Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 01:41 AM JST

PDB ID	:	7CWT
EMDB ID	:	EMD-30487
Title	:	SARS-CoV-2 Spike protein in complex with hb27 and fc05 Fab cocktail
Authors	:	Cui, Z.; Wang, X.
Deposited on	:	2020-08-31
Resolution	:	3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

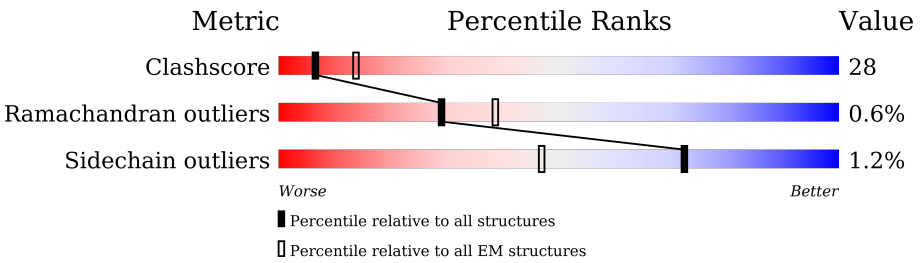
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1134	10% 63% 31% • 6%
1	B	1134	11% 62% 31% • 6%
1	C	1134	7% 60% 33% • 5%
2	D	111	62% 34% 63% •
2	F	111	89% 34% 63% •
2	J	111	46% 31% 62% 5% •
3	E	118	40% 31% 67% •
3	G	118	51% 36% 62% •

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Mol	Chain	Length	Quality of chain
3	I	118	29% 52% 45%
4	H	109	45% 58% 42%
4	K	109	40% 60% 40%
4	M	109	70% 61% 39%
5	L	120	65% 39% 60%
5	N	120	55% 40% 59%
5	P	120	57% 42% 58%

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	NAG	C	1201	X	-	-	-
6	NAG	C	1206	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 70206 atoms, of which 34568 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1065	16426	5307	8106	1385	1589	39	0	0
1	B	1071	16515	5333	8150	1395	1598	39	0	0
1	C	1074	16571	5352	8177	1401	1602	39	0	0

- Molecule 2 is a protein called Light chain Fab of HB27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	111	1639	522	803	145	166	3	0	0
2	F	111	1648	524	810	145	166	3	0	0
2	J	111	1648	524	810	145	166	3	0	0

- Molecule 3 is a protein called Heavy chain Fab of HB27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	118	1761	565	864	156	172	4	0	0
3	G	118	1761	565	864	156	172	4	0	0
3	I	118	1761	565	864	156	172	4	0	0

- Molecule 4 is a protein called Light chain Fab of FC05.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	H	109	1557	492	768	132	163	2	0	0

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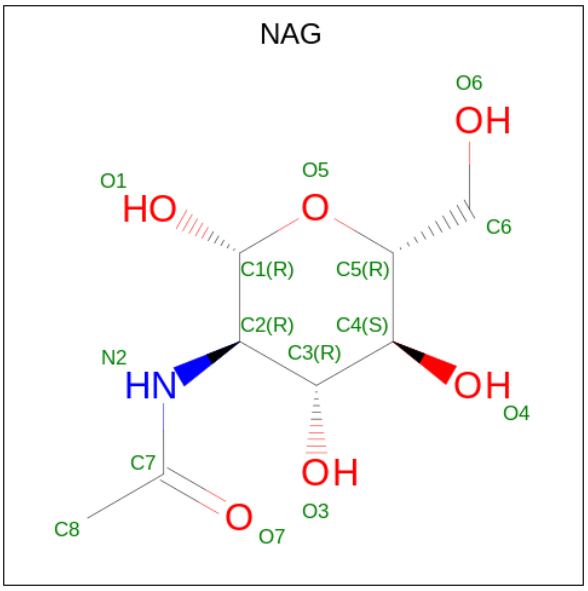
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	K	109	1557	492	768	132	163	2	0	0
			Total	C	H	N	O	S		
4	M	109	1557	492	768	132	163	2	0	0

- Molecule 5 is a protein called Heavy chain Fab of FC05.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	L	120	1809	587	878	149	188	7	0	0
			Total	C	H	N	O	S		
5	N	120	1809	587	878	149	188	7	0	0
			Total	C	H	N	O	S		
5	P	120	1809	587	878	149	188	7	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
6	A	1	135	40	65	5	25	0
			Total	C	H	N	O	
6	A	1	135	40	65	5	25	0
			Total	C	H	N	O	
6	A	1	135	40	65	5	25	0
			Total	C	H	N	O	
6	A	1	135	40	65	5	25	0

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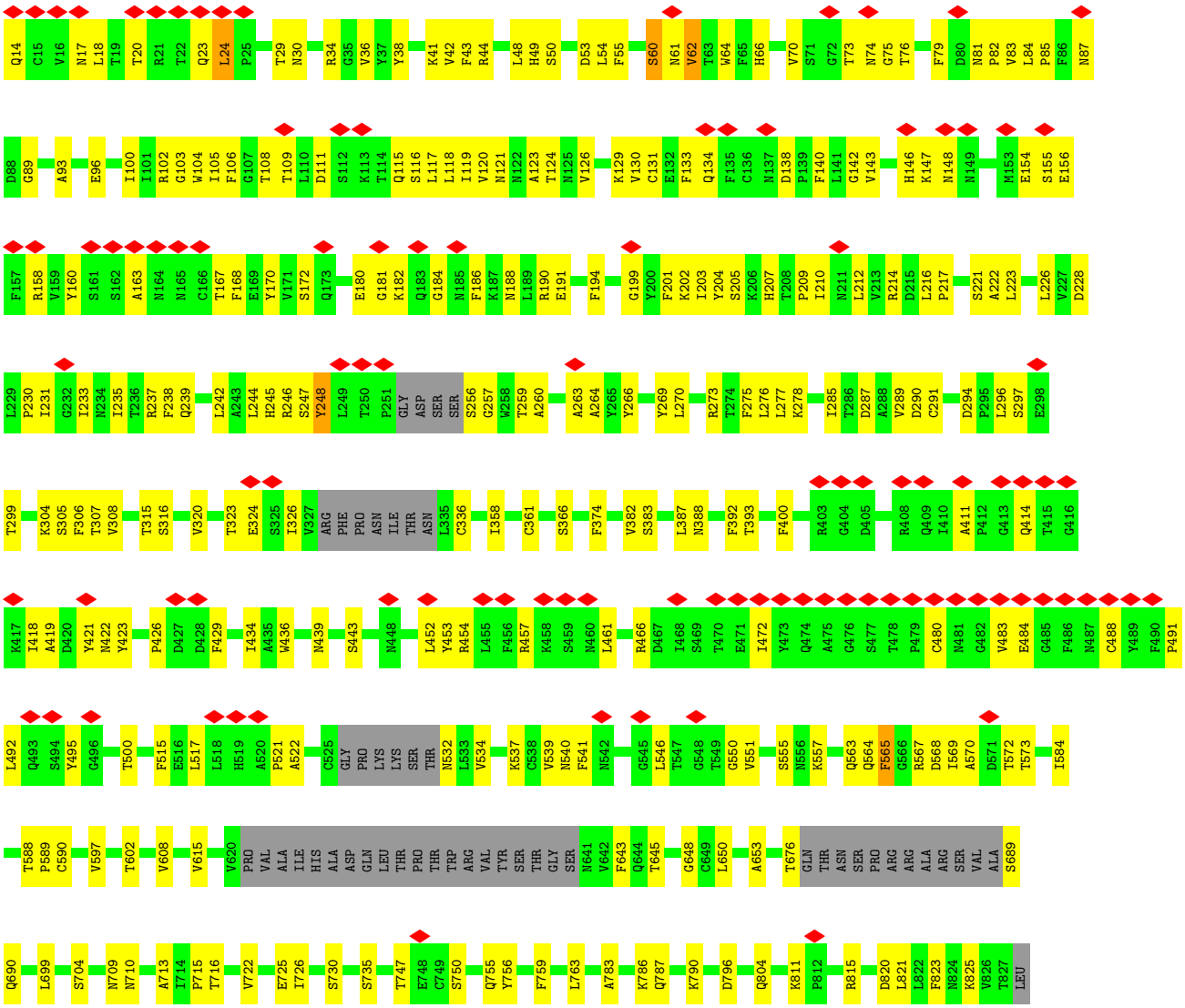
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
6	A	1	135	40	65	5	25	0
			Total	C	H	N	O	
6	B	1	81	24	39	3	15	0
			Total	C	H	N	O	
6	B	1	81	24	39	3	15	0
			Total	C	H	N	O	
6	B	1	81	24	39	3	15	0
			Total	C	H	N	O	
6	C	1	162	48	78	6	30	0
			Total	C	H	N	O	
6	C	1	162	48	78	6	30	0
			Total	C	H	N	O	
6	C	1	162	48	78	6	30	0
			Total	C	H	N	O	
6	C	1	162	48	78	6	30	0
			Total	C	H	N	O	
6	C	1	162	48	78	6	30	0
			Total	C	H	N	O	
6	C	1	162	48	78	6	30	0

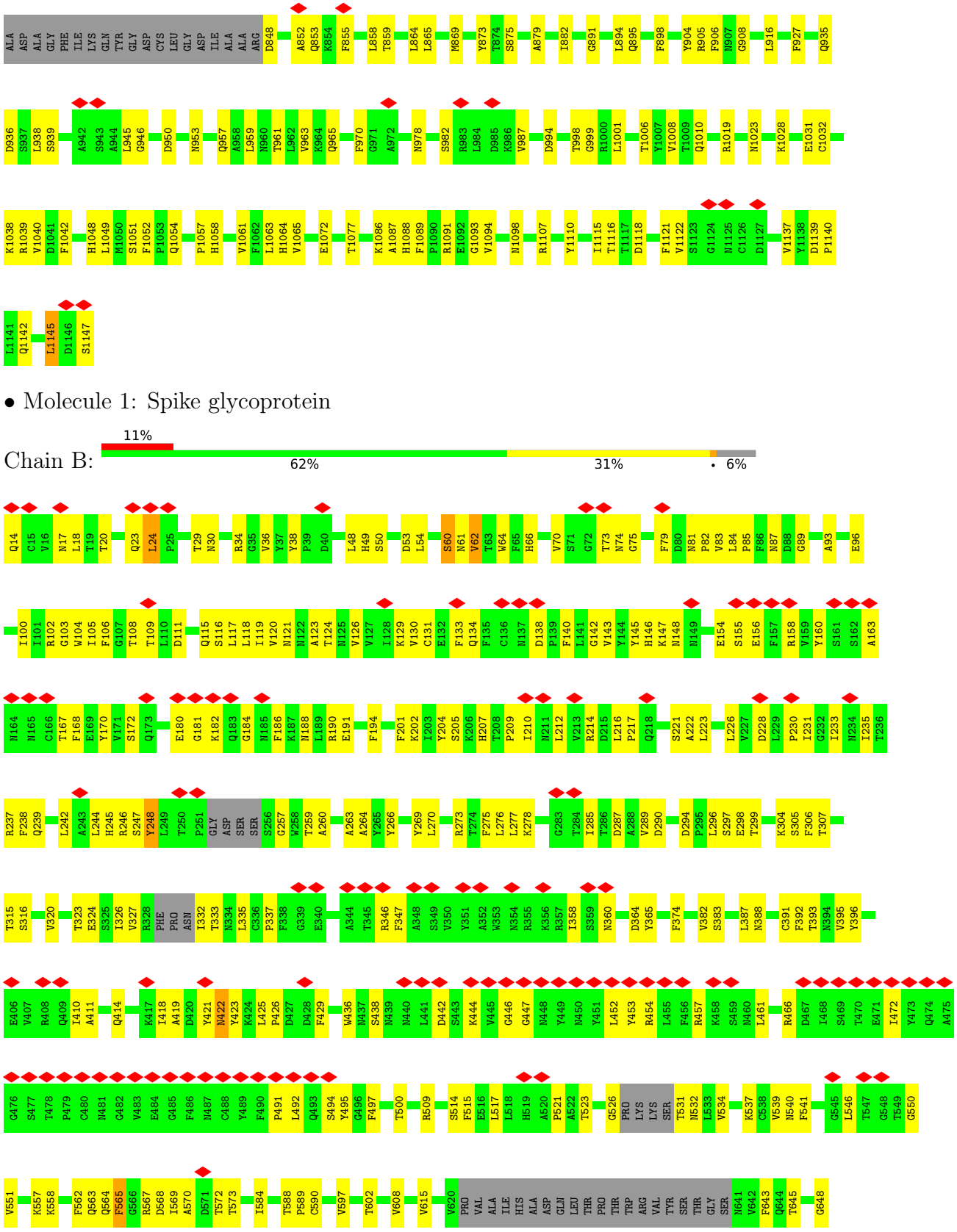
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Spike glycoprotein

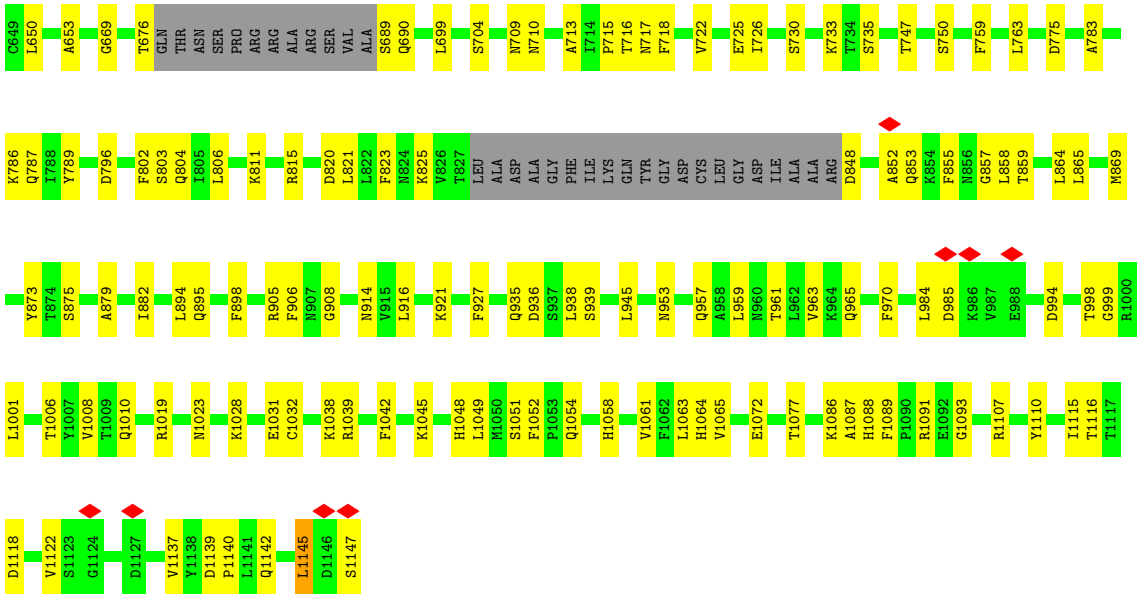
Chain A: 10% 63% 31% 6%





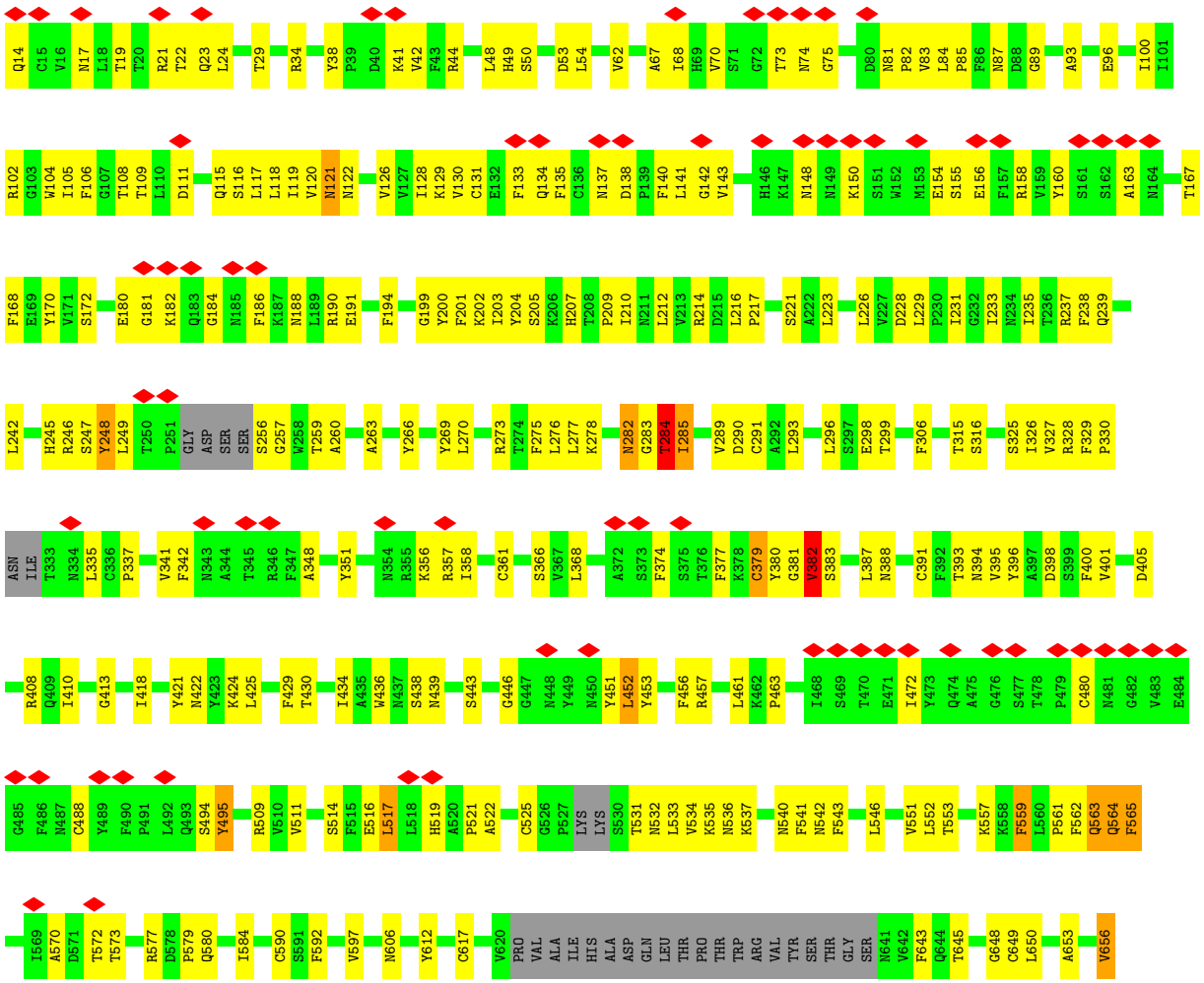
- Molecule 1: Spike glycoprotein

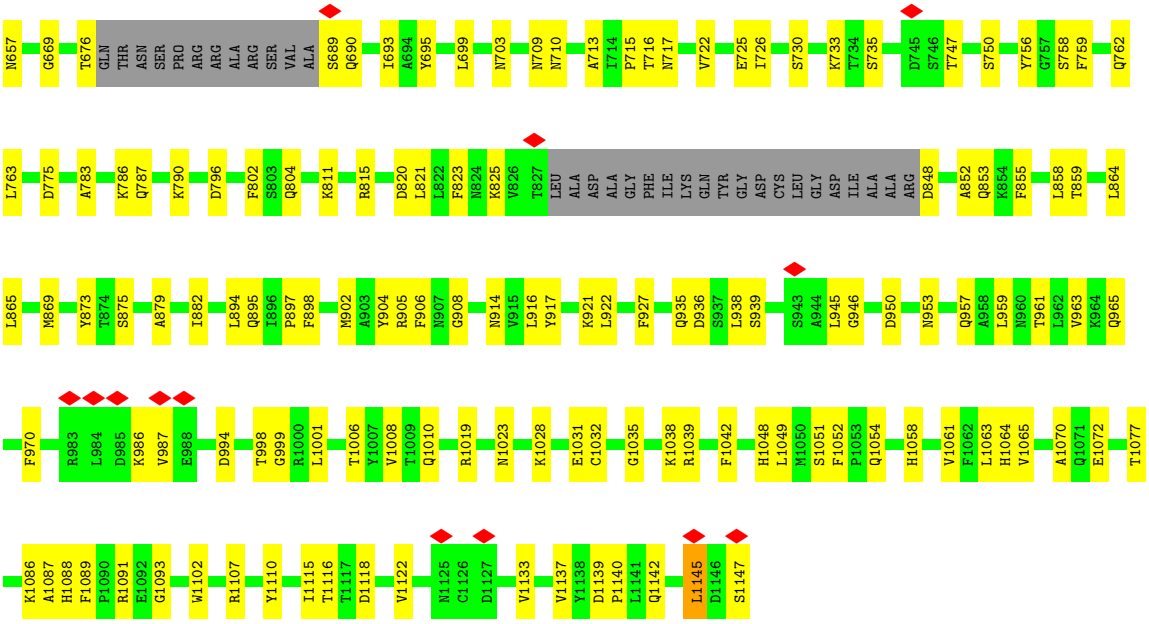
Chain B:



- Molecule 1: Spike glycoprotein

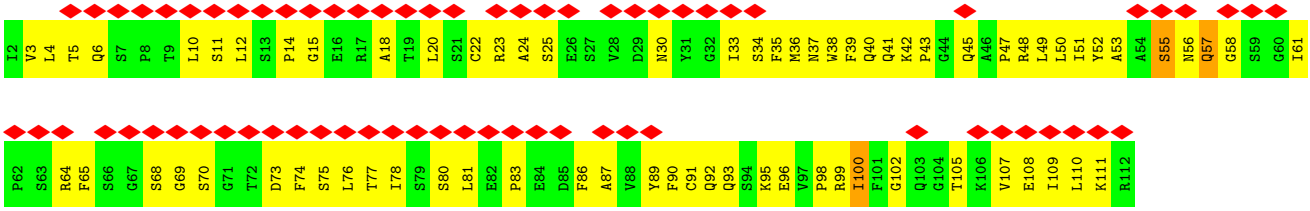
Chain C:





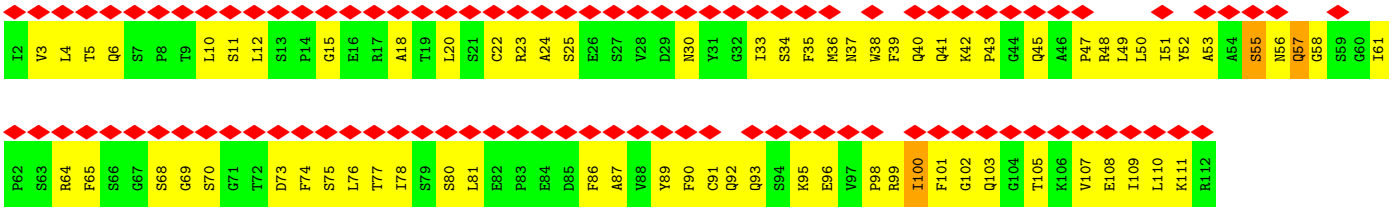
- Molecule 2: Light chain Fab of HB27

Chain D:



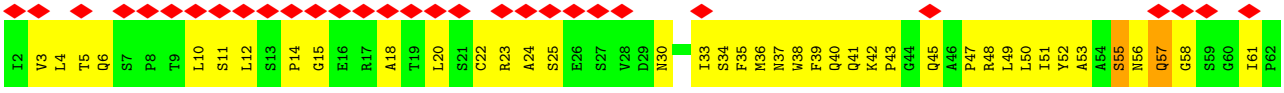
- Molecule 2: Light chain Fab of HB27

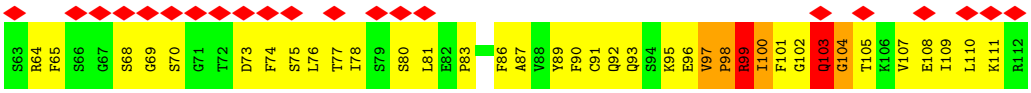
Chain F:



- Molecule 2: Light chain Fab of HB27

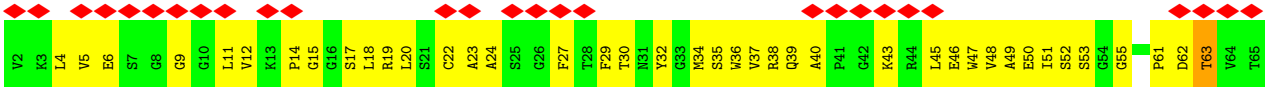
Chain J:





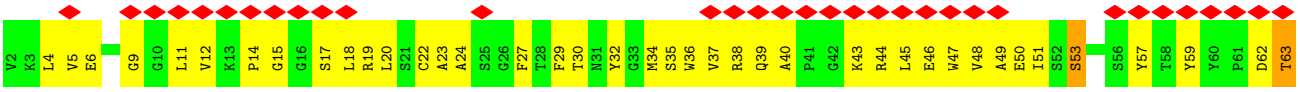
• Molecule 3: Heavy chain Fab of HB27

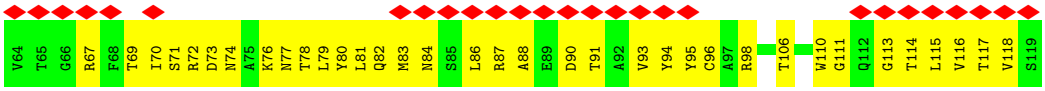
Chain E:



• Molecule 3: Heavy chain Fab of HB27

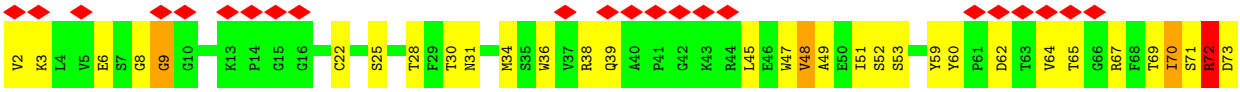
Chain G:

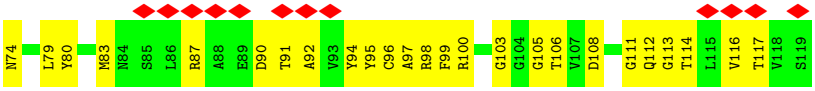




• Molecule 3: Heavy chain Fab of HB27

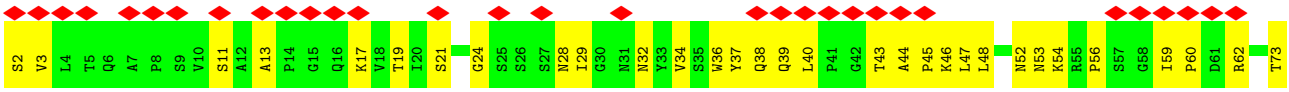
Chain I:

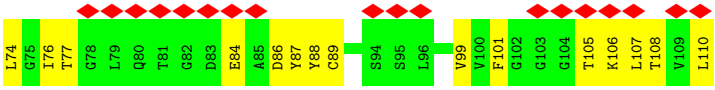




• Molecule 4: Light chain Fab of FC05

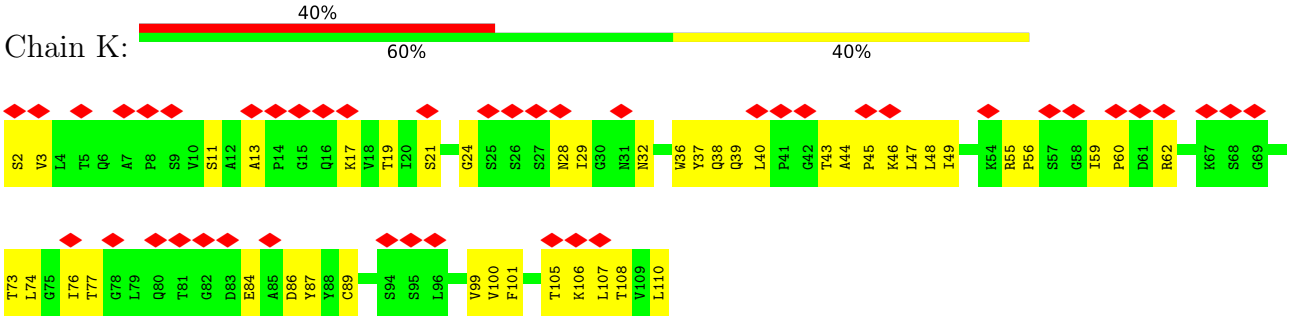
Chain H:





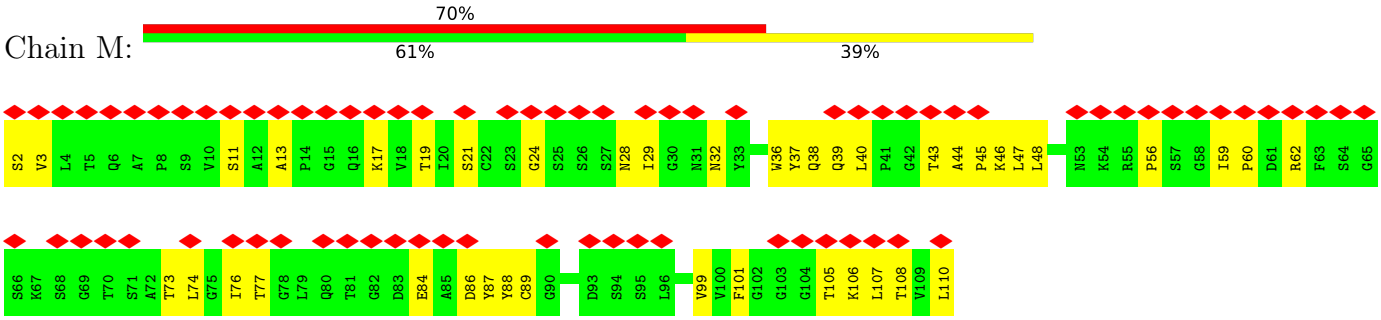
• Molecule 4: Light chain Fab of FC05

Chain K:



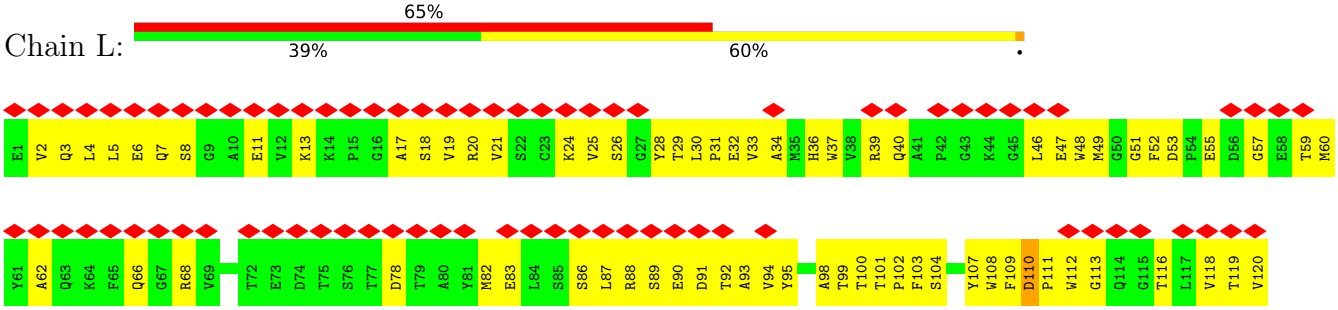
- Molecule 4: Light chain Fab of FC05

Chain M:



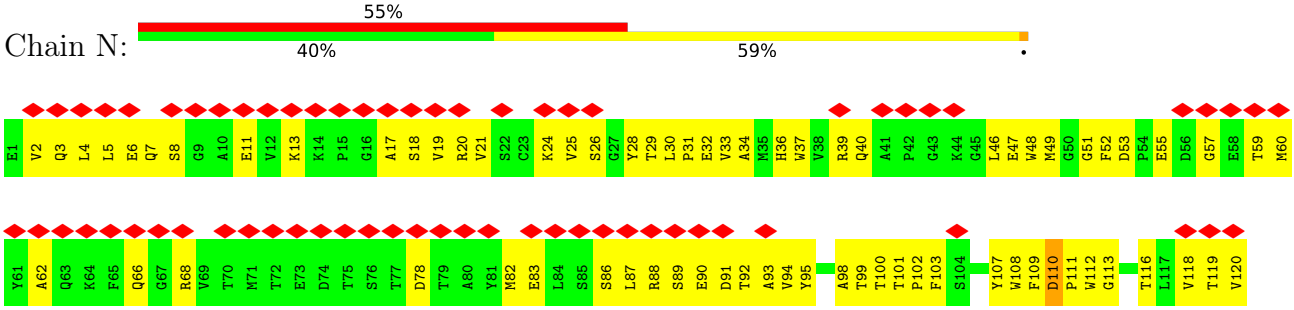
- Molecule 5: Heavy chain Fab of FC05

Chain L:



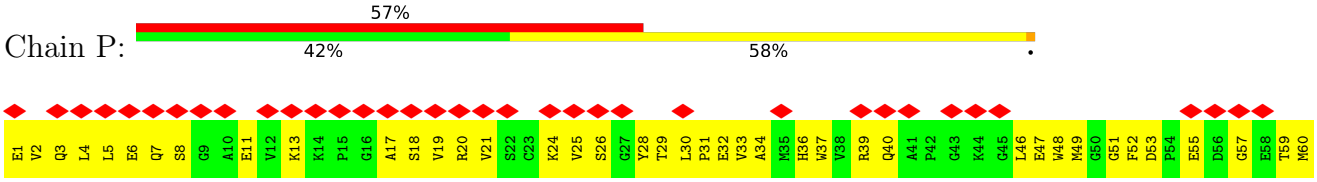
- Molecule 5: Heavy chain Fab of FC05

Chain N:



- Molecule 5: Heavy chain Fab of FC05

Chain P:



Y61
A62
Q63
K64
F65
Q66
G67
R68
V69
T70
M71
T72
E73
D74
T75
S76
T77
D78
T79
A80
Y81
M82
E83
L84
S85
S86
L87
R88
S89
E90
D91
T92
A93
V94
Y95
Y96
C97
A98
T101
P102
S105
S106
Y107
W108
F109
D110
P111
W112
G113
Q114
G115
T116
L117
V118
T119
V120

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	0/8508	0.59	1/11576 (0.0%)
1	B	0.50	0/8553	0.59	1/11637 (0.0%)
1	C	0.50	0/8585	0.62	4/11681 (0.0%)
2	D	0.36	0/853	0.66	0/1153
2	F	0.36	0/855	0.66	0/1156
2	J	0.46	0/855	0.76	2/1156 (0.2%)
3	E	0.49	0/917	0.65	0/1243
3	G	0.52	0/917	0.65	0/1243
3	I	0.65	0/917	0.71	1/1243 (0.1%)
4	H	0.29	0/805	0.49	0/1097
4	K	0.38	0/805	0.55	0/1097
4	M	0.33	0/805	0.52	0/1097
5	L	0.33	0/955	0.54	0/1299
5	N	0.33	0/955	0.54	0/1299
5	P	0.35	0/955	0.57	0/1299
All	All	0.48	0/36240	0.60	9/49276 (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	A	0	5
1	B	0	5
1	C	0	10
2	D	0	2
2	F	0	2
2	J	0	4
3	E	0	1
3	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	L	0	1
5	N	0	1
5	P	0	1
All	All	0	33

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	379	CYS	O-C-N	-7.16	111.24	122.70
3	I	72	ARG	CB-CA-C	6.01	122.42	110.40
2	J	98	PRO	N-CA-C	-5.51	97.78	112.10
2	J	103	GLN	C-N-CA	-5.25	111.28	122.30
1	B	848	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	848	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	848	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	380	TYR	N-CA-CB	5.03	119.65	110.60
1	C	495	TYR	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1145	LEU	Peptide
1	A	123	ALA	Peptide
1	A	248	TYR	Peptide
1	A	565	PHE	Peptide
1	A	60	SER	Peptide
1	B	1145	LEU	Peptide
1	B	123	ALA	Peptide
1	B	248	TYR	Peptide
1	B	565	PHE	Peptide
1	B	60	SER	Peptide
1	C	1145	LEU	Peptide
1	C	248	TYR	Peptide
1	C	282	ASN	Peptide
1	C	283	GLY	Peptide
1	C	284	THR	Peptide
1	C	379	CYS	Mainchain
1	C	381	GLY	Mainchain
1	C	382	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	C	565	PHE	Peptide
1	C	657	ASN	Peptide
2	D	55	SER	Peptide
2	D	57	GLN	Peptide
3	E	106	THR	Peptide
2	F	55	SER	Peptide
2	F	57	GLN	Peptide
3	I	105	GLY	Peptide
2	J	103	GLN	Peptide,Mainchain
2	J	55	SER	Peptide
2	J	57	GLN	Peptide
5	L	8	SER	Peptide
5	N	8	SER	Peptide
5	P	8	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8320	8106	8105	450	0
1	B	8365	8150	8151	411	0
1	C	8394	8177	8177	420	0
2	D	836	803	803	93	0
2	F	838	810	810	86	0
2	J	838	810	810	95	0
3	E	897	864	864	88	0
3	G	897	864	864	74	0
3	I	897	864	864	69	0
4	H	789	768	768	42	0
4	K	789	768	768	48	0
4	M	789	768	768	44	0
5	L	931	878	878	89	0
5	N	931	878	878	82	0
5	P	931	878	878	79	0
6	A	70	65	65	0	0
6	B	42	39	39	1	0
6	C	84	78	78	3	0
All	All	35638	34568	34568	1973	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 28.

All (1973) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HD11	1:B:306:PHE:CE1	1.32	1.62
1:A:276:LEU:HD11	1:A:306:PHE:CE1	1.32	1.60
1:A:147:LYS:HE3	5:L:52:PHE:CE2	1.40	1.55
1:A:64:TRP:CZ2	1:A:66:HIS:CE1	1.95	1.52
1:B:296:LEU:HD12	1:B:608:VAL:CG1	1.39	1.52
1:B:64:TRP:CZ2	1:B:66:HIS:CE1	1.95	1.51
1:B:392:PHE:CE1	1:B:517:LEU:HD21	1.45	1.51
1:A:296:LEU:HD12	1:A:608:VAL:CG1	1.39	1.50
1:C:410:ILE:HD11	1:C:418:ILE:CG2	1.37	1.50
1:B:276:LEU:CD1	1:B:306:PHE:HE1	1.23	1.47
1:A:276:LEU:CD1	1:A:306:PHE:HE1	1.23	1.46
1:B:296:LEU:CD1	1:B:608:VAL:HG13	1.45	1.46
1:A:64:TRP:CZ2	1:A:66:HIS:HE1	1.28	1.45
1:C:374:PHE:HE1	1:C:436:TRP:CZ3	1.32	1.44
1:B:426:PRO:CB	1:B:429:PHE:HD2	1.30	1.43
1:A:296:LEU:CD1	1:A:608:VAL:HG13	1.45	1.42
1:B:64:TRP:CZ2	1:B:66:HIS:HE1	1.28	1.40
1:B:296:LEU:CD1	1:B:608:VAL:CG1	1.97	1.38
1:B:18:LEU:O	1:B:18:LEU:HD12	1.24	1.38
1:A:296:LEU:CD1	1:A:608:VAL:CG1	1.97	1.37
1:B:392:PHE:CE1	1:B:517:LEU:CD2	2.04	1.37
1:A:426:PRO:CB	1:A:429:PHE:HD2	1.35	1.37
1:A:276:LEU:CD1	1:A:306:PHE:CE1	2.00	1.35
1:C:394:ASN:HB2	1:C:516:GLU:OE2	1.22	1.33
1:C:394:ASN:CB	1:C:516:GLU:OE2	1.78	1.32
1:C:394:ASN:HB2	1:C:516:GLU:CD	1.49	1.31
1:B:457:ARG:NE	1:B:461:LEU:HD21	1.45	1.31
1:C:374:PHE:CD1	1:C:434:ILE:HG22	1.63	1.31
1:C:457:ARG:NE	1:C:461:LEU:HD21	1.47	1.30
1:B:426:PRO:HB2	1:B:429:PHE:CD2	1.66	1.30
1:B:48:LEU:CD1	1:B:304:LYS:O	1.80	1.29
1:C:374:PHE:CE1	1:C:436:TRP:CZ3	2.21	1.29
3:I:95:TYR:CE1	3:I:112:GLN:O	1.85	1.29
3:I:95:TYR:CE1	3:I:113:GLY:CA	2.16	1.28
1:A:48:LEU:CD1	1:A:304:LYS:O	1.80	1.27
1:B:426:PRO:CB	1:B:429:PHE:CD2	2.15	1.27
1:A:230:PRO:CB	1:B:523:THR:HG22	1.63	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:PHE:CE1	1:C:436:TRP:CE3	2.22	1.27
1:A:147:LYS:CE	5:L:52:PHE:CE2	2.16	1.27
1:B:48:LEU:HD13	1:B:304:LYS:O	1.10	1.26
1:B:324:GLU:OE2	1:B:534:VAL:CG2	1.85	1.25
3:I:30:THR:CG2	3:I:74:ASN:HB3	1.65	1.25
1:A:324:GLU:OE2	1:A:534:VAL:CG2	1.85	1.24
1:A:358:ILE:CG2	1:A:361:CYS:SG	2.25	1.24
1:A:324:GLU:OE2	1:A:534:VAL:HG21	1.38	1.23
1:A:426:PRO:HB2	1:A:429:PHE:CD2	1.71	1.23
1:A:457:ARG:NE	1:A:461:LEU:HD21	1.50	1.23
3:I:95:TYR:HE1	3:I:112:GLN:O	0.93	1.23
1:A:18:LEU:HD12	1:A:18:LEU:O	1.24	1.22
1:A:426:PRO:CB	1:A:429:PHE:CD2	2.20	1.22
1:B:276:LEU:CD1	1:B:306:PHE:CE1	2.00	1.22
1:A:48:LEU:HD13	1:A:304:LYS:O	1.10	1.22
1:C:374:PHE:CD1	1:C:436:TRP:CE3	2.27	1.22
1:B:392:PHE:CD1	1:B:515:PHE:HB3	1.73	1.22
1:A:287:ASP:HB3	1:A:306:PHE:CE2	1.75	1.21
1:A:457:ARG:CZ	1:A:461:LEU:HD23	1.70	1.21
1:C:374:PHE:CG	1:C:434:ILE:CG2	2.23	1.21
1:C:410:ILE:CG2	1:C:425:LEU:HD12	1.69	1.21
1:B:457:ARG:CZ	1:B:461:LEU:HD23	1.70	1.21
1:B:287:ASP:HB3	1:B:306:PHE:CE2	1.75	1.19
1:A:296:LEU:HD11	1:A:608:VAL:HG13	1.20	1.19
1:C:457:ARG:CZ	1:C:461:LEU:HD23	1.71	1.18
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.06	1.18
1:A:64:TRP:CE2	1:A:66:HIS:CE1	2.32	1.17
1:A:147:LYS:HE2	5:L:52:PHE:CZ	1.80	1.16
1:B:64:TRP:CE2	1:B:66:HIS:CE1	2.32	1.16
1:C:374:PHE:CD1	1:C:434:ILE:CG2	2.29	1.16
1:A:421:TYR:O	1:A:461:LEU:HD12	1.45	1.16
1:A:147:LYS:CE	5:L:52:PHE:CZ	2.29	1.15
1:B:457:ARG:NE	1:B:461:LEU:CD2	2.09	1.15
1:B:324:GLU:OE2	1:B:534:VAL:HG21	1.38	1.14
1:B:296:LEU:HD11	1:B:608:VAL:HG13	1.20	1.14
3:I:30:THR:HG22	3:I:74:ASN:HB3	1.20	1.14
3:I:71:SER:OG	3:I:80:TYR:HB2	1.43	1.14
1:C:410:ILE:HD11	1:C:418:ILE:HG21	1.22	1.14
3:I:95:TYR:CE1	3:I:112:GLN:C	2.22	1.13
1:C:374:PHE:CG	1:C:434:ILE:HG21	1.81	1.13
1:A:42:VAL:HG22	1:B:565:PHE:HB2	1.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:TYR:O	1:A:461:LEU:CD1	1.96	1.13
1:A:457:ARG:NE	1:A:461:LEU:CD2	2.11	1.13
3:I:95:TYR:CD1	3:I:113:GLY:HA2	1.83	1.13
1:C:457:ARG:NE	1:C:461:LEU:CD2	2.11	1.12
1:C:394:ASN:CG	1:C:516:GLU:OE2	1.86	1.12
3:I:95:TYR:HE1	3:I:112:GLN:C	1.52	1.12
1:C:410:ILE:CD1	1:C:418:ILE:CG2	2.27	1.11
1:B:421:TYR:O	1:B:461:LEU:HD12	1.50	1.10
1:C:410:ILE:HG22	1:C:425:LEU:HD12	1.27	1.10
1:B:457:ARG:CZ	1:B:461:LEU:CD2	2.30	1.09
1:C:393:THR:HG22	1:C:522:ALA:HA	1.20	1.09
1:C:457:ARG:CZ	1:C:461:LEU:CD2	2.31	1.09
3:I:95:TYR:CD1	3:I:113:GLY:CA	2.36	1.08
1:A:147:LYS:HE2	5:L:52:PHE:CE1	1.87	1.08
2:J:4:LEU:HD11	2:J:102:GLY:HA2	1.22	1.08
1:C:410:ILE:CD1	1:C:418:ILE:HG21	1.84	1.07
1:A:457:ARG:CZ	1:A:461:LEU:CD2	2.32	1.07
1:B:299:THR:HG22	1:B:315:THR:OG1	1.54	1.07
1:C:278:LYS:HB2	1:C:306:PHE:CZ	1.90	1.06
1:A:393:THR:HG22	1:A:521:PRO:O	1.53	1.06
1:C:328:ARG:N	1:C:542:ASN:O	1.86	1.06
2:F:4:LEU:HD11	2:F:102:GLY:HA2	1.37	1.06
1:A:296:LEU:CD1	1:A:608:VAL:HG11	1.83	1.06
1:A:299:THR:HG22	1:A:315:THR:OG1	1.54	1.05
1:B:66:HIS:ND1	1:B:264:ALA:HB2	1.72	1.05
1:B:296:LEU:CD1	1:B:608:VAL:HG11	1.83	1.05
1:A:230:PRO:HB2	1:B:523:THR:HG22	1.07	1.04
1:C:536:ASN:OD1	1:C:553:THR:HG22	1.58	1.04
4:M:101:PHE:HZ	5:P:109:PHE:CE2	1.75	1.04
1:A:66:HIS:ND1	1:A:264:ALA:HB2	1.72	1.04
2:D:4:LEU:HD11	2:D:102:GLY:HA2	1.37	1.04
1:C:410:ILE:HD11	1:C:418:ILE:HG22	1.05	1.03
1:A:230:PRO:HB2	1:B:523:THR:CG2	1.87	1.03
1:B:426:PRO:CG	1:B:429:PHE:CD2	2.42	1.03
1:A:358:ILE:HG22	1:A:361:CYS:SG	1.96	1.02
1:B:426:PRO:HG2	1:B:429:PHE:CD2	1.94	1.02
1:C:201:PHE:HB3	1:C:231:ILE:HG13	1.41	1.02
1:C:374:PHE:HD1	1:C:436:TRP:HE3	1.07	1.02
1:C:394:ASN:CB	1:C:516:GLU:CD	2.22	1.02
1:B:296:LEU:HD12	1:B:608:VAL:CG2	1.89	1.02
1:C:393:THR:HG22	1:C:522:ALA:CA	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:6:GLN:HB2	2:J:103:GLN:HB3	1.42	1.01
1:A:296:LEU:HD12	1:A:608:VAL:CG2	1.89	1.01
1:B:201:PHE:HB3	1:B:231:ILE:HG13	1.40	1.01
1:A:201:PHE:HB3	1:A:231:ILE:HG13	1.40	1.01
1:B:287:ASP:HB3	1:B:306:PHE:HE2	1.06	1.00
3:I:22:CYS:HB2	3:I:96:CYS:SG	2.02	1.00
3:I:95:TYR:CE1	3:I:113:GLY:HA3	1.93	1.00
3:I:30:THR:HG22	3:I:74:ASN:CB	1.92	0.99
1:C:421:TYR:O	1:C:461:LEU:CD1	2.10	0.99
1:A:500:THR:HG21	2:D:99:ARG:NH2	1.77	0.99
1:B:296:LEU:HD12	1:B:608:VAL:CB	1.93	0.99
1:A:64:TRP:CE2	1:A:66:HIS:HE1	1.76	0.99
1:C:374:PHE:CD2	1:C:434:ILE:HG21	1.96	0.99
1:C:329:PHE:HE1	1:C:391:CYS:SG	1.87	0.98
1:B:287:ASP:CB	1:B:306:PHE:CE2	2.46	0.98
1:B:392:PHE:CD1	1:B:515:PHE:CB	2.47	0.98
1:A:393:THR:HG22	1:A:522:ALA:HA	1.42	0.98
1:C:421:TYR:O	1:C:461:LEU:HD12	1.63	0.97
3:I:22:CYS:CB	3:I:96:CYS:SG	2.52	0.97
1:A:287:ASP:CB	1:A:306:PHE:CE2	2.46	0.97
1:A:472:ILE:HD13	1:A:484:GLU:HA	1.44	0.97
1:A:296:LEU:HD12	1:A:608:VAL:CB	1.93	0.97
1:C:374:PHE:CD1	1:C:436:TRP:HE3	1.74	0.97
1:B:18:LEU:O	1:B:18:LEU:CD1	2.13	0.97
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.00	0.97
1:A:18:LEU:O	1:A:18:LEU:CD1	2.13	0.96
4:M:101:PHE:HZ	5:P:109:PHE:HE2	1.09	0.96
3:I:95:TYR:CD1	3:I:113:GLY:N	2.34	0.96
1:C:328:ARG:CB	1:C:543:PHE:CD1	2.49	0.96
1:A:147:LYS:CE	5:L:52:PHE:CD2	2.47	0.96
1:A:987:VAL:HG11	1:C:413:GLY:CA	1.96	0.96
1:B:64:TRP:CE2	1:B:66:HIS:HE1	1.76	0.95
1:A:296:LEU:HD12	1:A:608:VAL:HG11	1.43	0.95
1:A:393:THR:CG2	1:A:521:PRO:O	2.15	0.95
1:A:426:PRO:HB2	1:A:429:PHE:HD2	0.80	0.95
1:A:147:LYS:HE3	5:L:52:PHE:CD2	2.02	0.94
1:A:500:THR:HG21	2:D:99:ARG:HH22	1.28	0.94
1:C:248:TYR:HB3	5:P:101:THR:HG21	1.50	0.94
3:I:95:TYR:CE1	3:I:113:GLY:N	2.36	0.94
1:C:328:ARG:HB2	1:C:543:PHE:CD1	2.02	0.93
1:A:147:LYS:HE3	5:L:52:PHE:CZ	1.96	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:HIS:HD1	1:C:565:PHE:HE2	1.02	0.93
1:B:64:TRP:CH2	1:B:66:HIS:NE2	2.37	0.93
1:B:147:LYS:NZ	5:N:52:PHE:CG	2.29	0.93
1:A:64:TRP:CH2	1:A:66:HIS:NE2	2.37	0.93
2:D:37:ASN:HD22	2:D:92:GLN:HB2	1.34	0.93
1:A:66:HIS:ND1	1:A:264:ALA:CB	2.32	0.93
2:J:6:GLN:HB2	2:J:103:GLN:CB	1.99	0.93
1:B:66:HIS:ND1	1:B:264:ALA:CB	2.32	0.92
1:B:963:VAL:HG11	1:C:570:ALA:HB1	1.52	0.92
3:I:73:ASP:OD2	3:I:80:TYR:HE2	1.52	0.92
1:C:329:PHE:CE1	1:C:391:CYS:SG	2.63	0.92
3:I:73:ASP:OD2	3:I:80:TYR:CE2	2.23	0.92
2:F:37:ASN:HD22	2:F:92:GLN:HB2	1.34	0.92
1:A:41:LYS:HB3	1:B:564:GLN:N	1.84	0.91
1:A:987:VAL:HG11	1:C:413:GLY:HA3	1.52	0.91
1:C:853:GLN:OE1	1:C:959:LEU:HB3	1.71	0.91
4:M:101:PHE:CZ	5:P:109:PHE:HE2	1.88	0.90
3:I:94:TYR:CE2	3:I:116:VAL:HG11	2.05	0.90
1:A:853:GLN:OE1	1:A:959:LEU:HB3	1.72	0.90
1:B:853:GLN:OE1	1:B:959:LEU:HB3	1.72	0.90
1:B:426:PRO:HB2	1:B:429:PHE:HD2	0.75	0.90
1:A:987:VAL:HG21	1:C:413:GLY:HA2	1.54	0.89
1:A:382:VAL:HG11	1:A:387:LEU:CD2	2.02	0.89
1:A:118:LEU:CD2	1:A:120:VAL:HG23	2.03	0.89
1:A:426:PRO:CG	1:A:429:PHE:CD2	2.54	0.89
1:B:392:PHE:HE1	1:B:517:LEU:CD2	1.62	0.89
1:B:287:ASP:OD2	1:B:306:PHE:CD2	2.26	0.89
1:B:64:TRP:CH2	1:B:66:HIS:CE1	2.61	0.89
1:A:287:ASP:OD2	1:A:306:PHE:CD2	2.26	0.88
1:B:118:LEU:CD2	1:B:120:VAL:HG23	2.03	0.88
1:A:1039:ARG:NE	1:C:1031:GLU:OE2	2.06	0.88
1:B:421:TYR:O	1:B:461:LEU:CD1	2.20	0.88
1:A:64:TRP:CH2	1:A:66:HIS:CE1	2.61	0.88
1:B:299:THR:HG22	1:B:315:THR:HG1	1.28	0.88
3:E:49:ALA:HB1	3:E:70:ILE:HD11	1.56	0.87
1:A:426:PRO:HG2	1:A:429:PHE:CD2	2.10	0.87
1:A:452:LEU:HD21	1:A:492:LEU:HB3	1.55	0.87
1:C:1102:TRP:CZ2	1:C:1133:VAL:HG21	2.10	0.87
1:C:410:ILE:CD1	1:C:418:ILE:HG22	1.97	0.86
1:A:572:THR:HG21	1:C:855:PHE:HD2	1.40	0.86
1:B:64:TRP:CZ2	1:B:66:HIS:NE2	2.43	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:853:GLN:OE1	1:C:959:LEU:CB	2.24	0.86
1:A:147:LYS:NZ	5:L:52:PHE:CD2	2.43	0.86
1:B:392:PHE:CE1	1:B:517:LEU:HD23	2.10	0.86
3:G:49:ALA:HB1	3:G:70:ILE:HD11	1.56	0.86
1:A:853:GLN:OE1	1:A:959:LEU:CB	2.24	0.85
1:B:392:PHE:CD1	1:B:517:LEU:CD2	2.58	0.85
1:C:328:ARG:HB3	1:C:543:PHE:CD1	2.11	0.85
1:C:394:ASN:ND2	1:C:516:GLU:OE2	2.10	0.85
1:A:64:TRP:CZ2	1:A:66:HIS:NE2	2.43	0.85
1:A:41:LYS:O	1:B:563:GLN:HB3	1.77	0.85
1:C:299:THR:HG21	1:C:597:VAL:HB	1.56	0.85
1:A:534:VAL:HG11	1:A:539:VAL:CG1	2.07	0.85
1:C:246:ARG:NH1	5:P:28:TYR:HD1	1.75	0.85
1:A:1031:GLU:OE2	1:B:1039:ARG:NE	2.08	0.84
1:B:382:VAL:HG11	1:B:387:LEU:CD2	2.07	0.84
1:B:534:VAL:HG11	1:B:539:VAL:CG1	2.07	0.84
1:A:299:THR:CG2	1:A:315:THR:OG1	2.26	0.84
1:A:895:GLN:NE2	1:B:713:ALA:HB2	1.92	0.84
1:B:853:GLN:OE1	1:B:959:LEU:CB	2.25	0.84
1:A:392:PHE:CD1	1:A:517:LEU:HA	2.12	0.84
1:C:394:ASN:HB2	1:C:516:GLU:CG	2.08	0.84
1:B:299:THR:CG2	1:B:315:THR:OG1	2.25	0.83
1:C:327:VAL:HG12	1:C:542:ASN:HB3	1.57	0.83
1:C:328:ARG:CB	1:C:543:PHE:HD1	1.90	0.83
1:A:393:THR:CG2	1:A:522:ALA:HA	2.09	0.83
1:A:500:THR:HG22	3:E:99:PHE:CD2	2.14	0.83
1:A:296:LEU:CG	1:A:608:VAL:HG11	2.09	0.83
1:C:393:THR:CG2	1:C:522:ALA:HA	2.07	0.83
5:L:98:ALA:HB1	5:L:109:PHE:HB2	1.61	0.83
2:J:30:ASN:HA	2:J:95:LYS:HE2	1.60	0.83
2:D:30:ASN:HA	2:D:95:LYS:HE2	1.60	0.82
1:B:147:LYS:NZ	5:N:34:ALA:HB2	1.94	0.82
1:A:534:VAL:CB	1:A:539:VAL:HG11	2.10	0.82
1:A:287:ASP:CG	1:A:306:PHE:CE2	2.53	0.82
1:B:287:ASP:CG	1:B:306:PHE:CE2	2.53	0.82
3:E:39:GLN:NE2	3:E:43:LYS:O	2.13	0.82
5:N:98:ALA:HB1	5:N:109:PHE:HB2	1.61	0.82
1:B:296:LEU:HD12	1:B:608:VAL:HG11	1.43	0.82
1:B:296:LEU:CG	1:B:608:VAL:HG11	2.09	0.82
1:C:329:PHE:HE1	1:C:391:CYS:HG	1.17	0.82
1:A:411:ALA:HB3	1:A:414:GLN:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:NZ	5:L:52:PHE:CG	2.48	0.82
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.13	0.82
3:I:95:TYR:CE1	3:I:113:GLY:HA2	2.02	0.81
2:F:30:ASN:HA	2:F:95:LYS:HE2	1.60	0.81
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.13	0.81
1:A:472:ILE:HG21	1:A:488:CYS:HB3	1.62	0.81
1:B:534:VAL:CB	1:B:539:VAL:HG11	2.10	0.81
1:A:41:LYS:HB3	1:B:564:GLN:H	1.45	0.81
1:A:472:ILE:HD12	1:A:483:VAL:C	2.00	0.81
1:A:64:TRP:HZ2	1:A:66:HIS:HE1	1.24	0.81
1:A:230:PRO:CB	1:B:523:THR:CG2	2.52	0.81
1:A:358:ILE:HG23	1:A:361:CYS:SG	2.20	0.81
1:B:457:ARG:CD	1:B:461:LEU:HD21	2.10	0.81
1:A:392:PHE:HD1	1:A:517:LEU:N	1.79	0.81
4:K:44:ALA:HB1	5:N:112:TRP:HE1	1.45	0.81
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.13	0.80
1:C:278:LYS:HB2	1:C:306:PHE:HZ	1.44	0.80
1:C:457:ARG:HE	1:C:461:LEU:HD21	1.45	0.80
3:G:32:TYR:O	3:G:72:ARG:NH2	2.15	0.80
1:A:44:ARG:NH2	1:B:567:ARG:HD2	1.96	0.80
1:A:230:PRO:CG	1:B:523:THR:HG22	2.12	0.80
1:A:563:GLN:HG2	1:C:41:LYS:O	1.80	0.80
1:C:299:THR:CG2	1:C:597:VAL:HB	2.11	0.80
1:A:572:THR:HG21	1:C:855:PHE:CD2	2.17	0.79
1:B:118:LEU:HD23	1:B:120:VAL:HG23	1.63	0.79
2:J:38:TRP:N	2:J:51:ILE:O	2.15	0.79
3:G:39:GLN:NE2	3:G:43:LYS:O	2.13	0.79
2:F:38:TRP:N	2:F:51:ILE:O	2.15	0.79
1:A:118:LEU:HD23	1:A:120:VAL:HG23	1.63	0.79
3:E:32:TYR:O	3:E:72:ARG:NH2	2.15	0.79
3:I:95:TYR:CD1	3:I:111:GLY:O	2.36	0.79
1:A:248:TYR:HB3	5:L:101:THR:HG21	1.65	0.79
1:B:392:PHE:CG	1:B:515:PHE:HB3	2.16	0.79
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.62	0.79
3:I:94:TYR:CD2	3:I:116:VAL:HG11	2.18	0.78
2:D:38:TRP:N	2:D:51:ILE:O	2.15	0.78
1:A:457:ARG:CD	1:A:461:LEU:HD21	2.14	0.78
1:A:41:LYS:O	1:B:563:GLN:CB	2.30	0.78
1:A:324:GLU:OE2	1:A:534:VAL:HG22	1.83	0.78
1:A:392:PHE:CD1	1:A:517:LEU:CA	2.67	0.78
1:B:392:PHE:CD1	1:B:517:LEU:HG	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:PHE:CE1	1:B:517:LEU:CG	2.67	0.78
3:I:34:MET:CE	3:I:97:ALA:O	2.32	0.78
5:P:39:ARG:HB2	5:P:47:GLU:HB3	1.66	0.78
3:G:5:VAL:HB	3:G:23:ALA:HB3	1.66	0.77
2:J:20:LEU:HB2	2:J:76:LEU:HB3	1.66	0.77
5:N:39:ARG:HB2	5:N:47:GLU:HB3	1.66	0.77
1:A:472:ILE:CD1	1:A:484:GLU:HA	2.14	0.77
3:E:5:VAL:HB	3:E:23:ALA:HB3	1.66	0.77
1:A:500:THR:HG22	3:E:99:PHE:CE2	2.19	0.77
1:A:358:ILE:HG21	1:A:361:CYS:SG	2.23	0.77
1:C:299:THR:HG21	1:C:597:VAL:CB	2.13	0.77
1:A:457:ARG:HE	1:A:461:LEU:HD21	1.49	0.77
2:D:20:LEU:HB2	2:D:76:LEU:HB3	1.66	0.77
2:F:20:LEU:HB2	2:F:76:LEU:HB3	1.66	0.77
1:B:324:GLU:OE2	1:B:534:VAL:HG22	1.83	0.77
1:A:534:VAL:HB	1:A:539:VAL:HG11	1.67	0.77
4:M:101:PHE:CZ	5:P:109:PHE:CE2	2.65	0.77
2:F:89:TYR:N	2:F:105:THR:O	2.17	0.77
2:J:37:ASN:HD22	2:J:52:TYR:HA	1.49	0.77
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.17	0.76
1:B:457:ARG:HE	1:B:461:LEU:HD21	1.46	0.76
3:I:95:TYR:CD1	3:I:112:GLN:C	2.58	0.76
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.18	0.76
1:B:287:ASP:OD2	1:B:306:PHE:CE2	2.39	0.76
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.18	0.76
1:A:287:ASP:OD2	1:A:306:PHE:CE2	2.39	0.76
3:G:24:ALA:HB3	3:G:77:ASN:HB3	1.68	0.76
4:K:44:ALA:HB1	5:N:112:TRP:NE1	2.01	0.76
3:I:36:TRP:CH2	3:I:96:CYS:SG	2.79	0.76
4:K:38:GLN:HB2	4:K:48:LEU:HD11	1.68	0.76
1:B:534:VAL:HB	1:B:539:VAL:HG11	1.67	0.75
1:B:963:VAL:CG1	1:C:570:ALA:HB1	2.16	0.75
2:J:89:TYR:N	2:J:105:THR:O	2.17	0.75
1:A:534:VAL:CG1	1:A:539:VAL:HG11	2.16	0.75
1:B:534:VAL:CG1	1:B:539:VAL:HG11	2.16	0.75
3:E:24:ALA:HB3	3:E:77:ASN:HB3	1.67	0.75
1:B:550:GLY:HA2	1:B:589:PRO:HA	1.66	0.75
1:C:327:VAL:HG12	1:C:542:ASN:CB	2.17	0.75
3:I:38:ARG:NH2	3:I:83:MET:CE	2.49	0.75
1:B:392:PHE:HE1	1:B:517:LEU:HD21	0.94	0.75
1:C:48:LEU:HD11	1:C:306:PHE:CD2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:963:VAL:HG11	1:C:570:ALA:CB	2.15	0.75
5:N:13:LYS:H	5:N:119:THR:HB	1.52	0.75
1:B:855:PHE:HD2	1:C:572:THR:HG21	1.52	0.75
5:L:39:ARG:HB2	5:L:47:GLU:HB3	1.66	0.75
1:C:249:LEU:HD13	5:P:110:ASP:OD1	1.87	0.75
3:G:20:LEU:N	3:G:81:LEU:O	2.20	0.75
3:I:71:SER:OG	3:I:80:TYR:CB	2.31	0.75
3:E:20:LEU:N	3:E:81:LEU:O	2.20	0.74
1:C:457:ARG:CD	1:C:461:LEU:HD21	2.17	0.74
2:F:5:THR:N	2:F:23:ARG:O	2.18	0.74
1:B:382:VAL:HG11	1:B:387:LEU:HD21	1.68	0.74
3:I:95:TYR:HD1	3:I:111:GLY:O	1.69	0.74
5:L:13:LYS:H	5:L:119:THR:HB	1.52	0.74
1:A:550:GLY:HA2	1:A:589:PRO:HA	1.67	0.74
1:B:457:ARG:NH1	1:B:461:LEU:HD23	2.03	0.74
1:B:147:LYS:HZ1	5:N:34:ALA:HB2	1.52	0.73
1:C:328:ARG:HB2	1:C:543:PHE:CE1	2.23	0.73
1:B:147:LYS:NZ	5:N:34:ALA:CB	2.51	0.73
1:C:656:VAL:HG23	1:C:695:TYR:HB3	1.69	0.73
2:D:98:PRO:HG3	3:E:61:PRO:HB3	1.70	0.73
5:P:13:LYS:H	5:P:119:THR:HB	1.52	0.73
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.22	0.73
3:G:22:CYS:HB3	3:G:79:LEU:HB3	1.70	0.73
3:I:34:MET:HE2	3:I:97:ALA:O	1.88	0.73
2:J:102:GLY:C	2:J:104:GLY:H	1.90	0.73
1:A:715:PRO:HD3	1:C:894:LEU:HD13	1.71	0.73
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.71	0.73
2:D:89:TYR:N	2:D:105:THR:O	2.17	0.73
1:B:118:LEU:HD21	1:B:120:VAL:HG23	1.71	0.73
2:J:5:THR:N	2:J:23:ARG:O	2.18	0.73
2:D:91:CYS:O	2:D:102:GLY:N	2.22	0.73
1:A:457:ARG:NH1	1:A:461:LEU:HD23	2.03	0.72
1:C:299:THR:HG23	1:C:597:VAL:HG21	1.71	0.72
1:A:382:VAL:HG11	1:A:387:LEU:HD21	1.70	0.72
1:A:392:PHE:CG	1:A:515:PHE:HB3	2.24	0.72
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.22	0.72
3:E:36:TRP:HB2	3:E:49:ALA:HB3	1.71	0.72
1:A:299:THR:HG21	1:A:597:VAL:HB	1.70	0.72
1:B:296:LEU:HG	1:B:608:VAL:HG11	1.71	0.72
2:D:95:LYS:NZ	2:D:96:GLU:OE2	2.20	0.72
3:G:36:TRP:HB2	3:G:49:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:TYR:HB3	5:N:101:THR:HG21	1.71	0.72
3:E:22:CYS:HB3	3:E:79:LEU:HB3	1.70	0.72
3:I:3:LYS:HB2	3:I:25:SER:OG	1.88	0.72
1:A:534:VAL:HG11	1:A:539:VAL:HG11	1.71	0.72
1:B:299:THR:HG21	1:B:597:VAL:HB	1.70	0.72
2:F:91:CYS:O	2:F:102:GLY:N	2.22	0.72
1:B:985:ASP:N	1:C:383:SER:OG	2.22	0.72
2:F:95:LYS:NZ	2:F:96:GLU:OE2	2.19	0.72
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.22	0.72
3:I:30:THR:HG23	3:I:74:ASN:HB3	1.72	0.72
4:K:38:GLN:OE1	4:K:48:LEU:HD21	1.89	0.72
1:A:963:VAL:HG11	1:B:570:ALA:HB1	1.70	0.72
1:B:299:THR:CG2	1:B:597:VAL:HG21	2.19	0.72
1:B:143:VAL:HG22	1:B:154:GLU:HG2	1.72	0.71
1:B:296:LEU:HD11	1:B:608:VAL:CG1	1.92	0.71
1:B:64:TRP:HZ2	1:B:66:HIS:HE1	1.24	0.71
1:A:855:PHE:HD2	1:B:572:THR:HG21	1.55	0.71
1:C:143:VAL:HG22	1:C:154:GLU:HG2	1.72	0.71
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.71	0.71
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.72	0.71
1:B:147:LYS:HZ1	5:N:34:ALA:CB	2.03	0.71
2:D:5:THR:N	2:D:23:ARG:O	2.18	0.71
1:A:48:LEU:HD12	1:A:304:LYS:O	1.87	0.71
1:B:382:VAL:HG11	1:B:387:LEU:HD23	1.73	0.71
2:D:40:GLN:HE21	2:D:87:ALA:HB3	1.55	0.71
1:B:276:LEU:CD1	1:B:306:PHE:CZ	2.72	0.71
1:B:457:ARG:CD	1:B:461:LEU:CD2	2.67	0.71
1:C:100:ILE:HG21	1:C:263:ALA:HB2	1.72	0.71
1:C:330:PRO:HG2	1:C:522:ALA:O	1.90	0.71
1:C:410:ILE:CG2	1:C:425:LEU:CD1	2.61	0.71
1:A:296:LEU:HG	1:A:608:VAL:HG11	1.71	0.71
3:I:38:ARG:NH2	3:I:83:MET:HE2	2.06	0.71
4:K:28:ASN:OD1	4:K:29:ILE:N	2.24	0.71
5:L:68:ARG:NH1	5:L:86:SER:O	2.24	0.71
2:J:95:LYS:NZ	2:J:96:GLU:OE2	2.19	0.71
1:A:143:VAL:HG22	1:A:154:GLU:HG2	1.72	0.71
1:A:457:ARG:CD	1:A:461:LEU:CD2	2.69	0.71
1:B:726:ILE:HD13	1:B:945:LEU:HD23	1.73	0.71
1:C:374:PHE:HD1	1:C:436:TRP:CE3	1.85	0.71
3:E:19:ARG:HG2	3:E:82:GLN:HG2	1.73	0.71
1:A:118:LEU:HD21	1:A:120:VAL:HG23	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.71	0.70
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.73	0.70
5:P:68:ARG:NH1	5:P:86:SER:O	2.24	0.70
1:A:392:PHE:HD1	1:A:517:LEU:CA	2.04	0.70
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.72	0.70
1:A:472:ILE:CD1	1:A:483:VAL:C	2.60	0.70
2:J:40:GLN:HE21	2:J:87:ALA:HB3	1.56	0.70
1:A:296:LEU:HD12	1:A:608:VAL:HG13	1.19	0.70
1:B:102:ARG:NH1	1:B:154:GLU:OE2	2.25	0.70
1:B:121:ASN:HA	1:B:126:VAL:HG22	1.74	0.70
1:C:534:VAL:HG11	1:C:537:LYS:HE2	1.73	0.70
1:A:299:THR:CG2	1:A:597:VAL:HG21	2.19	0.70
2:F:4:LEU:HD23	2:F:93:GLN:HG3	1.74	0.70
1:B:276:LEU:HD13	1:B:306:PHE:CE1	2.21	0.70
1:B:815:ARG:HD2	1:B:823:PHE:HE2	1.57	0.70
1:C:73:THR:HG23	1:C:74:ASN:H	1.57	0.70
1:A:276:LEU:CD1	1:A:306:PHE:CZ	2.72	0.70
1:A:121:ASN:HA	1:A:126:VAL:HG22	1.73	0.70
3:E:52:SER:OG	3:E:55:GLY:O	2.09	0.70
2:F:40:GLN:HE21	2:F:87:ALA:HB3	1.55	0.70
1:B:392:PHE:CD1	1:B:517:LEU:HD23	2.24	0.70
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.72	0.70
1:C:299:THR:CG2	1:C:597:VAL:CB	2.69	0.70
1:C:327:VAL:HA	1:C:542:ASN:HB3	1.72	0.70
1:A:815:ARG:HD2	1:A:823:PHE:HE2	1.57	0.70
3:G:19:ARG:HG2	3:G:82:GLN:HG2	1.73	0.70
1:B:34:ARG:NH1	1:B:221:SER:OG	2.25	0.69
5:N:68:ARG:NH1	5:N:86:SER:O	2.24	0.69
1:A:73:THR:HG23	1:A:74:ASN:H	1.57	0.69
1:C:815:ARG:HD2	1:C:823:PHE:HE2	1.57	0.69
1:B:534:VAL:HG11	1:B:539:VAL:HG11	1.71	0.69
5:L:39:ARG:N	5:L:47:GLU:O	2.25	0.69
5:P:39:ARG:N	5:P:47:GLU:O	2.25	0.69
1:B:180:GLU:HG3	1:B:181:GLY:H	1.58	0.69
1:C:457:ARG:NH1	1:C:461:LEU:HD23	2.06	0.69
4:M:28:ASN:OD1	4:M:29:ILE:N	2.24	0.69
1:A:726:ILE:HD13	1:A:945:LEU:HD23	1.73	0.69
1:B:118:LEU:HD21	1:B:120:VAL:CG2	2.22	0.69
1:C:34:ARG:NH1	1:C:221:SER:OG	2.25	0.69
3:E:14:PRO:HB3	3:E:87:ARG:HA	1.74	0.69
5:N:21:VAL:HB	5:N:82:MET:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:39:ARG:N	5:N:47:GLU:O	2.25	0.69
1:A:118:LEU:HD21	1:A:120:VAL:CG2	2.22	0.69
1:B:392:PHE:CZ	1:B:517:LEU:HD21	2.22	0.69
3:G:34:MET:HB3	3:G:79:LEU:HD22	1.74	0.69
5:L:21:VAL:HB	5:L:82:MET:HB3	1.75	0.69
5:P:21:VAL:HB	5:P:82:MET:HB3	1.75	0.69
1:A:34:ARG:NH1	1:A:221:SER:OG	2.25	0.69
1:A:180:GLU:HG3	1:A:181:GLY:H	1.58	0.69
1:A:299:THR:HG22	1:A:315:THR:HG1	1.58	0.69
1:C:246:ARG:HH11	5:P:28:TYR:HD1	1.40	0.69
2:D:35:PHE:CE1	3:E:104:GLY:HA2	2.28	0.69
1:A:472:ILE:CD1	1:A:484:GLU:N	2.56	0.69
1:C:299:THR:HG21	1:C:597:VAL:CG1	2.23	0.69
1:C:394:ASN:N	1:C:516:GLU:OE1	2.26	0.69
2:F:39:PHE:HB2	2:F:90:PHE:HB2	1.76	0.69
3:G:14:PRO:HB3	3:G:87:ARG:HA	1.75	0.69
2:J:5:THR:O	2:J:23:ARG:N	2.21	0.69
1:B:73:THR:HG23	1:B:74:ASN:H	1.57	0.68
1:A:102:ARG:NH1	1:A:154:GLU:OE2	2.25	0.68
1:C:536:ASN:HA	1:C:551:VAL:CG1	2.23	0.68
1:A:500:THR:CG2	2:D:99:ARG:NH2	2.56	0.68
3:E:34:MET:HB3	3:E:79:LEU:HD22	1.74	0.68
2:J:4:LEU:HD23	2:J:93:GLN:HG3	1.74	0.68
4:H:28:ASN:OD1	4:H:29:ILE:N	2.24	0.68
2:J:39:PHE:HB2	2:J:90:PHE:HB2	1.75	0.68
5:N:53:ASP:HB2	5:N:60:MET:HG2	1.76	0.68
1:A:276:LEU:HD12	1:A:306:PHE:CE1	2.25	0.68
1:C:180:GLU:HG3	1:C:181:GLY:H	1.58	0.68
2:D:39:PHE:HB2	2:D:90:PHE:HB2	1.76	0.68
1:B:296:LEU:HB2	1:B:608:VAL:HG21	1.76	0.68
1:A:296:LEU:HD12	1:A:608:VAL:HG22	1.75	0.68
5:P:53:ASP:HB2	5:P:60:MET:HG2	1.76	0.68
2:D:4:LEU:HD23	2:D:93:GLN:HG3	1.74	0.67
1:A:276:LEU:HD13	1:A:306:PHE:CE1	2.21	0.67
1:B:676:THR:H	1:B:690:GLN:HG2	1.60	0.67
2:D:5:THR:O	2:D:23:ARG:N	2.21	0.67
1:B:320:VAL:HB	1:B:590:CYS:HB2	1.77	0.67
5:L:13:LYS:HE3	5:L:17:ALA:HB1	1.77	0.67
1:A:472:ILE:CD1	1:A:484:GLU:CA	2.73	0.67
5:N:91:ASP:O	5:N:95:TYR:OH	2.12	0.67
1:B:452:LEU:HD21	1:B:492:LEU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LEU:HD12	1:B:608:VAL:HG22	1.75	0.67
5:P:91:ASP:O	5:P:95:TYR:OH	2.12	0.67
1:A:565:PHE:HB2	1:C:42:VAL:HG22	1.77	0.67
1:B:276:LEU:HD12	1:B:306:PHE:CE1	2.25	0.67
1:B:392:PHE:HD1	1:B:517:LEU:HG	1.58	0.67
1:A:320:VAL:HB	1:A:590:CYS:HB2	1.77	0.67
1:C:102:ARG:NH1	1:C:154:GLU:OE2	2.25	0.67
4:K:48:LEU:HD11	4:K:87:TYR:CD1	2.30	0.67
1:A:676:THR:H	1:A:690:GLN:HG2	1.60	0.66
2:D:56:ASN:OD1	2:D:57:GLN:N	2.27	0.66
2:J:103:GLN:C	2:J:104:GLY:O	2.33	0.66
1:B:116:SER:N	1:B:131:CYS:O	2.29	0.66
5:P:13:LYS:HE3	5:P:17:ALA:HB1	1.77	0.66
1:A:42:VAL:HG11	1:B:567:ARG:HG3	1.77	0.66
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.76	0.66
1:A:299:THR:HG21	1:A:597:VAL:CB	2.26	0.66
1:B:48:LEU:HD12	1:B:304:LYS:O	1.87	0.66
1:B:299:THR:HG21	1:B:597:VAL:CB	2.26	0.66
1:C:116:SER:N	1:C:131:CYS:O	2.29	0.66
3:I:87:ARG:H	3:I:90:ASP:HB2	1.60	0.66
3:G:22:CYS:N	3:G:79:LEU:O	2.27	0.66
1:A:296:LEU:HD11	1:A:608:VAL:CG1	1.92	0.66
1:C:546:LEU:HD21	1:C:573:THR:HG21	1.77	0.66
1:A:100:ILE:HG21	1:A:263:ALA:HB2	1.77	0.66
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.29	0.66
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.29	0.66
1:B:100:ILE:HG21	1:B:263:ALA:HB2	1.77	0.66
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.77	0.66
3:E:22:CYS:N	3:E:79:LEU:O	2.27	0.66
1:A:713:ALA:HB2	1:C:895:GLN:NE2	2.11	0.66
1:C:676:THR:H	1:C:690:GLN:HG2	1.60	0.66
2:J:56:ASN:OD1	2:J:57:GLN:N	2.27	0.66
5:L:53:ASP:HB2	5:L:60:MET:HG2	1.76	0.65
4:H:86:ASP:HB2	4:H:106:LYS:HG2	1.78	0.65
2:J:35:PHE:CE2	2:J:95:LYS:HB2	2.32	0.65
1:C:326:ILE:HA	1:C:531:THR:OG1	1.97	0.65
1:C:457:ARG:CD	1:C:461:LEU:CD2	2.73	0.65
4:K:46:LYS:HA	5:N:112:TRP:CH2	2.31	0.65
1:A:392:PHE:HD1	1:A:517:LEU:H	1.43	0.65
2:J:102:GLY:O	2:J:104:GLY:N	2.27	0.65
5:N:13:LYS:HE3	5:N:17:ALA:HB1	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:HG22	1:A:522:ALA:CA	2.21	0.65
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.30	0.65
1:C:68:ILE:HG23	1:C:259:THR:HB	1.78	0.65
1:C:327:VAL:CG1	1:C:542:ASN:HB3	2.25	0.65
1:C:519:HIS:ND1	1:C:565:PHE:HE2	1.85	0.65
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.29	0.65
3:G:15:GLY:N	3:G:86:LEU:O	2.29	0.65
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.30	0.65
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.30	0.65
2:F:35:PHE:CE2	2:F:95:LYS:HB2	2.32	0.65
1:A:116:SER:N	1:A:131:CYS:O	2.29	0.65
1:C:472:ILE:HG21	1:C:488:CYS:HB3	1.79	0.65
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.30	0.65
4:K:19:THR:HG22	4:K:76:ILE:H	1.61	0.65
5:L:91:ASP:O	5:L:95:TYR:OH	2.12	0.65
4:M:19:THR:HG22	4:M:76:ILE:H	1.61	0.65
4:M:39:GLN:NE2	4:M:43:THR:O	2.30	0.65
1:C:121:ASN:HA	1:C:126:VAL:HA	1.78	0.65
2:D:35:PHE:CE2	2:D:95:LYS:HB2	2.32	0.65
2:F:5:THR:O	2:F:23:ARG:N	2.21	0.65
2:F:56:ASN:OD1	2:F:57:GLN:N	2.27	0.65
4:M:86:ASP:HB2	4:M:106:LYS:HG2	1.79	0.65
1:A:546:LEU:HD21	1:A:573:THR:HG21	1.77	0.65
3:E:15:GLY:N	3:E:86:LEU:O	2.29	0.65
4:K:86:ASP:HB2	4:K:106:LYS:HG2	1.79	0.65
2:J:20:LEU:HD12	2:J:76:LEU:HD23	1.80	0.64
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.30	0.64
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.79	0.64
2:F:70:SER:N	2:F:73:ASP:O	2.29	0.64
1:B:392:PHE:CD1	1:B:517:LEU:CG	2.80	0.64
3:I:38:ARG:NH2	3:I:83:MET:HE1	2.12	0.64
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.61	0.64
3:G:37:VAL:O	3:G:95:TYR:N	2.29	0.64
3:I:38:ARG:HH22	3:I:83:MET:HE2	1.62	0.64
1:A:336:CYS:SG	1:A:358:ILE:HG21	2.38	0.64
2:D:20:LEU:HD12	2:D:76:LEU:HD23	1.80	0.64
3:E:6:GLU:OE1	3:E:114:THR:OG1	2.13	0.64
4:M:44:ALA:HB1	5:P:112:TRP:HE1	1.63	0.64
1:A:987:VAL:HG11	1:C:413:GLY:HA2	1.75	0.64
4:H:62:ARG:O	4:H:77:THR:OG1	2.16	0.64
1:A:299:THR:HG23	1:A:597:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.29	0.64
3:E:37:VAL:O	3:E:95:TYR:N	2.30	0.64
1:B:299:THR:HG23	1:B:597:VAL:HG21	1.78	0.64
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.80	0.64
4:H:39:GLN:NE2	4:H:43:THR:O	2.30	0.64
3:G:6:GLU:OE1	3:G:114:THR:OG1	2.13	0.64
4:H:19:THR:HG22	4:H:76:ILE:H	1.61	0.64
2:F:39:PHE:N	2:F:90:PHE:O	2.30	0.63
2:J:39:PHE:N	2:J:90:PHE:O	2.30	0.63
1:A:42:VAL:HA	1:B:565:PHE:O	1.98	0.63
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.80	0.63
2:D:70:SER:N	2:D:73:ASP:O	2.29	0.63
4:M:99:VAL:HG13	5:P:107:TYR:CE1	2.32	0.63
1:A:44:ARG:HH21	1:B:567:ARG:HD2	1.63	0.63
1:A:326:ILE:HD11	1:A:534:VAL:HG23	1.79	0.63
1:A:891:GLY:HA2	1:B:1045:LYS:NZ	2.14	0.63
1:A:336:CYS:HB3	1:A:358:ILE:HG21	1.80	0.63
1:A:426:PRO:HB3	1:A:429:PHE:CD2	2.28	0.63
4:K:39:GLN:NE2	4:K:43:THR:O	2.30	0.63
1:B:326:ILE:HD11	1:B:534:VAL:HG23	1.79	0.63
1:C:329:PHE:CD1	1:C:525:CYS:SG	2.92	0.63
1:C:410:ILE:HG22	1:C:425:LEU:CD1	2.16	0.63
3:E:20:LEU:HB2	3:E:81:LEU:HB3	1.80	0.63
5:L:92:THR:HA	5:L:118:VAL:HG23	1.80	0.63
5:N:92:THR:HA	5:N:118:VAL:HG23	1.80	0.63
2:J:70:SER:N	2:J:73:ASP:O	2.29	0.63
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.30	0.63
4:K:60:PRO:HB2	4:K:62:ARG:HG2	1.81	0.63
5:P:34:ALA:HB1	5:P:52:PHE:HB3	1.81	0.63
1:A:987:VAL:CG2	1:C:413:GLY:HA2	2.27	0.63
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.29	0.63
3:G:20:LEU:HB2	3:G:81:LEU:HB3	1.80	0.63
2:J:6:GLN:HG3	2:J:103:GLN:H	1.64	0.63
1:A:147:LYS:CE	5:L:52:PHE:CE1	2.69	0.62
4:H:44:ALA:HB1	5:L:112:TRP:NE1	2.14	0.62
2:J:37:ASN:HB2	2:J:92:GLN:H	1.64	0.62
1:C:140:PHE:HB2	1:C:242:LEU:HB2	1.82	0.62
1:C:276:LEU:CD1	1:C:306:PHE:CE1	2.82	0.62
4:H:44:ALA:HB1	5:L:112:TRP:HE1	1.63	0.62
1:B:426:PRO:HB3	1:B:429:PHE:CD2	2.30	0.62
3:I:22:CYS:HG	3:I:96:CYS:CB	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:62:ARG:O	4:K:77:THR:OG1	2.16	0.62
4:M:44:ALA:HB1	5:P:112:TRP:NE1	2.14	0.62
1:A:855:PHE:CD2	1:B:572:THR:HG21	2.35	0.62
1:C:645:THR:OG1	1:C:648:GLY:O	2.13	0.62
2:F:4:LEU:HA	2:F:24:ALA:HA	1.81	0.62
3:G:47:TRP:CZ2	3:G:50:GLU:HB2	2.35	0.62
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.80	0.62
2:J:4:LEU:HA	2:J:24:ALA:HA	1.81	0.62
1:C:330:PRO:HD3	1:C:525:CYS:SG	2.39	0.62
2:D:4:LEU:HA	2:D:24:ALA:HA	1.82	0.62
5:N:34:ALA:HB1	5:N:52:PHE:HB3	1.81	0.62
5:N:68:ARG:NH2	5:N:91:ASP:OD2	2.33	0.62
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.82	0.62
1:C:1115:ILE:HG22	1:C:1137:VAL:HG13	1.82	0.62
5:L:34:ALA:HB1	5:L:52:PHE:HB3	1.81	0.62
5:P:92:THR:HA	5:P:118:VAL:HG23	1.80	0.62
2:D:10:LEU:O	2:D:108:GLU:N	2.32	0.62
5:P:68:ARG:NH2	5:P:91:ASP:OD2	2.33	0.62
1:C:148:ASN:C	1:C:150:LYS:H	2.02	0.62
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.82	0.62
2:F:20:LEU:HD12	2:F:76:LEU:HD23	1.80	0.62
1:A:894:LEU:HD13	1:B:715:PRO:HD3	1.82	0.61
1:B:392:PHE:HE1	1:B:517:LEU:CG	2.08	0.61
3:E:47:TRP:CZ2	3:E:50:GLU:HB2	2.35	0.61
4:M:17:LYS:HG3	4:M:77:THR:HG22	1.83	0.61
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.82	0.61
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.82	0.61
1:C:394:ASN:N	1:C:516:GLU:CD	2.53	0.61
1:A:41:LYS:O	1:B:563:GLN:HG2	1.99	0.61
1:A:393:THR:HG22	1:A:521:PRO:C	2.20	0.61
1:A:699:LEU:HD21	1:C:869:MET:HB3	1.82	0.61
1:A:1039:ARG:HB3	1:C:1031:GLU:OE2	2.00	0.61
3:E:30:THR:O	3:E:53:SER:OG	2.10	0.61
5:L:68:ARG:NH2	5:L:91:ASP:OD2	2.33	0.61
1:C:329:PHE:CD1	1:C:525:CYS:HB3	2.36	0.61
3:I:34:MET:HE3	3:I:97:ALA:O	2.01	0.61
4:K:17:LYS:HG3	4:K:77:THR:HG22	1.83	0.61
3:I:94:TYR:CE2	3:I:116:VAL:CG1	2.81	0.61
3:I:95:TYR:CZ	3:I:113:GLY:HA3	2.34	0.61
4:H:38:GLN:O	4:H:46:LYS:N	2.25	0.61
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.82	0.61
2:J:37:ASN:ND2	2:J:52:TYR:HA	2.15	0.61
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.82	0.61
4:M:62:ARG:O	4:M:77:THR:OG1	2.16	0.61
1:B:426:PRO:CB	1:B:429:PHE:CE2	2.83	0.61
1:B:853:GLN:OE1	1:B:959:LEU:HD13	2.01	0.61
1:C:327:VAL:HA	1:C:542:ASN:O	2.01	0.61
2:F:6:GLN:NE2	2:F:91:CYS:SG	2.70	0.61
4:K:99:VAL:HB	5:N:48:TRP:CG	2.36	0.61
1:A:382:VAL:HG11	1:A:387:LEU:HD23	1.83	0.60
1:B:140:PHE:HB2	1:B:242:LEU:HB2	1.81	0.60
1:B:299:THR:CG2	1:B:597:VAL:CG2	2.79	0.60
1:A:147:LYS:HE2	5:L:52:PHE:CD1	2.35	0.60
1:A:299:THR:CG2	1:A:597:VAL:CG2	2.79	0.60
2:F:10:LEU:O	2:F:108:GLU:N	2.32	0.60
4:H:99:VAL:HB	5:L:48:TRP:CG	2.36	0.60
3:I:72:ARG:HD3	3:I:74:ASN:HD21	1.65	0.60
5:P:110:ASP:HB3	5:P:111:PRO:HD2	1.84	0.60
1:B:645:THR:OG1	1:B:648:GLY:O	2.13	0.60
1:C:326:ILE:O	1:C:326:ILE:HG22	2.01	0.60
2:D:40:GLN:O	2:D:48:ARG:N	2.34	0.60
1:A:140:PHE:HB2	1:A:242:LEU:HB2	1.81	0.60
1:C:410:ILE:HD12	1:C:418:ILE:HG21	1.82	0.60
4:M:99:VAL:HB	5:P:48:TRP:CG	2.36	0.60
1:A:853:GLN:OE1	1:A:959:LEU:HD13	2.01	0.60
4:K:36:TRP:CH2	4:K:89:CYS:HB3	2.37	0.60
1:A:326:ILE:HD12	1:A:532:ASN:O	2.02	0.60
1:C:256:SER:HG	5:P:28:TYR:HE1	1.48	0.60
1:C:351:TYR:HE2	1:C:452:LEU:HB3	1.65	0.60
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.29	0.60
2:D:6:GLN:NE2	2:D:91:CYS:SG	2.70	0.60
3:I:30:THR:HG22	3:I:74:ASN:CG	2.21	0.60
4:H:36:TRP:CH2	4:H:89:CYS:HB3	2.37	0.60
3:I:100:ARG:HB2	3:I:108:ASP:HB2	1.84	0.60
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.82	0.60
1:C:421:TYR:O	1:C:461:LEU:CG	2.49	0.60
1:C:853:GLN:OE1	1:C:959:LEU:HD13	2.02	0.60
2:J:102:GLY:C	2:J:104:GLY:N	2.55	0.60
1:A:853:GLN:OE1	1:A:959:LEU:CD1	2.50	0.59
1:B:853:GLN:OE1	1:B:959:LEU:CD1	2.50	0.59
4:H:37:TYR:HD1	4:H:47:LEU:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:92:THR:HB	5:N:120:VAL:HG13	1.84	0.59
1:A:472:ILE:CG2	1:A:488:CYS:HB3	2.30	0.59
2:D:39:PHE:N	2:D:90:PHE:O	2.30	0.59
3:I:95:TYR:CG	3:I:113:GLY:HA2	2.34	0.59
5:P:92:THR:HB	5:P:120:VAL:HG13	1.84	0.59
1:B:299:THR:HG21	1:B:597:VAL:CG2	2.32	0.59
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.35	0.59
4:H:17:LYS:HG3	4:H:77:THR:HG22	1.83	0.59
2:J:10:LEU:O	2:J:108:GLU:N	2.32	0.59
1:A:66:HIS:ND1	1:A:264:ALA:HB1	2.16	0.59
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.35	0.59
2:F:50:LEU:HD11	2:F:89:TYR:HD1	1.67	0.59
4:M:36:TRP:CH2	4:M:89:CYS:HB3	2.37	0.59
1:A:500:THR:CG2	3:E:99:PHE:CD2	2.85	0.59
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.35	0.59
5:L:92:THR:HB	5:L:120:VAL:HG13	1.84	0.59
1:A:41:LYS:O	1:B:563:GLN:CG	2.51	0.59
1:A:336:CYS:HB3	1:A:358:ILE:HD13	1.85	0.59
1:A:1089:PHE:CE2	1:C:914:ASN:HA	2.37	0.59
1:A:472:ILE:HD11	1:A:484:GLU:N	2.18	0.59
1:B:326:ILE:HD12	1:B:532:ASN:O	2.02	0.59
1:C:328:ARG:HB2	1:C:543:PHE:HD1	1.55	0.59
3:E:36:TRP:CD1	3:E:81:LEU:HD13	2.38	0.59
4:H:99:VAL:HB	5:L:48:TRP:CD2	2.38	0.59
1:A:472:ILE:HD12	1:A:483:VAL:O	2.03	0.59
2:J:50:LEU:HD11	2:J:89:TYR:HD1	1.67	0.59
4:K:99:VAL:HB	5:N:48:TRP:CD2	2.38	0.59
1:B:410:ILE:HD11	1:B:418:ILE:HG21	1.85	0.59
3:G:27:PHE:HB2	3:G:32:TYR:HE2	1.67	0.59
1:B:66:HIS:ND1	1:B:264:ALA:HB1	2.16	0.58
2:F:68:SER:H	2:F:75:SER:HG	1.51	0.58
1:A:299:THR:HG21	1:A:597:VAL:CG2	2.32	0.58
2:D:68:SER:H	2:D:75:SER:HG	1.50	0.58
3:E:27:PHE:HB2	3:E:32:TYR:HE2	1.67	0.58
5:L:39:ARG:NH2	5:L:91:ASP:HA	2.18	0.58
4:M:37:TYR:HD1	4:M:47:LEU:HA	1.67	0.58
1:A:540:ASN:OD1	1:A:541:PHE:N	2.37	0.58
2:F:30:ASN:HB2	2:F:35:PHE:HB2	1.86	0.58
5:N:39:ARG:NH2	5:N:91:ASP:HA	2.18	0.58
2:D:50:LEU:HD11	2:D:89:TYR:HD1	1.67	0.58
3:E:4:LEU:HB2	3:E:111:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:87:LEU:HD13	5:L:120:VAL:HA	1.85	0.58
5:P:39:ARG:NH2	5:P:91:ASP:HA	2.18	0.58
1:B:540:ASN:OD1	1:B:541:PHE:N	2.37	0.58
1:C:328:ARG:HB3	1:C:543:PHE:HD1	1.56	0.58
3:G:36:TRP:CD1	3:G:81:LEU:HD13	2.38	0.58
1:A:891:GLY:HA2	1:B:1045:LYS:HZ1	1.67	0.58
4:M:99:VAL:HB	5:P:48:TRP:CD2	2.38	0.58
1:A:392:PHE:CD1	1:A:515:PHE:CB	2.82	0.58
1:C:326:ILE:HD12	1:C:532:ASN:O	2.04	0.58
2:D:30:ASN:HB2	2:D:35:PHE:HB2	1.86	0.58
1:B:392:PHE:CE1	1:B:515:PHE:CB	2.85	0.58
1:C:559:PHE:HB2	1:C:563:GLN:CG	2.34	0.58
1:C:853:GLN:OE1	1:C:959:LEU:CD1	2.51	0.58
2:D:20:LEU:HD22	2:D:105:THR:HG21	1.86	0.58
3:G:19:ARG:HA	3:G:82:GLN:HA	1.86	0.58
1:A:199:GLY:HA3	1:B:521:PRO:HB3	1.86	0.57
1:C:540:ASN:OD1	1:C:541:PHE:N	2.37	0.57
3:I:39:GLN:HB2	3:I:45:LEU:HD23	1.85	0.57
5:L:36:HIS:HA	5:L:51:GLY:HA2	1.86	0.57
5:L:89:SER:OG	5:L:90:GLU:OE1	2.22	0.57
2:J:20:LEU:HD22	2:J:105:THR:HG21	1.86	0.57
1:B:147:LYS:HZ2	5:N:34:ALA:HB2	1.69	0.57
2:D:38:TRP:CD2	2:D:76:LEU:HB2	2.39	0.57
2:F:38:TRP:CD2	2:F:76:LEU:HB2	2.39	0.57
5:P:87:LEU:HD13	5:P:120:VAL:HA	1.85	0.57
1:A:393:THR:HG21	1:A:521:PRO:O	2.04	0.57
1:B:84:LEU:N	1:B:238:PHE:O	2.29	0.57
1:B:115:GLN:HB2	1:B:233:ILE:HD12	1.86	0.57
1:B:392:PHE:CE1	1:B:517:LEU:HG	2.38	0.57
1:C:709:ASN:N	1:C:709:ASN:OD1	2.37	0.57
3:I:34:MET:HG2	3:I:98:ARG:HA	1.85	0.57
5:P:98:ALA:HB1	5:P:109:PHE:HB3	1.87	0.57
1:A:41:LYS:HB3	1:B:563:GLN:HA	1.85	0.57
1:C:231:ILE:HG22	1:C:233:ILE:HG22	1.86	0.57
2:J:30:ASN:HB2	2:J:35:PHE:HB2	1.86	0.57
2:J:40:GLN:O	2:J:48:ARG:N	2.34	0.57
1:C:115:GLN:HB2	1:C:233:ILE:HD12	1.86	0.57
1:C:246:ARG:NH1	5:P:28:TYR:CD1	2.63	0.57
1:C:327:VAL:CB	1:C:542:ASN:HB3	2.34	0.57
2:D:39:PHE:O	2:D:90:PHE:N	2.21	0.57
2:F:37:ASN:HB2	2:F:92:GLN:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:LEU:HB2	3:G:111:GLY:HA2	1.85	0.57
5:N:36:HIS:HA	5:N:51:GLY:HA2	1.86	0.57
2:J:68:SER:H	2:J:75:SER:HG	1.52	0.57
1:B:985:ASP:OD1	1:C:383:SER:HB3	2.04	0.57
1:C:521:PRO:HD3	1:C:564:GLN:HB2	1.87	0.57
2:F:20:LEU:HD22	2:F:105:THR:HG21	1.86	0.57
2:F:57:GLN:HG3	2:F:58:GLY:N	2.20	0.57
5:N:87:LEU:HD13	5:N:120:VAL:HA	1.85	0.57
1:A:105:ILE:HG12	1:A:239:GLN:H	1.70	0.57
1:A:382:VAL:HG12	1:A:383:SER:N	2.20	0.57
1:B:105:ILE:HG12	1:B:239:GLN:H	1.70	0.57
1:B:426:PRO:CG	1:B:429:PHE:CE2	2.86	0.57
1:B:709:ASN:N	1:B:709:ASN:OD1	2.37	0.57
1:C:105:ILE:HG12	1:C:239:GLN:H	1.70	0.57
3:I:91:THR:HG23	3:I:117:THR:HA	1.87	0.57
5:P:36:HIS:HA	5:P:51:GLY:HA2	1.86	0.57
1:A:230:PRO:CG	1:B:360:ASN:OD1	2.53	0.56
1:A:563:GLN:HA	1:C:41:LYS:HB3	1.86	0.56
1:B:212:LEU:HD23	1:B:214:ARG:H	1.70	0.56
1:C:374:PHE:CB	1:C:434:ILE:CG2	2.82	0.56
4:K:38:GLN:CB	4:K:48:LEU:HD21	2.35	0.56
2:D:37:ASN:HB2	2:D:92:GLN:H	1.70	0.56
2:D:57:GLN:HG3	2:D:58:GLY:N	2.20	0.56
4:K:38:GLN:HB2	4:K:48:LEU:HD21	1.85	0.56
1:A:709:ASN:OD1	1:A:709:ASN:N	2.37	0.56
1:A:936:ASP:HA	1:A:939:SER:HB2	1.87	0.56
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.37	0.56
1:C:53:ASP:OD1	1:C:54:LEU:N	2.37	0.56
2:F:40:GLN:O	2:F:48:ARG:N	2.34	0.56
3:G:35:SER:O	3:G:96:CYS:HA	2.05	0.56
2:J:38:TRP:CD2	2:J:76:LEU:HB2	2.39	0.56
1:A:563:GLN:CG	1:C:41:LYS:O	2.50	0.56
1:B:426:PRO:HG2	1:B:429:PHE:CE2	2.39	0.56
3:E:35:SER:O	3:E:96:CYS:HA	2.05	0.56
2:F:37:ASN:ND2	2:F:92:GLN:OE1	2.38	0.56
5:N:89:SER:OG	5:N:90:GLU:OE1	2.22	0.56
1:A:1040:VAL:HG21	1:C:1035:GLY:HA3	1.88	0.56
1:B:332:ILE:CG2	1:B:335:LEU:HD21	2.36	0.56
2:D:37:ASN:ND2	2:D:92:GLN:OE1	2.39	0.56
2:F:18:ALA:HB2	2:F:81:LEU:HD21	1.87	0.56
4:H:86:ASP:OD1	4:H:105:THR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:95:TYR:HD1	3:I:113:GLY:N	2.01	0.56
1:A:336:CYS:CB	1:A:358:ILE:HG21	2.36	0.56
4:M:86:ASP:OD1	4:M:105:THR:N	2.39	0.56
5:P:89:SER:OG	5:P:90:GLU:OE1	2.22	0.56
1:A:1019:ARG:NH2	1:A:1023:ASN:OD1	2.35	0.56
1:C:118:LEU:HD12	1:C:135:PHE:CE1	2.41	0.56
1:C:936:ASP:HA	1:C:939:SER:HB2	1.88	0.56
1:A:147:LYS:CE	5:L:52:PHE:CG	2.86	0.56
1:A:421:TYR:O	1:A:461:LEU:HD11	1.96	0.56
2:F:15:GLY:HA2	2:F:80:SER:HA	1.87	0.56
4:K:62:ARG:NH1	4:K:77:THR:O	2.37	0.56
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.88	0.56
4:K:86:ASP:OD1	4:K:105:THR:N	2.39	0.56
1:A:115:GLN:HB2	1:A:233:ILE:HD12	1.86	0.56
1:A:421:TYR:O	1:A:461:LEU:CG	2.55	0.56
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.37	0.56
1:B:936:ASP:HA	1:B:939:SER:HB2	1.88	0.56
1:B:1031:GLU:OE2	1:C:1039:ARG:NE	2.36	0.56
1:C:759:PHE:HD2	1:C:1001:LEU:HD21	1.71	0.56
1:C:1102:TRP:CE2	1:C:1133:VAL:HG21	2.41	0.56
1:A:212:LEU:HD23	1:A:214:ARG:H	1.70	0.55
1:A:650:LEU:HD21	1:A:653:ALA:HB3	1.88	0.55
1:B:346:ARG:HH12	1:B:442:ASP:HA	1.71	0.55
4:M:38:GLN:O	4:M:46:LYS:N	2.25	0.55
1:B:759:PHE:HD2	1:B:1001:LEU:HD21	1.71	0.55
3:E:19:ARG:HA	3:E:82:GLN:HA	1.86	0.55
3:E:100:ARG:NH1	3:E:103:GLY:HA3	2.21	0.55
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.88	0.55
1:A:534:VAL:CG1	1:A:539:VAL:CG1	2.78	0.55
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.88	0.55
1:C:424:LYS:HB3	1:C:463:PRO:HA	1.89	0.55
1:C:536:ASN:HA	1:C:551:VAL:HG13	1.86	0.55
3:G:93:VAL:HA	3:G:114:THR:O	2.06	0.55
5:L:36:HIS:N	5:L:98:ALA:O	2.40	0.55
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.37	0.55
2:D:15:GLY:HA2	2:D:80:SER:HA	1.87	0.55
2:D:18:ALA:HB2	2:D:81:LEU:HD21	1.88	0.55
2:D:86:PHE:CD2	2:D:109:ILE:HD12	2.42	0.55
2:J:57:GLN:HG3	2:J:58:GLY:N	2.20	0.55
4:M:101:PHE:HZ	5:P:109:PHE:CZ	2.23	0.55
1:B:1019:ARG:NH2	1:B:1023:ASN:OD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.88	0.55
1:A:53:ASP:OD1	1:A:54:LEU:N	2.37	0.55
1:A:759:PHE:HD2	1:A:1001:LEU:HD21	1.71	0.55
1:A:1089:PHE:HE2	1:C:914:ASN:HA	1.71	0.55
1:C:421:TYR:O	1:C:461:LEU:HG	2.06	0.55
3:G:17:SER:HA	3:G:83:MET:O	2.07	0.55
3:G:39:GLN:HB3	3:G:95:TYR:HE2	1.72	0.55
2:J:15:GLY:HA2	2:J:80:SER:HA	1.87	0.55
5:N:2:VAL:HG13	5:N:26:SER:O	2.07	0.55
1:B:1087:ALA:HB1	1:B:1089:PHE:HE1	1.72	0.55
1:C:410:ILE:HG21	1:C:425:LEU:HD12	1.79	0.55
2:J:6:GLN:NE2	2:J:91:CYS:SG	2.70	0.55
5:P:36:HIS:N	5:P:98:ALA:O	2.40	0.55
1:A:84:LEU:N	1:A:238:PHE:O	2.29	0.55
2:F:39:PHE:O	2:F:90:PHE:N	2.21	0.55
2:F:39:PHE:CD1	2:F:49:LEU:HA	2.42	0.55
2:F:86:PHE:CD2	2:F:109:ILE:HD12	2.42	0.55
4:H:99:VAL:HG13	5:L:107:TYR:CE1	2.42	0.55
2:J:6:GLN:HB2	2:J:103:GLN:HB2	1.82	0.55
2:J:18:ALA:HB2	2:J:81:LEU:HD21	1.87	0.55
2:J:39:PHE:O	2:J:90:PHE:N	2.21	0.55
2:J:86:PHE:CD2	2:J:109:ILE:HD12	2.42	0.55
5:N:36:HIS:N	5:N:98:ALA:O	2.40	0.55
5:P:2:VAL:HG21	5:P:28:TYR:CD2	2.42	0.55
1:A:546:LEU:HD22	1:A:565:PHE:CE1	2.42	0.55
1:B:23:GLN:O	1:B:24:LEU:HB2	2.06	0.55
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.88	0.55
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.88	0.55
1:C:337:PRO:HD2	1:C:358:ILE:HG23	1.87	0.55
3:E:36:TRP:CE2	3:E:81:LEU:HB2	2.42	0.55
3:E:39:GLN:HB3	3:E:95:TYR:HE2	1.72	0.55
3:G:20:LEU:HD12	3:G:81:LEU:HB3	1.89	0.55
4:K:48:LEU:HD11	4:K:87:TYR:CE1	2.42	0.55
1:A:853:GLN:CD	1:A:959:LEU:HD13	2.28	0.54
1:B:858:LEU:HD23	1:B:959:LEU:HD22	1.90	0.54
1:C:212:LEU:HD23	1:C:214:ARG:H	1.70	0.54
3:G:36:TRP:CE2	3:G:81:LEU:HB2	2.42	0.54
4:K:99:VAL:HG13	5:N:107:TYR:CE1	2.42	0.54
1:C:299:THR:HG21	1:C:597:VAL:HG11	1.88	0.54
3:E:93:VAL:HA	3:E:114:THR:O	2.06	0.54
1:B:853:GLN:CD	1:B:959:LEU:HD13	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASN:C	1:C:121:ASN:HD22	2.09	0.54
1:C:559:PHE:HB2	1:C:563:GLN:CB	2.37	0.54
1:C:875:SER:O	1:C:879:ALA:N	2.41	0.54
4:H:38:GLN:HB2	4:H:48:LEU:HD21	1.89	0.54
1:A:230:PRO:HG3	1:B:523:THR:HA	1.89	0.54
2:D:35:PHE:HE1	3:E:104:GLY:HA2	1.69	0.54
2:F:38:TRP:CE2	2:F:76:LEU:HB2	2.43	0.54
5:L:2:VAL:HG21	5:L:28:TYR:CD2	2.42	0.54
1:A:42:VAL:CG1	1:B:567:ARG:HG3	2.38	0.54
1:C:986:LYS:O	1:C:987:VAL:C	2.45	0.54
3:E:6:GLU:OE2	3:E:111:GLY:HA3	2.08	0.54
3:E:36:TRP:CD1	3:E:81:LEU:HB2	2.43	0.54
3:I:95:TYR:CZ	3:I:113:GLY:CA	2.88	0.54
2:J:64:ARG:O	2:J:78:ILE:HA	2.07	0.54
4:K:37:TYR:HE1	4:K:47:LEU:HD13	1.72	0.54
5:L:2:VAL:HG13	5:L:26:SER:O	2.07	0.54
5:N:2:VAL:HG21	5:N:28:TYR:CD2	2.42	0.54
1:A:103:GLY:HA3	1:A:119:ILE:O	2.08	0.54
1:B:546:LEU:HD22	1:B:565:PHE:CE1	2.42	0.54
3:E:17:SER:HA	3:E:83:MET:O	2.07	0.54
2:J:22:CYS:HB2	2:J:38:TRP:CH2	2.43	0.54
1:B:53:ASP:OD1	1:B:54:LEU:N	2.37	0.54
1:B:650:LEU:HD21	1:B:653:ALA:HB3	1.88	0.54
2:D:64:ARG:O	2:D:78:ILE:HA	2.07	0.54
3:E:11:LEU:HA	3:E:117:THR:O	2.08	0.54
2:F:64:ARG:O	2:F:78:ILE:HA	2.07	0.54
3:G:11:LEU:HA	3:G:117:THR:O	2.08	0.54
5:N:88:ARG:NH1	5:N:90:GLU:OE2	2.38	0.54
5:P:110:ASP:HB3	5:P:111:PRO:CD	2.38	0.54
1:C:546:LEU:HD22	1:C:565:PHE:CE1	2.42	0.54
2:D:22:CYS:HB2	2:D:38:TRP:CH2	2.43	0.54
3:E:20:LEU:HD12	3:E:81:LEU:HB3	1.90	0.54
2:F:22:CYS:HB2	2:F:38:TRP:CH2	2.43	0.54
1:A:108:THR:O	1:A:237:ARG:NH2	2.41	0.54
1:A:1006:THR:HG21	1:C:762:GLN:HE22	1.73	0.54
1:B:108:THR:O	1:B:237:ARG:NH2	2.41	0.54
1:B:118:LEU:HD22	1:B:129:LYS:HD2	1.90	0.54
1:B:145:TYR:CG	5:N:103:PHE:CE2	2.96	0.54
3:G:36:TRP:CD1	3:G:81:LEU:HB2	2.43	0.54
5:L:110:ASP:HB3	5:L:111:PRO:HD2	1.90	0.54
5:N:20:ARG:HG2	5:N:83:GLU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:O	1:A:24:LEU:HB2	2.06	0.54
1:A:118:LEU:HD22	1:A:129:LYS:HD2	1.90	0.54
4:M:62:ARG:NH1	4:M:77:THR:O	2.37	0.54
5:P:39:ARG:HA	5:P:95:TYR:HD1	1.73	0.54
1:C:1019:ARG:NH2	1:C:1023:ASN:OD1	2.34	0.53
1:B:170:TYR:CE2	1:B:172:SER:HB2	2.44	0.53
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.88	0.53
1:C:853:GLN:CD	1:C:959:LEU:HD13	2.28	0.53
2:D:39:PHE:CD1	2:D:49:LEU:HA	2.42	0.53
2:J:38:TRP:CE2	2:J:76:LEU:HB2	2.43	0.53
5:P:11:GLU:HG3	5:P:19:VAL:HG21	1.90	0.53
4:M:38:GLN:HB2	4:M:48:LEU:HD21	1.89	0.53
1:C:19:THR:HG23	1:C:138:ASP:OD2	2.07	0.53
1:C:119:ILE:HG22	1:C:128:ILE:HG23	1.90	0.53
1:C:563:GLN:HG3	1:C:577:ARG:NH1	2.24	0.53
2:D:38:TRP:CE2	2:D:76:LEU:HB2	2.43	0.53
5:N:39:ARG:HA	5:N:95:TYR:HD1	1.73	0.53
1:A:42:VAL:HG11	1:B:567:ARG:CG	2.37	0.53
1:B:276:LEU:HD11	1:B:306:PHE:HE1	0.40	0.53
2:J:39:PHE:CD1	2:J:49:LEU:HA	2.42	0.53
5:L:39:ARG:HA	5:L:95:TYR:HD1	1.73	0.53
5:P:2:VAL:HG13	5:P:26:SER:O	2.07	0.53
1:A:645:THR:OG1	1:A:648:GLY:O	2.13	0.53
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.91	0.53
1:C:519:HIS:HA	1:C:565:PHE:CE2	2.44	0.53
3:E:32:TYR:CD2	3:E:98:ARG:HD2	2.43	0.53
5:L:99:THR:O	5:L:110:ASP:HB2	2.08	0.53
1:A:230:PRO:HG2	1:B:360:ASN:OD1	2.08	0.53
1:A:1087:ALA:HB1	1:A:1089:PHE:HE1	1.72	0.53
1:B:103:GLY:HA3	1:B:119:ILE:O	2.08	0.53
1:C:170:TYR:CE2	1:C:172:SER:HB2	2.44	0.53
5:N:11:GLU:HG3	5:N:19:VAL:HG21	1.91	0.53
1:A:858:LEU:HD23	1:A:959:LEU:HD22	1.90	0.53
1:B:276:LEU:HD12	1:B:306:PHE:CZ	2.43	0.53
1:C:1087:ALA:HB1	1:C:1089:PHE:HE1	1.72	0.53
5:L:37:TRP:HB3	5:L:49:MET:HE2	1.90	0.53
1:C:446:GLY:HA2	2:J:95:LYS:HA	1.89	0.53
3:G:6:GLU:OE2	3:G:111:GLY:HA3	2.08	0.53
3:G:29:PHE:CE1	3:G:34:MET:HG3	2.44	0.53
5:N:110:ASP:HB3	5:N:111:PRO:HD2	1.90	0.53
1:B:66:HIS:HA	1:B:264:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:ASN:ND2	2:D:92:GLN:HB2	2.15	0.53
2:D:99:ARG:HH12	3:E:105:GLY:HA2	1.74	0.53
1:A:716:THR:HA	1:A:1110:TYR:HB3	1.90	0.52
1:B:875:SER:O	1:B:879:ALA:N	2.41	0.52
1:C:34:ARG:NE	1:C:216:LEU:HD23	2.24	0.52
1:C:108:THR:O	1:C:237:ARG:NH2	2.41	0.52
5:P:20:ARG:HG2	5:P:83:GLU:HB2	1.90	0.52
1:A:66:HIS:HA	1:A:264:ALA:HA	1.90	0.52
1:A:147:LYS:HZ2	5:L:34:ALA:HB2	1.74	0.52
1:B:34:ARG:NE	1:B:216:LEU:HD23	2.24	0.52
2:D:50:LEU:HA	2:D:61:ILE:HD12	1.91	0.52
2:J:43:PRO:HD3	2:J:87:ALA:HB1	1.91	0.52
1:A:202:LYS:HG2	1:A:228:ASP:HA	1.91	0.52
1:A:689:SER:OG	1:A:690:GLN:N	2.42	0.52
1:B:382:VAL:CG1	1:B:387:LEU:HD21	2.38	0.52
1:C:374:PHE:HE1	1:C:436:TRP:HZ3	1.34	0.52
1:C:410:ILE:HG13	1:C:418:ILE:HB	1.92	0.52
3:I:36:TRP:HB2	3:I:49:ALA:HB3	1.91	0.52
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.90	0.52
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.91	0.52
1:B:145:TYR:CG	5:N:103:PHE:HE2	2.26	0.52
2:F:43:PRO:HD3	2:F:87:ALA:HB1	1.92	0.52
3:I:6:GLU:OE2	3:I:96:CYS:N	2.42	0.52
5:L:20:ARG:HG2	5:L:83:GLU:HB2	1.90	0.52
1:B:210:ILE:HD12	1:B:217:PRO:HD3	1.92	0.52
1:C:202:LYS:HG2	1:C:228:ASP:HA	1.91	0.52
3:E:29:PHE:CE1	3:E:34:MET:HG3	2.44	0.52
2:F:65:PHE:CE1	2:F:78:ILE:HD11	2.45	0.52
1:C:210:ILE:HD12	1:C:217:PRO:HD3	1.92	0.52
1:C:328:ARG:HB3	1:C:543:PHE:HA	1.92	0.52
3:E:98:ARG:HH21	3:E:109:TYR:HD2	1.56	0.52
2:F:57:GLN:HG2	2:F:61:ILE:HG13	1.91	0.52
4:H:56:PRO:HD2	4:H:59:ILE:HG13	1.92	0.52
1:C:329:PHE:HD1	1:C:525:CYS:SG	2.31	0.52
2:J:57:GLN:HG2	2:J:61:ILE:HG13	1.92	0.52
5:N:99:THR:O	5:N:110:ASP:HB2	2.08	0.52
1:A:34:ARG:NE	1:A:216:LEU:HD23	2.24	0.52
1:A:704:SER:HB3	1:C:790:LYS:HE2	1.92	0.52
1:B:202:LYS:HG2	1:B:228:ASP:HA	1.91	0.52
1:B:551:VAL:N	1:B:588:THR:O	2.43	0.52
1:C:374:PHE:CE1	1:C:434:ILE:CG2	2.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:SER:OG	1:C:690:GLN:N	2.42	0.52
1:C:858:LEU:HD23	1:C:959:LEU:HD22	1.90	0.52
3:G:95:TYR:CE1	3:G:113:GLY:HA2	2.45	0.52
2:J:65:PHE:CE1	2:J:78:ILE:HD11	2.45	0.52
5:L:11:GLU:HG3	5:L:19:VAL:HG21	1.91	0.52
5:L:88:ARG:NH1	5:L:90:GLU:OE2	2.38	0.52
1:A:170:TYR:CE2	1:A:172:SER:HB2	2.44	0.52
1:A:186:PHE:CD1	1:A:209:PRO:HB3	2.45	0.52
1:C:643:PHE:CE2	1:C:645:THR:HG22	2.45	0.52
2:D:43:PRO:HD3	2:D:87:ALA:HB1	1.91	0.52
3:I:22:CYS:SG	3:I:96:CYS:CB	2.98	0.52
4:M:56:PRO:HD2	4:M:59:ILE:HG13	1.92	0.52
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.44	0.52
1:B:337:PRO:HD2	1:B:358:ILE:HG23	1.92	0.52
1:C:29:THR:HG22	1:C:62:VAL:O	2.09	0.52
2:J:3:VAL:O	2:J:25:SER:N	2.39	0.52
5:N:52:PHE:HD1	5:N:59:THR:HG22	1.75	0.52
1:C:186:PHE:CD1	1:C:209:PRO:HB3	2.45	0.51
1:C:328:ARG:HG3	1:C:579:PRO:HG2	1.92	0.51
1:C:396:TYR:HB2	1:C:514:SER:HB3	1.92	0.51
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.91	0.51
2:D:57:GLN:HG2	2:D:61:ILE:HG13	1.92	0.51
1:A:147:LYS:NZ	5:L:34:ALA:CB	2.73	0.51
3:E:95:TYR:CE1	3:E:113:GLY:HA2	2.45	0.51
1:A:276:LEU:HD12	1:A:306:PHE:CZ	2.43	0.51
1:A:299:THR:HG21	1:A:597:VAL:HG21	1.90	0.51
1:A:643:PHE:CE2	1:A:645:THR:HG22	2.45	0.51
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.44	0.51
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.92	0.51
1:B:689:SER:OG	1:B:690:GLN:N	2.42	0.51
1:C:131:CYS:HB2	1:C:133:PHE:CE2	2.44	0.51
2:D:65:PHE:CE1	2:D:78:ILE:HD11	2.45	0.51
2:F:3:VAL:O	2:F:25:SER:N	2.39	0.51
1:A:43:PHE:CE1	1:B:558:LYS:O	2.64	0.51
1:A:147:LYS:NZ	5:L:34:ALA:HB2	2.25	0.51
1:C:438:SER:HB3	1:C:509:ARG:HG3	1.93	0.51
2:J:50:LEU:HA	2:J:61:ILE:HD12	1.91	0.51
5:N:13:LYS:HD3	5:N:19:VAL:HB	1.92	0.51
1:B:230:PRO:HG3	1:C:357:ARG:CZ	2.40	0.51
1:B:244:LEU:HD22	1:B:259:THR:HA	1.92	0.51
1:C:716:THR:HA	1:C:1110:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:46:GLU:O	3:G:48:VAL:HG23	2.11	0.51
1:C:81:ASN:O	1:C:239:GLN:OE1	2.29	0.51
3:E:46:GLU:O	3:E:48:VAL:HG23	2.11	0.51
2:J:36:MET:HA	2:J:92:GLN:O	2.11	0.51
1:A:210:ILE:HD12	1:A:217:PRO:HD3	1.92	0.51
1:A:276:LEU:HD11	1:A:306:PHE:HE1	0.40	0.51
1:A:534:VAL:HG11	1:A:539:VAL:HG13	1.87	0.51
1:B:534:VAL:HG11	1:B:539:VAL:HG13	1.87	0.51
1:C:374:PHE:CE1	1:C:436:TRP:HZ3	2.15	0.51
2:D:3:VAL:O	2:D:25:SER:N	2.39	0.51
3:G:40:ALA:HB3	3:G:43:LYS:HG3	1.93	0.51
5:L:13:LYS:HD3	5:L:19:VAL:HB	1.92	0.51
1:A:244:LEU:HD22	1:A:259:THR:HA	1.92	0.51
1:B:115:GLN:HE21	1:B:167:THR:HG21	1.76	0.51
1:C:48:LEU:CD1	1:C:306:PHE:CD2	2.93	0.51
1:C:148:ASN:C	1:C:150:LYS:N	2.64	0.51
1:C:296:LEU:HD11	1:C:606:ASN:O	2.11	0.51
1:C:327:VAL:CA	1:C:542:ASN:HB3	2.39	0.51
1:C:853:GLN:NE2	1:C:959:LEU:HD13	2.26	0.51
3:G:34:MET:SD	3:G:98:ARG:HA	2.51	0.51
2:J:97:VAL:HG22	2:J:98:PRO:HD2	1.93	0.51
5:P:88:ARG:NH1	5:P:90:GLU:OE2	2.38	0.51
1:A:81:ASN:O	1:A:239:GLN:OE1	2.29	0.51
1:A:551:VAL:N	1:A:588:THR:O	2.43	0.51
1:B:643:PHE:CE2	1:B:645:THR:HG22	2.45	0.51
3:E:6:GLU:HG2	3:E:96:CYS:SG	2.51	0.51
3:G:6:GLU:HG2	3:G:96:CYS:SG	2.51	0.51
1:B:81:ASN:O	1:B:239:GLN:OE1	2.29	0.51
1:B:245:HIS:CD2	1:B:260:ALA:HB2	2.46	0.51
2:F:10:LEU:HB2	2:F:107:VAL:HG22	1.93	0.51
2:F:47:PRO:HD3	3:G:95:TYR:CZ	2.46	0.51
3:I:72:ARG:NH2	3:I:74:ASN:OD1	2.44	0.51
2:J:10:LEU:HB2	2:J:107:VAL:HG22	1.93	0.51
5:P:13:LYS:HD3	5:P:19:VAL:HB	1.92	0.51
1:B:392:PHE:CD1	1:B:515:PHE:HB2	2.44	0.50
1:C:118:LEU:HD22	1:C:129:LYS:HD2	1.93	0.50
1:C:735:SER:O	1:C:859:THR:OG1	2.27	0.50
2:F:50:LEU:HA	2:F:61:ILE:HD12	1.91	0.50
3:G:69:THR:HB	3:G:82:GLN:HB2	1.93	0.50
5:L:52:PHE:HD1	5:L:59:THR:HG22	1.75	0.50
1:B:186:PHE:CD1	1:B:209:PRO:HB3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:THR:HG22	1:C:522:ALA:CB	2.42	0.50
2:D:48:ARG:HH22	2:D:61:ILE:HD13	1.76	0.50
2:F:98:PRO:O	2:F:100:ILE:HG23	2.11	0.50
5:N:37:TRP:HB3	5:N:49:MET:HE3	1.93	0.50
1:A:64:TRP:CZ3	1:A:66:HIS:NE2	2.69	0.50
1:A:115:GLN:HE21	1:A:167:THR:HG21	1.76	0.50
1:A:521:PRO:HG2	1:C:199:GLY:HA3	1.92	0.50
1:B:382:VAL:HG12	1:B:383:SER:N	2.25	0.50
2:F:36:MET:HA	2:F:92:GLN:O	2.10	0.50
1:C:453:TYR:HB3	1:C:495:TYR:CZ	2.46	0.50
2:F:40:GLN:HB2	2:F:50:LEU:HD11	1.94	0.50
1:A:853:GLN:NE2	1:A:959:LEU:HD13	2.27	0.50
1:B:332:ILE:HG23	1:B:335:LEU:HD21	1.93	0.50
1:B:419:ALA:HA	1:B:423:TYR:O	2.12	0.50
3:E:114:THR:HG22	3:E:116:VAL:HG23	1.93	0.50
5:N:30:LEU:HB2	5:N:78:ASP:HA	1.93	0.50
1:A:296:LEU:CD1	1:A:608:VAL:CG2	2.79	0.50
1:B:759:PHE:CD2	1:B:1001:LEU:HD21	2.47	0.50
3:I:36:TRP:CZ3	3:I:96:CYS:SG	3.04	0.50
2:J:48:ARG:HH22	2:J:61:ILE:HD13	1.76	0.50
5:P:37:TRP:HB3	5:P:49:MET:HE3	1.93	0.50
1:A:953:ASN:O	1:A:957:GLN:N	2.39	0.50
1:B:914:ASN:HA	1:C:1089:PHE:HE2	1.76	0.50
1:C:922:LEU:HD21	6:C:1201:NAG:O3	2.11	0.50
1:A:790:LYS:HE2	1:B:704:SER:HB3	1.93	0.50
1:B:935:GLN:O	1:B:939:SER:N	2.40	0.50
1:C:759:PHE:CD2	1:C:1001:LEU:HD21	2.46	0.50
2:D:98:PRO:O	2:D:100:ILE:HG23	2.11	0.50
3:E:53:SER:HA	3:E:72:ARG:HH12	1.75	0.50
4:H:46:LYS:HA	5:L:112:TRP:CH2	2.47	0.50
4:K:2:SER:OG	4:K:3:VAL:N	2.45	0.50
5:P:52:PHE:HD1	5:P:59:THR:HG22	1.75	0.50
1:A:38:TYR:HD2	1:B:562:PHE:CZ	2.30	0.50
1:A:1006:THR:HG21	1:C:762:GLN:NE2	2.27	0.50
1:C:19:THR:CG2	1:C:138:ASP:OD2	2.60	0.50
1:C:117:LEU:HD11	1:C:119:ILE:HG23	1.94	0.50
1:C:245:HIS:CD2	1:C:260:ALA:HB2	2.47	0.50
1:C:366:SER:HB3	1:C:388:ASN:HD21	1.77	0.50
5:L:62:ALA:O	5:L:66:GLN:N	2.45	0.50
5:N:93:ALA:H	5:N:118:VAL:HG22	1.77	0.50
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:PHE:CD2	1:A:1001:LEU:HD21	2.47	0.49
1:A:970:PHE:CD1	1:C:756:TYR:HA	2.47	0.49
2:F:48:ARG:HH22	2:F:61:ILE:HD13	1.76	0.49
4:H:62:ARG:NH1	4:H:77:THR:O	2.37	0.49
1:A:245:HIS:CD2	1:A:260:ALA:HB2	2.46	0.49
1:A:875:SER:O	1:A:879:ALA:N	2.41	0.49
1:B:382:VAL:CG1	1:B:387:LEU:CD2	2.85	0.49
2:D:36:MET:HA	2:D:92:GLN:O	2.11	0.49
3:G:114:THR:HG22	3:G:116:VAL:HG23	1.93	0.49
1:A:715:PRO:HD3	1:C:894:LEU:CD1	2.40	0.49
1:B:853:GLN:NE2	1:B:959:LEU:HD13	2.27	0.49
3:E:40:ALA:HB3	3:E:43:LYS:HG3	1.93	0.49
2:J:40:GLN:HB2	2:J:50:LEU:HD11	1.94	0.49
4:M:46:LYS:HA	5:P:112:TRP:CH2	2.47	0.49
1:A:366:SER:HB3	1:A:388:ASN:HD21	1.78	0.49
1:A:869:MET:HB3	1:B:699:LEU:HD21	1.94	0.49
1:B:717:ASN:OD1	1:B:718:PHE:N	2.43	0.49
3:E:100:ARG:HH12	3:E:103:GLY:HA3	1.76	0.49
5:P:93:ALA:H	5:P:118:VAL:HG22	1.77	0.49
1:C:17:ASN:HD22	1:C:137:ASN:HD21	1.60	0.49
1:C:118:LEU:HD12	1:C:135:PHE:CZ	2.47	0.49
1:C:299:THR:CG2	1:C:597:VAL:CG2	2.91	0.49
2:D:10:LEU:HB2	2:D:107:VAL:HG22	1.93	0.49
3:E:32:TYR:CG	3:E:98:ARG:HD2	2.48	0.49
4:K:38:GLN:O	4:K:45:PRO:HA	2.12	0.49
1:A:147:LYS:HZ2	5:L:34:ALA:CB	2.25	0.49
3:E:62:ASP:O	3:E:63:THR:C	2.51	0.49
5:L:30:LEU:HB2	5:L:78:ASP:HA	1.93	0.49
5:P:62:ALA:O	5:P:66:GLN:N	2.45	0.49
1:A:1089:PHE:CD2	1:C:917:TYR:HD2	2.30	0.49
1:B:182:LYS:HG3	1:B:186:PHE:CD2	2.48	0.49
1:B:246:ARG:NH1	5:N:28:TYR:HD1	2.11	0.49
1:B:276:LEU:HG	1:B:289:VAL:HB	1.95	0.49
3:I:94:TYR:HE2	3:I:116:VAL:CG1	2.25	0.49
5:P:29:THR:O	5:P:32:GLU:HG2	2.13	0.49
1:A:89:GLY:HA3	1:A:270:LEU:HD12	1.95	0.49
1:A:290:ASP:O	1:A:297:SER:HB3	2.13	0.49
1:A:904:TYR:CE1	1:B:1107:ARG:HD3	2.47	0.49
1:B:20:THR:OG1	1:B:79:PHE:HB3	2.13	0.49
2:D:40:GLN:HB2	2:D:50:LEU:HD11	1.94	0.49
3:E:39:GLN:CB	3:E:95:TYR:HE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:GLN:CB	3:G:95:TYR:HE2	2.26	0.49
3:G:73:ASP:HB3	3:G:76:LYS:HB2	1.94	0.49
3:I:103:GLY:HA3	3:I:106:THR:HG22	1.95	0.49
2:J:6:GLN:CG	2:J:103:GLN:H	2.24	0.49
5:P:87:LEU:HD22	5:P:120:VAL:HG12	1.95	0.49
1:A:182:LYS:HG3	1:A:186:PHE:CD2	2.48	0.49
1:C:299:THR:CG2	1:C:597:VAL:HG21	2.39	0.49
1:C:535:LYS:HA	1:C:552:LEU:O	2.13	0.49
4:H:48:LEU:HD11	4:H:87:TYR:CD1	2.48	0.49
4:M:48:LEU:HD11	4:M:87:TYR:CD1	2.48	0.49
1:A:336:CYS:SG	1:A:358:ILE:CG2	3.00	0.49
1:A:1145:LEU:O	1:A:1147:SER:N	2.46	0.49
1:B:290:ASP:O	1:B:297:SER:HB3	2.12	0.49
2:D:93:GLN:O	2:D:99:ARG:HB2	2.13	0.49
5:N:87:LEU:HD22	5:N:120:VAL:HG12	1.95	0.49
1:A:41:LYS:CB	1:B:564:GLN:H	2.20	0.48
1:A:276:LEU:HG	1:A:289:VAL:HB	1.95	0.48
1:C:115:GLN:HE21	1:C:167:THR:HG21	1.76	0.48
3:E:73:ASP:HB3	3:E:76:LYS:HB2	1.94	0.48
4:H:60:PRO:HB2	4:H:62:ARG:HG2	1.95	0.48
5:N:3:GLN:O	5:N:26:SER:OG	2.27	0.48
5:N:62:ALA:O	5:N:66:GLN:N	2.45	0.48
1:A:41:LYS:HB3	1:B:563:GLN:C	2.32	0.48
1:A:324:GLU:CD	1:A:534:VAL:HG21	2.27	0.48
1:B:278:LYS:HE3	1:B:287:ASP:HB3	1.95	0.48
2:F:93:GLN:O	2:F:99:ARG:HB2	2.13	0.48
3:G:71:SER:OG	3:G:80:TYR:HD2	1.97	0.48
5:N:21:VAL:N	5:N:82:MET:O	2.46	0.48
1:A:419:ALA:HA	1:A:423:TYR:O	2.13	0.48
1:B:803:SER:HB3	6:B:1202:NAG:C7	2.43	0.48
1:B:853:GLN:OE1	1:B:959:LEU:HB2	2.12	0.48
1:C:326:ILE:CA	1:C:531:THR:OG1	2.60	0.48
2:D:22:CYS:O	2:D:73:ASP:HA	2.14	0.48
2:J:37:ASN:OD1	2:J:92:GLN:NE2	2.40	0.48
4:M:37:TYR:HE1	4:M:47:LEU:HD13	1.77	0.48
1:A:796:ASP:OD1	1:A:796:ASP:N	2.46	0.48
1:A:987:VAL:CG1	1:C:413:GLY:HA2	2.42	0.48
1:B:231:ILE:HG22	1:B:233:ILE:HG22	1.96	0.48
4:H:37:TYR:HE1	4:H:47:LEU:HD13	1.77	0.48
5:L:87:LEU:HD22	5:L:120:VAL:HG12	1.95	0.48
5:N:111:PRO:HA	5:N:112:TRP:CE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.96	0.48
1:C:67:ALA:O	1:C:68:ILE:C	2.50	0.48
1:C:563:GLN:HG3	1:C:563:GLN:H	1.35	0.48
1:C:1032:CYS:SG	1:C:1048:HIS:NE2	2.87	0.48
3:E:73:ASP:O	3:E:77:ASN:N	2.47	0.48
1:A:278:LYS:HE3	1:A:287:ASP:HB3	1.95	0.48
1:C:180:GLU:HG3	1:C:181:GLY:N	2.27	0.48
1:C:935:GLN:O	1:C:939:SER:N	2.39	0.48
3:I:49:ALA:HB1	3:I:70:ILE:HD13	1.95	0.48
5:L:29:THR:O	5:L:32:GLU:HG2	2.13	0.48
1:A:64:TRP:HZ2	1:A:66:HIS:CE1	2.06	0.48
1:B:296:LEU:CD1	1:B:608:VAL:CG2	2.79	0.48
1:B:1032:CYS:SG	1:B:1048:HIS:NE2	2.87	0.48
1:B:1145:LEU:O	1:B:1147:SER:N	2.46	0.48
1:C:120:VAL:HG13	1:C:141:LEU:HD11	1.96	0.48
1:C:717:ASN:HB3	1:C:1070:ALA:HB3	1.96	0.48
1:C:1145:LEU:O	1:C:1147:SER:N	2.47	0.48
1:A:147:LYS:CE	5:L:52:PHE:CD1	2.95	0.48
1:A:231:ILE:HG22	1:A:233:ILE:HG22	1.96	0.48
1:A:1032:CYS:SG	1:A:1048:HIS:NE2	2.87	0.48
1:C:374:PHE:CE2	1:C:434:ILE:HG21	2.47	0.48
1:C:394:ASN:HB2	1:C:516:GLU:HG3	1.92	0.48
2:D:35:PHE:HB3	2:D:36:MET:H	1.52	0.48
3:E:71:SER:OG	3:E:80:TYR:HD2	1.97	0.48
2:J:69:GLY:HA2	2:J:74:PHE:HA	1.96	0.48
5:N:29:THR:O	5:N:32:GLU:HG2	2.13	0.48
5:P:30:LEU:HB2	5:P:78:ASP:HA	1.93	0.48
1:A:20:THR:OG1	1:A:79:PHE:HB3	2.13	0.48
1:A:168:PHE:CD1	1:B:360:ASN:ND2	2.82	0.48
1:A:961:THR:HG23	1:C:758:SER:OG	2.14	0.48
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.94	0.48
1:C:84:LEU:N	1:C:238:PHE:O	2.29	0.48
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.94	0.48
4:M:60:PRO:HB2	4:M:62:ARG:HG2	1.95	0.48
1:A:14:GLN:HB3	1:A:158:ARG:HD3	1.96	0.48
1:A:895:GLN:CD	1:B:713:ALA:HB2	2.34	0.48
1:C:14:GLN:HB3	1:C:158:ARG:HD3	1.96	0.48
1:C:182:LYS:HG3	1:C:186:PHE:CD2	2.48	0.48
3:E:9:GLY:HA2	3:E:115:LEU:O	2.14	0.48
2:F:12:LEU:O	2:F:110:LEU:N	2.33	0.48
2:J:42:LYS:HB2	2:J:45:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:40:GLN:NE2	5:L:46:LEU:HD12	2.29	0.48
1:A:563:GLN:CB	1:C:41:LYS:O	2.62	0.47
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.49	0.47
1:C:89:GLY:HA3	1:C:270:LEU:HD12	1.95	0.47
1:C:156:GLU:OE1	1:C:156:GLU:N	2.44	0.47
1:C:194:PHE:HB3	1:C:201:PHE:CZ	2.49	0.47
3:E:30:THR:HG22	3:E:74:ASN:CG	2.34	0.47
3:G:53:SER:HA	3:G:72:ARG:HH12	1.78	0.47
4:H:2:SER:OG	4:H:3:VAL:N	2.45	0.47
1:A:194:PHE:HB3	1:A:201:PHE:CZ	2.49	0.47
1:B:89:GLY:HA3	1:B:270:LEU:HD12	1.95	0.47
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.50	0.47
1:C:717:ASN:OD1	6:C:1201:NAG:H3	2.14	0.47
3:G:9:GLY:HA2	3:G:115:LEU:O	2.14	0.47
3:G:30:THR:HG22	3:G:74:ASN:CG	2.34	0.47
2:J:12:LEU:O	2:J:110:LEU:N	2.33	0.47
2:J:50:LEU:O	2:J:61:ILE:HG13	2.14	0.47
5:L:21:VAL:N	5:L:82:MET:O	2.46	0.47
1:A:439:ASN:O	1:A:443:SER:HB2	2.14	0.47
1:B:410:ILE:HG23	1:B:425:LEU:HD11	1.96	0.47
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.96	0.47
3:G:62:ASP:O	3:G:63:THR:C	2.52	0.47
5:L:39:ARG:HG2	5:L:95:TYR:CE1	2.49	0.47
5:N:40:GLN:NE2	5:N:46:LEU:HD12	2.29	0.47
5:P:39:ARG:HG2	5:P:95:TYR:CE1	2.49	0.47
1:B:17:ASN:HB2	1:B:138:ASP:OD2	2.15	0.47
1:C:109:THR:HG22	1:C:111:ASP:HB3	1.97	0.47
5:L:111:PRO:HA	5:L:112:TRP:CE3	2.48	0.47
5:P:21:VAL:N	5:P:82:MET:O	2.46	0.47
1:B:180:GLU:HG3	1:B:181:GLY:N	2.27	0.47
1:B:735:SER:O	1:B:859:THR:OG1	2.27	0.47
1:C:23:GLN:O	1:C:24:LEU:HB2	2.15	0.47
1:C:248:TYR:CB	5:P:101:THR:HG21	2.33	0.47
1:C:1088:HIS:CE1	1:C:1122:VAL:HG22	2.50	0.47
3:E:20:LEU:HD11	3:E:94:TYR:CD2	2.50	0.47
3:E:97:ALA:HB1	3:E:107:VAL:CG1	2.45	0.47
2:F:42:LYS:HB2	2:F:45:GLN:HB3	1.96	0.47
3:G:36:TRP:NE1	3:G:81:LEU:HB2	2.30	0.47
3:G:73:ASP:O	3:G:77:ASN:N	2.47	0.47
4:H:2:SER:OG	4:H:101:PHE:O	2.25	0.47
4:H:84:GLU:HG3	4:H:107:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:TYR:CD1	1:B:388:ASN:OD1	2.67	0.47
1:B:1088:HIS:CE1	1:B:1122:VAL:HG22	2.50	0.47
1:C:374:PHE:CE1	1:C:434:ILE:HG22	2.37	0.47
2:D:50:LEU:O	2:D:61:ILE:HG13	2.14	0.47
2:D:69:GLY:HA2	2:D:74:PHE:HA	1.96	0.47
2:F:50:LEU:O	2:F:61:ILE:HG13	2.14	0.47
2:F:69:GLY:HA2	2:F:74:PHE:HA	1.96	0.47
2:J:22:CYS:O	2:J:73:ASP:HA	2.14	0.47
4:K:37:TYR:HE2	4:K:101:PHE:HE1	1.63	0.47
5:L:93:ALA:H	5:L:118:VAL:HG22	1.77	0.47
5:L:100:THR:HG22	5:L:108:TRP:O	2.15	0.47
1:A:109:THR:HG22	1:A:111:ASP:HB3	1.96	0.47
1:A:853:GLN:OE1	1:A:959:LEU:HB2	2.12	0.47
1:A:906:PHE:CE2	1:A:916:LEU:HB2	2.50	0.47
1:B:180:GLU:O	1:B:182:LYS:HG2	2.15	0.47
1:C:180:GLU:O	1:C:182:LYS:HG2	2.15	0.47
1:C:246:ARG:HH12	5:P:28:TYR:HA	1.80	0.47
2:D:12:LEU:O	2:D:110:LEU:N	2.33	0.47
2:D:51:ILE:CG2	2:D:56:ASN:H	2.28	0.47
3:I:8:GLY:O	3:I:9:GLY:C	2.53	0.47
2:J:36:MET:SD	2:J:93:GLN:HA	2.55	0.47
2:J:51:ILE:CG2	2:J:56:ASN:H	2.28	0.47
5:L:7:GLN:HG3	5:L:113:GLY:O	2.15	0.47
5:P:7:GLN:HG3	5:P:113:GLY:O	2.15	0.47
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.50	0.47
1:B:783:ALA:HB2	1:B:873:TYR:CZ	2.50	0.47
1:C:783:ALA:HB2	1:C:873:TYR:CZ	2.50	0.47
2:D:10:LEU:HB2	2:D:107:VAL:HG13	1.96	0.47
2:D:57:GLN:HG3	2:D:58:GLY:H	1.80	0.47
2:J:35:PHE:HB3	2:J:36:MET:H	1.52	0.47
5:N:92:THR:OG1	5:N:118:VAL:O	2.33	0.47
5:N:100:THR:HG22	5:N:108:TRP:O	2.15	0.47
1:A:180:GLU:O	1:A:182:LYS:HG2	2.15	0.47
1:A:755:GLN:O	1:B:970:PHE:N	2.43	0.47
1:A:935:GLN:O	1:A:939:SER:N	2.40	0.47
1:B:534:VAL:CG1	1:B:539:VAL:CG1	2.78	0.47
1:B:1116:THR:HB	1:B:1140:PRO:HD3	1.97	0.47
1:C:276:LEU:HG	1:C:289:VAL:HB	1.95	0.47
1:C:328:ARG:HD2	1:C:580:GLN:HG3	1.97	0.47
2:D:42:LYS:HB2	2:D:45:GLN:HB3	1.96	0.47
2:D:56:ASN:CG	2:D:57:GLN:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:39:GLN:HB2	3:E:45:LEU:HD23	1.97	0.47
2:F:22:CYS:O	2:F:73:ASP:HA	2.14	0.47
2:F:57:GLN:HG3	2:F:58:GLY:H	1.80	0.47
4:K:38:GLN:HB2	4:K:48:LEU:CD1	2.41	0.47
1:A:38:TYR:CD1	1:A:285:ILE:HD12	2.50	0.47
1:A:382:VAL:CG1	1:A:383:SER:N	2.78	0.47
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.96	0.47
1:B:296:LEU:HD12	1:B:608:VAL:HG13	1.19	0.47
1:C:1116:THR:HB	1:C:1140:PRO:HD3	1.97	0.47
2:F:36:MET:SD	2:F:93:GLN:HA	2.55	0.47
4:H:37:TYR:HE2	4:H:101:PHE:HE1	1.63	0.47
4:K:21:SER:HA	4:K:73:THR:HA	1.97	0.47
4:M:84:GLU:HG3	4:M:107:LEU:O	2.15	0.47
5:N:39:ARG:HG2	5:N:95:TYR:CE1	2.50	0.47
1:A:48:LEU:CD1	1:A:305:SER:HA	2.46	0.46
1:A:382:VAL:HG12	1:A:387:LEU:HG	1.96	0.46
1:C:710:ASN:O	1:C:1077:THR:HG22	2.16	0.46
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.96	0.46
3:E:27:PHE:CD1	3:E:32:TYR:HD2	2.33	0.46
3:E:94:TYR:CD2	3:E:116:VAL:HG21	2.50	0.46
3:G:27:PHE:CD1	3:G:32:TYR:HD2	2.33	0.46
4:K:84:GLU:HG3	4:K:107:LEU:O	2.15	0.46
1:A:961:THR:O	1:A:965:GLN:HG2	2.15	0.46
1:B:109:THR:HG22	1:B:111:ASP:HB3	1.97	0.46
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.50	0.46
2:F:37:ASN:ND2	2:F:92:GLN:HB2	2.15	0.46
3:G:83:MET:HB3	3:G:83:MET:HE2	1.75	0.46
3:G:94:TYR:CD2	3:G:116:VAL:HG21	2.50	0.46
5:P:94:VAL:HA	5:P:116:THR:O	2.15	0.46
1:A:180:GLU:HG3	1:A:181:GLY:N	2.27	0.46
1:B:38:TYR:CD1	1:B:285:ILE:HD12	2.50	0.46
1:B:48:LEU:CD1	1:B:305:SER:HA	2.46	0.46
1:C:49:HIS:O	1:C:277:LEU:N	2.43	0.46
1:C:452:LEU:HG	1:C:494:SER:HA	1.97	0.46
4:K:38:GLN:O	4:K:46:LYS:N	2.48	0.46
5:N:94:VAL:HA	5:N:116:THR:O	2.15	0.46
5:P:40:GLN:NE2	5:P:46:LEU:HD12	2.29	0.46
5:P:52:PHE:HA	5:P:59:THR:HA	1.98	0.46
1:B:14:GLN:HB3	1:B:158:ARG:HD3	1.96	0.46
1:B:421:TYR:O	1:B:461:LEU:CG	2.64	0.46
1:B:716:THR:HA	1:B:1110:TYR:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:HE1	1:C:285:ILE:HB	1.80	0.46
1:C:327:VAL:CA	1:C:542:ASN:O	2.63	0.46
3:E:91:THR:OG1	3:E:118:VAL:N	2.46	0.46
4:M:2:SER:OG	4:M:3:VAL:N	2.45	0.46
5:N:39:ARG:HA	5:N:95:TYR:CD1	2.50	0.46
1:A:38:TYR:HD2	1:B:562:PHE:HZ	1.64	0.46
1:B:568:ASP:OD1	1:B:569:ILE:N	2.45	0.46
1:B:961:THR:O	1:B:965:GLN:HG2	2.15	0.46
1:C:23:GLN:HG2	1:C:24:LEU:N	2.30	0.46
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.98	0.46
1:C:335:LEU:C	1:C:361:CYS:HB2	2.36	0.46
1:C:342:PHE:CE2	1:C:368:LEU:HD21	2.51	0.46
1:C:430:THR:HG21	1:C:517:LEU:HD21	1.98	0.46
1:C:953:ASN:O	1:C:957:GLN:N	2.39	0.46
2:D:40:GLN:HB2	2:D:50:LEU:HD21	1.97	0.46
3:E:36:TRP:NE1	3:E:81:LEU:HB2	2.30	0.46
2:F:10:LEU:HB2	2:F:107:VAL:HG13	1.96	0.46
2:F:103:GLN:HA	3:G:44:ARG:HE	1.80	0.46
4:H:28:ASN:O	4:H:32:ASN:HB2	2.16	0.46
3:I:6:GLU:OE1	3:I:114:THR:OG1	2.33	0.46
5:L:6:GLU:HG3	5:L:7:GLN:H	1.81	0.46
4:M:37:TYR:HE2	4:M:101:PHE:HE1	1.63	0.46
5:N:7:GLN:HG3	5:N:113:GLY:O	2.15	0.46
1:A:17:ASN:HB2	1:A:138:ASP:OD2	2.15	0.46
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.50	0.46
1:C:451:TYR:O	1:C:495:TYR:HB2	2.14	0.46
3:I:28:THR:OG1	3:I:31:ASN:HB3	2.15	0.46
2:J:10:LEU:HB2	2:J:107:VAL:HG13	1.97	0.46
4:K:99:VAL:HG13	5:N:107:TYR:CZ	2.51	0.46
5:L:11:GLU:O	5:L:11:GLU:HG2	2.16	0.46
4:M:28:ASN:O	4:M:32:ASN:HB2	2.16	0.46
5:N:52:PHE:HA	5:N:59:THR:HA	1.98	0.46
1:A:1107:ARG:HD3	1:C:904:TYR:CE1	2.51	0.46
2:F:35:PHE:CE2	2:F:95:LYS:HD3	2.51	0.46
2:F:40:GLN:HB2	2:F:50:LEU:HD21	1.97	0.46
3:G:20:LEU:HD11	3:G:94:TYR:CD2	2.50	0.46
3:G:22:CYS:O	3:G:78:THR:HA	2.16	0.46
4:H:99:VAL:HG13	5:L:107:TYR:CZ	2.51	0.46
3:I:22:CYS:HG	3:I:96:CYS:HB2	1.80	0.46
5:P:11:GLU:HG2	5:P:11:GLU:O	2.16	0.46
5:P:92:THR:OG1	5:P:118:VAL:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:HA	1:B:531:THR:OG1	2.16	0.46
1:B:710:ASN:O	1:B:1077:THR:HG22	2.16	0.46
1:B:1028:LYS:O	1:B:1032:CYS:N	2.46	0.46
1:C:247:SER:H	1:C:257:GLY:HA3	1.81	0.46
2:D:35:PHE:CE2	2:D:95:LYS:HD3	2.51	0.46
4:H:84:GLU:HG3	4:H:108:THR:HA	1.98	0.46
4:M:21:SER:HA	4:M:73:THR:HA	1.97	0.46
1:A:104:TRP:HB2	1:A:106:PHE:CE2	2.51	0.46
1:A:783:ALA:HB2	1:A:873:TYR:CZ	2.50	0.46
1:B:796:ASP:OD1	1:B:796:ASP:N	2.46	0.46
1:B:953:ASN:O	1:B:957:GLN:N	2.39	0.46
1:C:284:THR:HG22	1:C:285:ILE:O	2.15	0.46
1:C:342:PHE:HD2	6:C:1204:NAG:H82	1.81	0.46
1:C:377:PHE:CZ	1:C:434:ILE:HD11	2.51	0.46
1:C:906:PHE:CE2	1:C:916:LEU:HB2	2.51	0.46
3:E:22:CYS:O	3:E:78:THR:HA	2.16	0.46
2:J:35:PHE:CE2	2:J:95:LYS:HD3	2.51	0.46
5:L:39:ARG:HA	5:L:95:TYR:CD1	2.51	0.46
5:N:11:GLU:HG2	5:N:11:GLU:O	2.16	0.46
1:A:1088:HIS:CE1	1:A:1122:VAL:HG22	2.50	0.46
1:B:87:ASN:HB2	1:B:269:TYR:CD1	2.51	0.46
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.98	0.46
1:B:188:ASN:O	1:B:190:ARG:HG3	2.16	0.46
1:C:21:ARG:HG3	1:C:22:THR:N	2.31	0.46
1:C:188:ASN:O	1:C:190:ARG:HG3	2.16	0.46
1:C:961:THR:O	1:C:965:GLN:HG2	2.15	0.46
2:D:36:MET:SD	2:D:93:GLN:HA	2.55	0.46
3:E:30:THR:HG22	3:E:74:ASN:ND2	2.31	0.46
2:F:51:ILE:CG2	2:F:56:ASN:H	2.28	0.46
3:G:51:ILE:HG21	3:G:72:ARG:HE	1.81	0.46
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.98	0.45
1:B:815:ARG:HD2	1:B:823:PHE:CE2	2.45	0.45
1:C:87:ASN:HB2	1:C:269:TYR:CD1	2.51	0.45
5:L:92:THR:OG1	5:L:118:VAL:O	2.33	0.45
5:L:94:VAL:HA	5:L:116:THR:O	2.15	0.45
5:P:39:ARG:HA	5:P:95:TYR:CD1	2.50	0.45
1:A:426:PRO:CB	1:A:429:PHE:CE2	2.89	0.45
1:A:564:GLN:H	1:C:41:LYS:HB3	1.81	0.45
1:C:472:ILE:CG2	1:C:488:CYS:HB3	2.45	0.45
2:F:12:LEU:O	2:F:109:ILE:HA	2.17	0.45
3:G:36:TRP:HB2	3:G:49:ALA:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:5:LEU:HD13	5:L:24:LYS:HB2	1.99	0.45
1:A:41:LYS:CB	1:B:563:GLN:HA	2.46	0.45
1:A:188:ASN:O	1:A:190:ARG:HG3	2.16	0.45
1:C:382:VAL:HB	1:C:387:LEU:HD21	1.97	0.45
1:C:439:ASN:O	1:C:443:SER:HB2	2.16	0.45
2:D:24:ALA:HB1	2:D:93:GLN:HE21	1.81	0.45
2:D:69:GLY:CA	2:D:74:PHE:HA	2.47	0.45
3:G:30:THR:HG22	3:G:74:ASN:ND2	2.31	0.45
3:G:94:TYR:HD2	3:G:116:VAL:HG21	1.81	0.45
3:I:92:ALA:O	3:I:116:VAL:HB	2.16	0.45
1:A:87:ASN:HB2	1:A:269:TYR:CD1	2.51	0.45
1:A:382:VAL:CG1	1:A:387:LEU:HG	2.47	0.45
1:A:472:ILE:HG22	1:A:480:CYS:SG	2.57	0.45
1:A:710:ASN:O	1:A:1077:THR:HG22	2.15	0.45
1:A:864:LEU:HG	1:A:865:LEU:HD12	1.99	0.45
1:A:970:PHE:CD1	1:C:756:TYR:HD1	2.34	0.45
1:C:104:TRP:HB2	1:C:106:PHE:CE2	2.51	0.45
1:C:358:ILE:HB	1:C:395:VAL:HB	1.99	0.45
2:F:24:ALA:HB1	2:F:93:GLN:HE21	1.81	0.45
3:G:39:GLN:HB2	3:G:45:LEU:HD23	1.97	0.45
4:H:21:SER:HA	4:H:73:THR:HA	1.97	0.45
4:H:39:GLN:HG2	4:H:40:LEU:O	2.17	0.45
4:K:2:SER:OG	4:K:101:PHE:O	2.25	0.45
5:P:5:LEU:HD13	5:P:24:LYS:HB2	1.99	0.45
5:P:6:GLU:HG3	5:P:7:GLN:H	1.81	0.45
5:P:37:TRP:O	5:P:49:MET:N	2.49	0.45
1:B:100:ILE:HD13	1:B:263:ALA:HB2	1.98	0.45
1:B:104:TRP:HB2	1:B:106:PHE:CE2	2.51	0.45
1:B:106:PHE:HB2	1:B:117:LEU:HD23	1.99	0.45
1:B:287:ASP:OD2	1:B:306:PHE:CG	2.68	0.45
1:C:342:PHE:HE2	1:C:368:LEU:HD21	1.82	0.45
1:C:422:ASN:C	1:C:461:LEU:HD12	2.37	0.45
3:E:51:ILE:HG21	3:E:72:ARG:HE	1.81	0.45
3:E:94:TYR:HD2	3:E:116:VAL:HG21	1.81	0.45
2:F:86:PHE:HD2	2:F:109:ILE:HD12	1.80	0.45
2:J:40:GLN:HB2	2:J:50:LEU:HD21	1.97	0.45
4:K:13:ALA:HA	4:K:110:LEU:HB2	1.99	0.45
5:L:52:PHE:HA	5:L:59:THR:HA	1.98	0.45
5:N:6:GLU:HG3	5:N:7:GLN:H	1.81	0.45
1:A:106:PHE:HB2	1:A:117:LEU:HD23	1.99	0.45
1:B:299:THR:HG21	1:B:597:VAL:HG21	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:24:GLY:HA3	4:K:29:ILE:HD12	1.99	0.45
5:L:4:LEU:HD22	5:L:25:VAL:HG12	1.99	0.45
1:A:1072:GLU:N	1:A:1072:GLU:OE1	2.50	0.45
1:A:1093:GLY:HA2	1:A:1107:ARG:HG3	1.99	0.45
1:C:747:THR:HA	1:C:750:SER:HB3	1.99	0.45
2:D:64:ARG:HB2	2:D:78:ILE:HG23	1.98	0.45
5:L:11:GLU:OE1	5:L:11:GLU:N	2.50	0.45
1:A:882:ILE:O	1:A:898:PHE:HD1	2.00	0.45
1:B:864:LEU:HG	1:B:865:LEU:HD12	1.98	0.45
1:C:299:THR:CG2	1:C:597:VAL:HG11	2.47	0.45
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.50	0.45
2:F:11:SER:HA	2:F:108:GLU:HB2	1.99	0.45
2:J:12:LEU:O	2:J:109:ILE:HA	2.17	0.45
2:J:24:ALA:HB1	2:J:93:GLN:HE21	1.81	0.45
2:J:57:GLN:HG3	2:J:58:GLY:H	1.81	0.45
4:M:13:ALA:HA	4:M:110:LEU:HB2	1.99	0.45
1:A:156:GLU:OE1	1:A:156:GLU:N	2.44	0.45
1:A:1116:THR:HB	1:A:1140:PRO:HD3	1.97	0.45
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.40	0.45
1:C:1102:TRP:CH2	1:C:1133:VAL:HG21	2.52	0.45
2:D:86:PHE:HD2	2:D:109:ILE:HD12	1.80	0.45
2:J:11:SER:HA	2:J:108:GLU:HB2	1.99	0.45
2:J:69:GLY:CA	2:J:74:PHE:HA	2.47	0.45
4:M:39:GLN:HG2	4:M:40:LEU:O	2.17	0.45
5:N:37:TRP:O	5:N:49:MET:N	2.49	0.45
1:B:142:GLY:O	1:B:155:SER:N	2.50	0.45
1:B:332:ILE:HG22	1:B:333:THR:N	2.32	0.45
1:B:346:ARG:HA	1:B:346:ARG:HD3	1.79	0.45
1:C:201:PHE:CB	1:C:231:ILE:HG13	2.29	0.45
1:C:853:GLN:OE1	1:C:959:LEU:HB2	2.11	0.45
1:C:864:LEU:HG	1:C:865:LEU:HD12	1.99	0.45
2:F:64:ARG:HB2	2:F:78:ILE:HG23	1.98	0.45
2:J:43:PRO:HD3	2:J:87:ALA:CB	2.47	0.45
5:N:33:VAL:HA	5:N:102:PRO:HD3	1.99	0.45
1:A:366:SER:HB3	1:A:388:ASN:ND2	2.32	0.44
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.40	0.44
1:B:882:ILE:O	1:B:898:PHE:HD1	2.00	0.44
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.50	0.44
2:D:35:PHE:HE2	2:D:95:LYS:HB2	1.82	0.44
1:A:41:LYS:HB3	1:B:563:GLN:CA	2.45	0.44
1:A:43:PHE:N	1:B:565:PHE:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLY:O	1:A:155:SER:N	2.50	0.44
1:A:747:THR:HA	1:A:750:SER:HB3	1.99	0.44
1:A:756:TYR:HA	1:B:970:PHE:HD1	1.81	0.44
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.98	0.44
1:B:446:GLY:HA2	2:F:95:LYS:HG3	1.99	0.44
1:B:747:THR:HA	1:B:750:SER:HB3	1.99	0.44
1:B:1139:ASP:CG	1:B:1142:GLN:H	2.21	0.44
1:C:100:ILE:HD13	1:C:263:ALA:HB2	1.99	0.44
1:C:142:GLY:O	1:C:155:SER:N	2.50	0.44
1:C:882:ILE:O	1:C:898:PHE:HD1	2.00	0.44
2:J:36:MET:O	2:J:37:ASN:ND2	2.50	0.44
4:K:39:GLN:HG2	4:K:40:LEU:O	2.17	0.44
4:M:2:SER:OG	4:M:101:PHE:O	2.25	0.44
5:P:11:GLU:OE1	5:P:11:GLU:N	2.50	0.44
1:A:1121:PHE:HE1	1:C:914:ASN:HB3	1.82	0.44
1:B:347:PHE:HE2	1:B:509:ARG:HD3	1.82	0.44
1:C:315:THR:HG22	1:C:316:SER:N	2.33	0.44
1:C:329:PHE:CD1	1:C:525:CYS:CB	3.00	0.44
2:D:10:LEU:HD13	2:D:12:LEU:HD11	2.00	0.44
3:E:36:TRP:HB2	3:E:49:ALA:CB	2.45	0.44
3:E:88:ALA:HA	3:E:118:VAL:O	2.17	0.44
4:H:53:ASN:OD1	4:H:54:LYS:HG2	2.17	0.44
3:I:94:TYR:CD2	3:I:116:VAL:CG1	2.95	0.44
2:J:37:ASN:OD1	2:J:92:GLN:HB2	2.17	0.44
4:K:28:ASN:O	4:K:32:ASN:HB2	2.16	0.44
5:N:4:LEU:HD22	5:N:25:VAL:HG12	1.99	0.44
5:N:11:GLU:OE1	5:N:11:GLU:N	2.50	0.44
1:A:29:THR:HG22	1:A:62:VAL:O	2.17	0.44
1:B:452:LEU:CD2	1:B:492:LEU:HB3	2.46	0.44
2:D:12:LEU:O	2:D:109:ILE:HA	2.17	0.44
4:H:13:ALA:HA	4:H:110:LEU:HB2	1.99	0.44
2:J:4:LEU:HD11	2:J:102:GLY:CA	2.16	0.44
4:K:45:PRO:O	5:N:109:PHE:HZ	2.00	0.44
4:K:84:GLU:HG3	4:K:108:THR:HA	1.98	0.44
5:N:5:LEU:HD13	5:N:24:LYS:HB2	1.99	0.44
1:A:296:LEU:CD1	1:A:608:VAL:HG22	2.46	0.44
1:A:454:ARG:HD2	1:A:457:ARG:HB2	2.00	0.44
1:A:756:TYR:HA	1:B:970:PHE:CD1	2.53	0.44
1:A:970:PHE:CD2	1:A:999:GLY:HA3	2.53	0.44
1:B:184:GLY:C	1:B:186:PHE:H	2.21	0.44
1:B:396:TYR:HB2	1:B:514:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:GLY:C	1:C:186:PHE:H	2.21	0.44
2:F:69:GLY:CA	2:F:74:PHE:HA	2.47	0.44
3:G:67:ARG:HB3	3:G:84:ASN:HB2	1.99	0.44
3:G:94:TYR:HE2	3:G:116:VAL:HG11	1.82	0.44
4:H:24:GLY:HA3	4:H:29:ILE:HD12	1.98	0.44
3:I:73:ASP:OD2	3:I:80:TYR:CD2	2.70	0.44
4:M:24:GLY:HA3	4:M:29:ILE:HD12	1.99	0.44
1:A:422:ASN:HD22	1:A:454:ARG:H	1.65	0.44
1:B:29:THR:HG22	1:B:62:VAL:O	2.17	0.44
1:B:894:LEU:HD13	1:C:715:PRO:HD3	1.99	0.44
1:B:914:ASN:HA	1:C:1089:PHE:CE2	2.53	0.44
2:F:35:PHE:HE2	2:F:95:LYS:HB2	1.82	0.44
1:A:83:VAL:HA	1:A:239:GLN:HB2	2.00	0.44
1:A:100:ILE:HD13	1:A:263:ALA:HB2	1.98	0.44
1:A:143:VAL:O	1:A:245:HIS:HA	2.18	0.44
1:B:156:GLU:OE1	1:B:156:GLU:N	2.44	0.44
1:B:895:GLN:NE2	1:C:713:ALA:HB2	2.33	0.44
1:C:70:VAL:HG23	1:C:75:GLY:O	2.18	0.44
1:C:106:PHE:HB2	1:C:117:LEU:HD23	1.99	0.44
2:D:43:PRO:HD3	2:D:87:ALA:CB	2.48	0.44
3:I:51:ILE:HD12	3:I:70:ILE:HB	1.99	0.44
2:J:35:PHE:HD1	2:J:35:PHE:HA	1.73	0.44
1:A:184:GLY:C	1:A:186:PHE:H	2.21	0.44
1:B:143:VAL:O	1:B:245:HIS:HA	2.18	0.44
1:C:143:VAL:O	1:C:245:HIS:HA	2.18	0.44
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.47	0.44
4:K:48:LEU:CD1	4:K:87:TYR:CD1	3.00	0.44
1:A:246:ARG:HG3	5:L:32:GLU:OE1	2.18	0.44
1:C:205:SER:HB3	1:C:226:LEU:HD11	1.99	0.44
1:C:351:TYR:CE2	1:C:452:LEU:HB3	2.51	0.44
1:C:398:ASP:O	1:C:511:VAL:HA	2.18	0.44
2:F:37:ASN:HB3	2:F:39:PHE:CE2	2.53	0.44
5:P:33:VAL:HA	5:P:102:PRO:HD3	1.99	0.44
1:C:34:ARG:HE	1:C:216:LEU:HD23	1.83	0.43
1:C:374:PHE:CB	1:C:434:ILE:HG23	2.48	0.43
4:K:56:PRO:HD2	4:K:59:ILE:HG13	1.99	0.43
1:A:205:SER:HB3	1:A:226:LEU:HD11	1.99	0.43
1:A:1054:GLN:N	1:A:1061:VAL:O	2.50	0.43
1:A:1139:ASP:CG	1:A:1142:GLN:H	2.21	0.43
1:B:34:ARG:HE	1:B:216:LEU:HD23	1.83	0.43
1:B:315:THR:HG22	1:B:316:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:PHE:O	1:B:763:LEU:HG	2.19	0.43
1:B:970:PHE:CD2	1:B:999:GLY:HA3	2.53	0.43
1:C:341:VAL:HG22	1:C:356:LYS:HD3	2.00	0.43
2:D:37:ASN:HB3	2:D:39:PHE:CE2	2.53	0.43
3:E:18:LEU:HB2	3:E:86:LEU:HD11	2.00	0.43
3:E:32:TYR:HH	3:E:101:TYR:HH	1.62	0.43
2:J:37:ASN:HB3	2:J:39:PHE:CE2	2.54	0.43
4:M:84:GLU:HG3	4:M:108:THR:HA	1.98	0.43
1:A:256:SER:HG	5:L:28:TYR:HE1	1.66	0.43
1:A:759:PHE:O	1:A:763:LEU:HG	2.18	0.43
1:A:1089:PHE:CE2	1:C:917:TYR:HD2	2.36	0.43
1:B:83:VAL:HA	1:B:239:GLN:HB2	2.00	0.43
1:C:327:VAL:HA	1:C:542:ASN:CB	2.45	0.43
1:C:815:ARG:HD2	1:C:823:PHE:CE2	2.45	0.43
1:C:970:PHE:CD2	1:C:999:GLY:HA3	2.53	0.43
2:D:11:SER:HA	2:D:108:GLU:HB2	1.99	0.43
3:E:51:ILE:HB	3:E:70:ILE:HG21	2.00	0.43
3:E:68:PHE:HA	3:E:83:MET:HA	1.99	0.43
3:G:38:ARG:HA	3:G:94:TYR:HA	2.01	0.43
5:L:33:VAL:HA	5:L:102:PRO:HD3	1.99	0.43
4:M:11:SER:HB3	4:M:110:LEU:HD21	2.00	0.43
1:A:96:GLU:HB2	1:A:190:ARG:NH1	2.33	0.43
1:A:323:THR:OG1	1:A:537:LYS:HE3	2.18	0.43
1:A:426:PRO:HB3	1:A:429:PHE:CE2	2.53	0.43
1:A:1032:CYS:SG	1:A:1051:SER:OG	2.77	0.43
1:A:1077:THR:HG21	1:C:897:PRO:HG2	2.00	0.43
1:B:246:ARG:HH11	5:N:28:TYR:HD1	1.66	0.43
3:E:32:TYR:HB3	3:E:98:ARG:HG3	2.01	0.43
2:F:10:LEU:HD13	2:F:12:LEU:HD11	2.00	0.43
3:G:88:ALA:HA	3:G:118:VAL:O	2.17	0.43
1:A:567:ARG:HD2	1:C:44:ARG:NH2	2.33	0.43
1:A:946:GLY:O	1:A:950:ASP:N	2.44	0.43
1:B:422:ASN:HA	1:B:454:ARG:HE	1.83	0.43
1:B:1093:GLY:HA2	1:B:1107:ARG:HG3	1.99	0.43
1:C:256:SER:N	5:P:1:GLU:HA	2.33	0.43
2:F:35:PHE:HE2	2:F:95:LYS:HD3	1.84	0.43
4:H:36:TRP:CE2	4:H:74:LEU:HB2	2.54	0.43
2:J:64:ARG:HB2	2:J:78:ILE:HG23	1.99	0.43
5:P:4:LEU:HD22	5:P:25:VAL:HG12	1.99	0.43
5:P:68:ARG:HH22	5:P:88:ARG:HD3	1.84	0.43
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:OG1	1:B:537:LYS:HE3	2.18	0.43
1:B:364:ASP:OD1	1:B:388:ASN:ND2	2.52	0.43
1:C:83:VAL:HA	1:C:239:GLN:HB2	2.00	0.43
1:C:405:ASP:HB3	1:C:408:ARG:HH21	1.84	0.43
1:C:1032:CYS:SG	1:C:1051:SER:OG	2.77	0.43
3:E:94:TYR:HE2	3:E:116:VAL:HG11	1.83	0.43
2:F:43:PRO:HD3	2:F:87:ALA:CB	2.48	0.43
4:H:47:LEU:HG	4:H:56:PRO:HG2	2.01	0.43
2:J:86:PHE:HD2	2:J:109:ILE:HD12	1.80	0.43
4:K:44:ALA:CB	5:N:112:TRP:HE1	2.25	0.43
1:A:34:ARG:HD2	1:A:191:GLU:OE2	2.19	0.43
1:A:70:VAL:HG23	1:A:75:GLY:O	2.18	0.43
1:A:821:LEU:O	1:A:825:LYS:HG2	2.19	0.43
1:B:34:ARG:HD2	1:B:191:GLU:OE2	2.19	0.43
1:B:147:LYS:CE	5:N:52:PHE:CD1	2.99	0.43
1:B:1054:GLN:N	1:B:1061:VAL:O	2.50	0.43
1:C:1093:GLY:HA2	1:C:1107:ARG:HG3	1.99	0.43
3:E:97:ALA:HB1	3:E:107:VAL:HG11	2.00	0.43
2:J:98:PRO:O	2:J:100:ILE:HG23	2.19	0.43
5:N:109:PHE:HE1	5:N:112:TRP:CG	2.36	0.43
1:A:146:HIS:C	1:A:148:ASN:H	2.22	0.43
1:B:869:MET:HB3	1:C:699:LEU:HD21	2.01	0.43
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.19	0.43
1:C:821:LEU:O	1:C:825:LYS:HG2	2.19	0.43
1:C:1139:ASP:CG	1:C:1142:GLN:H	2.21	0.43
3:E:91:THR:HG23	3:E:117:THR:HA	2.01	0.43
2:F:34:SER:O	2:F:35:PHE:CD1	2.72	0.43
3:G:38:ARG:HB3	3:G:94:TYR:CD1	2.53	0.43
3:G:91:THR:HG23	3:G:117:THR:HA	2.01	0.43
2:J:34:SER:O	2:J:35:PHE:CD1	2.72	0.43
4:K:36:TRP:CE2	4:K:74:LEU:HB2	2.54	0.43
5:L:3:GLN:O	5:L:26:SER:OG	2.27	0.43
4:M:47:LEU:HG	4:M:56:PRO:HG2	2.01	0.43
1:A:66:HIS:CE1	1:A:264:ALA:CB	2.98	0.43
1:A:676:THR:HG23	1:A:690:GLN:HG2	2.01	0.43
1:A:1028:LYS:O	1:A:1032:CYS:N	2.46	0.43
1:B:70:VAL:HG23	1:B:75:GLY:O	2.18	0.43
1:B:96:GLU:HB2	1:B:190:ARG:NH1	2.34	0.43
1:B:205:SER:HB3	1:B:226:LEU:HD11	1.99	0.43
1:B:287:ASP:CG	1:B:306:PHE:CZ	2.91	0.43
1:B:393:THR:O	1:B:523:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ALA:HB3	1:B:414:GLN:HB3	2.00	0.43
1:C:759:PHE:O	1:C:763:LEU:HG	2.18	0.43
3:E:99:PHE:HA	3:E:106:THR:O	2.19	0.43
3:G:12:VAL:O	3:G:118:VAL:HG13	2.19	0.43
5:N:6:GLU:HG3	5:N:7:GLN:N	2.34	0.43
1:A:307:THR:HA	1:A:602:THR:HG21	2.01	0.43
1:A:315:THR:HG22	1:A:316:SER:N	2.33	0.43
1:B:298:GLU:OE2	1:B:316:SER:OG	2.21	0.43
1:B:307:THR:HA	1:B:602:THR:HG21	2.01	0.43
1:B:985:ASP:OD1	1:C:383:SER:CB	2.66	0.43
1:C:96:GLU:HB2	1:C:190:ARG:NH1	2.34	0.43
1:C:120:VAL:HG12	1:C:122:ASN:N	2.34	0.43
3:E:38:ARG:HB3	3:E:94:TYR:CD1	2.54	0.43
2:J:10:LEU:HD13	2:J:12:LEU:HD11	2.00	0.43
5:L:6:GLU:HG3	5:L:7:GLN:N	2.34	0.43
5:L:68:ARG:HH22	5:L:88:ARG:HD3	1.84	0.43
5:L:109:PHE:HE1	5:L:112:TRP:CG	2.36	0.43
1:A:287:ASP:CG	1:A:306:PHE:CZ	2.91	0.42
1:B:1032:CYS:SG	1:B:1051:SER:OG	2.77	0.42
2:F:23:ARG:HH11	2:F:73:ASP:CG	2.22	0.42
1:A:49:HIS:O	1:A:277:LEU:N	2.43	0.42
1:A:294:ASP:OD1	1:A:297:SER:N	2.45	0.42
1:B:676:THR:HG23	1:B:690:GLN:HG2	2.01	0.42
1:B:1088:HIS:C	1:B:1089:PHE:HD1	2.23	0.42
1:C:656:VAL:HG21	1:C:693:ILE:HD12	2.01	0.42
1:C:1028:LYS:O	1:C:1032:CYS:N	2.46	0.42
2:D:34:SER:O	2:D:35:PHE:CD1	2.72	0.42
3:E:39:GLN:HB2	3:E:45:LEU:CD2	2.49	0.42
3:G:39:GLN:HB2	3:G:45:LEU:CD2	2.49	0.42
1:B:30:ASN:HA	1:B:60:SER:O	2.19	0.42
1:B:821:LEU:O	1:B:825:LYS:HG2	2.19	0.42
1:C:186:PHE:C	1:C:188:ASN:H	2.22	0.42
2:D:35:PHE:HE2	2:D:95:LYS:HD3	1.84	0.42
2:F:101:PHE:CZ	3:G:37:VAL:HG11	2.54	0.42
4:H:34:VAL:HB	4:H:52:ASN:ND2	2.34	0.42
5:L:18:SER:HB3	5:L:83:GLU:OE2	2.19	0.42
5:N:18:SER:HB3	5:N:83:GLU:OE2	2.19	0.42
5:N:55:GLU:C	5:N:57:GLY:H	2.23	0.42
1:A:115:GLN:NE2	1:A:167:THR:HG21	2.34	0.42
1:B:294:ASP:OD1	1:B:297:SER:N	2.45	0.42
1:B:994:ASP:O	1:B:998:THR:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:PRO:HA	1:C:237:ARG:HA	2.02	0.42
1:C:327:VAL:C	1:C:542:ASN:O	2.53	0.42
2:D:37:ASN:OD1	2:D:52:TYR:HA	2.19	0.42
3:G:86:LEU:HA	3:G:90:ASP:OD2	2.20	0.42
2:J:23:ARG:HH11	2:J:73:ASP:CG	2.22	0.42
1:A:815:ARG:HD2	1:A:823:PHE:CE2	2.45	0.42
1:A:869:MET:CE	1:B:669:GLY:HA3	2.49	0.42
1:A:1088:HIS:C	1:A:1089:PHE:HD1	2.23	0.42
1:B:66:HIS:CE1	1:B:264:ALA:CB	2.98	0.42
1:B:115:GLN:NE2	1:B:167:THR:HG21	2.34	0.42
1:B:422:ASN:ND2	1:B:454:ARG:H	2.18	0.42
1:B:825:LYS:HE3	1:B:938:LEU:O	2.19	0.42
1:C:330:PRO:CD	1:C:525:CYS:SG	3.07	0.42
1:C:825:LYS:HE3	1:C:938:LEU:O	2.19	0.42
2:D:23:ARG:HH11	2:D:73:ASP:CG	2.22	0.42
3:G:51:ILE:HB	3:G:70:ILE:HG21	2.00	0.42
4:M:36:TRP:CE2	4:M:74:LEU:HB2	2.54	0.42
1:A:825:LYS:HE3	1:A:938:LEU:O	2.19	0.42
1:B:146:HIS:C	1:B:148:ASN:H	2.22	0.42
1:B:247:SER:HB3	1:B:257:GLY:HA3	2.02	0.42
1:B:327:VAL:O	1:B:531:THR:N	2.52	0.42
1:C:394:ASN:CA	1:C:516:GLU:CD	2.85	0.42
2:D:50:LEU:O	2:D:51:ILE:HD13	2.20	0.42
3:E:38:ARG:HA	3:E:94:TYR:HA	2.01	0.42
3:E:86:LEU:HA	3:E:90:ASP:OD2	2.20	0.42
2:F:37:ASN:OD1	2:F:52:TYR:HA	2.20	0.42
3:G:20:LEU:HD12	3:G:81:LEU:HD23	2.02	0.42
3:I:2:VAL:HG12	3:I:3:LYS:HG3	2.02	0.42
5:L:30:LEU:HB3	5:L:31:PRO:HD3	2.02	0.42
5:L:55:GLU:C	5:L:57:GLY:H	2.23	0.42
5:P:55:GLU:C	5:P:57:GLY:H	2.23	0.42
1:A:287:ASP:OD2	1:A:306:PHE:CG	2.68	0.42
1:B:452:LEU:HG	1:B:494:SER:HA	2.00	0.42
1:B:730:SER:O	1:B:1058:HIS:HB3	2.20	0.42
1:C:34:ARG:HD2	1:C:191:GLU:OE2	2.19	0.42
2:F:41:GLN:HA	2:F:47:PRO:HA	2.01	0.42
2:F:50:LEU:O	2:F:51:ILE:HD13	2.20	0.42
2:J:41:GLN:HA	2:J:47:PRO:HA	2.01	0.42
5:P:6:GLU:HG3	5:P:7:GLN:N	2.34	0.42
1:A:34:ARG:HE	1:A:216:LEU:HD23	1.83	0.42
1:A:85:PRO:HA	1:A:237:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLN:N	1:C:41:LYS:HB3	2.34	0.42
1:A:1094:VAL:HG11	1:C:904:TYR:OH	2.20	0.42
1:B:160:TYR:HE2	1:B:163:ALA:HB2	1.85	0.42
1:C:115:GLN:NE2	1:C:167:THR:HG21	2.34	0.42
4:H:11:SER:HB3	4:H:110:LEU:HD21	2.00	0.42
2:J:35:PHE:HE2	2:J:95:LYS:HD3	1.83	0.42
5:P:18:SER:HB3	5:P:83:GLU:OE2	2.19	0.42
1:B:186:PHE:C	1:B:188:ASN:H	2.22	0.42
1:C:676:THR:HG23	1:C:690:GLN:HG2	2.01	0.42
2:D:41:GLN:HA	2:D:47:PRO:HA	2.01	0.42
3:E:12:VAL:O	3:E:118:VAL:HG13	2.19	0.42
3:G:18:LEU:HB2	3:G:86:LEU:HD11	2.00	0.42
1:A:75:GLY:O	1:A:76:THR:OG1	2.35	0.42
1:A:160:TYR:HE2	1:A:163:ALA:HB2	1.85	0.42
1:B:444:LYS:HB2	1:B:447:GLY:H	1.85	0.42
1:B:453:TYR:HB3	1:B:495:TYR:CZ	2.54	0.42
1:B:852:ALA:HA	1:B:855:PHE:CE2	2.54	0.42
1:C:276:LEU:HD11	1:C:306:PHE:CE1	2.53	0.42
1:C:852:ALA:HA	1:C:855:PHE:CE2	2.54	0.42
1:C:1088:HIS:C	1:C:1089:PHE:HD1	2.23	0.42
2:J:50:LEU:O	2:J:51:ILE:HD13	2.19	0.42
1:A:730:SER:O	1:A:1058:HIS:HB3	2.20	0.41
1:C:921:LYS:HA	1:C:921:LYS:HD2	1.90	0.41
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.19	0.41
4:H:39:GLN:OE1	4:H:45:PRO:HG3	2.20	0.41
5:L:103:PHE:HA	5:L:104:SER:HA	1.67	0.41
4:M:39:GLN:OE1	4:M:45:PRO:HG3	2.20	0.41
1:A:30:ASN:HA	1:A:60:SER:O	2.19	0.41
1:A:570:ALA:HB1	1:C:963:VAL:HG11	2.02	0.41
1:A:713:ALA:HB2	1:C:895:GLN:CD	2.40	0.41
1:B:806:LEU:HA	1:B:806:LEU:HD23	1.82	0.41
1:C:50:SER:HA	1:C:275:PHE:O	2.21	0.41
1:C:100:ILE:HG21	1:C:263:ALA:CB	2.46	0.41
1:C:291:CYS:O	1:C:298:GLU:HG3	2.19	0.41
1:C:472:ILE:HG22	1:C:480:CYS:SG	2.60	0.41
3:I:22:CYS:HB3	3:I:79:LEU:HB3	2.00	0.41
4:K:11:SER:HB3	4:K:110:LEU:HD21	2.01	0.41
5:L:37:TRP:O	5:L:49:MET:N	2.49	0.41
5:N:68:ARG:HH22	5:N:88:ARG:HD3	1.84	0.41
1:A:199:GLY:HA3	1:B:521:PRO:HG3	2.02	0.41
1:A:418:ILE:HG23	1:A:422:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LYS:O	1:A:584:ILE:HG13	2.21	0.41
1:A:852:ALA:HA	1:A:855:PHE:CE2	2.54	0.41
1:B:324:GLU:CD	1:B:534:VAL:HG21	2.27	0.41
1:B:382:VAL:CG1	1:B:383:SER:N	2.82	0.41
1:C:559:PHE:HB2	1:C:563:GLN:HB3	2.03	0.41
2:D:18:ALA:O	2:D:77:THR:HA	2.20	0.41
3:I:47:TRP:HH2	3:I:99:PHE:CZ	2.38	0.41
1:A:453:TYR:HB3	1:A:495:TYR:CZ	2.55	0.41
1:A:555:SER:OG	1:A:584:ILE:O	2.34	0.41
1:C:160:TYR:HE2	1:C:163:ALA:HB2	1.85	0.41
1:C:203:ILE:HG22	1:C:226:LEU:HD12	2.03	0.41
1:C:802:PHE:HE1	1:C:927:PHE:CE2	2.39	0.41
1:C:1054:GLN:N	1:C:1061:VAL:O	2.50	0.41
5:N:30:LEU:HB3	5:N:31:PRO:HD3	2.01	0.41
1:A:38:TYR:CD2	1:B:562:PHE:HZ	2.39	0.41
1:C:200:TYR:HA	1:C:229:LEU:O	2.20	0.41
1:C:329:PHE:HD1	1:C:525:CYS:HG	1.66	0.41
2:D:35:PHE:HD1	2:D:35:PHE:HA	1.72	0.41
2:D:53:ALA:O	2:D:55:SER:N	2.53	0.41
3:I:47:TRP:HH2	3:I:99:PHE:CE1	2.39	0.41
1:A:36:VAL:O	1:A:222:ALA:HA	2.21	0.41
1:A:64:TRP:CZ2	1:A:214:ARG:HD2	2.56	0.41
1:B:358:ILE:HB	1:B:395:VAL:HB	2.02	0.41
1:B:447:GLY:HA2	1:B:497:PHE:O	2.20	0.41
1:B:864:LEU:O	1:C:669:GLY:N	2.51	0.41
1:C:327:VAL:HG12	1:C:542:ASN:HB2	1.99	0.41
1:C:536:ASN:N	1:C:552:LEU:O	2.39	0.41
1:C:902:MET:HE1	1:C:1049:LEU:HD13	2.03	0.41
2:F:18:ALA:O	2:F:77:THR:HA	2.20	0.41
4:H:38:GLN:O	4:H:45:PRO:HA	2.21	0.41
4:H:86:ASP:HA	4:H:106:LYS:HA	2.03	0.41
4:K:37:TYR:HD1	4:K:47:LEU:HA	1.84	0.41
4:M:38:GLN:O	4:M:45:PRO:HA	2.21	0.41
1:A:568:ASP:OD1	1:A:569:ILE:N	2.45	0.41
1:A:735:SER:O	1:A:859:THR:OG1	2.27	0.41
1:A:927:PHE:HE1	1:A:1065:VAL:HG21	1.86	0.41
1:B:857:GLY:HA2	1:C:592:PHE:CE2	2.55	0.41
1:C:557:LYS:O	1:C:584:ILE:HG13	2.21	0.41
1:C:796:ASP:N	1:C:796:ASP:OD1	2.46	0.41
3:I:28:THR:OG1	3:I:31:ASN:CB	2.68	0.41
4:K:49:ILE:HD13	4:K:55:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:86:ASP:HA	4:K:106:LYS:HA	2.02	0.41
5:P:30:LEU:HB3	5:P:31:PRO:HD3	2.01	0.41
1:B:857:GLY:HA2	1:C:592:PHE:HE2	1.86	0.41
1:C:118:LEU:CD2	1:C:129:LYS:HD2	2.51	0.41
1:C:994:ASP:O	1:C:998:THR:N	2.46	0.41
2:F:35:PHE:HB3	2:F:36:MET:H	1.52	0.41
2:F:51:ILE:HD12	2:F:56:ASN:O	2.21	0.41
2:F:53:ALA:O	2:F:55:SER:N	2.53	0.41
5:L:48:TRP:CZ2	5:L:51:GLY:HA3	2.56	0.41
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.56	0.41
1:A:203:ILE:HG22	1:A:226:LEU:HD12	2.03	0.41
1:A:247:SER:HB3	1:A:257:GLY:HA3	2.02	0.41
1:B:50:SER:HA	1:B:275:PHE:O	2.21	0.41
1:B:85:PRO:HA	1:B:237:ARG:HA	2.01	0.41
1:B:147:LYS:HZ2	5:N:34:ALA:CB	2.25	0.41
1:B:190:ARG:HG2	1:B:207:HIS:ND1	2.36	0.41
1:B:296:LEU:CD1	1:B:608:VAL:HG22	2.46	0.41
1:B:391:CYS:HB3	1:B:526:GLY:H	1.85	0.41
1:B:392:PHE:CE1	1:B:515:PHE:HB2	2.55	0.41
1:B:557:LYS:O	1:B:584:ILE:HG13	2.21	0.41
1:B:927:PHE:HE1	1:B:1065:VAL:HG21	1.86	0.41
1:B:1052:PHE:HB2	1:B:1063:LEU:HB2	2.03	0.41
1:C:82:PRO:HG2	1:C:84:LEU:HD21	2.03	0.41
1:C:328:ARG:HD3	1:C:328:ARG:HA	1.70	0.41
1:C:1089:PHE:N	1:C:1089:PHE:CD1	2.89	0.41
2:D:48:ARG:NH2	2:D:61:ILE:HD13	2.36	0.41
3:G:94:TYR:CE2	3:G:116:VAL:HG11	2.56	0.41
2:J:110:LEU:O	2:J:111:LYS:HB3	2.21	0.41
4:K:44:ALA:HA	4:K:45:PRO:HD3	1.98	0.41
1:A:186:PHE:C	1:A:188:ASN:H	2.22	0.41
1:A:308:VAL:H	1:A:602:THR:CG2	2.34	0.41
1:B:36:VAL:O	1:B:222:ALA:HA	2.21	0.41
1:B:82:PRO:HG2	1:B:84:LEU:HD21	2.03	0.41
1:B:201:PHE:CB	1:B:231:ILE:HG13	2.30	0.41
1:C:19:THR:HG22	1:C:138:ASP:OD1	2.21	0.41
1:C:293:LEU:HD12	1:C:293:LEU:HA	1.84	0.41
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	2.03	0.41
3:E:53:SER:HA	3:E:72:ARG:NH1	2.36	0.41
2:J:48:ARG:NH2	2:J:61:ILE:HD13	2.36	0.41
5:N:48:TRP:CZ2	5:N:51:GLY:HA3	2.56	0.41
5:P:3:GLN:O	5:P:26:SER:OG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HG2	1:A:207:HIS:ND1	2.36	0.40
1:A:205:SER:O	1:A:223:LEU:HG	2.21	0.40
1:A:534:VAL:CG1	1:A:537:LYS:HE2	2.51	0.40
1:A:563:GLN:HB3	1:C:41:LYS:O	2.20	0.40
1:B:921:LYS:HA	1:B:921:LYS:HD2	1.89	0.40
1:C:730:SER:O	1:C:1058:HIS:HB3	2.20	0.40
4:H:36:TRP:HA	4:H:88:TYR:O	2.21	0.40
4:K:100:VAL:O	5:N:107:TYR:OH	2.39	0.40
4:M:86:ASP:HA	4:M:106:LYS:HA	2.02	0.40
1:A:290:ASP:OD1	1:A:291:CYS:N	2.54	0.40
1:B:64:TRP:CZ2	1:B:214:ARG:HD2	2.56	0.40
1:C:205:SER:O	1:C:223:LEU:HG	2.21	0.40
2:D:14:PRO:HG3	2:D:83:PRO:HD3	2.04	0.40
2:D:51:ILE:HD12	2:D:56:ASN:O	2.21	0.40
2:D:110:LEU:O	2:D:111:LYS:HB3	2.21	0.40
2:J:18:ALA:O	2:J:77:THR:HA	2.20	0.40
2:J:53:ALA:O	2:J:55:SER:N	2.53	0.40
4:M:36:TRP:HA	4:M:88:TYR:O	2.21	0.40
5:P:48:TRP:CZ2	5:P:51:GLY:HA3	2.56	0.40
1:A:82:PRO:HG2	1:A:84:LEU:HD21	2.03	0.40
1:A:426:PRO:CG	1:A:429:PHE:CE2	3.01	0.40
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	2.03	0.40
1:B:534:VAL:CG1	1:B:537:LYS:HE2	2.51	0.40
1:B:802:PHE:HE1	1:B:927:PHE:CE2	2.39	0.40
1:C:394:ASN:CG	1:C:516:GLU:CD	2.65	0.40
2:F:110:LEU:O	2:F:111:LYS:HB3	2.21	0.40
2:J:99:ARG:O	2:J:100:ILE:HG13	2.21	0.40
5:P:21:VAL:O	5:P:82:MET:N	2.47	0.40
1:A:246:ARG:HH11	5:L:28:TYR:HD1	1.69	0.40
1:A:823:PHE:CD1	1:A:1057:PRO:HG3	2.57	0.40
1:A:994:ASP:O	1:A:998:THR:N	2.46	0.40
1:B:1089:PHE:N	1:B:1089:PHE:CD1	2.89	0.40
1:C:190:ARG:HG2	1:C:207:HIS:ND1	2.36	0.40
1:C:612:TYR:O	1:C:649:CYS:N	2.53	0.40
1:C:946:GLY:O	1:C:950:ASP:N	2.44	0.40
2:J:14:PRO:HG3	2:J:83:PRO:HD3	2.04	0.40
1:A:50:SER:HA	1:A:275:PHE:O	2.21	0.40
1:A:970:PHE:HD1	1:C:756:TYR:HA	1.87	0.40
1:A:978:ASN:O	1:A:982:SER:N	2.52	0.40
1:B:49:HIS:O	1:B:277:LEU:N	2.43	0.40
1:B:472:ILE:HA	1:B:491:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:TYR:HA	1:C:703:ASN:O	2.21	0.40
1:C:73:THR:HG23	1:C:74:ASN:N	2.33	0.40
1:C:290:ASP:OD1	1:C:291:CYS:N	2.54	0.40
1:C:348:ALA:O	1:C:400:PHE:HA	2.22	0.40
3:E:20:LEU:HD12	3:E:81:LEU:HD23	2.01	0.40
3:E:50:GLU:OE1	3:E:99:PHE:HZ	2.04	0.40
3:G:81:LEU:HD12	3:G:81:LEU:HA	1.92	0.40
5:P:69:VAL:HA	5:P:83:GLU:O	2.22	0.40
5:P:98:ALA:CB	5:P:109:PHE:CD1	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1051/1134 (93%)	986 (94%)	62 (6%)	3 (0%)	41	74
1	B	1057/1134 (93%)	990 (94%)	64 (6%)	3 (0%)	41	74
1	C	1060/1134 (94%)	982 (93%)	74 (7%)	4 (0%)	34	69
2	D	109/111 (98%)	93 (85%)	14 (13%)	2 (2%)	8	41
2	F	109/111 (98%)	93 (85%)	14 (13%)	2 (2%)	8	41
2	J	109/111 (98%)	90 (83%)	14 (13%)	5 (5%)	2	23
3	E	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	54
3	G	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	17	54
3	I	116/118 (98%)	99 (85%)	15 (13%)	2 (2%)	9	42
4	H	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
4	K	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
4	M	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
5	L	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	19	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	N	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	19	56
5	P	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	19	56
All	All	4518/4776 (95%)	4180 (92%)	312 (7%)	26 (1%)	29	62

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	B	62	VAL
1	C	561	PRO
2	D	33	ILE
3	E	63	THR
2	F	33	ILE
3	G	63	THR
2	J	33	ILE
2	J	100	ILE
2	J	103	GLN
2	J	104	GLY
1	C	284	THR
1	C	617	CYS
3	I	9	GLY
2	J	99	ARG
5	P	110	ASP
2	D	100	ILE
2	F	100	ILE
1	A	124	THR
1	B	124	THR
1	C	517	LEU
1	A	24	LEU
1	B	24	LEU
3	I	48	VAL
5	L	110	ASP
5	N	110	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	929/985 (94%)	923 (99%)	6 (1%)	86	93
1	B	934/985 (95%)	928 (99%)	6 (1%)	86	93
1	C	938/985 (95%)	923 (98%)	15 (2%)	62	80
2	D	91/95 (96%)	91 (100%)	0	100	100
2	F	92/95 (97%)	92 (100%)	0	100	100
2	J	92/95 (97%)	89 (97%)	3 (3%)	38	64
3	E	92/93 (99%)	92 (100%)	0	100	100
3	G	92/93 (99%)	87 (95%)	5 (5%)	22	54
3	I	92/93 (99%)	80 (87%)	12 (13%)	4	22
4	H	88/88 (100%)	88 (100%)	0	100	100
4	K	88/88 (100%)	88 (100%)	0	100	100
4	M	88/88 (100%)	88 (100%)	0	100	100
5	L	101/101 (100%)	101 (100%)	0	100	100
5	N	101/101 (100%)	101 (100%)	0	100	100
5	P	101/101 (100%)	101 (100%)	0	100	100
All	All	3919/4086 (96%)	3872 (99%)	47 (1%)	72	84

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	400	PHE
1	A	434	ILE
1	A	466	ARG
1	A	615	VAL
1	A	1098	ASN
1	B	61	ASN
1	B	422	ASN
1	B	466	ARG
1	B	500	THR
1	B	615	VAL
1	B	984	LEU
1	C	121	ASN
1	C	282	ASN
1	C	285	ILE
1	C	325	SER
1	C	382	VAL
1	C	429	PHE

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Mol	Chain	Res	Type
1	C	452	LEU
1	C	456	PHE
1	C	533	LEU
1	C	559	PHE
1	C	562	PHE
1	C	563	GLN
1	C	564	GLN
1	C	590	CYS
1	C	656	VAL
3	G	53	SER
3	G	57	TYR
3	G	59	TYR
3	G	106	THR
3	G	110	TRP
3	I	48	VAL
3	I	52	SER
3	I	53	SER
3	I	59	TYR
3	I	60	TYR
3	I	62	ASP
3	I	64	VAL
3	I	65	THR
3	I	67	ARG
3	I	69	THR
3	I	70	ILE
3	I	72	ARG
2	J	97	VAL
2	J	99	ARG
2	J	101	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands 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	$\#\|Z\| > 2$
6	NAG	A	1202	1	14,14,15	0.30	0	17,19,21	0.63	0
6	NAG	B	1201	1	14,14,15	0.31	0	17,19,21	0.55	0
6	NAG	C	1202	1	14,14,15	0.98	1 (7%)	17,19,21	1.83	3 (17%)
6	NAG	B	1203	1	14,14,15	0.27	0	17,19,21	0.57	0
6	NAG	C	1201	1	14,14,15	0.27	0	17,19,21	1.36	3 (17%)
6	NAG	C	1204	1	14,14,15	0.30	0	17,19,21	1.25	3 (17%)
6	NAG	C	1206	1	14,14,15	0.33	0	17,19,21	0.68	0
6	NAG	A	1204	1	14,14,15	0.35	0	17,19,21	0.64	0
6	NAG	B	1202	1	14,14,15	1.01	1 (7%)	17,19,21	2.47	5 (29%)
6	NAG	A	1203	1	14,14,15	1.10	1 (7%)	17,19,21	1.97	3 (17%)
6	NAG	A	1205	1	14,14,15	0.29	0	17,19,21	0.58	0
6	NAG	C	1205	1	14,14,15	0.52	0	17,19,21	1.65	2 (11%)
6	NAG	C	1203	1	14,14,15	0.30	0	17,19,21	0.63	0
6	NAG	A	1201	1	14,14,15	0.33	0	17,19,21	0.71	0

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
6	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1201	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1202	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1205	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1206	1	1/1/6/7	4/6/23/26	0/1/1/1
6	NAG	C	1204	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1204	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1202	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1201	1	1/1/6/7	3/6/23/26	0/1/1/1
6	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1201	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1203	NAG	C1-C2	3.98	1.58	1.52
6	B	1202	NAG	C1-C2	3.66	1.57	1.52
6	C	1202	NAG	C1-C2	3.55	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1202	NAG	O5-C1-C2	-7.02	100.20	111.29
6	A	1203	NAG	O5-C1-C2	-6.29	101.36	111.29
6	C	1202	NAG	O5-C1-C2	-5.93	101.93	111.29
6	C	1205	NAG	C1-O5-C5	5.91	120.19	112.19
6	B	1202	NAG	C2-N2-C7	4.17	128.84	122.90
6	B	1202	NAG	C4-C3-C2	-3.85	105.37	111.02
6	B	1202	NAG	C1-C2-N2	3.27	116.07	110.49
6	C	1202	NAG	C1-O5-C5	3.19	116.51	112.19
6	C	1201	NAG	C1-C2-N2	-2.98	105.39	110.49
6	A	1203	NAG	C1-O5-C5	2.95	116.19	112.19
6	C	1201	NAG	C2-N2-C7	-2.83	118.87	122.90
6	C	1201	NAG	O3-C3-C2	2.70	115.06	109.47
6	C	1204	NAG	C1-O5-C5	2.68	115.82	112.19
6	A	1203	NAG	C4-C3-C2	-2.38	107.53	111.02
6	C	1204	NAG	C1-C2-N2	-2.21	106.71	110.49
6	B	1202	NAG	C3-C4-C5	-2.16	106.39	110.24
6	C	1202	NAG	C4-C3-C2	-2.13	107.89	111.02
6	C	1204	NAG	C2-N2-C7	2.05	125.82	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1205	NAG	O5-C1-C2	-2.04	108.06	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	1201	NAG	C1
6	C	1206	NAG	C1

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1201	NAG	C8-C7-N2-C2
6	A	1201	NAG	O7-C7-N2-C2
6	B	1202	NAG	C8-C7-N2-C2
6	B	1202	NAG	O7-C7-N2-C2
6	C	1201	NAG	C8-C7-N2-C2
6	C	1201	NAG	O7-C7-N2-C2
6	C	1204	NAG	C3-C2-N2-C7
6	C	1204	NAG	C8-C7-N2-C2
6	C	1204	NAG	O7-C7-N2-C2
6	C	1205	NAG	C8-C7-N2-C2
6	C	1205	NAG	O7-C7-N2-C2
6	A	1205	NAG	C8-C7-N2-C2
6	A	1205	NAG	O7-C7-N2-C2
6	C	1202	NAG	C8-C7-N2-C2
6	C	1202	NAG	O7-C7-N2-C2
6	C	1206	NAG	C8-C7-N2-C2
6	C	1206	NAG	O7-C7-N2-C2
6	C	1206	NAG	O5-C5-C6-O6
6	C	1206	NAG	C4-C5-C6-O6
6	A	1202	NAG	C8-C7-N2-C2
6	B	1201	NAG	C8-C7-N2-C2
6	B	1201	NAG	O7-C7-N2-C2
6	B	1202	NAG	C1-C2-N2-C7
6	A	1202	NAG	O7-C7-N2-C2
6	A	1204	NAG	C8-C7-N2-C2
6	A	1204	NAG	O7-C7-N2-C2
6	A	1204	NAG	O5-C5-C6-O6
6	A	1205	NAG	O5-C5-C6-O6
6	B	1202	NAG	O5-C5-C6-O6
6	C	1201	NAG	C3-C2-N2-C7
6	C	1204	NAG	C1-C2-N2-C7

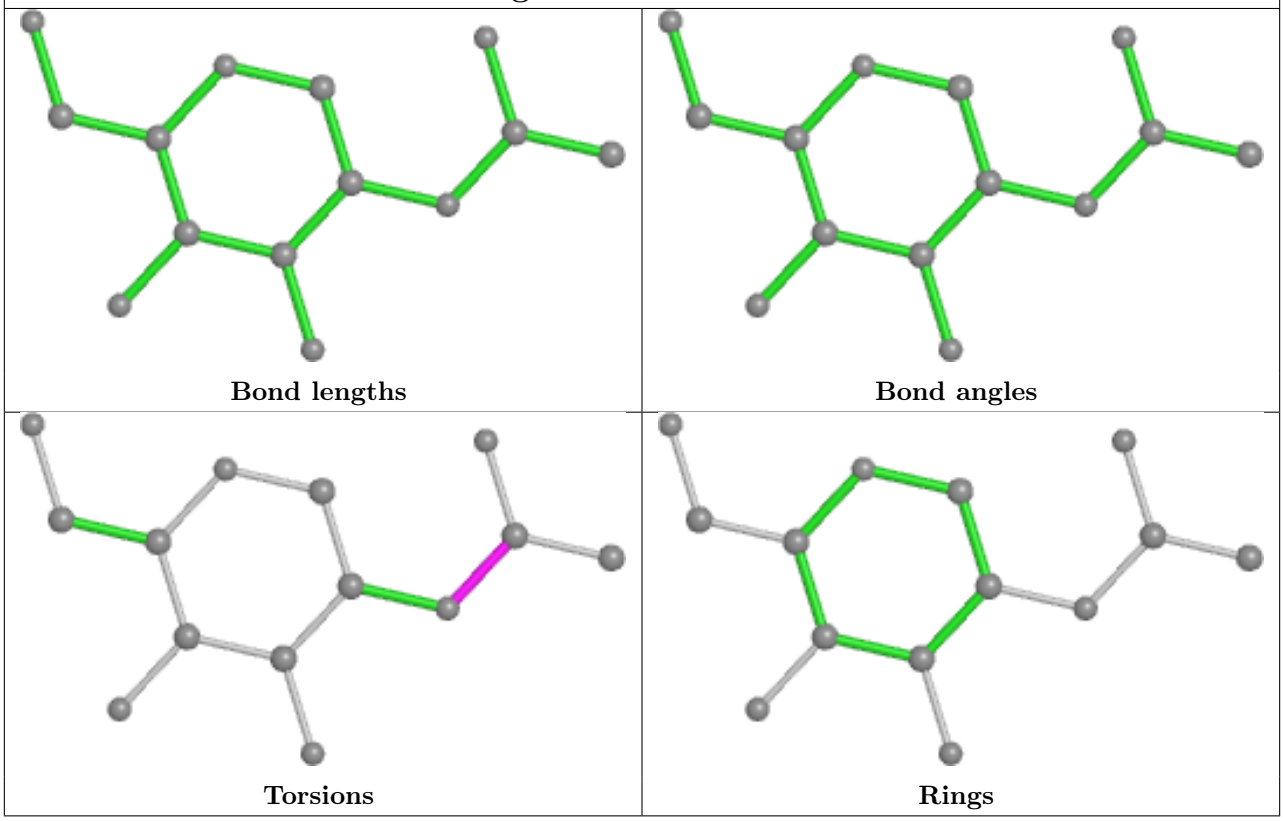
There are no ring outliers.

3 monomers are involved in 4 short contacts:

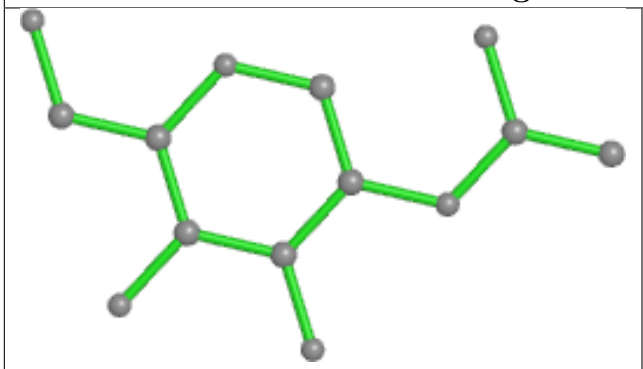
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1201	NAG	2	0
6	C	1204	NAG	1	0
6	B	1202	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

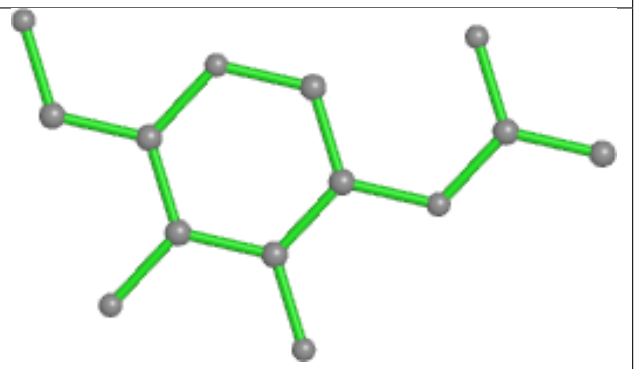
Ligand NAG A 1202



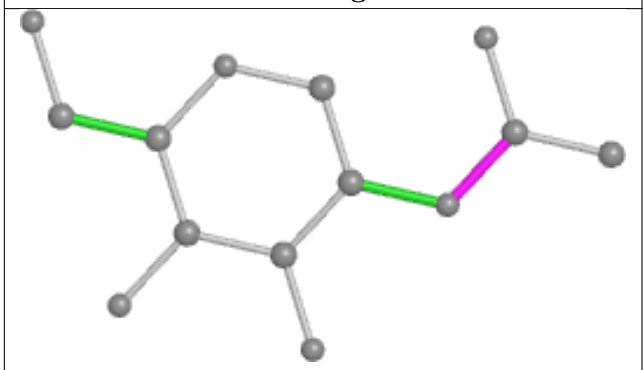
Ligand NAG B 1201



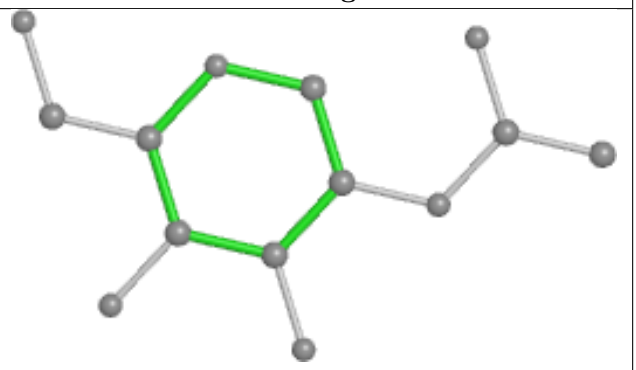
Bond lengths



Bond angles

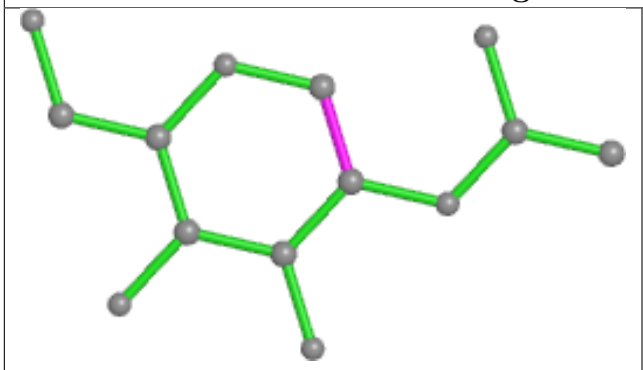


Torsions



Rings

Ligand NAG C 1202



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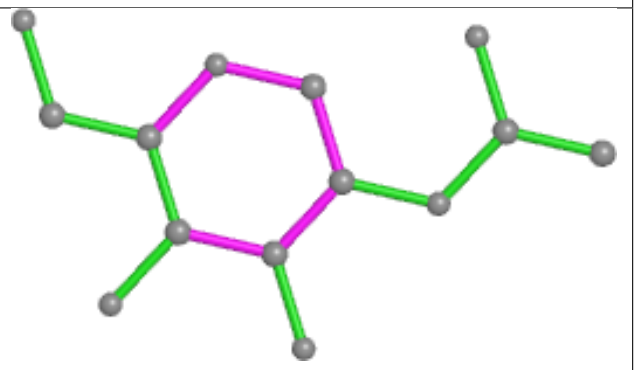
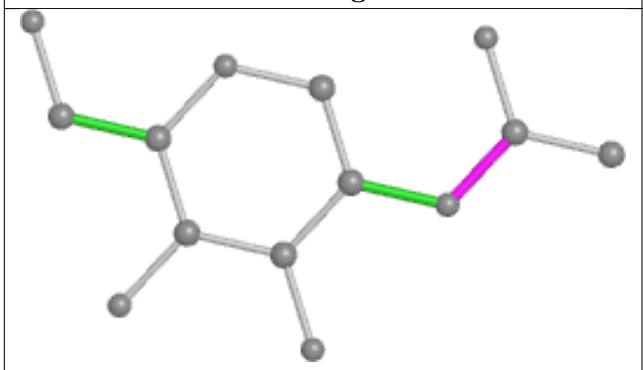


Bond angles



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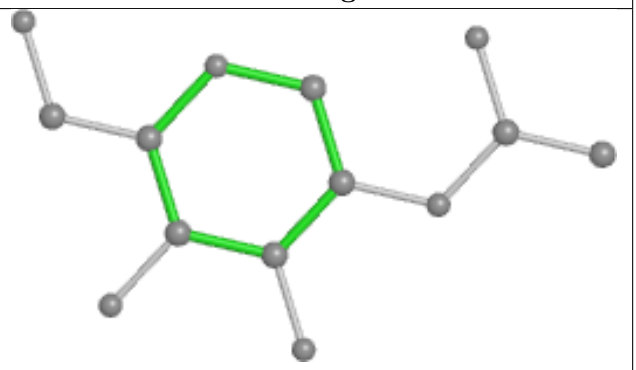
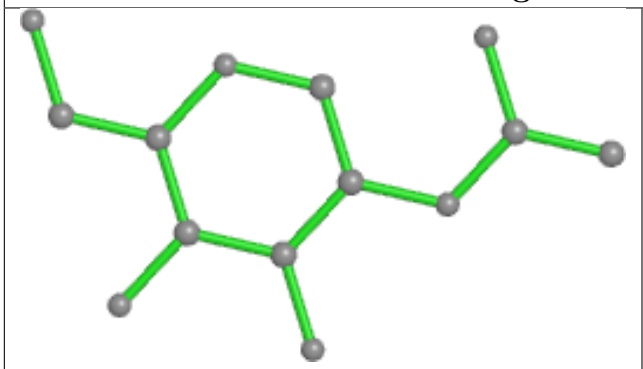
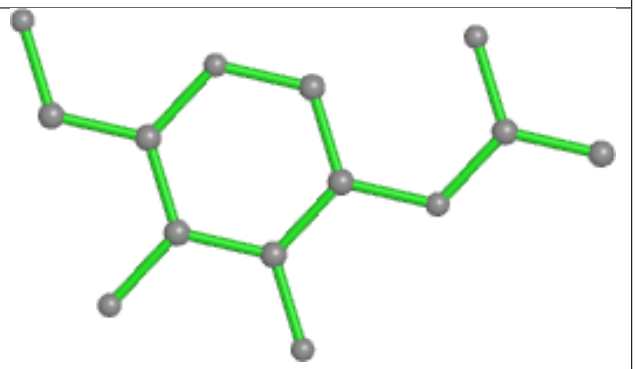


Rings

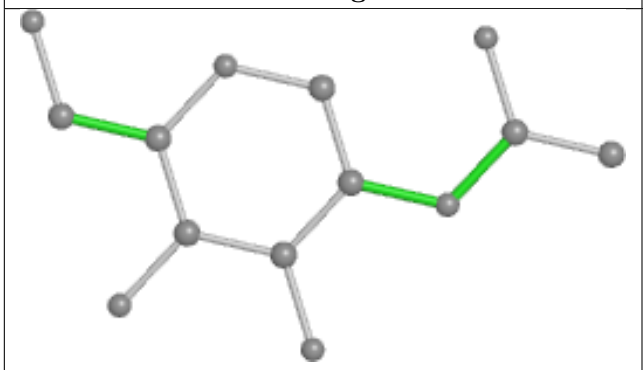
Ligand NAG B 1203



Bond lengths



Bond angles



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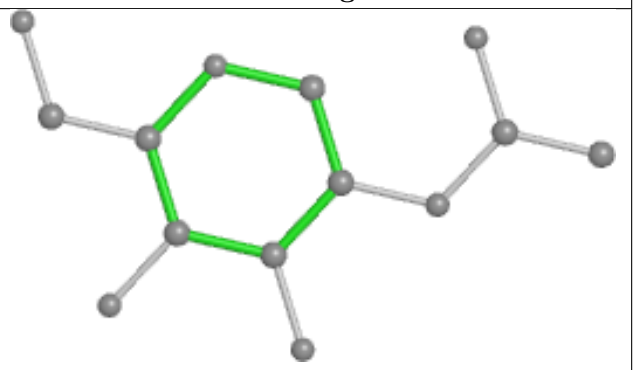
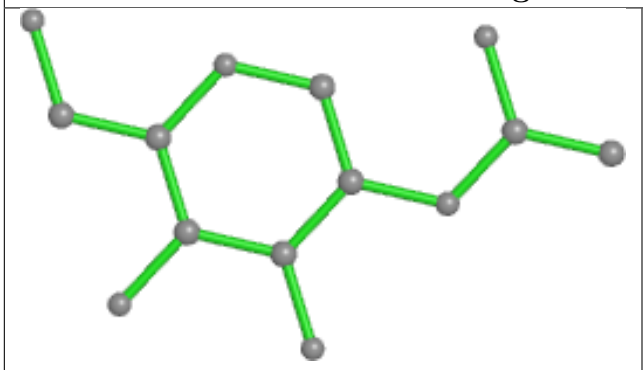
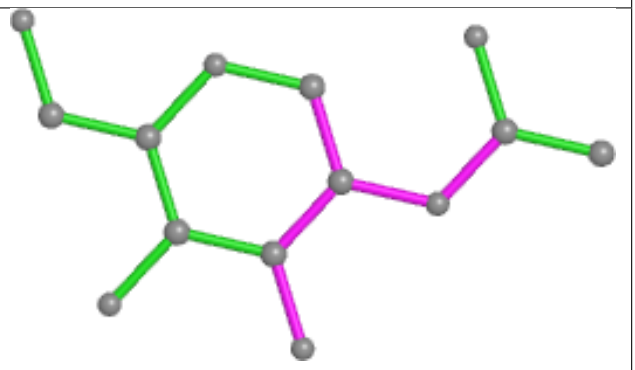


Rings

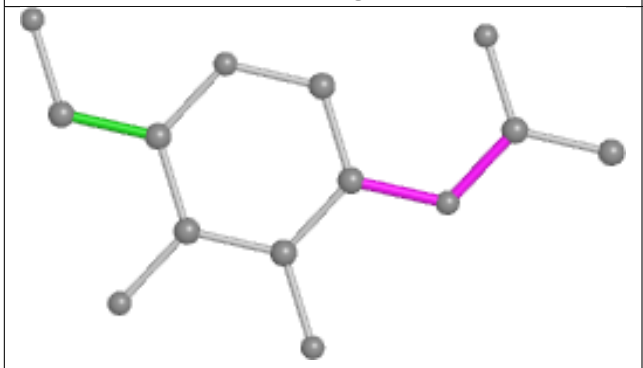
Ligand NAG C 1201



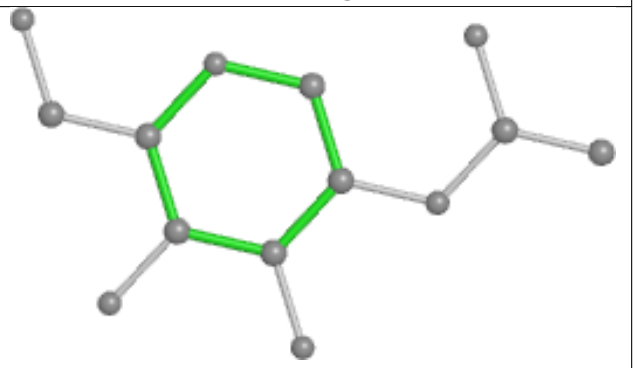
Bond lengths



Bond angles

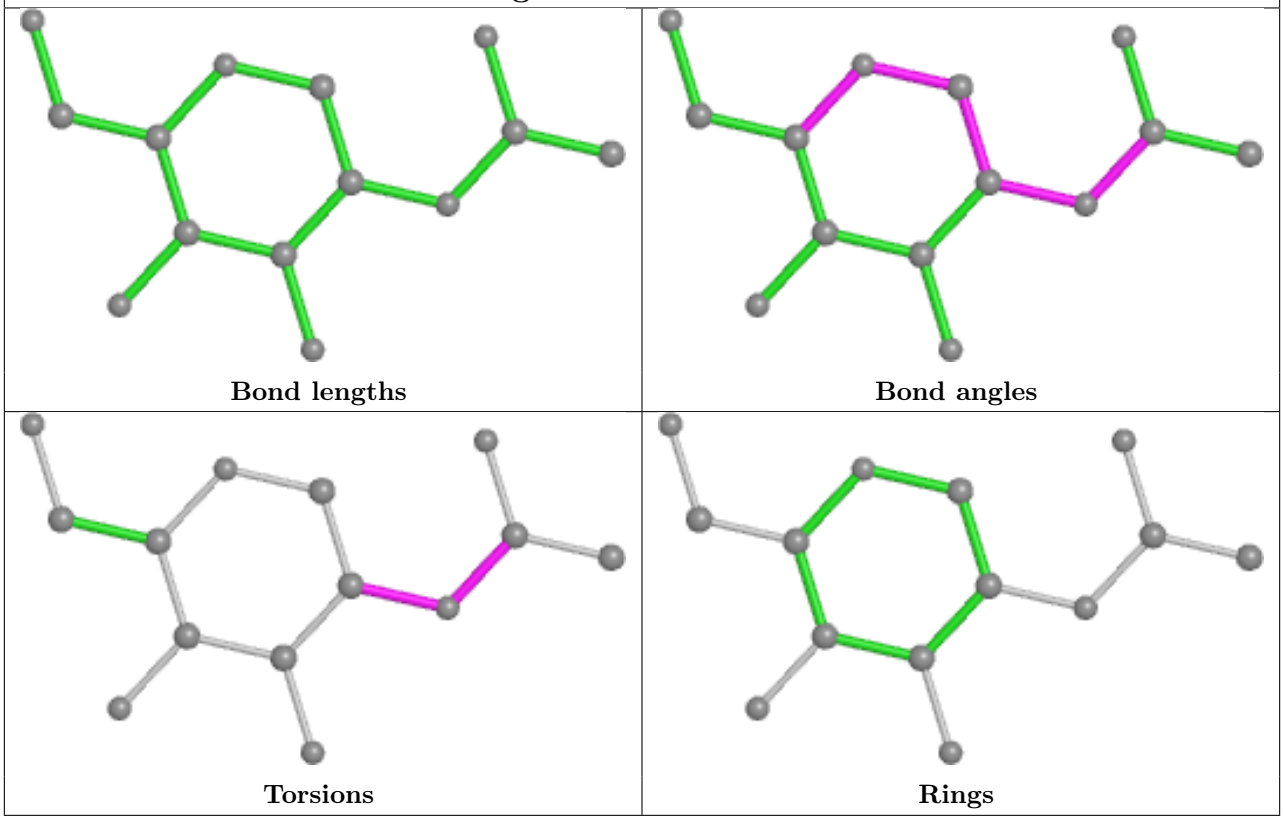


Torsions

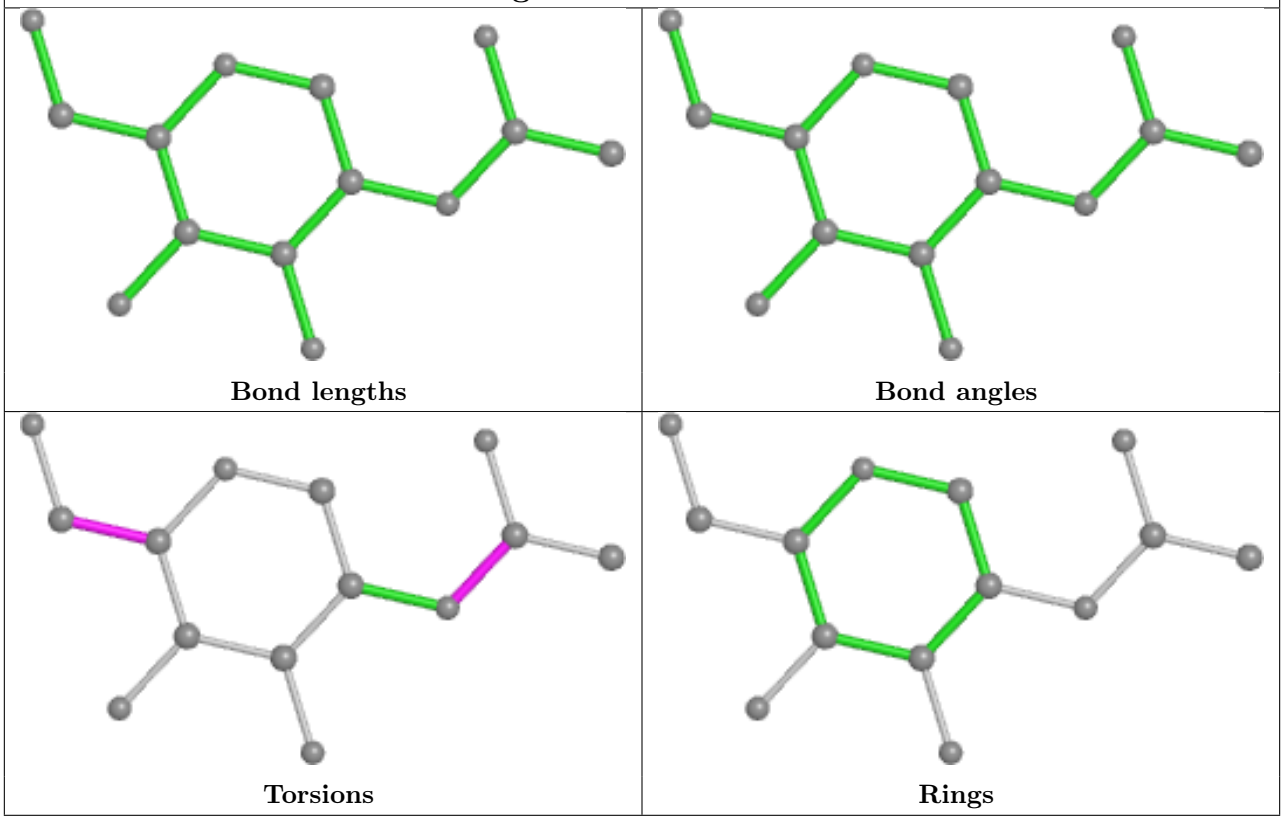


Rings

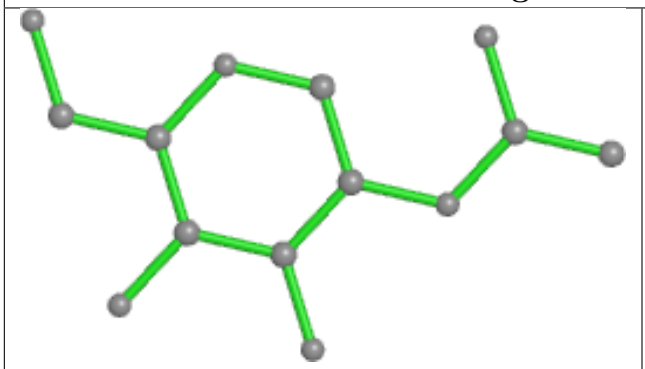
Ligand NAG C 1204



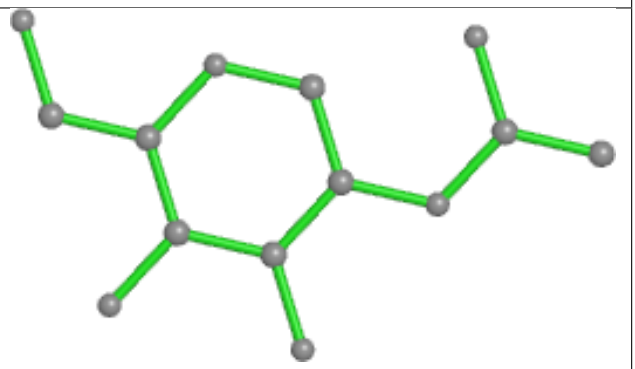
Ligand NAG C 1206



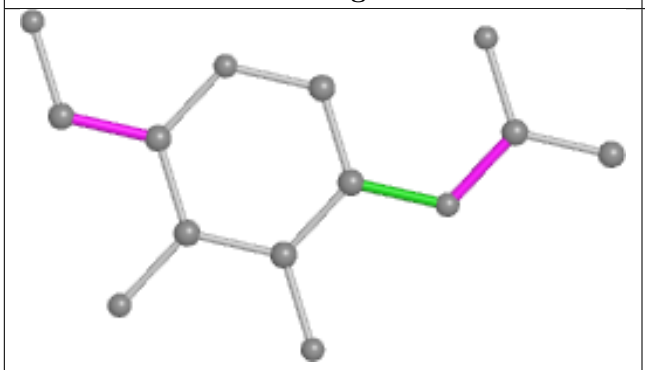
Ligand NAG A 1204



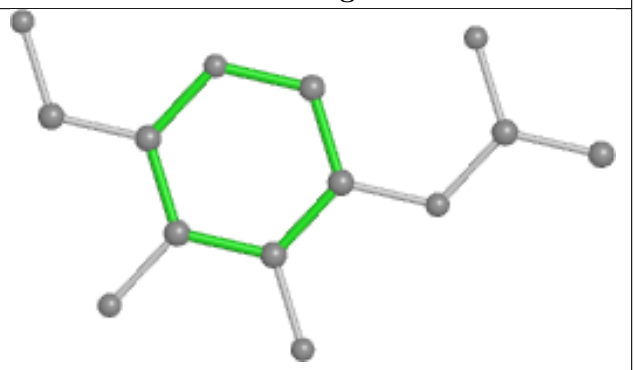
Bond lengths



Bond angles

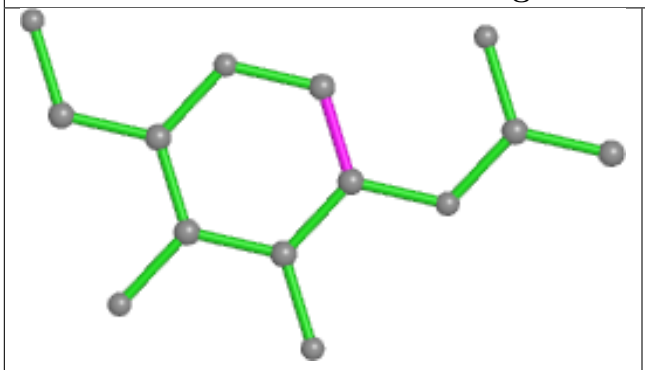


Torsions

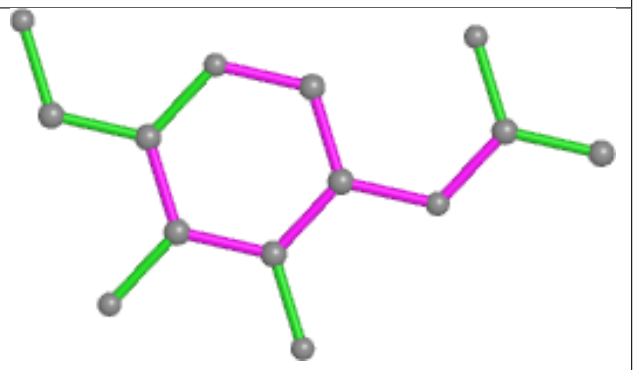


Rings

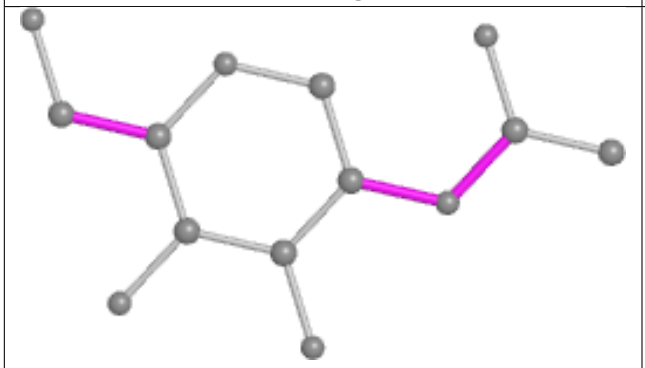
Ligand NAG B 1202



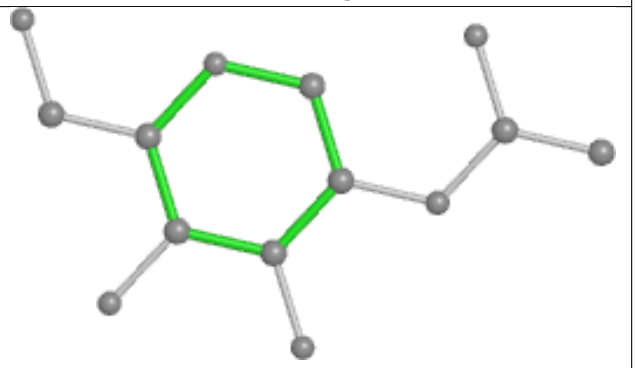
Bond lengths



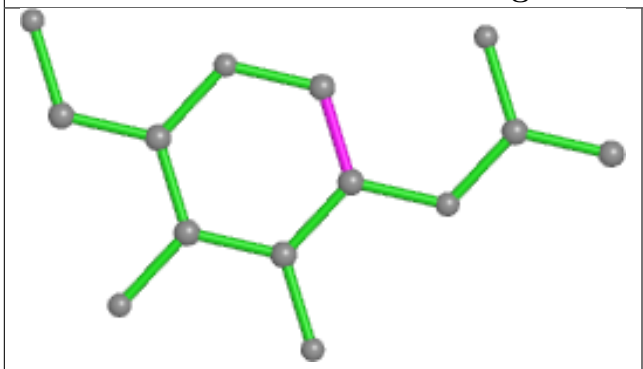
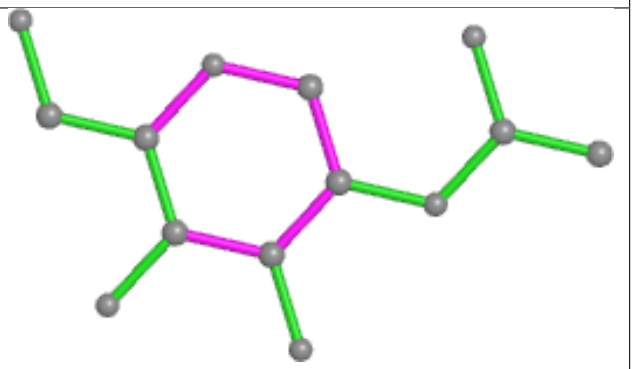
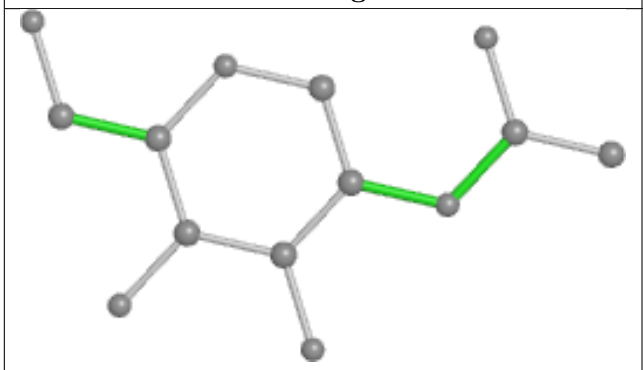
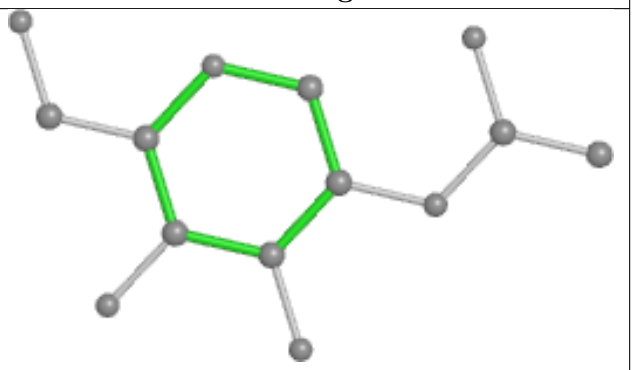
Bond angles

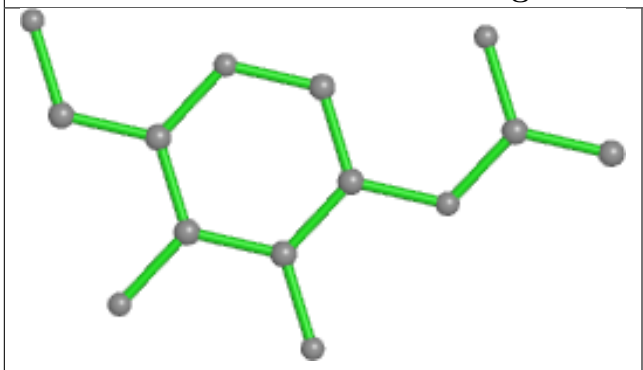
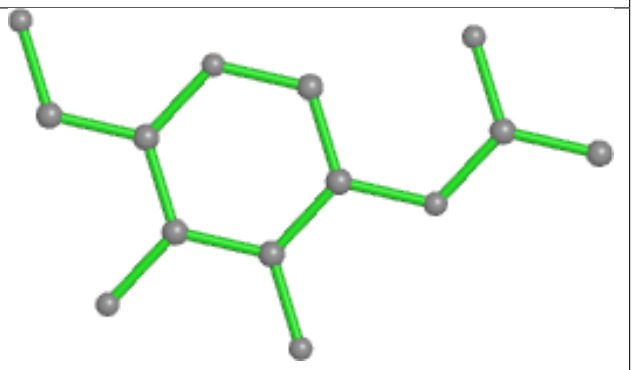
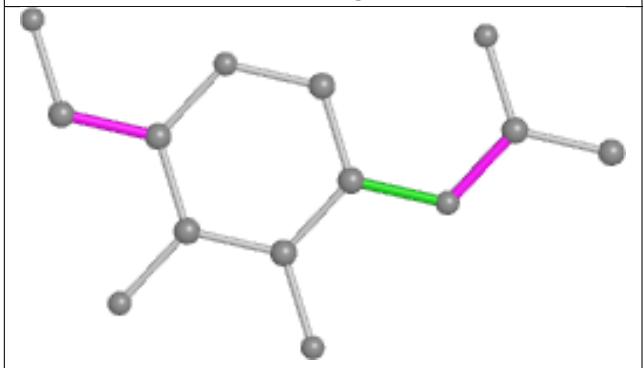
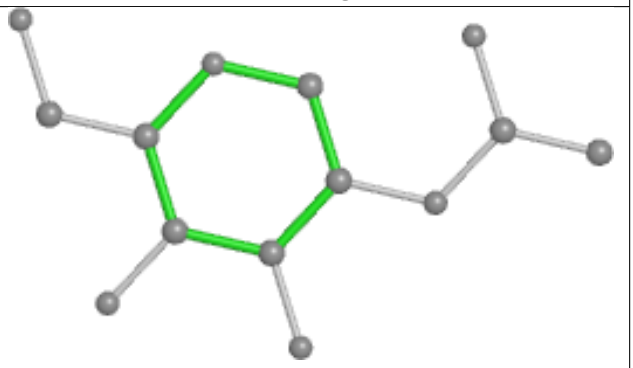


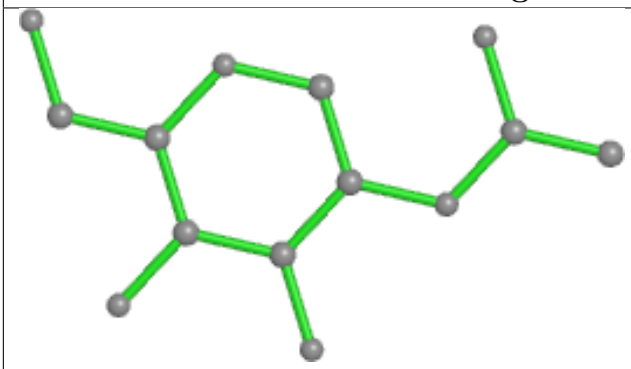
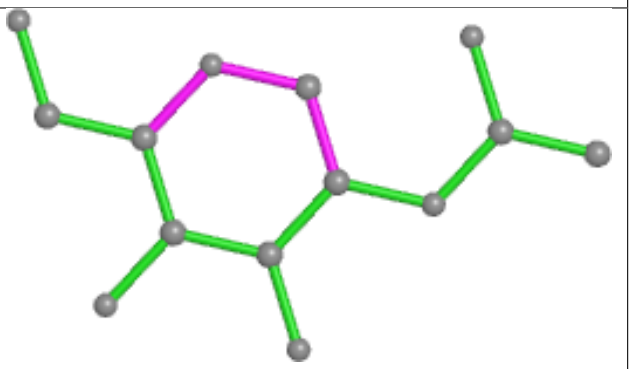
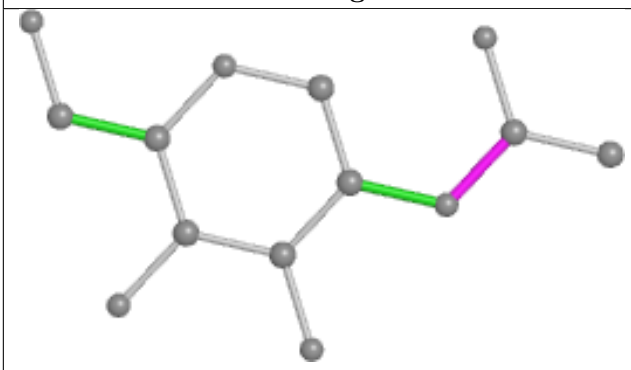
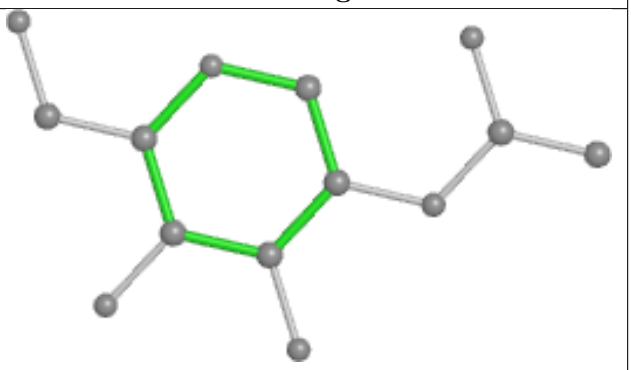
Torsions

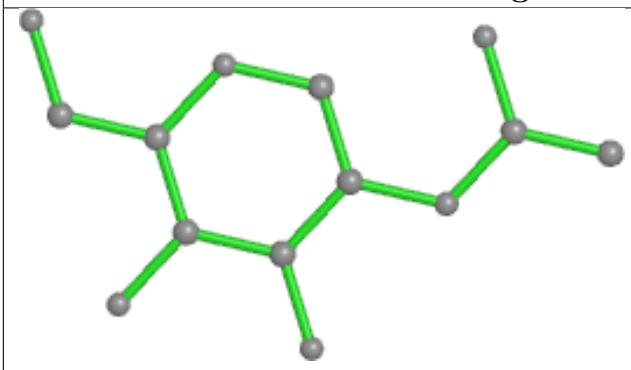
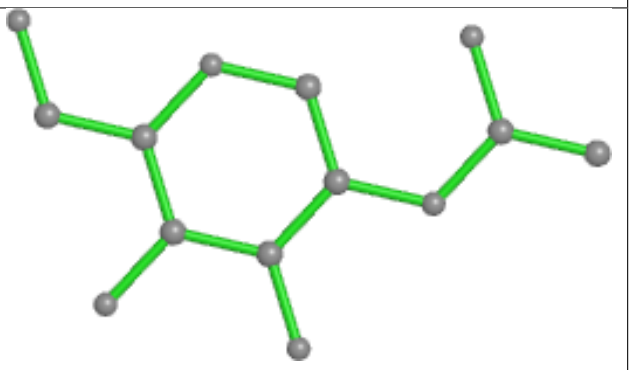
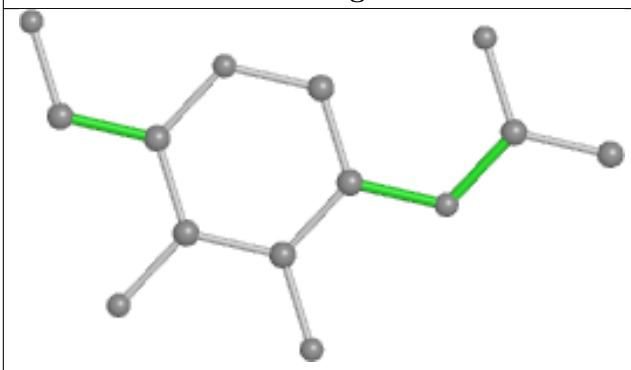
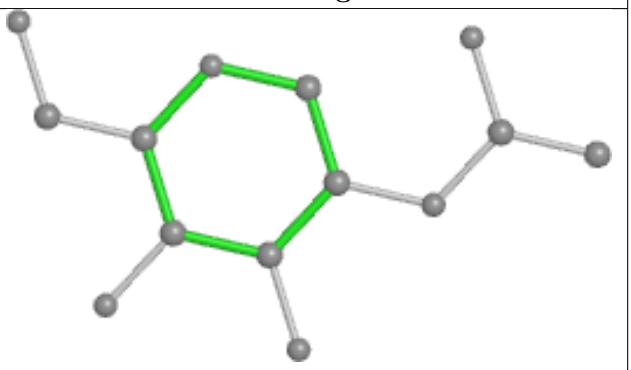


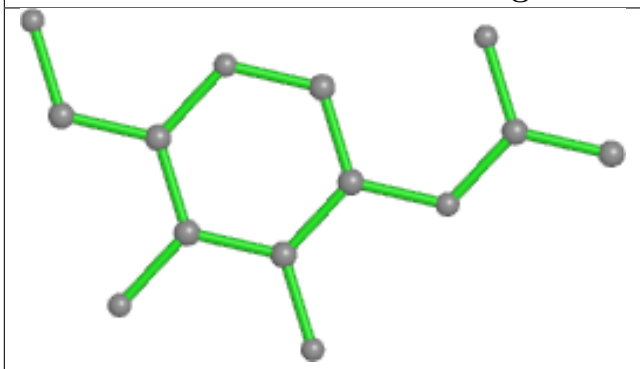
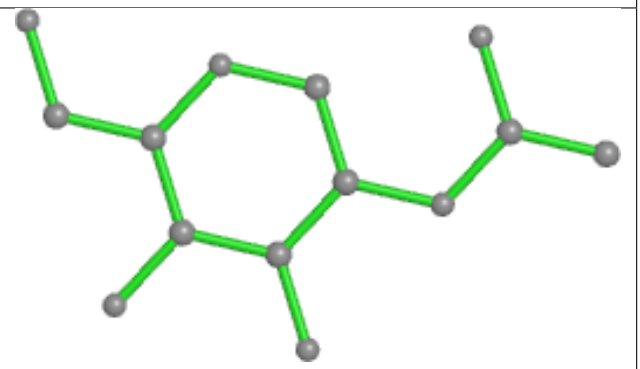
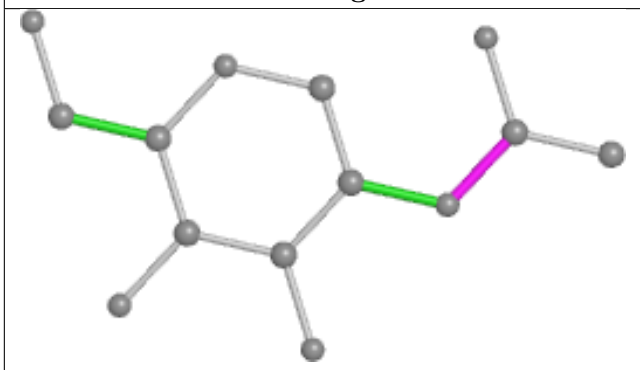
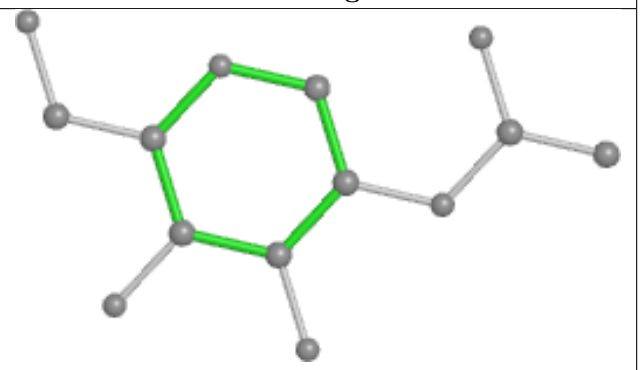
Rings

Ligand NAG A 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

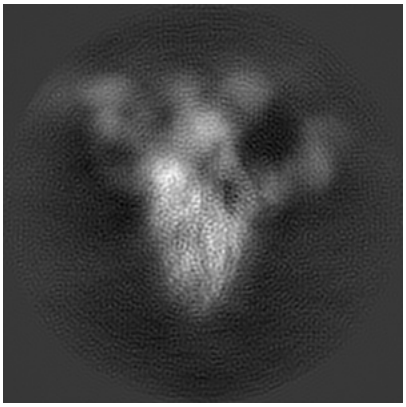
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30487. These allow visual inspection of the internal detail of the map and identification of artifacts.

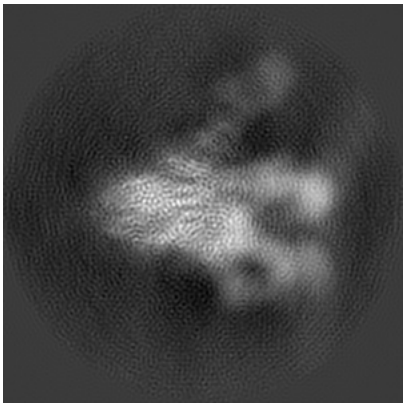
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

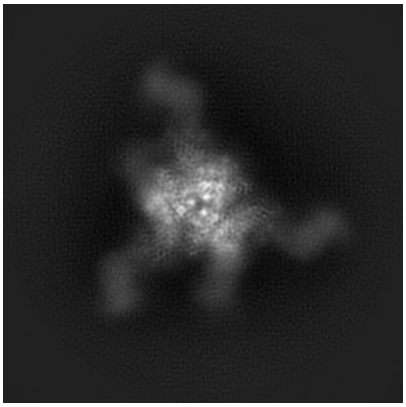
6.1.1 Primary map



X



Y

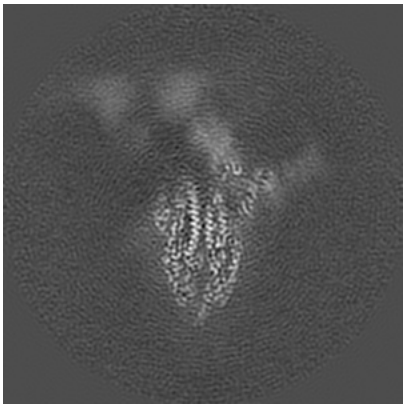


Z

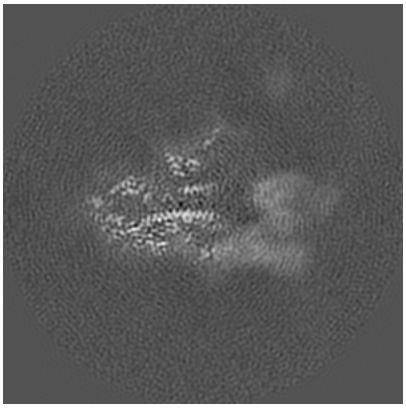
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

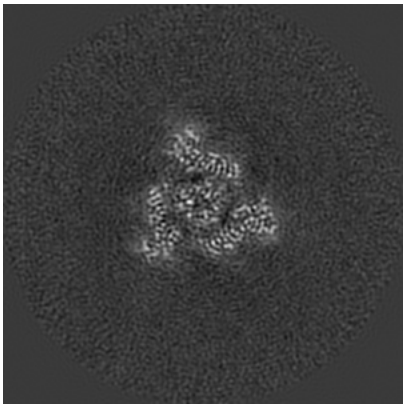
6.2.1 Primary map



X Index: 160



Y Index: 160

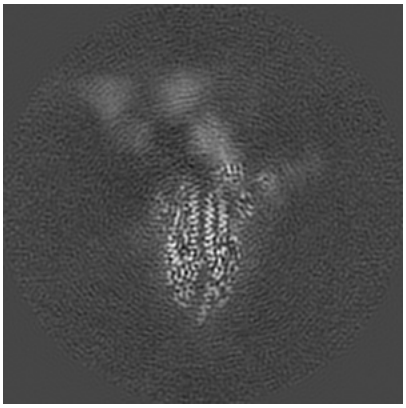


Z Index: 160

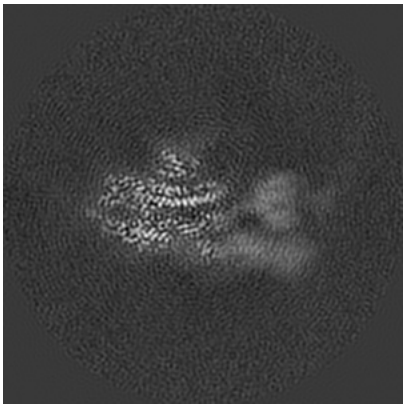
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

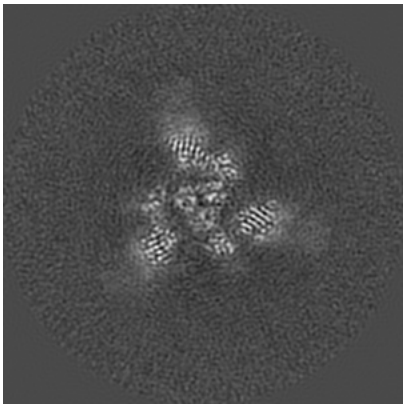
6.3.1 Primary map



X Index: 162



Y Index: 165



Z Index: 168

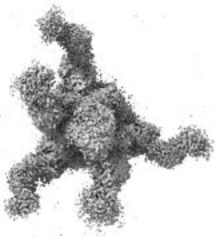
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

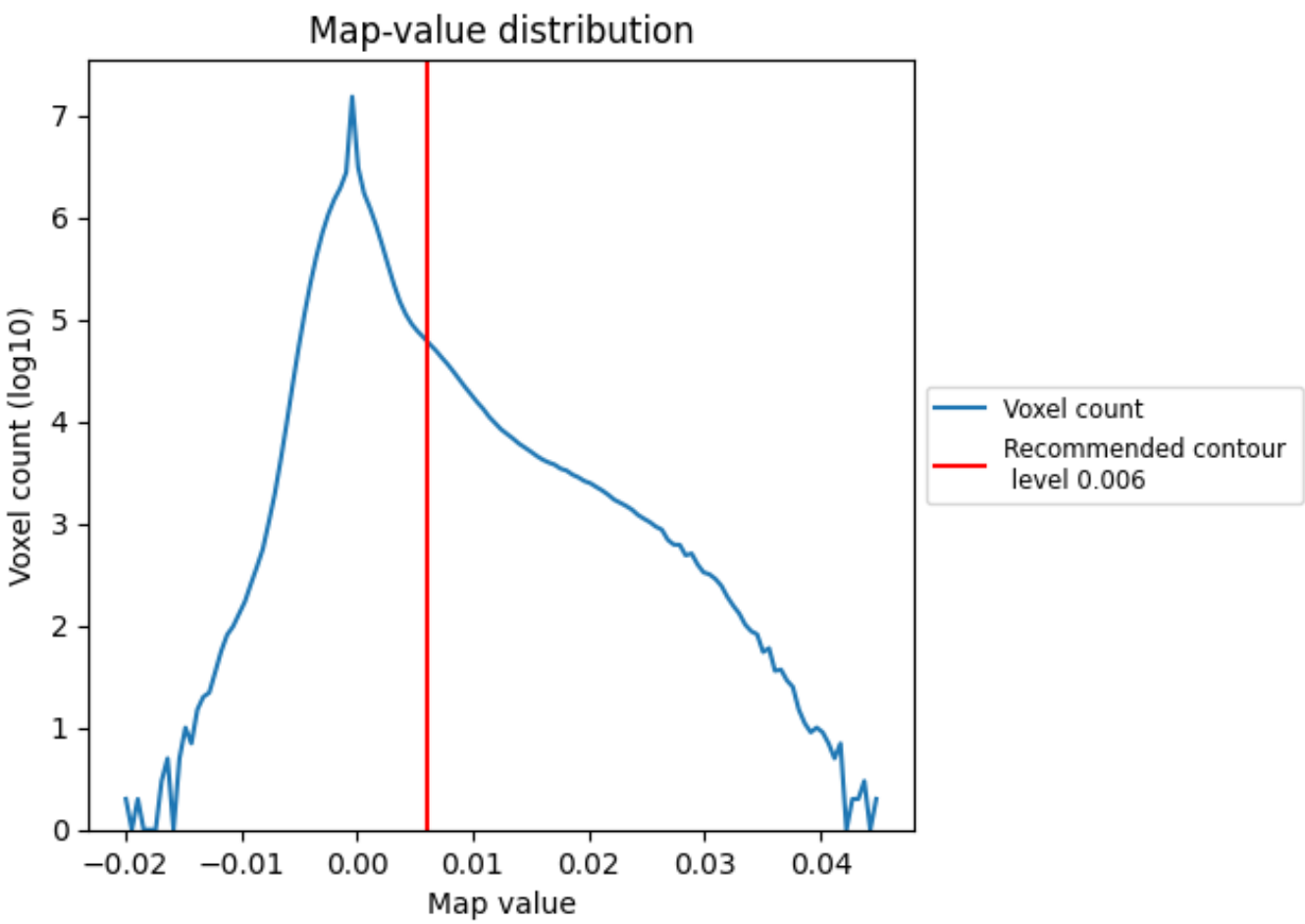
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

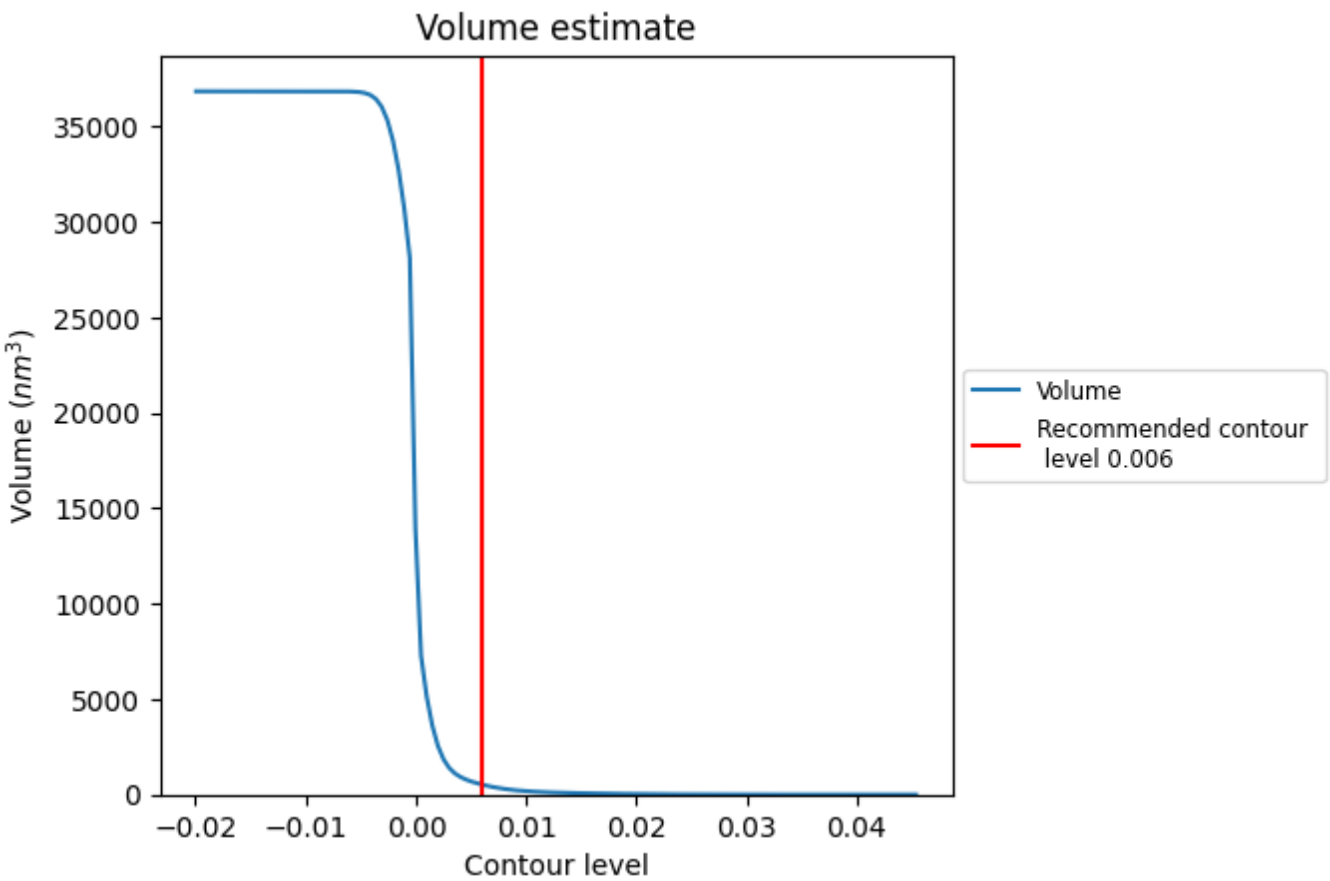
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

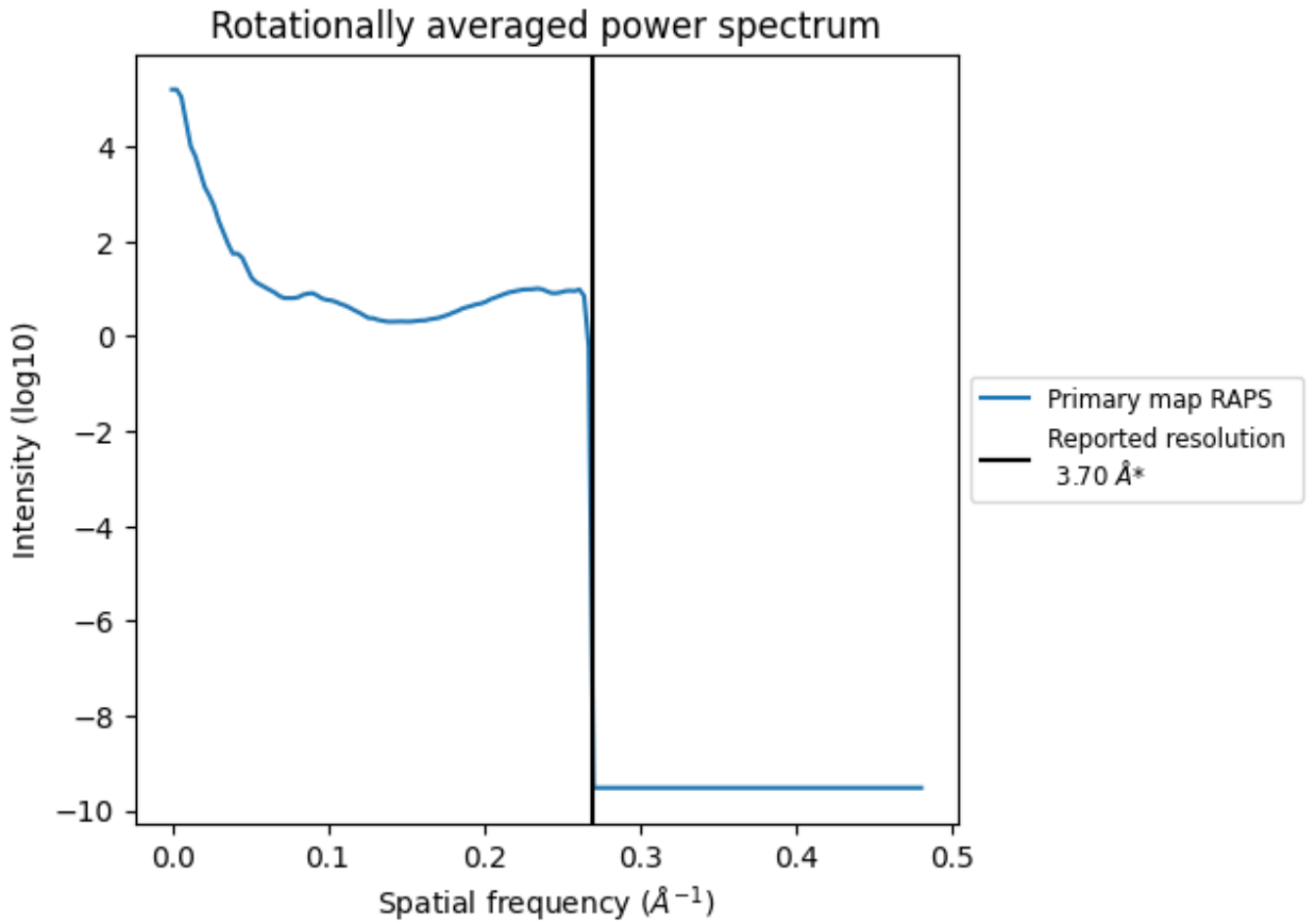
7.2 Volume estimate (i)



The volume at the recommended contour level is 520 nm^3; this corresponds to an approximate mass of 470 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

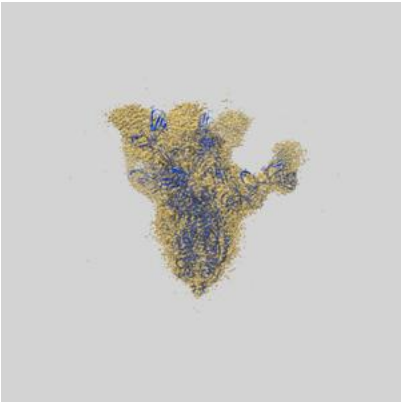
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

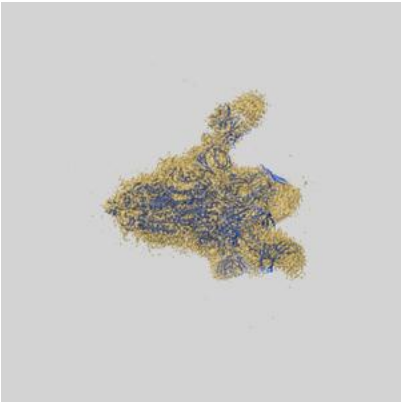
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30487 and PDB model 7CWT. Per-residue inclusion information can be found in section 3 on page 7.

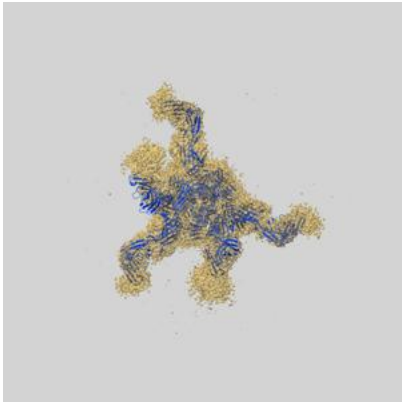
9.1 Map-model overlay (i)



X



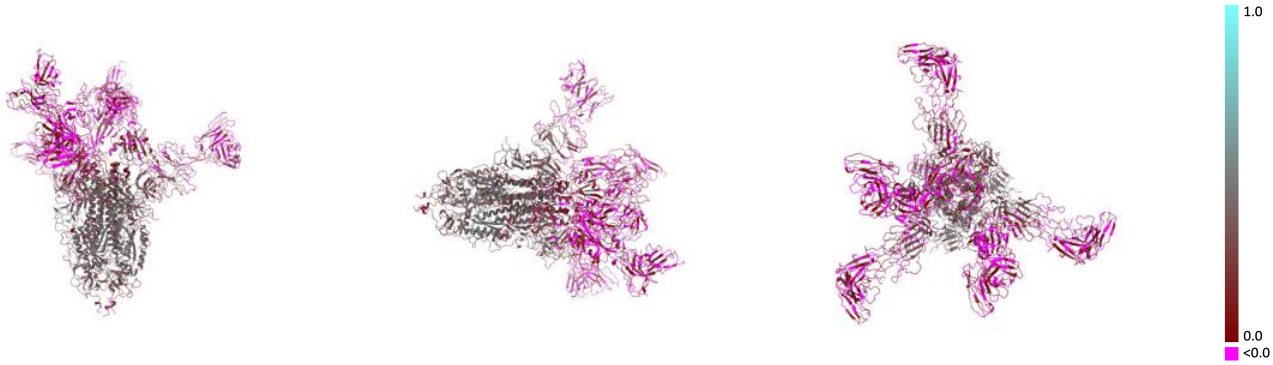
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

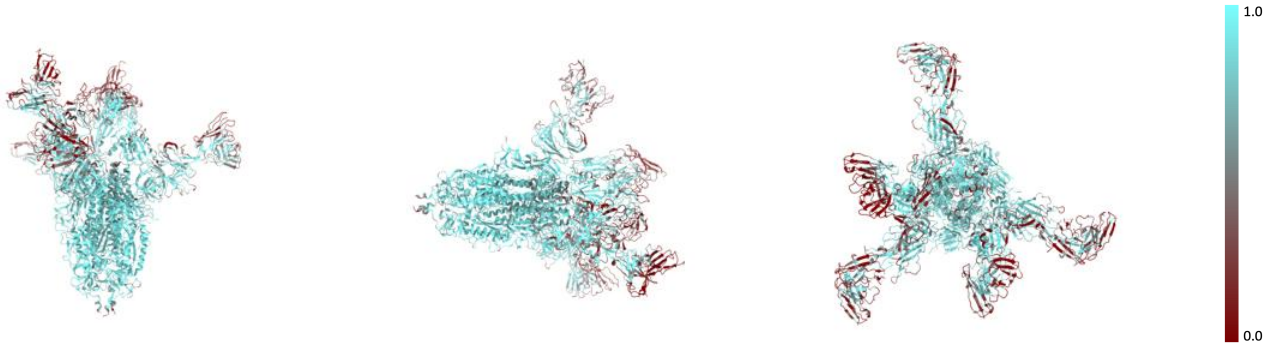
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

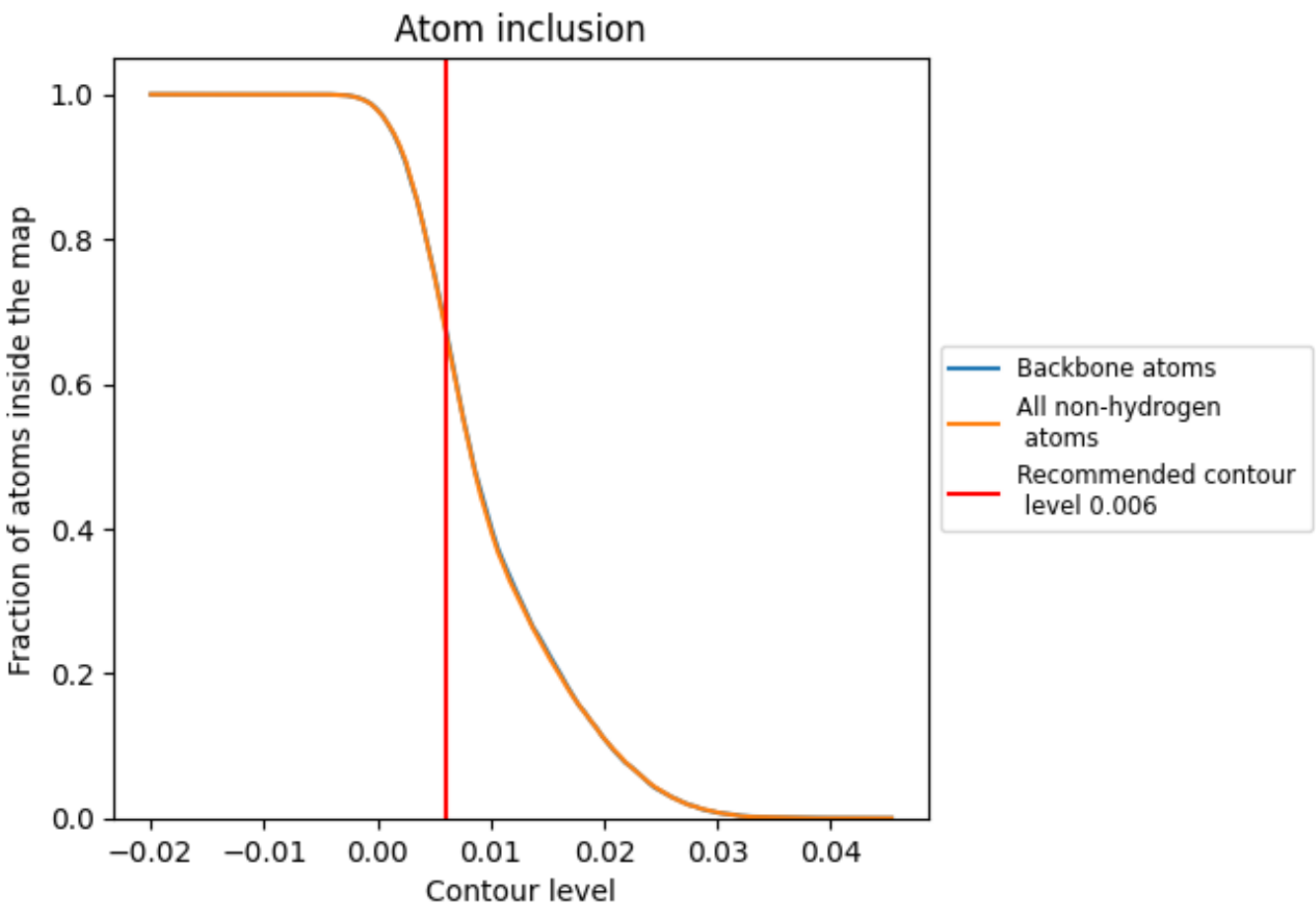
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6763	0.1810
A	0.7903	0.2470
B	0.7665	0.2270
C	0.7989	0.2620
D	0.3463	0.0370
E	0.5742	0.0290
F	0.1034	-0.0040
G	0.4384	0.0160
H	0.4794	0.0200
I	0.6375	0.0220
J	0.5353	0.0060
K	0.5180	0.0540
L	0.3165	0.0360
M	0.2995	0.0110
N	0.4283	0.0120
P	0.3812	0.0430