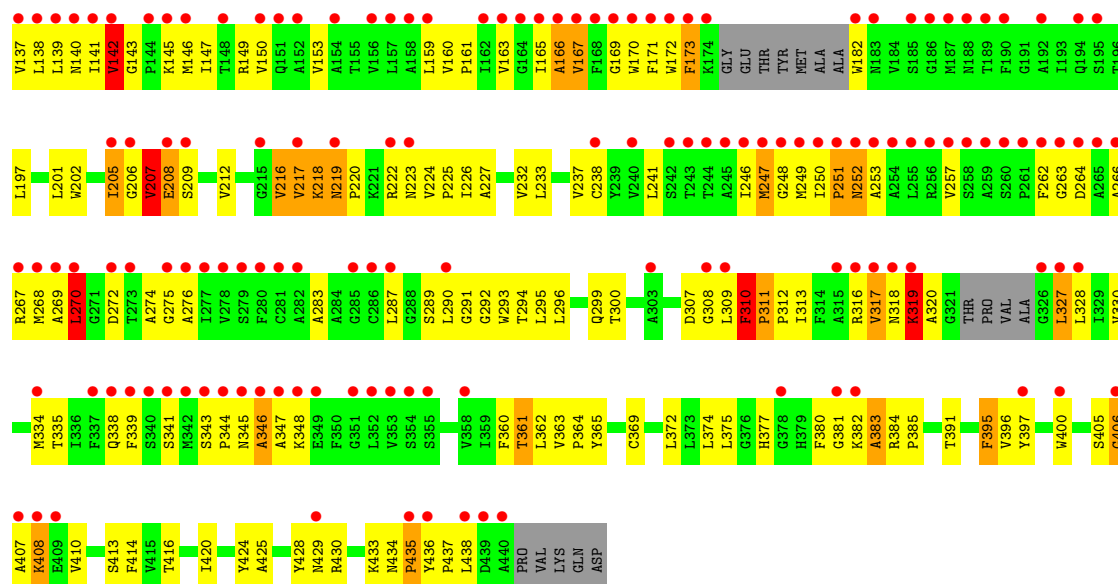
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: AdiC

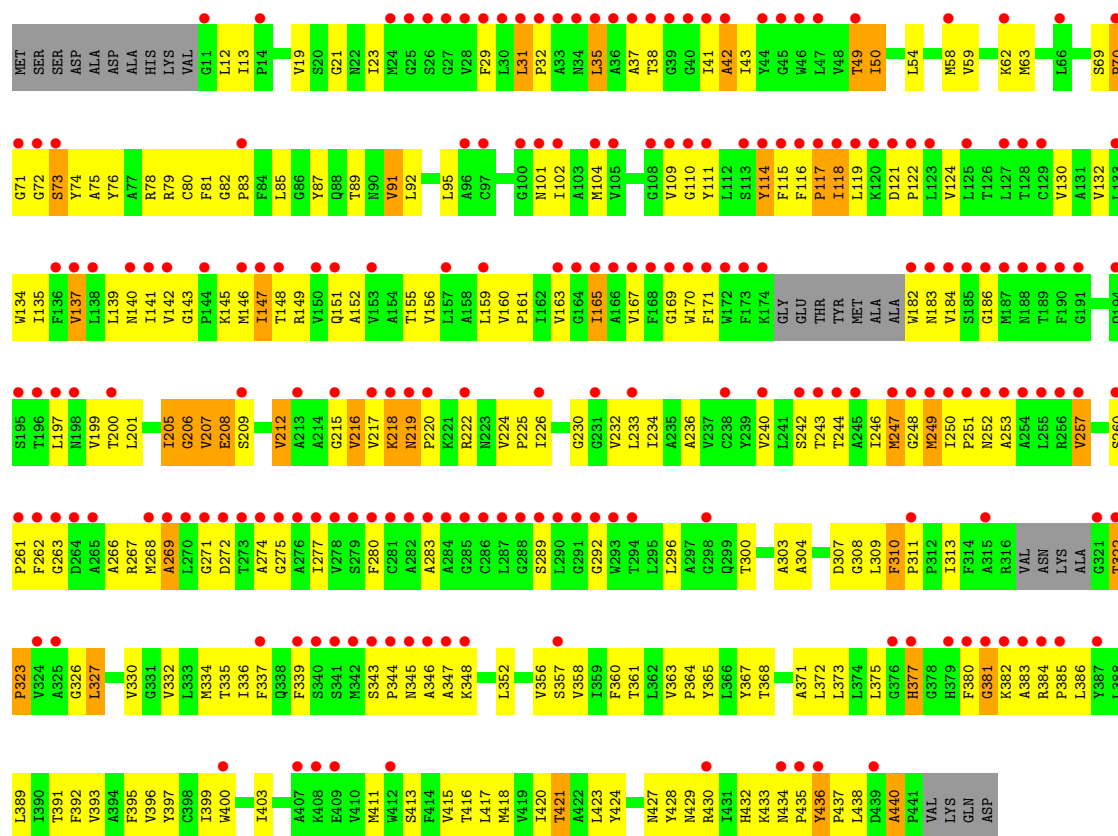
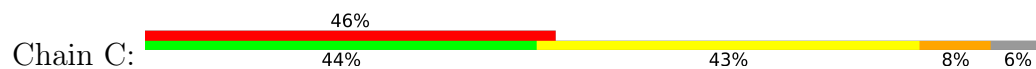


• Molecule 1: AdiC

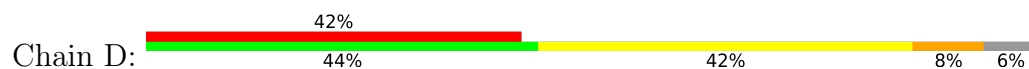


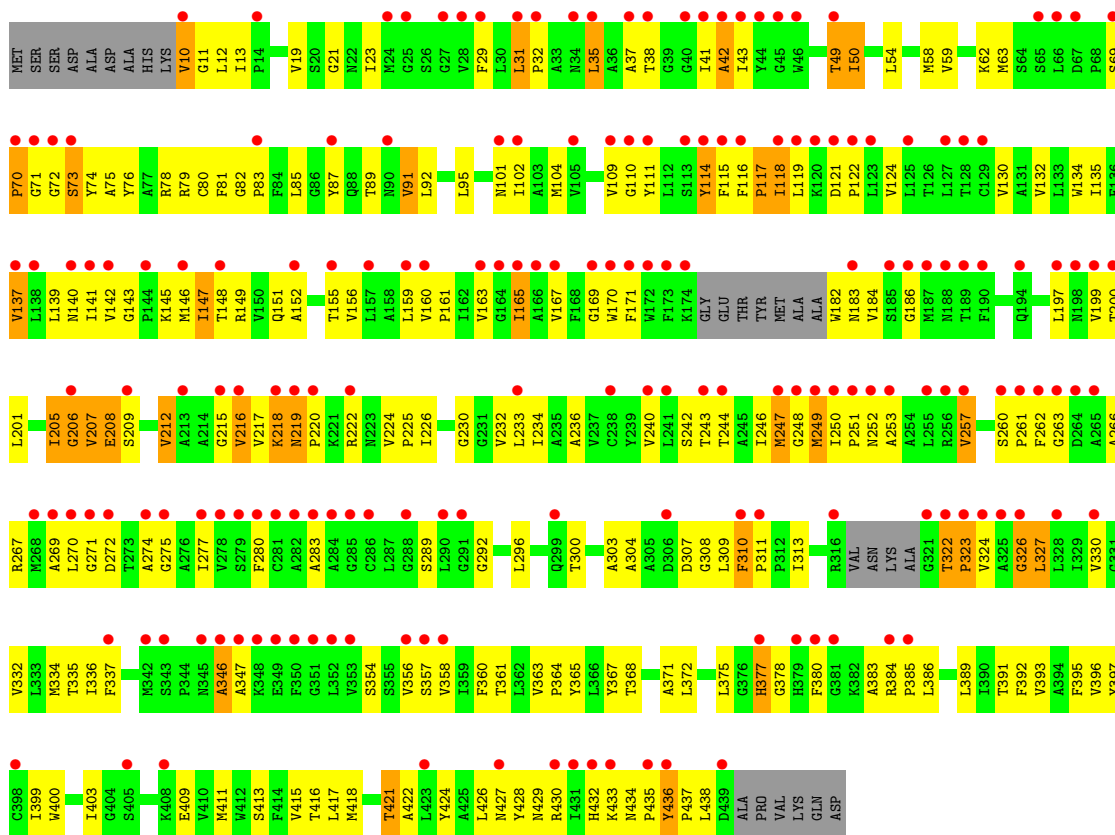


• Molecule 1: AdiC

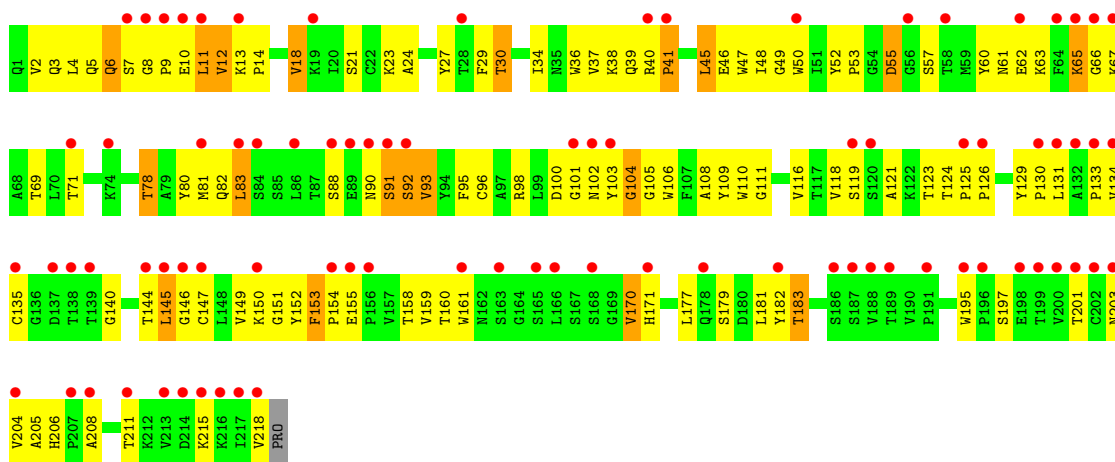


• Molecule 1: AdiC



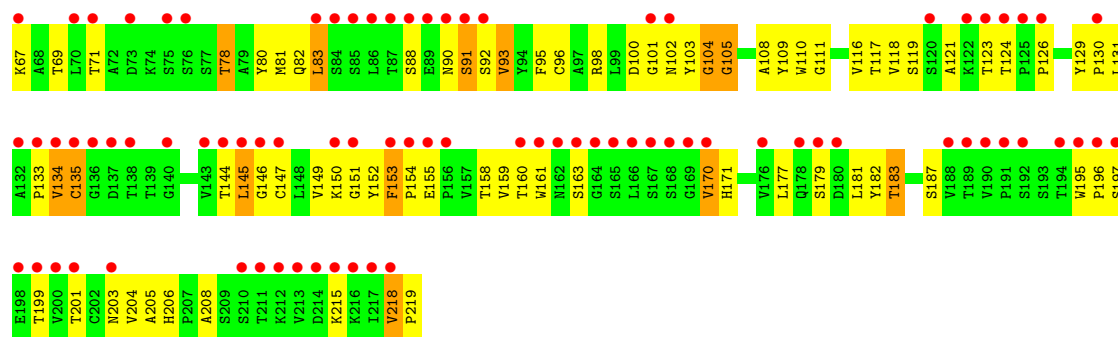


- Molecule 2: Fab Heavy chain

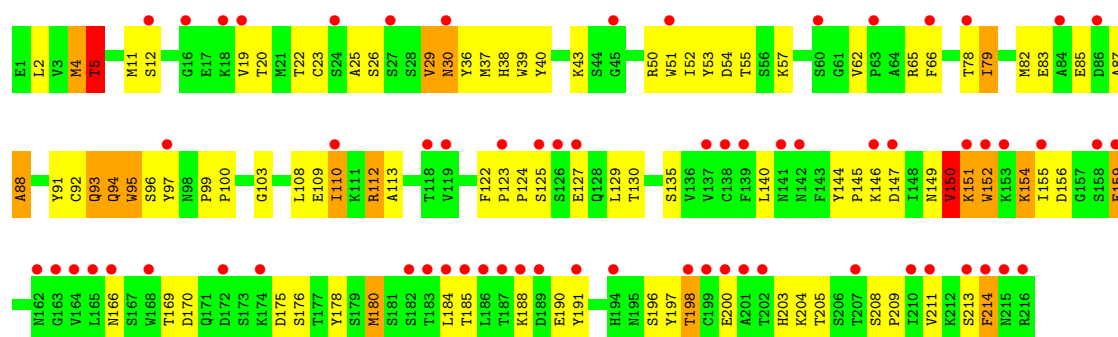


- Molecule 2: Fab Heavy chain

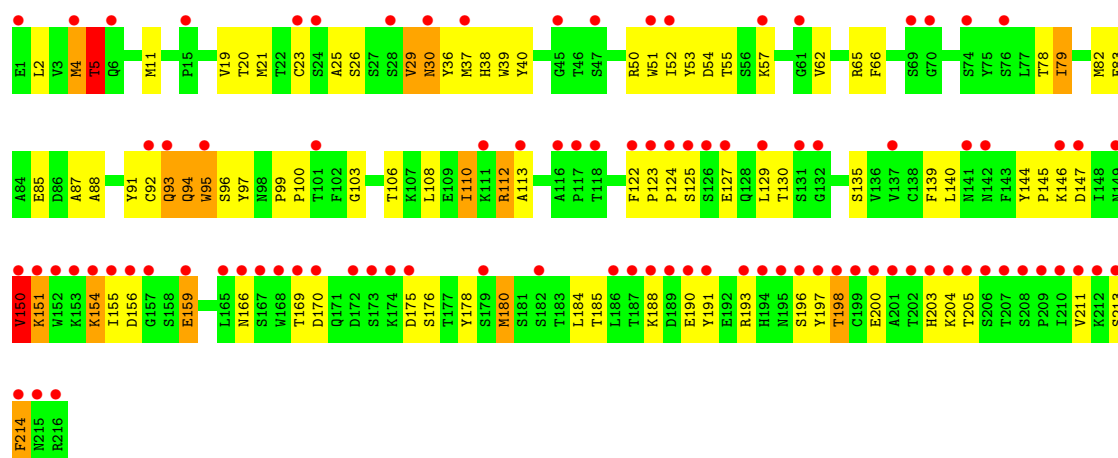




• Molecule 3: Fab Light chain



• Molecule 3: Fab Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.66Å 104.15Å 154.03Å 81.96° 75.93° 73.73°	Depositor
Resolution (Å)	33.23 – 3.20 33.23 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (33.23-3.20) 96.3 (33.23-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, REFMAC	Depositor
R, R_{free}	0.282 , 0.312 0.275 , 0.303	Depositor DCC
R_{free} test set	3612 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	18693	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/3125	0.78	7/4281 (0.2%)
1	B	0.30	0/3110	0.80	8/4257 (0.2%)
1	C	0.30	0/3107	0.78	7/4256 (0.2%)
1	D	0.30	0/3103	0.78	6/4250 (0.1%)
2	P	0.29	0/1694	0.75	1/2319 (0.0%)
2	Q	0.30	0/1686	0.77	1/2307 (0.0%)
3	S	0.27	0/1665	0.72	0/2260
3	W	0.27	0/1665	0.73	0/2260
All	All	0.29	0/19155	0.77	30/26190 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	LYS	N-CA-C	9.68	121.83	111.28
2	Q	92	SER	N-CA-C	-6.79	105.15	113.50
1	C	42	ALA	N-CA-C	-6.13	106.41	114.31
1	D	42	ALA	N-CA-C	-6.12	106.42	114.31
1	B	310	PHE	CA-C-N	5.59	126.14	120.38
1	B	310	PHE	C-N-CA	5.59	126.14	120.38
1	A	310	PHE	CA-C-N	5.57	126.11	120.38
1	A	310	PHE	C-N-CA	5.57	126.11	120.38
1	A	311	PRO	CA-C-N	5.56	125.39	119.28
1	A	311	PRO	C-N-CA	5.56	125.39	119.28
1	B	311	PRO	CA-C-N	5.54	125.38	119.28
1	B	311	PRO	C-N-CA	5.54	125.38	119.28
1	C	311	PRO	CA-C-N	5.54	125.37	119.28
1	C	311	PRO	C-N-CA	5.54	125.37	119.28
2	P	134	VAL	N-CA-C	-5.50	95.58	111.00
1	D	311	PRO	CA-C-N	5.50	125.33	119.28
1	D	311	PRO	C-N-CA	5.50	125.33	119.28
1	D	310	PHE	CA-C-N	5.43	125.98	120.38
1	D	310	PHE	C-N-CA	5.43	125.98	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	PHE	CA-C-N	5.33	125.87	120.38
1	C	310	PHE	C-N-CA	5.33	125.87	120.38
1	D	326	GLY	N-CA-C	-5.20	108.87	115.31
1	B	383	ALA	N-CA-C	-5.14	106.20	113.20
1	C	326	GLY	N-CA-C	-5.14	108.94	115.31
1	A	121	ASP	CA-C-N	5.08	126.20	119.84
1	A	121	ASP	C-N-CA	5.08	126.20	119.84
1	A	383	ALA	N-CA-C	-5.06	106.32	113.20
1	B	121	ASP	CA-C-N	5.05	126.16	119.84
1	B	121	ASP	C-N-CA	5.05	126.16	119.84
1	C	345	ASN	N-CA-C	5.02	116.50	108.41

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	3052	0	3120	212	0
1	B	3039	0	3112	203	0
1	C	3034	0	3098	206	0
1	D	3031	0	3102	213	0
2	P	1647	0	1601	133	0
2	Q	1640	0	1594	138	0
3	S	1625	0	1550	86	0
3	W	1625	0	1550	92	0
All	All	18693	0	18727	1211	0

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 33.

All (1211) 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:A:346:ALA:HA	1:A:347:ALA:CB	1.58	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ALA:CA	1:A:347:ALA:HB3	1.76	1.12
1:A:23:ILE:HG12	1:A:206:GLY:HA3	1.33	1.11
1:D:356:VAL:HG11	1:D:409:GLU:HB3	1.30	1.10
1:B:23:ILE:HG12	1:B:206:GLY:HA3	1.32	1.08
2:P:91:SER:HA	2:P:92:SER:HB3	1.36	1.07
2:P:9:PRO:HB3	2:P:10:GLU:HB3	1.37	1.05
1:B:346:ALA:CB	1:B:347:ALA:HA	1.91	1.01
1:B:346:ALA:HB3	1:B:347:ALA:CA	1.90	1.00
2:P:101:GLY:HA2	2:P:102:ASN:HB3	1.42	1.00
2:Q:101:GLY:HA2	2:Q:102:ASN:HB3	1.40	0.99
1:C:347:ALA:N	1:C:348:LYS:HA	1.75	0.99
1:B:346:ALA:HB3	1:B:347:ALA:HA	1.01	0.98
1:C:346:ALA:H	1:C:347:ALA:HA	1.26	0.96
1:D:72:GLY:HA3	1:D:74:TYR:N	1.80	0.96
1:C:72:GLY:HA3	1:C:74:TYR:N	1.81	0.95
1:B:39:GLY:HA3	1:B:247:MET:HG3	1.49	0.94
2:Q:10:GLU:HG2	2:Q:11:LEU:H	1.32	0.94
1:A:39:GLY:HA3	1:A:247:MET:HG3	1.50	0.94
2:Q:10:GLU:HG2	2:Q:11:LEU:N	1.83	0.92
2:Q:9:PRO:HB2	2:Q:10:GLU:HB2	1.52	0.90
2:P:90:ASN:HB3	2:P:118:VAL:HG12	1.53	0.90
1:D:72:GLY:HA3	1:D:74:TYR:H	1.35	0.90
2:Q:90:ASN:HB3	2:Q:118:VAL:HG12	1.53	0.89
1:C:134:TRP:HE1	1:C:335:THR:HG21	1.38	0.88
1:C:377:HIS:CD2	1:D:430:ARG:HG2	2.09	0.88
1:B:319:LYS:H	1:B:319:LYS:HD2	1.40	0.87
1:C:72:GLY:HA3	1:C:74:TYR:H	1.37	0.87
1:D:134:TRP:HE1	1:D:335:THR:HG21	1.39	0.87
1:A:343:SER:HB2	1:A:344:PRO:HD3	1.56	0.86
1:B:202:TRP:HE3	1:B:205:ILE:HD11	1.40	0.86
1:A:202:TRP:HE3	1:A:205:ILE:HD11	1.41	0.85
2:P:9:PRO:CB	2:P:10:GLU:HB3	2.06	0.84
1:A:313:ILE:HD12	1:A:313:ILE:H	1.42	0.84
2:Q:10:GLU:HG2	2:Q:11:LEU:HD23	1.59	0.84
1:C:346:ALA:N	1:C:347:ALA:HA	1.89	0.84
1:A:250:ILE:HB	1:A:251:PRO:HD3	1.59	0.83
1:B:313:ILE:HD12	1:B:313:ILE:H	1.42	0.83
1:B:250:ILE:HB	1:B:251:PRO:HD3	1.59	0.83
1:B:216:VAL:HG12	1:B:217:VAL:H	1.44	0.82
1:B:134:TRP:HE1	1:B:335:THR:HG21	1.44	0.82
1:A:38:THR:HG21	1:A:41:ILE:HG22	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:HG21	1:B:41:ILE:HG22	1.61	0.81
1:D:50:ILE:HD11	1:D:236:ALA:HB1	1.62	0.81
1:C:313:ILE:H	1:C:313:ILE:HD12	1.45	0.81
1:B:269:ALA:O	1:B:270:LEU:HB2	1.80	0.81
1:A:134:TRP:HE1	1:A:335:THR:HG21	1.45	0.80
1:A:216:VAL:HG12	1:A:217:VAL:H	1.45	0.80
1:D:356:VAL:CG1	1:D:409:GLU:HB3	2.11	0.80
1:C:346:ALA:H	1:C:347:ALA:CA	1.94	0.79
2:P:218:VAL:HG12	2:P:219:PRO:HD2	1.64	0.79
1:C:50:ILE:HD11	1:C:236:ALA:HB1	1.62	0.79
1:D:313:ILE:HD12	1:D:313:ILE:H	1.46	0.79
1:B:166:ALA:H	1:B:167:VAL:HB	1.48	0.79
1:A:166:ALA:H	1:A:167:VAL:HB	1.48	0.78
1:B:343:SER:HB3	1:B:344:PRO:HD3	1.63	0.78
1:B:252:ASN:HB2	1:B:253:ALA:HA	1.65	0.78
1:A:142:VAL:O	1:A:142:VAL:HG13	1.83	0.77
1:B:35:LEU:HD22	1:B:247:MET:HG2	1.66	0.77
1:B:72:GLY:HA3	1:B:74:TYR:N	2.00	0.77
1:B:142:VAL:O	1:B:142:VAL:HG13	1.82	0.77
1:A:72:GLY:HA3	1:A:74:TYR:N	1.99	0.77
1:C:322:THR:HB	1:C:323:PRO:HD3	1.66	0.77
1:A:35:LEU:HD22	1:A:247:MET:HG2	1.66	0.77
1:A:346:ALA:HA	1:A:347:ALA:HB3	0.79	0.76
3:S:4:MET:HE2	3:S:4:MET:HA	1.67	0.76
1:C:80:CYS:HA	1:D:434:ASN:HD21	1.48	0.76
2:Q:24:ALA:HB1	2:Q:27:TYR:HE1	1.51	0.76
2:P:24:ALA:HB1	2:P:27:TYR:HE1	1.51	0.76
2:P:91:SER:HB3	2:P:116:VAL:HB	1.66	0.76
1:A:252:ASN:HB2	1:A:253:ALA:HA	1.66	0.75
1:D:322:THR:HB	1:D:323:PRO:HD3	1.66	0.75
1:D:219:ASN:N	1:D:220:PRO:HD3	2.01	0.75
1:C:219:ASN:N	1:C:220:PRO:HD3	2.01	0.75
3:W:39:TRP:HB2	3:W:52:ILE:HB	1.68	0.75
1:B:31:LEU:HD13	1:B:246:ILE:HD12	1.69	0.75
3:W:4:MET:HE2	3:W:4:MET:HA	1.66	0.75
1:D:356:VAL:HG11	1:D:409:GLU:CB	2.16	0.75
2:Q:91:SER:HB3	2:Q:116:VAL:HB	1.68	0.74
1:A:85:LEU:HD11	1:B:85:LEU:HD11	1.68	0.74
2:P:150:LYS:NZ	3:S:185:THR:HG21	2.03	0.74
1:A:267:ARG:NE	1:A:274:ALA:HB2	2.03	0.74
3:W:94:GLN:HG2	3:W:96:SER:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD13	1:A:246:ILE:HD12	1.69	0.73
1:D:10:VAL:HG21	1:D:218:LYS:HD3	1.69	0.73
2:P:48:ILE:HG23	2:P:67:LYS:NZ	2.04	0.73
2:Q:159:VAL:HG22	2:Q:204:VAL:HG22	1.72	0.72
3:S:94:GLN:HG2	3:S:96:SER:H	1.52	0.72
1:D:435:PRO:HB3	2:Q:102:ASN:O	1.90	0.72
3:W:150:VAL:HG23	3:W:151:LYS:HA	1.72	0.72
1:A:346:ALA:CA	1:A:347:ALA:CB	2.42	0.72
1:A:381:GLY:N	1:A:382:LYS:HA	2.04	0.72
2:Q:48:ILE:HG23	2:Q:67:LYS:NZ	2.04	0.72
2:P:63:LYS:HZ2	2:P:63:LYS:HB2	1.54	0.72
3:S:39:TRP:HB2	3:S:52:ILE:HB	1.69	0.72
1:C:267:ARG:HH12	1:C:277:ILE:HG22	1.55	0.71
1:D:87:TYR:CE1	1:D:424:TYR:HB2	2.25	0.71
3:S:129:LEU:HD23	3:S:188:LYS:HZ2	1.53	0.71
1:A:269:ALA:O	1:A:270:LEU:HB2	1.91	0.71
1:D:250:ILE:HB	1:D:251:PRO:HD3	1.71	0.71
1:C:250:ILE:HB	1:C:251:PRO:HD3	1.71	0.71
1:D:267:ARG:HH12	1:D:277:ILE:HG22	1.55	0.71
2:Q:92:SER:O	2:Q:93:VAL:HB	1.91	0.71
1:A:72:GLY:HA3	1:A:73:SER:C	2.15	0.70
1:A:176:GLU:HA	1:A:182:TRP:N	2.06	0.70
3:S:40:TYR:CE2	3:S:93:GLN:HG2	2.26	0.70
1:D:207:VAL:HG12	1:D:232:VAL:HG22	1.73	0.70
1:B:202:TRP:CE3	1:B:205:ILE:HD11	2.26	0.70
1:D:224:VAL:HB	1:D:225:PRO:HD3	1.73	0.70
2:Q:10:GLU:CG	2:Q:11:LEU:H	1.95	0.70
1:B:72:GLY:HA3	1:B:73:SER:C	2.15	0.70
2:P:40:ARG:HD3	2:P:92:SER:HB2	1.72	0.70
2:P:159:VAL:HG22	2:P:204:VAL:HG22	1.73	0.70
2:P:129:TYR:HB3	3:S:125:SER:OG	1.91	0.70
3:W:40:TYR:CE2	3:W:93:GLN:HG2	2.27	0.70
1:A:202:TRP:CE3	1:A:205:ILE:HD11	2.26	0.70
1:B:381:GLY:N	1:B:382:LYS:HA	2.05	0.70
3:W:129:LEU:HD23	3:W:188:LYS:HZ2	1.57	0.70
2:P:11:LEU:HD12	2:P:117:THR:O	1.92	0.69
1:C:375:LEU:HD12	1:D:438:LEU:HG	1.74	0.69
1:D:10:VAL:CG2	1:D:218:LYS:HD3	2.22	0.69
1:A:212:VAL:HG23	1:A:296:LEU:HD22	1.75	0.69
1:C:49:THR:HG21	1:C:200:THR:HB	1.74	0.69
1:C:87:TYR:CE1	1:C:424:TYR:HB2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:THR:HG21	1:D:200:THR:HB	1.74	0.69
2:Q:10:GLU:CG	2:Q:11:LEU:HD23	2.22	0.69
2:Q:37:VAL:HG21	2:Q:110:TRP:HZ3	1.57	0.69
1:A:54:LEU:O	1:A:58:MET:HG2	1.93	0.69
2:P:39:GLN:O	2:P:92:SER:HA	1.91	0.69
1:C:31:LEU:HD12	1:C:32:PRO:HD3	1.74	0.69
1:D:262:PHE:CZ	1:D:266:ALA:HB2	2.28	0.69
1:B:212:VAL:HG23	1:B:296:LEU:HD22	1.75	0.68
1:C:262:PHE:CZ	1:C:266:ALA:HB2	2.28	0.68
1:C:31:LEU:HD23	1:C:243:THR:HG22	1.75	0.68
1:C:224:VAL:HB	1:C:225:PRO:HD3	1.74	0.68
1:D:171:PHE:HA	1:D:249:MET:HB3	1.75	0.68
1:C:207:VAL:HG12	1:C:232:VAL:HG22	1.74	0.68
2:Q:63:LYS:HB2	2:Q:63:LYS:HZ2	1.58	0.68
3:S:40:TYR:HE2	3:S:93:GLN:HG2	1.59	0.68
1:B:54:LEU:O	1:B:58:MET:HG2	1.94	0.68
1:A:274:ALA:HA	1:A:275:GLY:C	2.19	0.68
1:C:430:ARG:HG2	1:D:377:HIS:CD2	2.29	0.68
1:D:74:TYR:OH	1:D:309:LEU:HD12	1.94	0.68
1:A:414:PHE:HD1	1:B:410:VAL:HG13	1.59	0.67
1:D:31:LEU:HD23	1:D:243:THR:HG22	1.76	0.67
1:D:31:LEU:HD12	1:D:32:PRO:HD3	1.73	0.67
1:D:134:TRP:HA	1:D:137:VAL:HG12	1.76	0.67
1:A:29:PHE:O	1:A:32:PRO:HD2	1.94	0.67
1:B:29:PHE:O	1:B:32:PRO:HD2	1.95	0.67
2:P:37:VAL:HG21	2:P:110:TRP:HZ3	1.58	0.67
3:S:150:VAL:O	3:S:151:LYS:HB2	1.94	0.67
1:C:79:ARG:HA	1:D:436:TYR:H	1.60	0.67
3:W:40:TYR:HE2	3:W:93:GLN:HG2	1.59	0.67
1:A:171:PHE:HA	1:A:249:MET:HB3	1.77	0.67
1:A:439:ASP:O	1:A:440:ALA:HB2	1.95	0.67
1:B:319:LYS:HD2	1:B:319:LYS:N	2.08	0.67
1:A:435:PRO:HB3	2:P:103:TYR:HB3	1.77	0.67
1:B:10:VAL:HB	1:B:218:LYS:HD3	1.76	0.67
2:P:47:TRP:CZ2	2:P:49:GLY:HA2	2.30	0.67
1:C:171:PHE:HA	1:C:249:MET:HB3	1.75	0.67
2:Q:47:TRP:CZ2	2:Q:49:GLY:HA2	2.30	0.66
1:A:249:MET:N	1:A:249:MET:HE3	2.10	0.66
1:B:171:PHE:HA	1:B:249:MET:HB3	1.77	0.66
1:B:249:MET:HE3	1:B:249:MET:N	2.11	0.66
1:B:145:LYS:O	1:B:149:ARG:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:TRP:HA	1:C:137:VAL:HG12	1.76	0.66
1:C:268:MET:O	1:C:269:ALA:HB2	1.95	0.66
1:C:116:PHE:HB3	1:C:118:ILE:H	1.61	0.66
2:Q:134:VAL:HG21	3:W:123:PRO:HD3	1.76	0.66
1:A:145:LYS:O	1:A:149:ARG:HG3	1.96	0.65
2:Q:83:LEU:HD21	2:P:199:THR:HG23	1.78	0.65
1:A:10:VAL:HB	1:A:218:LYS:HD3	1.76	0.65
1:A:38:THR:HG1	1:A:182:TRP:N	1.95	0.65
1:D:116:PHE:HB3	1:D:118:ILE:H	1.61	0.65
2:Q:134:VAL:CG2	3:W:123:PRO:HD3	2.26	0.65
2:P:37:VAL:HG21	2:P:110:TRP:CZ3	2.32	0.65
1:A:439:ASP:O	1:A:440:ALA:CB	2.45	0.65
1:C:432:HIS:HD2	1:C:434:ASN:HB2	1.62	0.65
1:B:38:THR:HG1	1:B:182:TRP:N	1.94	0.64
2:P:91:SER:HA	2:P:92:SER:CB	2.15	0.64
2:P:154:PRO:HB2	2:P:206:HIS:NE2	2.11	0.64
3:S:38:HIS:CE1	3:S:54:ASP:H	2.16	0.64
1:D:432:HIS:HD2	1:D:434:ASN:HB2	1.62	0.64
2:Q:154:PRO:HB2	2:Q:206:HIS:NE2	2.11	0.64
1:C:74:TYR:OH	1:C:309:LEU:HD12	1.97	0.64
3:S:53:TYR:O	3:S:57:LYS:HB2	1.98	0.64
1:D:140:ASN:OD1	1:D:147:ILE:HG12	1.98	0.64
1:A:224:VAL:HB	1:A:225:PRO:HD3	1.79	0.64
1:B:224:VAL:HB	1:B:225:PRO:HD3	1.80	0.64
2:P:130:PRO:HG3	2:P:215:LYS:HB3	1.79	0.64
3:W:19:VAL:HB	3:W:79:ILE:HG13	1.79	0.64
1:B:237:VAL:HG13	1:B:241:LEU:HD12	1.80	0.64
2:Q:37:VAL:HG21	2:Q:110:TRP:CZ3	2.32	0.64
1:A:69:SER:HB3	1:A:70:PRO:HD2	1.80	0.63
2:Q:130:PRO:HG3	2:Q:215:LYS:HB3	1.78	0.63
1:A:237:VAL:HG13	1:A:241:LEU:HD12	1.79	0.63
1:C:438:LEU:HG	1:D:375:LEU:HD12	1.78	0.63
1:B:262:PHE:CE1	1:B:266:ALA:HB2	2.33	0.63
1:C:346:ALA:C	1:C:348:LYS:HA	2.23	0.63
1:A:249:MET:HE3	1:A:249:MET:H	1.63	0.63
3:S:198:THR:HG23	3:S:213:SER:HB2	1.79	0.63
1:D:161:PRO:O	1:D:165:ILE:HG12	1.98	0.63
3:W:124:PRO:HB2	3:W:129:LEU:HD11	1.80	0.63
1:A:343:SER:HB2	1:A:344:PRO:CD	2.29	0.63
1:C:434:ASN:HD21	1:D:80:CYS:HA	1.64	0.63
2:Q:48:ILE:HD13	2:Q:80:TYR:OH	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:HB3	1:B:70:PRO:HD2	1.80	0.63
1:D:415:VAL:HA	1:D:418:MET:HG3	1.81	0.63
1:A:262:PHE:CE1	1:A:266:ALA:HB2	2.33	0.63
3:S:19:VAL:HB	3:S:79:ILE:HG13	1.81	0.63
1:C:54:LEU:O	1:C:58:MET:HG2	1.99	0.62
1:B:249:MET:HE3	1:B:249:MET:H	1.64	0.62
1:C:140:ASN:OD1	1:C:147:ILE:HG12	1.98	0.62
1:C:161:PRO:O	1:C:165:ILE:HG12	1.98	0.62
3:W:53:TYR:O	3:W:57:LYS:HB2	1.98	0.62
3:W:38:HIS:CE1	3:W:54:ASP:H	2.18	0.62
1:C:347:ALA:N	1:C:348:LYS:CA	2.59	0.62
2:Q:83:LEU:HD21	2:P:199:THR:CG2	2.30	0.62
3:S:124:PRO:HB2	3:S:129:LEU:HD11	1.80	0.62
3:W:198:THR:HG23	3:W:213:SER:HB2	1.80	0.62
1:C:415:VAL:HA	1:C:418:MET:HG3	1.82	0.62
1:D:435:PRO:HA	1:D:437:PRO:HD3	1.82	0.62
2:Q:10:GLU:CD	2:Q:11:LEU:HD23	2.25	0.62
1:D:54:LEU:O	1:D:58:MET:HG2	2.00	0.61
1:D:135:ILE:O	1:D:139:LEU:HG	2.00	0.61
1:C:63:MET:HB2	1:C:372:LEU:HD12	1.82	0.61
1:A:273:THR:O	1:A:274:ALA:CB	2.48	0.61
1:C:395:PHE:O	1:C:399:ILE:HG13	2.00	0.61
1:C:218:LYS:O	1:C:219:ASN:HB2	2.00	0.61
2:P:34:ILE:HG21	2:P:78:THR:HG21	1.83	0.61
2:Q:39:GLN:O	2:Q:92:SER:HB3	2.00	0.61
2:P:48:ILE:HD13	2:P:80:TYR:OH	2.01	0.61
1:A:267:ARG:HE	1:A:274:ALA:HB2	1.64	0.61
1:B:205:ILE:HG22	1:B:205:ILE:O	2.01	0.61
1:C:135:ILE:O	1:C:139:LEU:HG	2.00	0.61
2:Q:34:ILE:HG21	2:Q:78:THR:HG21	1.82	0.61
1:C:361:THR:HG22	1:C:365:TYR:HE2	1.66	0.60
1:D:218:LYS:O	1:D:219:ASN:HB2	2.00	0.60
1:D:395:PHE:O	1:D:399:ILE:HG13	2.00	0.60
2:Q:124:THR:H	2:Q:154:PRO:HD3	1.65	0.60
1:A:166:ALA:HA	1:A:167:VAL:C	2.26	0.60
1:B:166:ALA:HA	1:B:167:VAL:C	2.26	0.60
1:D:63:MET:HB2	1:D:372:LEU:HD12	1.82	0.60
3:S:110:ILE:HD12	3:S:110:ILE:H	1.67	0.60
1:A:205:ILE:O	1:A:205:ILE:HG22	2.01	0.60
1:A:384:ARG:HB3	1:A:385:PRO:HD3	1.83	0.60
2:P:101:GLY:CA	2:P:102:ASN:HB3	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:177:LEU:H	2:P:177:LEU:HD23	1.66	0.60
2:P:124:THR:H	2:P:154:PRO:HD3	1.65	0.60
1:B:142:VAL:O	1:B:142:VAL:CG1	2.49	0.60
2:P:63:LYS:HB2	2:P:67:LYS:HZ3	1.67	0.60
1:B:165:ILE:O	1:B:166:ALA:HB2	2.01	0.60
1:C:435:PRO:HA	1:C:437:PRO:HD3	1.83	0.60
2:Q:177:LEU:HD23	2:Q:177:LEU:H	1.67	0.60
1:A:142:VAL:O	1:A:142:VAL:CG1	2.49	0.60
1:A:170:TRP:C	1:A:249:MET:HE2	2.27	0.60
1:B:13:ILE:HG22	1:B:14:PRO:HD3	1.84	0.60
1:A:160:VAL:HB	1:A:161:PRO:HD3	1.84	0.60
1:A:435:PRO:HB3	2:P:103:TYR:CB	2.32	0.60
1:B:166:ALA:N	1:B:167:VAL:HB	2.17	0.60
1:B:170:TRP:N	1:B:249:MET:HE2	2.17	0.60
1:B:268:MET:HG3	1:B:269:ALA:N	2.17	0.60
2:Q:14:PRO:O	2:P:163:SER:HB2	2.02	0.60
1:B:170:TRP:C	1:B:249:MET:HE2	2.27	0.59
1:B:384:ARG:HB3	1:B:385:PRO:HD3	1.83	0.59
1:D:269:ALA:O	1:D:270:LEU:C	2.44	0.59
1:D:361:THR:HG22	1:D:365:TYR:HE2	1.66	0.59
1:A:251:PRO:HB2	1:A:257:VAL:HG22	1.84	0.59
1:C:216:VAL:HG12	1:C:217:VAL:H	1.68	0.59
1:A:268:MET:HG3	1:A:269:ALA:N	2.17	0.59
1:D:364:PRO:O	1:D:368:THR:HG23	2.03	0.59
1:A:31:LEU:HB2	1:A:32:PRO:HD3	1.85	0.59
1:B:251:PRO:HB2	1:B:257:VAL:HG22	1.84	0.59
1:C:80:CYS:HA	1:D:434:ASN:ND2	2.17	0.59
2:Q:40:ARG:HB3	2:Q:41:PRO:HD2	1.84	0.59
2:P:40:ARG:HB3	2:P:41:PRO:HD2	1.84	0.59
3:W:110:ILE:HD12	3:W:110:ILE:H	1.68	0.59
2:Q:8:GLY:N	2:Q:9:PRO:CD	2.66	0.59
3:S:85:GLU:CD	3:S:85:GLU:H	2.11	0.59
1:A:13:ILE:HG22	1:A:14:PRO:HD3	1.85	0.58
1:B:16:THR:HG22	1:B:227:ALA:HA	1.85	0.58
1:B:160:VAL:HB	1:B:161:PRO:HD3	1.85	0.58
1:B:246:ILE:C	1:B:248:GLY:H	2.11	0.58
3:W:85:GLU:CD	3:W:85:GLU:H	2.10	0.58
1:A:165:ILE:O	1:A:166:ALA:HB2	2.01	0.58
1:C:43:ILE:HG12	1:C:244:THR:HG22	1.86	0.58
2:Q:18:VAL:HG23	2:Q:82:GLN:HB2	1.86	0.58
1:A:113:SER:HB2	1:A:119:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:PRO:HG3	2:Q:103:TYR:HD1	1.68	0.58
2:P:29:PHE:O	2:P:53:PRO:HG2	2.03	0.58
1:D:43:ILE:HG12	1:D:244:THR:HG22	1.86	0.58
1:A:170:TRP:N	1:A:249:MET:HE2	2.18	0.58
1:C:364:PRO:O	1:C:368:THR:HG23	2.04	0.58
1:C:377:HIS:HD2	1:D:430:ARG:HG2	1.62	0.58
2:Q:29:PHE:O	2:Q:53:PRO:HG2	2.03	0.58
3:S:156:ASP:HA	3:S:196:SER:HB3	1.86	0.58
1:A:246:ILE:C	1:A:248:GLY:H	2.11	0.58
1:B:31:LEU:HB2	1:B:32:PRO:HD3	1.85	0.58
1:D:10:VAL:HG22	1:D:145:LYS:HE3	1.84	0.58
1:D:216:VAL:HG12	1:D:217:VAL:H	1.67	0.57
3:S:30:ASN:O	3:S:36:TYR:HB2	2.03	0.57
1:A:219:ASN:N	1:A:220:PRO:HD3	2.19	0.57
1:A:374:LEU:HD21	1:B:425:ALA:HA	1.86	0.57
2:Q:47:TRP:CE3	3:W:100:PRO:HD2	2.39	0.57
2:P:150:LYS:HZ2	3:S:185:THR:HG21	1.68	0.57
1:A:274:ALA:HA	1:A:275:GLY:O	2.04	0.57
1:B:105:VAL:HG13	1:B:290:LEU:HD11	1.87	0.57
1:C:417:LEU:O	1:C:421:THR:HG23	2.04	0.57
2:P:11:LEU:HD13	2:P:117:THR:HB	1.86	0.57
1:A:31:LEU:O	1:A:35:LEU:HG	2.05	0.57
1:B:50:ILE:O	1:B:54:LEU:HB2	2.05	0.57
2:P:37:VAL:HG12	2:P:47:TRP:HA	1.86	0.57
1:A:16:THR:HG22	1:A:227:ALA:HA	1.86	0.57
3:W:4:MET:HB2	3:W:103:GLY:HA2	1.87	0.57
1:B:339:PHE:O	1:B:344:PRO:HD2	2.04	0.57
2:Q:37:VAL:HG12	2:Q:47:TRP:HA	1.85	0.57
3:W:156:ASP:HA	3:W:196:SER:HB3	1.86	0.57
1:B:113:SER:HB2	1:B:119:LEU:O	2.04	0.57
2:Q:24:ALA:HB1	2:Q:27:TYR:CE1	2.37	0.57
1:A:79:ARG:HB2	1:A:375:LEU:HD11	1.86	0.57
1:A:166:ALA:N	1:A:167:VAL:HB	2.17	0.57
1:D:417:LEU:O	1:D:421:THR:HG23	2.04	0.56
2:P:101:GLY:HA2	2:P:102:ASN:CB	2.19	0.56
3:W:151:LYS:O	3:W:151:LYS:HG2	2.04	0.56
1:A:31:LEU:CD1	1:A:246:ILE:HD12	2.36	0.56
1:A:71:GLY:O	1:A:212:VAL:HA	2.06	0.56
2:P:60:TYR:HD2	2:P:61:ASN:N	2.03	0.56
3:W:30:ASN:O	3:W:36:TYR:HB2	2.05	0.56
1:A:105:VAL:HG13	1:A:290:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:O	1:B:35:LEU:HG	2.05	0.56
1:C:118:ILE:HG22	1:C:119:LEU:HG	1.88	0.56
1:D:23:ILE:HG12	1:D:206:GLY:HA3	1.87	0.56
3:W:2:LEU:HD12	3:W:97:TYR:HD2	1.70	0.56
3:S:4:MET:HB2	3:S:103:GLY:HA2	1.87	0.56
1:B:219:ASN:N	1:B:220:PRO:HD3	2.19	0.56
1:C:436:TYR:H	1:D:79:ARG:HA	1.70	0.56
1:A:50:ILE:O	1:A:54:LEU:HB2	2.06	0.56
1:A:313:ILE:H	1:A:313:ILE:CD1	2.16	0.56
1:A:362:LEU:HD23	1:A:365:TYR:HD2	1.70	0.56
1:A:414:PHE:CD1	1:B:410:VAL:HG13	2.41	0.56
1:B:345:ASN:O	1:B:346:ALA:HB2	2.05	0.56
1:C:433:LYS:O	1:C:435:PRO:HD3	2.05	0.56
1:D:262:PHE:CG	1:D:263:GLY:N	2.73	0.56
2:P:45:LEU:HD12	2:P:45:LEU:H	1.71	0.56
2:P:48:ILE:HA	2:P:63:LYS:HZ3	1.69	0.56
1:A:313:ILE:HD12	1:A:313:ILE:N	2.19	0.56
1:C:383:ALA:HB1	1:C:386:LEU:HB3	1.88	0.56
2:Q:47:TRP:O	2:Q:60:TYR:HD1	1.88	0.56
3:S:140:LEU:H	3:S:140:LEU:HD12	1.69	0.56
1:C:262:PHE:CG	1:C:263:GLY:N	2.72	0.56
1:C:267:ARG:HA	1:C:272:ASP:HB3	1.88	0.56
1:A:62:LYS:HG3	1:A:372:LEU:HD11	1.88	0.56
1:B:79:ARG:HB2	1:B:375:LEU:HD11	1.87	0.56
2:Q:47:TRP:O	2:Q:60:TYR:CD1	2.59	0.56
2:Q:63:LYS:HB2	2:Q:67:LYS:HZ3	1.71	0.56
3:S:51:TRP:CZ3	3:S:62:VAL:HG13	2.41	0.56
1:A:102:ILE:HG22	1:A:338:GLN:OE1	2.06	0.55
1:C:72:GLY:H	1:C:75:ALA:H	1.54	0.55
1:C:330:VAL:HG12	1:C:334:MET:HE2	1.88	0.55
2:P:18:VAL:HG12	2:P:82:GLN:HB2	1.87	0.55
3:S:2:LEU:HD12	3:S:97:TYR:HD2	1.70	0.55
3:S:94:GLN:HG2	3:S:95:TRP:N	2.21	0.55
1:A:440:ALA:N	1:A:441:PRO:HD2	2.21	0.55
1:B:102:ILE:HG22	1:B:338:GLN:OE1	2.06	0.55
1:B:39:GLY:CA	1:B:247:MET:HG3	2.32	0.55
1:C:23:ILE:HG12	1:C:206:GLY:HA3	1.87	0.55
1:D:267:ARG:NH1	1:D:277:ILE:H	2.04	0.55
1:D:330:VAL:HG12	1:D:334:MET:HE2	1.88	0.55
2:P:36:TRP:O	2:P:48:ILE:HB	2.06	0.55
2:P:153:PHE:H	2:P:154:PRO:CD	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:87:ALA:HB2	3:W:110:ILE:HG13	1.88	0.55
1:B:220:PRO:C	1:B:222:ARG:H	2.15	0.55
1:C:62:LYS:HB3	1:C:372:LEU:HD11	1.88	0.55
1:D:433:LYS:O	1:D:435:PRO:HD3	2.06	0.55
2:Q:60:TYR:HD2	2:Q:61:ASN:N	2.05	0.55
2:Q:153:PHE:H	2:Q:154:PRO:CD	2.20	0.55
1:C:384:ARG:HB3	1:C:385:PRO:HD3	1.88	0.55
3:W:140:LEU:HD12	3:W:140:LEU:H	1.70	0.55
1:A:12:LEU:HB2	1:A:223:ASN:OD1	2.06	0.55
1:B:71:GLY:O	1:B:212:VAL:HA	2.07	0.55
1:D:69:SER:C	1:D:71:GLY:HA3	2.31	0.55
2:Q:101:GLY:CA	2:Q:102:ASN:HB3	2.25	0.55
1:B:12:LEU:HB2	1:B:223:ASN:OD1	2.07	0.55
1:B:62:LYS:HG3	1:B:372:LEU:HD11	1.89	0.55
1:C:69:SER:C	1:C:71:GLY:HA3	2.32	0.55
1:D:10:VAL:HA	1:D:217:VAL:O	2.06	0.55
1:D:377:HIS:HD1	1:D:378:GLY:N	2.05	0.55
2:Q:36:TRP:O	2:Q:48:ILE:HB	2.06	0.55
2:Q:48:ILE:HG21	2:Q:80:TYR:OH	2.07	0.55
2:P:92:SER:O	2:P:93:VAL:C	2.49	0.55
1:A:161:PRO:O	1:A:165:ILE:HG12	2.07	0.55
1:B:31:LEU:CD1	1:B:246:ILE:HD12	2.36	0.55
2:P:47:TRP:O	2:P:60:TYR:HD1	1.90	0.55
2:P:150:LYS:HZ3	3:S:185:THR:HG21	1.71	0.55
1:B:161:PRO:O	1:B:165:ILE:HG12	2.06	0.55
1:B:437:PRO:HG2	2:P:32:TYR:CZ	2.42	0.55
2:Q:45:LEU:HD12	2:Q:45:LEU:H	1.70	0.55
2:P:37:VAL:HG23	2:P:95:PHE:HB2	1.87	0.55
1:B:216:VAL:HG12	1:B:217:VAL:N	2.20	0.54
1:D:296:LEU:O	1:D:300:THR:HG22	2.07	0.54
3:W:94:GLN:HG2	3:W:95:TRP:N	2.23	0.54
3:S:87:ALA:HB2	3:S:110:ILE:HG13	1.88	0.54
1:B:362:LEU:HD23	1:B:365:TYR:HD2	1.71	0.54
1:C:37:ALA:O	1:C:184:VAL:HA	2.07	0.54
1:C:267:ARG:NH1	1:C:277:ILE:H	2.04	0.54
1:D:116:PHE:HB3	1:D:118:ILE:N	2.22	0.54
1:D:267:ARG:HA	1:D:272:ASP:HB3	1.88	0.54
2:Q:37:VAL:HG23	2:Q:95:PHE:HB2	1.88	0.54
3:W:38:HIS:HB2	3:W:93:GLN:HG3	1.89	0.54
1:D:118:ILE:HG22	1:D:119:LEU:HG	1.88	0.54
1:D:324:VAL:HG12	1:D:326:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:150:VAL:CG2	3:W:151:LYS:HA	2.37	0.54
3:S:36:TYR:HA	3:S:55:THR:OG1	2.07	0.54
3:S:38:HIS:HB2	3:S:93:GLN:HG3	1.88	0.54
1:D:78:ARG:HA	1:D:82:GLY:O	2.08	0.54
1:A:439:ASP:O	3:S:97:TYR:HB3	2.08	0.54
1:C:38:THR:HG23	1:C:42:ALA:HB2	1.89	0.54
1:C:343:SER:HB2	1:C:344:PRO:HD3	1.88	0.54
1:A:216:VAL:HG12	1:A:217:VAL:N	2.20	0.54
1:D:354:SER:C	1:D:356:VAL:H	2.16	0.54
2:Q:90:ASN:CB	2:Q:118:VAL:HG12	2.34	0.54
3:S:95:TRP:CH2	3:S:100:PRO:HD3	2.42	0.54
1:A:296:LEU:O	1:A:300:THR:HG22	2.08	0.54
1:C:116:PHE:HB3	1:C:118:ILE:N	2.22	0.54
1:B:135:ILE:O	1:B:139:LEU:HG	2.08	0.54
1:D:37:ALA:O	1:D:184:VAL:HA	2.07	0.54
1:A:273:THR:O	1:A:274:ALA:HB2	2.08	0.54
1:D:62:LYS:HB3	1:D:372:LEU:HD11	1.89	0.54
1:D:72:GLY:H	1:D:75:ALA:H	1.54	0.54
1:D:122:PRO:C	1:D:124:VAL:H	2.16	0.54
1:D:292:GLY:O	1:D:296:LEU:HG	2.08	0.54
1:B:313:ILE:H	1:B:313:ILE:CD1	2.16	0.53
1:C:274:ALA:HB1	1:C:275:GLY:HA2	1.90	0.53
2:Q:118:VAL:HG13	2:Q:118:VAL:O	2.08	0.53
2:P:118:VAL:HG13	2:P:118:VAL:O	2.08	0.53
1:C:296:LEU:O	1:C:300:THR:HG22	2.08	0.53
1:D:384:ARG:HB3	1:D:385:PRO:HD3	1.90	0.53
2:P:38:LYS:HB2	2:P:48:ILE:HD11	1.89	0.53
2:P:48:ILE:HG21	2:P:80:TYR:OH	2.08	0.53
1:A:289:SER:O	1:A:293:TRP:HD1	1.91	0.53
1:D:38:THR:HG23	1:D:42:ALA:HB2	1.89	0.53
2:P:47:TRP:O	2:P:60:TYR:CD1	2.61	0.53
1:A:220:PRO:C	1:A:222:ARG:H	2.15	0.53
3:W:36:TYR:HA	3:W:55:THR:OG1	2.07	0.53
1:C:78:ARG:HA	1:C:82:GLY:O	2.08	0.53
1:D:219:ASN:N	1:D:220:PRO:CD	2.70	0.53
1:D:277:ILE:O	1:D:280:PHE:HB2	2.08	0.53
2:Q:38:LYS:HB2	2:Q:48:ILE:HD11	1.90	0.53
1:A:135:ILE:O	1:A:139:LEU:HG	2.08	0.53
2:P:24:ALA:HB1	2:P:27:TYR:CE1	2.38	0.53
1:B:289:SER:O	1:B:293:TRP:HD1	1.91	0.53
1:B:313:ILE:HD12	1:B:313:ILE:N	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:45:LEU:HD12	2:Q:45:LEU:N	2.24	0.53
1:D:274:ALA:HB1	1:D:275:GLY:HA2	1.90	0.53
3:S:82:MET:SD	3:S:108:LEU:HD21	2.49	0.53
1:A:205:ILE:CG2	1:A:361:THR:HG21	2.39	0.53
1:B:80:CYS:SG	1:B:374:LEU:HD12	2.49	0.53
1:B:205:ILE:CG2	1:B:361:THR:HG21	2.39	0.53
3:W:51:TRP:CZ3	3:W:62:VAL:HG13	2.44	0.53
3:W:151:LYS:C	3:W:152:TRP:CG	2.85	0.53
1:D:160:VAL:N	1:D:161:PRO:HD2	2.24	0.52
1:B:117:PRO:O	1:B:118:ILE:C	2.53	0.52
1:B:346:ALA:CB	1:B:347:ALA:CA	2.67	0.52
1:B:377:HIS:CE1	3:S:30:ASN:HD21	2.28	0.52
1:C:277:ILE:O	1:C:280:PHE:HB2	2.08	0.52
1:C:346:ALA:H	1:C:347:ALA:C	2.17	0.52
1:A:216:VAL:HG23	1:A:299:GLN:NE2	2.24	0.52
1:B:207:VAL:HG23	1:B:365:TYR:CE1	2.45	0.52
1:D:399:ILE:O	1:D:403:ILE:HG13	2.09	0.52
2:P:12:VAL:HG12	2:P:13:LYS:N	2.25	0.52
1:B:59:VAL:HG22	1:B:391:THR:HG22	1.91	0.52
1:B:116:PHE:HB3	1:B:118:ILE:H	1.75	0.52
2:Q:63:LYS:HZ3	2:Q:67:LYS:NZ	2.08	0.52
1:A:262:PHE:HE1	1:A:266:ALA:HB2	1.74	0.52
1:B:262:PHE:HE1	1:B:266:ALA:HB2	1.74	0.52
1:C:19:VAL:O	1:C:23:ILE:HG13	2.09	0.52
1:D:63:MET:HE1	1:D:375:LEU:HG	1.90	0.52
2:Q:150:LYS:NZ	3:W:185:THR:HG21	2.24	0.52
1:A:117:PRO:O	1:A:118:ILE:C	2.53	0.52
1:A:308:GLY:O	1:A:428:TYR:HE1	1.91	0.52
1:B:296:LEU:O	1:B:300:THR:HG22	2.09	0.52
1:C:122:PRO:C	1:C:124:VAL:H	2.16	0.52
1:C:292:GLY:O	1:C:296:LEU:HG	2.08	0.52
1:D:19:VAL:O	1:D:23:ILE:HG13	2.10	0.52
1:D:71:GLY:O	1:D:212:VAL:HA	2.09	0.52
1:B:87:TYR:O	1:B:91:VAL:HG23	2.10	0.52
1:C:130:VAL:O	1:C:134:TRP:HD1	1.93	0.52
2:P:45:LEU:HD12	2:P:45:LEU:N	2.25	0.52
1:A:116:PHE:HB3	1:A:118:ILE:H	1.75	0.52
1:D:145:LYS:O	1:D:149:ARG:HG3	2.10	0.52
2:P:153:PHE:N	2:P:154:PRO:CD	2.73	0.52
1:A:80:CYS:SG	1:A:374:LEU:HD12	2.50	0.52
1:A:87:TYR:O	1:A:91:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLY:O	1:B:428:TYR:HE1	1.92	0.52
1:C:307:ASP:C	1:C:309:LEU:H	2.18	0.52
2:Q:2:VAL:HB	2:Q:109:TYR:CD1	2.45	0.52
3:W:23:CYS:HB2	3:W:39:TRP:CH2	2.45	0.52
1:C:71:GLY:O	1:C:212:VAL:HA	2.10	0.51
1:C:160:VAL:N	1:C:161:PRO:HD2	2.24	0.51
1:C:219:ASN:N	1:C:220:PRO:CD	2.70	0.51
1:D:307:ASP:C	1:D:309:LEU:H	2.17	0.51
3:S:151:LYS:CB	3:S:200:GLU:HB2	2.40	0.51
1:A:59:VAL:HG22	1:A:391:THR:HG22	1.92	0.51
1:A:119:LEU:HB3	1:A:124:VAL:HG11	1.92	0.51
1:D:207:VAL:C	1:D:209:SER:H	2.18	0.51
1:B:43:ILE:C	1:B:45:GLY:H	2.19	0.51
1:C:92:LEU:HD11	1:C:417:LEU:HD21	1.93	0.51
1:C:145:LYS:O	1:C:149:ARG:HG3	2.11	0.51
2:Q:50:TRP:O	2:Q:57:SER:HB2	2.10	0.51
3:W:155:ILE:HA	3:W:196:SER:O	2.10	0.51
3:S:197:TYR:HB2	3:S:214:PHE:CE2	2.44	0.51
1:A:207:VAL:HG23	1:A:365:TYR:CE1	2.46	0.51
1:B:216:VAL:HG23	1:B:299:GLN:NE2	2.25	0.51
3:W:197:TYR:HB2	3:W:214:PHE:CE2	2.45	0.51
1:C:41:ILE:HG22	1:C:41:ILE:O	2.11	0.51
1:C:147:ILE:HD12	1:C:148:THR:N	2.25	0.51
2:Q:153:PHE:N	2:Q:154:PRO:CD	2.73	0.51
1:A:267:ARG:HB3	1:A:272:ASP:HB2	1.92	0.51
1:C:395:PHE:CE2	1:D:422:ALA:HA	2.45	0.51
1:C:399:ILE:O	1:C:403:ILE:HG13	2.09	0.51
2:Q:9:PRO:CB	2:Q:10:GLU:HB2	2.35	0.51
1:D:308:GLY:O	1:D:428:TYR:HE1	1.94	0.51
2:Q:4:LEU:O	2:Q:111:GLY:HA2	2.11	0.51
2:Q:48:ILE:HG23	2:Q:67:LYS:HZ2	1.75	0.51
3:W:150:VAL:CB	3:W:151:LYS:HA	2.41	0.51
1:C:63:MET:HE1	1:C:375:LEU:HG	1.91	0.51
2:P:12:VAL:N	2:P:117:THR:O	2.43	0.51
3:S:155:ILE:HA	3:S:196:SER:O	2.11	0.51
1:B:159:LEU:HD11	1:B:238:CYS:SG	2.51	0.51
2:Q:150:LYS:HZ3	3:W:185:THR:HG21	1.75	0.51
2:P:47:TRP:CE3	3:S:100:PRO:HD2	2.46	0.51
2:P:66:GLY:HA2	2:P:83:LEU:HB3	1.93	0.51
2:Q:63:LYS:HD2	2:Q:67:LYS:HZ3	1.76	0.50
2:P:150:LYS:HG3	2:P:183:THR:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TYR:CE1	1:B:424:TYR:HB2	2.46	0.50
1:C:308:GLY:O	1:C:428:TYR:HE1	1.94	0.50
1:C:382:LYS:C	1:C:384:ARG:H	2.18	0.50
1:D:92:LEU:HD11	1:D:417:LEU:HD21	1.93	0.50
3:W:200:GLU:HG2	3:W:211:VAL:HG23	1.93	0.50
1:D:41:ILE:O	1:D:41:ILE:HG22	2.11	0.50
1:D:219:ASN:H	1:D:220:PRO:HD3	1.76	0.50
1:D:427:ASN:C	1:D:429:ASN:H	2.19	0.50
1:A:87:TYR:CE1	1:A:424:TYR:HB2	2.45	0.50
1:A:274:ALA:CA	1:A:275:GLY:C	2.84	0.50
1:C:251:PRO:HB2	1:C:257:VAL:HG22	1.94	0.50
1:D:147:ILE:HD12	1:D:148:THR:N	2.26	0.50
2:P:2:VAL:HB	2:P:109:TYR:CD1	2.46	0.50
2:P:4:LEU:O	2:P:111:GLY:HA2	2.12	0.50
2:P:187:SER:HB3	3:S:139:PHE:CE2	2.47	0.50
1:A:287:LEU:O	1:A:290:LEU:HB2	2.11	0.50
1:A:309:LEU:O	1:A:310:PHE:CB	2.60	0.50
2:Q:150:LYS:HG3	2:Q:183:THR:HB	1.94	0.50
2:P:135:CYS:SG	3:S:214:PHE:HB2	2.51	0.50
3:S:200:GLU:HG2	3:S:211:VAL:HG23	1.94	0.50
1:A:134:TRP:O	1:A:138:LEU:HG	2.12	0.50
1:B:119:LEU:HB3	1:B:124:VAL:HG11	1.92	0.50
1:B:343:SER:CB	1:B:344:PRO:HD3	2.36	0.50
1:D:313:ILE:H	1:D:313:ILE:CD1	2.21	0.50
2:P:144:THR:O	3:S:122:PHE:HZ	1.94	0.50
1:A:134:TRP:HE1	1:A:335:THR:CG2	2.20	0.50
1:A:166:ALA:HA	1:A:167:VAL:O	2.12	0.50
1:C:121:ASP:HB3	1:C:122:PRO:CD	2.42	0.50
1:D:222:ARG:O	1:D:226:ILE:HG13	2.12	0.50
1:A:37:ALA:O	1:A:38:THR:HG22	2.12	0.50
1:A:43:ILE:C	1:A:45:GLY:H	2.19	0.50
1:B:63:MET:HE2	1:B:76:TYR:HB3	1.93	0.50
1:B:287:LEU:O	1:B:290:LEU:HB2	2.11	0.50
1:D:436:TYR:N	1:D:436:TYR:CD2	2.80	0.50
2:P:50:TRP:O	2:P:57:SER:HB2	2.12	0.50
1:A:159:LEU:HD11	1:A:238:CYS:SG	2.52	0.50
1:A:246:ILE:O	1:A:251:PRO:HD2	2.12	0.50
1:D:251:PRO:HB2	1:D:257:VAL:HG22	1.94	0.50
2:Q:63:LYS:CB	2:Q:67:LYS:HZ3	2.24	0.50
2:Q:66:GLY:HA2	2:Q:83:LEU:HB3	1.93	0.50
2:Q:134:VAL:HG12	2:Q:135:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:51:TRP:HZ3	3:W:66:PHE:CD2	2.30	0.50
3:W:95:TRP:CH2	3:W:100:PRO:HD3	2.46	0.50
3:S:23:CYS:HB2	3:S:39:TRP:CH2	2.47	0.50
1:A:39:GLY:CA	1:A:247:MET:HG3	2.33	0.49
1:A:63:MET:HE2	1:A:76:TYR:HB3	1.94	0.49
1:D:130:VAL:O	1:D:134:TRP:HD1	1.93	0.49
2:P:158:THR:HB	2:P:205:ALA:HB3	1.94	0.49
1:A:216:VAL:C	1:A:218:LYS:H	2.20	0.49
1:A:430:ARG:HG2	1:B:377:HIS:ND1	2.27	0.49
1:B:363:VAL:N	1:B:364:PRO:HD2	2.27	0.49
1:C:418:MET:HE2	1:D:399:ILE:HA	1.93	0.49
1:D:81:PHE:HB3	1:D:85:LEU:HD12	1.94	0.49
1:D:111:TYR:HB3	1:D:283:ALA:HB2	1.94	0.49
1:B:37:ALA:O	1:B:38:THR:HG22	2.12	0.49
1:B:166:ALA:HA	1:B:167:VAL:O	2.12	0.49
2:Q:48:ILE:HA	2:Q:63:LYS:HZ3	1.76	0.49
2:P:11:LEU:CD1	2:P:117:THR:HB	2.42	0.49
2:P:60:TYR:C	2:P:60:TYR:CD2	2.91	0.49
2:P:63:LYS:NZ	2:P:67:LYS:HZ3	2.10	0.49
1:A:57:SER:HB3	1:A:232:VAL:HG21	1.94	0.49
1:A:159:LEU:O	1:A:163:VAL:HG12	2.13	0.49
1:D:69:SER:O	1:D:71:GLY:HA3	2.12	0.49
3:S:198:THR:CG2	3:S:213:SER:HB2	2.42	0.49
1:B:159:LEU:O	1:B:163:VAL:HG12	2.13	0.49
1:B:216:VAL:C	1:B:218:LYS:H	2.20	0.49
1:B:250:ILE:HG23	1:B:269:ALA:HB3	1.94	0.49
1:C:69:SER:O	1:C:71:GLY:HA3	2.13	0.49
1:C:111:TYR:HB3	1:C:283:ALA:HB2	1.94	0.49
1:C:339:PHE:O	1:C:344:PRO:HD2	2.12	0.49
1:A:363:VAL:N	1:A:364:PRO:HD2	2.27	0.49
1:B:309:LEU:O	1:B:310:PHE:CB	2.60	0.49
1:B:339:PHE:O	1:B:344:PRO:CD	2.60	0.49
1:D:121:ASP:HB3	1:D:122:PRO:CD	2.43	0.49
1:D:357:SER:O	1:D:360:PHE:HB2	2.11	0.49
1:D:377:HIS:HD1	1:D:378:GLY:H	1.60	0.49
2:P:30:THR:HG22	2:P:53:PRO:HB2	1.94	0.49
3:S:146:LYS:HE2	3:S:178:TYR:CE2	2.47	0.49
1:C:268:MET:O	1:C:269:ALA:CB	2.59	0.49
1:C:313:ILE:H	1:C:313:ILE:CD1	2.21	0.49
1:D:433:LYS:HE2	2:Q:52:TYR:CG	2.48	0.49
2:P:60:TYR:HD2	2:P:60:TYR:C	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:112:ARG:HD3	3:W:113:ALA:O	2.13	0.49
3:W:140:LEU:HD12	3:W:140:LEU:N	2.28	0.49
2:P:67:LYS:HB2	2:P:80:TYR:HE1	1.77	0.49
1:A:140:ASN:HD22	1:A:327:LEU:HD11	1.78	0.49
1:C:207:VAL:C	1:C:209:SER:H	2.19	0.49
1:C:429:ASN:OD1	1:C:430:ARG:HG3	2.13	0.49
3:W:149:ASN:ND2	3:W:151:LYS:HE2	2.28	0.49
1:A:250:ILE:HG23	1:A:269:ALA:HB3	1.94	0.49
1:B:57:SER:HB3	1:B:232:VAL:HG21	1.94	0.49
2:Q:30:THR:HG22	2:Q:53:PRO:HB2	1.95	0.49
2:Q:67:LYS:HB2	2:Q:80:TYR:HE1	1.77	0.49
2:P:90:ASN:CB	2:P:118:VAL:HG12	2.34	0.49
1:A:131:ALA:O	1:A:135:ILE:HG13	2.13	0.48
1:B:131:ALA:O	1:B:135:ILE:HG13	2.12	0.48
1:B:141:ILE:HD12	1:B:328:LEU:HD21	1.95	0.48
1:C:222:ARG:O	1:C:226:ILE:HG13	2.13	0.48
1:C:357:SER:O	1:C:360:PHE:HB2	2.12	0.48
1:C:436:TYR:N	1:C:436:TYR:CD2	2.81	0.48
1:D:159:LEU:O	1:D:163:VAL:HG12	2.13	0.48
3:W:146:LYS:HE2	3:W:178:TYR:CE2	2.48	0.48
3:S:144:TYR:CG	3:S:145:PRO:HA	2.48	0.48
1:A:147:ILE:HD11	1:A:291:GLY:C	2.38	0.48
1:A:330:VAL:HG12	1:A:334:MET:HE2	1.95	0.48
1:A:436:TYR:HE2	2:P:103:TYR:HE2	1.60	0.48
1:B:147:ILE:HD11	1:B:291:GLY:C	2.38	0.48
1:C:159:LEU:O	1:C:163:VAL:HG12	2.13	0.48
2:Q:92:SER:O	2:Q:93:VAL:CB	2.59	0.48
3:S:140:LEU:HD12	3:S:140:LEU:N	2.27	0.48
1:A:249:MET:H	1:A:249:MET:CE	2.26	0.48
1:B:140:ASN:HD22	1:B:327:LEU:HD11	1.78	0.48
1:C:343:SER:HB2	1:C:344:PRO:CD	2.42	0.48
2:Q:27:TYR:CE2	2:Q:98:ARG:HD2	2.48	0.48
2:Q:106:TRP:HB3	3:W:38:HIS:CE1	2.48	0.48
1:B:140:ASN:HD21	1:B:295:LEU:HA	1.78	0.48
3:W:82:MET:SD	3:W:108:LEU:HD21	2.52	0.48
3:W:198:THR:CG2	3:W:213:SER:HB2	2.43	0.48
3:S:166:ASN:HB3	3:S:180:MET:HE2	1.95	0.48
1:A:60:TYR:CE1	1:A:208:GLU:HB3	2.48	0.48
1:A:410:VAL:HG13	1:B:414:PHE:HD1	1.78	0.48
1:B:101:ASN:ND2	1:B:294:THR:HG23	2.29	0.48
1:B:246:ILE:O	1:B:251:PRO:HD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:VAL:HG22	1:C:391:THR:HG22	1.95	0.48
2:Q:131:LEU:HB2	2:Q:146:GLY:C	2.38	0.48
2:Q:158:THR:HB	2:Q:205:ALA:HB3	1.95	0.48
3:W:54:ASP:HB2	3:W:57:LYS:HD3	1.96	0.48
1:B:31:LEU:CB	1:B:32:PRO:HD3	2.43	0.48
1:D:110:GLY:O	1:D:114:TYR:HB2	2.13	0.48
2:Q:60:TYR:C	2:Q:60:TYR:CD2	2.92	0.48
3:S:51:TRP:HZ3	3:S:66:PHE:CD2	2.31	0.48
3:S:146:LYS:HE2	3:S:178:TYR:HE2	1.79	0.48
1:A:325:ALA:C	1:A:327:LEU:H	2.22	0.48
2:P:63:LYS:CB	2:P:67:LYS:HZ3	2.25	0.48
2:P:131:LEU:HB2	2:P:146:GLY:C	2.39	0.48
1:A:140:ASN:HD21	1:A:295:LEU:HA	1.79	0.48
1:A:169:GLY:HA2	1:A:170:TRP:HA	1.65	0.48
1:A:381:GLY:HA3	1:A:383:ALA:H	1.79	0.48
1:B:134:TRP:O	1:B:138:LEU:HG	2.12	0.48
1:D:59:VAL:HG22	1:D:391:THR:HG22	1.95	0.48
1:D:429:ASN:OD1	1:D:430:ARG:HG3	2.14	0.48
2:P:27:TYR:CE2	2:P:98:ARG:HD2	2.48	0.48
3:W:144:TYR:CG	3:W:145:PRO:HA	2.48	0.48
1:A:70:PRO:N	1:A:71:GLY:HA3	2.29	0.48
1:D:32:PRO:HG3	1:D:262:PHE:HB2	1.95	0.48
1:D:117:PRO:O	1:D:118:ILE:C	2.57	0.48
1:C:35:LEU:HA	1:C:38:THR:O	2.14	0.48
1:D:435:PRO:HG3	2:Q:103:TYR:CD1	2.49	0.48
2:Q:60:TYR:HD2	2:Q:60:TYR:C	2.22	0.48
2:P:152:TYR:CE1	2:P:182:TYR:HB2	2.49	0.48
3:S:20:THR:HG23	3:S:78:THR:HG22	1.96	0.48
1:A:433:LYS:O	1:A:435:PRO:HD3	2.14	0.47
1:B:73:SER:HB3	1:B:74:TYR:H	1.59	0.47
1:B:165:ILE:O	1:B:166:ALA:CB	2.62	0.47
1:C:141:ILE:HG23	1:C:141:ILE:O	2.14	0.47
1:D:141:ILE:HG23	1:D:141:ILE:O	2.14	0.47
2:P:61:ASN:O	2:P:62:GLU:C	2.57	0.47
2:P:134:VAL:O	2:P:135:CYS:HB2	2.13	0.47
3:S:54:ASP:HB2	3:S:57:LYS:HD3	1.96	0.47
3:S:112:ARG:HD3	3:S:113:ALA:O	2.14	0.47
1:A:165:ILE:O	1:A:166:ALA:CB	2.62	0.47
1:B:246:ILE:C	1:B:248:GLY:N	2.72	0.47
2:Q:60:TYR:CE2	3:W:99:PRO:HG2	2.49	0.47
1:A:101:ASN:ND2	1:A:294:THR:HG23	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD12	1:A:328:LEU:HD21	1.96	0.47
1:B:130:VAL:HG13	1:B:335:THR:HG22	1.96	0.47
1:C:399:ILE:HA	1:D:418:MET:HE2	1.96	0.47
2:Q:119:SER:HB3	2:Q:153:PHE:CZ	2.49	0.47
2:Q:152:TYR:CE1	2:Q:182:TYR:HB2	2.49	0.47
1:A:268:MET:HG3	1:A:269:ALA:H	1.79	0.47
1:B:10:VAL:HA	1:B:11:GLY:HA2	1.61	0.47
1:B:70:PRO:N	1:B:71:GLY:HA3	2.29	0.47
1:C:427:ASN:C	1:C:429:ASN:H	2.21	0.47
2:Q:10:GLU:HG2	2:Q:11:LEU:CD2	2.37	0.47
1:C:32:PRO:HG3	1:C:262:PHE:HB2	1.95	0.47
1:D:134:TRP:HA	1:D:137:VAL:CG1	2.43	0.47
2:P:50:TRP:CD1	2:P:50:TRP:C	2.92	0.47
1:B:60:TYR:CE1	1:B:208:GLU:HB3	2.49	0.47
1:B:134:TRP:HE1	1:B:335:THR:CG2	2.19	0.47
1:B:197:LEU:HB3	1:B:201:LEU:HG	1.96	0.47
1:C:165:ILE:O	1:C:165:ILE:HG22	2.15	0.47
1:D:35:LEU:HA	1:D:38:THR:O	2.14	0.47
1:D:80:CYS:SG	1:D:371:ALA:HA	2.55	0.47
2:P:48:ILE:HG23	2:P:67:LYS:HZ1	1.76	0.47
1:A:349:GLU:O	1:A:353:VAL:HG23	2.14	0.47
1:B:125:LEU:HD23	1:B:125:LEU:O	2.15	0.47
1:B:318:ASN:C	1:B:320:ALA:H	2.22	0.47
1:B:330:VAL:HG12	1:B:334:MET:HE2	1.96	0.47
1:C:73:SER:OG	1:C:364:PRO:HB3	2.14	0.47
1:C:110:GLY:O	1:C:114:TYR:HB2	2.14	0.47
1:D:248:GLY:HA3	1:D:249:MET:HA	1.70	0.47
2:Q:50:TRP:C	2:Q:50:TRP:CD1	2.92	0.47
2:Q:126:PRO:HA	2:Q:151:GLY:O	2.14	0.47
2:Q:145:LEU:HD23	2:Q:145:LEU:N	2.30	0.47
2:P:18:VAL:O	2:P:81:MET:HA	2.15	0.47
2:P:119:SER:HB3	2:P:153:PHE:CZ	2.50	0.47
2:P:154:PRO:HB3	2:P:208:ALA:CB	2.45	0.47
3:W:200:GLU:HG2	3:W:211:VAL:CG2	2.45	0.47
1:A:31:LEU:CB	1:A:32:PRO:HD3	2.44	0.47
1:C:117:PRO:O	1:C:118:ILE:C	2.57	0.47
1:C:134:TRP:HA	1:C:137:VAL:CG1	2.43	0.47
1:D:361:THR:O	1:D:365:TYR:HD2	1.97	0.47
3:W:166:ASN:HB3	3:W:180:MET:HE2	1.95	0.47
1:C:219:ASN:H	1:C:220:PRO:HD3	1.76	0.47
1:C:393:VAL:O	1:C:396:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLY:HA3	1:D:73:SER:C	2.33	0.47
1:D:73:SER:OG	1:D:364:PRO:HB3	2.14	0.47
1:D:346:ALA:HA	1:D:347:ALA:HA	1.56	0.47
2:P:12:VAL:CG1	2:P:13:LYS:N	2.78	0.47
3:W:20:THR:HG23	3:W:78:THR:HG22	1.96	0.47
1:A:141:ILE:HG12	1:A:141:ILE:O	2.15	0.47
1:C:49:THR:OG1	1:C:201:LEU:HD23	2.15	0.47
1:C:252:ASN:HA	1:C:253:ALA:HA	1.65	0.47
1:D:433:LYS:HE2	2:Q:52:TYR:CD2	2.50	0.47
1:A:377:HIS:ND1	1:B:430:ARG:HG2	2.29	0.46
1:B:381:GLY:HA3	1:B:383:ALA:H	1.80	0.46
1:C:332:VAL:O	1:C:336:ILE:HG13	2.15	0.46
1:D:247:MET:N	1:D:248:GLY:O	2.48	0.46
1:D:363:VAL:HB	1:D:364:PRO:HD3	1.97	0.46
2:Q:53:PRO:HA	2:Q:71:THR:HG21	1.98	0.46
3:W:65:ARG:CZ	3:W:83:GLU:HG3	2.45	0.46
3:S:65:ARG:CZ	3:S:83:GLU:HG3	2.45	0.46
1:A:69:SER:C	1:A:71:GLY:HA3	2.40	0.46
1:A:130:VAL:HG13	1:A:335:THR:HG22	1.97	0.46
1:A:205:ILE:HG23	1:A:361:THR:HG21	1.97	0.46
1:B:262:PHE:CG	1:B:263:GLY:N	2.83	0.46
1:C:81:PHE:HB3	1:C:85:LEU:HD12	1.96	0.46
1:C:361:THR:O	1:C:365:TYR:HD2	1.98	0.46
1:D:147:ILE:H	1:D:147:ILE:HG13	1.56	0.46
2:P:145:LEU:N	2:P:145:LEU:HD23	2.30	0.46
2:P:187:SER:HB3	3:S:139:PHE:CD2	2.50	0.46
3:W:146:LYS:HE2	3:W:178:TYR:HE2	1.79	0.46
1:A:109:VAL:C	1:A:111:TYR:H	2.23	0.46
1:A:121:ASP:HB3	1:A:122:PRO:HD2	1.97	0.46
1:B:317:VAL:O	1:B:318:ASN:C	2.58	0.46
2:P:126:PRO:HA	2:P:151:GLY:O	2.14	0.46
1:B:85:LEU:HD12	1:B:85:LEU:N	2.31	0.46
1:B:360:PHE:HE2	1:B:413:SER:HA	1.80	0.46
1:B:435:PRO:HA	1:B:436:TYR:HA	1.59	0.46
1:C:170:TRP:H	1:C:249:MET:HG3	1.80	0.46
1:C:363:VAL:HB	1:C:364:PRO:HD3	1.96	0.46
1:C:430:ARG:HG2	1:D:377:HIS:HD2	1.76	0.46
1:D:10:VAL:CG2	1:D:145:LYS:HE3	2.45	0.46
2:P:134:VAL:O	2:P:135:CYS:CB	2.62	0.46
3:W:110:ILE:H	3:W:110:ILE:CD1	2.26	0.46
1:A:125:LEU:O	1:A:125:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TRP:O	1:A:173:PHE:C	2.59	0.46
1:A:360:PHE:HE2	1:A:413:SER:HA	1.80	0.46
1:C:182:TRP:O	1:C:184:VAL:N	2.48	0.46
1:C:261:PRO:O	1:C:262:PHE:C	2.59	0.46
2:Q:154:PRO:HB3	2:Q:208:ALA:CB	2.45	0.46
2:P:53:PRO:HA	2:P:71:THR:HG21	1.97	0.46
3:S:4:MET:HE1	3:S:37:MET:HE1	1.98	0.46
1:B:222:ARG:O	1:B:226:ILE:HG13	2.16	0.46
1:B:248:GLY:HA2	1:B:249:MET:HA	1.63	0.46
1:B:268:MET:HG3	1:B:269:ALA:H	1.79	0.46
2:Q:63:LYS:NZ	2:Q:67:LYS:HZ3	2.14	0.46
2:Q:65:LYS:O	2:Q:67:LYS:HG2	2.15	0.46
1:C:70:PRO:HB3	1:C:215:GLY:CA	2.46	0.46
1:C:169:GLY:O	1:C:249:MET:HE3	2.16	0.46
2:Q:7:SER:C	2:Q:9:PRO:HD2	2.40	0.46
1:A:197:LEU:HB3	1:A:201:LEU:HG	1.96	0.46
1:A:216:VAL:O	1:A:217:VAL:HB	2.16	0.46
1:B:216:VAL:O	1:B:217:VAL:HB	2.15	0.46
1:B:249:MET:H	1:B:249:MET:CE	2.26	0.46
1:C:79:ARG:HB2	1:D:436:TYR:O	2.16	0.46
1:C:147:ILE:HD12	1:C:148:THR:H	1.81	0.46
1:D:250:ILE:HG23	1:D:269:ALA:CB	2.45	0.46
2:Q:18:VAL:O	2:Q:81:MET:HA	2.15	0.46
2:P:65:LYS:O	2:P:67:LYS:HG2	2.16	0.46
3:S:39:TRP:HA	3:S:91:TYR:O	2.15	0.46
1:A:117:PRO:HG2	1:A:120:LYS:HE2	1.98	0.46
1:B:109:VAL:C	1:B:111:TYR:H	2.22	0.46
1:C:403:ILE:HA	1:D:411:MET:CE	2.46	0.46
1:C:411:MET:CE	1:D:403:ILE:HA	2.46	0.46
1:D:165:ILE:HG22	1:D:165:ILE:O	2.15	0.46
2:Q:61:ASN:O	2:Q:62:GLU:C	2.58	0.46
3:W:4:MET:HE1	3:W:37:MET:HE1	1.98	0.46
3:W:154:LYS:HA	3:W:159:GLU:HA	1.98	0.46
3:S:4:MET:HA	3:S:4:MET:CE	2.40	0.46
1:A:72:GLY:HA3	1:A:75:ALA:H	1.81	0.46
1:A:85:LEU:N	1:A:85:LEU:HD12	2.31	0.46
1:A:222:ARG:O	1:A:226:ILE:HG13	2.16	0.46
1:A:440:ALA:O	1:A:441:PRO:C	2.58	0.46
1:B:69:SER:C	1:B:71:GLY:HA3	2.41	0.46
1:B:205:ILE:HG23	1:B:361:THR:HG21	1.97	0.46
1:C:403:ILE:HA	1:D:411:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:144:TYR:O	3:W:203:HIS:HE1	1.99	0.46
1:A:435:PRO:HB2	2:P:103:TYR:CD2	2.50	0.45
1:B:72:GLY:HA3	1:B:75:ALA:H	1.81	0.45
1:B:407:ALA:O	1:B:408:LYS:C	2.60	0.45
1:C:386:LEU:HD23	1:C:386:LEU:C	2.41	0.45
1:D:70:PRO:HB3	1:D:215:GLY:CA	2.46	0.45
1:D:207:VAL:O	1:D:209:SER:N	2.50	0.45
2:Q:134:VAL:HG12	2:Q:135:CYS:N	2.31	0.45
2:P:60:TYR:CE2	2:P:62:GLU:HB3	2.51	0.45
2:P:102:ASN:HA	2:P:103:TYR:HA	1.72	0.45
1:A:68:PRO:HB3	1:A:220:PRO:HB2	1.99	0.45
1:D:169:GLY:O	1:D:249:MET:HE3	2.16	0.45
1:D:332:VAL:O	1:D:336:ILE:HG13	2.16	0.45
1:D:386:LEU:C	1:D:386:LEU:HD23	2.41	0.45
2:Q:47:TRP:CG	3:W:100:PRO:HG2	2.52	0.45
2:Q:63:LYS:HD2	2:Q:67:LYS:NZ	2.32	0.45
3:S:200:GLU:HG2	3:S:211:VAL:CG2	2.45	0.45
1:A:246:ILE:C	1:A:248:GLY:N	2.72	0.45
1:A:339:PHE:O	1:A:344:PRO:HD2	2.16	0.45
1:D:49:THR:OG1	1:D:201:LEU:HD23	2.16	0.45
2:Q:63:LYS:HB3	2:Q:67:LYS:HE2	1.99	0.45
2:Q:129:TYR:HB3	3:W:125:SER:OG	2.16	0.45
1:B:68:PRO:HB3	1:B:220:PRO:HB2	1.99	0.45
1:D:29:PHE:O	1:D:29:PHE:CG	2.69	0.45
1:D:71:GLY:H	1:D:303:ALA:CB	2.30	0.45
3:S:144:TYR:O	3:S:203:HIS:HE1	2.00	0.45
1:B:172:TRP:O	1:B:173:PHE:C	2.59	0.45
1:C:411:MET:HE2	1:D:403:ILE:HA	1.97	0.45
1:D:147:ILE:HD12	1:D:148:THR:HG23	1.99	0.45
1:D:250:ILE:HG12	1:D:269:ALA:HB3	1.99	0.45
3:S:30:ASN:O	3:S:36:TYR:CB	2.64	0.45
1:A:134:TRP:HA	1:A:137:VAL:HB	1.99	0.45
1:C:71:GLY:H	1:C:303:ALA:CB	2.30	0.45
1:C:147:ILE:HD12	1:C:148:THR:HG23	1.98	0.45
1:C:260:SER:HA	1:C:261:PRO:HD3	1.79	0.45
1:D:147:ILE:HD12	1:D:148:THR:H	1.82	0.45
1:D:170:TRP:H	1:D:249:MET:HG3	1.80	0.45
1:A:10:VAL:HA	1:A:11:GLY:HA2	1.61	0.45
1:A:73:SER:O	1:A:74:TYR:C	2.60	0.45
1:B:53:ALA:HA	1:B:397:TYR:CE1	2.52	0.45
1:B:117:PRO:HG2	1:B:120:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:VAL:C	1:C:209:SER:N	2.75	0.45
1:D:74:TYR:CZ	1:D:304:ALA:HA	2.51	0.45
1:D:205:ILE:HG23	1:D:361:THR:HG21	1.99	0.45
1:D:261:PRO:O	1:D:262:PHE:C	2.59	0.45
1:D:361:THR:HG22	1:D:365:TYR:CE2	2.49	0.45
3:S:129:LEU:HD12	3:S:129:LEU:H	1.82	0.45
1:A:146:MET:O	1:A:150:VAL:HG23	2.17	0.45
1:A:262:PHE:CG	1:A:263:GLY:N	2.84	0.45
1:B:141:ILE:HG12	1:B:141:ILE:O	2.15	0.45
1:C:141:ILE:HA	1:C:142:VAL:HA	1.48	0.45
1:D:81:PHE:CB	1:D:85:LEU:HD12	2.47	0.45
1:D:143:GLY:O	1:D:146:MET:HB3	2.17	0.45
1:A:13:ILE:N	1:A:14:PRO:CD	2.80	0.45
1:B:13:ILE:N	1:B:14:PRO:CD	2.80	0.45
1:C:29:PHE:CG	1:C:29:PHE:O	2.69	0.45
1:C:85:LEU:HD21	1:D:85:LEU:HD11	1.98	0.45
1:C:121:ASP:HB3	1:C:122:PRO:HD2	1.98	0.45
1:C:143:GLY:O	1:C:146:MET:HB3	2.17	0.45
1:D:182:TRP:O	1:D:184:VAL:N	2.49	0.45
1:D:260:SER:HA	1:D:261:PRO:HD3	1.79	0.45
1:D:393:VAL:O	1:D:396:VAL:HG12	2.16	0.45
2:Q:60:TYR:CE2	2:Q:62:GLU:HB3	2.52	0.45
2:P:60:TYR:CE2	3:S:99:PRO:HG2	2.52	0.45
3:W:127:GLU:HA	3:W:130:THR:OG1	2.17	0.45
3:W:151:LYS:O	3:W:152:TRP:CD1	2.70	0.45
3:S:2:LEU:HD22	3:S:94:GLN:HE21	1.82	0.45
3:S:127:GLU:HA	3:S:130:THR:OG1	2.17	0.45
1:A:70:PRO:HB2	1:A:71:GLY:HA2	1.99	0.45
1:B:327:LEU:HD13	1:B:327:LEU:O	2.17	0.45
1:B:405:SER:O	1:B:406:GLY:C	2.60	0.45
1:C:132:VAL:HA	1:C:135:ILE:HD12	1.99	0.45
1:D:141:ILE:HA	1:D:142:VAL:HA	1.48	0.45
1:D:207:VAL:C	1:D:208:GLU:HG3	2.42	0.45
3:W:4:MET:HA	3:W:4:MET:CE	2.40	0.45
3:S:40:TYR:HD1	3:S:50:ARG:HA	1.82	0.45
1:A:23:ILE:HG12	1:A:206:GLY:CA	2.24	0.44
1:A:435:PRO:HA	1:A:436:TYR:HA	1.59	0.44
1:B:73:SER:O	1:B:74:TYR:C	2.60	0.44
1:B:434:ASN:O	1:B:437:PRO:HG3	2.17	0.44
1:C:428:TYR:N	1:C:428:TYR:CD2	2.85	0.44
2:Q:121:ALA:HB3	2:Q:153:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:191:TYR:HA	3:S:197:TYR:OH	2.17	0.44
1:B:121:ASP:HB3	1:B:122:PRO:HD2	1.98	0.44
1:B:433:LYS:HE2	2:P:52:TYR:CG	2.52	0.44
1:C:70:PRO:O	1:C:303:ALA:HB2	2.17	0.44
2:Q:12:VAL:O	2:Q:118:VAL:HA	2.17	0.44
3:W:129:LEU:HD12	3:W:129:LEU:N	2.32	0.44
1:B:70:PRO:HB2	1:B:71:GLY:HA2	1.99	0.44
1:C:373:LEU:CD1	1:D:426:LEU:HD23	2.47	0.44
1:C:435:PRO:HA	1:C:436:TYR:HA	1.68	0.44
1:D:252:ASN:HA	1:D:253:ALA:HA	1.66	0.44
1:D:397:TYR:CD2	1:D:397:TYR:C	2.96	0.44
2:P:121:ALA:HB3	2:P:153:PHE:CE2	2.53	0.44
1:A:222:ARG:C	1:A:225:PRO:HD2	2.42	0.44
1:A:327:LEU:O	1:A:327:LEU:HD13	2.18	0.44
1:A:405:SER:O	1:A:406:GLY:C	2.60	0.44
1:D:392:PHE:O	1:D:395:PHE:HB2	2.17	0.44
2:Q:151:GLY:O	2:Q:152:TYR:HB3	2.18	0.44
2:P:133:PRO:HG2	2:P:195:TRP:CH2	2.53	0.44
3:W:129:LEU:HD12	3:W:129:LEU:H	1.81	0.44
3:S:4:MET:O	3:S:5:THR:C	2.60	0.44
3:S:154:LYS:HA	3:S:159:GLU:HA	1.98	0.44
1:A:53:ALA:HA	1:A:397:TYR:CE1	2.52	0.44
1:A:292:GLY:O	1:A:296:LEU:HG	2.17	0.44
1:A:407:ALA:O	1:A:408:LYS:C	2.60	0.44
1:B:78:ARG:HA	1:B:82:GLY:O	2.17	0.44
1:C:361:THR:HG22	1:C:365:TYR:CE2	2.49	0.44
1:C:440:ALA:HB2	3:W:97:TYR:CD2	2.53	0.44
1:D:31:LEU:HB2	1:D:246:ILE:HD11	2.00	0.44
1:D:71:GLY:HA2	1:D:75:ALA:HB2	2.00	0.44
3:W:203:HIS:CE1	3:W:205:THR:HG23	2.52	0.44
1:A:60:TYR:CZ	1:A:208:GLU:HB3	2.53	0.44
1:A:377:HIS:HB3	1:B:429:ASN:OD1	2.16	0.44
1:C:247:MET:N	1:C:248:GLY:O	2.48	0.44
3:W:40:TYR:HD1	3:W:50:ARG:HA	1.82	0.44
1:A:78:ARG:HA	1:A:82:GLY:O	2.17	0.44
1:A:270:LEU:HD13	1:A:270:LEU:O	2.17	0.44
1:A:434:ASN:O	1:A:437:PRO:HG3	2.18	0.44
1:B:170:TRP:O	1:B:249:MET:HG3	2.18	0.44
1:B:311:PRO:HA	1:B:312:PRO:HD3	1.71	0.44
1:B:377:HIS:HE1	3:S:30:ASN:HD21	1.66	0.44
1:C:71:GLY:HA2	1:C:75:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:TYR:CZ	1:C:304:ALA:HA	2.52	0.44
1:C:80:CYS:SG	1:C:371:ALA:HA	2.58	0.44
1:C:207:VAL:O	1:C:209:SER:N	2.50	0.44
1:C:392:PHE:O	1:C:395:PHE:HB2	2.18	0.44
1:D:354:SER:C	1:D:356:VAL:N	2.76	0.44
2:Q:160:THR:O	2:Q:203:ASN:N	2.49	0.44
2:P:9:PRO:CB	2:P:10:GLU:CB	2.90	0.44
3:W:123:PRO:HB3	3:W:214:PHE:CE1	2.53	0.44
3:S:123:PRO:HB3	3:S:214:PHE:CE1	2.53	0.44
1:B:250:ILE:HB	1:B:251:PRO:CD	2.40	0.44
1:C:216:VAL:HG12	1:C:217:VAL:N	2.33	0.44
1:D:250:ILE:HG23	1:D:269:ALA:HB2	2.00	0.44
1:D:360:PHE:CZ	1:D:416:THR:HG21	2.53	0.44
2:Q:134:VAL:CG1	2:Q:135:CYS:N	2.80	0.44
2:P:4:LEU:HG	2:P:96:CYS:SG	2.57	0.44
3:W:112:ARG:HD2	3:W:144:TYR:HB2	2.00	0.44
3:S:175:ASP:O	3:S:176:SER:HB2	2.18	0.44
1:B:105:VAL:CG1	1:B:290:LEU:HD11	2.48	0.44
1:B:134:TRP:HA	1:B:137:VAL:HB	1.99	0.44
2:Q:34:ILE:O	2:Q:50:TRP:HA	2.18	0.44
2:Q:48:ILE:HG12	2:Q:67:LYS:HZ2	1.82	0.44
2:Q:101:GLY:HA2	2:Q:102:ASN:CB	2.18	0.44
3:W:191:TYR:HA	3:W:197:TYR:OH	2.17	0.44
1:B:433:LYS:O	1:B:435:PRO:HD3	2.18	0.43
1:D:10:VAL:HA	1:D:11:GLY:HA2	1.73	0.43
1:D:132:VAL:HA	1:D:135:ILE:HD12	2.00	0.43
2:P:34:ILE:O	2:P:50:TRP:HA	2.17	0.43
2:P:60:TYR:CD2	2:P:61:ASN:N	2.86	0.43
3:S:129:LEU:HD12	3:S:129:LEU:N	2.32	0.43
3:S:193:ARG:NH1	3:S:193:ARG:HA	2.33	0.43
1:C:205:ILE:HG23	1:C:361:THR:HG21	1.99	0.43
1:D:109:VAL:C	1:D:111:TYR:H	2.26	0.43
2:P:18:VAL:HG22	2:P:19:LYS:N	2.33	0.43
1:A:250:ILE:HB	1:A:251:PRO:CD	2.40	0.43
1:A:369:CYS:HB2	1:A:395:PHE:CE1	2.53	0.43
1:B:13:ILE:CG2	1:B:14:PRO:HD3	2.47	0.43
1:B:222:ARG:C	1:B:225:PRO:HD2	2.42	0.43
1:C:207:VAL:C	1:C:208:GLU:HG3	2.42	0.43
1:D:70:PRO:O	1:D:303:ALA:HB2	2.17	0.43
1:D:207:VAL:C	1:D:209:SER:N	2.74	0.43
1:D:250:ILE:HB	1:D:251:PRO:CD	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:10:GLU:OE2	2:Q:11:LEU:CD2	2.66	0.43
2:Q:41:PRO:HA	2:Q:92:SER:OG	2.19	0.43
1:A:262:PHE:CZ	1:A:266:ALA:HB2	2.54	0.43
1:A:270:LEU:HD22	1:A:270:LEU:HA	1.88	0.43
1:B:111:TYR:HB3	1:B:283:ALA:HB2	2.00	0.43
1:B:292:GLY:O	1:B:296:LEU:HG	2.18	0.43
1:B:369:CYS:HB2	1:B:395:PHE:CE1	2.53	0.43
2:Q:63:LYS:CD	2:Q:67:LYS:HZ3	2.31	0.43
3:W:30:ASN:O	3:W:36:TYR:CB	2.65	0.43
1:A:170:TRP:O	1:A:249:MET:HG3	2.19	0.43
1:A:292:GLY:O	1:A:295:LEU:HB3	2.19	0.43
1:B:377:HIS:HE1	3:S:30:ASN:ND2	2.16	0.43
2:Q:4:LEU:HG	2:Q:96:CYS:SG	2.58	0.43
2:Q:80:TYR:C	2:Q:80:TYR:CD1	2.95	0.43
3:W:2:LEU:HD22	3:W:94:GLN:HE21	1.83	0.43
1:A:105:VAL:CG1	1:A:290:LEU:HD11	2.48	0.43
1:A:111:TYR:HB3	1:A:283:ALA:HB2	2.00	0.43
1:C:91:VAL:O	1:C:95:LEU:HG	2.19	0.43
1:C:218:LYS:O	1:C:219:ASN:CB	2.67	0.43
1:C:381:GLY:HA2	1:C:382:LYS:HA	1.60	0.43
3:S:151:LYS:HB2	3:S:200:GLU:HB2	2.00	0.43
1:A:13:ILE:CG2	1:A:14:PRO:HD3	2.48	0.43
1:A:140:ASN:ND2	1:A:295:LEU:HA	2.33	0.43
1:A:207:VAL:C	1:A:208:GLU:HG3	2.44	0.43
1:B:140:ASN:ND2	1:B:295:LEU:HA	2.33	0.43
1:C:81:PHE:CB	1:C:85:LEU:HD12	2.48	0.43
1:C:240:VAL:C	1:C:242:SER:H	2.26	0.43
1:D:31:LEU:H	1:D:31:LEU:HG	1.38	0.43
1:D:313:ILE:HD12	1:D:313:ILE:N	2.25	0.43
2:Q:6:GLN:HB3	2:Q:21:SER:O	2.17	0.43
3:S:2:LEU:HD11	3:S:29:VAL:HG12	2.01	0.43
3:S:112:ARG:HD2	3:S:144:TYR:HB2	2.00	0.43
3:S:203:HIS:CE1	3:S:205:THR:HG23	2.53	0.43
1:D:216:VAL:HG12	1:D:217:VAL:N	2.33	0.43
3:S:38:HIS:O	3:S:92:CYS:HA	2.18	0.43
1:B:169:GLY:HA2	1:B:170:TRP:HA	1.65	0.43
1:B:262:PHE:CZ	1:B:266:ALA:HB2	2.54	0.43
1:C:70:PRO:HB3	1:C:215:GLY:HA3	2.00	0.43
1:C:109:VAL:C	1:C:111:TYR:H	2.27	0.43
1:D:91:VAL:O	1:D:95:LEU:HG	2.18	0.43
1:D:121:ASP:HB3	1:D:122:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:VAL:C	1:D:242:SER:H	2.26	0.43
1:D:435:PRO:HA	1:D:436:TYR:HA	1.69	0.43
2:Q:100:ASP:HB2	2:Q:108:ALA:HB2	2.01	0.43
2:P:6:GLN:HB3	2:P:21:SER:O	2.18	0.43
1:A:132:VAL:HA	1:A:135:ILE:HD12	2.01	0.43
1:B:60:TYR:CZ	1:B:208:GLU:HB3	2.53	0.43
1:B:207:VAL:C	1:B:208:GLU:HG3	2.44	0.43
1:B:267:ARG:HB3	1:B:272:ASP:O	2.19	0.43
1:B:382:LYS:C	1:B:384:ARG:H	2.26	0.43
2:Q:151:GLY:HA2	2:Q:181:LEU:HD23	2.01	0.43
2:P:170:VAL:C	2:P:171:HIS:HD2	2.27	0.43
1:B:146:MET:O	1:B:150:VAL:HG23	2.18	0.42
1:B:201:LEU:HD22	1:B:397:TYR:CE2	2.53	0.42
1:C:352:LEU:O	1:C:356:VAL:HG23	2.18	0.42
1:D:428:TYR:N	1:D:428:TYR:CD2	2.85	0.42
3:S:11:MET:HG3	3:S:108:LEU:HD12	2.01	0.42
1:A:201:LEU:HD22	1:A:397:TYR:CE2	2.53	0.42
1:C:85:LEU:HD11	1:D:85:LEU:HD21	2.01	0.42
1:C:389:LEU:O	1:C:392:PHE:HB3	2.18	0.42
1:D:267:ARG:CA	1:D:272:ASP:HB3	2.49	0.42
1:D:389:LEU:O	1:D:392:PHE:HB3	2.19	0.42
3:W:25:ALA:O	3:W:26:SER:C	2.62	0.42
3:W:154:LYS:HG3	3:W:159:GLU:HB3	2.01	0.42
1:B:34:ASN:OD1	1:B:34:ASN:C	2.61	0.42
1:C:63:MET:HE2	1:C:76:TYR:HB3	2.01	0.42
1:C:140:ASN:HB3	1:C:327:LEU:HD11	2.01	0.42
1:C:397:TYR:CD2	1:C:397:TYR:C	2.97	0.42
1:D:70:PRO:HB3	1:D:215:GLY:HA3	2.00	0.42
2:P:80:TYR:CD1	2:P:80:TYR:C	2.96	0.42
3:W:4:MET:O	3:W:5:THR:C	2.62	0.42
3:W:11:MET:HG3	3:W:108:LEU:HD12	2.01	0.42
3:S:198:THR:HG23	3:S:213:SER:CB	2.47	0.42
1:A:382:LYS:C	1:A:384:ARG:H	2.26	0.42
1:C:35:LEU:HD13	1:C:35:LEU:C	2.44	0.42
2:P:63:LYS:HZ3	2:P:67:LYS:NZ	2.17	0.42
2:P:151:GLY:O	2:P:152:TYR:HB3	2.19	0.42
1:B:38:THR:HG21	1:B:41:ILE:CG2	2.41	0.42
1:C:69:SER:HA	1:C:70:PRO:HD3	1.80	0.42
1:D:92:LEU:HD11	1:D:417:LEU:CD2	2.50	0.42
1:D:104:MET:HE2	1:D:289:SER:OG	2.19	0.42
1:D:151:GLN:HE22	1:D:289:SER:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:52:TYR:HD1	2:Q:53:PRO:HD2	1.84	0.42
2:Q:147:CYS:HB2	2:Q:161:TRP:CH2	2.55	0.42
2:P:63:LYS:HB3	2:P:67:LYS:HE2	2.00	0.42
2:P:153:PHE:H	2:P:154:PRO:HD3	1.84	0.42
3:W:149:ASN:CG	3:W:151:LYS:HB3	2.45	0.42
3:W:175:ASP:O	3:W:176:SER:HB2	2.18	0.42
1:A:248:GLY:HA2	1:A:249:MET:HA	1.63	0.42
1:D:63:MET:HE2	1:D:76:TYR:HB3	2.02	0.42
1:D:218:LYS:O	1:D:219:ASN:CB	2.67	0.42
1:D:230:GLY:O	1:D:234:ILE:HG13	2.19	0.42
2:Q:145:LEU:HD23	2:Q:145:LEU:H	1.85	0.42
2:Q:170:VAL:C	2:Q:171:HIS:HD2	2.27	0.42
2:P:52:TYR:HD1	2:P:53:PRO:HD2	1.84	0.42
2:P:145:LEU:HD23	2:P:145:LEU:H	1.85	0.42
1:B:31:LEU:H	1:B:31:LEU:HG	1.58	0.42
1:B:343:SER:N	1:B:344:PRO:CD	2.82	0.42
1:C:115:PHE:CE2	1:C:280:PHE:HE1	2.38	0.42
1:C:249:MET:SD	1:C:249:MET:N	2.90	0.42
1:D:35:LEU:C	1:D:35:LEU:HD13	2.45	0.42
1:D:140:ASN:HB3	1:D:327:LEU:HD11	2.00	0.42
2:P:195:TRP:HB3	2:P:196:PRO:HD3	2.01	0.42
3:W:135:SER:HA	3:W:184:LEU:O	2.20	0.42
1:A:10:VAL:CB	1:A:218:LYS:HD3	2.47	0.42
1:C:79:ARG:HD3	1:C:375:LEU:HD11	2.01	0.42
1:C:151:GLN:HE22	1:C:289:SER:HA	1.84	0.42
1:C:418:MET:HE3	1:C:418:MET:HB3	1.91	0.42
2:Q:60:TYR:CD2	2:Q:61:ASN:N	2.87	0.42
2:P:63:LYS:HD2	2:P:67:LYS:NZ	2.34	0.42
3:S:21:MET:HB3	3:S:106:THR:HG21	2.02	0.42
2:Q:40:ARG:HB3	2:Q:41:PRO:CD	2.49	0.42
2:Q:119:SER:HB3	2:Q:153:PHE:HZ	1.84	0.42
3:S:53:TYR:CZ	3:S:57:LYS:HB3	2.54	0.42
1:A:99:ILE:O	1:A:102:ILE:HG13	2.20	0.42
1:A:345:ASN:O	1:A:347:ALA:CB	2.67	0.42
1:B:292:GLY:O	1:B:295:LEU:HB3	2.19	0.42
1:C:92:LEU:HD11	1:C:417:LEU:CD2	2.49	0.42
1:C:230:GLY:O	1:C:234:ILE:HG13	2.20	0.42
1:C:313:ILE:HD12	1:C:313:ILE:N	2.25	0.42
1:D:249:MET:SD	1:D:249:MET:N	2.90	0.42
2:Q:106:TRP:HB3	3:W:38:HIS:CG	2.54	0.42
3:W:43:LYS:HG2	3:W:88:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:25:ALA:O	3:S:26:SER:C	2.63	0.42
3:S:135:SER:HA	3:S:184:LEU:O	2.19	0.42
1:A:149:ARG:O	1:A:153:VAL:HG23	2.21	0.41
1:B:307:ASP:C	1:B:309:LEU:H	2.28	0.41
1:C:31:LEU:HB2	1:C:246:ILE:HD11	2.01	0.41
1:C:423:LEU:HD12	1:C:423:LEU:HA	1.93	0.41
2:P:50:TRP:CD1	2:P:58:THR:H	2.38	0.41
3:W:208:SER:HA	3:W:209:PRO:HD3	1.92	0.41
1:B:99:ILE:O	1:B:102:ILE:HG13	2.20	0.41
1:B:165:ILE:O	1:B:165:ILE:HG22	2.20	0.41
1:B:267:ARG:CZ	1:B:276:ALA:HA	2.50	0.41
1:C:21:GLY:HA3	1:C:155:THR:HG21	2.02	0.41
1:D:197:LEU:C	1:D:199:VAL:N	2.79	0.41
2:Q:153:PHE:H	2:Q:154:PRO:HD3	1.85	0.41
2:P:119:SER:HB3	2:P:153:PHE:HZ	1.84	0.41
1:C:197:LEU:C	1:C:199:VAL:H	2.29	0.41
2:Q:41:PRO:N	2:Q:92:SER:HB2	2.36	0.41
2:Q:144:THR:O	3:W:122:PHE:HZ	2.03	0.41
3:W:38:HIS:O	3:W:92:CYS:HA	2.20	0.41
3:W:39:TRP:HA	3:W:91:TYR:O	2.19	0.41
3:S:110:ILE:H	3:S:110:ILE:CD1	2.25	0.41
3:S:154:LYS:HG3	3:S:159:GLU:HB3	2.02	0.41
1:B:132:VAL:HA	1:B:135:ILE:HD12	2.01	0.41
1:C:104:MET:HE2	1:C:289:SER:OG	2.20	0.41
1:D:21:GLY:HA3	1:D:155:THR:HG21	2.02	0.41
1:D:115:PHE:CE2	1:D:280:PHE:HE1	2.38	0.41
2:Q:10:GLU:OE2	2:Q:11:LEU:HD23	2.19	0.41
2:P:88:SER:C	2:P:90:ASN:H	2.28	0.41
2:P:100:ASP:HB2	2:P:108:ALA:HB2	2.02	0.41
2:P:151:GLY:HA2	2:P:181:LEU:HD23	2.01	0.41
3:W:53:TYR:CZ	3:W:57:LYS:HB3	2.56	0.41
1:A:267:ARG:CZ	1:A:276:ALA:HA	2.50	0.41
1:C:73:SER:HA	1:C:368:THR:CG2	2.50	0.41
1:C:91:VAL:HG11	1:C:420:ILE:HD12	2.01	0.41
1:C:267:ARG:CA	1:C:272:ASP:HB3	2.49	0.41
1:D:12:LEU:CD2	1:D:13:ILE:HD12	2.50	0.41
1:D:101:ASN:O	1:D:104:MET:HB2	2.20	0.41
2:Q:23:LYS:HE3	2:Q:23:LYS:HB2	1.88	0.41
2:P:48:ILE:HG23	2:P:67:LYS:CE	2.49	0.41
2:P:48:ILE:HG12	2:P:67:LYS:HZ2	1.84	0.41
1:B:380:PHE:HD2	1:B:380:PHE:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:147:CYS:HB2	2:P:161:TRP:CH2	2.55	0.41
1:A:436:TYR:CE2	2:P:103:TYR:HE2	2.37	0.41
1:B:207:VAL:C	1:B:209:SER:H	2.29	0.41
1:C:23:ILE:HG12	1:C:206:GLY:CA	2.50	0.41
1:D:73:SER:HA	1:D:368:THR:CG2	2.51	0.41
1:D:102:ILE:HD11	1:D:337:PHE:HB3	2.03	0.41
2:Q:48:ILE:HG23	2:Q:67:LYS:CE	2.50	0.41
2:Q:102:ASN:HA	2:Q:103:TYR:HA	1.73	0.41
2:Q:125:PRO:HB3	2:Q:211:THR:HG21	2.03	0.41
1:A:165:ILE:O	1:A:165:ILE:HG22	2.20	0.41
1:B:149:ARG:O	1:B:153:VAL:HG23	2.21	0.41
1:B:406:GLY:O	1:B:407:ALA:C	2.64	0.41
2:Q:133:PRO:HG2	2:Q:195:TRP:CH2	2.56	0.41
1:A:307:ASP:C	1:A:309:LEU:H	2.28	0.41
1:C:12:LEU:CD2	1:C:13:ILE:HD12	2.50	0.41
1:C:31:LEU:H	1:C:31:LEU:HG	1.37	0.41
1:C:89:THR:CG2	1:C:367:TYR:HD2	2.34	0.41
1:D:79:ARG:HD3	1:D:375:LEU:HD11	2.02	0.41
1:D:152:ALA:O	1:D:156:VAL:HG23	2.21	0.41
2:Q:3:GLN:HA	2:Q:3:GLN:OE1	2.21	0.41
3:W:37:MET:HE2	3:W:37:MET:HB2	1.93	0.41
3:W:198:THR:HG23	3:W:213:SER:CB	2.48	0.41
1:A:49:THR:HG21	1:A:200:THR:HB	2.03	0.41
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.94	0.41
1:C:152:ALA:O	1:C:156:VAL:HG23	2.21	0.41
1:D:87:TYR:HE1	1:D:424:TYR:HB2	1.82	0.41
2:Q:63:LYS:NZ	2:Q:67:LYS:NZ	2.69	0.41
2:Q:88:SER:C	2:Q:90:ASN:H	2.28	0.41
2:P:30:THR:HA	2:P:53:PRO:HB2	2.04	0.41
2:P:160:THR:O	2:P:203:ASN:N	2.48	0.41
1:B:416:THR:O	1:B:420:ILE:HG12	2.21	0.40
1:C:101:ASN:O	1:C:104:MET:HB2	2.21	0.40
1:C:119:LEU:HD13	1:C:124:VAL:CG1	2.51	0.40
1:D:119:LEU:HD13	1:D:124:VAL:CG1	2.50	0.40
1:D:356:VAL:HG12	1:D:356:VAL:O	2.20	0.40
2:Q:12:VAL:CG2	2:Q:13:LYS:N	2.84	0.40
2:P:104:GLY:HA2	2:P:105:GLY:HA2	1.85	0.40
1:A:43:ILE:HA	1:A:46:TRP:HD1	1.85	0.40
1:A:267:ARG:CB	1:A:272:ASP:HB2	2.51	0.40
1:C:220:PRO:C	1:C:222:ARG:H	2.29	0.40
1:C:433:LYS:HD3	2:Q:104:GLY:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:GLY:C	1:D:207:VAL:O	2.64	0.40
2:P:63:LYS:NZ	2:P:67:LYS:NZ	2.69	0.40
1:A:207:VAL:C	1:A:209:SER:H	2.29	0.40
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.94	0.40
1:D:70:PRO:N	1:D:71:GLY:HA3	2.35	0.40
3:W:2:LEU:HB3	3:W:94:GLN:HE22	1.86	0.40
3:W:12:SER:HA	3:W:109:GLU:O	2.21	0.40
1:A:34:ASN:OD1	1:A:34:ASN:C	2.62	0.40
1:A:260:SER:HA	1:A:261:PRO:HD3	1.91	0.40
1:B:69:SER:HB3	1:B:70:PRO:CD	2.50	0.40
1:C:122:PRO:C	1:C:124:VAL:N	2.80	0.40
1:C:222:ARG:O	1:C:225:PRO:HD2	2.21	0.40
1:C:360:PHE:CZ	1:C:416:THR:HG21	2.55	0.40
1:D:89:THR:CG2	1:D:367:TYR:HD2	2.34	0.40
2:P:3:GLN:OE1	2:P:3:GLN:HA	2.22	0.40
2:P:40:ARG:HA	2:P:92:SER:HB2	2.03	0.40
3:W:2:LEU:HD11	3:W:29:VAL:HG12	2.02	0.40
1:A:406:GLY:O	1:A:407:ALA:C	2.64	0.40
1:B:216:VAL:O	1:B:218:LYS:N	2.51	0.40
1:C:102:ILE:HD11	1:C:337:PHE:HB3	2.04	0.40
1:D:361:THR:O	1:D:365:TYR:CD2	2.74	0.40

There are no symmetry-related clashes.

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	416/445 (94%)	328 (79%)	59 (14%)	29 (7%)	1	6
1	B	414/445 (93%)	328 (79%)	57 (14%)	29 (7%)	1	6
1	C	414/445 (93%)	322 (78%)	68 (16%)	24 (6%)	1	10
1	D	413/445 (93%)	319 (77%)	71 (17%)	23 (6%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	217/219 (99%)	179 (82%)	27 (12%)	11 (5%)	1	13
2	Q	216/219 (99%)	180 (83%)	25 (12%)	11 (5%)	1	13
3	S	209/211 (99%)	174 (83%)	28 (13%)	7 (3%)	3	21
3	W	209/211 (99%)	173 (83%)	29 (14%)	7 (3%)	3	21
All	All	2508/2640 (95%)	2003 (80%)	364 (14%)	141 (6%)	1	11

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	PHE
1	A	118	ILE
1	A	166	ALA
1	A	270	LEU
1	A	274	ALA
1	A	440	ALA
1	B	116	PHE
1	B	118	ILE
1	B	166	ALA
1	B	270	LEU
1	B	317	VAL
1	B	346	ALA
1	C	70	PRO
1	C	118	ILE
1	C	186	GLY
1	C	219	ASN
1	C	271	GLY
1	D	70	PRO
1	D	118	ILE
1	D	186	GLY
1	D	271	GLY
1	D	383	ALA
2	Q	93	VAL
2	Q	140	GLY
2	P	135	CYS
3	W	152	TRP
3	S	151	LYS
1	A	38	THR
1	A	142	VAL
1	A	207	VAL
1	A	208	GLU
1	A	275	GLY

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Mol	Chain	Res	Type
1	A	406	GLY
1	A	435	PRO
1	B	38	THR
1	B	142	VAL
1	B	207	VAL
1	B	208	GLU
1	B	274	ALA
1	B	275	GLY
1	B	406	GLY
1	B	435	PRO
1	C	183	ASN
1	C	207	VAL
1	C	208	GLU
1	C	218	LYS
1	C	269	ALA
1	C	381	GLY
1	D	183	ASN
1	D	207	VAL
1	D	208	GLU
1	D	218	LYS
1	D	219	ASN
2	Q	55	ASP
2	Q	83	LEU
2	Q	104	GLY
2	Q	197	SER
2	P	55	ASP
2	P	83	LEU
2	P	93	VAL
2	P	104	GLY
2	P	197	SER
3	W	154	LYS
3	W	170	ASP
3	S	150	VAL
3	S	154	LYS
3	S	170	ASP
1	A	143	GLY
1	A	216	VAL
1	A	310	PHE
1	A	438	LEU
1	B	143	GLY
1	B	216	VAL
1	B	310	PHE

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Mol	Chain	Res	Type
1	B	438	LEU
1	C	216	VAL
1	C	247	MET
1	C	322	THR
1	C	380	PHE
1	D	216	VAL
1	D	247	MET
1	D	322	THR
1	D	346	ALA
1	D	380	PHE
3	S	5	THR
1	A	117	PRO
1	A	122	PRO
1	A	173	PHE
1	A	218	LYS
1	A	251	PRO
1	A	323	PRO
1	A	341	SER
1	B	117	PRO
1	B	122	PRO
1	B	173	PHE
1	B	218	LYS
1	B	251	PRO
1	B	319	LYS
1	B	341	SER
1	C	73	SER
1	C	83	PRO
1	C	205	ILE
1	C	310	PHE
1	D	73	SER
1	D	83	PRO
1	D	310	PHE
2	Q	149	VAL
2	P	149	VAL
3	W	5	THR
3	W	150	VAL
1	C	117	PRO
1	C	323	PRO
1	D	117	PRO
1	D	205	ILE
1	D	323	PRO
2	Q	41	PRO

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Mol	Chain	Res	Type
2	Q	179	SER
2	P	41	PRO
2	P	179	SER
3	W	88	ALA
3	W	204	LYS
3	S	88	ALA
3	S	204	LYS
1	A	167	VAL
1	A	347	ALA
1	B	167	VAL
1	C	206	GLY
1	D	206	GLY
1	A	205	ILE
1	C	165	ILE
1	D	165	ILE
2	Q	105	GLY
1	B	205	ILE
2	P	105	GLY
1	A	83	PRO
1	A	217	VAL
1	B	83	PRO
1	B	217	VAL
2	P	153	PHE
1	C	440	ALA
2	Q	153	PHE

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	308/343 (90%)	287 (93%)	21 (7%)	14	46
1	B	306/343 (89%)	284 (93%)	22 (7%)	13	44
1	C	305/343 (89%)	285 (93%)	20 (7%)	15	47
1	D	306/343 (89%)	285 (93%)	21 (7%)	14	45
2	P	187/187 (100%)	170 (91%)	17 (9%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	186/187 (100%)	166 (89%)	20 (11%)	6	27
3	S	185/185 (100%)	167 (90%)	18 (10%)	8	32
3	W	185/185 (100%)	165 (89%)	20 (11%)	6	27
All	All	1968/2116 (93%)	1809 (92%)	159 (8%)	11	39

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	34	ASN
1	A	56	LEU
1	A	73	SER
1	A	102	ILE
1	A	105	VAL
1	A	142	VAL
1	A	207	VAL
1	A	219	ASN
1	A	233	LEU
1	A	247	MET
1	A	252	ASN
1	A	264	ASP
1	A	270	LEU
1	A	316	ARG
1	A	327	LEU
1	A	361	THR
1	A	395	PHE
1	A	396	VAL
1	A	400	TRP
1	A	408	LYS
1	B	31	LEU
1	B	34	ASN
1	B	56	LEU
1	B	73	SER
1	B	102	ILE
1	B	105	VAL
1	B	142	VAL
1	B	207	VAL
1	B	219	ASN
1	B	233	LEU
1	B	247	MET
1	B	252	ASN

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Mol	Chain	Res	Type
1	B	264	ASP
1	B	270	LEU
1	B	316	ARG
1	B	319	LYS
1	B	327	LEU
1	B	361	THR
1	B	395	PHE
1	B	396	VAL
1	B	400	TRP
1	B	408	LYS
1	C	31	LEU
1	C	35	LEU
1	C	49	THR
1	C	50	ILE
1	C	91	VAL
1	C	114	TYR
1	C	137	VAL
1	C	147	ILE
1	C	167	VAL
1	C	212	VAL
1	C	233	LEU
1	C	249	MET
1	C	257	VAL
1	C	327	LEU
1	C	358	VAL
1	C	377	HIS
1	C	400	TRP
1	C	413	SER
1	C	421	THR
1	C	436	TYR
1	D	10	VAL
1	D	31	LEU
1	D	35	LEU
1	D	49	THR
1	D	50	ILE
1	D	91	VAL
1	D	114	TYR
1	D	137	VAL
1	D	147	ILE
1	D	167	VAL
1	D	212	VAL
1	D	233	LEU

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Mol	Chain	Res	Type
1	D	249	MET
1	D	257	VAL
1	D	327	LEU
1	D	358	VAL
1	D	377	HIS
1	D	400	TRP
1	D	413	SER
1	D	421	THR
1	D	436	TYR
2	Q	5	GLN
2	Q	6	GLN
2	Q	11	LEU
2	Q	12	VAL
2	Q	18	VAL
2	Q	30	THR
2	Q	45	LEU
2	Q	46	GLU
2	Q	55	ASP
2	Q	65	LYS
2	Q	69	THR
2	Q	78	THR
2	Q	91	SER
2	Q	123	THR
2	Q	145	LEU
2	Q	155	GLU
2	Q	170	VAL
2	Q	183	THR
2	Q	201	THR
2	Q	218	VAL
2	P	5	GLN
2	P	6	GLN
2	P	30	THR
2	P	45	LEU
2	P	46	GLU
2	P	55	ASP
2	P	65	LYS
2	P	69	THR
2	P	78	THR
2	P	91	SER
2	P	123	THR
2	P	145	LEU
2	P	155	GLU

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Mol	Chain	Res	Type
2	P	170	VAL
2	P	183	THR
2	P	201	THR
2	P	218	VAL
3	W	4	MET
3	W	5	THR
3	W	22	THR
3	W	29	VAL
3	W	30	ASN
3	W	79	ILE
3	W	93	GLN
3	W	94	GLN
3	W	95	TRP
3	W	110	ILE
3	W	112	ARG
3	W	147	ASP
3	W	150	VAL
3	W	151	LYS
3	W	159	GLU
3	W	169	THR
3	W	180	MET
3	W	190	GLU
3	W	198	THR
3	W	214	PHE
3	S	4	MET
3	S	5	THR
3	S	29	VAL
3	S	30	ASN
3	S	79	ILE
3	S	93	GLN
3	S	94	GLN
3	S	95	TRP
3	S	110	ILE
3	S	112	ARG
3	S	147	ASP
3	S	150	VAL
3	S	159	GLU
3	S	169	THR
3	S	180	MET
3	S	190	GLU
3	S	198	THR
3	S	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	151	GLN
1	A	427	ASN
1	B	140	ASN
1	B	151	GLN
1	B	377	HIS
1	B	427	ASN
1	C	90	ASN
1	C	151	GLN
1	C	223	ASN
1	C	299	GLN
1	C	434	ASN
1	D	299	GLN
3	W	30	ASN
3	W	94	GLN
3	W	98	ASN
3	W	203	HIS
3	S	30	ASN
3	S	94	GLN
3	S	98	ASN
3	S	203	HIS

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

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	422/445 (94%)	2.14	204 (48%)  	56, 127, 231, 339	0
1	B	419/445 (94%)	2.24	200 (47%)  	62, 126, 220, 332	0
1	C	419/445 (94%)	2.17	204 (48%)  	37, 104, 203, 283	0
1	D	416/445 (93%)	2.00	185 (44%)  	33, 105, 197, 283	0
2	P	218/219 (99%)	2.17	103 (47%)  	48, 104, 168, 224	2 (0%)
2	Q	216/219 (98%)	1.89	84 (38%)  	44, 108, 166, 278	2 (0%)
3	S	209/211 (99%)	1.99	94 (44%)  	30, 80, 169, 258	0
3	W	207/211 (98%)	1.59	66 (31%)  	23, 81, 166, 266	0
All	All	2526/2640 (95%)	2.06	1140 (45%)  	23, 109, 203, 339	4 (0%)

All (1140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	186	GLY	12.9
1	B	264	ASP	10.5
2	P	134	VAL	9.5
1	B	116	PHE	9.3
1	B	255	LEU	8.6
1	B	186	GLY	8.6
1	D	121	ASP	8.3
1	C	264	ASP	8.3
1	C	116	PHE	7.9
2	P	88	SER	7.9
1	A	175	GLY	7.7
2	Q	139	THR	7.7
1	B	248	GLY	7.5
2	Q	92	SER	7.5
2	Q	9	PRO	7.5
1	D	270	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASN	7.3
1	B	265	ALA	7.3
2	Q	8	GLY	7.3
1	C	255	LEU	7.2
1	B	263	GLY	7.2
3	W	199	CYS	7.2
2	Q	137	ASP	7.1
3	S	152	TRP	6.8
1	D	345	ASN	6.8
2	P	84	SER	6.8
1	D	250	ILE	6.7
1	C	194	GLN	6.7
1	B	190	PHE	6.7
1	B	326	GLY	6.6
1	D	381	GLY	6.6
1	B	185	SER	6.6
1	C	141	ILE	6.5
2	Q	138	THR	6.4
1	D	343	SER	6.4
1	C	252	ASN	6.3
1	D	252	ASN	6.3
3	S	207	THR	6.2
2	P	66	GLY	6.2
3	S	202	THR	6.2
1	B	347	ALA	6.1
1	B	140	ASN	6.1
1	C	185	SER	6.1
1	B	244	THR	6.0
2	P	195	TRP	6.0
1	B	269	ALA	5.9
1	B	381	GLY	5.9
3	S	199	CYS	5.9
3	S	165	LEU	5.9
1	B	189	THR	5.9
1	A	255	LEU	5.9
1	B	349	GLU	5.9
2	Q	134	VAL	5.8
2	P	199	THR	5.8
2	P	200	VAL	5.8
2	P	9	PRO	5.8
2	P	140	GLY	5.8
1	C	215	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
3	S	210	ILE	5.8
1	C	341	SER	5.8
1	B	275	GLY	5.8
1	B	247	MET	5.7
1	B	440	ALA	5.7
1	B	346	ALA	5.7
2	P	137	ASP	5.7
1	B	40	GLY	5.7
1	A	36	ALA	5.6
2	Q	132	ALA	5.6
1	C	70	PRO	5.6
2	P	138	THR	5.6
2	P	166	LEU	5.5
2	Q	135	CYS	5.5
1	B	41	ILE	5.5
1	B	341	SER	5.5
1	A	171	PHE	5.5
1	B	25	GLY	5.5
1	A	219	ASN	5.4
1	A	254	ALA	5.4
1	A	252	ASN	5.4
1	D	347	ALA	5.4
1	C	11	GLY	5.4
1	A	141	ILE	5.4
1	B	114	TYR	5.3
1	C	115	PHE	5.3
2	P	10	GLU	5.3
1	D	70	PRO	5.3
1	B	318	ASN	5.3
1	D	342	MET	5.3
1	C	262	PHE	5.3
1	C	270	LEU	5.3
1	B	173	PHE	5.2
1	D	260	SER	5.2
3	W	152	TRP	5.2
1	B	70	PRO	5.2
1	A	25	GLY	5.2
2	P	163	SER	5.2
3	S	159	GLU	5.2
1	B	171	PHE	5.2
2	P	135	CYS	5.2
1	A	265	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	116	PHE	5.1
1	D	262	PHE	5.1
1	D	164	GLY	5.1
1	D	38	THR	5.1
1	C	337	PHE	5.1
1	C	25	GLY	5.0
1	B	343	SER	5.0
1	B	254	ALA	5.0
1	B	10	VAL	5.0
1	D	268	MET	5.0
3	S	170	ASP	5.0
2	P	162	ASN	4.9
1	B	243	THR	4.9
1	D	337	PHE	4.9
1	B	150	VAL	4.9
1	A	128	THR	4.9
1	B	117	PRO	4.9
1	B	262	PHE	4.9
1	B	28	VAL	4.9
1	C	174	LYS	4.9
1	C	346	ALA	4.9
1	B	141	ILE	4.8
1	A	41	ILE	4.8
1	B	342	MET	4.8
1	C	287	LEU	4.8
2	P	83	LEU	4.8
1	B	187	MET	4.8
1	B	219	ASN	4.7
1	D	34	ASN	4.7
1	A	176	GLU	4.7
1	B	145	LYS	4.7
2	Q	133	PRO	4.7
2	P	194	THR	4.7
1	C	34	ASN	4.7
1	C	36	ALA	4.7
2	P	92	SER	4.7
2	P	178	GLN	4.7
1	D	285	GLY	4.7
1	B	249	MET	4.7
1	A	185	SER	4.7
2	Q	166	LEU	4.6
2	P	167	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	321	GLY	4.6
1	C	37	ALA	4.6
2	P	71	THR	4.6
1	D	281	CYS	4.6
1	B	29	PHE	4.6
1	D	114	TYR	4.6
2	P	198	GLU	4.6
3	S	200	GLU	4.6
2	P	8	GLY	4.6
1	A	264	ASP	4.6
1	A	26	SER	4.6
1	A	122	PRO	4.6
1	B	250	ILE	4.6
1	B	170	TRP	4.6
1	C	248	GLY	4.6
1	B	268	MET	4.6
1	A	343	SER	4.5
1	C	183	ASN	4.5
1	B	182	TRP	4.5
2	P	12	VAL	4.5
1	B	174	LYS	4.5
1	A	247	MET	4.5
1	C	114	TYR	4.5
3	W	123	PRO	4.5
1	B	345	ASN	4.5
1	D	215	GLY	4.5
1	B	44	TYR	4.5
1	C	113	SER	4.4
1	A	322	THR	4.4
1	B	123	LEU	4.4
1	B	138	LEU	4.4
1	C	125	LEU	4.4
1	B	163	VAL	4.4
1	D	167	VAL	4.4
1	D	247	MET	4.4
1	C	44	TYR	4.4
2	Q	218	VAL	4.4
2	Q	10	GLU	4.4
1	A	249	MET	4.4
1	D	325	ALA	4.4
1	A	16	THR	4.4
1	A	18	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	272	ASP	4.4
2	Q	91	SER	4.4
1	C	40	GLY	4.3
1	B	251	PRO	4.3
2	P	154	PRO	4.3
1	B	276	ALA	4.3
1	B	352	LEU	4.3
1	D	138	LEU	4.3
2	P	216	LYS	4.3
1	A	316	ARG	4.3
1	A	44	TYR	4.3
1	B	354	SER	4.3
1	C	129	CYS	4.3
1	C	275	GLY	4.3
2	Q	83	LEU	4.3
1	B	113	SER	4.3
1	B	252	ASN	4.3
1	D	122	PRO	4.3
1	C	379	HIS	4.2
1	C	32	PRO	4.2
1	A	189	THR	4.2
1	B	148	THR	4.2
1	C	260	SER	4.2
1	C	247	MET	4.2
1	C	342	MET	4.2
1	A	173	PHE	4.2
1	A	37	ALA	4.2
1	A	70	PRO	4.2
1	C	263	GLY	4.2
1	A	65	SER	4.2
2	Q	7	SER	4.2
1	C	277	ILE	4.2
3	S	191	TYR	4.2
1	D	408	LYS	4.2
1	A	409	GLU	4.2
3	W	159	GLU	4.2
1	C	46	TRP	4.2
1	C	250	ILE	4.2
1	D	37	ALA	4.2
1	C	381	GLY	4.2
1	D	322	THR	4.2
1	C	209	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	343	SER	4.1
1	B	222	ARG	4.1
3	S	198	THR	4.1
1	D	115	PHE	4.1
2	P	132	ALA	4.1
1	A	20	SER	4.1
2	P	168	SER	4.1
2	P	191	PRO	4.1
2	Q	120	SER	4.1
1	B	169	GLY	4.1
2	P	201	THR	4.1
1	C	249	MET	4.1
1	B	348	LYS	4.1
1	D	188	ASN	4.1
1	B	258	SER	4.1
1	C	226	ILE	4.1
1	B	119	LEU	4.0
1	C	119	LEU	4.0
1	D	264	ASP	4.0
2	P	180	ASP	4.0
1	C	120	LYS	4.0
3	S	166	ASN	4.0
1	D	141	ILE	4.0
1	C	42	ALA	4.0
3	W	200	GLU	4.0
1	B	344	PRO	4.0
1	A	215	GLY	4.0
1	B	27	GLY	4.0
3	W	188	LYS	4.0
3	S	151	LYS	4.0
1	A	183	ASN	4.0
1	D	439	ASP	4.0
1	A	19	VAL	4.0
1	A	13	ILE	4.0
1	A	280	PHE	4.0
1	A	345	ASN	4.0
3	S	149	ASN	4.0
1	A	408	LYS	4.0
3	S	153	LYS	4.0
1	B	39	GLY	4.0
1	D	263	GLY	4.0
1	C	170	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
3	W	162	ASN	4.0
3	S	142	ASN	4.0
1	A	123	LEU	4.0
1	B	256	ARG	3.9
2	Q	64	PHE	3.9
1	A	120	LYS	3.9
2	P	143	VAL	3.9
2	Q	208	ALA	3.9
1	A	119	LEU	3.9
1	B	16	THR	3.9
3	S	209	PRO	3.9
1	A	281	CYS	3.9
1	B	327	LEU	3.9
1	C	187	MET	3.9
1	C	279	SER	3.9
2	P	196	PRO	3.9
1	B	400	TRP	3.9
1	D	199	VAL	3.9
1	C	38	THR	3.9
1	B	429	ASN	3.9
1	A	272	ASP	3.9
1	A	279	SER	3.9
1	B	26	SER	3.9
1	B	273	THR	3.8
2	P	136	GLY	3.8
3	S	172	ASP	3.8
1	C	254	ALA	3.8
1	C	265	ALA	3.8
1	C	268	MET	3.8
1	C	291	GLY	3.8
1	C	321	GLY	3.8
1	C	280	PHE	3.8
1	B	125	LEU	3.8
1	A	57	SER	3.8
1	B	245	ALA	3.8
2	P	89	GLU	3.8
1	A	200	THR	3.8
1	A	47	LEU	3.8
1	D	219	ASN	3.8
1	D	120	LYS	3.8
1	A	165	ILE	3.8
2	P	144	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	34	ASN	3.8
1	C	219	ASN	3.8
1	A	27	GLY	3.8
1	C	71	GLY	3.8
1	A	138	LEU	3.8
1	B	194	GLN	3.7
1	B	172	TRP	3.7
3	S	4	MET	3.7
1	D	71	GLY	3.7
1	A	114	TYR	3.7
1	A	251	PRO	3.7
1	C	190	PHE	3.7
1	D	170	TRP	3.7
1	C	292	GLY	3.7
1	A	190	PHE	3.7
1	A	188	ASN	3.7
1	A	125	LEU	3.7
2	Q	214	ASP	3.7
2	P	101	GLY	3.7
3	S	123	PRO	3.7
3	S	188	LYS	3.7
1	A	49	THR	3.7
1	A	245	ALA	3.7
1	A	268	MET	3.7
3	W	210	ILE	3.7
2	P	145	LEU	3.7
1	A	186	GLY	3.7
3	W	182	SER	3.7
1	C	315	ALA	3.7
2	P	70	LEU	3.7
1	A	308	GLY	3.7
1	D	186	GLY	3.7
1	D	385	PRO	3.6
1	D	435	PRO	3.6
1	C	439	ASP	3.6
1	D	251	PRO	3.6
1	D	261	PRO	3.6
3	S	213	SER	3.6
2	P	214	ASP	3.6
1	B	126	THR	3.6
2	P	123	THR	3.6
1	B	47	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	118	ILE	3.6
1	D	27	GLY	3.6
3	S	92	CYS	3.6
1	D	282	ALA	3.6
2	Q	89	GLU	3.6
1	A	38	THR	3.6
1	A	243	THR	3.6
3	W	183	THR	3.6
3	S	168	TRP	3.6
1	A	241	LEU	3.6
1	B	287	LEU	3.6
1	A	274	ALA	3.6
1	C	274	ALA	3.6
1	C	288	GLY	3.5
1	C	109	VAL	3.5
1	A	269	ALA	3.5
1	B	270	LEU	3.5
2	P	90	ASN	3.5
1	C	243	THR	3.5
2	P	124	THR	3.5
1	B	11	GLY	3.5
1	A	174	LYS	3.5
2	P	190	VAL	3.5
1	A	270	LEU	3.5
1	D	244	THR	3.5
1	C	163	VAL	3.5
1	B	30	LEU	3.5
2	P	86	LEU	3.5
1	A	164	GLY	3.5
1	C	172	TRP	3.5
1	D	187	MET	3.5
1	C	128	THR	3.5
1	A	233	LEU	3.5
1	A	220	PRO	3.5
1	A	344	PRO	3.5
1	B	122	PRO	3.5
1	A	250	ILE	3.5
2	Q	195	TRP	3.5
1	D	10	VAL	3.4
1	D	352	LEU	3.4
2	P	87	THR	3.4
1	B	166	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
3	S	179	SER	3.4
1	D	353	VAL	3.4
3	S	137	VAL	3.4
1	A	52	GLY	3.4
1	A	275	GLY	3.4
1	D	283	ALA	3.4
1	B	355	SER	3.4
3	S	126	SER	3.4
1	A	400	TRP	3.4
1	A	121	ASP	3.4
1	D	29	PHE	3.4
1	D	123	LEU	3.4
1	D	200	THR	3.4
1	A	412	TRP	3.4
1	C	168	PHE	3.4
2	P	64	PHE	3.4
3	W	189	ASP	3.4
1	C	157	LEU	3.4
1	B	253	ALA	3.4
1	D	326	GLY	3.4
2	Q	101	GLY	3.4
1	A	348	LYS	3.4
1	C	151	GLN	3.4
1	C	189	THR	3.4
2	Q	178	GLN	3.4
3	W	185	THR	3.4
1	C	122	PRO	3.4
1	B	217	VAL	3.4
1	D	125	LEU	3.4
1	D	348	LYS	3.4
1	C	251	PRO	3.4
1	D	148	THR	3.4
1	A	337	PHE	3.3
1	B	280	PHE	3.3
1	C	121	ASP	3.3
1	A	111	TYR	3.3
1	A	248	GLY	3.3
2	Q	215	LYS	3.3
3	W	153	LYS	3.3
1	D	140	ASN	3.3
3	S	215	ASN	3.3
1	D	116	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	3.3
1	C	28	VAL	3.3
1	D	257	VAL	3.3
2	P	192	SER	3.3
1	C	144	PRO	3.3
1	D	220	PRO	3.3
1	A	273	THR	3.3
1	A	262	PHE	3.3
1	C	173	PHE	3.3
3	W	165	LEU	3.3
1	A	131	ALA	3.3
1	B	340	SER	3.3
2	Q	84	SER	3.3
1	B	121	ASP	3.3
3	S	156	ASP	3.3
3	W	194	HIS	3.3
1	C	123	LEU	3.3
1	C	138	LEU	3.3
1	D	249	MET	3.3
1	C	283	ALA	3.3
1	B	209	SER	3.3
3	W	12	SER	3.3
3	S	47	SER	3.3
3	S	131	SER	3.3
1	C	347	ALA	3.3
2	P	164	GLY	3.3
1	C	436	TYR	3.2
1	D	222	ARG	3.2
2	P	125	PRO	3.2
2	P	5	GLN	3.2
1	B	246	ILE	3.2
1	C	96	ALA	3.2
1	C	140	ASN	3.2
1	C	169	GLY	3.2
1	A	30	LEU	3.2
1	D	190	PHE	3.2
1	C	105	VAL	3.2
1	C	184	VAL	3.2
1	D	142	VAL	3.2
3	S	23	CYS	3.2
1	A	172	TRP	3.2
1	D	271	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	330	VAL	3.2
1	D	73	SER	3.2
2	P	85	SER	3.2
3	W	27	SER	3.2
1	B	286	CYS	3.2
1	D	243	THR	3.2
1	A	342	MET	3.2
1	B	102	ILE	3.2
1	A	378	GLY	3.2
1	C	108	GLY	3.2
1	D	46	TRP	3.2
1	D	436	TYR	3.2
1	D	350	PHE	3.2
2	Q	207	PRO	3.2
1	A	148	THR	3.2
1	A	347	ALA	3.2
1	B	351	GLY	3.2
1	B	378	GLY	3.2
1	C	31	LEU	3.2
2	Q	90	ASN	3.2
1	B	192	ALA	3.2
1	A	298	GLY	3.1
1	A	163	VAL	3.1
2	Q	213	VAL	3.1
2	P	153	PHE	3.1
1	A	323	PRO	3.1
3	W	216	ARG	3.1
1	B	33	ALA	3.1
2	P	215	LYS	3.1
1	C	148	THR	3.1
2	P	7	SER	3.1
2	Q	66	GLY	3.1
1	B	281	CYS	3.1
1	B	409	GLU	3.1
1	D	129	CYS	3.1
1	C	171	PHE	3.1
1	A	117	PRO	3.1
1	B	34	ASN	3.1
1	B	183	ASN	3.1
3	S	203	HIS	3.1
1	A	315	ALA	3.1
1	C	244	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	355	SER	3.1
1	B	164	GLY	3.1
3	S	189	ASP	3.1
2	P	62	GLU	3.1
1	D	127	LEU	3.1
2	P	11	LEU	3.1
1	A	191	GLY	3.1
1	C	45	GLY	3.1
1	C	164	GLY	3.1
1	D	25	GLY	3.1
1	D	128	THR	3.1
2	Q	146	GLY	3.1
1	D	405	SER	3.1
2	Q	187	SER	3.1
1	A	257	VAL	3.1
1	D	163	VAL	3.1
1	D	172	TRP	3.1
2	Q	50	TRP	3.1
2	P	67	LYS	3.1
1	B	18	MET	3.1
1	A	263	GLY	3.1
2	P	146	GLY	3.1
1	D	356	VAL	3.1
3	W	137	VAL	3.1
3	S	125	SER	3.1
1	D	171	PHE	3.1
2	Q	145	LEU	3.0
3	S	201	ALA	3.0
1	B	316	ARG	3.0
1	D	110	GLY	3.0
2	Q	40	ARG	3.0
2	Q	199	THR	3.0
1	D	324	VAL	3.0
3	W	146	LYS	3.0
1	C	118	ILE	3.0
1	C	146	MET	3.0
2	P	130	PRO	3.0
1	D	67	ASP	3.0
1	C	325	ALA	3.0
1	D	286	CYS	3.0
1	A	145	LYS	3.0
2	P	218	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	246	ILE	3.0
1	D	32	PRO	3.0
1	B	157	LEU	3.0
1	C	159	LEU	3.0
1	A	110	GLY	3.0
1	D	351	GLY	3.0
1	D	279	SER	3.0
1	D	328	LEU	3.0
3	W	158	SER	3.0
3	W	213	SER	3.0
1	A	53	ALA	3.0
1	A	169	GLY	3.0
1	A	351	GLY	3.0
3	S	157	GLY	3.0
1	B	317	VAL	3.0
1	D	330	VAL	3.0
3	S	150	VAL	3.0
3	S	30	ASN	3.0
1	D	119	LEU	3.0
2	Q	126	PRO	3.0
1	B	267	ARG	3.0
1	C	282	ALA	3.0
1	C	383	ALA	3.0
1	D	166	ALA	3.0
1	B	408	LYS	3.0
3	W	172	ASP	3.0
3	S	175	ASP	3.0
2	P	170	VAL	3.0
1	A	115	PHE	3.0
1	C	238	CYS	3.0
1	B	43	ILE	3.0
1	C	200	THR	3.0
3	S	155	ILE	3.0
1	A	278	VAL	2.9
1	B	206	GLY	2.9
2	Q	188	VAL	2.9
1	B	31	LEU	2.9
3	W	215	ASN	2.9
1	B	38	THR	2.9
3	S	216	ARG	2.9
3	W	174	LYS	2.9
1	A	276	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	209	SER	2.9
1	B	111	TYR	2.9
3	S	196	SER	2.9
3	W	163	GLY	2.9
1	A	43	ILE	2.9
1	D	118	ILE	2.9
1	D	255	LEU	2.9
3	W	166	ASN	2.9
1	C	14	PRO	2.9
1	C	142	VAL	2.9
1	C	167	VAL	2.9
3	S	208	SER	2.9
2	Q	13	LYS	2.9
1	D	83	PRO	2.9
1	D	183	ASN	2.9
3	W	141	ASN	2.9
2	P	50	TRP	2.9
3	W	51	TRP	2.9
1	B	278	VAL	2.9
1	C	137	VAL	2.9
3	S	214	PHE	2.9
1	A	69	SER	2.9
3	W	125	SER	2.9
1	C	117	PRO	2.9
3	S	124	PRO	2.9
1	B	137	VAL	2.9
1	C	217	VAL	2.9
1	C	278	VAL	2.9
1	A	40	GLY	2.9
1	A	326	GLY	2.9
1	B	136	PHE	2.9
1	C	72	GLY	2.9
1	C	111	TYR	2.9
1	C	30	LEU	2.9
1	A	151	GLN	2.8
1	B	69	SER	2.8
1	B	272	ASP	2.8
1	C	344	PRO	2.8
3	S	205	THR	2.8
1	C	110	GLY	2.8
2	Q	216	LYS	2.8
2	Q	103	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	274	ALA	2.8
1	B	167	VAL	2.8
3	S	51	TRP	2.8
1	D	174	LYS	2.8
3	S	129	LEU	2.8
1	C	276	ALA	2.8
1	D	269	ALA	2.8
1	C	261	PRO	2.8
2	Q	204	VAL	2.8
1	B	439	ASP	2.8
1	A	17	LEU	2.8
1	B	22	ASN	2.8
1	B	285	GLY	2.8
1	C	285	GLY	2.8
1	A	436	TYR	2.8
3	W	191	TYR	2.8
1	C	213	ALA	2.8
2	P	40	ARG	2.8
1	B	319	LYS	2.8
1	C	340	SER	2.8
1	C	435	PRO	2.8
2	P	133	PRO	2.8
2	P	156	PRO	2.8
1	C	66	LEU	2.8
2	Q	11	LEU	2.8
2	P	189	THR	2.8
2	Q	182	TYR	2.8
2	Q	202	CYS	2.8
1	A	325	ALA	2.8
1	C	382	LYS	2.8
1	A	64	SER	2.8
1	A	195	SER	2.8
1	D	65	SER	2.8
3	W	126	SER	2.8
2	Q	58	THR	2.8
1	B	58	MET	2.7
1	D	72	GLY	2.7
2	P	161	TRP	2.7
2	Q	65	LYS	2.7
2	Q	86	LEU	2.7
1	A	113	SER	2.7
1	B	146	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	260	SER	2.7
1	C	29	PHE	2.7
1	C	195	SER	2.7
1	D	209	SER	2.7
1	D	349	GLU	2.7
1	C	39	GLY	2.7
1	C	271	GLY	2.7
1	C	400	TRP	2.7
1	C	101	ASN	2.7
1	D	101	ASN	2.7
1	A	158	ALA	2.7
1	B	438	LEU	2.7
2	Q	81	MET	2.7
1	C	357	SER	2.7
3	S	69	SER	2.7
3	S	212	LYS	2.7
3	S	147	ASP	2.7
1	A	377	HIS	2.7
1	A	10	VAL	2.7
1	D	66	LEU	2.7
1	A	261	PRO	2.7
1	B	165	ILE	2.7
1	C	165	ILE	2.7
1	D	41	ILE	2.7
1	D	384	ARG	2.7
3	W	60	SER	2.7
1	B	266	ALA	2.7
2	Q	203	ASN	2.7
1	B	32	PRO	2.7
1	D	431	ILE	2.7
1	D	146	MET	2.7
3	W	139	PHE	2.7
1	B	215	GLY	2.7
1	C	273	THR	2.7
1	A	341	SER	2.7
2	Q	165	SER	2.7
2	P	91	SER	2.7
1	A	346	ALA	2.7
1	B	139	LEU	2.7
1	D	31	LEU	2.7
2	Q	102	ASN	2.7
1	C	218	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	409	GLU	2.6
3	S	132	GLY	2.6
1	C	281	CYS	2.6
3	W	202	THR	2.6
1	B	240	VAL	2.6
1	C	73	SER	2.6
1	C	153	VAL	2.6
2	Q	88	SER	2.6
3	S	113	ALA	2.6
1	D	377	HIS	2.6
1	A	439	ASP	2.6
1	A	32	PRO	2.6
1	D	310	PHE	2.6
1	D	323	PRO	2.6
2	P	61	ASN	2.6
1	B	308	GLY	2.6
3	W	198	THR	2.6
1	A	35	LEU	2.6
1	B	407	ALA	2.6
1	A	289	SER	2.6
1	A	24	MET	2.6
3	W	214	PHE	2.6
1	C	434	ASN	2.6
1	D	90	ASN	2.6
2	P	102	ASN	2.6
3	S	1	GLU	2.6
1	A	327	LEU	2.6
1	D	35	LEU	2.6
1	D	233	LEU	2.6
1	D	160	VAL	2.6
2	P	58	THR	2.6
3	W	138	CYS	2.6
1	D	185	SER	2.6
2	Q	186	SER	2.6
2	P	179	SER	2.6
1	B	168	PHE	2.6
1	C	83	PRO	2.6
3	W	86	ASP	2.6
1	A	381	GLY	2.6
1	C	345	ASN	2.6
2	P	169	GLY	2.6
3	S	195	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	197	LEU	2.6
1	D	218	LYS	2.6
1	A	187	MET	2.6
2	Q	119	SER	2.6
2	P	120	SER	2.6
1	D	248	GLY	2.6
1	B	35	LEU	2.6
1	D	159	LEU	2.6
1	B	37	ALA	2.6
1	D	213	ALA	2.6
2	Q	200	VAL	2.6
1	A	29	PHE	2.5
1	D	44	TYR	2.5
3	S	197	TYR	2.5
2	P	53	PRO	2.5
3	S	61	GLY	2.5
1	B	15	VAL	2.5
1	D	316	ARG	2.5
3	S	141	ASN	2.5
1	C	412	TRP	2.5
3	S	118	THR	2.5
1	D	380	PHE	2.5
3	W	63	PRO	2.5
1	A	292	GLY	2.5
1	C	298	GLY	2.5
1	D	113	SER	2.5
1	C	222	ARG	2.5
3	S	154	LYS	2.5
1	A	33	ALA	2.5
1	B	152	ALA	2.5
2	Q	198	GLU	2.5
2	Q	144	THR	2.5
1	A	206	GLY	2.5
1	A	238	CYS	2.5
1	C	231	GLY	2.5
2	Q	74	LYS	2.5
3	S	174	LYS	2.5
1	B	195	SER	2.5
1	A	217	VAL	2.5
1	D	105	VAL	2.5
1	D	346	ALA	2.5
1	A	277	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	104	MET	2.5
2	Q	71	THR	2.5
1	A	112	LEU	2.5
1	B	290	LEU	2.5
1	C	47	LEU	2.5
1	C	377	HIS	2.5
2	Q	171	HIS	2.5
1	A	129	CYS	2.5
1	D	398	CYS	2.5
3	S	167	SER	2.5
3	S	190	GLU	2.5
1	A	350	PHE	2.5
1	C	408	LYS	2.5
3	W	151	LYS	2.5
1	A	31	LEU	2.5
3	S	193	ARG	2.5
1	C	220	PRO	2.5
2	Q	41	PRO	2.5
1	A	45	GLY	2.5
1	B	105	VAL	2.5
2	P	188	VAL	2.5
1	B	36	ALA	2.4
1	B	259	ALA	2.4
1	C	289	SER	2.4
3	S	127	GLU	2.4
1	B	115	PHE	2.4
1	C	339	PHE	2.4
1	C	62	LYS	2.4
1	C	293	TRP	2.4
2	P	33	ASP	2.4
1	C	27	GLY	2.4
1	D	40	GLY	2.4
1	D	109	VAL	2.4
1	C	407	ALA	2.4
1	D	284	ALA	2.4
3	S	93	GLN	2.4
1	A	102	ILE	2.4
1	A	118	ILE	2.4
1	A	73	SER	2.4
1	B	242	SER	2.4
2	P	165	SER	2.4
1	A	426	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	2.4
1	B	46	TRP	2.4
1	D	198	ASN	2.4
2	Q	201	THR	2.4
3	S	95	TRP	2.4
2	Q	191	PRO	2.4
1	A	71	GLY	2.4
1	C	387	TYR	2.4
1	D	28	VAL	2.4
1	D	288	GLY	2.4
1	A	162	ILE	2.4
1	B	334	MET	2.4
1	A	149	ARG	2.4
1	B	382	LYS	2.4
1	A	204	PHE	2.4
2	Q	62	GLU	2.4
1	B	279	SER	2.4
1	B	159	LEU	2.4
1	A	161	PRO	2.4
2	Q	130	PRO	2.4
3	S	187	THR	2.4
1	B	142	VAL	2.4
1	B	358	VAL	2.4
1	B	282	ALA	2.4
1	C	33	ALA	2.4
1	C	284	ALA	2.4
2	Q	217	ILE	2.4
1	B	120	LYS	2.4
1	D	24	MET	2.4
2	Q	19	LYS	2.4
3	S	111	LYS	2.4
1	A	290	LEU	2.4
1	D	197	LEU	2.4
1	A	260	SER	2.4
2	Q	168	SER	2.4
1	C	286	CYS	2.4
1	A	28	VAL	2.4
1	A	126	THR	2.4
1	D	102	ILE	2.4
1	D	433	LYS	2.4
3	S	204	LYS	2.4
1	A	339	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	56	LEU	2.4
1	C	133	LEU	2.4
2	P	76	SER	2.4
3	S	206	SER	2.4
1	B	238	CYS	2.4
2	Q	156	PRO	2.4
2	P	160	THR	2.3
3	W	207	THR	2.3
1	B	158	ALA	2.3
1	C	348	LYS	2.3
1	D	43	ILE	2.3
1	D	427	ASN	2.3
2	P	217	ILE	2.3
1	D	137	VAL	2.3
2	P	197	SER	2.3
1	B	71	GLY	2.3
1	C	294	THR	2.3
2	Q	211	THR	2.3
3	S	57	LYS	2.3
1	A	104	MET	2.3
1	A	198	ASN	2.3
1	C	58	MET	2.3
1	B	151	GLN	2.3
1	B	339	PHE	2.3
3	S	186	LEU	2.3
1	D	194	GLN	2.3
1	A	433	LYS	2.3
1	A	170	TRP	2.3
1	A	166	ALA	2.3
1	C	26	SER	2.3
1	D	277	ILE	2.3
1	D	155	THR	2.3
2	P	75	SER	2.3
1	C	380	PHE	2.3
1	C	257	VAL	2.3
2	P	212	LYS	2.3
1	C	256	ARG	2.3
1	B	144	PRO	2.3
1	B	277	ILE	2.3
1	B	435	PRO	2.3
1	C	385	PRO	2.3
2	Q	154	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	182	TRP	2.3
1	C	376	GLY	2.3
3	W	45	GLY	2.3
1	A	192	ALA	2.3
1	C	166	ALA	2.3
1	C	269	ALA	2.3
1	B	49	THR	2.3
1	B	128	THR	2.3
1	C	24	MET	2.3
2	P	211	THR	2.3
3	W	78	THR	2.3
3	W	187	THR	2.3
1	A	223	ASN	2.3
1	A	222	ARG	2.3
1	B	156	VAL	2.3
1	D	14	PRO	2.3
1	D	45	GLY	2.3
3	W	168	TRP	2.3
1	C	35	LEU	2.3
1	D	357	SER	2.3
2	P	147	CYS	2.3
3	S	6	GLN	2.3
3	S	146	LYS	2.3
1	C	384	ARG	2.3
1	C	150	VAL	2.3
2	P	55	ASP	2.3
3	W	147	ASP	2.3
1	B	208	GLU	2.2
2	Q	155	GLU	2.2
1	C	41	ILE	2.2
1	B	45	GLY	2.2
2	P	41	PRO	2.2
3	S	15	PRO	2.2
1	B	328	LEU	2.2
1	C	233	LEU	2.2
1	A	391	THR	2.2
1	B	337	PHE	2.2
1	A	387	TYR	2.2
1	B	397	TYR	2.2
3	S	24	SER	2.2
1	B	353	VAL	2.2
1	C	324	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	299	GLN	2.2
2	Q	147	CYS	2.2
1	A	349	GLU	2.2
1	B	315	ALA	2.2
1	C	127	LEU	2.2
1	C	245	ALA	2.2
1	D	275	GLY	2.2
3	S	70	GLY	2.2
3	S	116	ALA	2.2
1	C	136	PHE	2.2
1	C	49	THR	2.2
2	Q	163	SER	2.2
3	S	28	SER	2.2
1	A	393	VAL	2.2
3	W	19	VAL	2.2
1	B	223	ASN	2.2
1	C	102	ILE	2.2
1	D	238	CYS	2.2
1	B	67	ASP	2.2
1	A	376	GLY	2.2
1	C	253	ALA	2.2
1	D	206	GLY	2.2
1	D	241	LEU	2.2
3	S	117	PRO	2.2
2	Q	189	THR	2.2
1	A	124	VAL	2.2
3	W	119	VAL	2.2
1	B	135	ILE	2.2
1	B	162	ILE	2.2
1	C	147	ILE	2.2
2	P	203	ASN	2.2
3	W	127	GLU	2.2
3	W	184	LEU	2.2
1	A	231	GLY	2.2
1	A	398	CYS	2.2
1	A	407	ALA	2.2
3	S	37	MET	2.2
1	C	97	CYS	2.2
1	C	100	GLY	2.2
3	S	45	GLY	2.2
1	D	430	ARG	2.2
1	C	182	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	196	THR	2.2
3	W	164	VAL	2.2
3	W	211	VAL	2.2
3	S	52	ILE	2.2
1	D	157	LEU	2.2
1	D	290	LEU	2.2
1	D	144	PRO	2.2
2	Q	150	LYS	2.2
2	P	126	PRO	2.2
2	P	150	LYS	2.2
3	W	84	ALA	2.2
3	W	142	ASN	2.2
1	A	72	GLY	2.2
1	C	191	GLY	2.2
1	D	432	HIS	2.2
1	D	216	VAL	2.1
1	D	423	LEU	2.1
1	A	211	SER	2.1
1	B	303	ALA	2.1
1	C	242	SER	2.1
1	D	69	SER	2.1
3	S	173	SER	2.1
3	S	182	SER	2.1
1	C	311	PRO	2.1
1	D	169	GLY	2.1
3	W	16	GLY	2.1
1	D	173	PHE	2.1
3	W	66	PHE	2.1
1	C	272	ASP	2.1
1	A	48	VAL	2.1
1	D	358	VAL	2.1
2	Q	28	THR	2.1
1	B	13	ILE	2.1
2	P	60	TYR	2.1
3	W	97	TYR	2.1
3	W	18	LYS	2.1
1	A	299	GLN	2.1
1	A	253	ALA	2.1
1	D	152	ALA	2.1
1	D	256	ARG	2.1
1	A	39	GLY	2.1
1	B	57	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	PHE	2.1
1	B	188	ASN	2.1
1	D	280	PHE	2.1
1	B	257	VAL	2.1
3	S	211	VAL	2.1
1	B	205	ILE	2.1
1	C	322	THR	2.1
1	D	165	ILE	2.1
1	B	436	TYR	2.1
1	D	87	TYR	2.1
1	C	430	ARG	2.1
1	A	194	GLN	2.1
1	B	154	ALA	2.1
1	D	253	ALA	2.1
1	D	291	GLY	2.1
1	D	311	PRO	2.1
2	P	155	GLU	2.1
3	S	76	SER	2.1
1	C	240	VAL	2.1
1	D	379	HIS	2.1
1	D	189	THR	2.1
3	S	101	THR	2.1
3	S	169	THR	2.1
1	D	265	ALA	2.1
1	B	406	GLY	2.1
2	P	151	GLY	2.1
2	Q	125	PRO	2.1
3	S	122	PHE	2.1
3	W	24	SER	2.1
1	C	188	ASN	2.1
2	P	122	LYS	2.1
1	A	362	LEU	2.1
3	S	194	HIS	2.1
1	B	87	TYR	2.1
1	D	111	TYR	2.1
1	A	152	ALA	2.1
1	A	236	ALA	2.1
1	D	42	ALA	2.1
1	B	338	GLN	2.1
1	B	261	PRO	2.1
1	A	240	VAL	2.0
2	P	213	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	242	SER	2.0
2	P	210	SER	2.0
1	C	290	LEU	2.0
3	W	186	LEU	2.0
2	Q	161	TRP	2.0
1	D	49	THR	2.0
1	D	306	ASP	2.0
2	P	73	ASP	2.0
2	Q	196	PRO	2.0
1	A	105	VAL	2.0
1	A	137	VAL	2.0
2	P	176	VAL	2.0
1	B	309	LEU	2.0
2	Q	131	LEU	2.0
3	S	74	SER	2.0
1	C	198	ASN	2.0
3	W	30	ASN	2.0
1	A	103	ALA	2.0
3	W	118	THR	2.0
3	W	201	ALA	2.0
1	A	369	CYS	2.0
2	Q	56	GLY	2.0
2	P	42	GLY	2.0
2	Q	67	LYS	2.0
2	P	3	GLN	2.0
1	A	430	ARG	2.0
1	B	109	VAL	2.0
1	D	240	VAL	2.0
1	D	278	VAL	2.0
1	A	375	LEU	2.0
3	W	110	ILE	2.0
3	W	155	ILE	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.