



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:27 am GMT

PDB ID : 3QUM  
Title : Crystal structure of human prostate specific antigen (PSA) in Fab sandwich with a high affinity and a PCa selective antibody  
Authors : Stura, E.A.; Muller, B.H.; Michel, S.; Ducancel, F.  
Deposited on : 2011-02-24  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

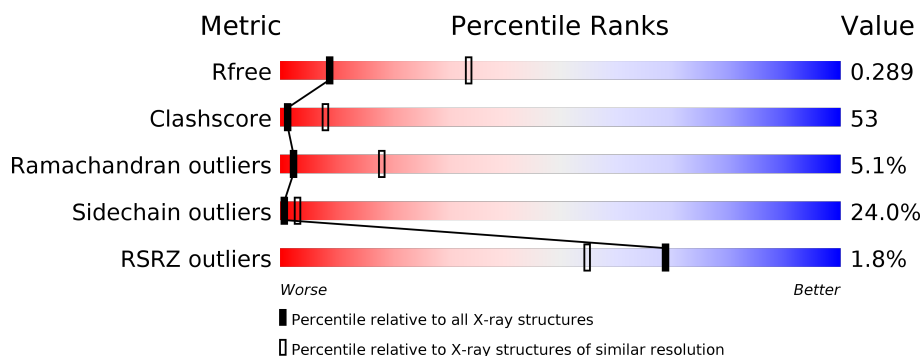
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	P	237	<div> <div>5%</div> <div>35%</div> <div>49%</div> <div>15%</div> <div>.</div> </div>
1	Q	237	<div> <div>5%</div> <div>26%</div> <div>54%</div> <div>18%</div> <div>.</div> </div>
2	L	219	<div> <div>31%</div> <div>54%</div> <div>15%</div> </div>
2	M	219	<div> <div>30%</div> <div>56%</div> <div>13%</div> <div>.</div> </div>
3	H	219	<div> <div>33%</div> <div>48%</div> <div>18%</div> <div>.</div> </div>
3	K	219	<div> <div>44%</div> <div>42%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	A	218	
4	C	218	
5	B	219	
5	D	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SIA	P	410	-	-	-	X
7	A2G	P	300	-	-	-	X
7	GAL	P	301	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17606 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 Prostate-specific antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	237	Total	C	N	O	S	4	0	0
			1832	1162	323	333	14			
1	Q	237	Total	C	N	O	S	0	0	0
			1832	1162	323	333	14			

- Molecule 2 is a protein called Fab 5D3D11 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	0	0
			1704	1063	289	343	9			
2	M	219	Total	C	N	O	S	0	0	0
			1704	1063	289	343	9			

- Molecule 3 is a protein called Fab 5D3D11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1637	1040	267	323	7			
3	K	219	Total	C	N	O	S	0	0	0
			1657	1050	272	328	7			

- Molecule 4 is a protein called Fab 5D5A5 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	218	Total	C	N	O	S	0	0	0
			1701	1062	287	345	7			
4	C	218	Total	C	N	O	S	0	0	0
			1701	1062	287	345	7			

- Molecule 5 is a protein called Fab 5D5A5 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	219	Total	C	N	O	S	0	0	0
			1655	1043	273	330	9			
5	D	219	Total	C	N	O	S	0	0	0
			1655	1043	273	330	9			

- Molecule 6 is a polymer of unknown type called SUGAR (15-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	P	15	Total	C	N	O	0	0
			206	115	8	83		
6	Q	15	Total	C	N	O	0	0
			206	115	8	83		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	P	2	Total	C	N	O	0	0
			25	14	1	10		

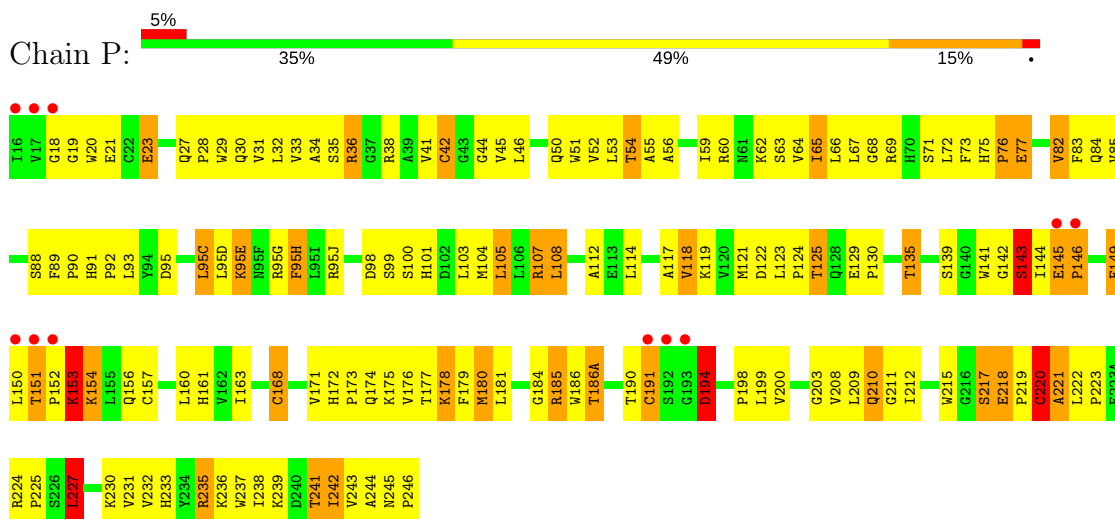
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	26	Total	O	0	0
			26	26		
8	L	4	Total	O	0	0
			4	4		
8	H	10	Total	O	0	0
			10	10		
8	A	4	Total	O	0	0
			4	4		
8	B	4	Total	O	0	0
			4	4		
8	Q	5	Total	O	0	0
			5	5		
8	M	6	Total	O	0	0
			6	6		
8	K	14	Total	O	0	0
			14	14		
8	C	11	Total	O	0	0
			11	11		
8	D	7	Total	O	0	0
			7	7		

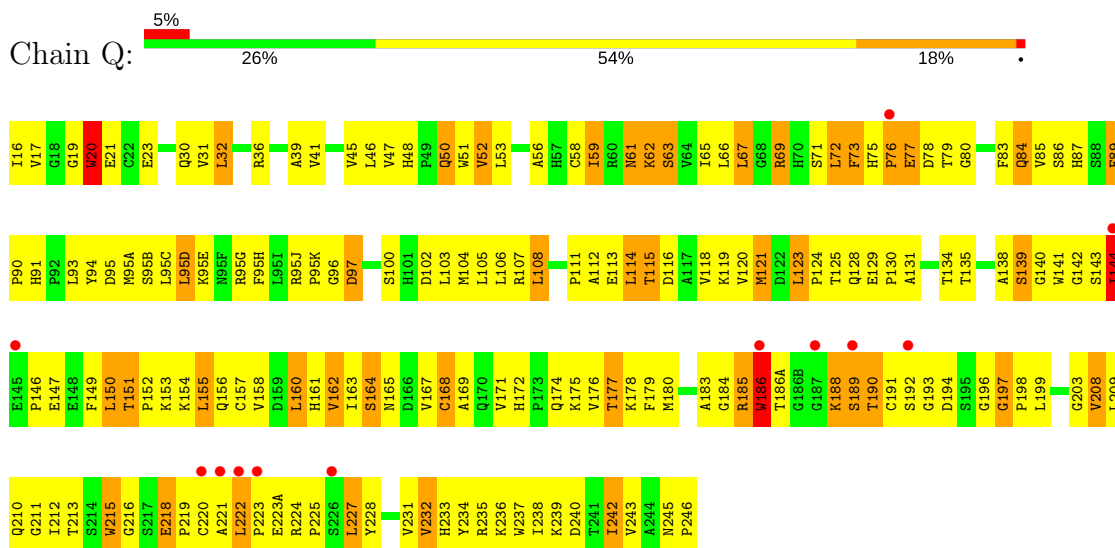
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

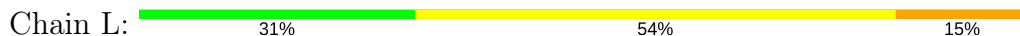
#### • Molecule 1: Prostate-specific antigen



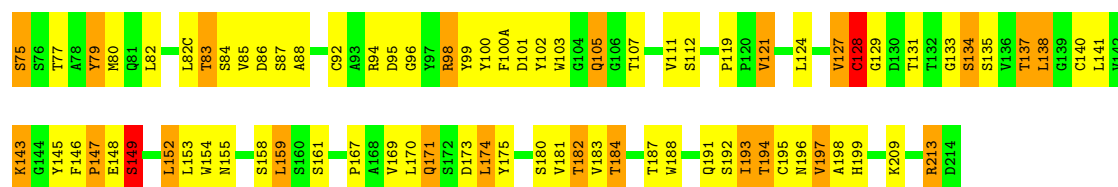
#### • Molecule 1: Prostate-specific antigen



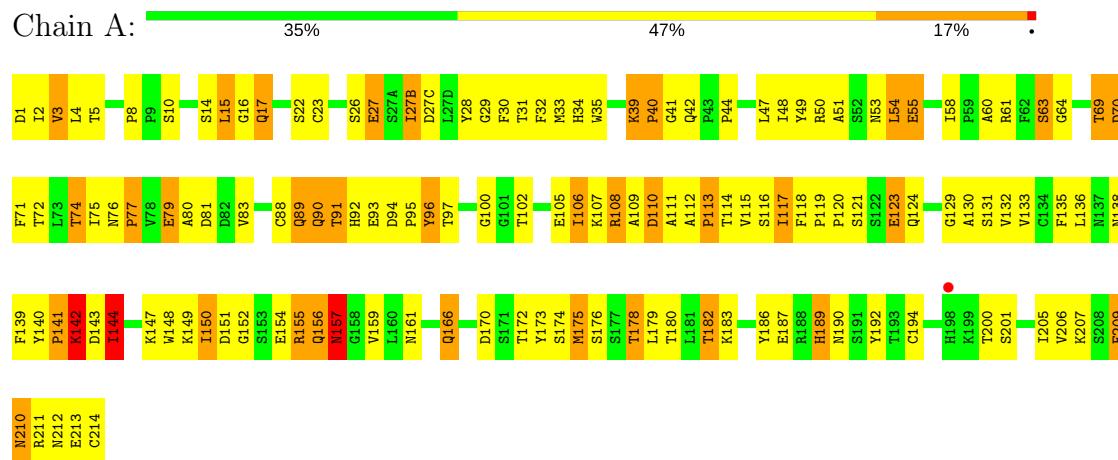
#### • Molecule 2: Fab 5D3D11 Light Chain



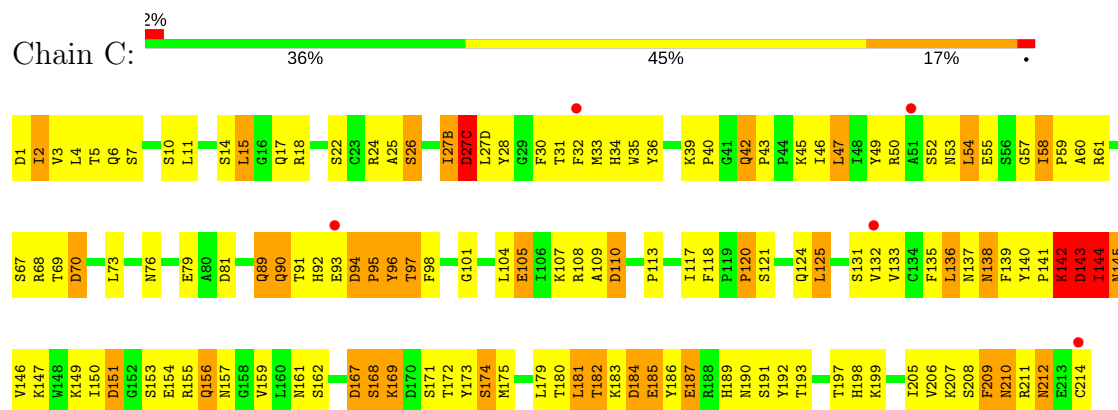




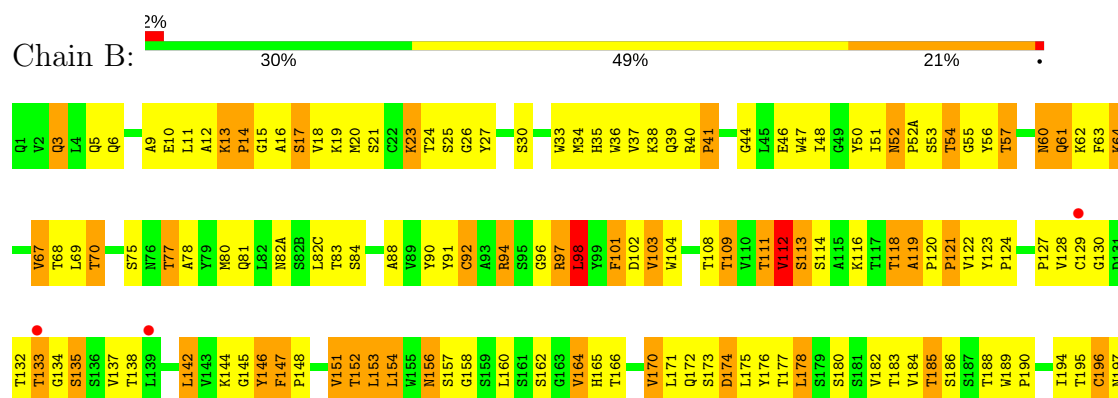
• Molecule 4: Fab 5D5A5 Light Chain



• Molecule 4: Fab 5D5A5 Light Chain



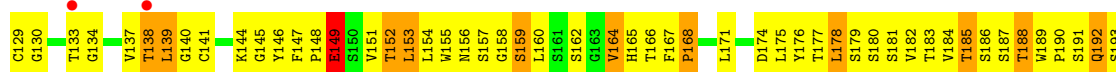
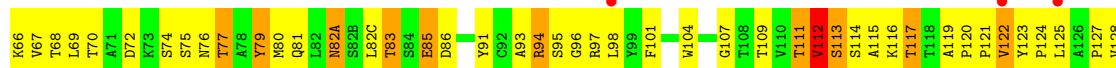
• Molecule 5: Fab 5D5A5 Heavy Chain







● Molecule 5: Fab 5D5A5 Heavy Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.31Å 226.88Å 118.69Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	58.97 – 3.20 81.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (58.97-3.20) 98.3 (81.76-3.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.198 , 0.294 0.193 , 0.289	Depositor DCC
$R_{free}$ test set	2369 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 75.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SIA, GAL, FUC, A2G, MAN

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	P	0.73	2/1883 (0.1%)	0.87	1/2564 (0.0%)
1	Q	0.45	0/1883	0.67	0/2564
2	L	0.58	0/1743	0.76	2/2366 (0.1%)
2	M	0.63	0/1743	0.76	0/2366
3	H	0.64	0/1680	0.80	1/2294 (0.0%)
3	K	0.71	0/1700	0.76	0/2319
4	A	0.53	0/1742	0.71	0/2368
4	C	0.58	0/1742	0.72	0/2368
5	B	0.57	0/1697	0.72	2/2316 (0.1%)
5	D	0.51	0/1697	0.72	0/2316
All	All	0.60	2/17510 (0.0%)	0.75	6/23841 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	2
2	M	0	1
3	H	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	168	CYS	CB-SG	-6.03	1.72	1.82
1	P	220	CYS	CA-C	-5.33	1.39	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	113	SER	N-CA-C	6.26	127.91	111.00
2	L	33	LEU	CA-CB-CG	5.68	128.37	115.30
5	B	98	LEU	CA-CB-CG	-5.64	102.33	115.30
2	L	27(C)	LEU	CA-CB-CG	5.44	127.82	115.30
3	H	45	LEU	CA-CB-CG	5.24	127.34	115.30
1	P	227	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	98	ARG	Sidechain
2	M	93	GLU	Peptide
1	P	153	LYS	Peptide
1	P	95(J)	ARG	Sidechain

## 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	P	1832	0	1802	208	0
1	Q	1832	0	1803	255	0
2	L	1704	0	1636	176	0
2	M	1704	0	1636	161	0
3	H	1637	0	1607	149	0
3	K	1657	0	1624	144	0
4	A	1701	0	1624	189	0
4	C	1701	0	1624	184	0
5	B	1655	0	1612	217	0
5	D	1655	0	1612	211	0
6	P	206	0	172	10	0
6	Q	206	0	172	13	0
7	P	25	0	22	1	0
8	A	4	0	0	0	0
8	B	4	0	0	3	0
8	C	11	0	0	0	0
8	D	7	0	0	2	0
8	H	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	K	14	0	0	1	0
8	L	4	0	0	3	0
8	M	6	0	0	2	0
8	P	26	0	0	5	0
8	Q	5	0	0	2	0
All	All	17606	0	16946	1821	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 53.

All (1821) 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)
5:D:120:PRO:HG2	5:D:146:TYR:CD1	1.76	1.20
1:P:161:HIS:CE1	1:P:185:ARG:HH21	1.64	1.15
1:Q:73:PHE:HE2	1:Q:153:LYS:HA	1.09	1.14
5:B:111:THR:O	5:B:112:VAL:HG12	1.48	1.14
1:P:237:TRP:O	1:P:241:THR:HG22	1.46	1.12
4:C:140:TYR:CD1	4:C:141:PRO:HA	1.88	1.08
5:D:120:PRO:HG2	5:D:146:TYR:HD1	0.97	1.07
5:B:98:LEU:N	5:B:98:LEU:HD23	1.52	1.07
1:Q:62:LYS:HD2	1:Q:62:LYS:H	1.19	1.06
2:M:131:SER:HB2	2:M:180:THR:HG22	1.38	1.06
2:L:24:ARG:HH21	2:L:70:ASP:HB2	1.11	1.05
4:A:27(B):ILE:HD11	4:A:32:PHE:N	1.71	1.05
5:D:120:PRO:CG	5:D:146:TYR:HD1	1.69	1.05
3:H:13:LYS:HD2	3:H:13:LYS:H	1.22	1.05
1:Q:72:LEU:HD12	4:C:28:TYR:HB3	1.37	1.04
5:D:111:THR:C	5:D:112:VAL:HG22	1.76	1.03
1:Q:19:GLY:HA3	1:Q:190:THR:OG1	1.58	1.03
5:D:111:THR:O	5:D:112:VAL:HG13	1.57	1.03
1:Q:161:HIS:HD2	1:Q:185:ARG:HB2	1.18	1.02
4:A:143:ASP:C	4:A:144:ILE:HG22	1.75	1.02
3:K:119:PRO:HB3	3:K:145:TYR:HB3	1.39	1.01
4:C:31:THR:O	4:C:50:ARG:HG2	1.59	1.01
4:C:125:LEU:H	4:C:125:LEU:HD22	1.21	1.01
5:D:111:THR:O	5:D:112:VAL:HG22	1.58	1.01
1:Q:94:TYR:CE1	1:Q:102:ASP:HB3	1.94	1.01
5:B:153:LEU:HD11	5:B:198:VAL:HG22	1.41	1.00
2:M:193:THR:HB	2:M:208:SER:HB3	1.38	1.00
5:B:111:THR:C	5:B:112:VAL:CG1	2.30	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:154:GLU:HG2	2:M:155:ARG:H	1.22	0.99
1:Q:222:LEU:HB2	1:Q:223:PRO:HD2	1.39	0.99
1:Q:123:LEU:H	1:Q:123:LEU:HD12	1.26	0.99
1:Q:63:SER:O	1:Q:85:VAL:HG23	1.63	0.99
3:H:31:SER:HB2	8:H:220:HOH:O	1.63	0.99
1:P:84:GLN:HE21	5:B:98:LEU:HD23	1.25	0.99
4:A:157:ASN:HD22	4:A:157:ASN:H	1.01	0.98
4:A:143:ASP:O	4:A:144:ILE:HG22	1.62	0.98
1:Q:222:LEU:HB2	1:Q:223:PRO:CD	1.94	0.97
4:A:108:ARG:HD2	4:A:140:TYR:HB2	1.46	0.97
4:A:27(B):ILE:HD11	4:A:32:PHE:H	1.21	0.97
5:B:133:THR:HG22	5:B:134:GLY:H	1.27	0.97
1:Q:144:ILE:HG22	1:Q:194:ASP:HA	1.44	0.97
4:C:47:LEU:O	4:C:54:LEU:HB3	1.65	0.97
2:L:136:LEU:HD12	2:L:136:LEU:N	1.77	0.96
1:Q:59:ILE:HD11	1:Q:104:MET:SD	2.05	0.96
1:Q:73:PHE:CE2	1:Q:153:LYS:HA	1.99	0.96
4:A:148:TRP:O	4:A:154:GLU:HB2	1.66	0.96
2:L:170:ASP:HB3	2:L:172:THR:HG23	1.42	0.96
1:P:130:PRO:HG3	1:P:210:GLN:HG2	1.44	0.96
4:C:190:ASN:HD21	4:C:212:ASN:HD21	1.05	0.96
5:D:145:GLY:HA2	5:D:175:LEU:HB3	1.48	0.95
5:B:6:GLN:NE2	5:B:92:CYS:H	1.63	0.95
5:B:54:THR:HG22	5:B:56:TYR:H	1.31	0.94
1:Q:186:TRP:CE3	1:Q:224:ARG:HD2	2.01	0.94
4:C:54:LEU:HD12	4:C:54:LEU:H	1.31	0.94
1:Q:140:GLY:HA3	1:Q:193:GLY:HA3	1.46	0.94
1:P:176:VAL:HA	1:P:180:MET:CE	1.97	0.94
3:K:143:LYS:HG3	3:K:143:LYS:O	1.68	0.94
2:L:51:MET:HE3	2:L:66:GLY:N	1.83	0.94
5:B:120:PRO:HD3	5:B:146:TYR:HB3	1.45	0.94
5:B:61:GLN:HA	5:B:61:GLN:HE21	1.30	0.94
1:P:84:GLN:HE21	5:B:98:LEU:CD2	1.79	0.94
3:H:60:ASN:HD22	3:H:61:GLY:N	1.66	0.94
2:M:124:GLN:HE22	2:M:131:SER:HB3	1.32	0.94
5:B:111:THR:C	5:B:112:VAL:HG12	1.88	0.93
1:P:72:LEU:HD21	1:P:141:TRP:CD1	2.02	0.93
3:K:148:GLU:HG3	3:K:149:SER:N	1.83	0.93
5:B:120:PRO:HG2	5:B:145:GLY:C	1.88	0.93
4:A:39:LYS:HB3	4:A:40:PRO:HD3	1.50	0.93
3:K:75:SER:O	3:K:77:THR:HG23	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:220:CYS:O	1:P:221:ALA:HB3	1.70	0.92
5:B:146:TYR:CE1	5:B:176:TYR:HB2	2.03	0.92
4:C:90:GLN:HE22	4:C:92:HIS:H	1.16	0.92
5:D:48:ILE:HG23	5:D:63:PHE:CD1	2.04	0.91
2:M:160:LEU:HD21	3:K:171:GLN:HG3	1.52	0.91
1:P:221:ALA:O	1:P:222:LEU:HG	1.71	0.91
4:C:90:GLN:NE2	4:C:92:HIS:H	1.68	0.91
3:H:13:LYS:CD	3:H:13:LYS:H	1.84	0.91
1:Q:218:GLU:O	1:Q:222:LEU:HD23	1.71	0.91
1:P:176:VAL:HA	1:P:180:MET:HE3	1.53	0.91
4:C:210:ASN:HD22	4:C:210:ASN:H	0.91	0.90
2:L:136:LEU:CD1	2:L:136:LEU:N	2.30	0.90
5:D:122:VAL:HG22	5:D:209:LYS:HG3	1.52	0.90
1:P:222:LEU:HB3	1:P:224:ARG:HB2	1.52	0.90
3:H:64:LYS:HD3	3:H:64:LYS:O	1.72	0.90
2:M:128:GLY:O	2:M:183:LYS:HB2	1.71	0.89
4:C:140:TYR:HD1	4:C:141:PRO:HA	1.31	0.89
4:C:27(B):ILE:HD13	4:C:27(B):ILE:H	1.38	0.89
1:Q:94:TYR:CD1	1:Q:102:ASP:HB3	2.08	0.89
5:D:156:ASN:OD1	5:D:194:ILE:HG22	1.73	0.89
2:L:188:ARG:O	2:L:188:ARG:HG3	1.71	0.89
3:K:60:ASN:HD22	3:K:61:GLY:N	1.70	0.88
5:D:156:ASN:HD22	5:D:159:SER:HB3	1.35	0.88
2:M:162:SER:OG	3:K:167:PRO:HD2	1.73	0.88
2:L:190:ASN:O	2:L:210:ASN:HA	1.74	0.88
4:C:210:ASN:HD22	4:C:210:ASN:N	1.70	0.87
3:H:124:LEU:HB2	3:H:139:GLY:O	1.74	0.87
1:P:150:LEU:HD23	1:P:152:PRO:HG2	1.56	0.87
5:B:98:LEU:N	5:B:98:LEU:CD2	2.30	0.87
4:C:210:ASN:H	4:C:210:ASN:ND2	1.72	0.87
5:D:61:GLN:HA	5:D:61:GLN:HE21	1.38	0.87
2:L:120:PRO:HB3	2:L:130:ALA:HB1	1.57	0.87
1:P:161:HIS:CE1	1:P:185:ARG:NH2	2.42	0.87
1:P:221:ALA:C	1:P:222:LEU:HG	1.95	0.87
5:B:6:GLN:HE22	5:B:92:CYS:H	1.20	0.87
2:M:136:LEU:HD13	2:M:175:MET:HG2	1.56	0.86
4:C:151:ASP:HB2	4:C:189:HIS:HD2	1.37	0.86
4:C:94:ASP:O	4:C:96:TYR:HD1	1.58	0.86
4:A:142:LYS:HD3	4:A:142:LYS:H	1.39	0.86
5:B:12:ALA:O	5:B:112:VAL:HA	1.75	0.86
1:Q:161:HIS:CD2	1:Q:185:ARG:HB2	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:140:TYR:CG	4:A:140:TYR:O	2.29	0.86
1:P:144:ILE:HD13	1:P:194:ASP:HB3	1.58	0.85
2:L:17:GLU:O	2:L:77:ARG:HA	1.75	0.85
2:L:24:ARG:NH2	2:L:70:ASP:HB2	1.90	0.85
4:A:39:LYS:HB2	4:A:42:GLN:HG3	1.57	0.85
4:A:27(B):ILE:HD12	4:A:27(B):ILE:O	1.77	0.85
4:C:61:ARG:HH12	4:C:79:GLU:HB2	1.40	0.85
2:M:36:PHE:CE2	2:M:46:LEU:HB2	2.12	0.84
5:B:13:LYS:O	5:B:16:ALA:HB3	1.75	0.84
1:Q:119:LYS:HD2	3:K:52:TYR:CE1	2.11	0.84
1:Q:47:VAL:HG23	1:Q:48:HIS:H	1.42	0.84
1:Q:59:ILE:CD1	1:Q:104:MET:SD	2.65	0.84
4:A:155:ARG:HH21	4:A:157:ASN:ND2	1.76	0.84
4:A:140:TYR:CD1	4:A:140:TYR:O	2.30	0.84
4:C:139:PHE:O	4:C:139:PHE:CD1	2.30	0.84
4:C:94:ASP:O	4:C:96:TYR:CD1	2.29	0.84
5:B:128:VAL:HG22	5:B:129:CYS:H	1.41	0.84
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.13	0.83
3:K:148:GLU:HG3	3:K:149:SER:H	1.41	0.83
1:P:150:LEU:HG	1:P:152:PRO:CD	2.08	0.83
5:B:174:ASP:O	5:B:175:LEU:HD12	1.77	0.83
1:P:143:SER:HA	1:P:191:CYS:SG	2.19	0.83
2:M:19:VAL:HG22	2:M:20:SER:H	1.42	0.82
5:B:61:GLN:HA	5:B:61:GLN:NE2	1.94	0.82
3:K:6:GLN:HE22	3:K:92:CYS:H	1.23	0.82
1:P:35:SER:HB3	1:P:62:LYS:O	1.78	0.82
4:C:144:ILE:HG13	4:C:145:ASN:H	1.45	0.82
4:C:67:SER:HB3	4:C:70:ASP:O	1.80	0.82
3:H:13:LYS:HD2	3:H:13:LYS:N	1.95	0.82
2:M:7:THR:O	2:M:9:PRO:HD3	1.78	0.82
4:A:14:SER:HA	4:A:107:LYS:HB2	1.60	0.82
2:L:90:GLN:HE21	2:L:93:GLU:H	1.27	0.82
4:C:61:ARG:NH1	4:C:79:GLU:HB2	1.94	0.82
5:D:156:ASN:ND2	5:D:159:SER:HB3	1.93	0.82
2:M:14:THR:OG1	2:M:107:LYS:HE3	1.77	0.82
3:K:6:GLN:NE2	3:K:92:CYS:H	1.76	0.82
4:A:79:GLU:HG3	4:A:80:ALA:N	1.94	0.82
4:C:108:ARG:HG3	4:C:140:TYR:CD2	2.14	0.82
5:B:60:ASN:HD22	5:B:61:GLN:N	1.77	0.81
5:D:149:GLU:OE2	5:D:149:GLU:HA	1.79	0.81
3:H:188:TRP:CZ2	3:H:210:ILE:HG13	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159:VAL:HA	2:L:178:THR:O	1.80	0.81
1:P:186:TRP:CZ2	1:P:219:PRO:HB3	2.15	0.81
4:A:90:GLN:NE2	4:A:92:HIS:H	1.78	0.81
5:D:120:PRO:CG	5:D:146:TYR:CD1	2.53	0.81
4:C:34:HIS:HD2	4:C:49:TYR:HB2	1.44	0.81
4:A:91:THR:HG21	5:B:98:LEU:HB3	1.62	0.81
2:L:108:ARG:N	2:L:140:TYR:CE1	2.48	0.81
4:A:156:GLN:H	4:A:156:GLN:HE21	1.29	0.81
3:H:188:TRP:HZ2	3:H:210:ILE:HG13	1.44	0.81
4:A:170:ASP:HB3	4:A:172:THR:HG23	1.60	0.81
5:B:146:TYR:HE1	5:B:176:TYR:HB2	1.41	0.81
1:P:56:ALA:O	1:P:59:ILE:HG22	1.81	0.80
5:B:119:ALA:HB3	5:B:205:THR:HG21	1.62	0.80
4:A:157:ASN:N	4:A:157:ASN:HD22	1.79	0.80
5:D:111:THR:O	5:D:112:VAL:CG1	2.30	0.80
5:D:24:THR:HG23	5:D:25:SER:N	1.96	0.80
1:Q:97:ASP:O	1:Q:175:LYS:HB2	1.82	0.80
5:B:156:ASN:HD21	5:B:194:ILE:HA	1.47	0.80
1:Q:87:HIS:HD2	5:D:54:THR:HG22	1.46	0.80
3:K:6:GLN:H	3:K:105:GLN:NE2	1.80	0.80
2:M:131:SER:CB	2:M:180:THR:HG22	2.11	0.80
1:P:71:SER:HB2	1:P:153:LYS:HB2	1.62	0.80
5:B:116:LYS:HB2	5:B:148:PRO:HG3	1.62	0.79
1:Q:21:GLU:HB2	1:Q:155:LEU:O	1.81	0.79
3:H:4:LEU:CD2	3:H:24:VAL:HG23	2.11	0.79
1:P:222:LEU:N	1:P:223:PRO:HD3	1.98	0.79
4:A:143:ASP:O	4:A:144:ILE:CG2	2.30	0.79
1:P:221:ALA:O	1:P:222:LEU:CD2	2.31	0.79
4:A:157:ASN:ND2	4:A:157:ASN:H	1.80	0.79
3:H:127:VAL:CG1	3:H:212:PRO:HB3	2.13	0.79
3:H:40:ARG:HH21	3:H:85:VAL:HA	1.48	0.79
1:Q:144:ILE:CG2	1:Q:194:ASP:HA	2.13	0.78
4:C:108:ARG:CG	4:C:140:TYR:CD2	2.67	0.78
5:D:111:THR:O	5:D:112:VAL:CG2	2.30	0.78
5:D:16:ALA:O	5:D:82(C):LEU:HD12	1.82	0.78
1:P:168:CYS:HB2	1:P:172:HIS:HD2	1.46	0.78
1:P:161:HIS:CE1	1:P:185:ARG:HD3	2.19	0.78
1:Q:185:ARG:O	1:Q:185:ARG:HG3	1.83	0.78
5:D:112:VAL:O	5:D:113:SER:CB	2.30	0.78
4:A:210:ASN:HB2	4:A:213:GLU:HG3	1.64	0.78
2:L:9:PRO:O	2:L:103:LYS:HG2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:115:VAL:O	4:A:207:LYS:HE3	1.84	0.78
4:C:192:TYR:HB2	4:C:209:PHE:CE2	2.18	0.78
2:L:170:ASP:HB3	2:L:172:THR:CG2	2.13	0.78
5:B:12:ALA:O	5:B:112:VAL:HB	1.84	0.78
1:P:221:ALA:O	1:P:222:LEU:CG	2.32	0.77
3:K:170:LEU:HD23	3:K:171:GLN:N	1.99	0.77
1:P:150:LEU:HG	1:P:152:PRO:HD3	1.66	0.77
4:C:144:ILE:CG1	4:C:145:ASN:H	1.97	0.77
1:Q:164:SER:O	1:Q:167:VAL:HG13	1.84	0.77
4:C:190:ASN:HD21	4:C:212:ASN:ND2	1.82	0.77
1:P:145:GLU:H	1:P:146:PRO:HD3	1.50	0.77
3:K:12:VAL:CG1	3:K:16:ALA:HB3	2.15	0.77
1:Q:21:GLU:HA	1:Q:156:GLN:HA	1.65	0.77
5:B:133:THR:HG22	5:B:134:GLY:N	2.00	0.77
3:H:153:LEU:HD12	3:H:196:ASN:HB2	1.67	0.77
3:H:51:ILE:O	3:H:52(A):PRO:HD3	1.85	0.77
1:P:18:GLY:HA2	1:P:190:THR:HG21	1.64	0.77
1:P:35:SER:CB	1:P:62:LYS:O	2.33	0.77
5:D:19:LYS:HE2	5:D:79:TYR:HD1	1.50	0.76
2:M:21:ILE:HD11	2:M:102:THR:HG21	1.66	0.76
5:D:128:VAL:HG22	5:D:129:CYS:H	1.50	0.76
3:K:6:GLN:H	3:K:105:GLN:HE22	1.31	0.76
3:H:173:ASP:O	3:H:174:LEU:HD23	1.85	0.76
1:P:130:PRO:HG3	1:P:210:GLN:CG	2.15	0.76
1:Q:72:LEU:HD22	1:Q:72:LEU:N	1.99	0.76
3:K:6:GLN:N	3:K:105:GLN:HE22	1.82	0.76
1:Q:129:GLU:HB2	1:Q:130:PRO:CD	2.15	0.76
4:A:142:LYS:O	4:A:144:ILE:HG22	1.85	0.76
5:D:12:ALA:C	5:D:13:LYS:HD3	2.06	0.76
3:H:57:THR:C	3:H:58:LYS:HG2	2.06	0.76
2:L:6:GLN:HE21	2:L:99:GLY:HA3	1.50	0.76
1:Q:162:VAL:HA	1:Q:183:ALA:HB2	1.68	0.76
1:Q:95:ASP:O	1:Q:95(C):LEU:HD13	1.85	0.76
5:B:98:LEU:H	5:B:98:LEU:HD23	1.48	0.76
1:P:186:TRP:HB2	1:P:223:PRO:HA	1.66	0.76
1:P:20:TRP:HA	1:P:20:TRP:CE3	2.19	0.76
4:A:15:LEU:HG	4:A:16:GLY:N	2.01	0.75
2:L:158:GLY:O	2:L:180:THR:HG22	1.86	0.75
1:P:64:VAL:HG12	1:P:84:GLN:HA	1.67	0.75
2:L:77:ARG:HH11	2:L:77:ARG:HB3	1.50	0.75
2:L:150:ILE:HG12	2:L:153:SER:HB3	1.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:405:NAG:H3	6:Q:405:NAG:H83	1.68	0.75
2:L:19:VAL:HG12	2:L:75:ILE:HB	1.69	0.75
4:C:118:PHE:HB2	4:C:133:VAL:HG12	1.69	0.75
2:L:173:TYR:O	2:L:174:SER:HB2	1.87	0.75
3:H:165:THR:HG23	3:H:179:SER:HB3	1.69	0.75
2:M:136:LEU:HD12	2:M:175:MET:O	1.87	0.75
1:Q:168:CYS:HA	1:Q:171:VAL:HG22	1.68	0.75
1:Q:144:ILE:HD11	1:Q:218:GLU:HA	1.66	0.75
5:D:199:ALA:HB1	5:D:206:LYS:HD2	1.67	0.75
1:Q:62:LYS:N	1:Q:62:LYS:HD2	1.97	0.75
2:L:136:LEU:CD1	2:L:136:LEU:H	1.97	0.74
4:A:90:GLN:HE22	4:A:92:HIS:H	1.34	0.74
5:B:36:TRP:CE3	5:B:80:MET:HE2	2.22	0.74
2:M:87:TYR:HE1	2:M:101:GLY:HA3	1.52	0.74
1:Q:47:VAL:HG23	1:Q:48:HIS:N	2.03	0.74
4:C:34:HIS:HD2	4:C:49:TYR:CB	2.01	0.74
1:Q:32:LEU:HD23	1:Q:141:TRP:CZ3	2.22	0.74
4:C:108:ARG:HG3	4:C:140:TYR:HD2	1.52	0.74
1:Q:211:GLY:HA2	1:Q:231:VAL:HG23	1.67	0.74
1:Q:218:GLU:O	1:Q:222:LEU:CD2	2.35	0.74
5:B:111:THR:O	5:B:112:VAL:CG1	2.30	0.74
2:L:213:GLU:HG3	2:L:214:CYS:N	2.02	0.74
6:P:410:SIA:H113	6:P:410:SIA:H4	1.70	0.74
1:P:151:THR:N	1:P:152:PRO:CD	2.50	0.74
6:Q:405:NAG:C8	6:Q:405:NAG:H3	2.18	0.74
1:Q:50:GLN:NE2	1:Q:111:PRO:HG3	2.03	0.73
5:B:116:LYS:CE	5:B:202:ALA:HB1	2.17	0.73
2:L:137:ASN:O	2:L:138:ASN:CG	2.26	0.73
1:P:95(G):ARG:CD	1:P:95(G):ARG:H	2.00	0.73
5:D:48:ILE:HD12	5:D:80:MET:HE1	1.70	0.73
4:A:149:LYS:HE3	4:A:152:GLY:H	1.53	0.73
5:B:123:TYR:HB2	5:B:142:LEU:HD22	1.70	0.73
5:D:11:LEU:HD13	5:D:111:THR:HB	1.70	0.73
1:P:154:LYS:NZ	2:L:28:ASN:O	2.20	0.73
2:M:150:ILE:HG22	2:M:151:ASP:OD2	1.87	0.73
5:B:112:VAL:HG23	5:B:113:SER:HB3	1.70	0.73
4:C:144:ILE:CG1	4:C:145:ASN:N	2.51	0.73
5:B:144:LYS:HG3	5:B:177:THR:HG22	1.71	0.73
2:M:89:MET:HB3	2:M:98:PHE:CD2	2.24	0.73
1:Q:203:GLY:HA3	8:K:222:HOH:O	1.89	0.73
3:K:35:ASN:CG	3:K:100(A):PHE:HE1	1.92	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:125:LEU:HD22	4:C:125:LEU:N	2.00	0.73
5:D:146:TYR:CE2	5:D:176:TYR:HB2	2.23	0.73
1:P:95(G):ARG:HD3	1:P:95(G):ARG:H	1.53	0.73
4:C:92:HIS:HD2	4:C:93:GLU:HG2	1.53	0.72
4:C:39:LYS:HB2	4:C:42:GLN:HG3	1.70	0.72
5:D:192:GLN:N	5:D:192:GLN:HE21	1.87	0.72
2:M:117:ILE:CD1	2:M:194:CYS:HB2	2.20	0.72
5:D:112:VAL:O	5:D:113:SER:HB3	1.88	0.72
1:P:208:VAL:HG21	7:P:300:A2G:H14	1.71	0.72
5:D:189:TRP:HD1	5:D:194:ILE:HD11	1.52	0.72
1:Q:215:TRP:HE3	1:Q:216:GLY:H	1.38	0.72
1:Q:65:ILE:HG22	1:Q:67:LEU:HD11	1.72	0.72
4:C:54:LEU:HD12	4:C:54:LEU:N	2.03	0.71
2:M:18:SER:HB3	2:M:76:SER:O	1.90	0.71
4:C:34:HIS:CD2	4:C:49:TYR:HB2	2.25	0.71
3:K:153:LEU:CD2	3:K:196:ASN:HB2	2.20	0.71
1:P:186:TRP:CH2	1:P:219:PRO:HB3	2.24	0.71
1:Q:141:TRP:CD2	1:Q:155:LEU:HD23	2.25	0.71
4:A:3:VAL:HB	4:A:97:THR:HG21	1.70	0.71
5:D:154:LEU:CB	5:D:197:ASN:HD22	2.02	0.71
1:P:149:PHE:CD2	1:P:149:PHE:N	2.58	0.71
2:L:36:PHE:HE1	2:L:89:MET:HE3	1.54	0.71
1:P:208:VAL:HA	8:P:264:HOH:O	1.90	0.71
2:L:193:THR:HA	2:L:208:SER:HB3	1.72	0.71
1:P:72:LEU:H	1:P:153:LYS:HB3	1.54	0.71
4:C:47:LEU:N	4:C:47:LEU:HD23	2.06	0.71
2:L:151:ASP:H	2:L:152:GLY:HA3	1.56	0.71
2:L:213:GLU:O	2:L:214:CYS:HB2	1.88	0.71
4:A:190:ASN:HB2	4:A:211:ARG:N	2.06	0.71
5:B:200:HIS:HB3	5:B:205:THR:HB	1.72	0.71
3:K:35:ASN:H	3:K:35:ASN:HD22	1.36	0.71
1:P:150:LEU:CG	1:P:152:PRO:HD2	2.21	0.71
4:A:120:PRO:HD3	4:A:132:VAL:HG22	1.73	0.70
2:M:87:TYR:CE1	2:M:101:GLY:HA3	2.25	0.70
5:D:190:PRO:HA	8:D:219:HOH:O	1.91	0.70
5:D:189:TRP:CD1	5:D:194:ILE:HD11	2.26	0.70
2:L:107:LYS:HA	2:L:140:TYR:HE1	1.55	0.70
2:L:147:LYS:HG2	2:L:195:GLU:HB3	1.73	0.70
1:P:221:ALA:O	1:P:222:LEU:HD23	1.91	0.70
5:B:145:GLY:O	5:B:175:LEU:HD23	1.91	0.70
2:M:159:VAL:O	2:M:160:LEU:HD12	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:27(D):HIS:ND1	2:M:28:ASN:HB3	2.07	0.70
2:M:36:PHE:HE2	2:M:46:LEU:HB2	1.51	0.70
1:P:84:GLN:NE2	5:B:98:LEU:HD23	2.03	0.70
5:D:111:THR:C	5:D:112:VAL:CG2	2.52	0.70
5:D:125:LEU:HD12	5:D:140:GLY:C	2.12	0.70
2:L:39:ARG:HG3	8:L:218:HOH:O	1.90	0.70
1:Q:160:LEU:HG	1:Q:184:GLY:HA2	1.74	0.70
4:A:39:LYS:HB3	4:A:40:PRO:CD	2.19	0.70
4:C:47:LEU:HD23	4:C:47:LEU:H	1.57	0.70
3:K:146:PHE:CD2	3:K:147:PRO:CA	2.74	0.70
2:L:175:MET:HG2	2:L:176:SER:N	2.07	0.70
2:L:90:GLN:NE2	2:L:93:GLU:H	1.88	0.70
2:M:136:LEU:N	2:M:136:LEU:HD12	2.05	0.70
3:H:116:THR:HG23	3:H:147:PRO:HD3	1.74	0.70
3:K:55:GLY:O	3:K:57:THR:HG22	1.91	0.70
1:Q:80:GLY:HA3	4:C:30:PHE:HE2	1.57	0.70
3:H:83:THR:CG2	3:H:84:SER:N	2.54	0.70
3:K:57:THR:HG1	3:K:59:TYR:HE2	1.36	0.70
3:H:152:LEU:HD12	3:H:153:LEU:N	2.05	0.70
5:B:97:ARG:O	5:B:98:LEU:HB2	1.91	0.69
4:C:179:LEU:HD11	4:C:181:LEU:CD2	2.22	0.69
1:P:23:GLU:HG2	3:H:99:TYR:HA	1.72	0.69
4:C:96:TYR:H	4:C:96:TYR:HD1	1.40	0.69
5:B:154:LEU:HD13	5:B:158:GLY:N	2.08	0.69
3:K:146:PHE:CD2	3:K:147:PRO:HA	2.27	0.69
4:A:108:ARG:HG3	4:A:140:TYR:CG	2.27	0.69
5:D:154:LEU:HD13	5:D:158:GLY:HA3	1.73	0.69
2:L:136:LEU:HD13	2:L:136:LEU:H	1.57	0.69
1:Q:69:ARG:HH21	1:Q:69:ARG:HA	1.57	0.69
3:K:57:THR:O	3:K:58:LYS:HG3	1.93	0.69
3:K:23:LYS:HG3	3:K:77:THR:HG22	1.75	0.69
5:D:120:PRO:HG3	5:D:146:TYR:HB3	1.75	0.69
3:H:156:SER:H	3:H:196:ASN:ND2	1.90	0.69
6:P:413:GAL:H4	8:P:268:HOH:O	1.93	0.69
3:H:127:VAL:HG12	3:H:212:PRO:HB3	1.74	0.69
2:M:17:GLU:O	2:M:77:ARG:HA	1.92	0.69
3:H:156:SER:H	3:H:196:ASN:HD21	1.40	0.69
4:C:108:ARG:H	4:C:140:TYR:HE2	1.39	0.69
5:D:48:ILE:HG23	5:D:63:PHE:CE1	2.28	0.69
5:D:83:THR:HG23	5:D:86:ASP:OD2	1.93	0.69
3:H:60:ASN:HD22	3:H:61:GLY:H	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:154:GLU:HG2	2:M:155:ARG:N	2.03	0.69
1:Q:215:TRP:HE3	1:Q:216:GLY:N	1.90	0.69
5:B:12:ALA:O	5:B:112:VAL:CA	2.40	0.68
5:D:186:SER:O	5:D:190:PRO:HD2	1.92	0.68
5:D:188:THR:O	5:D:192:GLN:HG2	1.92	0.68
5:D:148:PRO:CB	5:D:202:ALA:HB3	2.23	0.68
3:H:188:TRP:CD1	3:H:193:ILE:HD13	2.28	0.68
3:K:82(C):LEU:HD23	3:K:86:ASP:OD2	1.93	0.68
5:D:122:VAL:CG2	5:D:209:LYS:HG3	2.21	0.68
3:H:188:TRP:HB3	3:H:189:PRO:HD3	1.75	0.68
2:L:41:GLY:O	2:L:42:GLN:HG2	1.93	0.68
1:Q:188:LYS:HD3	1:Q:221:ALA:CB	2.22	0.68
4:A:182:THR:HG22	4:A:183:LYS:N	2.09	0.68
5:B:186:SER:O	5:B:190:PRO:HD2	1.93	0.68
3:H:170:LEU:O	3:H:170:LEU:HD22	1.94	0.68
2:M:199:LYS:HG3	2:M:200:THR:N	2.08	0.68
4:A:155:ARG:NH2	4:A:157:ASN:ND2	2.41	0.68
3:H:12:VAL:HG21	3:H:18:VAL:HG13	1.76	0.68
1:P:146:PRO:HG2	1:P:149:PHE:HA	1.74	0.68
4:A:143:ASP:O	4:A:144:ILE:CB	2.42	0.68
5:D:146:TYR:CD2	5:D:176:TYR:HB2	2.29	0.68
2:M:183:LYS:O	2:M:186:TYR:HB3	1.94	0.68
4:A:76:ASN:HB2	4:A:77:PRO:HD3	1.76	0.68
5:B:128:VAL:HG13	5:B:130:GLY:H	1.59	0.68
1:Q:47:VAL:CG2	1:Q:48:HIS:H	2.07	0.68
4:C:35:TRP:CD2	4:C:73:LEU:HD22	2.28	0.68
4:A:33:MET:O	4:A:34:HIS:CD2	2.47	0.68
1:Q:96:GLY:HA2	1:Q:175:LYS:HZ2	1.59	0.68
4:A:8:PRO:O	4:A:102:THR:HG23	1.94	0.67
4:A:174:SER:OG	5:B:165:HIS:CE1	2.47	0.67
3:H:4:LEU:HD23	3:H:24:VAL:HG23	1.76	0.67
2:M:121:SER:C	2:M:123:GLU:H	1.97	0.67
3:K:146:PHE:CG	3:K:147:PRO:HA	2.29	0.67
3:K:12:VAL:O	3:K:111:VAL:HA	1.94	0.67
3:K:11:LEU:HD22	3:K:147:PRO:HG3	1.77	0.67
1:Q:108:LEU:H	1:Q:108:LEU:HD23	1.60	0.67
4:A:159:VAL:HA	4:A:178:THR:O	1.95	0.67
4:A:210:ASN:HD21	2:M:74:ARG:HH22	1.43	0.67
5:B:120:PRO:HG2	5:B:145:GLY:CA	2.24	0.67
5:D:212:VAL:HG13	5:D:213:PRO:HD2	1.75	0.67
1:P:119:LYS:HD2	3:H:52:TYR:CD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:171:GLN:HA	3:H:171:GLN:OE1	1.94	0.67
3:K:188:TRP:HD1	3:K:193:ILE:HG22	1.59	0.67
4:C:144:ILE:HG23	4:C:145:ASN:N	2.09	0.67
2:M:38:GLN:HE22	3:K:39:GLN:HE22	1.41	0.67
1:P:82:VAL:HG13	1:P:83:PHE:N	2.09	0.67
5:B:17:SER:HA	5:B:82(C):LEU:HD23	1.76	0.67
4:A:34:HIS:HD2	4:A:49:TYR:HA	1.59	0.67
4:A:182:THR:HG22	4:A:183:LYS:H	1.60	0.67
5:B:111:THR:C	5:B:112:VAL:HG13	2.14	0.67
4:A:55:GLU:O	4:A:58:ILE:HD13	1.94	0.66
5:B:212:VAL:HG13	5:B:213:PRO:HD2	1.77	0.66
2:L:34:TYR:HB2	2:L:89:MET:HG2	1.77	0.66
3:K:40:ARG:HA	3:K:88:ALA:HB2	1.78	0.66
2:L:210:ASN:N	2:L:210:ASN:HD22	1.92	0.66
4:A:14:SER:CA	4:A:107:LYS:HB2	2.26	0.66
3:K:127:VAL:O	3:K:129:GLY:N	2.28	0.66
3:K:124:LEU:HD21	3:K:141:LEU:HB2	1.75	0.66
5:B:101:PHE:N	5:B:101:PHE:HD1	1.93	0.66
2:M:186:TYR:CD2	2:M:186:TYR:C	2.68	0.66
4:C:27(C):ASP:OD2	4:C:68:ARG:HA	1.93	0.66
2:M:46:LEU:HD22	3:K:99:TYR:CE1	2.30	0.66
1:Q:161:HIS:O	1:Q:183:ALA:HB1	1.95	0.66
5:B:133:THR:CG2	5:B:134:GLY:H	2.07	0.66
5:D:184:VAL:HG22	5:D:185:THR:N	2.11	0.66
2:L:163:TRP:N	2:L:163:TRP:CE3	2.64	0.66
1:Q:176:VAL:HG12	1:Q:176:VAL:O	1.94	0.66
5:B:30:SER:HB3	5:B:53:SER:HB2	1.77	0.66
2:L:195:GLU:HG3	2:L:206:VAL:HG22	1.77	0.66
1:P:222:LEU:N	1:P:223:PRO:CD	2.59	0.66
4:C:144:ILE:HG13	4:C:145:ASN:N	2.11	0.66
3:H:36:TRP:CD1	3:H:69:LEU:HD22	2.30	0.66
2:M:54:LEU:HD13	2:M:62:PHE:O	1.96	0.66
1:Q:186:TRP:CZ3	1:Q:224:ARG:HD2	2.30	0.66
1:P:119:LYS:CD	3:H:52:TYR:CD2	2.79	0.66
2:L:24:ARG:HH21	2:L:70:ASP:CB	1.98	0.66
2:M:160:LEU:HD21	3:K:171:GLN:CG	2.24	0.66
1:P:144:ILE:CD1	1:P:194:ASP:HB3	2.24	0.66
1:Q:73:PHE:HE2	1:Q:153:LYS:CA	1.99	0.66
4:C:142:LYS:O	4:C:143:ASP:C	2.34	0.65
3:H:6:GLN:H	3:H:105:GLN:NE2	1.94	0.65
2:M:164:THR:HG23	2:M:174:SER:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:220:CYS:O	1:P:221:ALA:CB	2.39	0.65
1:Q:67:LEU:HD12	1:Q:67:LEU:N	2.10	0.65
5:B:54:THR:HG22	5:B:56:TYR:N	2.09	0.65
3:K:188:TRP:CD1	3:K:193:ILE:CG2	2.78	0.65
2:L:77:ARG:O	2:L:77:ARG:HG3	1.97	0.65
4:C:151:ASP:HA	4:C:191:SER:OG	1.95	0.65
5:D:115:ALA:O	5:D:117:THR:N	2.27	0.65
2:M:142:LYS:HB2	2:M:173:TYR:CE1	2.32	0.65
1:Q:124:PRO:HG3	1:Q:209:LEU:O	1.96	0.65
1:Q:65:ILE:HG22	1:Q:67:LEU:CD1	2.25	0.65
4:C:94:ASP:O	4:C:96:TYR:N	2.29	0.65
5:D:36:TRP:CE3	5:D:80:MET:HE3	2.32	0.65
3:K:13:LYS:H	3:K:13:LYS:HD2	1.62	0.65
1:P:150:LEU:HG	1:P:152:PRO:HD2	1.77	0.65
3:H:73:LYS:O	3:H:75:SER:N	2.30	0.65
4:A:76:ASN:CB	4:A:77:PRO:HD3	2.27	0.65
5:B:6:GLN:HE22	5:B:92:CYS:N	1.93	0.65
5:D:154:LEU:HB2	5:D:197:ASN:HB2	1.77	0.65
3:K:127:VAL:CG2	3:K:128:CYS:N	2.59	0.65
2:M:159:VAL:C	2:M:160:LEU:HD12	2.17	0.65
2:M:136:LEU:HD13	2:M:175:MET:CG	2.25	0.65
1:P:151:THR:HG23	1:P:152:PRO:HD3	1.77	0.65
4:A:205:ILE:HA	2:M:67:SER:HB3	1.78	0.65
5:D:191:SER:C	5:D:192:GLN:HE21	2.00	0.65
3:H:154:TRP:CZ3	3:H:195:CYS:HB3	2.31	0.65
1:P:84:GLN:NE2	5:B:98:LEU:H	1.94	0.65
3:H:155:ASN:HB2	3:H:158:SER:OG	1.97	0.65
3:H:170:LEU:HD13	3:H:170:LEU:C	2.17	0.65
3:H:152:LEU:C	3:H:152:LEU:HD12	2.17	0.65
4:A:48:ILE:HG23	4:A:53:ASN:O	1.96	0.64
5:D:24:THR:CG2	5:D:25:SER:N	2.59	0.64
5:B:13:LYS:H	5:B:13:LYS:HD2	1.61	0.64
3:H:210:ILE:HG12	3:H:211:VAL:N	2.11	0.64
1:P:161:HIS:ND1	1:P:185:ARG:NH2	2.44	0.64
1:P:95(G):ARG:HG3	8:P:266:HOH:O	1.96	0.64
1:P:101:HIS:HE1	1:P:179:PHE:CE1	2.16	0.64
1:Q:100:SER:HB3	1:Q:177:THR:OG1	1.98	0.64
5:B:12:ALA:O	5:B:112:VAL:CB	2.44	0.64
4:C:155:ARG:NH1	4:C:157:ASN:HB2	2.13	0.64
4:C:187:GLU:CD	4:C:187:GLU:H	1.99	0.64
4:C:43:PRO:HB3	5:D:91:TYR:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:187:GLU:O	2:L:211:ARG:NH1	2.30	0.64
1:P:75:HIS:N	1:P:76:PRO:HD3	2.12	0.64
5:B:121:PRO:HB2	5:B:123:TYR:CZ	2.33	0.64
5:D:171:LEU:HD12	5:D:176:TYR:CZ	2.32	0.64
2:L:146:VAL:HA	2:L:195:GLU:O	1.96	0.64
5:B:39:GLN:HG3	5:B:44:GLY:O	1.97	0.64
2:M:39:ARG:O	2:M:42:GLN:HB2	1.98	0.64
4:A:154:GLU:HG2	4:A:154:GLU:O	1.96	0.64
5:B:147:PHE:O	5:B:147:PHE:CD2	2.51	0.64
5:B:36:TRP:CD2	5:B:80:MET:HE2	2.33	0.64
1:Q:140:GLY:CA	1:Q:193:GLY:HA3	2.25	0.64
4:A:150:ILE:HD13	4:A:192:TYR:CD1	2.32	0.64
5:D:198:VAL:HG12	5:D:199:ALA:N	2.13	0.64
1:P:72:LEU:CD2	1:P:141:TRP:CD1	2.79	0.64
4:C:108:ARG:HG2	4:C:140:TYR:CD2	2.32	0.64
5:D:148:PRO:HB3	5:D:202:ALA:HB3	1.80	0.64
1:Q:119:LYS:CD	3:K:52:TYR:CE1	2.81	0.64
4:C:193:THR:HG22	4:C:208:SER:HB3	1.80	0.63
5:D:48:ILE:HG23	5:D:63:PHE:HD1	1.55	0.63
1:Q:179:PHE:HD2	1:Q:233:HIS:CE1	2.16	0.63
5:B:195:THR:HG23	5:B:210:LYS:HB3	1.79	0.63
5:D:215:ASP:O	5:D:216:CYS:HB3	1.98	0.63
3:H:132:THR:HG23	3:H:133:GLY:N	2.13	0.63
3:K:12:VAL:HG13	3:K:16:ALA:HB3	1.80	0.63
1:P:125:THR:HG23	1:P:235:ARG:NH1	2.13	0.63
5:B:170:VAL:O	5:B:176:TYR:HA	1.97	0.63
3:K:127:VAL:HG23	3:K:128:CYS:N	2.12	0.63
1:P:151:THR:N	1:P:152:PRO:HD3	2.13	0.63
1:P:30:GLN:HE22	1:P:198:PRO:CD	2.10	0.63
1:P:36:ARG:N	1:P:36:ARG:HD3	2.12	0.63
1:Q:143:SER:HB3	1:Q:191:CYS:SG	2.39	0.63
4:A:190:ASN:O	4:A:210:ASN:HA	1.98	0.63
4:A:205:ILE:HA	2:M:67:SER:CB	2.29	0.63
2:L:38:GLN:HE22	3:H:39:GLN:HE22	1.45	0.63
3:K:69:LEU:O	3:K:70:THR:HG23	1.97	0.63
4:C:39:LYS:HB3	4:C:40:PRO:CD	2.28	0.63
3:H:64:LYS:HD3	3:H:64:LYS:C	2.16	0.63
4:A:190:ASN:HB2	4:A:211:ARG:H	1.63	0.63
3:K:127:VAL:HG23	3:K:128:CYS:SG	2.38	0.63
2:L:51:MET:HE3	2:L:66:GLY:H	1.59	0.63
4:A:170:ASP:HB3	4:A:172:THR:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:144:LYS:HG3	5:B:177:THR:CG2	2.29	0.63
5:B:153:LEU:CD2	5:B:178:LEU:HD21	2.29	0.63
4:C:58:ILE:HG22	4:C:59:PRO:HD2	1.81	0.63
2:L:181:LEU:HD23	2:L:182:THR:N	2.14	0.63
4:A:91:THR:CG2	4:A:91:THR:O	2.46	0.62
5:D:44:GLY:O	5:D:45:LEU:HD23	1.99	0.62
1:P:71:SER:HB2	1:P:153:LYS:CB	2.29	0.62
1:P:72:LEU:HD22	1:P:72:LEU:N	2.13	0.62
1:Q:50:GLN:HG3	1:Q:50:GLN:O	1.99	0.62
5:B:38:LYS:HD2	5:B:90:TYR:CE1	2.34	0.62
1:Q:66:LEU:HG	4:C:30:PHE:CE1	2.34	0.62
3:K:98:ARG:HG2	3:K:99:TYR:CD2	2.35	0.62
2:L:110:ASP:HA	2:L:141:PRO:HD3	1.81	0.62
2:M:115:VAL:HG12	2:M:207:LYS:HD2	1.81	0.62
5:D:36:TRP:O	5:D:48:ILE:HG13	1.99	0.62
2:M:137:ASN:HA	2:M:174:SER:HB3	1.80	0.62
4:A:34:HIS:HD2	4:A:49:TYR:CA	2.11	0.62
4:C:190:ASN:ND2	4:C:212:ASN:HD21	1.89	0.62
3:K:133:GLY:C	3:K:135:SER:H	2.03	0.62
5:D:154:LEU:HB2	5:D:197:ASN:HD22	1.63	0.62
3:H:192:SER:C	3:H:193:ILE:HD12	2.19	0.62
3:H:72:ASP:O	3:H:73:LYS:C	2.37	0.62
2:M:181:LEU:HD23	2:M:181:LEU:N	2.14	0.62
4:A:27(B):ILE:CD1	4:A:32:PHE:H	2.04	0.62
1:P:150:LEU:CG	1:P:152:PRO:CD	2.78	0.62
1:P:46:LEU:HD22	1:P:67:LEU:HD23	1.82	0.62
1:Q:142:GLY:HA3	1:Q:151:THR:HA	1.81	0.62
4:C:2:ILE:HD11	4:C:4:LEU:HG	1.82	0.62
5:D:153:LEU:HD22	5:D:180:SER:HB2	1.82	0.62
2:L:90:GLN:HE21	2:L:93:GLU:N	1.95	0.62
5:B:128:VAL:HG22	5:B:129:CYS:N	2.14	0.62
4:C:140:TYR:CD1	4:C:141:PRO:CA	2.75	0.62
3:K:30:SER:OG	3:K:73:LYS:HE3	2.00	0.62
1:P:144:ILE:HD13	1:P:194:ASP:CB	2.28	0.62
1:Q:199:LEU:HD13	1:Q:228:TYR:HE1	1.64	0.62
3:K:188:TRP:CD1	3:K:193:ILE:HG22	2.35	0.62
2:M:21:ILE:HG12	2:M:102:THR:OG1	1.99	0.62
4:A:135:PHE:C	4:A:136:LEU:HD12	2.20	0.61
4:C:59:PRO:O	4:C:61:ARG:N	2.33	0.61
2:L:151:ASP:N	2:L:152:GLY:HA3	2.15	0.61
5:D:13:LYS:HD3	5:D:13:LYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:137:THR:HB	3:H:182:THR:OG1	2.00	0.61
1:P:160:LEU:HD23	1:P:185:ARG:O	2.00	0.61
1:Q:72:LEU:HD12	4:C:28:TYR:CB	2.23	0.61
4:C:61:ARG:HH12	4:C:79:GLU:CB	2.13	0.61
3:H:6:GLN:H	3:H:105:GLN:HE22	1.46	0.61
3:K:40:ARG:HA	3:K:88:ALA:CB	2.29	0.61
2:L:126:THR:HG22	2:L:126:THR:O	2.00	0.61
2:L:151:ASP:HB2	2:L:152:GLY:CA	2.29	0.61
2:L:213:GLU:HG3	2:L:214:CYS:H	1.64	0.61
5:D:111:THR:O	5:D:112:VAL:CB	2.46	0.61
2:L:37:LEU:HB2	2:L:47:LEU:HD11	1.81	0.61
1:P:222:LEU:HD22	1:P:224:ARG:HD3	1.82	0.61
4:A:210:ASN:HD21	2:M:74:ARG:NH2	1.99	0.61
5:B:174:ASP:C	5:B:175:LEU:HD12	2.20	0.61
5:D:207:VAL:CG1	5:D:208:ASP:N	2.63	0.61
4:A:192:TYR:HB2	4:A:209:PHE:HE2	1.65	0.61
5:D:153:LEU:CD2	5:D:180:SER:HB2	2.30	0.61
3:K:66:LYS:HG3	3:K:66:LYS:O	2.01	0.61
4:A:143:ASP:C	4:A:144:ILE:CG2	2.50	0.61
3:H:150:VAL:HG23	3:H:198:ALA:O	2.00	0.61
2:L:140:TYR:CD2	2:L:140:TYR:C	2.74	0.61
2:L:122:SER:HA	2:L:125:LEU:HD12	1.82	0.61
2:M:186:TYR:C	2:M:186:TYR:HD2	2.04	0.61
5:B:196:CYS:O	5:B:208:ASP:HB2	2.01	0.61
5:D:215:ASP:O	5:D:216:CYS:CB	2.49	0.61
2:M:137:ASN:O	2:M:138:ASN:HB2	2.00	0.61
4:A:192:TYR:HB2	4:A:209:PHE:CE2	2.36	0.60
5:B:120:PRO:HB2	5:B:144:LYS:O	2.01	0.60
4:C:113:PRO:HD3	4:C:198:HIS:CD2	2.36	0.60
1:Q:84:GLN:HB2	5:D:33:TRP:CZ2	2.36	0.60
3:K:82:LEU:HD23	3:K:82:LEU:N	2.15	0.60
1:P:19:GLY:HA3	1:P:156:GLN:OE1	2.01	0.60
5:D:185:THR:HG22	5:D:187:SER:H	1.66	0.60
5:D:48:ILE:CG2	5:D:63:PHE:HD1	2.12	0.60
3:K:146:PHE:CE2	3:K:147:PRO:HB3	2.36	0.60
2:M:148:TRP:O	2:M:154:GLU:HA	2.01	0.60
2:M:46:LEU:HD23	2:M:46:LEU:O	2.02	0.60
1:Q:153:LYS:HD2	8:Q:247:HOH:O	2.01	0.60
1:Q:165:ASN:HD22	1:Q:178:LYS:HD2	1.65	0.60
4:C:27(B):ILE:CD1	4:C:27(B):ILE:H	2.12	0.60
5:D:148:PRO:HG2	5:D:200:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:137:THR:HB	3:K:182:THR:HB	1.82	0.60
2:M:93:GLU:CD	2:M:94:TYR:H	2.05	0.60
1:Q:113:GLU:O	1:Q:115:THR:HG23	2.01	0.60
4:A:27(C):ASP:HA	4:A:31:THR:HG22	1.82	0.60
2:L:41:GLY:C	2:L:42:GLN:HG2	2.21	0.60
1:Q:144:ILE:HD13	1:Q:219:PRO:HD2	1.83	0.60
5:B:5:GLN:OE1	5:B:5:GLN:HA	2.01	0.60
5:D:194:ILE:HD12	5:D:194:ILE:O	2.01	0.60
3:H:83:THR:HG23	3:H:84:SER:H	1.65	0.60
2:L:14:THR:O	2:L:17:GLU:HB2	2.02	0.60
1:Q:162:VAL:HA	1:Q:183:ALA:CB	2.31	0.60
1:Q:72:LEU:CD2	1:Q:72:LEU:N	2.64	0.60
5:B:185:THR:HB	5:B:188:THR:HG23	1.83	0.60
3:H:188:TRP:O	3:H:190:SER:N	2.34	0.60
1:Q:123:LEU:HD12	1:Q:123:LEU:N	2.08	0.60
1:Q:243:VAL:O	1:Q:246:PRO:HG3	2.01	0.60
5:B:171:LEU:HB2	5:B:176:TYR:CD1	2.36	0.60
3:K:12:VAL:HG11	3:K:16:ALA:HB3	1.84	0.60
3:K:35:ASN:N	3:K:35:ASN:ND2	2.49	0.60
2:M:149:LYS:HD2	2:M:195:GLU:OE1	2.01	0.60
4:A:118:PHE:HZ	5:B:138:THR:O	1.84	0.60
5:D:146:TYR:CZ	5:D:151:VAL:HG21	2.37	0.60
2:M:157:ASN:HD22	2:M:157:ASN:C	2.06	0.60
2:M:170:ASP:HB3	8:M:216:HOH:O	2.02	0.60
2:M:14:THR:O	2:M:17:GLU:HB2	2.02	0.60
1:P:20:TRP:HA	1:P:20:TRP:HE3	1.64	0.60
1:Q:130:PRO:HG3	1:Q:210:GLN:CG	2.31	0.60
1:Q:143:SER:O	1:Q:144:ILE:HG12	2.02	0.60
1:Q:77:GLU:HG2	1:Q:79:THR:H	1.67	0.60
4:C:209:PHE:HD2	4:C:209:PHE:O	1.82	0.60
4:C:18:ARG:HD3	4:C:76:ASN:ND2	2.17	0.60
2:M:193:THR:CB	2:M:208:SER:HB3	2.24	0.60
1:P:161:HIS:HE1	1:P:185:ARG:HH21	1.37	0.60
1:P:186:TRP:HZ2	1:P:219:PRO:HB3	1.66	0.60
1:Q:222:LEU:CB	1:Q:223:PRO:CD	2.73	0.60
5:D:29:PHE:CZ	5:D:77:THR:O	2.55	0.59
5:D:36:TRP:HE3	5:D:80:MET:HE3	1.66	0.59
3:H:172:SER:O	3:H:173:ASP:CB	2.49	0.59
2:L:90:GLN:NE2	2:L:93:GLU:N	2.49	0.59
1:P:114:LEU:H	1:P:114:LEU:HD12	1.66	0.59
1:Q:77:GLU:HG2	1:Q:78:ASP:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:124:PRO:HB2	1:Q:232:VAL:CG1	2.32	0.59
4:A:22:SER:HB3	4:A:72:THR:HG22	1.83	0.59
5:B:13:LYS:N	5:B:13:LYS:HD2	2.16	0.59
5:B:33:TRP:CZ3	5:B:52:ASN:HB2	2.38	0.59
3:H:6:GLN:NE2	3:H:106:GLY:H	2.01	0.59
1:Q:129:GLU:HB2	1:Q:130:PRO:HD3	1.85	0.59
5:B:154:LEU:O	5:B:197:ASN:HB2	2.03	0.59
4:C:96:TYR:CD1	4:C:96:TYR:N	2.70	0.59
5:D:195:THR:OG1	5:D:196:CYS:N	2.35	0.59
4:C:179:LEU:HD11	4:C:181:LEU:HD23	1.84	0.59
5:B:145:GLY:O	5:B:175:LEU:CD2	2.51	0.59
4:C:155:ARG:HH11	4:C:157:ASN:HB2	1.67	0.59
5:D:178:LEU:HD23	5:D:179:SER:N	2.18	0.59
5:D:35:HIS:HD2	5:D:47:TRP:HE1	1.50	0.59
3:K:153:LEU:HD21	3:K:196:ASN:HB2	1.83	0.59
2:L:90:GLN:HG2	2:L:91:HIS:N	2.18	0.59
1:P:144:ILE:HB	1:P:194:ASP:HA	1.85	0.59
1:Q:177:THR:O	1:Q:180:MET:HG3	2.03	0.59
1:Q:188:LYS:HD3	1:Q:221:ALA:HB2	1.85	0.59
3:K:72:ASP:OD2	3:K:75:SER:HB3	2.02	0.59
2:L:163:TRP:H	2:L:163:TRP:HE3	1.49	0.59
2:M:126:THR:C	2:M:128:GLY:H	2.06	0.59
1:P:21:GLU:OE1	1:P:154:LYS:HD2	2.02	0.59
1:P:130:PRO:CG	1:P:210:GLN:HG2	2.25	0.59
6:Q:401:NAG:H82	6:Q:401:NAG:O3	2.03	0.59
4:A:4:LEU:O	4:A:4:LEU:HD12	2.02	0.58
4:C:90:GLN:NE2	4:C:92:HIS:N	2.47	0.58
5:D:184:VAL:HG22	5:D:185:THR:H	1.67	0.58
2:L:107:LYS:HA	2:L:140:TYR:CE1	2.38	0.58
3:K:18:VAL:HG23	3:K:82(C):LEU:HD11	1.85	0.58
3:K:24:VAL:O	3:K:24:VAL:HG12	2.04	0.58
2:M:192:TYR:O	2:M:208:SER:HB2	2.02	0.58
1:P:217:SER:HB3	1:P:227:LEU:HD12	1.85	0.58
4:C:4:LEU:HD23	4:C:25:ALA:HA	1.85	0.58
2:M:33:LEU:HD12	2:M:51:MET:HA	1.84	0.58
5:B:196:CYS:HB2	5:B:209:LYS:O	2.03	0.58
4:C:192:TYR:HD2	4:C:209:PHE:HE2	1.51	0.58
5:D:155:TRP:CH2	5:D:196:CYS:SG	2.97	0.58
2:L:139:PHE:CD2	2:L:139:PHE:N	2.69	0.58
2:M:193:THR:HB	2:M:208:SER:CB	2.23	0.58
1:Q:23:GLU:OE1	2:M:34:TYR:OH	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:55:ALA:O	2:M:58:VAL:HG23	2.04	0.58
5:D:70:THR:OG1	5:D:79:TYR:HB2	2.04	0.58
5:D:19:LYS:CE	5:D:79:TYR:HD1	2.16	0.58
1:Q:234:TYR:O	1:Q:237:TRP:N	2.37	0.58
5:D:94:ARG:HG2	5:D:95:SER:N	2.18	0.58
1:Q:71:SER:OG	1:Q:154:LYS:HG2	2.02	0.58
5:B:16:ALA:O	5:B:82(C):LEU:HD23	2.04	0.58
5:B:201:PRO:O	5:B:202:ALA:O	2.20	0.58
1:Q:80:GLY:HA3	4:C:30:PHE:CE2	2.37	0.58
4:A:91:THR:HG22	4:A:91:THR:O	2.03	0.58
3:H:114:ALA:HB3	3:H:146:PHE:CE2	2.39	0.58
2:L:196:ALA:HB3	2:L:205:ILE:HB	1.86	0.58
1:P:65:ILE:HG12	1:P:108:LEU:HD11	1.86	0.58
5:D:198:VAL:HG12	5:D:199:ALA:H	1.70	0.57
3:K:47:TRP:CH2	3:K:49:GLY:HA2	2.39	0.57
1:Q:119:LYS:CD	3:K:52:TYR:CD1	2.87	0.57
1:P:150:LEU:CB	1:P:152:PRO:HD2	2.34	0.57
4:C:47:LEU:O	4:C:54:LEU:CB	2.48	0.57
4:C:54:LEU:HD22	4:C:58:ILE:O	2.04	0.57
1:Q:85:VAL:C	5:D:33:TRP:HH2	2.08	0.57
3:H:146:PHE:CG	3:H:147:PRO:HA	2.39	0.57
2:L:106:ILE:HB	2:L:166:GLN:HE22	1.68	0.57
1:P:28:PRO:HB3	1:P:119:LYS:H	1.69	0.57
1:Q:121:MET:HG3	1:Q:121:MET:O	2.04	0.57
4:C:108:ARG:HD3	4:C:140:TYR:HB2	1.85	0.57
3:K:85:VAL:O	3:K:85:VAL:HG23	2.04	0.57
1:Q:75:HIS:N	1:Q:76:PRO:HD3	2.19	0.57
4:A:175:MET:HG3	4:A:176:SER:N	2.19	0.57
4:C:2:ILE:HD13	4:C:26:SER:H	1.70	0.57
3:H:134:SER:O	3:H:184:THR:HA	2.05	0.57
3:K:193:ILE:O	3:K:193:ILE:HG12	2.04	0.57
2:L:56:SER:O	2:L:58:VAL:N	2.32	0.57
1:P:145:GLU:N	1:P:146:PRO:HD3	2.17	0.57
1:P:176:VAL:CA	1:P:180:MET:HE3	2.29	0.57
1:Q:188:LYS:HD3	1:Q:221:ALA:HB1	1.85	0.57
5:B:142:LEU:HD23	5:B:142:LEU:O	2.04	0.57
5:B:120:PRO:CD	5:B:146:TYR:HB3	2.27	0.57
5:B:97:ARG:O	5:B:98:LEU:CB	2.52	0.57
5:D:146:TYR:CE2	5:D:176:TYR:CB	2.87	0.57
3:H:199:HIS:ND1	3:H:202:SER:OG	2.38	0.57
1:P:186:TRP:CB	1:P:223:PRO:HA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:13:LYS:HB2	5:D:14:PRO:HD2	1.85	0.57
1:Q:84:GLN:HB2	5:D:33:TRP:CH2	2.39	0.57
5:B:120:PRO:HD3	5:B:146:TYR:CB	2.28	0.57
4:C:151:ASP:HB2	4:C:189:HIS:CD2	2.28	0.57
2:M:136:LEU:H	2:M:136:LEU:HD12	1.68	0.57
2:M:198:HIS:HD2	2:M:200:THR:OG1	1.87	0.57
5:D:193:SER:O	5:D:194:ILE:HG23	2.04	0.57
3:K:59:TYR:N	3:K:59:TYR:CD2	2.73	0.57
3:K:59:TYR:N	3:K:59:TYR:HD2	2.02	0.57
2:M:107:LYS:HA	2:M:140:TYR:OH	2.05	0.57
5:B:137:VAL:HG12	5:B:138:THR:N	2.19	0.57
5:B:189:TRP:CZ2	5:B:211:ILE:HD11	2.39	0.57
4:C:192:TYR:CD2	4:C:209:PHE:HE2	2.23	0.57
4:C:49:TYR:OH	4:C:55:GLU:OE1	2.22	0.57
5:B:54:THR:HG22	5:B:55:GLY:N	2.20	0.56
5:B:36:TRP:CD1	5:B:69:LEU:CD2	2.88	0.56
3:H:11:LEU:HD13	3:H:147:PRO:HG3	1.87	0.56
1:Q:119:LYS:HD2	3:K:52:TYR:CD1	2.39	0.56
4:A:190:ASN:HB2	4:A:212:ASN:H	1.69	0.56
2:L:151:ASP:HB2	2:L:152:GLY:HA3	1.86	0.56
1:P:150:LEU:HG	1:P:151:THR:H	1.71	0.56
1:Q:142:GLY:HA3	1:Q:151:THR:HB	1.85	0.56
4:A:210:ASN:O	4:A:213:GLU:HB2	2.05	0.56
4:A:54:LEU:N	4:A:54:LEU:CD1	2.67	0.56
5:B:11:LEU:HD12	5:B:12:ALA:H	1.69	0.56
5:B:152:THR:HG22	5:B:199:ALA:HB3	1.87	0.56
5:D:79:TYR:CD2	5:D:79:TYR:N	2.72	0.56
2:L:36:PHE:CE1	2:L:89:MET:HE3	2.38	0.56
2:M:33:LEU:C	2:M:33:LEU:HD13	2.26	0.56
5:B:101:PHE:N	5:B:101:PHE:CD1	2.65	0.56
5:D:51:ILE:O	5:D:51:ILE:HG23	2.05	0.56
3:H:172:SER:O	3:H:173:ASP:HB3	2.05	0.56
1:Q:77:GLU:CG	1:Q:79:THR:H	2.19	0.56
4:A:108:ARG:HD2	4:A:140:TYR:CB	2.29	0.56
5:B:3:GLN:HB3	8:B:220:HOH:O	2.05	0.56
5:D:171:LEU:HD23	5:D:171:LEU:C	2.25	0.56
2:L:147:LYS:HD3	2:L:147:LYS:N	2.21	0.56
2:M:108:ARG:HD3	2:M:172:THR:HG22	1.86	0.56
2:M:139:PHE:O	2:M:172:THR:HB	2.06	0.56
1:Q:59:ILE:HD13	1:Q:104:MET:SD	2.45	0.56
4:A:63:SER:HG	4:A:74:THR:HB	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:96:TYR:HD1	4:C:96:TYR:N	2.02	0.56
1:P:150:LEU:HD23	1:P:152:PRO:CG	2.32	0.56
6:P:410:SIA:C11	6:P:410:SIA:H4	2.35	0.56
1:Q:163:ILE:HD12	1:Q:167:VAL:HG21	1.87	0.56
1:Q:179:PHE:CD2	1:Q:233:HIS:CE1	2.94	0.56
2:L:71:PHE:CD1	2:L:71:PHE:N	2.73	0.56
4:C:35:TRP:O	4:C:46:ILE:HD12	2.05	0.56
1:P:32:LEU:HD23	1:P:66:LEU:HD22	1.88	0.56
5:B:194:ILE:HD12	5:B:194:ILE:C	2.25	0.56
4:C:27(B):ILE:HD13	4:C:27(C):ASP:OD1	2.04	0.56
3:K:145:TYR:HB2	3:K:199:HIS:CE1	2.41	0.56
4:A:156:GLN:N	4:A:156:GLN:HE21	2.01	0.56
5:D:137:VAL:HG12	5:D:138:THR:N	2.21	0.56
6:P:409:GAL:H4	6:P:410:SIA:O7	2.06	0.56
4:A:79:GLU:HG3	4:A:80:ALA:H	1.72	0.55
5:B:146:TYR:HE1	5:B:176:TYR:CB	2.16	0.55
5:B:194:ILE:HD12	5:B:194:ILE:O	2.06	0.55
4:C:179:LEU:HD12	4:C:180:THR:N	2.21	0.55
5:D:75:SER:O	5:D:76:ASN:HB2	2.07	0.55
3:K:35:ASN:N	3:K:35:ASN:HD22	2.01	0.55
1:P:45:VAL:CG2	1:P:198:PRO:HG3	2.36	0.55
1:P:76:PRO:C	1:P:77:GLU:HG3	2.26	0.55
1:P:95(G):ARG:CD	1:P:95(G):ARG:N	2.69	0.55
5:B:30:SER:HA	5:B:52(A):PRO:HB2	1.88	0.55
5:B:6:GLN:NE2	5:B:92:CYS:N	2.45	0.55
2:M:48:ILE:HD11	2:M:54:LEU:HD12	1.88	0.55
5:B:198:VAL:HG12	5:B:199:ALA:N	2.21	0.55
4:C:161:ASN:HB3	4:C:175:MET:HE3	1.88	0.55
2:L:106:ILE:CG2	2:L:107:LYS:N	2.69	0.55
3:K:134:SER:O	3:K:184:THR:HA	2.05	0.55
2:L:165:ASP:OD2	2:L:165:ASP:N	2.37	0.55
2:L:37:LEU:HD13	2:L:86:TYR:CZ	2.42	0.55
2:M:48:ILE:HG23	2:M:53:ASN:O	2.06	0.55
1:Q:141:TRP:CE2	1:Q:155:LEU:HD23	2.41	0.55
5:B:77:THR:OG1	5:B:78:ALA:N	2.40	0.55
4:C:39:LYS:NZ	4:C:81:ASP:HB2	2.22	0.55
3:H:83:THR:HG23	3:H:84:SER:N	2.19	0.55
2:L:124:GLN:NE2	2:L:130:ALA:HA	2.21	0.55
2:M:186:TYR:HD2	2:M:187:GLU:N	2.04	0.55
4:A:39:LYS:HB2	4:A:42:GLN:CG	2.32	0.55
5:B:165:HIS:O	5:B:166:THR:HB	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:83:THR:HG22	3:H:85:VAL:H	1.72	0.55
3:K:6:GLN:HE22	3:K:92:CYS:N	2.00	0.55
2:M:154:GLU:CG	2:M:155:ARG:H	2.03	0.55
4:C:124:GLN:NE2	4:C:131:SER:H	2.04	0.55
3:K:121:VAL:O	3:K:121:VAL:HG22	2.07	0.55
2:M:6:GLN:NE2	2:M:101:GLY:H	2.04	0.55
1:P:95(E):LYS:O	1:P:95(H):PHE:CE1	2.59	0.55
1:Q:50:GLN:O	1:Q:108:LEU:HD23	2.06	0.55
4:C:47:LEU:CD2	4:C:47:LEU:N	2.69	0.55
5:D:67:VAL:HG12	5:D:68:THR:N	2.22	0.55
4:A:174:SER:OG	5:B:165:HIS:HE1	1.90	0.55
5:B:37:VAL:HG11	5:B:104:TRP:CZ3	2.42	0.55
5:D:128:VAL:HG13	5:D:129:CYS:N	2.21	0.55
3:K:153:LEU:HD23	3:K:153:LEU:N	2.21	0.55
3:K:98:ARG:HG2	3:K:99:TYR:HD2	1.72	0.55
4:C:154:GLU:HG2	4:C:155:ARG:N	2.21	0.55
4:C:27(D):LEU:HD23	4:C:92:HIS:CE1	2.41	0.55
3:H:18:VAL:HG21	3:H:109:VAL:HG21	1.89	0.55
3:H:60:ASN:ND2	3:H:61:GLY:N	2.46	0.55
1:Q:134:THR:H	1:Q:162:VAL:HG23	1.72	0.55
4:A:183:LYS:NZ	4:A:187:GLU:HB2	2.22	0.54
4:C:206:VAL:HG12	4:C:207:LYS:N	2.21	0.54
3:K:57:THR:OG1	3:K:59:TYR:HE2	1.91	0.54
4:A:14:SER:HA	4:A:107:LYS:CB	2.35	0.54
1:Q:141:TRP:N	1:Q:193:GLY:HA2	2.23	0.54
4:C:168:SER:O	4:C:169:LYS:HG2	2.07	0.54
5:D:147:PHE:N	5:D:148:PRO:CD	2.70	0.54
2:M:83:VAL:HG22	2:M:84:GLY:N	2.22	0.54
1:Q:96:GLY:HA2	1:Q:175:LYS:NZ	2.22	0.54
5:B:13:LYS:O	5:B:16:ALA:CB	2.52	0.54
2:M:38:GLN:HG3	2:M:44:PRO:HG3	1.90	0.54
4:A:166:GLN:HG3	4:A:173:TYR:CE1	2.43	0.54
4:A:31:THR:O	4:A:50:ARG:HA	2.07	0.54
5:D:29:PHE:HZ	5:D:77:THR:O	1.90	0.54
3:H:105:GLN:HE21	3:H:105:GLN:H	1.54	0.54
3:K:173:ASP:O	3:K:174:LEU:HD23	2.08	0.54
1:Q:199:LEU:HD22	1:Q:228:TYR:CD1	2.43	0.54
1:Q:53:LEU:HD11	1:Q:103:LEU:CD1	2.38	0.54
1:Q:91:HIS:HE1	1:Q:93:LEU:HG	1.72	0.54
4:A:149:LYS:HD2	4:A:152:GLY:HA2	1.89	0.54
5:B:24:THR:HG23	5:B:27:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:48:ILE:CG2	5:D:63:PHE:CD1	2.84	0.54
1:Q:65:ILE:O	1:Q:66:LEU:HD12	2.06	0.54
5:D:164:VAL:HG23	5:D:165:HIS:N	2.23	0.54
5:D:119:ALA:HA	5:D:200:HIS:HD1	1.72	0.54
2:L:89:MET:HE2	2:L:98:PHE:CZ	2.42	0.54
4:A:117:ILE:HD11	4:A:194:CYS:HB2	1.90	0.54
4:A:141:PRO:O	4:A:143:ASP:N	2.40	0.54
5:B:116:LYS:HG3	5:B:116:LYS:O	2.06	0.54
5:B:52:ASN:ND2	5:B:52:ASN:C	2.60	0.54
4:C:27(C):ASP:OD2	4:C:68:ARG:HG2	2.08	0.54
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.89	0.54
2:L:162:SER:HA	2:L:163:TRP:CE3	2.42	0.54
1:Q:192:SER:HB3	1:Q:219:PRO:O	2.08	0.54
5:B:13:LYS:H	5:B:13:LYS:CD	2.21	0.54
5:D:128:VAL:HG13	5:D:130:GLY:H	1.73	0.54
1:Q:72:LEU:H	1:Q:72:LEU:CD2	2.20	0.54
5:B:189:TRP:HB3	5:B:190:PRO:HD3	1.90	0.54
1:Q:87:HIS:CD2	5:D:54:THR:HG22	2.37	0.54
4:A:39:LYS:CB	4:A:42:GLN:HG3	2.36	0.53
5:B:68:THR:O	5:B:68:THR:HG22	2.07	0.53
2:M:140:TYR:O	2:M:140:TYR:CG	2.60	0.53
1:P:91:HIS:CG	1:P:92:PRO:HD2	2.43	0.53
4:A:131:SER:HB3	4:A:180:THR:HA	1.89	0.53
5:B:52:ASN:HD22	5:B:52(A):PRO:N	2.05	0.53
3:H:101:ASP:OD1	3:H:102:TYR:N	2.42	0.53
3:H:11:LEU:HA	3:H:110:THR:O	2.09	0.53
3:H:29:ILE:HG12	3:H:29:ILE:O	2.08	0.53
2:M:80:ALA:O	2:M:83:VAL:HG12	2.07	0.53
1:P:114:LEU:N	1:P:114:LEU:HD12	2.23	0.53
1:P:161:HIS:HE1	1:P:185:ARG:NH2	1.97	0.53
1:Q:138:ALA:O	1:Q:157:CYS:HA	2.09	0.53
4:A:210:ASN:ND2	2:M:74:ARG:HH22	2.06	0.53
4:A:34:HIS:CD2	4:A:49:TYR:HA	2.43	0.53
5:D:96:GLY:O	5:D:97:ARG:HG3	2.08	0.53
6:P:411:MAN:H62	6:P:412:NAG:O3	2.08	0.53
4:C:142:LYS:HD3	4:C:173:TYR:OH	2.08	0.53
4:C:168:SER:C	4:C:169:LYS:HG2	2.27	0.53
3:K:170:LEU:HD12	3:K:175:TYR:CE1	2.43	0.53
3:K:2:VAL:HA	3:K:26:GLY:HA3	1.90	0.53
4:C:135:PHE:C	4:C:136:LEU:HD12	2.29	0.53
3:H:120:PRO:HD2	3:H:143:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:120:PRO:HG2	5:B:145:GLY:HA3	1.89	0.53
5:B:96:GLY:C	5:B:97:ARG:CG	2.75	0.53
1:Q:171:VAL:C	1:Q:223(A):GLU:HG3	2.29	0.53
1:Q:36:ARG:O	1:Q:36:ARG:HG2	2.08	0.53
1:Q:95(C):LEU:N	1:Q:95(C):LEU:HD12	2.24	0.53
4:C:120:PRO:HG2	4:C:186:TYR:CE1	2.43	0.53
5:D:144:LYS:HA	5:D:177:THR:HG23	1.90	0.53
1:P:211:GLY:HA2	1:P:231:VAL:HG23	1.91	0.53
1:Q:150:LEU:HD22	1:Q:151:THR:HG23	1.90	0.53
4:C:35:TRP:CG	4:C:73:LEU:HD22	2.44	0.53
3:H:119:PRO:HD2	3:H:204:THR:HG21	1.91	0.53
2:L:103:LYS:NZ	8:L:216:HOH:O	2.42	0.53
2:M:52:SER:HA	2:M:64:GLY:O	2.08	0.53
4:A:150:ILE:HD12	4:A:151:ASP:N	2.24	0.53
5:B:171:LEU:HB2	5:B:176:TYR:CE1	2.44	0.53
4:C:43:PRO:HB3	5:D:91:TYR:HE1	1.72	0.53
5:D:192:GLN:HE21	5:D:192:GLN:CA	2.22	0.53
5:D:124:PRO:HA	5:D:211:ILE:HD11	1.91	0.53
1:Q:147:GLU:OE1	1:Q:147:GLU:HA	2.09	0.53
5:B:197:ASN:HA	5:B:208:ASP:HB2	1.91	0.52
4:C:35:TRP:O	4:C:47:LEU:HD23	2.08	0.52
2:L:135:PHE:CE2	3:H:180:SER:OG	2.62	0.52
5:B:102:ASP:O	5:B:103:VAL:HG13	2.10	0.52
5:D:171:LEU:HD12	5:D:176:TYR:CE1	2.45	0.52
3:H:13:LYS:CD	3:H:13:LYS:N	2.61	0.52
2:M:121:SER:C	2:M:123:GLU:N	2.61	0.52
1:Q:130:PRO:HG3	1:Q:210:GLN:HG3	1.90	0.52
4:A:212:ASN:O	4:A:213:GLU:HG2	2.09	0.52
5:B:60:ASN:HD22	5:B:61:GLN:H	1.53	0.52
3:H:146:PHE:HE1	3:H:175:TYR:HE2	1.55	0.52
2:L:188:ARG:O	2:L:189:HIS:CG	2.62	0.52
1:P:30:GLN:HE22	1:P:198:PRO:CG	2.22	0.52
4:A:16:GLY:O	4:A:17:GLN:O	2.27	0.52
1:P:76:PRO:HG3	4:A:29:GLY:HA2	1.92	0.52
5:D:28:SER:HA	8:D:218:HOH:O	2.09	0.52
5:D:6:GLN:HE22	5:D:91:TYR:HA	1.74	0.52
2:L:188:ARG:O	2:L:189:HIS:CD2	2.62	0.52
1:P:150:LEU:HB3	1:P:152:PRO:HD2	1.91	0.52
1:Q:23:GLU:HG3	3:K:99:TYR:HA	1.91	0.52
4:A:142:LYS:O	4:A:144:ILE:CG2	2.57	0.52
5:B:154:LEU:HD13	5:B:157:SER:C	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:19:LYS:CE	5:D:79:TYR:CD1	2.93	0.52
2:M:150:ILE:HB	2:M:153:SER:HB3	1.91	0.52
4:C:206:VAL:CG1	4:C:207:LYS:N	2.72	0.52
5:D:153:LEU:HD12	5:D:153:LEU:N	2.25	0.52
3:K:60:ASN:C	3:K:60:ASN:HD22	2.09	0.52
2:L:118:PHE:HB2	2:L:133:VAL:HG22	1.92	0.52
1:Q:169:ALA:HA	1:Q:176:VAL:HG21	1.92	0.52
5:B:56:TYR:C	5:B:57:THR:HG22	2.30	0.52
3:H:57:THR:O	3:H:58:LYS:HG2	2.09	0.52
1:Q:94:TYR:C	1:Q:94:TYR:CD2	2.82	0.52
3:H:188:TRP:HD1	3:H:193:ILE:HD13	1.72	0.52
3:H:48:ILE:O	3:H:48:ILE:HG22	2.09	0.52
3:K:148:GLU:O	3:K:149:SER:HB2	2.10	0.52
2:L:159:VAL:C	2:L:160:LEU:HD12	2.30	0.52
1:Q:86:SER:OG	1:Q:107:ARG:NE	2.43	0.52
1:Q:233:HIS:HB3	1:Q:234:TYR:CD2	2.44	0.52
1:P:69:ARG:NH1	4:A:28:TYR:O	2.42	0.52
5:B:35:HIS:HD2	5:B:47:TRP:HE1	1.58	0.52
4:C:135:PHE:O	4:C:136:LEU:HD12	2.10	0.52
5:D:36:TRP:CE3	5:D:80:MET:CE	2.93	0.52
1:Q:85:VAL:O	5:D:33:TRP:CH2	2.63	0.52
4:C:180:THR:O	4:C:181:LEU:HD22	2.10	0.52
5:D:153:LEU:HD21	5:D:166:THR:HG23	1.91	0.52
2:L:183:LYS:HG2	2:L:184:ASP:N	2.25	0.52
1:P:161:HIS:CE1	1:P:185:ARG:CD	2.92	0.52
1:P:41:VAL:HG12	1:P:42:CYS:HB2	1.92	0.52
5:B:52:ASN:HD22	5:B:52:ASN:C	2.12	0.51
5:D:193:SER:OG	5:D:210:LYS:HE3	2.11	0.51
3:H:132:THR:CG2	3:H:133:GLY:N	2.73	0.51
2:L:181:LEU:CD2	2:L:185:GLU:HB2	2.40	0.51
1:P:150:LEU:CD2	1:P:152:PRO:HG2	2.33	0.51
4:A:139:PHE:O	4:A:139:PHE:CD1	2.63	0.51
5:B:60:ASN:HD22	5:B:60:ASN:C	2.09	0.51
2:L:116:SER:CB	2:L:118:PHE:HE1	2.24	0.51
2:L:38:GLN:HE21	2:L:87:TYR:HE2	1.56	0.51
1:Q:172:HIS:N	1:Q:223(A):GLU:HG3	2.24	0.51
1:Q:72:LEU:HD22	1:Q:72:LEU:H	1.70	0.51
2:L:160:LEU:HD21	3:H:171:GLN:HB2	1.92	0.51
2:M:55:ALA:HB3	2:M:58:VAL:HG21	1.93	0.51
1:Q:168:CYS:HA	1:Q:171:VAL:CG2	2.38	0.51
4:A:3:VAL:O	4:A:26:SER:OG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2:ILE:HD12	4:C:3:VAL:N	2.26	0.51
4:C:3:VAL:O	4:C:3:VAL:HG22	2.11	0.51
3:H:184:THR:C	3:H:186:SER:H	2.14	0.51
2:L:13:VAL:CG1	2:L:78:VAL:HG21	2.41	0.51
1:P:29:TRP:O	1:P:31:VAL:HG13	2.11	0.51
1:Q:47:VAL:CG2	1:Q:48:HIS:N	2.68	0.51
5:D:151:VAL:HG12	5:D:152:THR:N	2.26	0.51
5:D:153:LEU:HD21	5:D:166:THR:CG2	2.41	0.51
3:H:37:VAL:HG23	3:H:38:LYS:N	2.25	0.51
3:H:56:ASP:OD1	3:H:57:THR:N	2.44	0.51
2:L:108:ARG:NH2	2:L:140:TYR:HB2	2.26	0.51
6:Q:404:MAN:C1	6:Q:408:NAG:H2	2.41	0.51
4:A:90:GLN:HE22	4:A:93:GLU:H	1.57	0.51
4:C:144:ILE:O	4:C:145:ASN:HB2	2.10	0.51
3:H:188:TRP:HZ2	3:H:210:ILE:CG1	2.18	0.51
1:Q:63:SER:C	1:Q:85:VAL:HG23	2.31	0.51
4:A:135:PHE:O	4:A:136:LEU:HD12	2.11	0.51
5:B:189:TRP:CE2	5:B:211:ILE:HD11	2.45	0.51
5:B:37:VAL:HG23	5:B:46:GLU:O	2.11	0.51
4:C:27(D):LEU:O	4:C:27(D):LEU:HD12	2.10	0.51
5:D:113:SER:C	5:D:114:SER:OG	2.47	0.51
3:H:153:LEU:CD1	3:H:196:ASN:HB2	2.39	0.51
3:K:148:GLU:O	3:K:149:SER:CB	2.58	0.51
1:Q:65:ILE:CG2	1:Q:67:LEU:HD11	2.39	0.51
5:B:146:TYR:CE2	5:B:151:VAL:HG21	2.46	0.51
5:B:17:SER:HA	5:B:82(C):LEU:CD2	2.40	0.51
3:H:40:ARG:NH1	3:H:87:SER:O	2.44	0.51
2:L:151:ASP:CB	2:L:152:GLY:HA3	2.40	0.51
1:P:107:ARG:HH21	1:P:107:ARG:HG3	1.75	0.51
1:Q:196:GLY:H	1:Q:213:THR:HB	1.76	0.51
5:B:178:LEU:C	5:B:178:LEU:HD23	2.31	0.51
5:B:211:ILE:HD12	5:B:212:VAL:N	2.25	0.51
5:D:6:GLN:NE2	5:D:107:GLY:H	2.09	0.51
2:L:181:LEU:HD23	2:L:182:THR:H	1.72	0.51
2:L:35:TRP:CE3	2:L:88:CYS:HB3	2.45	0.51
2:L:6:GLN:NE2	2:L:99:GLY:HA3	2.23	0.51
1:Q:108:LEU:N	1:Q:108:LEU:HD23	2.24	0.51
5:B:61:GLN:CA	5:B:61:GLN:HE21	2.12	0.51
4:C:192:TYR:HB2	4:C:209:PHE:HE2	1.71	0.51
5:D:120:PRO:CG	5:D:146:TYR:HB3	2.39	0.51
3:K:6:GLN:NE2	3:K:92:CYS:SG	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:108:ARG:HG3	2:M:109:ALA:O	2.11	0.51
1:Q:75:HIS:CB	2:M:28:ASN:HA	2.41	0.51
5:B:142:LEU:C	5:B:142:LEU:HD23	2.30	0.50
5:D:199:ALA:O	5:D:201:PRO:HD3	2.12	0.50
3:H:74:SER:OG	3:H:74:SER:O	2.30	0.50
3:K:99:TYR:N	3:K:99:TYR:CD2	2.78	0.50
2:L:147:LYS:CD	2:L:147:LYS:N	2.74	0.50
2:M:83:VAL:CG2	2:M:84:GLY:N	2.74	0.50
1:P:142:GLY:O	1:P:143:SER:C	2.49	0.50
1:P:98:ASP:HB2	1:P:175:LYS:HD3	1.93	0.50
4:A:155:ARG:NH2	4:A:157:ASN:CG	2.64	0.50
4:A:27(B):ILE:HD11	4:A:32:PHE:CA	2.41	0.50
5:B:195:THR:HG23	5:B:210:LYS:CA	2.42	0.50
4:C:27(C):ASP:CG	4:C:68:ARG:HG2	2.31	0.50
5:D:189:TRP:O	5:D:190:PRO:C	2.46	0.50
2:M:83:VAL:HG23	2:M:104:VAL:O	2.10	0.50
2:M:8:ALA:O	2:M:102:THR:HG22	2.11	0.50
1:P:73:PHE:O	1:P:75:HIS:C	2.49	0.50
1:Q:85:VAL:O	5:D:33:TRP:HH2	1.93	0.50
5:D:198:VAL:O	5:D:199:ALA:HB2	2.12	0.50
5:D:19:LYS:HE2	5:D:79:TYR:CD1	2.39	0.50
2:L:46:LEU:CD2	3:H:99:TYR:CD1	2.95	0.50
4:A:205:ILE:HG23	2:M:67:SER:HB3	1.93	0.50
1:P:208:VAL:HG12	1:P:209:LEU:O	2.11	0.50
1:Q:16:ILE:HG12	1:Q:16:ILE:O	2.11	0.50
4:C:141:PRO:O	4:C:142:LYS:O	2.30	0.50
2:M:73:LEU:HG	2:M:74:ARG:N	2.27	0.50
4:A:154:GLU:CG	4:A:154:GLU:O	2.60	0.50
4:A:34:HIS:HD2	4:A:49:TYR:CB	2.22	0.50
4:A:8:PRO:HG2	4:A:10:SER:O	2.11	0.50
4:A:1:ASP:OD2	4:A:95:PRO:HB3	2.12	0.50
4:C:59:PRO:C	4:C:61:ARG:H	2.14	0.50
5:D:50:TYR:HE1	5:D:58:GLU:HG3	1.76	0.50
1:Q:95(A):MET:C	1:Q:95(C):LEU:H	2.15	0.50
4:A:156:GLN:NE2	4:A:156:GLN:H	2.04	0.50
4:C:142:LYS:HD3	4:C:173:TYR:CZ	2.46	0.50
1:P:35:SER:HB3	1:P:63:SER:HA	1.93	0.50
4:A:58:ILE:HD12	4:A:58:ILE:N	2.26	0.50
5:B:33:TRP:CE3	5:B:52:ASN:HB2	2.47	0.50
5:D:146:TYR:O	5:D:146:TYR:HD2	1.94	0.50
3:H:40:ARG:HH11	3:H:40:ARG:HG3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:108:ARG:HG2	2:M:140:TYR:CD1	2.46	0.50
5:B:37:VAL:HG13	5:B:91:TYR:HB2	1.93	0.50
5:D:125:LEU:HD12	5:D:140:GLY:CA	2.42	0.50
5:D:40:ARG:CZ	5:D:85:GLU:HG3	2.42	0.50
2:M:46:LEU:HD22	3:K:99:TYR:HE1	1.76	0.50
1:P:50:GLN:O	1:P:108:LEU:HD22	2.11	0.50
1:Q:190:THR:O	1:Q:190:THR:OG1	2.26	0.50
4:A:63:SER:OG	4:A:74:THR:HB	2.12	0.50
3:H:150:VAL:HG22	3:H:151:THR:N	2.27	0.50
2:M:117:ILE:HD13	2:M:194:CYS:HB2	1.93	0.50
1:P:238:ILE:O	1:P:239:LYS:C	2.48	0.50
1:Q:72:LEU:HB3	4:C:28:TYR:HA	1.92	0.49
5:D:125:LEU:HD12	5:D:140:GLY:HA3	1.93	0.49
5:D:156:ASN:O	5:D:157:SER:OG	2.23	0.49
5:D:112:VAL:O	5:D:113:SER:OG	2.30	0.49
3:H:138:LEU:N	3:H:138:LEU:HD23	2.27	0.49
2:M:160:LEU:HB3	3:K:169:VAL:HG11	1.95	0.49
2:L:170:ASP:CB	2:L:172:THR:HG23	2.30	0.49
2:L:91:HIS:CD2	2:L:91:HIS:O	2.65	0.49
1:Q:47:VAL:O	1:Q:120:VAL:HB	2.12	0.49
1:Q:72:LEU:HD21	1:Q:141:TRP:NE1	2.27	0.49
5:D:13:LYS:O	5:D:16:ALA:HB3	2.12	0.49
5:D:35:HIS:CD2	5:D:47:TRP:HE1	2.29	0.49
3:H:40:ARG:HG3	3:H:41:PRO:HD2	1.95	0.49
3:K:103:TRP:N	3:K:103:TRP:CD1	2.80	0.49
2:L:142:LYS:HG3	2:L:173:TYR:CE1	2.47	0.49
2:L:144:ILE:HB	2:L:197:THR:O	2.12	0.49
2:L:163:TRP:CD2	2:L:163:TRP:N	2.80	0.49
1:Q:139:SER:HA	1:Q:156:GLN:O	2.13	0.49
4:A:2:ILE:HG22	4:A:26:SER:HB3	1.95	0.49
5:B:189:TRP:CE3	5:B:190:PRO:HG3	2.48	0.49
5:D:146:TYR:O	5:D:146:TYR:CD2	2.65	0.49
1:P:176:VAL:HA	1:P:180:MET:HE1	1.90	0.49
1:Q:19:GLY:HA3	1:Q:190:THR:HG1	1.74	0.49
1:Q:46:LEU:HD12	1:Q:51:TRP:O	2.13	0.49
4:C:155:ARG:HH12	4:C:181:LEU:HD21	1.78	0.49
5:D:157:SER:N	5:D:197:ASN:HD21	2.10	0.49
3:H:137:THR:C	3:H:138:LEU:HD23	2.33	0.49
1:P:174:GLN:HG2	1:P:175:LYS:N	2.27	0.49
4:A:131:SER:HA	4:A:179:LEU:O	2.13	0.49
5:D:114:SER:O	5:D:147:PHE:HD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:LYS:CE	3:H:13:LYS:H	2.25	0.49
2:L:77:ARG:O	2:L:77:ARG:CG	2.59	0.49
2:L:2:ILE:HD13	2:L:93:GLU:HB2	1.95	0.49
4:A:206:VAL:O	2:M:66:GLY:HA2	2.13	0.49
1:P:65:ILE:HG22	1:P:67:LEU:CD1	2.42	0.49
4:A:106:ILE:HG23	4:A:107:LYS:N	2.27	0.49
5:B:173:SER:O	5:B:175:LEU:N	2.46	0.49
5:D:121:PRO:HB2	5:D:123:TYR:CE2	2.48	0.49
5:D:124:PRO:HA	5:D:211:ILE:CD1	2.43	0.49
3:H:146:PHE:CD1	3:H:147:PRO:HA	2.48	0.49
3:K:13:LYS:N	3:K:13:LYS:HD2	2.27	0.49
2:L:136:LEU:O	2:L:137:ASN:OD1	2.30	0.49
2:M:62:PHE:CE1	2:M:75:ILE:HG13	2.48	0.49
1:P:30:GLN:HE22	1:P:198:PRO:HG2	1.78	0.49
1:P:36:ARG:H	1:P:36:ARG:HD3	1.77	0.49
1:P:35:SER:HB2	1:P:62:LYS:O	2.11	0.49
1:P:95(G):ARG:NH2	8:P:267:HOH:O	2.46	0.49
1:Q:165:ASN:ND2	1:Q:178:LYS:HD2	2.27	0.49
1:Q:20:TRP:HB2	3:K:98:ARG:NH1	2.28	0.49
2:L:195:GLU:HG3	2:L:206:VAL:CG2	2.42	0.49
1:P:28:PRO:CB	1:P:119:LYS:H	2.26	0.49
1:Q:188:LYS:HG2	1:Q:224:ARG:HH12	1.78	0.49
1:Q:186:TRP:HE3	1:Q:224:ARG:HD2	1.67	0.49
1:Q:231:VAL:O	1:Q:233:HIS:N	2.45	0.49
6:Q:403:MAN:H3	6:Q:411:MAN:O2	2.13	0.49
4:A:108:ARG:CG	4:A:140:TYR:CG	2.95	0.49
4:A:157:ASN:N	4:A:157:ASN:ND2	2.48	0.49
4:C:33:MET:O	4:C:50:ARG:N	2.43	0.49
5:D:113:SER:O	5:D:114:SER:OG	2.30	0.49
3:H:20:ILE:HD12	3:H:107:THR:HG21	1.95	0.49
3:K:182:THR:C	3:K:183:VAL:HG13	2.32	0.49
3:K:154:TRP:CZ3	3:K:195:CYS:HB3	2.48	0.49
2:L:116:SER:HB2	2:L:118:PHE:HE1	1.75	0.49
1:P:150:LEU:HG	1:P:151:THR:N	2.28	0.49
1:Q:83:PHE:CZ	1:Q:112:ALA:HA	2.48	0.49
1:Q:128:GLN:CG	1:Q:129:GLU:N	2.76	0.49
5:D:154:LEU:HB2	5:D:197:ASN:ND2	2.27	0.48
5:D:52:ASN:C	5:D:52:ASN:HD22	2.15	0.48
2:M:27:LYS:HE3	2:M:27:LYS:HB3	1.64	0.48
1:P:153:LYS:HE2	1:P:154:LYS:NZ	2.28	0.48
1:Q:125:THR:HG22	1:Q:128:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:51:ALA:O	4:A:64:GLY:HA3	2.12	0.48
2:M:38:GLN:NE2	3:K:39:GLN:HE22	2.09	0.48
4:A:123:GLU:OE1	4:A:123:GLU:N	2.46	0.48
5:B:64:LYS:HE3	5:B:64:LYS:HB3	1.47	0.48
4:C:142:LYS:O	4:C:143:ASP:O	2.29	0.48
3:H:159:LEU:H	3:H:159:LEU:HD23	1.78	0.48
2:L:178:THR:O	2:L:178:THR:HG22	2.12	0.48
1:Q:239:LYS:O	1:Q:239:LYS:HG3	2.12	0.48
5:B:116:LYS:HE3	5:B:202:ALA:HB1	1.95	0.48
5:B:83:THR:HG22	5:B:84:SER:N	2.27	0.48
3:H:50:ARG:NH1	3:H:95:ASP:OD2	2.46	0.48
4:A:205:ILE:CG2	2:M:67:SER:HB3	2.44	0.48
1:P:238:ILE:O	1:P:242:ILE:HB	2.13	0.48
5:B:35:HIS:CD2	5:B:47:TRP:HE1	2.32	0.48
4:C:11:LEU:HD12	4:C:11:LEU:HA	1.60	0.48
4:C:39:LYS:HZ3	4:C:81:ASP:HB2	1.76	0.48
2:L:133:VAL:HG21	3:H:124:LEU:HD23	1.95	0.48
3:K:33:TRP:CE3	3:K:50:ARG:HG3	2.48	0.48
3:K:94:ARG:HH21	3:K:101:ASP:CG	2.17	0.48
2:L:135:PHE:C	2:L:136:LEU:HD12	2.32	0.48
2:M:48:ILE:HD12	2:M:54:LEU:HA	1.96	0.48
1:P:215:TRP:HA	1:P:215:TRP:CE3	2.49	0.48
1:P:93:LEU:HB2	1:P:101:HIS:CD2	2.47	0.48
4:A:108:ARG:CG	4:A:140:TYR:CD1	2.96	0.48
4:A:156:GLN:O	4:A:159:VAL:HG22	2.13	0.48
4:A:206:VAL:H	2:M:67:SER:H	1.61	0.48
5:B:154:LEU:HD12	5:B:154:LEU:C	2.34	0.48
4:C:193:THR:HA	4:C:208:SER:HB3	1.96	0.48
4:C:2:ILE:O	4:C:97:THR:HG21	2.13	0.48
1:Q:84:GLN:NE2	5:D:33:TRP:CD2	2.82	0.48
3:H:152:LEU:HD11	3:H:195:CYS:HB2	1.95	0.48
3:H:194:THR:HG23	3:H:208:LYS:O	2.13	0.48
3:K:124:LEU:HD23	3:K:140:CYS:N	2.29	0.48
6:P:414:SIA:H8	6:P:414:SIA:N5	2.29	0.48
4:C:184:ASP:HA	4:C:187:GLU:CD	2.34	0.48
3:K:155:ASN:HD22	3:K:159:LEU:CD1	2.27	0.48
2:L:95:PRO:O	2:L:97:THR:HG23	2.14	0.48
1:P:124:PRO:HG3	1:P:209:LEU:O	2.14	0.48
1:P:151:THR:H	1:P:152:PRO:HD3	1.79	0.48
1:Q:72:LEU:HD21	1:Q:141:TRP:CD1	2.48	0.48
4:C:125:LEU:CD2	4:C:125:LEU:H	2.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:VAL:CG2	3:H:38:LYS:N	2.77	0.48
3:K:101:ASP:C	3:K:101:ASP:OD1	2.51	0.48
2:L:166:GLN:O	2:L:167:ASP:O	2.32	0.48
6:Q:405:NAG:H83	6:Q:405:NAG:C3	2.42	0.48
5:D:144:LYS:HD3	5:D:144:LYS:C	2.34	0.48
3:K:69:LEU:HD23	3:K:80:MET:HG2	1.95	0.48
2:L:189:HIS:O	2:L:211:ARG:NE	2.47	0.48
1:P:157:CYS:O	3:H:98:ARG:NH1	2.47	0.48
1:P:73:PHE:HD1	1:P:153:LYS:HG2	1.78	0.48
4:A:156:GLN:NE2	4:A:156:GLN:N	2.61	0.48
4:A:90:GLN:HE22	4:A:92:HIS:N	2.09	0.48
5:B:195:THR:CG2	5:B:210:LYS:HB3	2.43	0.48
2:L:183:LYS:H	2:L:183:LYS:HD2	1.78	0.48
2:M:27(B):LEU:HD21	2:M:90:GLN:HB2	1.95	0.48
1:P:123:LEU:N	1:P:123:LEU:CD1	2.76	0.48
1:P:218:GLU:HA	1:P:219:PRO:HD3	1.43	0.48
1:P:71:SER:O	1:P:72:LEU:HD13	2.14	0.48
1:Q:231:VAL:C	1:Q:233:HIS:N	2.67	0.48
4:A:150:ILE:HD13	4:A:192:TYR:CE1	2.49	0.47
4:A:205:ILE:HG23	2:M:67:SER:CB	2.44	0.47
5:B:24:THR:CG2	5:B:25:SER:N	2.76	0.47
4:C:146:VAL:CG1	4:C:147:LYS:N	2.76	0.47
5:D:66:LYS:HD3	5:D:82(A):ASN:O	2.14	0.47
3:H:105:GLN:HE21	3:H:105:GLN:N	2.12	0.47
3:K:83:THR:OG1	3:K:84:SER:N	2.45	0.47
2:L:183:LYS:CD	2:L:183:LYS:H	2.27	0.47
2:M:47:LEU:O	2:M:48:ILE:HD13	2.15	0.47
1:Q:67:LEU:CD1	1:Q:67:LEU:N	2.77	0.47
4:A:94:ASP:HA	4:A:96:TYR:CE1	2.49	0.47
5:B:14:PRO:O	5:B:16:ALA:N	2.46	0.47
3:K:153:LEU:O	3:K:153:LEU:HG	2.14	0.47
3:K:98:ARG:CG	3:K:99:TYR:HD2	2.26	0.47
2:M:206:VAL:O	2:M:206:VAL:HG12	2.13	0.47
1:Q:124:PRO:HB2	1:Q:232:VAL:HG12	1.95	0.47
4:A:23:CYS:HB2	4:A:35:TRP:CH2	2.49	0.47
5:B:60:ASN:ND2	5:B:62:LYS:HG2	2.29	0.47
5:D:207:VAL:HG12	5:D:208:ASP:N	2.29	0.47
5:D:61:GLN:HA	5:D:61:GLN:NE2	2.18	0.47
5:D:75:SER:CB	5:D:77:THR:HG23	2.45	0.47
2:L:36:PHE:HE1	2:L:89:MET:CE	2.25	0.47
4:A:112:ALA:O	4:A:113:PRO:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:184:VAL:CG2	5:D:185:THR:N	2.77	0.47
5:D:198:VAL:CG1	5:D:199:ALA:N	2.78	0.47
2:L:108:ARG:HG2	2:L:109:ALA:H	1.78	0.47
1:P:75:HIS:N	1:P:76:PRO:CD	2.77	0.47
1:Q:234:TYR:O	1:Q:236:LYS:N	2.47	0.47
1:Q:95(E):LYS:HZ2	6:Q:410:SIA:H111	1.79	0.47
4:A:142:LYS:CD	4:A:142:LYS:H	2.15	0.47
1:P:76:PRO:CG	4:A:29:GLY:HA2	2.44	0.47
5:B:195:THR:HG23	5:B:210:LYS:CB	2.45	0.47
4:C:157:ASN:HD22	4:C:157:ASN:H	1.62	0.47
4:C:89:GLN:NE2	4:C:98:PHE:CZ	2.82	0.47
2:L:131:SER:HB3	2:L:180:THR:CB	2.44	0.47
6:Q:404:MAN:H4	6:Q:408:NAG:H4	1.97	0.47
4:C:121:SER:HB3	4:C:124:GLN:HB2	1.96	0.47
4:C:136:LEU:HD21	4:C:146:VAL:CG2	2.45	0.47
4:C:54:LEU:H	4:C:54:LEU:CD1	2.03	0.47
5:D:157:SER:CA	5:D:197:ASN:HD21	2.27	0.47
5:D:196:CYS:O	5:D:208:ASP:HA	2.14	0.47
3:H:147:PRO:HB2	3:H:148:GLU:H	1.53	0.47
2:L:135:PHE:CE2	3:H:180:SER:HB3	2.49	0.47
3:K:133:GLY:C	3:K:135:SER:N	2.68	0.47
1:P:130:PRO:HG3	1:P:210:GLN:CD	2.34	0.47
1:Q:119:LYS:HE3	3:K:52:TYR:HD1	1.79	0.47
4:A:141:PRO:O	4:A:142:LYS:C	2.53	0.47
4:A:151:ASP:OD2	4:A:189:HIS:CB	2.62	0.47
4:C:7:SER:O	4:C:22:SER:N	2.41	0.47
5:D:50:TYR:CD1	5:D:58:GLU:HB2	2.50	0.47
3:H:146:PHE:CE1	3:H:175:TYR:HE2	2.32	0.47
3:K:13:LYS:HA	3:K:112:SER:O	2.15	0.47
1:P:95(E):LYS:H	1:P:95(H):PHE:HE1	1.63	0.47
1:Q:66:LEU:HG	4:C:30:PHE:CD1	2.50	0.47
4:A:192:TYR:HD2	4:A:209:PHE:CE2	2.32	0.47
4:A:27(B):ILE:HA	4:A:92:HIS:ND1	2.29	0.47
4:A:89:GLN:HG2	4:A:90:GLN:N	2.30	0.47
5:B:120:PRO:O	5:B:121:PRO:O	2.33	0.47
4:C:137:ASN:HA	4:C:174:SER:HB3	1.97	0.47
4:C:190:ASN:O	4:C:211:ARG:N	2.39	0.47
4:C:193:THR:HG22	4:C:208:SER:CB	2.44	0.47
3:K:29:ILE:HG12	3:K:29:ILE:O	2.14	0.47
3:K:96:GLY:HA3	3:K:101:ASP:OD2	2.14	0.47
2:L:137:ASN:O	2:L:138:ASN:OD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:48:ILE:CD1	2:M:54:LEU:HA	2.44	0.47
1:Q:143:SER:C	1:Q:144:ILE:HG23	2.34	0.47
5:B:118:THR:O	5:B:120:PRO:CD	2.63	0.47
5:B:60:ASN:HB3	5:B:63:PHE:CD1	2.50	0.47
5:B:75:SER:O	5:B:77:THR:HG22	2.15	0.47
4:C:156:GLN:O	4:C:159:VAL:HG12	2.15	0.47
4:C:27(B):ILE:CD1	4:C:27(B):ILE:N	2.78	0.47
2:L:173:TYR:O	2:L:174:SER:CB	2.60	0.47
1:P:242:ILE:HG22	1:P:243:VAL:N	2.30	0.47
1:Q:91:HIS:CE1	1:Q:93:LEU:HG	2.48	0.47
5:B:153:LEU:HD12	5:B:153:LEU:HA	1.63	0.47
4:C:157:ASN:HD22	4:C:157:ASN:N	2.13	0.47
5:D:75:SER:HB2	5:D:77:THR:HG23	1.97	0.47
3:K:13:LYS:CD	3:K:13:LYS:H	2.26	0.47
2:L:155:ARG:HG2	2:L:155:ARG:HH21	1.80	0.47
2:L:67:SER:O	2:L:69:THR:N	2.48	0.47
2:L:94:TYR:OH	3:H:50:ARG:HD3	2.15	0.47
2:M:19:VAL:HG22	2:M:20:SER:N	2.20	0.47
5:B:197:ASN:HA	5:B:208:ASP:CB	2.45	0.47
5:B:60:ASN:HB3	5:B:63:PHE:HD1	1.80	0.47
5:D:114:SER:O	5:D:147:PHE:CD1	2.68	0.47
5:D:33:TRP:N	5:D:33:TRP:HE3	2.13	0.47
2:M:167:ASP:OD1	2:M:170:ASP:HB2	2.14	0.47
5:B:69:LEU:O	5:B:70:THR:HG23	2.15	0.46
3:H:111:VAL:O	3:H:112:SER:HB3	2.15	0.46
3:H:18:VAL:HG22	3:H:82(C):LEU:HD11	1.98	0.46
2:M:182:THR:OG1	2:M:185:GLU:OE1	2.29	0.46
2:M:38:GLN:HE22	3:K:39:GLN:NE2	2.10	0.46
4:A:170:ASP:CB	4:A:172:THR:HG23	2.40	0.46
4:A:47:LEU:HA	4:A:58:ILE:HG12	1.96	0.46
4:C:155:ARG:CZ	4:C:155:ARG:HB3	2.45	0.46
4:C:113:PRO:HD3	4:C:198:HIS:HD2	1.77	0.46
3:H:83:THR:HG22	3:H:84:SER:N	2.29	0.46
2:L:10:SER:OG	2:L:11:VAL:N	2.48	0.46
1:Q:61:ASN:OD1	6:Q:401:NAG:N2	2.48	0.46
4:A:143:ASP:O	4:A:144:ILE:HB	2.13	0.46
4:A:190:ASN:HB3	4:A:212:ASN:OD1	2.15	0.46
5:B:14:PRO:C	5:B:16:ALA:N	2.68	0.46
5:B:208:ASP:OD2	5:B:208:ASP:O	2.33	0.46
5:B:211:ILE:O	5:B:212:VAL:HG23	2.16	0.46
4:C:117:ILE:HG12	4:C:118:PHE:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:48:ILE:O	3:H:48:ILE:CG2	2.63	0.46
3:K:152:LEU:O	3:K:152:LEU:HD23	2.15	0.46
2:M:132:VAL:CG1	2:M:133:VAL:N	2.78	0.46
1:P:33:VAL:HG12	1:P:34:ALA:N	2.30	0.46
5:B:63:PHE:CD1	5:B:63:PHE:N	2.84	0.46
5:D:148:PRO:HB3	5:D:202:ALA:CB	2.45	0.46
5:D:164:VAL:CG2	5:D:165:HIS:N	2.76	0.46
3:H:60:ASN:C	3:H:60:ASN:HD22	2.09	0.46
3:K:194:THR:HB	3:K:209:LYS:HA	1.97	0.46
2:L:2:ILE:HD11	2:L:93:GLU:HG3	1.97	0.46
2:M:160:LEU:HD23	3:K:169:VAL:CG1	2.45	0.46
2:M:47:LEU:O	2:M:55:ALA:CB	2.64	0.46
5:B:36:TRP:CE3	5:B:80:MET:CE	2.95	0.46
5:D:212:VAL:HG13	5:D:213:PRO:CD	2.43	0.46
3:H:12:VAL:CG2	3:H:18:VAL:HG13	2.46	0.46
3:H:24:VAL:HG12	3:H:76:SER:HB3	1.97	0.46
3:H:51:ILE:HA	3:H:56:ASP:O	2.16	0.46
2:M:214:CYS:C	3:K:213:ARG:HG3	2.36	0.46
1:P:194:ASP:OD2	1:P:194:ASP:N	2.46	0.46
1:P:52:VAL:CG1	1:P:53:LEU:N	2.78	0.46
1:Q:95(H):PHE:HA	8:Q:251:HOH:O	2.16	0.46
4:A:132:VAL:HG12	4:A:148:TRP:CH2	2.50	0.46
5:B:112:VAL:CG2	5:B:113:SER:HB3	2.43	0.46
4:C:179:LEU:HD12	4:C:180:THR:H	1.81	0.46
5:D:97:ARG:O	5:D:98:LEU:HB2	2.14	0.46
1:P:72:LEU:HD21	1:P:141:TRP:NE1	2.29	0.46
1:Q:208:VAL:HG23	1:Q:209:LEU:N	2.28	0.46
5:B:112:VAL:HG23	5:B:113:SER:N	2.30	0.46
5:B:120:PRO:O	5:B:121:PRO:C	2.53	0.46
5:B:164:VAL:CG2	5:B:165:HIS:N	2.78	0.46
5:B:38:LYS:HB2	5:B:90:TYR:CE1	2.51	0.46
4:C:146:VAL:HG13	4:C:147:LYS:N	2.31	0.46
4:C:2:ILE:HD11	4:C:4:LEU:CG	2.45	0.46
3:H:75:SER:O	3:H:77:THR:HG23	2.16	0.46
2:M:25:SER:HB2	2:M:26:SER:H	1.36	0.46
1:Q:199:LEU:HD22	1:Q:228:TYR:HD1	1.80	0.46
1:Q:86:SER:HB2	5:D:31:SER:HA	1.97	0.46
1:Q:95(C):LEU:N	1:Q:95(C):LEU:CD1	2.79	0.46
4:A:27(C):ASP:CA	4:A:31:THR:HG22	2.46	0.46
5:B:23:LYS:HD3	5:B:24:THR:N	2.31	0.46
5:B:63:PHE:HB3	5:B:67:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:118:PHE:O	4:C:132:VAL:HG13	2.16	0.46
3:H:188:TRP:CB	3:H:189:PRO:HD3	2.43	0.46
2:L:106:ILE:HG23	2:L:107:LYS:H	1.79	0.46
1:Q:169:ALA:HA	1:Q:176:VAL:CG2	2.46	0.46
5:B:121:PRO:CB	5:B:123:TYR:CZ	2.98	0.46
5:D:184:VAL:CG2	5:D:185:THR:H	2.29	0.46
5:D:199:ALA:CB	5:D:206:LYS:HD2	2.41	0.46
3:H:40:ARG:HG3	3:H:40:ARG:NH1	2.31	0.46
2:M:162:SER:OG	3:K:167:PRO:CD	2.55	0.46
4:A:55:GLU:O	4:A:58:ILE:CD1	2.63	0.46
4:C:104:LEU:HD23	4:C:105:GLU:O	2.15	0.46
1:P:68:GLY:HA2	1:P:117:ALA:O	2.16	0.46
1:Q:144:ILE:CD1	1:Q:219:PRO:HD2	2.45	0.46
5:B:84:SER:HA	8:B:218:HOH:O	2.16	0.45
5:D:144:LYS:HD3	5:D:144:LYS:O	2.16	0.45
2:M:47:LEU:O	2:M:55:ALA:HB2	2.16	0.45
2:M:93:GLU:CG	2:M:94:TYR:H	2.28	0.45
1:Q:174:GLN:HE22	1:Q:227:LEU:HD11	1.80	0.45
1:Q:46:LEU:HD13	1:Q:52:VAL:HG23	1.98	0.45
5:B:182:VAL:HG13	5:B:183:THR:N	2.32	0.45
2:L:56:SER:C	2:L:58:VAL:H	2.16	0.45
1:P:186:TRP:HB2	1:P:223:PRO:CA	2.43	0.45
1:Q:222:LEU:HD11	1:Q:223(A):GLU:O	2.17	0.45
5:D:194:ILE:CD1	5:D:194:ILE:O	2.64	0.45
5:D:198:VAL:CG1	5:D:199:ALA:H	2.29	0.45
3:K:20:ILE:N	3:K:20:ILE:HD13	2.31	0.45
1:P:52:VAL:HG12	1:P:53:LEU:N	2.31	0.45
1:Q:129:GLU:HB2	1:Q:130:PRO:HD2	1.98	0.45
1:Q:199:LEU:HD13	1:Q:228:TYR:CE1	2.49	0.45
1:Q:222:LEU:HD12	1:Q:223(A):GLU:H	1.80	0.45
5:B:182:VAL:HG22	5:B:183:THR:H	1.81	0.45
4:C:186:TYR:CD2	4:C:186:TYR:C	2.89	0.45
3:H:26:GLY:O	3:H:27:TYR:HB3	2.16	0.45
2:L:124:GLN:HG2	2:L:129:GLY:O	2.16	0.45
2:L:129:GLY:HA2	2:L:183:LYS:N	2.31	0.45
2:L:27(A):SER:HA	2:L:68:GLY:O	2.16	0.45
2:M:126:THR:C	2:M:128:GLY:N	2.70	0.45
2:M:186:TYR:HD2	2:M:187:GLU:HA	1.82	0.45
1:P:217:SER:OG	1:P:217:SER:O	2.30	0.45
1:Q:105:LEU:HD23	1:Q:105:LEU:HA	1.60	0.45
1:Q:119:LYS:HE3	3:K:52:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:144:ILE:C	1:Q:146:PRO:HD3	2.37	0.45
4:A:40:PRO:HD2	4:A:41:GLY:H	1.82	0.45
5:B:156:ASN:O	5:B:197:ASN:ND2	2.50	0.45
5:D:2:VAL:HA	5:D:25:SER:O	2.17	0.45
5:D:51:ILE:HA	5:D:56:TYR:O	2.17	0.45
6:P:414:SIA:H8	6:P:414:SIA:C10	2.47	0.45
1:Q:94:TYR:HE1	1:Q:102:ASP:HB3	1.69	0.45
4:A:91:THR:CG2	5:B:98:LEU:HD13	2.46	0.45
4:C:149:LYS:HA	4:C:154:GLU:HA	1.99	0.45
4:C:15:LEU:C	4:C:15:LEU:HD12	2.37	0.45
4:C:173:TYR:CD1	4:C:173:TYR:N	2.84	0.45
4:C:121:SER:OG	5:D:124:PRO:HD2	2.17	0.45
2:M:211:ARG:NE	8:M:218:HOH:O	2.34	0.45
2:M:88:CYS:O	2:M:98:PHE:HA	2.16	0.45
5:D:178:LEU:C	5:D:178:LEU:HD23	2.37	0.45
5:D:32:TYR:N	5:D:32:TYR:CD1	2.84	0.45
3:H:69:LEU:CD2	3:H:80:MET:HG3	2.45	0.45
3:K:155:ASN:HD22	3:K:159:LEU:HD12	1.82	0.45
1:P:121:MET:HG3	1:P:122:ASP:N	2.31	0.45
1:P:95(E):LYS:HD3	1:P:95(G):ARG:O	2.16	0.45
1:Q:160:LEU:HA	1:Q:185:ARG:HB3	1.98	0.45
1:Q:17:VAL:HG22	1:Q:20:TRP:HA	1.98	0.45
6:Q:405:NAG:C8	6:Q:405:NAG:C3	2.90	0.45
1:Q:66:LEU:HG	4:C:30:PHE:HE1	1.81	0.45
4:A:178:THR:HG22	4:A:178:THR:O	2.16	0.45
5:B:52:ASN:O	5:B:55:GLY:N	2.48	0.45
1:P:101:HIS:HE1	1:P:179:PHE:CD1	2.34	0.45
4:C:183:LYS:O	4:C:183:LYS:HG2	2.15	0.45
4:C:209:PHE:HD2	4:C:209:PHE:C	2.20	0.45
3:H:136:VAL:HG22	3:H:138:LEU:HD22	1.99	0.45
2:L:25:SER:C	2:L:27:LYS:H	2.20	0.45
2:M:166:GLN:HA	2:M:173:TYR:CE2	2.52	0.45
2:M:198:HIS:CD2	2:M:200:THR:OG1	2.69	0.45
1:Q:234:TYR:CD2	1:Q:234:TYR:N	2.84	0.45
4:A:108:ARG:HG3	4:A:140:TYR:CD1	2.52	0.45
4:A:33:MET:O	4:A:34:HIS:CG	2.69	0.45
3:K:127:VAL:O	3:K:128:CYS:C	2.54	0.45
2:M:106:ILE:CG2	2:M:107:LYS:N	2.80	0.45
2:M:134:CYS:HB2	2:M:148:TRP:CH2	2.52	0.45
1:P:31:VAL:HG23	1:P:32:LEU:N	2.32	0.45
1:P:63:SER:O	1:P:85:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:95(B):SER:HB3	1:Q:95(C):LEU:HD12	1.97	0.45
4:A:22:SER:CB	4:A:72:THR:HG22	2.45	0.44
5:B:33:TRP:HZ3	5:B:52:ASN:OD1	2.00	0.44
4:C:192:TYR:O	4:C:208:SER:HB2	2.17	0.44
5:D:13:LYS:CB	5:D:14:PRO:HD2	2.46	0.44
3:H:170:LEU:HB3	3:H:175:TYR:CD1	2.52	0.44
6:P:402:NAG:O3	6:P:403:MAN:H5	2.17	0.44
1:Q:94:TYR:CD2	1:Q:95:ASP:N	2.85	0.44
4:A:14:SER:N	4:A:107:LYS:HB2	2.33	0.44
4:A:4:LEU:HD13	4:A:88:CYS:SG	2.56	0.44
5:D:29:PHE:CE2	5:D:76:ASN:C	2.90	0.44
5:D:23:LYS:HA	5:D:77:THR:HA	1.99	0.44
3:K:146:PHE:CD2	3:K:147:PRO:N	2.85	0.44
2:L:119:PRO:O	2:L:120:PRO:C	2.56	0.44
2:L:95:PRO:O	2:L:96:VAL:C	2.52	0.44
2:M:161:ASN:OD1	2:M:177:SER:HA	2.17	0.44
1:P:215:TRP:HA	1:P:215:TRP:HE3	1.82	0.44
1:P:59:ILE:HD12	1:P:90:PRO:HG3	1.98	0.44
1:Q:103:LEU:HD12	1:Q:212:ILE:HD11	1.99	0.44
1:Q:131:ALA:HB3	1:Q:134:THR:OG1	2.17	0.44
4:C:167:ASP:OD1	4:C:168:SER:N	2.50	0.44
3:H:170:LEU:HB3	3:H:175:TYR:CE1	2.53	0.44
3:K:105:GLN:H	3:K:105:GLN:HG3	1.49	0.44
2:M:23:CYS:O	2:M:71:PHE:HD1	1.99	0.44
4:A:124:GLN:HG2	4:A:129:GLY:O	2.17	0.44
4:A:132:VAL:HG12	4:A:148:TRP:HH2	1.82	0.44
4:A:39:LYS:CB	4:A:40:PRO:CD	2.93	0.44
4:C:14:SER:HA	4:C:107:LYS:HB2	2.00	0.44
5:D:122:VAL:HG11	5:D:198:VAL:HG21	2.00	0.44
4:C:121:SER:HB2	5:D:124:PRO:HD2	2.00	0.44
5:D:199:ALA:HA	5:D:205:THR:O	2.17	0.44
2:L:210:ASN:ND2	2:L:210:ASN:N	2.62	0.44
1:P:56:ALA:HA	1:P:104:MET:HB2	2.00	0.44
1:P:89:PHE:CD1	1:P:89:PHE:N	2.86	0.44
1:Q:143:SER:O	1:Q:144:ILE:HG23	2.18	0.44
5:B:173:SER:C	5:B:175:LEU:N	2.70	0.44
5:B:146:TYR:CD1	5:B:176:TYR:HB2	2.50	0.44
5:B:98:LEU:HD22	5:B:98:LEU:HA	1.61	0.44
4:C:149:LYS:HG2	4:C:154:GLU:CA	2.48	0.44
4:C:209:PHE:CD2	4:C:209:PHE:C	2.91	0.44
2:M:197:THR:HG22	2:M:198:HIS:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:181:LEU:HG	1:P:230:LYS:HB2	1.99	0.44
5:B:36:TRP:CD1	5:B:69:LEU:HD21	2.52	0.44
5:B:96:GLY:C	5:B:97:ARG:HG2	2.38	0.44
5:D:133:THR:CG2	5:D:133:THR:O	2.66	0.44
5:D:148:PRO:HD2	5:D:200:HIS:CE1	2.52	0.44
3:H:164:HIS:O	3:H:179:SER:HB2	2.17	0.44
3:H:193:ILE:HD12	3:H:193:ILE:N	2.32	0.44
3:K:79:TYR:CD2	3:K:79:TYR:N	2.84	0.44
2:L:13:VAL:HG12	2:L:78:VAL:HG21	1.98	0.44
1:Q:46:LEU:HD12	1:Q:46:LEU:HA	1.78	0.44
4:A:48:ILE:HG12	4:A:53:ASN:O	2.18	0.44
4:A:49:TYR:CD2	4:A:49:TYR:O	2.71	0.44
5:B:52:ASN:HD22	5:B:52(A):PRO:CD	2.31	0.44
4:C:27(B):ILE:HD13	4:C:27(C):ASP:H	1.82	0.44
5:D:93:ALA:HB2	5:D:104:TRP:HA	1.98	0.44
3:K:4:LEU:CD2	3:K:24:VAL:HG22	2.47	0.44
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.52	0.44
3:K:66:LYS:HE3	3:K:86:ASP:OD1	2.17	0.44
2:L:106:ILE:CG2	2:L:107:LYS:H	2.31	0.44
2:L:5:THR:HA	8:L:217:HOH:O	2.17	0.44
2:L:21:ILE:O	2:L:72:THR:HG23	2.17	0.44
1:Q:95(J):ARG:HA	1:Q:95(K):PRO:HD3	1.82	0.44
5:B:112:VAL:HG11	8:B:218:HOH:O	2.18	0.44
1:P:84:GLN:HE21	5:B:98:LEU:H	1.64	0.44
4:C:167:ASP:CG	4:C:168:SER:N	2.72	0.44
4:C:32:PHE:HB3	4:C:91:THR:OG1	2.18	0.44
2:L:135:PHE:CE2	3:H:180:SER:CB	3.01	0.44
1:P:145:GLU:N	1:P:146:PRO:CD	2.80	0.44
1:P:185:ARG:HG2	1:P:186(A):THR:HG23	2.00	0.44
1:P:83:PHE:CZ	1:P:112:ALA:HA	2.52	0.44
1:Q:50:GLN:HE21	1:Q:111:PRO:HG3	1.79	0.44
4:A:69:THR:CG2	4:A:69:THR:O	2.66	0.43
5:B:36:TRP:CZ3	5:B:92:CYS:HB3	2.53	0.43
3:H:206:VAL:HG23	3:H:207:ASP:N	2.33	0.43
3:K:22:CYS:SG	3:K:34:MET:HE1	2.57	0.43
2:L:48:ILE:N	2:L:48:ILE:HD13	2.33	0.43
2:M:186:TYR:HD2	2:M:187:GLU:CA	2.31	0.43
1:P:75:HIS:N	1:P:75:HIS:CD2	2.85	0.43
1:Q:114:LEU:HA	1:Q:114:LEU:HD12	1.70	0.43
1:Q:242:ILE:HG22	1:Q:243:VAL:N	2.33	0.43
4:C:46:ILE:HD12	4:C:47:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:171:LEU:HD12	5:D:176:TYR:OH	2.18	0.43
2:L:36:PHE:CE2	2:L:46:LEU:HB2	2.54	0.43
2:M:17:GLU:HB3	2:M:18:SER:H	1.73	0.43
2:M:58:VAL:CG1	2:M:59:PRO:HD2	2.48	0.43
4:A:210:ASN:ND2	2:M:74:ARG:NH2	2.63	0.43
1:P:129:GLU:OE1	1:P:230:LYS:HD2	2.18	0.43
1:Q:51:TRP:CZ3	1:Q:107:ARG:HB2	2.53	0.43
1:Q:45:VAL:HG21	1:Q:198:PRO:HB3	1.99	0.43
4:A:33:MET:C	4:A:34:HIS:CG	2.92	0.43
5:B:9:ALA:HB2	5:B:109:THR:HG23	2.00	0.43
5:B:60:ASN:O	5:B:61:GLN:C	2.56	0.43
5:D:153:LEU:HA	5:D:197:ASN:O	2.17	0.43
5:D:201:PRO:C	5:D:203:SER:H	2.21	0.43
3:H:153:LEU:HD13	3:H:196:ASN:HD22	1.82	0.43
2:L:181:LEU:HD22	2:L:185:GLU:HB2	2.00	0.43
4:A:48:ILE:HD13	4:A:64:GLY:CA	2.48	0.43
5:B:118:THR:O	5:B:120:PRO:N	2.52	0.43
5:B:96:GLY:O	5:B:97:ARG:HG2	2.18	0.43
5:D:77:THR:OG1	5:D:79:TYR:CE2	2.71	0.43
3:H:154:TRP:O	3:H:155:ASN:C	2.56	0.43
3:H:202:SER:HB2	3:H:204:THR:OG1	2.18	0.43
1:P:154:LYS:HG3	1:P:154:LYS:H	1.48	0.43
1:P:30:GLN:NE2	1:P:198:PRO:HG2	2.33	0.43
1:P:44:GLY:CA	1:P:54:THR:HG23	2.49	0.43
1:Q:142:GLY:HA3	1:Q:151:THR:CA	2.47	0.43
1:Q:139:SER:HB3	1:Q:157:CYS:SG	2.58	0.43
4:C:47:LEU:HB3	4:C:58:ILE:HG13	2.01	0.43
2:L:199:LYS:HA	2:L:199:LYS:HD2	1.60	0.43
2:M:27(B):LEU:CD2	2:M:90:GLN:HB2	2.48	0.43
1:Q:174:GLN:NE2	1:Q:227:LEU:HD11	2.34	0.43
5:D:139:LEU:HD12	5:D:139:LEU:N	2.32	0.43
5:D:66:LYS:HE2	5:D:66:LYS:HB2	1.86	0.43
2:L:144:ILE:HD12	2:L:145:ASN:N	2.33	0.43
2:L:89:MET:CE	2:L:98:PHE:CZ	3.01	0.43
4:A:119:PRO:HB3	4:A:209:PHE:CE1	2.54	0.43
4:A:3:VAL:C	4:A:26:SER:OG	2.57	0.43
5:B:189:TRP:O	5:B:190:PRO:C	2.57	0.43
5:B:124:PRO:HB3	5:B:211:ILE:HG22	2.00	0.43
5:B:40:ARG:O	5:B:41:PRO:C	2.56	0.43
2:L:149:LYS:HE3	2:L:149:LYS:HB2	1.78	0.43
2:L:193:THR:CA	2:L:208:SER:HB3	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:56:SER:C	2:L:58:VAL:N	2.72	0.43
1:P:178:LYS:HD3	1:P:178:LYS:HA	1.71	0.43
1:Q:46:LEU:CD1	1:Q:52:VAL:HG23	2.48	0.43
3:H:193:ILE:O	3:H:210:ILE:HG22	2.19	0.43
2:L:118:PHE:HA	2:L:119:PRO:HD3	1.70	0.43
2:L:19:VAL:HG22	2:L:20:SER:H	1.83	0.43
2:M:169:LYS:HB2	2:M:169:LYS:HE3	1.74	0.43
1:P:244:ALA:C	1:P:246:PRO:HD3	2.39	0.43
1:P:71:SER:HB2	1:P:153:LYS:HD2	2.00	0.43
1:Q:94:TYR:CE2	1:Q:95:ASP:O	2.71	0.43
4:A:130:ALA:HB3	4:A:182:THR:O	2.19	0.43
5:B:189:TRP:CZ2	5:B:211:ILE:CD1	3.02	0.43
4:C:34:HIS:HD2	4:C:49:TYR:CA	2.31	0.43
5:D:27:TYR:CD1	5:D:28:SER:N	2.87	0.43
3:K:138:LEU:CD2	3:K:193:ILE:HD13	2.48	0.43
3:K:33:TRP:HB2	3:K:95:ASP:HB2	2.00	0.43
2:M:124:GLN:NE2	2:M:131:SER:HB3	2.14	0.43
1:P:144:ILE:O	1:P:144:ILE:HG23	2.19	0.43
1:Q:167:VAL:O	1:Q:167:VAL:HG23	2.19	0.43
4:A:108:ARG:HG2	4:A:140:TYR:CD1	2.53	0.43
4:C:32:PHE:O	4:C:90:GLN:HA	2.19	0.43
5:D:160:LEU:HG	5:D:162:SER:OG	2.19	0.43
3:H:73:LYS:C	3:H:75:SER:H	2.22	0.43
1:P:135:THR:HA	1:P:161:HIS:HB3	2.01	0.43
1:Q:50:GLN:HE22	1:Q:111:PRO:HG3	1.80	0.43
1:Q:208:VAL:CG2	1:Q:209:LEU:N	2.81	0.43
1:Q:53:LEU:HD12	1:Q:104:MET:O	2.19	0.43
3:H:153:LEU:CD1	3:H:196:ASN:HD22	2.32	0.42
3:H:123:PRO:HG3	3:H:208:LYS:CG	2.48	0.42
2:M:36:PHE:HD2	2:M:46:LEU:HA	1.84	0.42
1:P:139:SER:HA	1:P:156:GLN:O	2.18	0.42
1:Q:171:VAL:HB	1:Q:223(A):GLU:HB3	2.01	0.42
1:Q:95(H):PHE:CD2	6:Q:410:SIA:H91	2.54	0.42
4:A:131:SER:CB	4:A:180:THR:HA	2.49	0.42
5:D:120:PRO:HB3	5:D:144:LYS:O	2.19	0.42
4:C:121:SER:CB	5:D:124:PRO:HD2	2.49	0.42
3:H:195:CYS:O	3:H:207:ASP:HA	2.19	0.42
2:L:117:ILE:C	2:L:118:PHE:CD1	2.93	0.42
1:P:177:THR:H	1:P:180:MET:HE3	1.84	0.42
6:P:403:MAN:O2	6:P:411:MAN:C1	2.67	0.42
1:P:82:VAL:O	1:P:83:PHE:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:95(C):LEU:HD13	1:P:99:SER:HB3	2.01	0.42
1:Q:168:CYS:O	1:Q:172:HIS:HB2	2.19	0.42
5:B:116:LYS:CG	5:B:116:LYS:O	2.67	0.42
5:B:116:LYS:HZ1	5:B:202:ALA:HB1	1.83	0.42
4:C:139:PHE:O	4:C:139:PHE:CG	2.68	0.42
1:P:119:LYS:HD3	3:H:52:TYR:CD2	2.54	0.42
3:K:56:ASP:C	3:K:57:THR:HG22	2.40	0.42
2:L:36:PHE:CE1	2:L:89:MET:CE	3.02	0.42
2:M:13:VAL:HG11	2:M:78:VAL:HG11	2.02	0.42
1:P:119:LYS:HD2	3:H:52:TYR:CE2	2.54	0.42
1:Q:140:GLY:O	1:Q:155:LEU:HD22	2.20	0.42
1:Q:20:TRP:HB2	3:K:98:ARG:CZ	2.49	0.42
1:Q:56:ALA:HA	1:Q:104:MET:HE1	2.00	0.42
4:C:1:ASP:HB3	4:C:95:PRO:HB2	2.00	0.42
2:L:121:SER:OG	3:H:123:PRO:HD2	2.20	0.42
3:K:87:SER:O	3:K:88:ALA:HB2	2.20	0.42
2:L:153:SER:OG	2:L:154:GLU:N	2.53	0.42
2:L:39:ARG:HB3	2:L:40:PRO:CD	2.49	0.42
2:M:131:SER:HB2	2:M:180:THR:CG2	2.28	0.42
2:M:32:TYR:N	2:M:32:TYR:CD2	2.87	0.42
1:P:105:LEU:HD21	1:P:238:ILE:HG23	2.01	0.42
1:P:231:VAL:O	1:P:233:HIS:N	2.52	0.42
1:Q:130:PRO:HG3	1:Q:210:GLN:HG2	1.98	0.42
1:Q:144:ILE:O	1:Q:146:PRO:HD3	2.19	0.42
1:Q:188:LYS:HE2	1:Q:224:ARG:CZ	2.50	0.42
1:Q:95(A):MET:HG3	1:Q:95(D):LEU:CD1	2.50	0.42
5:B:116:LYS:NZ	5:B:202:ALA:HB1	2.35	0.42
4:C:136:LEU:N	4:C:136:LEU:CD1	2.82	0.42
2:L:106:ILE:HG22	2:L:107:LYS:N	2.35	0.42
2:L:118:PHE:CD1	2:L:118:PHE:N	2.87	0.42
2:L:181:LEU:HD21	2:L:185:GLU:OE2	2.18	0.42
2:M:167:ASP:CG	2:M:170:ASP:HB2	2.39	0.42
2:M:142:LYS:HA	2:M:173:TYR:HD1	1.84	0.42
2:M:15:PRO:C	2:M:17:GLU:H	2.22	0.42
1:P:124:PRO:HB3	1:P:208:VAL:HG11	2.00	0.42
1:Q:75:HIS:HB3	2:M:28:ASN:HA	2.01	0.42
4:A:109:ALA:O	4:A:110:ASP:C	2.58	0.42
4:C:141:PRO:HD2	4:C:198:HIS:HE1	1.84	0.42
5:D:33:TRP:N	5:D:33:TRP:CE3	2.88	0.42
3:K:18:VAL:HG23	3:K:82(C):LEU:CD1	2.49	0.42
1:P:184:GLY:O	1:P:185:ARG:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:134:THR:O	1:Q:161:HIS:HB2	2.19	0.42
1:Q:213:THR:HA	1:Q:228:TYR:CD2	2.54	0.42
4:A:141:PRO:O	4:A:143:ASP:O	2.38	0.42
5:B:133:THR:CG2	5:B:134:GLY:N	2.70	0.42
5:B:174:ASP:N	5:B:174:ASP:OD2	2.52	0.42
5:B:195:THR:HG23	5:B:210:LYS:N	2.35	0.42
4:C:190:ASN:ND2	4:C:212:ASN:ND2	2.59	0.42
5:D:72:ASP:OD1	5:D:74:SER:HB3	2.19	0.42
3:K:83:THR:OG1	3:K:85:VAL:HG13	2.20	0.42
2:L:131:SER:HB3	2:L:180:THR:HA	2.01	0.42
2:M:132:VAL:HG13	2:M:133:VAL:N	2.34	0.42
1:P:231:VAL:C	1:P:233:HIS:N	2.71	0.42
1:P:71:SER:C	1:P:72:LEU:HD13	2.39	0.42
1:P:95(G):ARG:CD	8:P:266:HOH:O	2.68	0.42
1:Q:69:ARG:NH1	1:Q:77:GLU:OE1	2.52	0.42
4:C:138:ASN:HD22	4:C:172:THR:HG21	1.84	0.42
2:L:91:HIS:O	2:L:91:HIS:HD2	2.03	0.42
2:M:140:TYR:C	2:M:140:TYR:CD2	2.92	0.42
1:Q:153:LYS:HB3	1:Q:154:LYS:H	1.64	0.42
1:Q:86:SER:HA	5:D:33:TRP:HZ3	1.85	0.42
5:B:118:THR:HG23	5:B:119:ALA:N	2.33	0.42
5:B:19:LYS:HB2	5:B:81:GLN:HG3	2.02	0.42
5:B:17:SER:HB2	5:B:82(A):ASN:HA	2.01	0.42
5:D:101:PHE:CD1	5:D:101:PHE:N	2.83	0.42
3:H:12:VAL:O	3:H:111:VAL:HA	2.20	0.42
3:H:51:ILE:HD13	3:H:71:VAL:HG13	2.01	0.42
2:M:115:VAL:HG12	2:M:207:LYS:CD	2.48	0.42
1:P:153:LYS:HG3	1:P:153:LYS:H	1.67	0.42
1:Q:238:ILE:O	1:Q:240:ASP:N	2.53	0.42
4:A:213:GLU:O	4:A:214:CYS:HB3	2.20	0.42
4:A:34:HIS:CD2	4:A:49:TYR:CB	3.03	0.42
5:B:188:THR:OG1	5:B:189:TRP:N	2.53	0.42
5:D:51:ILE:O	5:D:51:ILE:CG2	2.67	0.42
3:H:211:VAL:HA	3:H:212:PRO:HD3	1.78	0.42
3:H:62:LYS:HB3	3:H:62:LYS:HE2	1.93	0.42
2:M:150:ILE:HD12	2:M:150:ILE:N	2.35	0.42
1:Q:215:TRP:CE3	1:Q:216:GLY:N	2.80	0.42
4:C:141:PRO:O	4:C:142:LYS:C	2.56	0.41
3:K:181:VAL:HG22	3:K:182:THR:N	2.34	0.41
2:L:13:VAL:CG1	2:L:14:THR:N	2.83	0.41
2:L:159:VAL:HG12	2:L:179:LEU:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:ARG:NH1	2:L:77:ARG:HB3	2.25	0.41
2:M:182:THR:O	2:M:185:GLU:OE1	2.38	0.41
2:M:186:TYR:CD2	2:M:187:GLU:N	2.86	0.41
2:M:18:SER:HB2	2:M:75:ILE:O	2.20	0.41
1:Q:94:TYR:CD1	1:Q:102:ASP:CB	2.92	0.41
4:A:186:TYR:HD1	4:A:192:TYR:HH	1.64	0.41
4:A:26:SER:O	4:A:27:GLU:HB3	2.20	0.41
5:B:147:PHE:H	5:B:148:PRO:CD	2.33	0.41
5:B:33:TRP:HZ3	5:B:52:ASN:CG	2.24	0.41
3:K:153:LEU:HD23	3:K:153:LEU:H	1.84	0.41
3:K:18:VAL:HG12	3:K:19:LYS:N	2.34	0.41
2:L:110:ASP:OD1	2:L:110:ASP:N	2.53	0.41
2:L:89:MET:HE3	2:L:89:MET:HB3	1.68	0.41
1:Q:163:ILE:HG12	1:Q:183:ALA:HA	2.03	0.41
1:Q:45:VAL:CG2	1:Q:198:PRO:HB3	2.49	0.41
1:Q:224:ARG:HB3	1:Q:225:PRO:HD3	2.02	0.41
4:A:149:LYS:CE	4:A:152:GLY:H	2.28	0.41
4:A:27(C):ASP:HA	4:A:30:PHE:O	2.20	0.41
4:A:70:ASP:C	4:A:71:PHE:CD1	2.94	0.41
4:C:124:GLN:NE2	4:C:131:SER:N	2.67	0.41
5:D:6:GLN:HE21	5:D:107:GLY:H	1.66	0.41
5:D:167:PHE:HA	5:D:168:PRO:HD2	1.71	0.41
5:D:155:TRP:CG	5:D:182:VAL:HG21	2.55	0.41
5:D:36:TRP:HB3	5:D:80:MET:HE2	2.02	0.41
5:D:4:LEU:N	5:D:4:LEU:HD23	2.35	0.41
3:H:136:VAL:N	3:H:183:VAL:O	2.50	0.41
1:Q:196:GLY:O	1:Q:197:GLY:C	2.58	0.41
1:Q:58:CYS:O	1:Q:59:ILE:HG12	2.19	0.41
5:B:148:PRO:HD2	5:B:200:HIS:CE1	2.55	0.41
4:C:109:ALA:O	4:C:110:ASP:C	2.58	0.41
5:D:121:PRO:HB2	5:D:123:TYR:CZ	2.55	0.41
5:D:18:VAL:HG12	5:D:19:LYS:N	2.35	0.41
3:K:54:ASP:C	3:K:54:ASP:OD1	2.59	0.41
2:L:2:ILE:CD1	2:L:2:ILE:H	2.33	0.41
2:M:166:GLN:OE1	2:M:173:TYR:CZ	2.72	0.41
2:M:142:LYS:HA	2:M:173:TYR:CD1	2.56	0.41
1:P:98:ASP:OD1	1:P:98:ASP:C	2.57	0.41
1:Q:165:ASN:CB	1:Q:178:LYS:HD2	2.50	0.41
1:Q:228:TYR:HD2	1:Q:228:TYR:HA	1.69	0.41
2:M:89:MET:HA	2:M:97:THR:O	2.21	0.41
1:P:45:VAL:HG22	1:P:198:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:89:PHE:HA	1:Q:90:PRO:HD3	1.90	0.41
5:B:134:GLY:O	5:B:186:SER:HB3	2.20	0.41
4:C:149:LYS:HG2	4:C:154:GLU:N	2.36	0.41
5:D:115:ALA:O	5:D:117:THR:HG22	2.21	0.41
1:Q:123:LEU:HD21	1:Q:238:ILE:HG21	2.02	0.41
1:Q:32:LEU:HD23	1:Q:141:TRP:CE3	2.55	0.41
1:Q:65:ILE:C	1:Q:66:LEU:HD12	2.40	0.41
4:A:132:VAL:N	4:A:179:LEU:O	2.48	0.41
4:A:182:THR:CG2	4:A:183:LYS:N	2.79	0.41
4:A:69:THR:HG22	4:A:70:ASP:OD2	2.21	0.41
5:B:198:VAL:CG1	5:B:199:ALA:N	2.84	0.41
4:C:135:PHE:C	4:C:136:LEU:CD1	2.89	0.41
2:M:46:LEU:CD2	3:K:99:TYR:CE1	3.03	0.41
2:L:188:ARG:O	2:L:188:ARG:CG	2.49	0.41
2:L:192:TYR:HB2	2:L:209:PHE:CE2	2.55	0.41
2:L:90:GLN:CG	2:L:91:HIS:N	2.84	0.41
2:M:135:PHE:C	2:M:136:LEU:HG	2.40	0.41
2:M:138:ASN:HA	2:M:172:THR:OG1	2.20	0.41
2:M:211:ARG:HD3	2:M:211:ARG:HA	1.87	0.41
1:P:54:THR:HB	1:P:55:ALA:H	1.64	0.41
1:Q:53:LEU:HD11	1:Q:103:LEU:HG	2.03	0.41
1:Q:95(A):MET:C	1:Q:95(C):LEU:N	2.74	0.41
4:A:142:LYS:HD3	4:A:142:LYS:N	2.21	0.41
4:A:201:SER:CB	4:A:205:ILE:HD11	2.49	0.41
5:B:94:ARG:HD2	5:B:103:VAL:CG2	2.50	0.41
4:C:179:LEU:HD11	4:C:181:LEU:HD22	2.00	0.41
3:K:187:THR:HB	3:K:191:GLN:NE2	2.36	0.41
3:K:60:ASN:HD22	3:K:61:GLY:H	1.59	0.41
1:P:69:ARG:NH2	1:P:76:PRO:HA	2.36	0.41
4:A:47:LEU:O	4:A:54:LEU:HA	2.21	0.41
5:B:13:LYS:HA	5:B:14:PRO:HD3	1.93	0.41
3:H:133:GLY:O	3:H:135:SER:N	2.53	0.41
3:K:51:ILE:O	3:K:52(A):PRO:HD3	2.20	0.41
1:P:51:TRP:CZ3	1:P:107:ARG:HB2	2.56	0.41
1:P:56:ALA:O	1:P:59:ILE:CG2	2.61	0.41
1:P:95:ASP:HB3	1:P:95(C):LEU:HD12	2.03	0.41
1:Q:50:GLN:HE21	1:Q:50:GLN:HB2	1.49	0.41
1:Q:46:LEU:HD22	1:Q:67:LEU:HD23	2.02	0.41
4:C:181:LEU:HD13	4:C:181:LEU:HA	1.59	0.41
4:C:185:GLU:HG3	4:C:185:GLU:O	2.21	0.41
3:K:138:LEU:HD23	3:K:193:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:197:VAL:HG12	3:K:198:ALA:H	1.86	0.41
3:K:19:LYS:HG2	3:K:19:LYS:O	2.21	0.41
2:L:26:SER:O	2:L:26:SER:OG	2.38	0.41
2:L:2:ILE:N	2:L:2:ILE:HD12	2.35	0.41
1:P:144:ILE:HD12	1:P:144:ILE:HA	1.98	0.41
1:P:224:ARG:HA	1:P:225:PRO:HD2	1.70	0.41
1:P:232:VAL:O	1:P:232:VAL:HG22	2.21	0.41
1:P:245:ASN:N	1:P:246:PRO:HD3	2.35	0.41
1:P:53:LEU:HD12	1:P:53:LEU:HA	1.90	0.41
1:P:59:ILE:HD13	1:P:59:ILE:HG21	1.79	0.41
1:P:65:ILE:HG12	1:P:108:LEU:CD1	2.49	0.41
1:Q:128:GLN:HG2	1:Q:129:GLU:N	2.35	0.41
1:Q:234:TYR:C	1:Q:236:LYS:N	2.74	0.41
4:A:33:MET:O	4:A:50:ARG:N	2.44	0.41
5:B:134:GLY:O	5:B:135:SER:C	2.58	0.41
5:B:26:GLY:O	5:B:27:TYR:HB3	2.22	0.41
5:B:94:ARG:HB3	5:B:103:VAL:HG23	2.02	0.41
2:L:182:THR:OG1	2:L:183:LYS:N	2.53	0.41
2:L:58:VAL:HA	2:L:59:PRO:HD3	1.70	0.41
2:M:202:THR:HG22	2:M:202:THR:H	1.56	0.41
6:P:402:NAG:H4	6:P:403:MAN:H2	1.74	0.41
1:P:84:GLN:CD	5:B:33:TRP:CD1	2.95	0.41
1:Q:32:LEU:HD11	1:Q:39:ALA:CB	2.51	0.41
1:Q:85:VAL:C	5:D:33:TRP:CH2	2.93	0.41
4:A:148:TRP:CD1	4:A:159:VAL:HG11	2.55	0.40
4:A:209:PHE:O	4:A:209:PHE:CD2	2.74	0.40
5:B:116:LYS:HE2	5:B:202:ALA:HB1	2.02	0.40
5:B:207:VAL:HG23	5:B:208:ASP:N	2.36	0.40
4:C:36:TYR:CE1	4:C:46:ILE:HB	2.56	0.40
5:D:37:VAL:HA	5:D:48:ILE:HG13	2.03	0.40
1:P:203:GLY:HA3	3:H:28:ALA:HB3	2.02	0.40
2:M:138:ASN:N	2:M:173:TYR:O	2.52	0.40
1:P:123:LEU:HA	1:P:124:PRO:HD3	1.80	0.40
1:P:236:LYS:HD3	1:P:236:LYS:HA	1.84	0.40
6:Q:412:NAG:H4	6:Q:413:GAL:H2	1.80	0.40
4:A:117:ILE:CG2	4:A:117:ILE:O	2.67	0.40
5:B:14:PRO:C	5:B:16:ALA:H	2.24	0.40
5:D:134:GLY:O	5:D:186:SER:HB3	2.21	0.40
3:H:194:THR:HG23	3:H:208:LYS:C	2.41	0.40
3:K:20:ILE:HD12	3:K:107:THR:HG21	2.02	0.40
3:K:80:MET:SD	3:K:82:LEU:HD21	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:193:THR:CG2	2:L:206:VAL:HG13	2.50	0.40
1:P:172:HIS:HA	1:P:173:PRO:HD3	1.89	0.40
1:Q:95(H):PHE:HD2	6:Q:410:SIA:H91	1.87	0.40
1:Q:89:PHE:CD1	1:Q:89:PHE:N	2.89	0.40
1:Q:91:HIS:HE1	1:Q:93:LEU:CG	2.31	0.40
5:B:23:LYS:C	5:B:23:LYS:HD3	2.41	0.40
5:B:52:ASN:HD22	5:B:52(A):PRO:HD2	1.86	0.40
5:D:139:LEU:HD21	5:D:189:TRP:CD2	2.56	0.40
5:D:3:GLN:C	5:D:4:LEU:HD23	2.41	0.40
3:H:36:TRP:CZ3	3:H:92:CYS:HB3	2.56	0.40
3:H:19:LYS:HG3	3:H:81:GLN:HG3	2.04	0.40
1:P:103:LEU:HD12	1:P:103:LEU:HA	1.86	0.40
1:Q:231:VAL:O	1:Q:232:VAL:C	2.58	0.40
4:A:183:LYS:HZ2	4:A:187:GLU:HB2	1.85	0.40
4:A:83:VAL:HG13	4:A:83:VAL:O	2.21	0.40
5:B:203:SER:O	5:B:205:THR:N	2.48	0.40
2:L:136:LEU:CD2	2:L:144:ILE:HD11	2.51	0.40
1:P:83:PHE:CE2	1:P:112:ALA:HB2	2.57	0.40
1:Q:119:LYS:CD	3:K:52:TYR:HE1	2.30	0.40
1:Q:174:GLN:NE2	1:Q:227:LEU:HD21	2.37	0.40
1:Q:32:LEU:HD11	1:Q:39:ALA:HB1	2.04	0.40
4:A:106:ILE:CG2	4:A:107:LYS:N	2.83	0.40
4:A:111:ALA:HB3	4:A:140:TYR:H	1.87	0.40
4:A:149:LYS:HA	4:A:154:GLU:HA	2.04	0.40
4:C:6:GLN:HE22	4:C:101:GLY:HA2	1.87	0.40
5:D:119:ALA:HA	5:D:120:PRO:HD3	1.79	0.40
3:H:135:SER:HA	3:H:184:THR:HA	2.02	0.40
3:H:170:LEU:HD12	3:H:170:LEU:H	1.87	0.40
2:L:198:HIS:CG	2:L:199:LYS:H	2.39	0.40
1:P:44:GLY:HA2	1:P:54:THR:HG23	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	235/237 (99%)	195 (83%)	31 (13%)	9 (4%)	4	25
1	Q	235/237 (99%)	186 (79%)	39 (17%)	10 (4%)	3	23
2	L	217/219 (99%)	166 (76%)	39 (18%)	12 (6%)	2	16
2	M	217/219 (99%)	177 (82%)	31 (14%)	9 (4%)	3	24
3	H	215/219 (98%)	186 (86%)	18 (8%)	11 (5%)	2	18
3	K	217/219 (99%)	181 (83%)	32 (15%)	4 (2%)	10	47
4	A	216/218 (99%)	177 (82%)	22 (10%)	17 (8%)	1	7
4	C	216/218 (99%)	173 (80%)	30 (14%)	13 (6%)	2	14
5	B	217/219 (99%)	166 (76%)	35 (16%)	16 (7%)	1	8
5	D	217/219 (99%)	163 (75%)	42 (19%)	12 (6%)	2	16
All	All	2202/2224 (99%)	1770 (80%)	319 (14%)	113 (5%)	2	18

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	95	PRO
2	L	167	ASP
2	L	174	SER
3	H	173	ASP
4	A	17	GLN
4	A	39	LYS
4	A	40	PRO
4	A	113	PRO
4	A	144	ILE
5	B	41	PRO
5	B	127	PRO
5	B	202	ALA
5	B	213	PRO
1	Q	144	ILE
2	M	59	PRO
2	M	153	SER
3	K	128	CYS
3	K	149	SER
4	C	17	GLN
4	C	142	LYS
5	D	112	VAL
5	D	116	LYS

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Mol	Chain	Res	Type
1	P	118	VAL
1	P	143	SER
1	P	146	PRO
1	P	194	ASP
2	L	68	GLY
2	L	110	ASP
3	H	74	SER
3	H	190	SER
4	A	142	LYS
5	B	48	ILE
5	B	98	LEU
5	B	112	VAL
5	B	133	THR
1	Q	20	TRP
2	M	16	GLY
4	C	57	GLY
4	C	60	ALA
4	C	110	ASP
4	C	143	ASP
5	D	29	PHE
5	D	113	SER
5	D	149	GLU
5	D	159	SER
5	D	199	ALA
1	P	76	PRO
1	P	220	CYS
1	P	221	ALA
2	L	188	ARG
3	H	62	LYS
4	A	96	TYR
4	A	100	GLY
4	A	182	THR
5	B	15	GLY
5	B	88	ALA
5	B	121	PRO
5	B	204	SER
1	Q	41	VAL
1	Q	76	PRO
1	Q	152	PRO
1	Q	189	SER
1	Q	235	ARG
2	M	95	PRO

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Mol	Chain	Res	Type
3	K	54	ASP
3	K	100	TYR
4	C	27(C)	ASP
4	C	53	ASN
4	C	138	ASN
5	D	168	PRO
1	P	185	ARG
2	L	119	PRO
2	L	157	ASN
3	H	134	SER
4	A	60	ALA
4	A	157	ASN
5	B	147	PHE
5	B	174	ASP
1	Q	186	TRP
1	Q	197	GLY
2	M	25	SER
4	C	144	ILE
4	C	182	THR
2	L	39	ARG
2	L	57	GLY
2	L	65	SER
2	L	120	PRO
3	H	126	PRO
4	A	27	GLU
4	A	110	ASP
4	A	138	ASN
5	B	119	ALA
2	M	19	VAL
2	M	94	TYR
5	D	41	PRO
1	P	145	GLU
3	H	188	TRP
4	A	141	PRO
5	D	127	PRO
5	D	185	THR
4	A	77	PRO
4	C	95	PRO
3	H	167	PRO
5	B	14	PRO
1	Q	232	VAL
2	M	119	PRO

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Mol	Chain	Res	Type
3	H	119	PRO
2	M	140	TYR
5	D	51	ILE
3	H	189	PRO
4	A	44	PRO
4	C	120	PRO
3	H	147	PRO

### 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	P	205/205 (100%)	161 (78%)	44 (22%)	1	6
1	Q	205/205 (100%)	150 (73%)	55 (27%)	0	2
2	L	196/196 (100%)	160 (82%)	36 (18%)	2	9
2	M	196/196 (100%)	146 (74%)	50 (26%)	0	2
3	H	187/189 (99%)	135 (72%)	52 (28%)	0	1
3	K	189/189 (100%)	148 (78%)	41 (22%)	1	6
4	A	193/193 (100%)	152 (79%)	41 (21%)	1	6
4	C	193/193 (100%)	143 (74%)	50 (26%)	0	2
5	B	189/189 (100%)	135 (71%)	54 (29%)	0	1
5	D	189/189 (100%)	145 (77%)	44 (23%)	1	4
All	All	1942/1944 (100%)	1475 (76%)	467 (24%)	1	3

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	23	GLU
1	P	27	GLN
1	P	36	ARG
1	P	38	ARG
1	P	42	CYS
1	P	54	THR

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Mol	Chain	Res	Type
1	P	60	ARG
1	P	65	ILE
1	P	77	GLU
1	P	82	VAL
1	P	88	SER
1	P	95(C)	LEU
1	P	95(D)	LEU
1	P	95(E)	LYS
1	P	95(H)	PHE
1	P	100	SER
1	P	105	LEU
1	P	107	ARG
1	P	108	LEU
1	P	118	VAL
1	P	125	THR
1	P	135	THR
1	P	143	SER
1	P	149	PHE
1	P	151	THR
1	P	153	LYS
1	P	154	LYS
1	P	163	ILE
1	P	171	VAL
1	P	178	LYS
1	P	180	MET
1	P	186(A)	THR
1	P	191	CYS
1	P	194	ASP
1	P	199	LEU
1	P	200	VAL
1	P	210	GLN
1	P	212	ILE
1	P	217	SER
1	P	218	GLU
1	P	227	LEU
1	P	235	ARG
1	P	241	THR
1	P	242	ILE
2	L	1	ASP
2	L	3	VAL
2	L	7	THR
2	L	17	GLU

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Mol	Chain	Res	Type
2	L	23	CYS
2	L	24	ARG
2	L	26	SER
2	L	31	THR
2	L	33	LEU
2	L	42	GLN
2	L	48	ILE
2	L	65	SER
2	L	71	PHE
2	L	77	ARG
2	L	89	MET
2	L	92	LEU
2	L	94	TYR
2	L	96	VAL
2	L	103	LYS
2	L	105	GLU
2	L	122	SER
2	L	132	VAL
2	L	134	CYS
2	L	136	LEU
2	L	139	PHE
2	L	147	LYS
2	L	155	ARG
2	L	163	TRP
2	L	165	ASP
2	L	167	ASP
2	L	176	SER
2	L	178	THR
2	L	182	THR
2	L	183	LYS
2	L	210	ASN
2	L	212	ASN
3	H	1	GLN
3	H	11	LEU
3	H	13	LYS
3	H	18	VAL
3	H	21	SER
3	H	23	LYS
3	H	24	VAL
3	H	30	SER
3	H	32	SER
3	H	35	ASN

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Mol	Chain	Res	Type
3	H	37	VAL
3	H	45	LEU
3	H	50	ARG
3	H	58	LYS
3	H	60	ASN
3	H	64	LYS
3	H	74	SER
3	H	80	MET
3	H	82	LEU
3	H	82(B)	SER
3	H	83	THR
3	H	105	GLN
3	H	109	VAL
3	H	113	SER
3	H	115	LYS
3	H	117	THR
3	H	121	VAL
3	H	130	ASP
3	H	131	THR
3	H	132	THR
3	H	135	SER
3	H	137	THR
3	H	138	LEU
3	H	140	CYS
3	H	153	LEU
3	H	159	LEU
3	H	163	VAL
3	H	170	LEU
3	H	171	GLN
3	H	177	LEU
3	H	184	THR
3	H	186	SER
3	H	191	GLN
3	H	192	SER
3	H	202	SER
3	H	203	SER
3	H	204	THR
3	H	205	LYS
3	H	206	VAL
3	H	209	LYS
3	H	210	ILE
3	H	211	VAL

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Mol	Chain	Res	Type
4	A	3	VAL
4	A	5	THR
4	A	15	LEU
4	A	27(B)	ILE
4	A	54	LEU
4	A	55	GLU
4	A	61	ARG
4	A	63	SER
4	A	69	THR
4	A	70	ASP
4	A	74	THR
4	A	75	ILE
4	A	79	GLU
4	A	81	ASP
4	A	89	GLN
4	A	90	GLN
4	A	91	THR
4	A	105	GLU
4	A	106	ILE
4	A	108	ARG
4	A	114	THR
4	A	116	SER
4	A	117	ILE
4	A	121	SER
4	A	123	GLU
4	A	133	VAL
4	A	142	LYS
4	A	144	ILE
4	A	147	LYS
4	A	150	ILE
4	A	155	ARG
4	A	156	GLN
4	A	157	ASN
4	A	161	ASN
4	A	166	GLN
4	A	175	MET
4	A	178	THR
4	A	189	HIS
4	A	200	THR
4	A	209	PHE
4	A	210	ASN
5	B	3	GLN

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Mol	Chain	Res	Type
5	B	10	GLU
5	B	13	LYS
5	B	17	SER
5	B	18	VAL
5	B	20	MET
5	B	21	SER
5	B	23	LYS
5	B	34	MET
5	B	50	TYR
5	B	51	ILE
5	B	52	ASN
5	B	54	THR
5	B	57	THR
5	B	60	ASN
5	B	61	GLN
5	B	64	LYS
5	B	67	VAL
5	B	70	THR
5	B	77	THR
5	B	92	CYS
5	B	94	ARG
5	B	97	ARG
5	B	98	LEU
5	B	101	PHE
5	B	103	VAL
5	B	108	THR
5	B	109	THR
5	B	111	THR
5	B	112	VAL
5	B	114	SER
5	B	118	THR
5	B	122	VAL
5	B	132	THR
5	B	135	SER
5	B	142	LEU
5	B	146	TYR
5	B	151	VAL
5	B	152	THR
5	B	153	LEU
5	B	154	LEU
5	B	156	ASN
5	B	160	LEU

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Mol	Chain	Res	Type
5	B	162	SER
5	B	164	VAL
5	B	170	VAL
5	B	172	GLN
5	B	178	LEU
5	B	180	SER
5	B	184	VAL
5	B	185	THR
5	B	196	CYS
5	B	207	VAL
5	B	216	CYS
1	Q	20	TRP
1	Q	30	GLN
1	Q	31	VAL
1	Q	32	LEU
1	Q	50	GLN
1	Q	52	VAL
1	Q	59	ILE
1	Q	61	ASN
1	Q	62	LYS
1	Q	63	SER
1	Q	67	LEU
1	Q	69	ARG
1	Q	72	LEU
1	Q	73	PHE
1	Q	77	GLU
1	Q	84	GLN
1	Q	89	PHE
1	Q	95(D)	LEU
1	Q	95(G)	ARG
1	Q	97	ASP
1	Q	106	LEU
1	Q	108	LEU
1	Q	114	LEU
1	Q	115	THR
1	Q	116	ASP
1	Q	118	VAL
1	Q	121	MET
1	Q	123	LEU
1	Q	135	THR
1	Q	139	SER
1	Q	144	ILE

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Mol	Chain	Res	Type
1	Q	149	PHE
1	Q	150	LEU
1	Q	151	THR
1	Q	155	LEU
1	Q	158	VAL
1	Q	160	LEU
1	Q	162	VAL
1	Q	164	SER
1	Q	168	CYS
1	Q	177	THR
1	Q	185	ARG
1	Q	186	TRP
1	Q	186(A)	THR
1	Q	188	LYS
1	Q	189	SER
1	Q	190	THR
1	Q	208	VAL
1	Q	215	TRP
1	Q	218	GLU
1	Q	220	CYS
1	Q	222	LEU
1	Q	227	LEU
1	Q	242	ILE
1	Q	245	ASN
2	M	5	THR
2	M	10	SER
2	M	25	SER
2	M	27(E)	SER
2	M	28	ASN
2	M	31	THR
2	M	33	LEU
2	M	43	SER
2	M	45	GLN
2	M	46	LEU
2	M	53	ASN
2	M	60	ASP
2	M	65	SER
2	M	69	THR
2	M	71	PHE
2	M	89	MET
2	M	94	TYR
2	M	97	THR

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Mol	Chain	Res	Type
2	M	105	GLU
2	M	108	ARG
2	M	110	ASP
2	M	116	SER
2	M	117	ILE
2	M	125	LEU
2	M	127	SER
2	M	131	SER
2	M	136	LEU
2	M	142	LYS
2	M	143	ASP
2	M	144	ILE
2	M	156	GLN
2	M	157	ASN
2	M	159	VAL
2	M	168	SER
2	M	169	LYS
2	M	172	THR
2	M	174	SER
2	M	176	SER
2	M	181	LEU
2	M	184	ASP
2	M	186	TYR
2	M	187	GLU
2	M	190	ASN
2	M	191	SER
2	M	193	THR
2	M	199	LYS
2	M	202	THR
2	M	205	ILE
2	M	211	ARG
2	M	213	GLU
3	K	7	SER
3	K	13	LYS
3	K	17	SER
3	K	25	SER
3	K	30	SER
3	K	35	ASN
3	K	57	THR
3	K	59	TYR
3	K	60	ASN
3	K	68	THR

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Mol	Chain	Res	Type
3	K	73	LYS
3	K	75	SER
3	K	79	TYR
3	K	83	THR
3	K	98	ARG
3	K	102	TYR
3	K	105	GLN
3	K	121	VAL
3	K	127	VAL
3	K	128	CYS
3	K	131	THR
3	K	134	SER
3	K	137	THR
3	K	138	LEU
3	K	143	LYS
3	K	147	PRO
3	K	149	SER
3	K	152	LEU
3	K	158	SER
3	K	159	LEU
3	K	161	SER
3	K	171	GLN
3	K	174	LEU
3	K	180	SER
3	K	182	THR
3	K	184	THR
3	K	192	SER
3	K	193	ILE
3	K	194	THR
3	K	197	VAL
3	K	213	ARG
4	C	2	ILE
4	C	5	THR
4	C	10	SER
4	C	15	LEU
4	C	24	ARG
4	C	26	SER
4	C	27(B)	ILE
4	C	27(C)	ASP
4	C	42	GLN
4	C	45	LYS
4	C	47	LEU

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Mol	Chain	Res	Type
4	C	52	SER
4	C	54	LEU
4	C	58	ILE
4	C	69	THR
4	C	70	ASP
4	C	89	GLN
4	C	90	GLN
4	C	94	ASP
4	C	96	TYR
4	C	97	THR
4	C	105	GLU
4	C	125	LEU
4	C	136	LEU
4	C	142	LYS
4	C	143	ASP
4	C	144	ILE
4	C	145	ASN
4	C	150	ILE
4	C	151	ASP
4	C	153	SER
4	C	156	GLN
4	C	162	SER
4	C	167	ASP
4	C	168	SER
4	C	169	LYS
4	C	171	SER
4	C	174	SER
4	C	181	LEU
4	C	182	THR
4	C	184	ASP
4	C	185	GLU
4	C	187	GLU
4	C	197	THR
4	C	199	LYS
4	C	205	ILE
4	C	209	PHE
4	C	210	ASN
4	C	212	ASN
4	C	214	CYS
5	D	3	GLN
5	D	11	LEU
5	D	13	LYS

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Mol	Chain	Res	Type
5	D	21	SER
5	D	24	THR
5	D	28	SER
5	D	33	TRP
5	D	34	MET
5	D	37	VAL
5	D	43	GLN
5	D	48	ILE
5	D	52	ASN
5	D	54	THR
5	D	57	THR
5	D	59	ASN
5	D	61	GLN
5	D	69	LEU
5	D	77	THR
5	D	79	TYR
5	D	81	GLN
5	D	82(A)	ASN
5	D	83	THR
5	D	85	GLU
5	D	94	ARG
5	D	109	THR
5	D	111	THR
5	D	112	VAL
5	D	117	THR
5	D	122	VAL
5	D	138	THR
5	D	139	LEU
5	D	141	CYS
5	D	149	GLU
5	D	152	THR
5	D	153	LEU
5	D	164	VAL
5	D	174	ASP
5	D	178	LEU
5	D	181	SER
5	D	183	THR
5	D	188	THR
5	D	192	GLN
5	D	195	THR
5	D	211	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such



sidechains are listed below:

Mol	Chain	Res	Type
1	P	27	GLN
1	P	30	GLN
1	P	84	GLN
1	P	101	HIS
1	P	210	GLN
2	L	6	GLN
2	L	28	ASN
2	L	38	GLN
2	L	90	GLN
2	L	91	HIS
2	L	124	GLN
2	L	166	GLN
2	L	189	HIS
2	L	210	ASN
3	H	6	GLN
3	H	35	ASN
3	H	60	ASN
3	H	81	GLN
3	H	105	GLN
3	H	196	ASN
4	A	34	HIS
4	A	38	GLN
4	A	89	GLN
4	A	90	GLN
4	A	156	GLN
4	A	157	ASN
4	A	189	HIS
4	A	198	HIS
4	A	210	ASN
5	B	6	GLN
5	B	35	HIS
5	B	52	ASN
5	B	60	ASN
5	B	61	GLN
5	B	156	ASN
5	B	165	HIS
5	B	197	ASN
1	Q	30	GLN
1	Q	50	GLN
1	Q	70	HIS
1	Q	128	GLN
1	Q	161	HIS

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Mol	Chain	Res	Type
1	Q	174	GLN
1	Q	202	ASN
1	Q	233	HIS
2	M	6	GLN
2	M	30	ASN
2	M	38	GLN
2	M	124	GLN
2	M	138	ASN
2	M	156	GLN
2	M	157	ASN
2	M	190	ASN
2	M	198	HIS
3	K	5	GLN
3	K	6	GLN
3	K	35	ASN
3	K	39	GLN
3	K	60	ASN
3	K	105	GLN
3	K	191	GLN
4	C	17	GLN
4	C	34	HIS
4	C	38	GLN
4	C	90	GLN
4	C	92	HIS
4	C	124	GLN
4	C	138	ASN
4	C	145	ASN
4	C	156	GLN
4	C	157	ASN
4	C	189	HIS
4	C	190	ASN
4	C	198	HIS
4	C	210	ASN
5	D	6	GLN
5	D	35	HIS
5	D	52	ASN
5	D	60	ASN
5	D	61	GLN
5	D	76	ASN
5	D	172	GLN
5	D	192	GLN
5	D	197	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

32 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	A2G	P	300	1,7	14,14,15	0.70	0	15,19,21	1.16	2 (13%)
7	GAL	P	301	7	11,11,12	0.74	0	13,15,17	1.43	3 (23%)
6	NAG	P	401	1,6	14,14,15	1.12	0	15,19,21	2.03	4 (26%)
6	NAG	P	402	6	14,14,15	0.58	0	15,19,21	1.19	2 (13%)
6	MAN	P	403	6	11,11,12	1.17	1 (9%)	13,15,17	2.24	5 (38%)
6	MAN	P	404	6	11,11,12	0.68	0	13,15,17	2.61	4 (30%)
6	NAG	P	405	6	14,14,15	0.70	0	15,19,21	1.65	2 (13%)
6	GAL	P	406	6	11,11,12	1.30	2 (18%)	13,15,17	0.54	0
6	SIA	P	407	6	17,20,21	2.11	5 (29%)	19,28,31	1.31	2 (10%)
6	NAG	P	408	6	14,14,15	0.53	0	15,19,21	0.77	0
6	GAL	P	409	6	11,11,12	0.55	0	13,15,17	1.82	4 (30%)
6	SIA	P	410	6	17,20,21	0.61	0	19,28,31	1.96	5 (26%)
6	MAN	P	411	6	11,11,12	0.73	0	13,15,17	1.52	2 (15%)
6	NAG	P	412	6	14,14,15	0.82	1 (7%)	15,19,21	1.99	3 (20%)
6	GAL	P	413	6	11,11,12	0.67	0	13,15,17	1.18	1 (7%)
6	SIA	P	414	6	17,20,21	0.81	0	19,28,31	0.95	1 (5%)
6	FUC	P	415	6	9,10,11	0.70	0	13,14,16	0.71	0
6	NAG	Q	401	1,6	14,14,15	0.56	0	15,19,21	2.20	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	Q	402	6	14,14,15	0.55	0	15,19,21	1.77	4 (26%)
6	MAN	Q	403	6	11,11,12	0.73	0	13,15,17	2.62	6 (46%)
6	MAN	Q	404	6	11,11,12	0.73	0	13,15,17	2.32	3 (23%)
6	NAG	Q	405	6	14,14,15	0.56	0	15,19,21	2.73	7 (46%)
6	GAL	Q	406	6	11,11,12	0.96	1 (9%)	13,15,17	1.27	1 (7%)
6	SIA	Q	407	6	17,20,21	0.69	0	19,28,31	1.58	2 (10%)
6	NAG	Q	408	6	14,14,15	1.33	1 (7%)	15,19,21	1.72	5 (33%)
6	GAL	Q	409	6	11,11,12	0.83	0	13,15,17	2.02	5 (38%)
6	SIA	Q	410	6	17,20,21	0.52	0	19,28,31	1.13	1 (5%)
6	MAN	Q	411	6	11,11,12	0.68	0	13,15,17	1.44	2 (15%)
6	NAG	Q	412	6	14,14,15	0.64	0	15,19,21	1.74	5 (33%)
6	GAL	Q	413	6	11,11,12	0.74	0	13,15,17	1.21	1 (7%)
6	SIA	Q	414	6	17,20,21	0.70	0	19,28,31	0.80	0
6	FUC	Q	415	6	9,10,11	0.68	0	13,14,16	1.94	4 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	A2G	P	300	1,7	-	0/6/23/26	0/1/1/1
7	GAL	P	301	7	-	0/2/19/22	0/1/1/1
6	NAG	P	401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	402	6	-	0/6/23/26	0/1/1/1
6	MAN	P	403	6	-	0/2/19/22	0/1/1/1
6	MAN	P	404	6	-	0/2/19/22	0/1/1/1
6	NAG	P	405	6	-	0/6/23/26	0/1/1/1
6	GAL	P	406	6	-	0/2/19/22	0/1/1/1
6	SIA	P	407	6	-	0/14/34/38	0/1/1/1
6	NAG	P	408	6	-	0/6/23/26	0/1/1/1
6	GAL	P	409	6	-	0/2/19/22	0/1/1/1
6	SIA	P	410	6	-	0/14/34/38	0/1/1/1
6	MAN	P	411	6	-	0/2/19/22	1/1/1/1
6	NAG	P	412	6	-	0/6/23/26	0/1/1/1
6	GAL	P	413	6	-	0/2/19/22	0/1/1/1
6	SIA	P	414	6	-	0/14/34/38	0/1/1/1
6	FUC	P	415	6	-	0/0/17/20	0/1/1/1
6	NAG	Q	401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	402	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	Q	403	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	404	6	-	0/2/19/22	0/1/1/1
6	NAG	Q	405	6	-	0/6/23/26	0/1/1/1
6	GAL	Q	406	6	-	0/2/19/22	0/1/1/1
6	SIA	Q	407	6	-	0/14/34/38	0/1/1/1
6	NAG	Q	408	6	-	0/6/23/26	0/1/1/1
6	GAL	Q	409	6	-	0/2/19/22	0/1/1/1
6	SIA	Q	410	6	-	0/14/34/38	0/1/1/1
6	MAN	Q	411	6	-	0/2/19/22	0/1/1/1
6	NAG	Q	412	6	-	0/6/23/26	0/1/1/1
6	GAL	Q	413	6	-	0/2/19/22	0/1/1/1
6	SIA	Q	414	6	-	0/14/34/38	0/1/1/1
6	FUC	Q	415	6	-	0/0/17/20	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	407	SIA	C11-C10	-4.71	1.40	1.50
6	P	407	SIA	O10-C10	-4.45	1.12	1.23
6	Q	408	NAG	O5-C1	-4.42	1.36	1.43
6	P	407	SIA	C9-C8	2.10	1.58	1.52
6	P	407	SIA	C7-C6	2.12	1.55	1.52
6	P	406	GAL	C2-C3	2.20	1.55	1.52
6	Q	406	GAL	C2-C3	2.42	1.55	1.52
6	P	412	NAG	C1-C2	2.56	1.56	1.52
6	P	403	MAN	C2-C3	2.86	1.56	1.52
6	P	406	GAL	O3-C3	3.03	1.49	1.43
6	P	407	SIA	C10-N5	3.52	1.47	1.34

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	401	NAG	O5-C1-C2	-5.78	103.43	111.47
6	Q	405	NAG	O4-C4-C3	-3.46	102.83	110.36
6	P	411	MAN	C3-C4-C5	-3.44	104.16	110.22
6	P	404	MAN	C1-C2-C3	-3.42	105.32	109.65
6	Q	401	NAG	C2-N2-C7	-3.41	117.97	122.94
6	Q	409	GAL	O5-C1-C2	-3.25	105.70	110.79
6	Q	409	GAL	C1-C2-C3	-3.05	105.78	109.65
6	P	409	GAL	C3-C4-C5	-2.91	105.09	110.22
6	Q	401	NAG	O5-C1-C2	-2.84	107.52	111.47
6	Q	403	MAN	C6-C5-C4	-2.74	106.58	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	402	NAG	O5-C1-C2	-2.62	107.83	111.47
6	Q	408	NAG	C1-C2-N2	-2.49	106.23	110.49
6	Q	401	NAG	C1-C2-N2	-2.44	106.33	110.49
6	P	401	NAG	C1-C2-N2	-2.21	106.71	110.49
6	Q	412	NAG	C3-C4-C5	-2.14	106.44	110.22
6	P	401	NAG	C3-C4-C5	-2.06	106.58	110.22
6	P	402	NAG	O3-C3-C2	-2.05	104.99	109.39
6	Q	405	NAG	O7-C7-C8	-2.01	118.41	122.06
7	P	300	A2G	C1-O-C5	2.02	114.94	112.17
6	Q	402	NAG	C1-O5-C5	2.03	114.96	112.17
6	P	404	MAN	O2-C2-C3	2.04	114.18	110.17
7	P	300	A2G	O4-C4-C5	2.06	114.47	109.28
6	Q	412	NAG	C8-C7-N2	2.06	119.84	116.11
6	P	407	SIA	C4-C3-C2	2.09	113.68	109.75
6	P	401	NAG	C1-O5-C5	2.13	115.10	112.17
6	Q	408	NAG	C1-O5-C5	2.14	115.11	112.17
6	Q	408	NAG	O4-C4-C3	2.14	115.01	110.36
6	P	403	MAN	O3-C3-C4	2.14	115.02	110.36
6	P	411	MAN	C6-C5-C4	2.18	118.11	113.00
6	P	409	GAL	O5-C1-C2	2.22	114.26	110.79
6	Q	403	MAN	O5-C1-C2	2.26	114.33	110.79
6	Q	415	FUC	O5-C1-C2	2.28	114.36	110.79
6	P	402	NAG	C4-C3-C2	2.31	114.40	111.02
6	P	407	SIA	C6-C5-N5	2.32	115.09	111.00
6	P	412	NAG	O4-C4-C3	2.41	115.59	110.36
7	P	301	GAL	C1-C2-C3	2.46	112.77	109.65
6	Q	402	NAG	C4-C3-C2	2.52	114.71	111.02
7	P	301	GAL	C3-C4-C5	2.55	114.72	110.22
7	P	301	GAL	C2-C3-C4	2.61	115.44	110.88
6	Q	408	NAG	C2-N2-C7	2.77	126.99	122.94
6	Q	404	MAN	O5-C1-C2	2.78	115.15	110.79
6	Q	412	NAG	C1-O5-C5	2.79	116.01	112.17
6	P	403	MAN	O5-C1-C2	2.79	115.16	110.79
6	Q	409	GAL	O3-C3-C2	2.79	115.10	110.02
6	Q	412	NAG	O5-C1-C2	2.80	115.37	111.47
6	Q	409	GAL	C1-O5-C5	2.83	116.06	112.17
6	P	414	SIA	C8-C7-C6	2.85	118.58	113.04
6	Q	413	GAL	C1-C2-C3	2.87	113.28	109.65
6	P	410	SIA	C5-N5-C10	2.89	130.50	123.19
6	P	404	MAN	C3-C4-C5	2.91	115.34	110.22
6	P	410	SIA	C11-C10-N5	2.92	121.37	116.11
6	P	410	SIA	C4-C3-C2	2.93	115.24	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	403	MAN	O3-C3-C2	2.99	115.46	110.02
6	P	412	NAG	C2-N2-C7	3.02	127.35	122.94
6	Q	411	MAN	C1-C2-C3	3.08	113.56	109.65
6	Q	405	NAG	C8-C7-N2	3.10	121.71	116.11
6	Q	415	FUC	C3-C4-C5	3.11	114.57	109.68
6	P	403	MAN	O3-C3-C2	3.13	115.71	110.02
6	Q	411	MAN	C1-O5-C5	3.17	116.53	112.17
6	Q	405	NAG	C4-C3-C2	3.21	115.72	111.02
6	Q	412	NAG	C4-C3-C2	3.35	115.93	111.02
6	P	405	NAG	C4-C3-C2	3.40	116.00	111.02
6	P	410	SIA	C3-C4-C5	3.41	115.59	111.46
6	Q	401	NAG	C1-O5-C5	3.41	116.87	112.17
6	Q	407	SIA	C3-C4-C5	3.44	115.62	111.46
6	P	405	NAG	C1-O5-C5	3.56	117.07	112.17
6	Q	415	FUC	O5-C5-C4	3.59	115.54	109.62
6	P	413	GAL	C1-C2-C3	3.59	114.20	109.65
6	Q	406	GAL	O3-C3-C2	3.62	116.61	110.02
6	Q	402	NAG	C2-N2-C7	3.63	128.24	122.94
6	P	409	GAL	C1-O5-C5	3.63	117.17	112.17
6	Q	410	SIA	C4-C3-C2	3.64	116.57	109.75
6	Q	409	GAL	C3-C4-C5	3.66	116.67	110.22
6	P	409	GAL	O3-C3-C2	3.70	116.75	110.02
6	Q	403	MAN	C1-C2-C3	3.73	114.38	109.65
6	Q	408	NAG	C4-C3-C2	3.79	116.58	111.02
6	Q	415	FUC	C1-O5-C5	3.82	120.85	112.39
6	Q	403	MAN	C3-C4-C5	3.93	117.14	110.22
6	Q	405	NAG	O4-C4-C5	4.00	119.36	109.28
6	P	410	SIA	C4-C5-C6	4.02	119.45	108.89
6	P	403	MAN	C1-C2-C3	4.12	114.88	109.65
6	P	403	MAN	C1-O5-C5	4.27	118.05	112.17
6	Q	404	MAN	C1-O5-C5	4.59	118.50	112.17
6	Q	401	NAG	C4-C3-C2	4.82	118.08	111.02
6	Q	405	NAG	C2-N2-C7	4.95	130.16	122.94
6	Q	407	SIA	C4-C3-C2	5.29	119.66	109.75
6	P	412	NAG	C1-O5-C5	5.62	119.91	112.17
6	Q	405	NAG	C1-O5-C5	5.69	120.01	112.17
6	Q	404	MAN	O2-C2-C1	5.81	121.00	109.18
6	Q	403	MAN	C1-O5-C5	6.00	120.43	112.17
6	P	404	MAN	C1-O5-C5	7.47	122.47	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	411	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	300	A2G	1	0
6	P	402	NAG	2	0
6	P	403	MAN	3	0
6	P	409	GAL	1	0
6	P	410	SIA	3	0
6	P	411	MAN	2	0
6	P	412	NAG	1	0
6	P	413	GAL	1	0
6	P	414	SIA	2	0
6	Q	401	NAG	2	0
6	Q	403	MAN	1	0
6	Q	404	MAN	2	0
6	Q	405	NAG	4	0
6	Q	408	NAG	2	0
6	Q	410	SIA	3	0
6	Q	411	MAN	1	0
6	Q	412	NAG	1	0
6	Q	413	GAL	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	P	237/237 (100%)	0.01	11 (4%) 33 20	28, 49, 123, 155	4 (1%)
1	Q	237/237 (100%)	0.22	12 (5%) 29 16	58, 94, 155, 193	0
2	L	219/219 (100%)	-0.03	1 (0%) 90 85	36, 76, 123, 155	0
2	M	219/219 (100%)	-0.21	0 100 100	46, 71, 104, 154	0
3	H	217/219 (99%)	-0.16	1 (0%) 90 85	27, 52, 139, 172	0
3	K	219/219 (100%)	-0.28	0 100 100	33, 56, 83, 142	0
4	A	218/218 (100%)	-0.03	1 (0%) 90 85	51, 79, 104, 141	0
4	C	218/218 (100%)	0.03	5 (2%) 61 46	50, 76, 109, 150	0
5	B	219/219 (100%)	0.04	4 (1%) 69 55	48, 84, 118, 157	0
5	D	219/219 (100%)	0.01	6 (2%) 55 40	53, 85, 113, 140	0
All	All	2222/2224 (99%)	-0.04	41 (1%) 69 55	27, 74, 124, 193	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	152	PRO	9.4
1	P	192	SER	7.3
1	Q	192	SER	5.4
1	P	150	LEU	4.9
1	P	146	PRO	4.6
1	Q	221	ALA	4.0
1	Q	222	LEU	3.8
2	L	153	SER	3.7
1	P	151	THR	3.7
1	Q	220	CYS	3.6
4	C	214	CYS	3.6
3	H	138	LEU	3.5
5	B	211	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
5	D	125	LEU	3.0
1	Q	144	ILE	2.9
5	D	98	LEU	2.7
1	Q	189	SER	2.7
1	P	17	VAL	2.6
1	Q	223	PRO	2.6
1	P	145	GLU	2.5
5	D	138	THR	2.4
5	B	139	LEU	2.4
1	Q	186	TRP	2.4
4	C	51	ALA	2.4
1	P	193	GLY	2.3
1	Q	226	SER	2.3
4	C	93	GLU	2.2
5	D	122	VAL	2.2
5	D	133	THR	2.2
1	P	16	ILE	2.2
1	P	191	CYS	2.2
1	Q	145	GLU	2.2
4	C	132	VAL	2.2
5	D	211	ILE	2.2
1	Q	187	GLY	2.1
5	B	129	CYS	2.1
4	A	198	HIS	2.1
1	P	18	GLY	2.1
1	Q	76	PRO	2.0
5	B	133	THR	2.0
4	C	32	PHE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GAL	P	301	11/12	0.80	0.43	8.94	65,66,66,66	11
6	SIA	P	410	20/21	0.51	0.43	8.88	106,108,110,110	20
7	A2G	P	300	14/15	0.77	0.36	8.42	60,63,65,65	14
6	GAL	P	409	11/12	0.80	0.29	-	111,112,112,112	11
6	SIA	Q	414	20/21	0.36	0.54	-	116,118,118,118	20
6	GAL	Q	406	11/12	0.45	0.79	-	141,142,143,143	0
6	GAL	Q	409	11/12	0.64	0.53	-	131,132,132,132	11
6	SIA	Q	410	20/21	0.68	0.35	-	131,132,133,133	20
6	MAN	Q	411	11/12	0.39	0.52	-	119,121,122,122	11
6	NAG	Q	405	14/15	0.39	0.36	-	134,136,137,139	14
6	GAL	Q	413	11/12	0.42	0.45	-	116,117,118,118	11
6	GAL	P	406	11/12	0.49	0.48	-	118,119,119,119	11
6	NAG	Q	401	14/15	0.82	0.19	-	96,99,101,104	0
6	MAN	P	404	11/12	0.78	0.25	-	117,119,120,120	11
6	SIA	Q	407	20/21	0.50	0.52	-	144,145,146,146	0
6	NAG	P	401	14/15	0.90	0.15	-	73,77,83,89	0
6	MAN	P	403	11/12	0.41	0.23	-	112,114,118,118	0
6	SIA	P	414	20/21	0.60	0.41	-	117,119,120,120	20
6	NAG	P	412	14/15	0.75	0.35	-	123,123,124,124	0
6	MAN	P	411	11/12	0.45	0.37	-	120,121,122,122	0
6	NAG	Q	402	14/15	0.70	0.41	-	112,114,116,120	14
6	FUC	P	415	10/11	0.95	0.11	-	88,88,89,89	0
6	NAG	P	405	14/15	0.48	0.45	-	119,121,121,121	14
6	NAG	Q	412	14/15	0.41	0.40	-	115,117,117,118	14
6	GAL	P	413	11/12	0.62	0.37	-	122,122,123,123	11
6	MAN	Q	403	11/12	0.54	0.32	-	123,124,127,129	0
6	MAN	Q	404	11/12	0.55	0.39	-	130,132,133,134	11
6	NAG	Q	408	14/15	0.40	0.49	-	130,131,132,132	14
6	NAG	P	408	14/15	0.62	0.47	-	114,116,117,117	14
6	NAG	P	402	14/15	0.83	0.19	-	97,99,102,107	0
6	FUC	Q	415	10/11	0.86	0.33	-	100,101,101,101	0
6	SIA	P	407	20/21	0.49	0.47	-	115,119,119,119	20

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.