



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:52 AM GMT

PDB ID : 3NCY  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

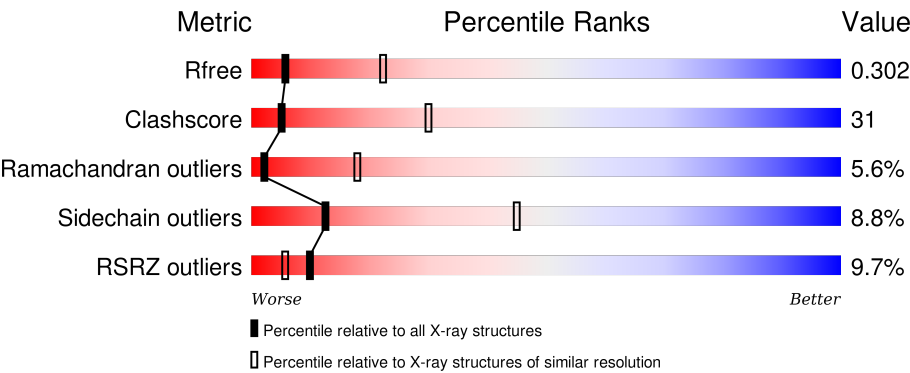
# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	<div><div>13%</div><div><div></div><div>47%</div><div>40%</div><div>8%</div><div>5%</div></div></div>
1	B	445	<div><div>9%</div><div><div></div><div>46%</div><div>40%</div><div>7%</div><div>6%</div></div></div>
1	C	445	<div><div>7%</div><div><div></div><div>47%</div><div>41%</div><div>7%</div><div>6%</div></div></div>
1	D	445	<div><div>9%</div><div><div></div><div>47%</div><div>41%</div><div>7%</div><div>6%</div></div></div>
2	P	219	<div><div>6%</div><div><div></div><div>46%</div><div>45%</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	Q	219	
3	S	211	
3	W	211	

## 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			

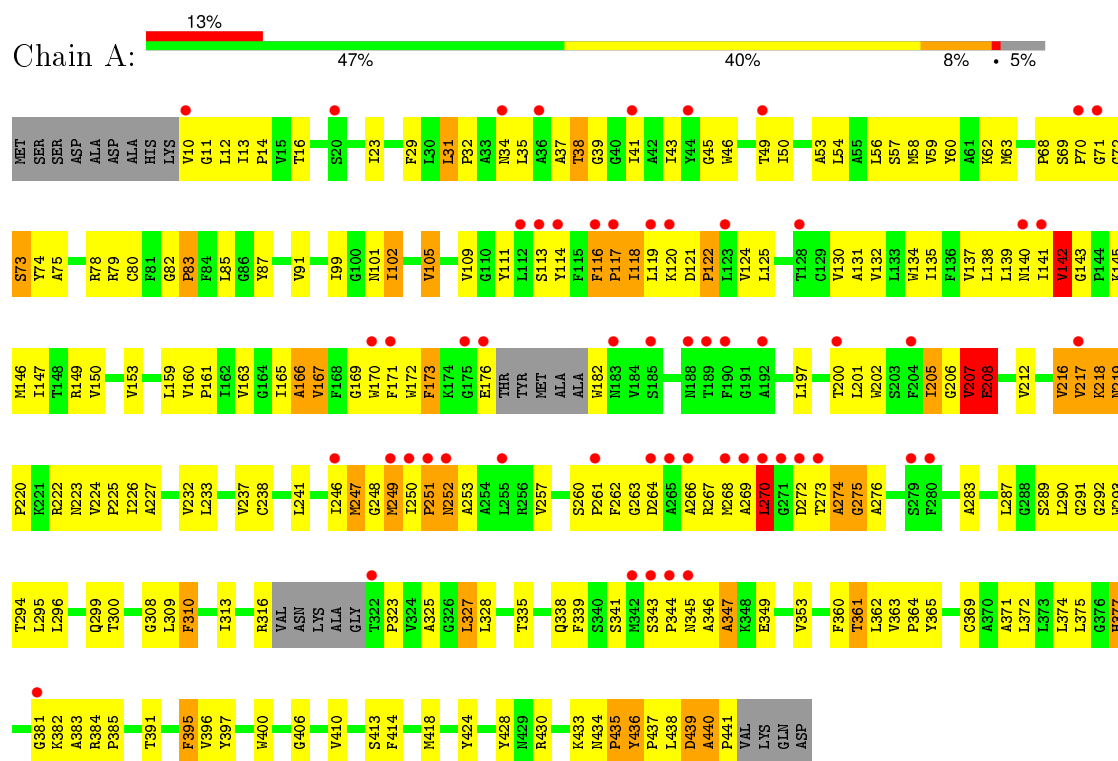
- Molecule 3 is a protein called Fab Light chain.

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			

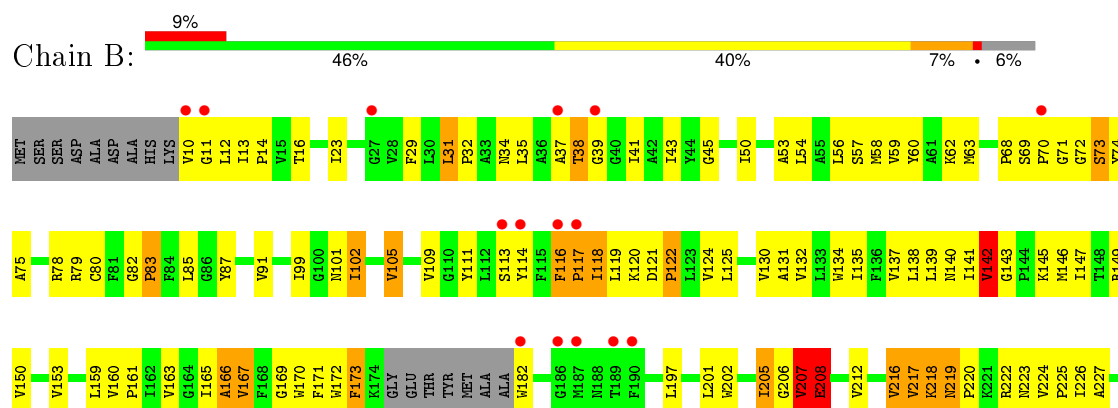
### 3 Residue-property plots

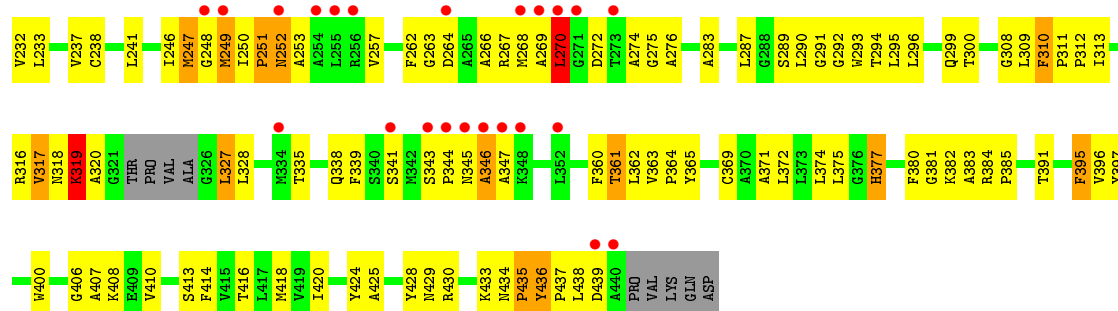
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

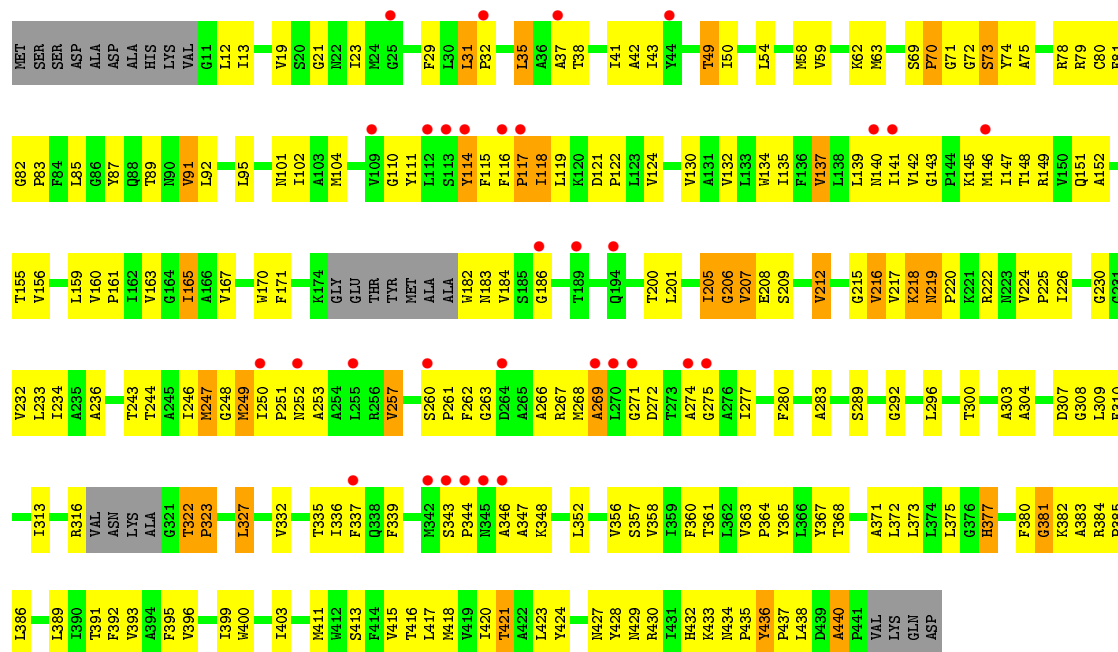


#### • Molecule 1: AdiC

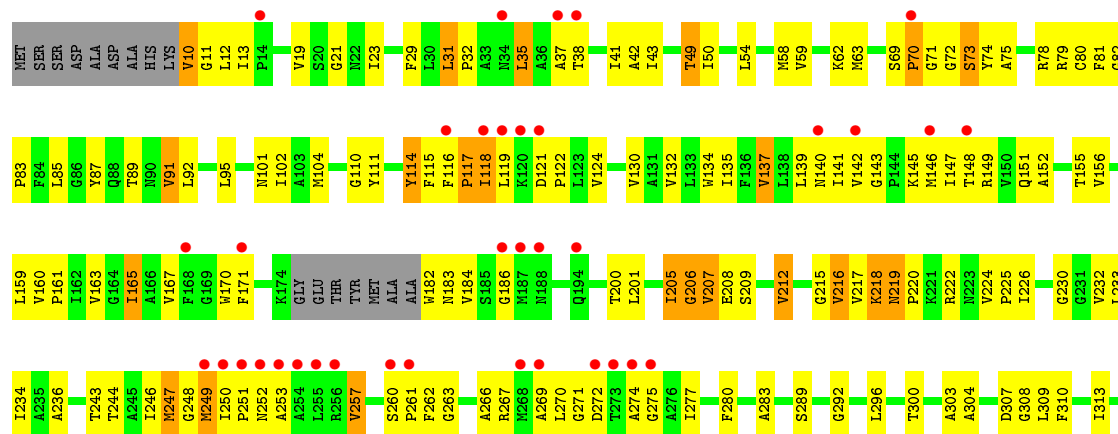


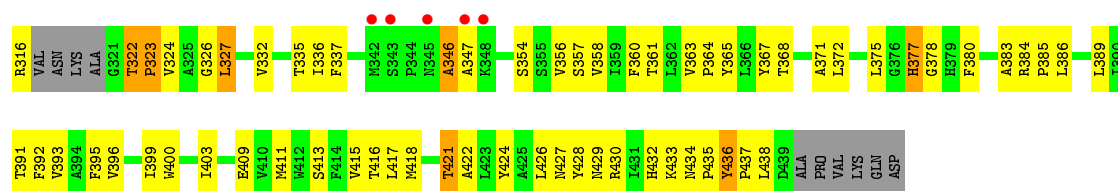


• Molecule 1: AdiC

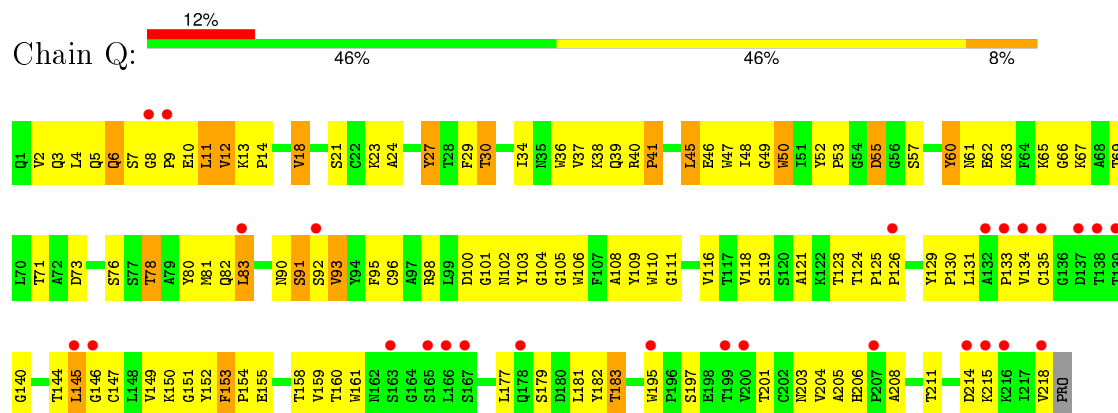


• Molecule 1: AdiC

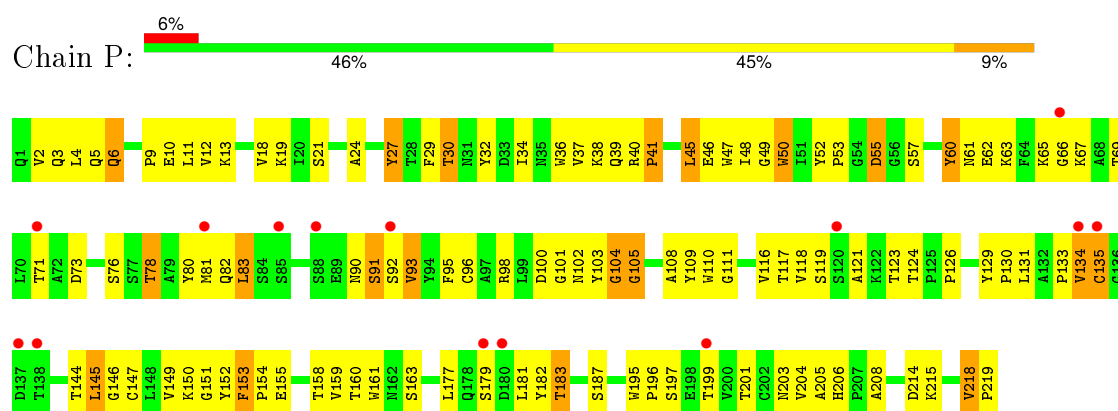




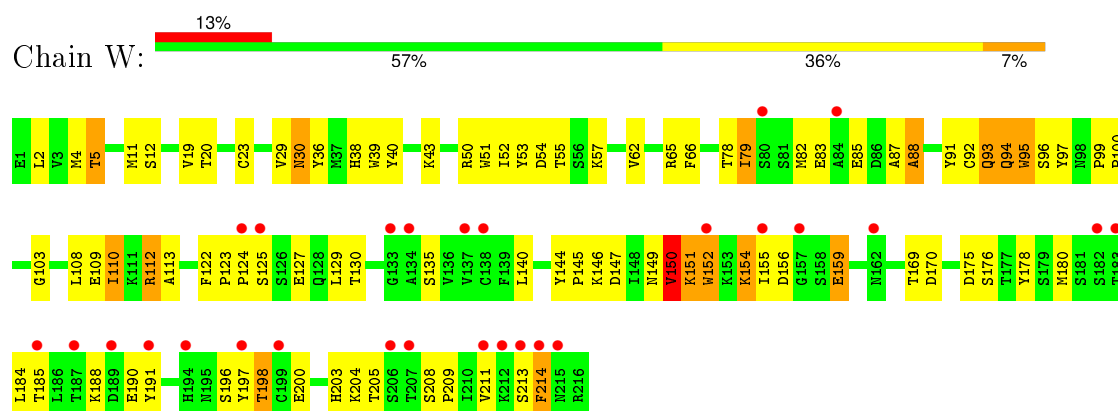
• Molecule 2: Fab Heavy chain



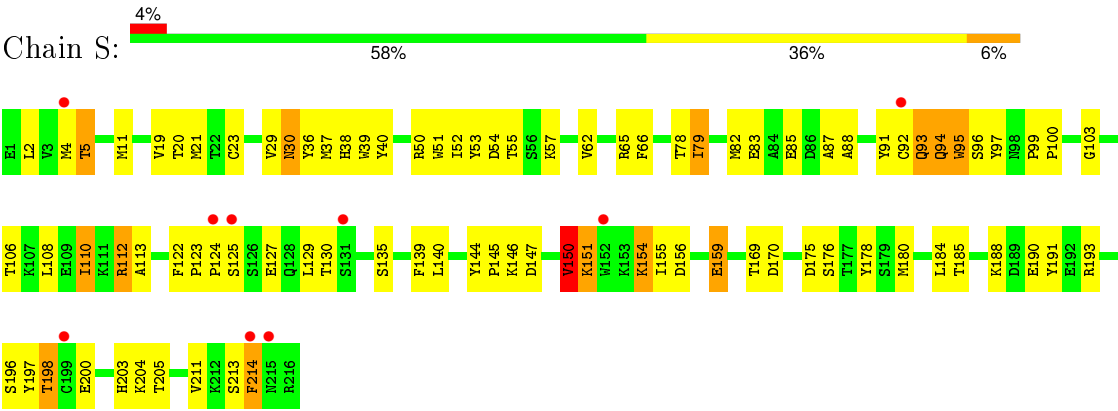
• Molecule 2: Fab Heavy chain



• 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, $\alpha$ , $\beta$ , $\gamma$	79.66 Å   104.15 Å   154.03 Å 81.96°   75.93°   73.73°	Depositor
Resolution (Å)	33.23 – 3.20 45.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (33.23-3.20) 94.1 (45.88-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 3.19 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.282   ,   0.312 0.274   ,   0.302	Depositor DCC
$R_{free}$ test set	3612 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 84.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 73033 reflections	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	18693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.22	0/3125	0.42	0/4281
1	B	0.22	0/3110	0.43	0/4257
1	C	0.22	0/3107	0.43	0/4256
1	D	0.22	0/3103	0.42	0/4250
2	P	0.22	0/1694	0.46	1/2319 (0.0%)
2	Q	0.23	0/1686	0.46	0/2307
3	S	0.23	0/1665	0.42	0/2260
3	W	0.23	0/1665	0.43	0/2260
All	All	0.22	0/19155	0.43	1/26190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	134	VAL	N-CA-C	-5.71	95.58	111.00

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	201	0
1	B	3039	0	3112	191	0
1	C	3034	0	3098	190	0
1	D	3031	0	3102	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1647	0	1601	128	0
2	Q	1640	0	1594	135	0
3	S	1625	0	1550	83	0
3	W	1625	0	1550	85	0
All	All	18693	0	18727	1142	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 31.

All (1142) 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
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
2:Q:10:GLU:HG2	2:Q:11:LEU:H	1.32	0.94
1:B:39:GLY:HA3	1:B:247:MET:HG3	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:313:ILE:HD12	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
1:D:50:ILE:HD11	1:D:236:ALA:HB1	1.62	0.81
1:B:38:THR:HG21	1:B:41:ILE:HG22	1.61	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:D:356:VAL:CG1	1:D:409:GLU:HB3	2.11	0.80
1:A:216:VAL:HG12	1:A:217:VAL:H	1.45	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
2:Q:154:PRO:HB2	2:Q:206:HIS:HE2	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:142:VAL:HG13	1:B:142:VAL:O	1.82	0.78
1:B:252:ASN:HB2	1:B:253:ALA:HA	1.65	0.78
1:B:35:LEU:HD22	1:B:247:MET:HG2	1.66	0.77
1:A:142:VAL:O	1:A:142:VAL:HG13	1.83	0.77
1:B:72:GLY:HA3	1:B:74:TYR:N	2.00	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
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:Q:63:LYS:HZ3	2:Q:67:LYS:NZ	1.84	0.76
2:P:24:ALA:HB1	2:P:27:TYR:HE1	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:Q:48:ILE:HG23	2:Q:67:LYS:NZ	2.04	0.72
1:A:381:GLY:N	1:A:382:LYS:HA	2.04	0.72
3:S:39:TRP:HB2	3:S:52:ILE:HB	1.69	0.72
1:D:87:TYR:CE1	1:D:424:TYR:HB2	2.25	0.71
1:C:267:ARG:HH12	1:C:277:ILE:HG22	1.55	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
2:Q:92:SER:O	2:Q:93:VAL:HB	1.91	0.71
1:D:267:ARG:HH12	1:D:277:ILE:HG22	1.55	0.71
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
2:Q:10:GLU:CG	2:Q:11:LEU:H	1.95	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:P:40:ARG:HD3	2:P:92:SER:HB2	1.72	0.70
3:W:129:LEU:HD23	3:W:188:LYS:HZ2	1.57	0.70
2:P:159:VAL:HG22	2:P:204:VAL:HG22	1.73	0.70
3:W:40:TYR:CE2	3:W:93:GLN:HG2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:129:TYR:HB3	3:S:125:SER:OG	1.91	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
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:D:49:THR:HG21	1:D:200:THR:HB	1.74	0.69
1:C:87:TYR:CE1	1:C:424:TYR:HB2	2.26	0.69
1:C:49:THR:HG21	1:C: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
2:P:39:GLN:O	2:P:92:SER:HA	1.91	0.69
1:A:54:LEU:O	1:A:58:MET:HG2	1.93	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
2:Q:63:LYS:HZ3	2:Q:67:LYS:HZ3	1.40	0.68
1:C:262:PHE:CZ	1:C:266:ALA:HB2	2.28	0.68
1:B:212:VAL:HG23	1:B:296:LEU:HD22	1.75	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
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:D:74:TYR:OH	1:D:309:LEU:HD12	1.94	0.68
1:C:430:ARG:HG2	1:D:377:HIS:CD2	2.29	0.68
1:D:134:TRP:HA	1:D:137:VAL:HG12	1.76	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:A:414:PHE:HD1	1:B:410:VAL:HG13	1.59	0.67
1:B:29:PHE:O	1:B:32:PRO:HD2	1.95	0.67
1:A:29:PHE:O	1:A:32:PRO:HD2	1.94	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:B:319:LYS:N	1:B:319:LYS:HD2	2.08	0.67
1:A:439:ASP:O	1:A:440:ALA:HB2	1.95	0.67
1:A:435:PRO:HB3	2:P:103:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:171:PHE:HA	1:B:249:MET:HB3	1.77	0.66
1:B:145:LYS:O	1:B:149:ARG:HG3	1.96	0.66
1:C:134:TRP:HA	1:C:137:VAL:HG12	1.76	0.66
1:A:72:GLY:HA3	1:A:73:SER:C	2.15	0.66
1:C:268:MET:O	1:C:269:ALA:HB2	1.95	0.66
2:Q:134:VAL:HG21	3:W:123:PRO:HD3	1.76	0.66
1:C:116:PHE:HB3	1:C:118:ILE:H	1.61	0.66
2:Q:83:LEU:HD21	2:P:199:THR:HG23	1.78	0.65
1:A:145:LYS:O	1:A:149:ARG:HG3	1.96	0.65
1:A:38:THR:HG1	1:A:182:TRP:N	1.95	0.65
1:A:10:VAL:HB	1:A:218:LYS:HD3	1.76	0.65
1:D:116:PHE:HB3	1:D:118:ILE:H	1.61	0.65
1:B:72:GLY:HA3	1:B:73:SER:C	2.15	0.65
2:Q:134:VAL:CG2	3:W:123:PRO:HD3	2.26	0.65
2:P:63:LYS:HZ3	2:P:67:LYS:NZ	1.94	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
2:P:91:SER:HA	2:P:92:SER:CB	2.15	0.64
3:S:38:HIS:CE1	3:S:54:ASP:H	2.16	0.64
2:P:154:PRO:HB2	2:P:206:HIS:NE2	2.11	0.64
1:D:432:HIS:HD2	1:D:434:ASN:HB2	1.62	0.64
1:C:74:TYR:OH	1:C:309:LEU:HD12	1.97	0.64
1:B:38:THR:HG1	1:B:182:TRP:N	1.95	0.64
2:Q:154:PRO:HB2	2:Q:206:HIS:NE2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:CE1	1:B:266:ALA:HB2	2.33	0.63
3:S:198:THR:HG23	3:S:213:SER:HB2	1.79	0.63
1:A:274:ALA:HA	1:A:275:GLY:C	2.19	0.63
3:W:124:PRO:HB2	3:W:129:LEU:HD11	1.80	0.63
1:D:161:PRO:O	1:D:165:ILE:HG12	1.98	0.63
1:A:343:SER:HB2	1:A:344:PRO:CD	2.29	0.63
2:Q:48:ILE:HD13	2:Q:80:TYR:OH	1.99	0.63
1:C:434:ASN:HD21	1:D:80:CYS:HA	1.64	0.63
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
3:S:19:VAL:HB	3:S:79:ILE:HG13	1.81	0.63
1:A:262:PHE:CE1	1:A:266:ALA:HB2	2.33	0.63
1:C:54:LEU:O	1:C:58:MET:HG2	1.99	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
2:P:63:LYS:HB2	2:P:67:LYS:HZ3	1.65	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:D:435:PRO:HA	1:D:437:PRO:HD3	1.82	0.62
1:C:415:VAL:HA	1:C:418:MET:HG3	1.82	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:B:165:ILE:O	1:B:166:ALA:HB2	2.01	0.61
1:C:218:LYS:O	1:C:219:ASN:HB2	2.00	0.61
1:D:218:LYS:O	1:D:219:ASN:HB2	2.00	0.61
2:P:34:ILE:HG21	2:P:78:THR:HG21	1.83	0.61
2:P:48:ILE:HD13	2:P:80:TYR:OH	2.01	0.61
2:Q:39:GLN:O	2:Q:92:SER:HB3	2.00	0.61
1:B:205:ILE:O	1:B:205:ILE:HG22	2.01	0.61
1:A:267:ARG:HE	1:A:274:ALA:HB2	1.64	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:D:395:PHE:O	1:D:399:ILE:HG13	2.00	0.60
1:C:361:THR:HG22	1:C:365:TYR:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:124:THR:H	2:Q:154:PRO:HD3	1.65	0.60
3:S:110:ILE:HD12	3:S:110:ILE:H	1.67	0.60
1:D:63:MET:HB2	1:D:372:LEU:HD12	1.82	0.60
2:P:101:GLY:CA	2:P:102:ASN:HB3	2.26	0.60
1:A:205:ILE:HG22	1:A:205:ILE:O	2.01	0.60
1:A:384:ARG:HB3	1:A:385:PRO:HD3	1.83	0.60
2:P:177:LEU:HD23	2:P:177:LEU:H	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
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:B:13:ILE:HG22	1:B:14:PRO:HD3	1.84	0.60
1:A:435:PRO:HB3	2:P:103:TYR:CB	2.32	0.60
1:B:268:MET:HG3	1:B:269:ALA:N	2.17	0.60
1:B:166:ALA:N	1:B:167:VAL:HB	2.17	0.60
1:A:160:VAL:HB	1:A:161:PRO:HD3	1.84	0.60
2:Q:14:PRO:O	2:P:163:SER:HB2	2.02	0.60
1:B:384:ARG:HB3	1:B:385:PRO:HD3	1.83	0.59
1:A:165:ILE:O	1:A:166:ALA:HB2	2.01	0.59
2:P:48:ILE:HG23	2:P:67:LYS:HZ1	1.66	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:D:364:PRO:O	1:D:368:THR:HG23	2.03	0.59
1:B:170:TRP:N	1:B:249:MET:HE1	2.18	0.59
1:A:268:MET:HG3	1:A:269:ALA:N	2.17	0.59
1:B:63:MET:HE2	1:B:371:ALA:HB1	1.85	0.59
1:B:251:PRO:HB2	1:B:257:VAL:HG22	1.84	0.59
1:A:31:LEU:HB2	1:A:32:PRO:HD3	1.85	0.59
2:P:40:ARG:HB3	2:P:41:PRO:HD2	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
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
1:C:346:ALA:C	1:C:348:LYS:HA	2.23	0.58
1:A:13:ILE:HG22	1:A:14:PRO:HD3	1.85	0.58
1:B:160:VAL:HB	1:B:161:PRO:HD3	1.85	0.58
1:B:16:THR:HG22	1:B:227:ALA:HA	1.85	0.58
2:Q:18:VAL:HG23	2:Q:82:GLN:HB2	1.86	0.58
1:C:43:ILE:HG12	1:C:244:THR:HG22	1.86	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
1:A:113:SER:HB2	1:A:119:LEU:O	2.04	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:C:364:PRO:O	1:C:368:THR:HG23	2.04	0.58
2:Q:29:PHE:O	2:Q:53:PRO:HG2	2.03	0.58
1:C:377:HIS:HD2	1:D:430:ARG:HG2	1.62	0.58
3:S:156:ASP:HA	3:S:196:SER:HB3	1.86	0.58
1:B:31:LEU:HB2	1:B:32:PRO:HD3	1.85	0.58
3:S:30:ASN:O	3:S:36:TYR:HB2	2.03	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
2:P:150:LYS:HZ2	3:S:185:THR:HG21	1.68	0.57
2:Q:47:TRP:CE3	3:W:100:PRO:HD2	2.39	0.57
1:A:374:LEU:HD21	1:B:425:ALA:HA	1.86	0.57
1:A:219:ASN:N	1:A:220:PRO:HD3	2.19	0.57
1:A:274:ALA:HA	1:A:275:GLY:O	2.04	0.57
2:P:11:LEU:HD13	2:P:117:THR:HB	1.86	0.57
1:C:417:LEU:O	1:C:421:THR:HG23	2.04	0.57
1:A:63:MET:HE2	1:A:371:ALA:HB1	1.86	0.57
1:B:105:VAL:HG13	1:B:290:LEU:HD11	1.87	0.57
1:A:31:LEU:O	1:A:35:LEU:HG	2.05	0.57
2:P:37:VAL:HG12	2:P:47:TRP:HA	1.86	0.57
1:B:50:ILE:O	1:B:54:LEU:HB2	2.05	0.57
3:W:4:MET:HB2	3:W:103:GLY:HA2	1.87	0.57
1:A:16:THR:HG22	1:A:227:ALA:HA	1.86	0.57
2:Q:10:GLU:CD	2:Q:11:LEU:HD23	2.25	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
2:Q:63:LYS:HB2	2:Q:67:LYS:HZ3	1.69	0.57
3:W:156:ASP:HA	3:W:196:SER:HB3	1.86	0.57
3:S:129:LEU:HD23	3:S:188:LYS:HZ2	1.68	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:166:ALA:N	1:A:167:VAL:HB	2.17	0.57
1:A:79:ARG:HB2	1:A:375:LEU:HD11	1.86	0.57
2:P:101:GLY:HA2	2:P:102:ASN:CB	2.19	0.56
3:W:151:LYS:HG2	3:W:151:LYS:O	2.04	0.56
1:C:399:ILE:HA	1:D:418:MET:HE2	1.87	0.56
3:S:129:LEU:HB3	3:S:188:LYS:HZ2	1.70	0.56
1:C:418:MET:HE2	1:D:399:ILE:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:LEU:O	1:D:421:THR:HG23	2.04	0.56
1:A:31:LEU:CD1	1:A:246:ILE:HD12	2.36	0.56
2:P:60:TYR:HD2	2:P:61:ASN:N	2.03	0.56
1:A:71:GLY:O	1:A:212:VAL:HA	2.06	0.56
3:W:30:ASN:O	3:W:36:TYR:HB2	2.05	0.56
1:B:31:LEU:O	1:B:35:LEU:HG	2.05	0.56
3:W:2:LEU:HD12	3:W:97:TYR:HD2	1.70	0.56
1:C:118:ILE:HG22	1:C:119:LEU:HG	1.88	0.56
3:S:4:MET:HB2	3:S:103:GLY:HA2	1.87	0.56
1:A:105:VAL:HG13	1:A:290:LEU:HD11	1.87	0.56
1:D:23:ILE:HG12	1:D:206:GLY:HA3	1.87	0.56
1:C:262:PHE:CG	1:C:263:GLY:N	2.72	0.56
1:B:219:ASN:N	1:B:220:PRO:HD3	2.19	0.56
2:P:63:LYS:HZ3	2:P:67:LYS:HZ3	1.53	0.56
1:C:436:TYR:H	1:D:79:ARG:HA	1.70	0.56
1:B:345:ASN:O	1:B:346:ALA:HB2	2.05	0.56
1:A:313:ILE:H	1:A:313:ILE:CD1	2.16	0.56
1:A:50:ILE:O	1:A:54:LEU:HB2	2.06	0.56
1:D:262:PHE:CG	1:D:263:GLY:N	2.73	0.56
1:A:414:PHE:CD1	1:B:410:VAL:HG13	2.41	0.56
1:C:433:LYS:O	1:C:435:PRO:HD3	2.05	0.56
1:A:362:LEU:HD23	1:A:365:TYR:HD2	1.70	0.56
2:P:45:LEU:HD12	2:P:45:LEU:H	1.71	0.56
1:A:313:ILE:N	1:A:313:ILE:HD12	2.19	0.56
2:Q:47:TRP:O	2:Q:60:TYR:HD1	1.88	0.56
3:S:140:LEU:HD12	3:S:140:LEU:H	1.69	0.56
1:C:383:ALA:HB1	1:C:386:LEU:HB3	1.88	0.56
1:B:166:ALA:HA	1:B:167:VAL:C	2.26	0.56
1:C:267:ARG:HA	1:C:272:ASP:HB3	1.88	0.56
2:Q:47:TRP:O	2:Q:60:TYR:CD1	2.59	0.56
3:S:51:TRP:CZ3	3:S:62:VAL:HG13	2.41	0.56
1:B:79:ARG:HB2	1:B:375:LEU:HD11	1.87	0.56
1:A:62:LYS:HG3	1:A:372:LEU:HD11	1.88	0.56
1:C:72:GLY:H	1:C:75:ALA:H	1.54	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
2:P:18:VAL:HG12	2:P:82:GLN:HB2	1.87	0.55
1:A:102:ILE:HG22	1:A:338:GLN:OE1	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:36:TRP:O	2:P:48:ILE:HB	2.06	0.55
1:D:267:ARG:NH1	1:D:277:ILE:H	2.04	0.55
2:P:153:PHE:H	2:P:154:PRO:CD	2.19	0.55
3:W:87:ALA:HB2	3:W:110:ILE:HG13	1.88	0.55
1:C:23:ILE:HG12	1:C:206:GLY:HA3	1.87	0.55
1:D:433:LYS:O	1:D:435:PRO:HD3	2.06	0.55
2:Q:153:PHE:H	2:Q:154:PRO:CD	2.20	0.55
2:Q:60:TYR:HD2	2:Q:61:ASN:N	2.05	0.55
1:C:62:LYS:HB3	1:C:372:LEU:HD11	1.88	0.55
1:A:166:ALA:HA	1:A:167:VAL:C	2.26	0.55
3:W:140:LEU:H	3:W:140:LEU:HD12	1.70	0.55
1:C:384:ARG:HB3	1:C:385:PRO:HD3	1.88	0.55
2:Q:101:GLY:CA	2:Q:102:ASN:HB3	2.25	0.55
1:B:71:GLY:O	1:B:212:VAL:HA	2.07	0.55
1:A:12:LEU:HB2	1:A:223:ASN:OD1	2.06	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
1:D:10:VAL:HA	1:D:217:VAL:O	2.06	0.55
1:D:269:ALA:O	1:D:270:LEU:C	2.44	0.55
1:D:377:HIS:HD1	1:D:378:GLY:N	2.05	0.55
1:B:62:LYS:HG3	1:B:372:LEU:HD11	1.89	0.55
1:B:12:LEU:HB2	1:B:223:ASN:OD1	2.07	0.55
1:B:31:LEU:CD1	1:B:246:ILE:HD12	2.36	0.55
1:A:161:PRO:O	1:A:165:ILE:HG12	2.07	0.55
2:P:150:LYS:HZ3	3:S:185:THR:HG21	1.71	0.55
2:P:47:TRP:O	2:P:60:TYR:HD1	1.90	0.55
1:B:161:PRO:O	1:B:165:ILE:HG12	2.06	0.55
2:P:37:VAL:HG23	2:P:95:PHE:HB2	1.87	0.55
1:B:437:PRO:HG2	2:P:32:TYR:CZ	2.42	0.55
2:Q:45:LEU:H	2:Q:45:LEU:HD12	1.70	0.55
1:B:216:VAL:HG12	1:B:217:VAL:N	2.20	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:D:296:LEU:O	1:D:300:THR:HG22	2.07	0.54
2:Q:37:VAL:HG23	2:Q:95:PHE:HB2	1.88	0.54
1:C:267:ARG:NH1	1:C:277:ILE:H	2.04	0.54
1:D:267:ARG:HA	1:D:272:ASP:HB3	1.88	0.54
3:W:38:HIS:HB2	3:W:93:GLN:HG3	1.89	0.54
1:D:116:PHE:HB3	1:D:118:ILE:N	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ILE:HG22	1:D:119:LEU:HG	1.88	0.54
3:W:150:VAL:CG2	3:W:151:LYS:HA	2.37	0.54
3:S:38:HIS:HB2	3:S:93:GLN:HG3	1.88	0.54
3:S:36:TYR:HA	3:S:55:THR:OG1	2.07	0.54
1:D:324:VAL:HG12	1:D:326:GLY:H	1.72	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:343:SER:HB2	1:C:344:PRO:HD3	1.88	0.54
1:C:38:THR:HG23	1:C:42:ALA:HB2	1.89	0.54
3:S:85:GLU:H	3:S:85:GLU:CD	2.11	0.54
1:A:246:ILE:C	1:A:248:GLY:H	2.11	0.54
2:Q:90:ASN:CB	2:Q:118:VAL:HG12	2.34	0.54
1:A:216:VAL:HG12	1:A:217:VAL:N	2.20	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
3:W:85:GLU:CD	3:W:85:GLU:H	2.10	0.54
1:B:246:ILE:C	1:B:248:GLY:H	2.11	0.54
1:D:37:ALA:O	1:D:184:VAL:HA	2.07	0.54
1:B:135:ILE:O	1:B:139:LEU:HG	2.08	0.54
1:D:72:GLY:H	1:D:75:ALA:H	1.54	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:292:GLY:O	1:D:296:LEU:HG	2.08	0.54
2:P:118:VAL:O	2:P:118:VAL:HG13	2.08	0.53
2:Q:118:VAL:O	2:Q:118:VAL:HG13	2.08	0.53
1:B:313:ILE:CD1	1:B:313:ILE:H	2.16	0.53
1:C:274:ALA:HB1	1:C:275:GLY:HA2	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: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:47:TRP:O	2:P:60:TYR:CD1	2.61	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
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
2:Q:38:LYS:HB2	2:Q:48:ILE:HD11	1.90	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:P:24:ALA:HB1	2:P:27:TYR:CE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:O	1:A:139:LEU:HG	2.08	0.53
1:B:313:ILE:HD12	1:B:313:ILE:N	2.18	0.53
2:Q:45:LEU:N	2:Q:45:LEU:HD12	2.24	0.53
1:B:289:SER:O	1:B:293:TRP:HD1	1.91	0.53
3:S:82:MET:SD	3:S:108:LEU:HD21	2.49	0.53
1:D:274:ALA:HB1	1:D:275:GLY:HA2	1.90	0.53
1:B:205:ILE:CG2	1:B:361:THR:HG21	2.39	0.53
1:A:205:ILE:CG2	1:A:361:THR:HG21	2.39	0.53
3:W:51:TRP:CZ3	3:W:62:VAL:HG13	2.44	0.53
1:B:80:CYS:SG	1:B:374:LEU:HD12	2.49	0.53
1:D:160:VAL:N	1:D:161:PRO:HD2	2.24	0.52
1:B:346:ALA:CB	1:B:347:ALA:CA	2.67	0.52
1:C:277:ILE:O	1:C:280:PHE:HB2	2.08	0.52
1:B:377:HIS:CE1	3:S:30:ASN:HD21	2.28	0.52
1:A:216:VAL:HG23	1:A:299:GLN:NE2	2.24	0.52
2:P:63:LYS:HZ2	2:P:63:LYS:HB2	1.73	0.52
2:P:12:VAL:HG12	2:P:13:LYS:N	2.25	0.52
1:D:399:ILE:O	1:D:403:ILE:HG13	2.09	0.52
1:B:207:VAL:HG23	1:B:365:TYR:CE1	2.45	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
1:B:262:PHE:HE1	1:B:266:ALA:HB2	1.74	0.52
1:A:262:PHE:HE1	1:A:266:ALA:HB2	1.74	0.52
1:C:19:VAL:O	1:C:23:ILE:HG13	2.09	0.52
2:Q:150:LYS:NZ	3:W:185:THR:HG21	2.24	0.52
1:D:71:GLY:O	1:D:212:VAL:HA	2.09	0.52
1:B:296:LEU:O	1:B:300:THR:HG22	2.09	0.52
1:D:19:VAL:O	1:D:23:ILE:HG13	2.10	0.52
1:C:292:GLY:O	1:C:296:LEU:HG	2.08	0.52
1:A:308:GLY:O	1:A:428:TYR:HE1	1.91	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:B:87:TYR:O	1:B:91:VAL:HG23	2.10	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
3:W:4:MET:CE	3:W:4:MET:HA	2.40	0.52
1:A:116:PHE:HB3	1:A:118:ILE:H	1.75	0.52
3:W:23:CYS:HB2	3:W:39:TRP:CH2	2.45	0.52
2:P:63:LYS:NZ	2:P:67:LYS:HZ3	2.07	0.52
1:A:80:CYS:SG	1:A:374:LEU:HD12	2.50	0.52
2:Q:2:VAL:HB	2:Q:109:TYR:CD1	2.45	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:A:87:TYR:O	1:A:91:VAL:HG23	2.10	0.52
1:C:71:GLY:O	1:C:212:VAL:HA	2.10	0.51
1:C:219:ASN:N	1:C:220:PRO:CD	2.70	0.51
3:S:151:LYS:CB	3:S:200:GLU:HB2	2.40	0.51
1:C:160:VAL:N	1:C:161:PRO:HD2	2.24	0.51
1:A:119:LEU:HB3	1:A:124:VAL:HG11	1.92	0.51
1:A:59:VAL:HG22	1:A:391:THR:HG22	1.92	0.51
2:Q:50:TRP:O	2:Q:57:SER:HB2	2.10	0.51
1:C:92:LEU:HD11	1:C:417:LEU:HD21	1.93	0.51
3:W:155:ILE:HA	3:W:196:SER:O	2.10	0.51
1:C:145:LYS:O	1:C:149:ARG:HG3	2.11	0.51
3:S:197:TYR:HB2	3:S:214:PHE:CE2	2.44	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:A:207:VAL:HG23	1:A:365:TYR:CE1	2.46	0.51
2:Q:153:PHE:N	2:Q:154:PRO:CD	2.73	0.51
1:C:147:ILE:HD12	1:C:148:THR:N	2.25	0.51
3:S:4:MET:HA	3:S:4:MET:CE	2.40	0.51
1:C:41:ILE:HG22	1:C:41:ILE:O	2.11	0.51
2:Q:9:PRO:CB	2:Q:10:GLU:HB2	2.35	0.51
1:A:267:ARG:HB3	1:A:272:ASP:HB2	1.92	0.51
1:C:399:ILE:O	1:C:403:ILE:HG13	2.09	0.51
1:C:395:PHE:CE2	1:D:422:ALA:HA	2.45	0.51
3:W:150:VAL:CB	3:W:151:LYS:HA	2.41	0.51
2:Q:4:LEU:O	2:Q:111:GLY:HA2	2.11	0.51
1:D:308:GLY:O	1:D:428:TYR:HE1	1.94	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:P:47:TRP:CE3	3:S:100:PRO:HD2	2.46	0.51
1:B:220:PRO:C	1:B:222:ARG:H	2.15	0.51
2:P:66:GLY:HA2	2:P:83:LEU:HB3	1.93	0.51
2:P:150:LYS:HG3	2:P:183:THR:HB	1.94	0.50
1:D:92:LEU:HD11	1:D:417:LEU:HD21	1.93	0.50
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
3:W:200:GLU:HG2	3:W:211:VAL:HG23	1.93	0.50
1:D:69:SER:C	1:D:71:GLY:HA3	2.31	0.50
1:D:219:ASN:H	1:D:220:PRO:HD3	1.76	0.50
1:D:41:ILE:HG22	1:D:41:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:92:SER:O	2:P:93:VAL:C	2.49	0.50
1:C:69:SER:C	1:C:71:GLY:HA3	2.32	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
1:A:87:TYR:CE1	1:A:424:TYR:HB2	2.45	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
2:P:2:VAL:HB	2:P:109:TYR:CD1	2.46	0.50
3:W:151:LYS:C	3:W:152:TRP:CG	2.85	0.50
3:S:200:GLU:HG2	3:S:211:VAL:HG23	1.94	0.50
1:A:287:LEU:O	1:A:290:LEU:HB2	2.11	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
1:A:309:LEU:O	1:A:310:PHE:CB	2.60	0.50
1:A:134:TRP:O	1:A:138:LEU:HG	2.12	0.50
1:D:313:ILE:CD1	1:D:313:ILE:H	2.21	0.50
1:B:343:SER:CB	1:B:344:PRO:HD3	2.36	0.50
1:B:119:LEU:HB3	1:B:124:VAL:HG11	1.92	0.50
2:P:144:THR:O	3:S:122:PHE:HZ	1.94	0.50
1:A:170:TRP:N	1:A:249:MET:HE1	2.27	0.50
1:A:249:MET:HE3	1:A:249:MET:H	1.76	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
2:Q:63:LYS:CB	2:Q:67:LYS:HZ3	2.24	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:D:436:TYR:N	1:D:436:TYR:CD2	2.80	0.50
1:A:37:ALA:O	1:A:38:THR:HG22	2.12	0.50
2:P:50:TRP:O	2:P:57:SER:HB2	2.12	0.50
1:B:287:LEU:O	1:B:290:LEU:HB2	2.11	0.50
1:A:246:ILE:O	1:A:251:PRO:HD2	2.12	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:D:251:PRO:HB2	1:D:257:VAL:HG22	1.94	0.50
2:Q:134:VAL:HG12	2:Q:135:CYS:SG	2.52	0.50
2:Q:66:GLY:HA2	2:Q:83:LEU:HB3	1.93	0.50
3:W:51:TRP:HZ3	3:W:66:PHE:CD2	2.30	0.50
1:A:159:LEU:HD11	1:A:238:CYS:SG	2.52	0.50
1:A:39:GLY:CA	1:A:247:MET:HG3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HG2	1:B:377:HIS:ND1	2.27	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:363:VAL:N	1:B:364:PRO:HD2	2.27	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:P:11:LEU:CD1	2:P:117:THR:HB	2.42	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:A:159:LEU:O	1:A:163:VAL:HG12	2.13	0.49
1:A:57:SER:HB3	1:A:232:VAL:HG21	1.94	0.49
1:C:69:SER:O	1:C:71:GLY:HA3	2.13	0.49
1:B:250:ILE:HG23	1:B:269:ALA:HB3	1.94	0.49
1:C:339:PHE:O	1:C:344:PRO:HD2	2.12	0.49
1:B:159:LEU:O	1:B:163:VAL:HG12	2.13	0.49
1:C:111:TYR:HB3	1:C:283:ALA:HB2	1.94	0.49
1:A:249:MET:H	1:A:249:MET:CE	2.26	0.49
1:B:339:PHE:O	1:B:344:PRO:CD	2.60	0.49
1:D:377:HIS:HD1	1:D:378:GLY:H	1.60	0.49
1:D:121:ASP:HB3	1:D:122:PRO:CD	2.43	0.49
2:P:30:THR:HG22	2:P:53:PRO:HB2	1.94	0.49
1:A:363:VAL:N	1:A:364:PRO:HD2	2.27	0.49
1:D:357:SER:O	1:D:360:PHE:HB2	2.11	0.49
3:S:146:LYS:HE2	3:S:178:TYR:CE2	2.47	0.49
1:B:309:LEU:O	1:B:310:PHE:CB	2.60	0.49
1:D:433:LYS:HE2	2:Q:52:TYR:CG	2.48	0.49
1:C:313:ILE:CD1	1:C:313:ILE:H	2.21	0.49
1:C:268:MET:O	1:C:269:ALA:CB	2.59	0.49
3:W:140:LEU:N	3:W:140:LEU:HD12	2.28	0.49
3:W:112:ARG:HD3	3:W:113:ALA:O	2.13	0.49
2:P:67:LYS:HB2	2:P:80:TYR:HE1	1.77	0.49
1:D:122:PRO:C	1:D:124:VAL:H	2.16	0.49
3:W:149:ASN:ND2	3:W:151:LYS:HE2	2.28	0.49
1:A:140:ASN:HD22	1:A:327:LEU:HD11	1.78	0.49
1:C:429:ASN:OD1	1:C:430:ARG:HG3	2.13	0.49
2:Q:30:THR:HG22	2:Q:53:PRO:HB2	1.95	0.49
1:A:250:ILE:HG23	1:A:269:ALA:HB3	1.94	0.49
2:P:90:ASN:CB	2:P:118:VAL:HG12	2.34	0.49
2:Q:67:LYS:HB2	2:Q:80:TYR:HE1	1.77	0.49
1:B:57:SER:HB3	1:B:232:VAL:HG21	1.94	0.49
1:C:222:ARG:O	1:C:226:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TYR:CD2	1:C:436:TYR:N	2.81	0.48
1:B:131:ALA:O	1:B:135:ILE:HG13	2.12	0.48
1:A:131:ALA:O	1:A:135:ILE:HG13	2.13	0.48
1:B:141:ILE:HD12	1:B:328:LEU:HD21	1.95	0.48
3:S:144:TYR:CG	3:S:145:PRO:HA	2.48	0.48
3:W:146:LYS:HE2	3:W:178:TYR:CE2	2.48	0.48
1:D:159:LEU:O	1:D:163:VAL:HG12	2.13	0.48
1:C:357:SER:O	1:C:360:PHE:HB2	2.12	0.48
1:A:436:TYR:HE2	2:P:103:TYR:HE2	1.60	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:C:159:LEU:O	1:C:163:VAL:HG12	2.13	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:HD22	1:B:327:LEU:HD11	1.78	0.48
1:C:343:SER:HB2	1:C:344:PRO:CD	2.42	0.48
1:B:140:ASN:HD21	1:B:295:LEU:HA	1.78	0.48
3:W:198:THR:CG2	3:W:213:SER:HB2	2.43	0.48
3:W:82:MET:SD	3:W:108:LEU:HD21	2.52	0.48
1:D:354:SER:C	1:D:356:VAL:H	2.16	0.48
1:B:246:ILE:O	1:B:251:PRO:HD2	2.12	0.48
3:W:54:ASP:HB2	3:W:57:LYS:HD3	1.96	0.48
1:A:220:PRO:C	1:A:222:ARG:H	2.15	0.48
2:Q:158:THR:HB	2:Q:205:ALA:HB3	1.95	0.48
1:A:60:TYR:CE1	1:A:208:GLU:HB3	2.48	0.48
1:B:101:ASN:ND2	1:B:294:THR:HG23	2.29	0.48
1:C:59:VAL:HG22	1:C:391:THR:HG22	1.95	0.48
1:A:410:VAL:HG13	1:B:414:PHE:HD1	1.78	0.48
1:B:31:LEU:CB	1:B:32:PRO:HD3	2.43	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:D:110:GLY:O	1:D:114:TYR:HB2	2.13	0.48
1:A:169:GLY:HA2	1:A:170:TRP:HA	1.65	0.48
1:D:429:ASN:OD1	1:D:430:ARG:HG3	2.14	0.48
1:B:134:TRP:O	1:B:138:LEU:HG	2.12	0.48
2:P:27:TYR:CE2	2:P:98:ARG:HD2	2.48	0.48
1:A:381:GLY:HA3	1:A:383:ALA:H	1.79	0.48
1:A:140:ASN:HD21	1:A:295:LEU:HA	1.79	0.48
3:W:144:TYR:CG	3:W:145:PRO:HA	2.48	0.48
1:D:59:VAL:HG22	1:D:391:THR:HG22	1.95	0.48
1:A:70:PRO:N	1:A:71:GLY:HA3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:PRO:HG3	1:D:262:PHE:HB2	1.95	0.48
1:D:435:PRO:HG3	2:Q:103:TYR:CD1	2.49	0.48
1:C:35:LEU:HA	1:C:38:THR:O	2.14	0.48
1:B:117:PRO:O	1:B:118:ILE:C	2.53	0.48
3:S:20:THR:HG23	3:S:78:THR:HG22	1.96	0.48
2:P:152:TYR:CE1	2:P:182:TYR:HB2	2.49	0.48
1:A:433:LYS:O	1:A:435:PRO:HD3	2.14	0.47
1:C:346:ALA:H	1:C:347:ALA:C	2.17	0.47
1:B:165:ILE:O	1:B:166:ALA:CB	2.62	0.47
1:B:73:SER:HB3	1:B:74:TYR:H	1.59	0.47
3:S:54:ASP:HB2	3:S:57:LYS:HD3	1.96	0.47
2:P:134:VAL:O	2:P:135:CYS:HB2	2.13	0.47
3:S:112:ARG:HD3	3:S:113:ALA:O	2.14	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
1:D:307:ASP:C	1:D:309:LEU:H	2.17	0.47
1:A:165:ILE:O	1:A:166:ALA:CB	2.62	0.47
2:Q:60:TYR:CE2	3:W:99:PRO:HG2	2.49	0.47
1:B:249:MET:CE	1:B:249:MET:H	2.26	0.47
1:B:130:VAL:HG13	1:B:335:THR:HG22	1.96	0.47
2:Q:119:SER:HB3	2:Q:153:PHE:CZ	2.49	0.47
1:A:101:ASN:ND2	1:A:294:THR:HG23	2.29	0.47
2:Q:152:TYR:CE1	2:Q:182:TYR:HB2	2.49	0.47
1:A:141:ILE:HD12	1:A:328:LEU:HD21	1.96	0.47
2:Q:10:GLU:HG2	2:Q:11:LEU:CD2	2.37	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:D:134:TRP:HA	1:D:137:VAL:CG1	2.43	0.47
1:C:32:PRO:HG3	1:C:262:PHE:HB2	1.95	0.47
1:C:122:PRO:C	1:C:124:VAL:H	2.16	0.47
1:A:117:PRO:O	1:A:118:ILE:C	2.53	0.47
1:B:134:TRP:HE1	1:B:335:THR:CG2	2.19	0.47
1:D:80:CYS:SG	1:D:371:ALA:HA	2.55	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:B:197:LEU:HB3	1:B:201:LEU:HG	1.96	0.47
1:B:60:TYR:CE1	1:B:208:GLU:HB3	2.49	0.47
1:C:307:ASP:C	1:C:309:LEU:H	2.18	0.47
2:Q:63:LYS:NZ	2:Q:67:LYS:HZ3	2.12	0.47
1:D:248:GLY:HA3	1:D:249:MET:HA	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:154:PRO:HB3	2:P:208:ALA:CB	2.45	0.47
2:P:119:SER:HB3	2:P:153:PHE:CZ	2.50	0.47
1:C:73:SER:OG	1:C:364:PRO:HB3	2.14	0.47
2:P:18:VAL:O	2:P:81:MET:HA	2.15	0.47
3:W:200:GLU:HG2	3:W:211:VAL:CG2	2.45	0.47
2:Q:126:PRO:HA	2:Q:151:GLY:O	2.14	0.47
1:A:349:GLU:O	1:A:353:VAL:HG23	2.14	0.47
2:Q:145:LEU:N	2:Q:145:LEU:HD23	2.30	0.47
1:B:125:LEU:HD23	1:B:125:LEU:O	2.15	0.47
1:C:110:GLY:O	1:C:114:TYR:HB2	2.14	0.47
1:A:31:LEU:CB	1:A:32:PRO:HD3	2.44	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
1:D:73:SER:OG	1:D:364:PRO:HB3	2.14	0.47
2:Q:48:ILE:HG23	2:Q:67:LYS:HZ2	1.80	0.47
1:C:219:ASN:H	1:C:220:PRO:HD3	1.76	0.47
1:D:207:VAL:C	1:D:209:SER:H	2.18	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:D:346:ALA:HA	1:D:347:ALA:HA	1.56	0.47
1:C:393:VAL:O	1:C:396:VAL:HG12	2.15	0.47
1:D:433:LYS:HE2	2:Q:52:TYR:CD2	2.50	0.47
1:C:49:THR:OG1	1:C:201:LEU:HD23	2.15	0.47
1:A:141:ILE:HG12	1:A:141:ILE:O	2.15	0.47
1:C:252:ASN:HA	1:C:253:ALA:HA	1.65	0.47
2:Q:53:PRO:HA	2:Q:71:THR:HG21	1.98	0.46
1:D:363:VAL:HB	1:D:364:PRO:HD3	1.97	0.46
2:Q:63:LYS:HD2	2:Q:67:LYS:HZ3	1.80	0.46
2:P:63:LYS:CB	2:P:67:LYS:HZ3	2.27	0.46
1:B:381:GLY:HA3	1:B:383:ALA:H	1.80	0.46
1:D:247:MET:N	1:D:248:GLY:O	2.48	0.46
3:W:65:ARG:CZ	3:W:83:GLU:HG3	2.45	0.46
1:C:332:VAL:O	1:C:336:ILE:HG13	2.15	0.46
1:A:377:HIS:ND1	1:B:430:ARG:HG2	2.29	0.46
3:S:65:ARG:CZ	3:S:83:GLU:HG3	2.45	0.46
1:A:205:ILE:HG23	1:A:361:THR:HG21	1.97	0.46
1:A:130:VAL:HG13	1:A:335:THR:HG22	1.97	0.46
1:D:147:ILE:H	1:D:147:ILE:HG13	1.56	0.46
1:B:262:PHE:CG	1:B:263:GLY:N	2.83	0.46
1:C:361:THR:O	1:C:365:TYR:HD2	1.98	0.46
2:P:187:SER:HB3	3:S:139:PHE:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:PHE:HB3	1:C:85:LEU:HD12	1.96	0.46
3:W:146:LYS:HE2	3:W:178:TYR:HE2	1.79	0.46
2:P:145:LEU:HD23	2:P:145:LEU:N	2.30	0.46
2:P:126:PRO:HA	2:P:151:GLY:O	2.14	0.46
1:A:121:ASP:HB3	1:A:122:PRO:HD2	1.97	0.46
1:D:10:VAL:CG2	1:D:145:LYS:HE3	2.45	0.46
1:B:85:LEU:HD12	1:B:85:LEU:N	2.31	0.46
1:C:430:ARG:HG2	1:D:377:HIS:HD2	1.76	0.46
1:C:170:TRP:H	1:C:249:MET:HG3	1.80	0.46
3:W:110:ILE:CD1	3:W:110:ILE:H	2.26	0.46
1:B:435:PRO:HA	1:B:436:TYR:HA	1.59	0.46
1:C:363:VAL:HB	1:C:364:PRO:HD3	1.96	0.46
2:P:134:VAL:O	2:P:135:CYS:CB	2.62	0.46
1:B:360:PHE:HE2	1:B:413:SER:HA	1.80	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
1:C:182:TRP:O	1:C:184:VAL:N	2.48	0.46
1:A:360:PHE:HE2	1:A:413:SER:HA	1.80	0.46
1:A:125:LEU:O	1:A:125:LEU:HD23	2.15	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:65:LYS:O	2:Q:67:LYS:HG2	2.15	0.46
1:B:222:ARG:O	1:B:226:ILE:HG13	2.16	0.46
1:C:70:PRO:HB3	1:C:215:GLY:CA	2.46	0.46
1:B:43:ILE:C	1:B:45:GLY:H	2.19	0.46
1:C:79:ARG:HB2	1:D:436:TYR:O	2.16	0.46
1:B:216:VAL:O	1:B:217:VAL:HB	2.15	0.46
1:A:216:VAL:O	1:A:217:VAL:HB	2.16	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:D:250:ILE:HG23	1:D:269:ALA:CB	2.45	0.46
1:C:147:ILE:HD12	1:C:148:THR:H	1.81	0.46
2:Q:18:VAL:O	2:Q:81:MET:HA	2.15	0.46
1:A:197:LEU:HB3	1:A:201:LEU:HG	1.96	0.46
1:D:165:ILE:HG22	1:D:165:ILE:O	2.15	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:A:117:PRO:HG2	1:A:120:LYS:HE2	1.98	0.46
3:W:154:LYS:HA	3:W:159:GLU:HA	1.98	0.46
1:D:427:ASN:C	1:D:429:ASN:H	2.19	0.46
1:B:205:ILE:HG23	1:B:361:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:P:102:ASN:HA	2:P:103:TYR:HA	1.72	0.45
1:D:70:PRO:HB3	1:D:215:GLY:CA	2.46	0.45
1:B:72:GLY:HA3	1:B:75:ALA:H	1.81	0.45
2:P:60:TYR:CE2	2:P:62:GLU:HB3	2.51	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:Q:63:LYS:HD2	2:Q:67:LYS:NZ	2.32	0.45
2:Q:47:TRP:CG	3:W:100:PRO:HG2	2.52	0.45
3:S:200:GLU:HG2	3:S:211:VAL:CG2	2.45	0.45
1:A:68:PRO:HB3	1:A:220:PRO:HB2	1.99	0.45
1:D:332:VAL:O	1:D:336:ILE:HG13	2.16	0.45
1:A:339:PHE:O	1:A:344:PRO:HD2	2.16	0.45
2:Q:63:LYS:HB3	2:Q:67:LYS:HE2	1.99	0.45
1:D:49:THR:OG1	1:D:201:LEU:HD23	2.16	0.45
2:Q:129:TYR:HB3	3:W:125:SER:OG	2.16	0.45
1:D:71:GLY:H	1:D:303:ALA:CB	2.30	0.45
1:A:274:ALA:CA	1:A:275:GLY:C	2.84	0.45
1:B:68:PRO:HB3	1:B:220:PRO:HB2	1.99	0.45
1:C:382:LYS:C	1:C:384:ARG:H	2.18	0.45
3:S:144:TYR:O	3:S:203:HIS:HE1	2.00	0.45
1:A:43:ILE:C	1:A:45:GLY:H	2.19	0.45
1:D:29:PHE:CG	1:D:29:PHE:O	2.69	0.45
1:D:250:ILE:HG12	1:D:269:ALA:HB3	1.99	0.45
1:D:147:ILE:HD12	1:D:148:THR:HG23	1.99	0.45
3:S:30:ASN:O	3:S:36:TYR:CB	2.64	0.45
1:C:71:GLY:H	1:C:303:ALA:CB	2.30	0.45
1:A:134:TRP:HA	1:A:137:VAL:HB	1.99	0.45
1:C:260:SER:HA	1:C:261:PRO:HD3	1.79	0.45
1:D:170:TRP:H	1:D:249:MET:HG3	1.80	0.45
1:D:147:ILE:HD12	1:D:148:THR:H	1.82	0.45
1:C:147:ILE:HD12	1:C:148:THR:HG23	1.98	0.45
1:D:74:TYR:CZ	1:D:304:ALA:HA	2.51	0.45
1:A:10:VAL:HA	1:A:11:GLY:HA2	1.61	0.45
3:S:129:LEU:H	3:S:129:LEU:HD12	1.82	0.45
1:D:205:ILE:HG23	1:D:361:THR:HG21	1.99	0.45
1:D:361:THR:HG22	1:D:365:TYR:CE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:PRO:HG2	1:B:120:LYS:HE2	1.98	0.45
1:B:141:ILE:HG12	1:B:141:ILE:O	2.15	0.45
1:B:53:ALA:HA	1:B:397:TYR:CE1	2.52	0.45
1:A:216:VAL:C	1:A:218:LYS:H	2.20	0.45
1:A:262:PHE:CG	1:A:263:GLY:N	2.84	0.45
1:D:81:PHE:CB	1:D:85:LEU:HD12	2.47	0.45
1:C:141:ILE:HA	1:C:142:VAL:HA	1.48	0.45
1:A:146:MET:O	1:A:150:VAL:HG23	2.17	0.45
1:D:143:GLY:O	1:D:146:MET:HB3	2.17	0.45
2:Q:60:TYR:CE2	2:Q:62:GLU:HB3	2.52	0.45
2:P:60:TYR:C	2:P:60:TYR:CD2	2.91	0.45
3:S:2:LEU:HD22	3:S:94:GLN:HE21	1.82	0.45
2:P:60:TYR:CE2	3:S:99:PRO:HG2	2.52	0.45
3:W:151:LYS:O	3:W:152:TRP:CD1	2.70	0.45
1:D:260:SER:HA	1:D:261:PRO:HD3	1.79	0.45
1:C:121:ASP:HB3	1:C:122:PRO:HD2	1.98	0.45
1:B:13:ILE:N	1:B:14:PRO:CD	2.80	0.45
1:A:13:ILE:N	1:A:14:PRO:CD	2.80	0.45
1:D:182:TRP:O	1:D:184:VAL:N	2.49	0.45
1:C:85:LEU:HD21	1:D:85:LEU:HD11	1.98	0.45
1:D:393:VAL:O	1:D:396:VAL:HG12	2.16	0.45
1:C:143:GLY:O	1:C:146:MET:HB3	2.17	0.45
3:S:127:GLU:HA	3:S:130:THR:OG1	2.17	0.45
3:W:127:GLU:HA	3:W:130:THR:OG1	2.17	0.45
1:C:29:PHE:O	1:C:29:PHE:CG	2.69	0.45
3:S:40:TYR:HD1	3:S:50:ARG:HA	1.82	0.45
1:A:70:PRO:HB2	1:A:71:GLY:HA2	1.99	0.45
1:B:327:LEU:O	1:B:327:LEU:HD13	2.17	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: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:216:VAL:C	1:B:218:LYS:H	2.20	0.44
2:Q:121:ALA:HB3	2:Q:153:PHE:CE2	2.52	0.44
1:B:434:ASN:O	1:B:437:PRO:HG3	2.17	0.44
3:S:191:TYR:HA	3:S:197:TYR:OH	2.17	0.44
1:C:428:TYR:CD2	1:C:428:TYR:N	2.85	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:433:LYS:HE2	2:P:52:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASP:HB3	1:B:122:PRO:HD2	1.98	0.44
2:P:60:TYR:C	2:P:60:TYR:HD2	2.21	0.44
1:B:70:PRO:HB2	1:B:71:GLY:HA2	1.99	0.44
2:P:121:ALA:HB3	2:P:153:PHE:CE2	2.53	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:C:373:LEU:CD1	1:D:426:LEU:HD23	2.47	0.44
3:W:129:LEU:HD12	3:W:129:LEU:H	1.81	0.44
1:A:327:LEU:O	1:A:327:LEU:HD13	2.18	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:S:154:LYS:HA	3:S:159:GLU:HA	1.98	0.44
1:D:71:GLY:HA2	1:D:75:ALA:HB2	2.00	0.44
1:C:440:ALA:HB2	3:W:97:TYR:CD2	2.53	0.44
1:A:292:GLY:O	1:A:296:LEU:HG	2.17	0.44
1:D:31:LEU:HB2	1:D:246:ILE:HD11	2.00	0.44
1:C:207:VAL:C	1:C:209:SER:H	2.19	0.44
1:C:361:THR:HG22	1:C:365:TYR:CE2	2.49	0.44
3:W:203:HIS:CE1	3:W:205:THR:HG23	2.52	0.44
1:A:53:ALA:HA	1:A:397:TYR:CE1	2.52	0.44
1:B:147:ILE:HD11	1:B:291:GLY:C	2.38	0.44
1:B:78:ARG:HA	1:B:82:GLY:O	2.17	0.44
3:W:40:TYR:HD1	3:W:50:ARG:HA	1.82	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
2:P:9:PRO:CB	2:P:10:GLU:CB	2.90	0.44
1:C:74:TYR:CZ	1:C:304:ALA:HA	2.52	0.44
1:C:71:GLY:HA2	1:C:75:ALA:HB2	2.00	0.44
1:B:170:TRP:O	1:B:249:MET:HG3	2.18	0.44
1:A:270:LEU:O	1:A:270:LEU:HD13	2.17	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
3:W:123:PRO:HB3	3:W:214:PHE:CE1	2.53	0.44
1:C:392:PHE:O	1:C:395:PHE:HB2	2.18	0.44
1:B:377:HIS:HE1	3:S:30:ASN:HD21	1.66	0.44
3:S:123:PRO:HB3	3:S:214:PHE:CE1	2.53	0.44
1:A:434:ASN:O	1:A:437:PRO:HG3	2.18	0.44
1:A:78:ARG:HA	1:A:82:GLY:O	2.17	0.44
2:Q:160:THR:O	2:Q:203:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PRO:HA	1:B:312:PRO:HD3	1.71	0.44
1:B:250:ILE:HB	1:B:251:PRO:CD	2.40	0.44
1:D:250:ILE:HG23	1:D:269:ALA:HB2	2.00	0.44
2:Q:134:VAL:CG1	2:Q:135:CYS:N	2.80	0.44
1:C:216:VAL:HG12	1:C:217:VAL:N	2.33	0.44
2:P:4:LEU:HG	2:P:96:CYS:SG	2.57	0.44
1:D:360:PHE:CZ	1:D:416:THR:HG21	2.53	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:A:147:ILE:HD11	1:A:291:GLY:C	2.38	0.44
2:Q:101:GLY:HA2	2:Q:102:ASN:CB	2.18	0.44
1:B:134:TRP:HA	1:B:137:VAL:HB	1.99	0.44
3:W:191:TYR:HA	3:W:197:TYR:OH	2.17	0.44
2:Q:34:ILE:O	2:Q:50:TRP:HA	2.18	0.44
1:B:105:VAL:CG1	1:B:290:LEU:HD11	2.48	0.44
1:D:10:VAL:HA	1:D:11:GLY:HA2	1.73	0.43
2:P:60:TYR:CD2	2:P:61:ASN:N	2.86	0.43
3:S:129:LEU:N	3:S:129:LEU:HD12	2.32	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
1:B:433:LYS:O	1:B:435:PRO:HD3	2.18	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
2:P:18:VAL:HG22	2:P:19:LYS:N	2.33	0.43
2:Q:131:LEU:HB2	2:Q:146:GLY:C	2.38	0.43
1:D:70:PRO:O	1:D:303:ALA:HB2	2.17	0.43
2:Q:10:GLU:OE2	2:Q:11:LEU:CD2	2.66	0.43
1:A:250:ILE:HB	1:A:251:PRO:CD	2.40	0.43
1:D:250:ILE:HB	1:D:251:PRO:CD	2.45	0.43
2:Q:41:PRO:HA	2:Q:92:SER:OG	2.19	0.43
1:B:13:ILE:CG2	1:B:14:PRO:HD3	2.47	0.43
1:A:369:CYS:HB2	1:A:395:PHE:CE1	2.53	0.43
1:A:270:LEU:HA	1:A:270:LEU:HD22	1.88	0.43
1:A:325:ALA:C	1:A:327:LEU:H	2.22	0.43
1:B:292:GLY:O	1:B:296:LEU:HG	2.18	0.43
1:A:262:PHE:CZ	1:A:266:ALA:HB2	2.54	0.43
3:W:30:ASN:O	3:W:36:TYR:CB	2.65	0.43
1:B:369:CYS:HB2	1:B:395:PHE:CE1	2.53	0.43
2:P:131:LEU:HB2	2:P:146:GLY:C	2.39	0.43
1:B:111:TYR:HB3	1:B:283:ALA:HB2	2.00	0.43
1:A:170:TRP:O	1:A:249:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:2:LEU:HD22	3:W:94:GLN:HE21	1.83	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
1:C:218:LYS:O	1:C:219:ASN:CB	2.67	0.43
2:Q:60:TYR:CD2	2:Q:60:TYR:C	2.92	0.43
3:S:151:LYS:HB2	3:S:200:GLU:HB2	2.00	0.43
1:D:117:PRO:O	1:D:118:ILE:C	2.57	0.43
1:A:105:VAL:CG1	1:A:290:LEU:HD11	2.48	0.43
1:C:381:GLY:HA2	1:C:382:LYS:HA	1.60	0.43
1:C:91:VAL:O	1:C:95:LEU:HG	2.19	0.43
1:A:111:TYR:HB3	1:A:283:ALA:HB2	2.00	0.43
1:D:313:ILE:HD12	1:D:313:ILE:N	2.25	0.43
2:Q:60:TYR:C	2:Q:60:TYR:HD2	2.22	0.43
3:S:2:LEU:HD11	3:S:29:VAL:HG12	2.01	0.43
1:A:140:ASN:ND2	1:A:295:LEU:HA	2.33	0.43
1:D:31:LEU:HG	1:D:31:LEU:H	1.38	0.43
1:B:140:ASN:ND2	1:B:295:LEU:HA	2.33	0.43
1:A:13:ILE:CG2	1:A:14:PRO:HD3	2.48	0.43
1:C:81:PHE:CB	1:C:85:LEU:HD12	2.48	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
2:Q:6:GLN:HB3	2:Q:21:SER:O	2.17	0.43
1:D:216:VAL:HG12	1:D:217:VAL:N	2.33	0.43
2:P:61:ASN:O	2:P:62:GLU:C	2.57	0.43
3:S:38:HIS:O	3:S:92:CYS:HA	2.18	0.43
1:D:435:PRO:HA	1:D:436:TYR:HA	1.69	0.43
1:C:70:PRO:HB3	1:C:215:GLY:HA3	2.00	0.43
1:B:169:GLY:HA2	1:B:170:TRP:HA	1.65	0.43
1:D:121:ASP:HB3	1:D:122:PRO:HD2	1.99	0.43
1:B:262:PHE:CZ	1:B:266:ALA:HB2	2.54	0.43
2:Q:100:ASP:HB2	2:Q:108:ALA:HB2	2.01	0.43
1:D:91:VAL:O	1:D:95:LEU:HG	2.18	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
2:Q:151:GLY:HA2	2:Q:181:LEU:HD23	2.01	0.43
1:B:60:TYR:CZ	1:B:208:GLU:HB3	2.53	0.43
1:B:267:ARG:HB3	1:B:272:ASP:O	2.19	0.43
1:C:427:ASN:C	1:C:429:ASN:H	2.21	0.42
3:S:11:MET:HG3	3:S:108:LEU:HD12	2.01	0.42
1:D:428:TYR:N	1:D:428:TYR:CD2	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:HD22	1:B:397:TYR:CE2	2.53	0.42
1:B:146:MET:O	1:B:150:VAL:HG23	2.18	0.42
1:C:352:LEU:O	1:C:356:VAL:HG23	2.18	0.42
1:A:246:ILE:C	1:A:248:GLY:N	2.72	0.42
1:D:267:ARG:CA	1:D:272:ASP:HB3	2.49	0.42
1:C:389:LEU:O	1:C:392:PHE:HB3	2.18	0.42
1:D:389:LEU:O	1:D:392:PHE:HB3	2.19	0.42
2:P:50:TRP:CD1	2:P:50:TRP:C	2.92	0.42
1:C:85:LEU:HD11	1:D:85:LEU:HD21	2.01	0.42
1:A:201:LEU:HD22	1:A:397:TYR:CE2	2.53	0.42
3:W:154:LYS:HG3	3:W:159:GLU:HB3	2.01	0.42
3:W:175:ASP:O	3:W:176:SER:HB2	2.18	0.42
1:D:70:PRO:HB3	1:D:215:GLY:HA3	2.00	0.42
3:S:198:THR:HG23	3:S:213:SER:CB	2.47	0.42
1:C:140:ASN:HB3	1:C:327:LEU:HD11	2.01	0.42
3:W:11:MET:HG3	3:W:108:LEU:HD12	2.01	0.42
2:Q:48:ILE:HG12	2:Q:67:LYS:HZ2	1.83	0.42
2:Q:50:TRP:CD1	2:Q:50:TRP:C	2.92	0.42
2:P:151:GLY:O	2:P:152:TYR:HB3	2.19	0.42
3:S:37:MET:HB2	3:S:37:MET:HE2	1.80	0.42
2:Q:52:TYR:HD1	2:Q:53:PRO:HD2	1.84	0.42
1:C:69:SER:HA	1:C:70:PRO:HD3	1.80	0.42
1:B:38:THR:HG21	1:B:41:ILE:CG2	2.41	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
1:D:92:LEU:HD11	1:D:417:LEU:CD2	2.50	0.42
1:D:151:GLN:HE22	1:D:289:SER:HA	1.84	0.42
2:Q:147:CYS:HB2	2:Q:161:TRP:CH2	2.55	0.42
1:B:318:ASN:C	1:B:320:ALA:H	2.22	0.42
1:A:248:GLY:HA2	1:A:249:MET:HA	1.63	0.42
1:D:218:LYS:O	1:D:219:ASN:CB	2.67	0.42
1:C:117:PRO:O	1:C:118:ILE:C	2.57	0.42
2:P:52:TYR:HD1	2:P:53:PRO:HD2	1.84	0.42
2:Q:145:LEU:HD23	2:Q:145:LEU:H	1.85	0.42
2:P:145:LEU:HD23	2:P:145:LEU:H	1.85	0.42
1:A:109:VAL:C	1:A:111:TYR:H	2.23	0.42
1:D:230:GLY:O	1:D:234:ILE:HG13	2.19	0.42
1:B:31:LEU:HG	1:B:31:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:79:ARG:HD3	1:C:375:LEU:HD11	2.01	0.42
1:D:72:GLY:HA3	1:D:73:SER:C	2.33	0.42
1:B:246:ILE:C	1:B:248:GLY:N	2.72	0.42
1:A:10:VAL:CB	1:A:218:LYS:HD3	2.47	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
1:C:151:GLN:HE22	1:C:289:SER:HA	1.84	0.42
3:S:21:MET:HB3	3:S:106:THR:HG21	2.02	0.42
2:Q:119:SER:HB3	2:Q:153:PHE:HZ	1.84	0.42
2:Q:40:ARG:HB3	2:Q:41:PRO:CD	2.49	0.42
3:S:53:TYR:CZ	3:S:57:LYS:HB3	2.54	0.42
2:Q:150:LYS:HZ3	3:W:185:THR:HG21	1.85	0.42
1:A:345:ASN:O	1:A:347:ALA:CB	2.67	0.42
1:C:313:ILE:HD12	1:C:313:ILE:N	2.25	0.42
2:Q:106:TRP:HB3	3:W:38:HIS:CG	2.54	0.42
1:B:292:GLY:O	1:B:295:LEU:HB3	2.19	0.42
1:D:249:MET:SD	1:D:249:MET:N	2.90	0.42
1:C:92:LEU:HD11	1:C:417:LEU:CD2	2.49	0.42
1:A:99:ILE:O	1:A:102:ILE:HG13	2.20	0.42
1:C:230:GLY:O	1:C:234:ILE:HG13	2.20	0.42
3:S:135:SER:HA	3:S:184:LEU:O	2.19	0.42
3:W:43:LYS:HG2	3:W:88:ALA:HB2	2.01	0.42
1:A:69:SER:C	1:A:71:GLY:HA3	2.40	0.41
1:C:31:LEU:HB2	1:C:246:ILE:HD11	2.01	0.41
1:A:149:ARG:O	1:A:153:VAL:HG23	2.21	0.41
1:B:317:VAL:O	1:B:318:ASN:C	2.58	0.41
3:W:208:SER:HA	3:W:209:PRO:HD3	1.92	0.41
1:C:423:LEU:HA	1:C:423:LEU:HD12	1.93	0.41
2:Q:153:PHE:H	2:Q:154:PRO:HD3	1.85	0.41
1:B:165:ILE:O	1:B:165:ILE:HG22	2.20	0.41
2:P:119:SER:HB3	2:P:153:PHE:HZ	1.84	0.41
1:B:99:ILE:O	1:B:102:ILE:HG13	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
3:W:39:TRP:HA	3:W:91:TYR:O	2.19	0.41
2:Q:41:PRO:N	2:Q:92:SER:HB2	2.36	0.41
3:W:38:HIS:O	3:W:92:CYS:HA	2.20	0.41
3:S:110:ILE:CD1	3:S:110:ILE:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:154:LYS:HG3	3:S:159:GLU:HB3	2.02	0.41
2:Q:144:THR:O	3:W:122:PHE:HZ	2.03	0.41
2:Q:10:GLU:OE2	2:Q:11:LEU:HD23	2.19	0.41
1:A:170:TRP:C	1:A:249:MET:HE2	2.40	0.41
1:D:115:PHE:CE2	1:D:280:PHE:HE1	2.38	0.41
3:W:53:TYR:CZ	3:W:57:LYS:HB3	2.56	0.41
1:C:261:PRO:O	1:C:262:PHE:C	2.59	0.41
1:B:132:VAL:HA	1:B:135:ILE:HD12	2.01	0.41
2:P:151:GLY:HA2	2:P:181:LEU:HD23	2.01	0.41
1:A:172:TRP:O	1:A:173:PHE:C	2.59	0.41
1:D:21:GLY:HA3	1:D:155:THR:HG21	2.02	0.41
2:P:100:ASP:HB2	2:P:108:ALA:HB2	2.02	0.41
2:Q:7:SER:C	2:Q:9:PRO:HD2	2.40	0.41
2:Q:48:ILE:HG23	2:Q:67:LYS:HZ1	1.82	0.41
1:A:267:ARG:CZ	1:A:276:ALA:HA	2.50	0.41
2:P:48:ILE:HG23	2:P:67:LYS:CE	2.49	0.41
1:C:267:ARG:CA	1:C:272:ASP:HB3	2.49	0.41
1:C:73:SER:HA	1:C:368:THR:CG2	2.50	0.41
1:B:109:VAL:C	1:B:111:TYR:H	2.22	0.41
1:C:91:VAL:HG11	1:C:420:ILE:HD12	2.01	0.41
1:D:101:ASN:O	1:D:104:MET:HB2	2.20	0.41
1:D:12:LEU:CD2	1:D:13:ILE:HD12	2.50	0.41
2:Q:23:LYS:HB2	2:Q:23:LYS:HE3	1.88	0.41
2:P:147:CYS:HB2	2:P:161:TRP:CH2	2.55	0.41
1:B:380:PHE:HD2	1:B:380:PHE:HA	1.76	0.41
1:A:436:TYR:CE2	2:P:103:TYR:HE2	2.37	0.41
2:Q:102:ASN:HA	2:Q:103:TYR:HA	1.73	0.41
1:D:73:SER:HA	1:D:368:THR:CG2	2.51	0.41
2:Q:48:ILE:HG23	2:Q:67:LYS:CE	2.50	0.41
2:Q:63:LYS:HB2	2:Q:63:LYS:NZ	2.34	0.41
1:C:23:ILE:HG12	1:C:206:GLY:CA	2.50	0.41
1:D:102:ILE:HD11	1:D:337:PHE:HB3	2.03	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
2:Q:61:ASN:O	2:Q:62:GLU:C	2.58	0.41
2:P:63:LYS:NZ	2:P:63:LYS:HB2	2.36	0.41
1:A:440:ALA:O	1:A:441:PRO:C	2.58	0.41
1:B:69:SER:C	1:B:71:GLY:HA3	2.41	0.41
1:B:149:ARG:O	1:B:153:VAL:HG23	2.21	0.41
2:Q:133:PRO:HG2	2:Q:195:TRP:CH2	2.56	0.41
1:C:31:LEU:HG	1:C:31:LEU:H	1.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ARG:HD3	1:D:375:LEU:HD11	2.02	0.41
3:W:198:THR:HG23	3:W:213:SER:CB	2.48	0.41
1:C:386:LEU:HD23	1:C:386:LEU:C	2.41	0.41
1:C:12:LEU:CD2	1:C:13:ILE:HD12	2.50	0.41
2:Q:3:GLN:OE1	2:Q:3:GLN:HA	2.21	0.41
1:B:407:ALA:O	1:B:408:LYS:C	2.60	0.41
1:C:89:THR:CG2	1:C:367:TYR:HD2	2.34	0.41
1:D:152:ALA:O	1:D:156:VAL:HG23	2.21	0.41
1:D:386:LEU:C	1:D:386:LEU:HD23	2.41	0.41
1:D:87:TYR:HE1	1:D:424:TYR:HB2	1.82	0.41
1:D:207:VAL:C	1:D:209:SER:N	2.74	0.41
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.94	0.41
2:P:30:THR:HA	2:P:53:PRO:HB2	2.04	0.41
1:C:152:ALA:O	1:C:156:VAL:HG23	2.21	0.41
2:P:160:THR:O	2:P:203:ASN:N	2.48	0.41
1:A:49:THR:HG21	1:A:200:THR:HB	2.03	0.41
1:D:356:VAL:O	1:D:356:VAL:HG12	2.20	0.40
1:C:70:PRO:N	1:C:71:GLY:HA3	2.35	0.40
2:Q:12:VAL:CG2	2:Q:13:LYS:N	2.84	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: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
2:P:104:GLY:HA2	2:P:105:GLY:HA2	1.85	0.40
2:Q:63:LYS:CD	2:Q:67:LYS:HZ3	2.34	0.40
1:A:267:ARG:CB	1:A:272:ASP:HB2	2.51	0.40
1:A:43:ILE:HA	1:A:46:TRP:HD1	1.85	0.40
1:B:172:TRP:O	1:B:173:PHE:C	2.59	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
1:A:241:LEU:HA	1:A:241:LEU:HD23	1.94	0.40
1:C:403:ILE:HA	1:D:411:MET:HE1	2.03	0.40
3:W:12:SER:HA	3:W:109:GLU:O	2.21	0.40
2:P:40:ARG:HA	2:P:92:SER:HB2	2.03	0.40
1:B:249:MET:HE3	1:B:249:MET:H	1.86	0.40
1:A:73:SER:O	1:A:74:TYR:C	2.60	0.40
3:W:2:LEU:HD11	3:W:29:VAL:HG12	2.02	0.40
1:D:261:PRO:O	1:D:262:PHE:C	2.59	0.40
1:B:69:SER:HB3	1:B:70:PRO:CD	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:SER:HA	1:A:261:PRO:HD3	1.91	0.40
1:D:89:THR:CG2	1:D:367:TYR:HD2	2.34	0.40
2:P:3:GLN:HA	2:P:3:GLN:OE1	2.22	0.40
1:B:216:VAL:O	1:B:218:LYS:N	2.51	0.40
1:D:361:THR:O	1:D:365:TYR:CD2	2.74	0.40
1:C:102:ILE:HD11	1:C:337:PHE:HB3	2.04	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	10
1	B	414/445 (93%)	328 (79%)	57 (14%)	29 (7%)	1	10
1	C	414/445 (93%)	322 (78%)	68 (16%)	24 (6%)	2	17
1	D	413/445 (93%)	319 (77%)	71 (17%)	23 (6%)	2	18
2	P	217/219 (99%)	179 (82%)	27 (12%)	11 (5%)	2	20
2	Q	216/219 (99%)	180 (83%)	25 (12%)	11 (5%)	2	20
3	S	209/211 (99%)	174 (83%)	28 (13%)	7 (3%)	5	32
3	W	209/211 (99%)	173 (83%)	29 (14%)	7 (3%)	5	32
All	All	2508/2640 (95%)	2003 (80%)	364 (14%)	141 (6%)	2	18

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	280 (91%)	28 (9%)	12	42
1	B	306/343 (89%)	277 (90%)	29 (10%)	11	40
1	C	305/343 (89%)	286 (94%)	19 (6%)	23	64
1	D	306/343 (89%)	286 (94%)	20 (6%)	21	61
2	P	187/187 (100%)	166 (89%)	21 (11%)	7	32
2	Q	186/187 (100%)	162 (87%)	24 (13%)	5	24
3	S	185/185 (100%)	169 (91%)	16 (9%)	13	46
3	W	185/185 (100%)	168 (91%)	17 (9%)	11	41
All	All	1968/2116 (93%)	1794 (91%)	174 (9%)	12	45

All (174) 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

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Mol	Chain	Res	Type
1	A	83	PRO
1	A	102	ILE
1	A	105	VAL
1	A	114	TYR
1	A	142	VAL
1	A	207	VAL
1	A	208	GLU
1	A	219	ASN
1	A	233	LEU
1	A	247	MET
1	A	249	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	377	HIS
1	A	395	PHE
1	A	396	VAL
1	A	400	TRP
1	A	418	MET
1	A	436	TYR
1	A	439	ASP
1	B	31	LEU
1	B	34	ASN
1	B	56	LEU
1	B	73	SER
1	B	83	PRO
1	B	102	ILE
1	B	105	VAL
1	B	114	TYR
1	B	142	VAL
1	B	207	VAL
1	B	208	GLU
1	B	219	ASN
1	B	233	LEU
1	B	247	MET
1	B	249	MET
1	B	252	ASN
1	B	264	ASP
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	316	ARG
1	B	319	LYS
1	B	327	LEU
1	B	361	THR
1	B	377	HIS
1	B	395	PHE
1	B	396	VAL
1	B	400	TRP
1	B	418	MET
1	B	436	TYR
1	B	439	ASP
1	C	31	LEU
1	C	35	LEU
1	C	49	THR
1	C	91	VAL
1	C	114	TYR
1	C	137	VAL
1	C	167	VAL
1	C	212	VAL
1	C	233	LEU
1	C	249	MET
1	C	257	VAL
1	C	316	ARG
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	91	VAL
1	D	114	TYR
1	D	137	VAL
1	D	167	VAL
1	D	212	VAL
1	D	233	LEU
1	D	249	MET
1	D	257	VAL

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Mol	Chain	Res	Type
1	D	316	ARG
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	27	TYR
2	Q	30	THR
2	Q	45	LEU
2	Q	46	GLU
2	Q	50	TRP
2	Q	55	ASP
2	Q	60	TYR
2	Q	69	THR
2	Q	73	ASP
2	Q	76	SER
2	Q	78	THR
2	Q	91	SER
2	Q	123	THR
2	Q	145	LEU
2	Q	155	GLU
2	Q	183	THR
2	Q	201	THR
2	Q	214	ASP
2	Q	218	VAL
2	P	5	GLN
2	P	6	GLN
2	P	27	TYR
2	P	30	THR
2	P	45	LEU
2	P	46	GLU
2	P	50	TRP
2	P	55	ASP
2	P	60	TYR
2	P	69	THR

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Mol	Chain	Res	Type
2	P	73	ASP
2	P	76	SER
2	P	78	THR
2	P	91	SER
2	P	123	THR
2	P	145	LEU
2	P	155	GLU
2	P	183	THR
2	P	201	THR
2	P	214	ASP
2	P	218	VAL
3	W	5	THR
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	5	THR
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

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Mol	Chain	Res	Type
3	S	198	THR
3	S	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	B	140	ASN
1	B	299	GLN
1	B	377	HIS
1	C	299	GLN
1	C	434	ASN
1	D	299	GLN
3	W	30	ASN
3	W	94	GLN
3	S	41	GLN
3	S	94	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	422/445 (94%)	0.72	57 (13%) 4 2	56, 127, 231, 339	0
1	B	419/445 (94%)	0.42	38 (9%) 11 6	62, 126, 220, 332	0
1	C	420/445 (94%)	0.33	32 (7%) 17 9	37, 105, 203, 283	0
1	D	416/445 (93%)	0.53	41 (9%) 9 5	33, 105, 197, 283	0
2	P	218/219 (99%)	0.47	14 (6%) 23 13	48, 104, 168, 282	2 (0%)
2	Q	216/219 (98%)	0.71	27 (12%) 5 3	44, 108, 171, 278	2 (0%)
3	S	209/211 (99%)	0.34	9 (4%) 39 25	30, 80, 169, 258	0
3	W	207/211 (98%)	0.58	28 (13%) 4 2	23, 81, 166, 266	0
All	All	2527/2640 (95%)	0.51	246 (9%) 10 6	23, 109, 203, 339	4 (0%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	135	CYS	22.4
1	D	250	ILE	12.7
2	Q	137	ASP	12.2
1	B	264	ASP	8.4
1	B	117	PRO	8.0
1	A	268	MET	7.9
1	C	186	GLY	7.2
1	A	175	GLY	7.0
1	A	264	ASP	6.9
1	A	269	ALA	6.2
1	D	252	ASN	6.1
1	A	36	ALA	6.0
1	B	116	PHE	5.6
2	Q	92	SER	5.6
1	C	264	ASP	5.6
1	A	114	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	5.4
1	A	343	SER	5.3
1	B	249	MET	5.3
1	A	344	PRO	5.2
1	D	268	MET	5.2
3	S	152	TRP	5.2
1	A	171	PHE	5.0
1	D	343	SER	4.9
1	D	38	THR	4.9
1	D	272	ASP	4.9
2	P	138	THR	4.8
3	W	189	ASP	4.8
1	D	249	MET	4.8
3	W	215	ASN	4.8
1	A	255	LEU	4.8
2	P	137	ASP	4.7
1	C	344	PRO	4.7
2	P	88	SER	4.6
1	D	255	LEU	4.6
1	C	113	SER	4.6
1	A	119	LEU	4.6
1	A	189	THR	4.4
3	W	162	ASN	4.4
1	D	342	MET	4.3
1	D	186	GLY	4.3
1	A	116	PHE	4.2
1	C	346	ALA	4.2
1	C	116	PHE	4.2
2	P	66	GLY	4.2
1	B	345	ASN	4.1
2	Q	166	LEU	4.1
3	W	214	PHE	4.1
1	A	265	ALA	4.1
1	A	249	MET	4.0
2	P	180	ASP	4.0
1	A	185	SER	4.0
1	C	345	ASN	4.0
3	S	125	SER	3.9
1	A	279	SER	3.9
2	Q	139	THR	3.8
1	D	345	ASN	3.8
3	W	152	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	ASN	3.8
1	C	269	ALA	3.8
1	D	269	ALA	3.8
3	W	191	TYR	3.8
3	W	157	GLY	3.8
1	D	261	PRO	3.7
1	D	273	THR	3.7
2	Q	132	ALA	3.7
2	P	134	VAL	3.6
1	D	140	ASN	3.6
1	D	171	PHE	3.6
1	A	251	PRO	3.6
1	D	251	PRO	3.6
2	Q	145	LEU	3.5
1	A	141	ILE	3.5
1	A	70	PRO	3.5
1	C	250	ILE	3.5
1	A	176	GLU	3.5
1	B	186	GLY	3.5
1	B	439	ASP	3.5
1	D	260	SER	3.4
1	B	187	MET	3.4
1	D	142	VAL	3.4
2	Q	83	LEU	3.3
1	C	275	GLY	3.3
2	Q	133	PRO	3.3
1	A	20	SER	3.3
1	C	114	TYR	3.3
1	D	34	ASN	3.3
1	A	266	ALA	3.3
1	C	343	SER	3.3
1	C	252	ASN	3.2
2	P	85	SER	3.2
1	B	70	PRO	3.2
2	Q	126	PRO	3.2
1	B	346	ALA	3.2
1	A	41	ILE	3.2
1	A	250	ILE	3.2
1	D	253	ALA	3.2
1	B	189	THR	3.1
3	W	183	THR	3.1
3	S	131	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	348	LYS	3.1
1	A	261	PRO	3.1
2	Q	8	GLY	3.1
1	D	120	LYS	3.0
1	B	440	ALA	3.0
1	C	342	MET	3.0
1	B	269	ALA	3.0
1	A	120	LYS	3.0
1	A	271	GLY	3.0
1	B	273	THR	3.0
1	D	187	MET	3.0
1	A	190	PHE	3.0
1	D	254	ALA	3.0
1	A	44	TYR	2.9
1	A	252	ASN	2.9
1	C	141	ILE	2.9
2	Q	218	VAL	2.9
1	B	348	LYS	2.9
3	S	199	CYS	2.9
1	B	344	PRO	2.9
3	W	187	THR	2.9
1	B	11	GLY	2.9
2	P	135	CYS	2.9
3	W	197	TYR	2.9
1	A	183	ASN	2.8
3	W	207	THR	2.8
2	Q	165	SER	2.8
1	D	347	ALA	2.8
1	C	146	MET	2.8
1	A	140	ASN	2.8
1	D	70	PRO	2.8
1	B	113	SER	2.8
2	Q	178	GLN	2.8
1	C	271	GLY	2.8
1	D	274	ALA	2.8
1	B	10	VAL	2.8
1	D	275	GLY	2.8
2	Q	216	LYS	2.8
1	B	270	LEU	2.7
1	A	10	VAL	2.7
1	C	337	PHE	2.7
1	C	37	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	268	MET	2.7
3	W	185	THR	2.7
2	Q	163	SER	2.7
1	A	280	PHE	2.7
1	A	342	MET	2.7
2	Q	214	ASP	2.7
1	D	119	LEU	2.7
3	W	182	SER	2.6
1	C	140	ASN	2.6
3	W	80	SER	2.6
3	W	138	CYS	2.6
1	A	381	GLY	2.6
3	W	212	LYS	2.6
3	W	137	VAL	2.6
1	C	109	VAL	2.6
2	Q	134	VAL	2.6
1	B	255	LEU	2.6
2	P	199	THR	2.6
1	D	188	ASN	2.6
1	D	121	ASP	2.5
1	A	117	PRO	2.5
2	Q	167	SER	2.5
1	C	25	GLY	2.5
3	S	215	ASN	2.5
1	B	248	GLY	2.5
1	A	128	THR	2.4
1	A	217	VAL	2.4
3	W	199	CYS	2.4
2	Q	199	THR	2.4
2	P	92	SER	2.4
2	P	120	SER	2.4
1	A	71	GLY	2.4
1	D	37	ALA	2.4
1	A	200	THR	2.4
1	B	347	ALA	2.4
1	C	260	SER	2.4
1	A	34	ASN	2.4
1	D	14	PRO	2.3
1	B	190	PHE	2.3
1	D	194	GLN	2.3
3	W	213	SER	2.3
1	A	192	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	274	ALA	2.3
3	W	194	HIS	2.3
1	D	116	PHE	2.3
2	Q	138	THR	2.3
3	W	84	ALA	2.3
3	W	134	ALA	2.3
1	B	352	LEU	2.3
1	A	322	THR	2.3
1	A	170	TRP	2.3
1	C	117	PRO	2.3
1	C	194	GLN	2.3
2	Q	215	LYS	2.3
1	B	343	SER	2.3
1	D	148	THR	2.3
1	C	32	PRO	2.3
1	A	49	THR	2.3
3	W	133	GLY	2.3
3	S	214	PHE	2.3
1	B	256	ARG	2.3
1	A	204	PHE	2.3
1	C	255	LEU	2.3
3	W	211	VAL	2.3
3	W	124	PRO	2.2
1	A	345	ASN	2.2
1	A	272	ASP	2.2
2	Q	207	PRO	2.2
3	W	125	SER	2.2
1	B	252	ASN	2.2
1	C	112	LEU	2.2
2	Q	195	TRP	2.2
1	B	271	GLY	2.2
2	Q	200	VAL	2.2
3	W	155	ILE	2.2
1	A	112	LEU	2.2
1	A	113	SER	2.2
1	D	146	MET	2.2
2	Q	9	PRO	2.2
1	A	246	ILE	2.2
3	W	206	SER	2.2
2	P	71	THR	2.2
1	D	118	ILE	2.2
1	B	114	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	S	4	MET	2.1
1	C	189	THR	2.1
1	D	256	ARG	2.1
1	B	334	MET	2.1
3	S	92	CYS	2.1
1	B	39	GLY	2.1
2	Q	146	GLY	2.1
1	B	254	ALA	2.1
1	B	37	ALA	2.1
1	B	27	GLY	2.1
1	D	168	PHE	2.0
1	B	341	SER	2.0
2	P	81	MET	2.0
3	S	124	PRO	2.0
1	A	270	LEU	2.0
1	C	270	LEU	2.0
1	B	182	TRP	2.0
1	C	44	TYR	2.0
2	P	179	SER	2.0
1	A	273	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.