



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 07:31 PM EST

PDB ID : 7KEK
EMDB ID : EMD-22840
Title : Structure of the free outer-arm dynein in pre-parallel state
Authors : Rao, Q.; Zhang, K.
Deposited on : 2020-10-11
Resolution : 8.00 Å (reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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) : 2.31.2

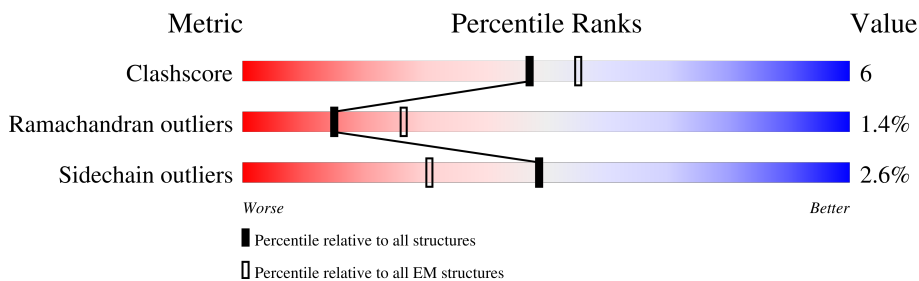
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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 $\leq 5\%$. 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	4620	
2	C	4168	
3	Q	202	
4	B	4595	
5	I	110	
6	H	92	
7	G	159	
8	F	133	

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Mol	Chain	Length	Quality of chain
9	N	117	<p>8% 85% 13%</p>
10	O	132	<p>75% 14% 9%</p>
11	E	670	<p>73% 9% 17%</p>
12	D	667	<p>73% 12% 13%</p>
13	P	122	<p>81% 8% 11%</p>
14	L	111	<p>76% 11% 12%</p>
15	K	93	<p>92%</p>
16	J	111	<p>79% 6% 14%</p>
17	M	87	<p>82% 17%</p>

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 117936 atoms, of which 0 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 Dynein alpha heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4443	33894	21519	5788	6429	158	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4488	LYS	GLY	conflict	UNP Q22A67

- Molecule 2 is a protein called Dynein gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	3943	30436	19390	5162	5735	149	0	0

- Molecule 3 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Q	192	1002	607	202	193	2	0

- Molecule 4 is a protein called Dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	4516	34604	21978	5928	6547	151	0	0

- Molecule 5 is a protein called Dynein light chain LC8_1a (LC10).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	106	827	526	134	161	6	0	0

- Molecule 6 is a protein called Dynein light chain LC8_1b (DLC82).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 7 is a protein called Dynein light chain roadblock LC7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	96	Total	C	N	O	S	0	0
			749	471	129	148	1		

- Molecule 8 is a protein called Dynein light chain roadblock LC7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	110	Total	C	N	O	S	0	0
			863	544	152	165	2		

- Molecule 9 is a protein called Dynein light chain Tctex_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	114	Total	C	N	O	S	0	0
			855	543	143	166	3		

- Molecule 10 is a protein called Dynein light chain Tctex_a (LC2A).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	120	Total	C	N	O	S	0	0
			986	634	172	177	3		

- Molecule 11 is a protein called Dynein intermediate chain DIC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	555	Total	C	N	O	S	0	0
			4423	2786	759	856	22		

- Molecule 12 is a protein called Dynein intermediate chain DIC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	579	Total	C	N	O	S	0	0
			4664	2964	787	883	30		

- Molecule 13 is a protein called Thioredoxin LC3BL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	P	109	541	323	109	109	0	0

- Molecule 14 is a protein called Dynein light chain LC8_3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	98	783	511	132	137	3	0	0

- Molecule 15 is a protein called Dynein light chain LC8_2a (LC8E).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	90	754	489	124	137	4	0	0

- Molecule 16 is a protein called Dynein light chain LC8_2b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	95	806	527	135	140	4	0	0

- Molecule 17 is a protein called Dynein light chain LC8_3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	87	735	477	123	130	5	0	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
18	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
18	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
18	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
18	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
18	B	1	Total	C	N	O	P	0
			54	20	10	20	4	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	A	1	31	10	5	13	3	0
19	C	1	31	10	5	13	3	0
19	B	1	31	10	5	13	3	0

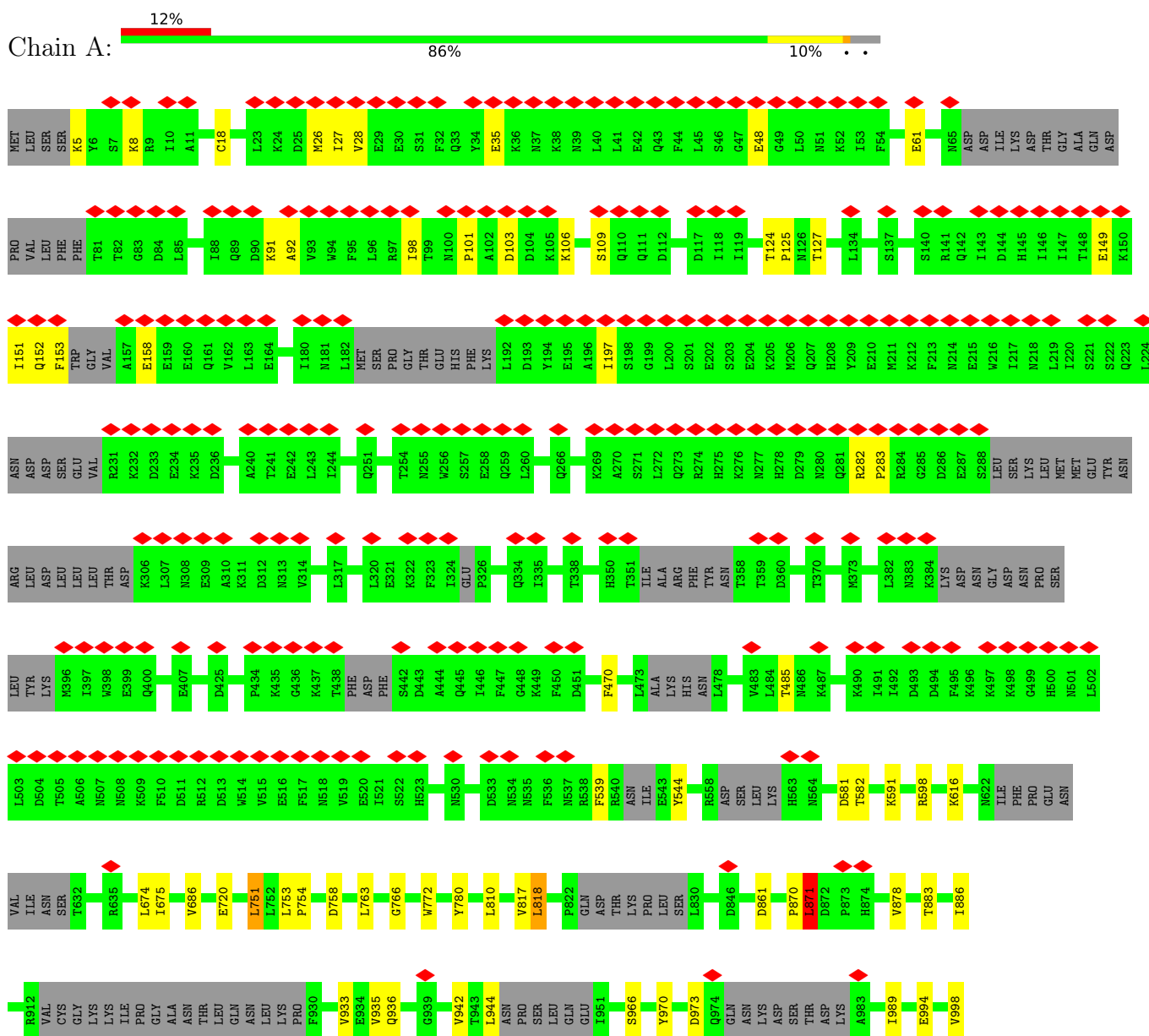
- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

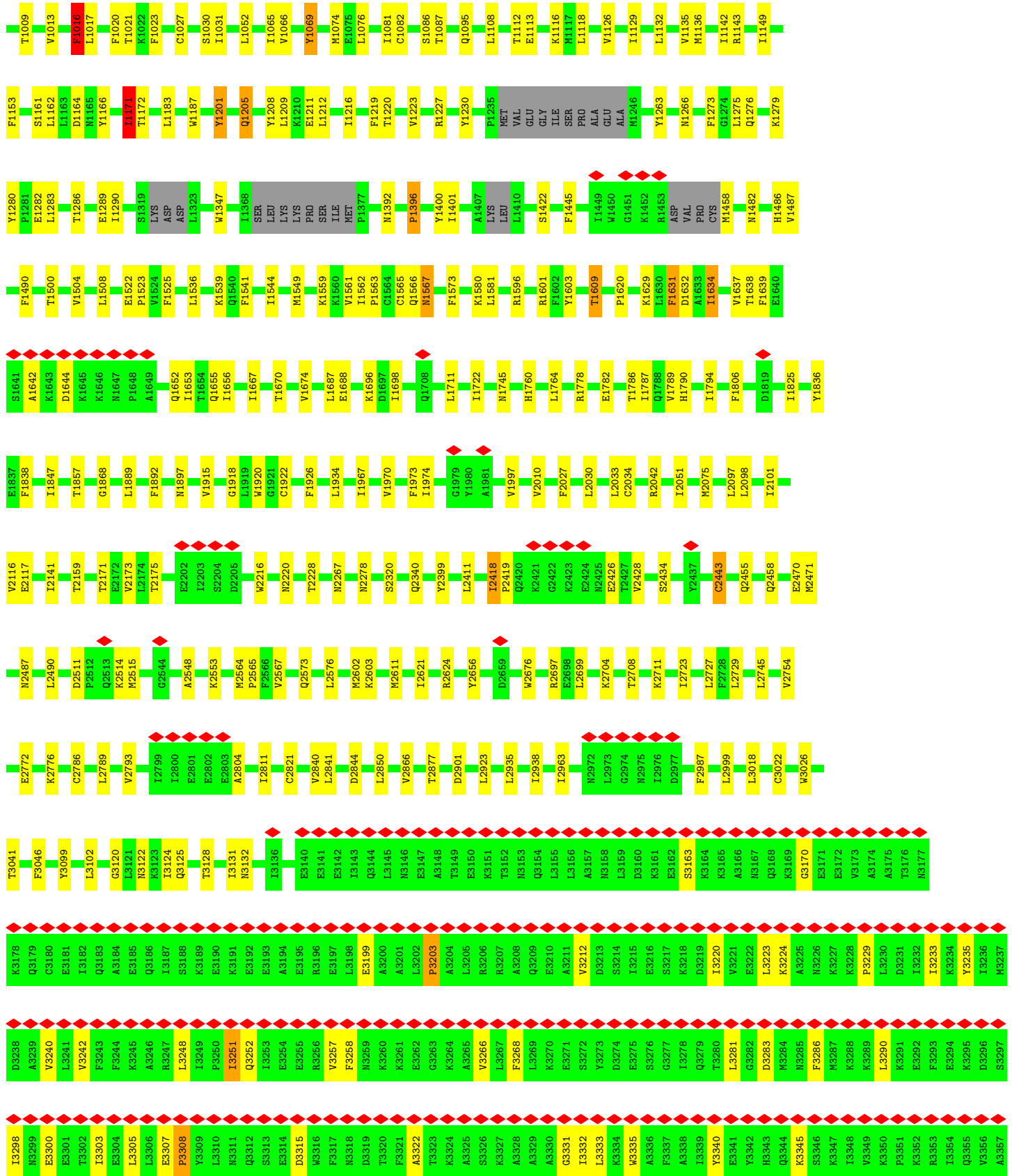
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
20	A	3	3	3	0
20	C	3	3	3	0
20	B	3	3	3	0

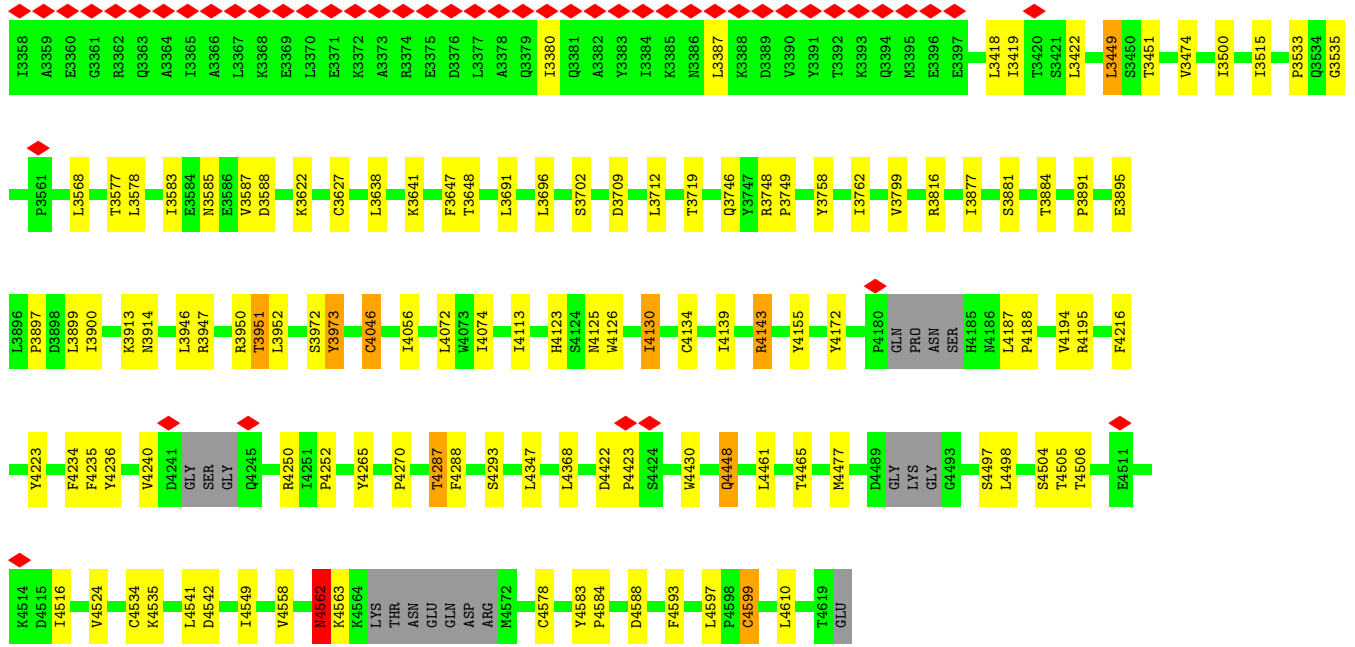
3 Residue-property plots [i](#)

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.

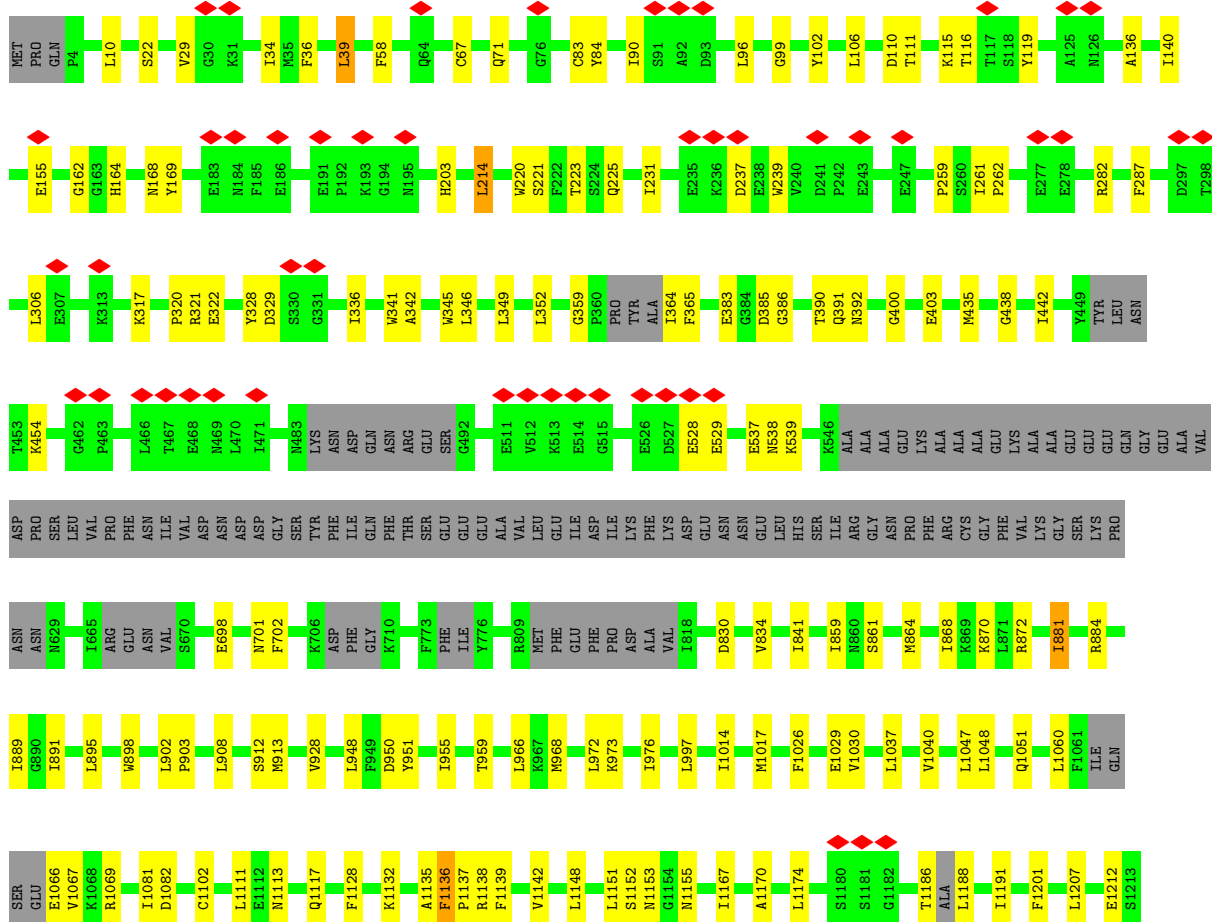
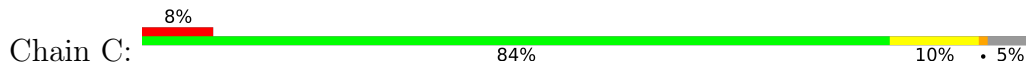
- Molecule 1: Dynein alpha heavy chain

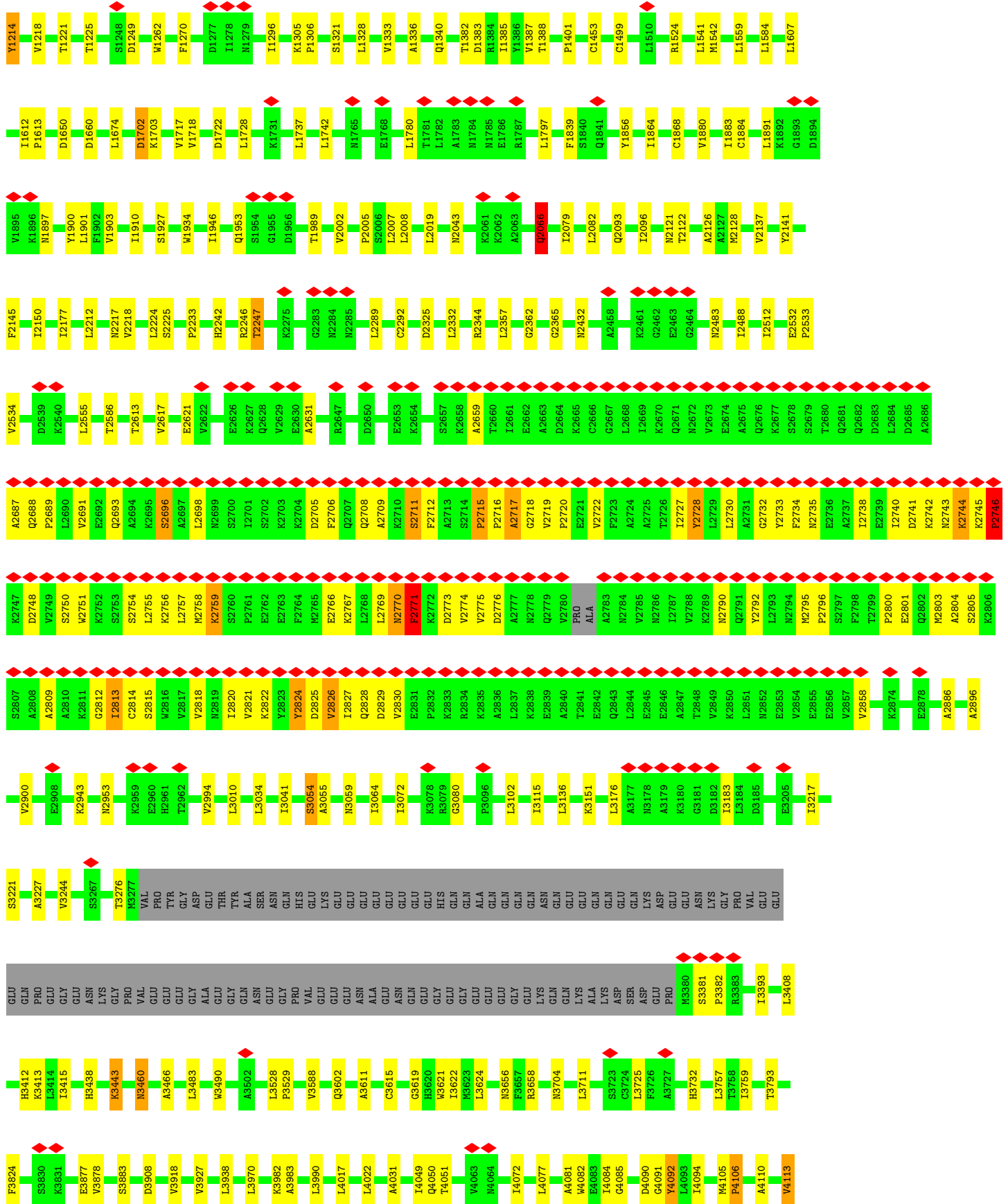


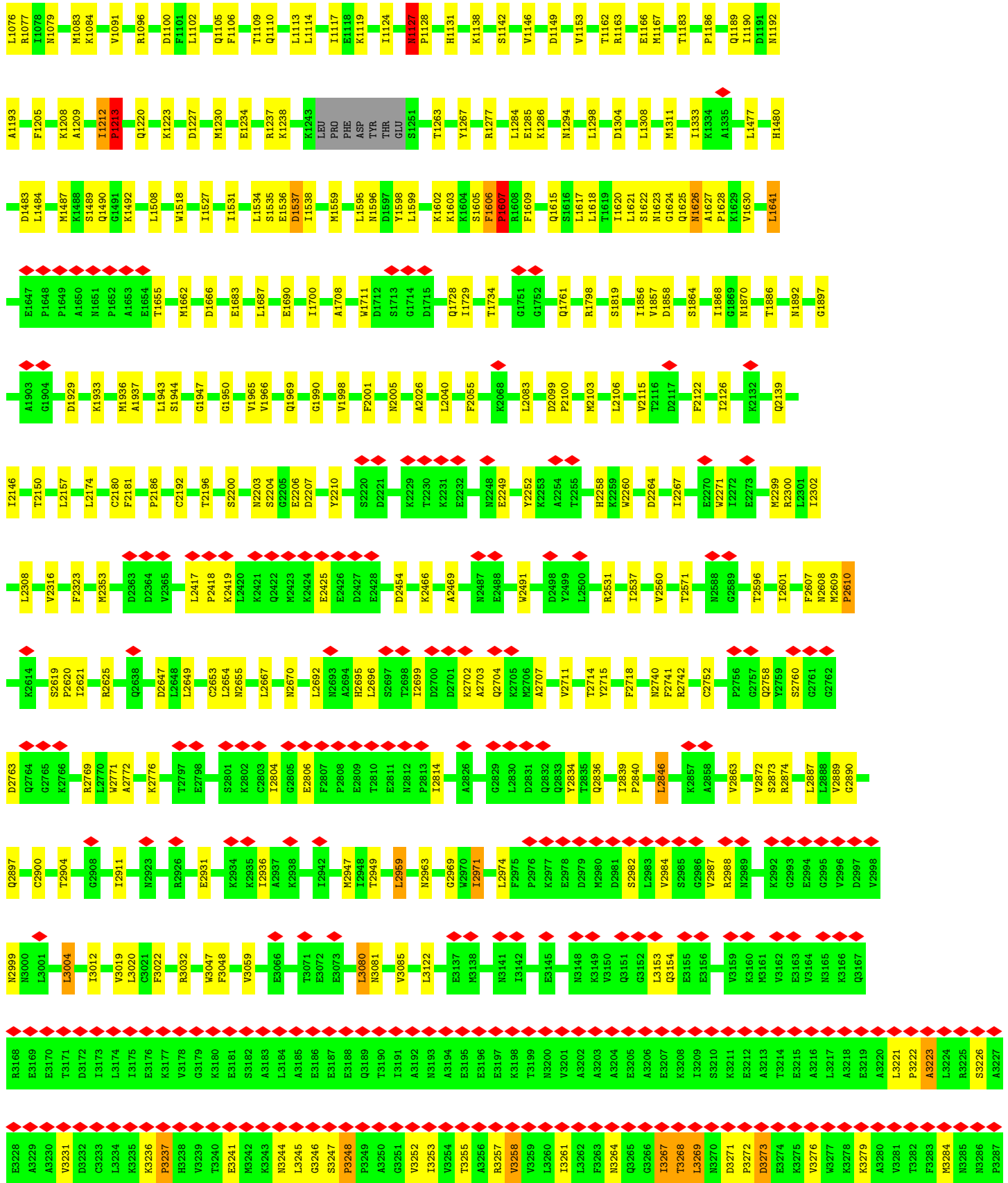


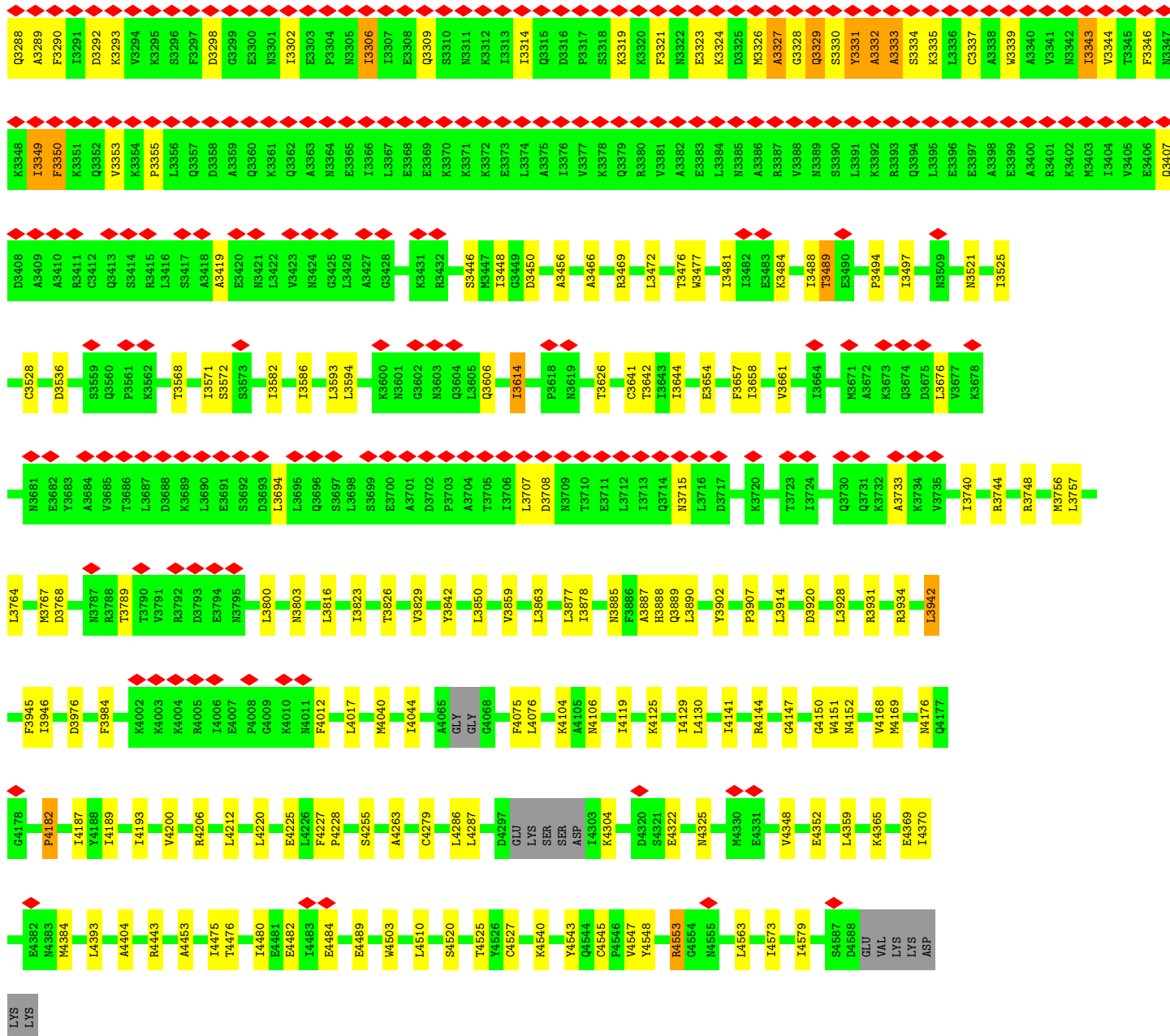


● Molecule 2: Dynein gamma heavy chain

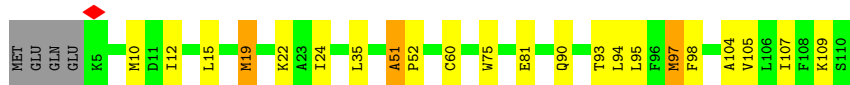
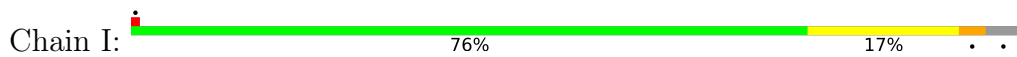




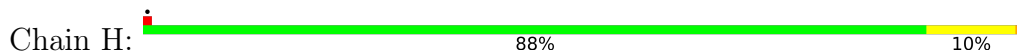




- Molecule 5: Dynein light chain LC8_1a (LC10)

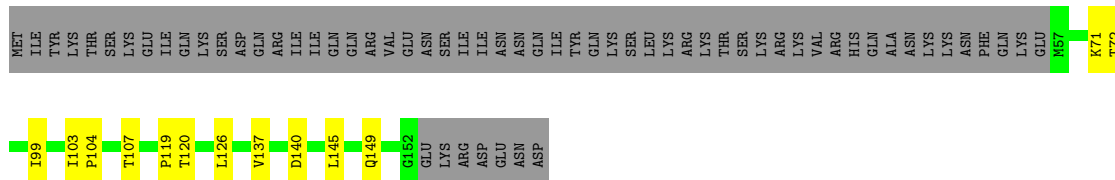


- Molecule 6: Dynein light chain LC8_1b (DLC82)

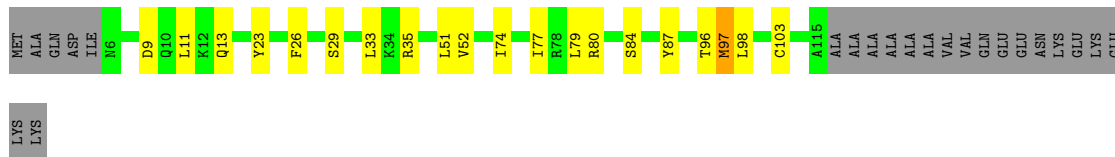




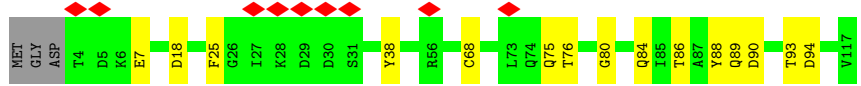
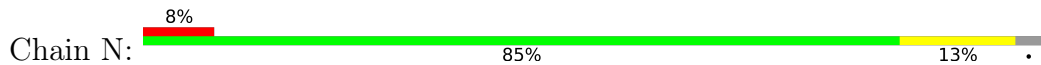
• Molecule 7: Dynein light chain roadblock LC7B



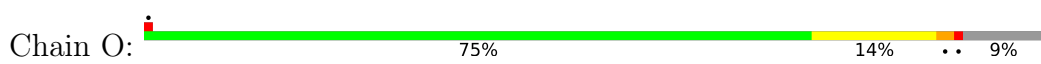
• Molecule 8: Dynein light chain roadblock LC7A



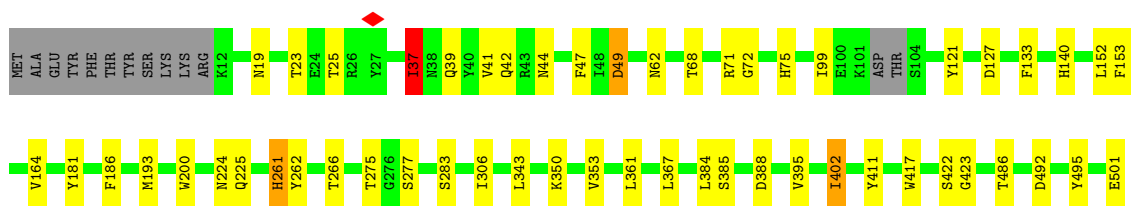
• Molecule 9: Dynein light chain Tctex_b

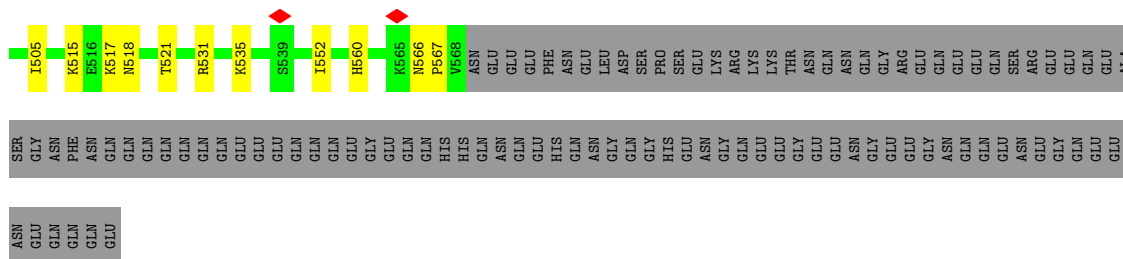


• Molecule 10: Dynein light chain Tctex_a (LC2A)

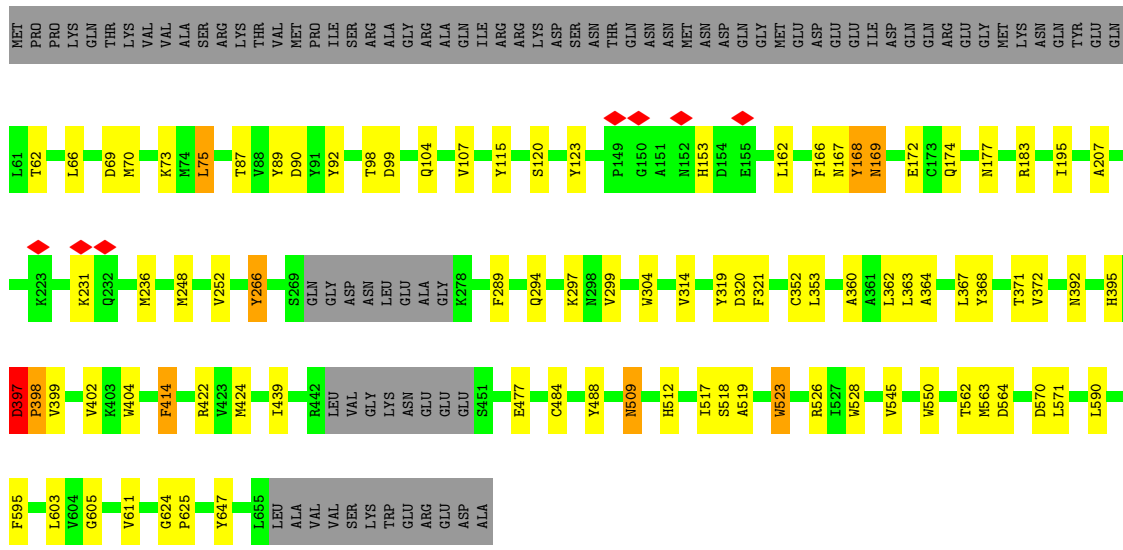


• Molecule 11: Dynein intermediate chain DIC3

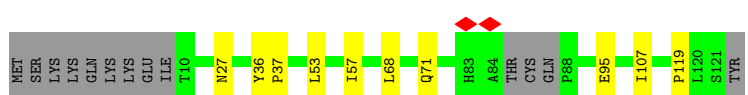
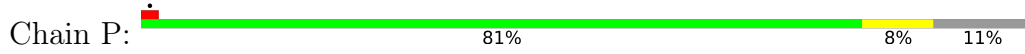




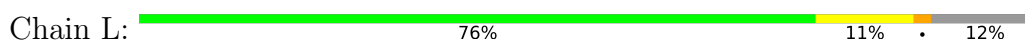
• Molecule 12: Dynein intermediate chain DIC2



• Molecule 13: Thioredoxin LC3BL




• Molecule 14: Dynein light chain LC8_3b

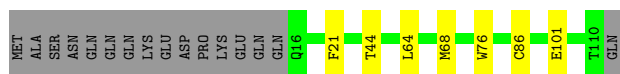


• Molecule 15: Dynein light chain LC8_2a (LC8E)




- Molecule 16: Dynein light chain LC8_2b

Chain J:  79% 6% 14%



- Molecule 17: Dynein light chain LC8_3a

Chain M:  82% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.3	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	9.863	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	1015.746, 1061.068, 970.42395	wwPDB
Map dimensions	381, 398, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.666, 2.666, 2.666	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: ADP, MG, ATP

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	0.69	0/34464	0.78	1/46623 (0.0%)
2	C	0.69	1/31037 (0.0%)	0.80	5/42000 (0.0%)
3	Q	0.86	0/1005	0.84	0/1388
4	B	0.70	2/35205 (0.0%)	0.81	7/47647 (0.0%)
5	I	0.68	0/838	0.77	0/1131
6	H	0.67	0/767	0.77	0/1031
7	G	0.69	0/755	0.77	0/1018
8	F	0.68	0/875	0.77	0/1178
9	N	0.69	0/867	0.78	0/1179
10	O	0.67	0/1004	0.80	0/1349
11	E	0.67	0/4522	0.78	0/6114
12	D	0.66	0/4772	0.78	1/6458 (0.0%)
13	P	0.87	0/538	0.86	0/746
14	L	0.66	0/800	0.76	0/1076
15	K	0.66	0/776	0.73	0/1038
16	J	0.63	0/831	0.74	0/1118
17	M	0.65	0/752	0.76	0/1006
All	All	0.69	3/119808 (0.0%)	0.79	14/162100 (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	2
2	C	0	3
4	B	0	4
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1606	PHE	C-N	20.47	1.73	1.34
2	C	1136	PHE	C-N	16.22	1.65	1.34
4	B	730	LEU	C-O	5.28	1.33	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1136	PHE	O-C-N	26.30	171.08	121.10
2	C	1136	PHE	C-N-CD	23.12	176.95	128.40
4	B	1606	PHE	O-C-N	-20.88	81.42	121.10
4	B	1606	PHE	C-N-CD	-20.37	75.80	120.60
2	C	1136	PHE	CA-C-N	-18.02	66.65	117.10
2	C	1136	PHE	C-N-CA	-13.06	67.16	122.00
4	B	1606	PHE	CA-C-N	10.97	147.81	117.10
4	B	1606	PHE	C-N-CA	10.59	166.47	122.00
4	B	3248	PRO	N-CA-CB	-6.34	95.62	102.60
4	B	533	ARG	CB-CA-C	6.17	122.75	110.40
4	B	1127	ASN	CB-CA-C	5.70	121.79	110.40
12	D	397	ASP	CB-CA-C	5.15	120.71	110.40
2	C	2824	TYR	CB-CA-C	-5.14	100.11	110.40
1	A	1016	PHE	CB-CA-C	5.10	120.61	110.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	GLU	Peptide
1	A	4250	ARG	Peptide
4	B	1864	SER	Peptide
4	B	2466	LYS	Peptide
4	B	3319	LYS	Peptide
4	B	3536	ASP	Peptide
2	C	2717	ALA	Peptide
2	C	2746	PRO	Peptide
2	C	528	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33894	0	32284	319	0
2	C	30436	0	29388	319	0
3	Q	1002	0	498	6	0
4	B	34604	0	33084	703	0
5	I	827	0	829	17	0
6	H	750	0	735	7	0
7	G	749	0	772	10	0
8	F	863	0	881	9	0
9	N	855	0	800	13	0
10	O	986	0	1002	11	0
11	E	4423	0	4291	40	0
12	D	4664	0	4484	65	0
13	P	541	0	220	2	0
14	L	783	0	811	9	0
15	K	754	0	716	3	0
16	J	806	0	769	2	0
17	M	735	0	738	9	0
18	A	54	0	24	2	0
18	B	54	0	24	0	0
18	C	54	0	24	3	0
19	A	31	0	12	0	0
19	B	31	0	12	1	0
19	C	31	0	12	0	0
20	A	3	0	0	0	0
20	B	3	0	0	0	0
20	C	3	0	0	0	0
All	All	117936	0	112410	1466	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 6.

All (1466) 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)
4:B:1223:LYS:HE2	4:B:1277:ARG:CB	1.23	1.63
4:B:1599:LEU:HB3	4:B:1617:LEU:CG	1.18	1.61
1:A:1219:PHE:HZ	1:A:1263:TYR:CD2	1.17	1.60
1:A:1219:PHE:CE1	1:A:1263:TYR:HA	1.26	1.60
1:A:1219:PHE:CZ	1:A:1263:TYR:CD2	1.89	1.60
4:B:1223:LYS:CE	4:B:1277:ARG:CB	1.81	1.58
4:B:1603:LYS:CG	4:B:1609:PHE:CB	1.82	1.57
2:C:1132:LYS:CE	2:C:1151:LEU:HD22	1.12	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1595:LEU:HB3	4:B:1618:LEU:CD2	1.09	1.57
4:B:1606:PHE:CZ	4:B:1690:GLU:HB2	1.36	1.56
2:C:1132:LYS:HE2	2:C:1151:LEU:CD2	1.26	1.56
4:B:1599:LEU:HD23	4:B:1621:LEU:CD2	1.28	1.56
4:B:1599:LEU:HB3	4:B:1617:LEU:CD2	1.08	1.55
4:B:1599:LEU:CD2	4:B:1621:LEU:HD22	1.30	1.55
4:B:1595:LEU:CB	4:B:1618:LEU:CD2	1.80	1.54
4:B:1606:PHE:CD1	4:B:1687:LEU:HA	1.43	1.53
4:B:1212:ILE:HG23	4:B:1284:LEU:CB	1.37	1.53
4:B:808:PRO:HG2	4:B:1077:ARG:CD	1.39	1.51
4:B:1603:LYS:HG2	4:B:1609:PHE:CB	1.05	1.50
2:C:1132:LYS:CE	2:C:1151:LEU:CD2	1.81	1.50
4:B:1599:LEU:CB	4:B:1617:LEU:CD2	1.88	1.49
1:A:1223:VAL:HG11	1:A:1282:GLU:C	1.17	1.47
4:B:1599:LEU:CG	4:B:1617:LEU:HG	1.41	1.45
4:B:1606:PHE:CE1	4:B:1687:LEU:HA	1.50	1.43
4:B:1599:LEU:CB	4:B:1617:LEU:CG	1.97	1.41
4:B:898:PRO:HD3	4:B:1073:ILE:CG2	1.47	1.40
4:B:1602:LYS:HD2	4:B:1683:GLU:CD	1.40	1.40
4:B:1606:PHE:C	4:B:1607:PRO:N	1.73	1.38
2:C:364:ILE:O	2:C:365:PHE:CB	1.68	1.38
2:C:1136:PHE:HD2	2:C:1139:PHE:N	1.20	1.38
4:B:1531:ILE:CG2	4:B:1622:SER:OG	1.72	1.36
1:A:1219:PHE:HE1	1:A:1263:TYR:CA	1.36	1.36
4:B:1606:PHE:CZ	4:B:1690:GLU:CB	2.06	1.36
4:B:1603:LYS:HE2	4:B:1609:PHE:O	1.26	1.35
4:B:1603:LYS:CG	4:B:1609:PHE:HB3	1.46	1.34
1:A:1219:PHE:CZ	1:A:1263:TYR:HD2	1.30	1.33
4:B:1490:GLN:CD	4:B:3614:ILE:HG21	1.48	1.33
4:B:1606:PHE:C	4:B:1607:PRO:CD	1.97	1.33
4:B:1606:PHE:CD1	4:B:1687:LEU:CD1	2.12	1.32
4:B:1237:ARG:NE	4:B:1263:THR:CB	1.92	1.32
4:B:1606:PHE:CD1	4:B:1687:LEU:CA	2.13	1.31
1:A:1223:VAL:CG1	1:A:1282:GLU:O	1.76	1.31
4:B:1599:LEU:CB	4:B:1617:LEU:HG	1.52	1.31
4:B:1535:SER:HB2	4:B:1622:SER:O	1.22	1.31
4:B:1595:LEU:CB	4:B:1618:LEU:HD22	1.47	1.30
4:B:1603:LYS:CG	4:B:1609:PHE:HB2	1.49	1.30
4:B:1606:PHE:CD1	4:B:1687:LEU:HD12	1.67	1.29
4:B:1220:GLN:HG2	4:B:1294:ASN:CB	1.61	1.29
4:B:1212:ILE:CG2	4:B:1284:LEU:CB	2.10	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:899:LEU:HD21	4:B:1075:TRP:NE1	1.47	1.28
4:B:1606:PHE:HD1	4:B:1687:LEU:CD1	1.45	1.27
4:B:1490:GLN:OE1	4:B:3614:ILE:CG2	1.82	1.27
4:B:764:GLN:O	4:B:765:PHE:C	1.73	1.26
2:C:1136:PHE:CD2	2:C:1139:PHE:N	2.05	1.24
4:B:1603:LYS:HE2	4:B:1609:PHE:C	1.56	1.24
4:B:1599:LEU:HD13	4:B:1617:LEU:CB	1.67	1.24
4:B:1490:GLN:NE2	4:B:3572:SER:CB	2.01	1.23
4:B:1212:ILE:HG12	4:B:1284:LEU:CA	1.66	1.23
4:B:1238:LYS:HE3	4:B:1308:LEU:CA	1.69	1.22
4:B:1599:LEU:HD11	4:B:1618:LEU:N	1.55	1.21
4:B:1606:PHE:HZ	4:B:1690:GLU:CB	1.43	1.21
4:B:1237:ARG:HE	4:B:1263:THR:CB	1.53	1.20
4:B:1238:LYS:CE	4:B:1308:LEU:HA	1.72	1.19
1:A:1223:VAL:HG11	1:A:1283:LEU:N	1.26	1.19
4:B:1234:GLU:OE2	4:B:1304:ASP:CB	1.90	1.19
4:B:1490:GLN:NE2	4:B:3568:THR:O	1.74	1.19
4:B:1531:ILE:O	4:B:1622:SER:HB3	1.39	1.18
1:A:1223:VAL:HG11	1:A:1282:GLU:O	1.34	1.18
4:B:1490:GLN:NE2	4:B:3572:SER:HB3	1.57	1.17
4:B:898:PRO:CD	4:B:1073:ILE:CG2	2.22	1.17
4:B:808:PRO:CG	4:B:1077:ARG:HD2	1.76	1.15
2:C:1067:VAL:HG21	2:C:1148:LEU:O	1.45	1.15
1:A:1219:PHE:CE1	1:A:1263:TYR:CA	2.18	1.15
4:B:1606:PHE:CE1	4:B:1690:GLU:HB3	1.82	1.14
1:A:1223:VAL:CG1	1:A:1282:GLU:C	2.10	1.14
4:B:1599:LEU:CD2	4:B:1617:LEU:HG	1.76	1.14
4:B:898:PRO:HB2	4:B:1077:ARG:N	1.63	1.14
4:B:1531:ILE:HG22	4:B:1622:SER:OG	1.37	1.14
4:B:764:GLN:O	4:B:766:ILE:N	1.79	1.14
2:C:1132:LYS:HE3	2:C:1151:LEU:CD2	1.70	1.13
4:B:1599:LEU:CD2	4:B:1617:LEU:O	1.97	1.13
4:B:1212:ILE:HG12	4:B:1284:LEU:HA	1.20	1.12
4:B:1490:GLN:NE2	4:B:3572:SER:OG	1.81	1.11
2:C:1132:LYS:HG2	2:C:1151:LEU:HD11	1.18	1.11
4:B:1599:LEU:HA	4:B:1621:LEU:HD21	1.29	1.11
4:B:898:PRO:CD	4:B:1073:ILE:HG21	1.79	1.10
4:B:898:PRO:HG3	4:B:1073:ILE:HG12	1.18	1.10
4:B:900:PHE:CB	4:B:1076:LEU:HD12	1.81	1.10
4:B:1599:LEU:CB	4:B:1617:LEU:HD21	1.59	1.10
4:B:1599:LEU:HD13	4:B:1617:LEU:HB3	1.25	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1606:PHE:CE1	4:B:1690:GLU:CB	2.33	1.10
4:B:900:PHE:HB3	4:B:1076:LEU:HD12	1.30	1.09
1:A:1276:GLN:HG2	12:D:153:HIS:CE1	1.87	1.08
2:C:1135:ALA:HB1	2:C:1212:GLU:CG	1.83	1.08
4:B:1602:LYS:CD	4:B:1683:GLU:CD	2.22	1.08
4:B:1602:LYS:NZ	4:B:1683:GLU:OE1	1.85	1.08
4:B:1212:ILE:HG12	4:B:1284:LEU:CB	1.83	1.08
4:B:1531:ILE:HD13	4:B:1618:LEU:HB3	1.36	1.07
4:B:1531:ILE:HG23	4:B:1622:SER:OG	1.49	1.06
4:B:1238:LYS:CE	4:B:1308:LEU:CA	2.32	1.06
4:B:1602:LYS:HD2	4:B:1683:GLU:CG	1.85	1.06
2:C:454:LYS:CB	2:C:701:ASN:CB	2.33	1.06
4:B:899:LEU:HD11	4:B:1075:TRP:CZ2	1.90	1.06
4:B:1535:SER:CB	4:B:1622:SER:O	2.04	1.06
4:B:1595:LEU:HB2	4:B:1618:LEU:CD2	1.81	1.06
4:B:1490:GLN:OE1	4:B:3614:ILE:HG21	0.88	1.05
2:C:403:GLU:O	4:B:2988:ARG:NH1	1.89	1.05
4:B:808:PRO:HG2	4:B:1077:ARG:HD3	1.35	1.05
4:B:750:PRO:O	4:B:752:ILE:N	1.89	1.05
4:B:1537:ASP:HA	4:B:1625:GLN:HG3	1.36	1.05
4:B:899:LEU:HD21	4:B:1075:TRP:CD1	1.90	1.05
4:B:1223:LYS:HE3	4:B:1277:ARG:CB	1.82	1.04
4:B:1602:LYS:HD2	4:B:1683:GLU:OE1	1.57	1.04
4:B:1602:LYS:HB3	4:B:1683:GLU:HB3	1.33	1.04
1:A:1219:PHE:CE2	1:A:1263:TYR:HD2	1.73	1.04
2:C:1066:GLU:N	2:C:1153:ASN:OD1	1.89	1.04
4:B:1599:LEU:HB3	4:B:1617:LEU:HD21	1.11	1.03
4:B:3255:THR:OG1	4:B:3337:CYS:SG	2.13	1.03
2:C:1132:LYS:HG2	2:C:1151:LEU:CD1	1.88	1.03
4:B:1606:PHE:HD1	4:B:1687:LEU:CB	1.71	1.03
4:B:1490:GLN:HE21	4:B:3572:SER:CB	1.66	1.02
4:B:1606:PHE:CD1	4:B:1687:LEU:CB	2.42	1.02
4:B:1595:LEU:CB	4:B:1618:LEU:HD21	1.87	1.02
2:C:1067:VAL:N	2:C:1152:SER:OG	1.92	1.02
4:B:899:LEU:H	4:B:1076:LEU:HA	1.22	1.02
1:A:1230:TYR:CB	1:A:1289:GLU:C	2.29	1.01
4:B:1599:LEU:CD1	4:B:1617:LEU:HG	1.91	1.01
4:B:1492:LYS:HZ1	4:B:3606:GLN:HB2	1.24	1.01
4:B:1492:LYS:NZ	4:B:3606:GLN:HB2	1.74	1.01
4:B:1602:LYS:CD	4:B:1683:GLU:OE1	2.08	1.01
1:A:1230:TYR:CB	1:A:1289:GLU:O	2.09	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:808:PRO:CG	4:B:1077:ARG:CD	2.36	1.01
4:B:1599:LEU:HD22	4:B:1617:LEU:O	1.59	1.01
2:C:1136:PHE:CD2	2:C:1138:ARG:CA	2.21	1.00
1:A:1219:PHE:HZ	1:A:1263:TYR:CG	1.78	1.00
4:B:1537:ASP:CA	4:B:1625:GLN:HG3	1.91	1.00
1:A:1276:GLN:HG2	12:D:153:HIS:HE1	1.26	1.00
1:A:1536:LEU:CD2	4:B:3888:HIS:HB2	1.92	1.00
2:C:1132:LYS:CE	2:C:1151:LEU:HD21	1.88	1.00
4:B:1535:SER:HB2	4:B:1622:SER:C	1.81	1.00
4:B:1599:LEU:CD1	4:B:1618:LEU:N	2.23	1.00
2:C:539:LYS:CB	2:C:702:PHE:HA	1.92	0.99
4:B:898:PRO:CG	4:B:1073:ILE:HG12	1.93	0.99
4:B:898:PRO:HD3	4:B:1073:ILE:HG21	1.01	0.99
4:B:1599:LEU:CG	4:B:1617:LEU:CG	2.34	0.99
4:B:1603:LYS:CE	4:B:1609:PHE:O	2.10	0.99
4:B:1606:PHE:C	4:B:1607:PRO:HD3	1.80	0.98
1:A:1219:PHE:CE2	1:A:1263:TYR:CD2	2.50	0.98
2:C:1136:PHE:CD2	2:C:1138:ARG:C	2.37	0.98
4:B:1603:LYS:HG3	4:B:1609:PHE:CB	1.92	0.97
4:B:1606:PHE:O	4:B:1607:PRO:N	1.96	0.97
4:B:1238:LYS:HE3	4:B:1308:LEU:CB	1.95	0.97
2:C:2826:VAL:O	2:C:2829:ASP:N	1.96	0.97
4:B:1531:ILE:CG2	4:B:1622:SER:HG	1.78	0.97
4:B:1599:LEU:HA	4:B:1621:LEU:CD2	1.94	0.96
4:B:1599:LEU:CD2	4:B:1617:LEU:C	2.34	0.96
4:B:1238:LYS:HE2	4:B:1308:LEU:HA	1.47	0.96
4:B:765:PHE:O	4:B:766:ILE:C	2.00	0.95
1:A:1219:PHE:HE2	1:A:1280:TYR:HA	1.29	0.95
4:B:1606:PHE:HE1	4:B:1690:GLU:HB3	1.20	0.95
4:B:898:PRO:CB	4:B:1077:ARG:N	2.28	0.95
4:B:1531:ILE:O	4:B:1622:SER:CB	2.14	0.95
4:B:1603:LYS:HG3	4:B:1609:PHE:HB3	1.49	0.94
4:B:1606:PHE:CD1	4:B:1687:LEU:HD13	2.01	0.94
4:B:1599:LEU:HD21	4:B:1617:LEU:O	1.65	0.94
2:C:1136:PHE:CD2	2:C:1138:ARG:N	2.36	0.94
4:B:1490:GLN:CD	4:B:3614:ILE:CG2	2.32	0.93
4:B:891:ILE:HD13	4:B:1075:TRP:HA	1.49	0.93
4:B:1598:TYR:HD2	4:B:1621:LEU:HD23	1.33	0.93
4:B:1212:ILE:CG1	4:B:1284:LEU:CA	2.36	0.93
4:B:751:GLY:O	4:B:754:GLU:N	2.01	0.93
4:B:1212:ILE:CG1	4:B:1284:LEU:CB	2.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1602:LYS:CE	4:B:1683:GLU:OE1	2.16	0.93
1:A:1223:VAL:HG12	1:A:1282:GLU:O	1.69	0.93
1:A:1536:LEU:HD22	4:B:3888:HIS:HB2	1.51	0.92
4:B:1606:PHE:CE1	4:B:1687:LEU:CA	2.46	0.92
4:B:1599:LEU:HD13	4:B:1617:LEU:CG	1.98	0.92
4:B:1606:PHE:HD1	4:B:1687:LEU:CG	1.81	0.92
4:B:1606:PHE:CE1	4:B:1687:LEU:HD12	2.03	0.92
1:A:1276:GLN:CG	12:D:153:HIS:CE1	2.53	0.92
4:B:1238:LYS:HE3	4:B:1308:LEU:HA	1.34	0.91
4:B:898:PRO:CD	4:B:1073:ILE:HG23	1.99	0.91
4:B:1602:LYS:CB	4:B:1683:GLU:HB3	1.99	0.91
4:B:1603:LYS:N	4:B:1609:PHE:HD2	1.69	0.91
2:C:1132:LYS:CG	2:C:1151:LEU:HD21	2.00	0.91
4:B:900:PHE:HB2	4:B:1076:LEU:HB2	1.51	0.91
4:B:1595:LEU:HB3	4:B:1618:LEU:HD23	0.93	0.90
4:B:808:PRO:HG2	4:B:1077:ARG:HD2	0.92	0.90
4:B:1599:LEU:HB2	4:B:1617:LEU:CD2	1.99	0.90
4:B:1527:ILE:CG2	4:B:1615:GLN:OE1	2.20	0.89
4:B:1603:LYS:HG2	4:B:1609:PHE:HB3	1.04	0.89
4:B:1599:LEU:HD22	4:B:1617:LEU:HG	1.52	0.89
2:C:391:GLN:HA	4:B:2596:THR:HG22	1.54	0.89
4:B:1237:ARG:NH2	4:B:1263:THR:N	2.21	0.89
4:B:1599:LEU:CB	4:B:1617:LEU:HD23	2.02	0.89
4:B:750:PRO:O	4:B:751:GLY:C	2.09	0.88
4:B:1527:ILE:HG21	4:B:1615:GLN:OE1	1.72	0.87
2:C:1067:VAL:N	2:C:1152:SER:CA	2.31	0.87
4:B:1212:ILE:CG1	4:B:1284:LEU:HA	1.97	0.87
4:B:1599:LEU:HD11	4:B:1618:LEU:CA	2.05	0.87
2:C:261:ILE:HB	2:C:385:ASP:CB	2.04	0.87
1:A:1219:PHE:CE2	1:A:1280:TYR:HA	2.10	0.86
4:B:1537:ASP:HB2	4:B:1624:GLY:N	1.91	0.86
2:C:1136:PHE:HD2	2:C:1139:PHE:H	0.87	0.86
2:C:1135:ALA:HB1	2:C:1212:GLU:HG2	1.56	0.86
4:B:1490:GLN:CD	4:B:3568:THR:O	2.14	0.86
1:A:1219:PHE:CZ	1:A:1263:TYR:CG	2.58	0.85
4:B:716:ASP:O	4:B:717:MET:C	2.11	0.85
4:B:1598:TYR:CD2	4:B:1621:LEU:HD23	2.11	0.85
4:B:1599:LEU:HD22	4:B:1617:LEU:C	1.95	0.85
4:B:1599:LEU:CD1	4:B:1617:LEU:CG	2.53	0.85
9:N:38:TYR:CB	9:N:75:GLN:HE22	1.89	0.85
4:B:1531:ILE:HG23	4:B:1622:SER:HG	1.35	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1603:LYS:CB	4:B:1609:PHE:HB2	2.07	0.84
4:B:1599:LEU:HD22	4:B:1617:LEU:CG	2.08	0.83
4:B:1538:ILE:HB	4:B:1622:SER:O	1.78	0.83
4:B:1606:PHE:HA	4:B:1687:LEU:HD13	1.61	0.83
1:A:1209:LEU:HA	1:A:1273:PHE:CE1	2.13	0.83
4:B:900:PHE:HB2	4:B:1076:LEU:CB	2.08	0.83
4:B:1603:LYS:HG2	4:B:1609:PHE:HB2	0.83	0.83
4:B:1603:LYS:HG2	4:B:1609:PHE:CA	2.06	0.82
4:B:898:PRO:CB	4:B:1077:ARG:CA	2.57	0.82
4:B:1599:LEU:HD11	4:B:1618:LEU:HG	1.59	0.82
4:B:898:PRO:HB2	4:B:1077:ARG:CA	2.10	0.81
1:A:1276:GLN:OE1	12:D:153:HIS:CE1	2.34	0.81
4:B:898:PRO:CB	4:B:1073:ILE:HG23	2.10	0.81
2:C:1135:ALA:CB	2:C:1212:GLU:CG	2.58	0.81
2:C:1014:ILE:HD11	2:C:1037:LEU:HD12	1.62	0.81
4:B:898:PRO:CD	4:B:1073:ILE:HD13	2.11	0.81
4:B:1227:ASP:OD1	4:B:1298:LEU:HA	1.80	0.81
2:C:1132:LYS:CG	2:C:1151:LEU:HD11	2.08	0.80
4:B:1212:ILE:CB	4:B:1284:LEU:CB	2.59	0.80
4:B:1599:LEU:CA	4:B:1621:LEU:HD21	2.09	0.80
9:N:76:THR:HG21	11:E:39:GLN:HE22	1.47	0.80
4:B:2887:LEU:HD13	4:B:3020:LEU:HD11	1.62	0.80
4:B:901:ASP:HA	4:B:1077:ARG:O	1.80	0.80
4:B:900:PHE:HB2	4:B:1076:LEU:HD12	1.64	0.80
4:B:349:ASN:HA	4:B:416:LEU:HD21	1.64	0.80
4:B:1599:LEU:CD1	4:B:1618:LEU:HG	2.12	0.80
4:B:1205:PHE:HZ	4:B:1285:GLU:CB	1.95	0.79
4:B:898:PRO:HD3	4:B:1073:ILE:CB	2.12	0.79
4:B:898:PRO:HD3	4:B:1073:ILE:CG1	2.13	0.79
4:B:1237:ARG:NH2	4:B:1263:THR:H	1.79	0.79
4:B:1595:LEU:CD1	4:B:1618:LEU:HD22	2.11	0.79
4:B:660:LEU:CB	4:B:755:ILE:HD12	2.13	0.79
4:B:900:PHE:H	4:B:1076:LEU:HB2	1.47	0.79
4:B:1606:PHE:CZ	4:B:1690:GLU:CG	2.66	0.79
2:C:1069:ARG:HG2	2:C:1155:ASN:ND2	1.98	0.79
4:B:1599:LEU:C	4:B:1617:LEU:HD21	2.02	0.78
4:B:900:PHE:CB	4:B:1076:LEU:HB2	2.13	0.78
4:B:904:LEU:HG	4:B:1083:MET:HG3	1.66	0.78
4:B:1595:LEU:HB2	4:B:1618:LEU:HD22	1.46	0.78
2:C:2066:GLN:HE21	2:C:2066:GLN:HA	1.48	0.78
4:B:1599:LEU:CA	4:B:1617:LEU:HD21	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1606:PHE:HB2	4:B:1687:LEU:HB2	1.66	0.78
4:B:1595:LEU:HB3	4:B:1618:LEU:HD22	1.10	0.78
2:C:1066:GLU:N	2:C:1152:SER:HG	1.82	0.78
4:B:1490:GLN:CB	4:B:3614:ILE:HG23	2.14	0.78
1:A:1536:LEU:HD21	4:B:3888:HIS:HB2	1.66	0.77
4:B:1599:LEU:HD23	4:B:1621:LEU:CG	2.13	0.77
1:A:1208:TYR:HD1	1:A:1273:PHE:CE2	2.03	0.77
2:C:538:ASN:O	2:C:702:PHE:CB	2.33	0.77
4:B:1534:LEU:O	4:B:1623:ASN:OD1	2.02	0.77
4:B:1599:LEU:HB3	4:B:1617:LEU:CD1	2.12	0.77
2:C:2659:ALA:HB1	2:C:2858:VAL:HG22	1.65	0.77
4:B:899:LEU:HD21	4:B:1075:TRP:CE2	2.20	0.77
4:B:1238:LYS:CE	4:B:1308:LEU:N	2.48	0.77
4:B:1237:ARG:CZ	4:B:1263:THR:CB	2.63	0.77
12:D:397:ASP:HB3	12:D:398:PRO:HD3	1.67	0.77
4:B:1599:LEU:CD2	4:B:1617:LEU:CG	2.60	0.77
2:C:391:GLN:HA	4:B:2596:THR:CG2	2.15	0.76
4:B:1595:LEU:CG	4:B:1618:LEU:HD22	2.15	0.76
4:B:1599:LEU:CA	4:B:1621:LEU:CD2	2.63	0.76
2:C:1066:GLU:N	2:C:1153:ASN:CG	2.38	0.75
4:B:1537:ASP:HB3	4:B:1624:GLY:CA	2.14	0.75
1:A:1223:VAL:HG13	1:A:1283:LEU:C	1.95	0.75
2:C:10:LEU:HD12	2:C:349:LEU:HD23	1.66	0.75
4:B:899:LEU:HD11	4:B:1075:TRP:CE2	2.21	0.75
4:B:1602:LYS:HB3	4:B:1609:PHE:HE2	1.50	0.75
4:B:1603:LYS:CD	4:B:1609:PHE:HB3	2.16	0.75
2:C:2687:ALA:HB1	2:C:2830:VAL:HG22	1.67	0.75
4:B:715:LEU:O	4:B:716:ASP:C	2.22	0.75
4:B:900:PHE:HB2	4:B:1076:LEU:CD1	2.16	0.74
4:B:900:PHE:N	4:B:1076:LEU:HB2	2.01	0.74
2:C:1067:VAL:CG2	2:C:1148:LEU:O	2.30	0.74
4:B:1223:LYS:NZ	4:B:1277:ARG:CB	2.50	0.74
4:B:3253:ILE:O	4:B:3253:ILE:HG22	1.88	0.74
1:A:1016:PHE:CZ	1:A:1069:TYR:HB2	2.22	0.74
1:A:1212:LEU:HD21	1:A:1275:LEU:CD1	2.17	0.73
1:A:1209:LEU:HB2	1:A:1273:PHE:HE1	1.51	0.73
11:E:395:VAL:CG2	11:E:402:ILE:HD12	2.18	0.73
4:B:1234:GLU:CD	4:B:1304:ASP:CB	2.43	0.73
1:A:933:VAL:HG11	1:A:944:LEU:HD12	1.68	0.73
2:C:2613:THR:HG21	2:C:3176:LEU:HD22	1.70	0.72
4:B:1490:GLN:CB	4:B:3614:ILE:CG2	2.66	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2717:ALA:HB1	2:C:2803:MET:SD	2.29	0.72
4:B:1490:GLN:HB3	4:B:3614:ILE:HG23	1.71	0.72
2:C:1132:LYS:HG2	2:C:1151:LEU:HD21	1.71	0.72
4:B:1599:LEU:CG	4:B:1621:LEU:HD22	2.15	0.72
2:C:1128:PHE:HZ	2:C:1151:LEU:HB3	1.53	0.72
2:C:2812:GLY:O	2:C:2815:SER:N	2.23	0.72
4:B:898:PRO:HD3	4:B:1073:ILE:HD13	1.71	0.72
4:B:899:LEU:CD2	4:B:1075:TRP:NE1	2.42	0.72
4:B:900:PHE:CB	4:B:1076:LEU:CD1	2.63	0.72
2:C:898:TRP:O	2:C:902:LEU:HD13	1.90	0.72
4:B:808:PRO:HD2	4:B:1077:ARG:HH11	1.54	0.71
4:B:1537:ASP:CB	4:B:1624:GLY:N	2.52	0.71
4:B:1599:LEU:HD22	4:B:1617:LEU:CD1	2.20	0.71
4:B:898:PRO:CG	4:B:1073:ILE:HG23	2.20	0.71
4:B:1602:LYS:CE	4:B:1683:GLU:CD	2.56	0.71
4:B:891:ILE:CD1	4:B:1075:TRP:HA	2.21	0.71
1:A:1220:THR:HG23	1:A:1279:LYS:CB	2.20	0.71
4:B:2621:ILE:HG23	4:B:2667:LEU:CD1	2.20	0.71
2:C:2766:GLU:O	2:C:2769:LEU:N	2.23	0.71
1:A:3212:VAL:HG13	1:A:3335:TRP:NE1	2.06	0.70
4:B:751:GLY:O	4:B:753:GLU:N	2.24	0.70
4:B:898:PRO:CD	4:B:1073:ILE:CG1	2.69	0.70
2:C:1067:VAL:N	2:C:1152:SER:CB	2.50	0.70
4:B:719:VAL:O	4:B:720:ASP:C	2.29	0.70
4:B:898:PRO:HB2	4:B:1077:ARG:HB2	1.73	0.70
4:B:1537:ASP:CB	4:B:1624:GLY:CA	2.70	0.70
2:C:2617:VAL:CG1	2:C:2900:VAL:HG22	2.21	0.70
1:A:1209:LEU:CB	1:A:1273:PHE:HE1	2.04	0.70
4:B:1595:LEU:HB2	4:B:1618:LEU:HD21	1.57	0.70
2:C:1135:ALA:CB	2:C:1212:GLU:HG3	2.22	0.69
2:C:1135:ALA:CB	2:C:1212:GLU:HG2	2.20	0.69
4:B:660:LEU:CB	4:B:752:ILE:HG23	2.22	0.69
4:B:1599:LEU:HD21	4:B:1617:LEU:C	2.08	0.69
4:B:764:GLN:O	4:B:767:SER:N	2.26	0.69
4:B:1606:PHE:HZ	4:B:1690:GLU:HB2	0.65	0.69
1:A:1212:LEU:HD21	1:A:1275:LEU:HD13	1.74	0.69
1:A:1220:THR:CG2	1:A:1279:LYS:CB	2.71	0.69
2:C:1136:PHE:CG	2:C:1138:ARG:N	2.58	0.69
4:B:1531:ILE:HD13	4:B:1618:LEU:CB	2.17	0.69
1:A:3583:ILE:HG22	1:A:3627:CYS:HA	1.74	0.69
4:B:3331:TYR:O	4:B:3334:SER:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1599:LEU:CD1	4:B:1617:LEU:C	2.62	0.68
4:B:3273:ASP:O	4:B:3276:VAL:N	2.24	0.68
2:C:1135:ALA:HB1	2:C:1212:GLU:HG3	1.72	0.68
4:B:1220:GLN:CG	4:B:1294:ASN:CB	2.56	0.68
1:A:1500:THR:HG23	1:A:1566:GLN:HE22	1.58	0.68
2:C:1067:VAL:N	2:C:1152:SER:C	2.42	0.68
2:C:2617:VAL:HG22	2:C:3183:ILE:HD13	1.75	0.68
2:C:3970:LEU:HD23	2:C:3990:LEU:HD21	1.75	0.68
4:B:2696:LEU:HD12	4:B:2707:ALA:HB2	1.74	0.68
1:A:1276:GLN:CD	12:D:153:HIS:CE1	2.67	0.68
4:B:898:PRO:HD2	4:B:1073:ILE:HD13	1.76	0.68
9:N:38:TYR:CB	9:N:75:GLN:NE2	2.57	0.68
4:B:1606:PHE:HZ	4:B:1690:GLU:CG	2.06	0.68
2:C:359:GLY:O	2:C:386:GLY:C	2.18	0.68
4:B:900:PHE:CA	4:B:1076:LEU:HB2	2.24	0.67
4:B:898:PRO:HG3	4:B:1073:ILE:CG1	2.12	0.67
2:C:972:LEU:HD21	2:C:1017:MET:CE	2.25	0.67
4:B:1603:LYS:CE	4:B:1609:PHE:HB3	2.25	0.67
2:C:2177:ILE:HG22	2:C:2233:PRO:HA	1.77	0.67
1:A:1016:PHE:CZ	1:A:1076:LEU:HD12	2.30	0.67
1:A:2443:CYS:O	1:A:2443:CYS:SG	2.53	0.67
4:B:1603:LYS:N	4:B:1609:PHE:CD2	2.58	0.67
2:C:539:LYS:CB	2:C:702:PHE:CA	2.71	0.67
2:C:1132:LYS:HE2	2:C:1151:LEU:CG	2.19	0.67
4:B:1230:MET:CE	4:B:1267:TYR:HA	2.25	0.67
4:B:1599:LEU:HD11	4:B:1618:LEU:H	1.54	0.66
4:B:899:LEU:CD2	4:B:1075:TRP:CD1	2.75	0.66
4:B:1237:ARG:CD	4:B:1263:THR:CB	2.73	0.66
2:C:834:VAL:HG22	2:C:881:ILE:HD11	1.78	0.66
4:B:898:PRO:HG2	4:B:1077:ARG:HB2	1.77	0.66
4:B:1102:LEU:HD23	4:B:1105:GLN:HB2	1.78	0.66
2:C:1132:LYS:HG2	2:C:1151:LEU:CD2	2.26	0.66
2:C:2790:ASN:CB	2:C:2821:VAL:HG22	2.25	0.66
4:B:898:PRO:HD3	4:B:1073:ILE:CD1	2.26	0.66
4:B:1490:GLN:HB3	4:B:3614:ILE:CG2	2.26	0.66
4:B:1603:LYS:CA	4:B:1609:PHE:HD2	2.09	0.66
1:A:1013:VAL:HG13	1:A:1076:LEU:HD11	1.78	0.66
2:C:39:LEU:HD12	2:C:345:TRP:CZ2	2.31	0.66
1:A:751:LEU:HG	1:A:886:ILE:HD11	1.77	0.65
4:B:1606:PHE:CD1	4:B:1687:LEU:HB2	2.31	0.65
11:E:395:VAL:HG21	11:E:402:ILE:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1634:ILE:HD13	1:A:1656:ILE:HG23	1.78	0.65
4:B:898:PRO:CD	4:B:1073:ILE:CD1	2.75	0.65
4:B:1595:LEU:CB	4:B:1618:LEU:HD23	1.86	0.65
2:C:2801:GLU:O	2:C:2804:ALA:HB3	1.96	0.65
4:B:1602:LYS:CB	4:B:1609:PHE:HE2	2.10	0.65
4:B:4168:VAL:HG11	4:B:4189:ILE:HG21	1.77	0.65
4:B:808:PRO:CG	4:B:1077:ARG:HD3	2.17	0.65
1:A:1209:LEU:CA	1:A:1273:PHE:CE1	2.80	0.65
2:C:1060:LEU:HD11	2:C:1148:LEU:HD22	1.77	0.65
2:C:1069:ARG:HG2	2:C:1155:ASN:CG	2.17	0.65
2:C:1132:LYS:CD	2:C:1151:LEU:CD2	2.72	0.65
4:B:898:PRO:HA	4:B:1075:TRP:O	1.97	0.65
4:B:1238:LYS:HE2	4:B:1308:LEU:CA	2.14	0.65
4:B:898:PRO:HB2	4:B:1077:ARG:H	1.60	0.65
4:B:1537:ASP:HB2	4:B:1624:GLY:H	1.62	0.65
4:B:3289:ALA:O	4:B:3292:ASP:HB2	1.97	0.65
4:B:898:PRO:HB2	4:B:1077:ARG:CB	2.27	0.65
2:C:2812:GLY:O	2:C:2815:SER:OG	2.08	0.64
1:A:1219:PHE:CD1	1:A:1266:ASN:CB	2.81	0.64
1:A:2418:ILE:HG22	1:A:2419:PRO:HD2	1.80	0.64
4:B:871:ILE:HD11	4:B:944:ILE:HD11	1.79	0.64
4:B:886:ILE:HA	4:B:1075:TRP:CD1	2.33	0.64
4:B:2157:LEU:HB2	19:B:4701:ATP:N1	2.12	0.64
5:I:94:LEU:HD21	12:D:195:ILE:HD13	1.80	0.64
1:A:1631:PHE:HB2	1:A:1634:ILE:CG2	2.27	0.64
1:A:3290:LEU:HD22	1:A:3335:TRP:CZ2	2.33	0.64
4:B:898:PRO:CG	4:B:1077:ARG:HB2	2.28	0.64
4:B:898:PRO:HB3	4:B:1077:ARG:N	2.13	0.64
1:A:3702:SER:CB	1:A:3712:LEU:HD11	2.28	0.63
4:B:3332:ALA:O	4:B:3335:LYS:N	2.31	0.63
1:A:1219:PHE:CE1	1:A:1263:TYR:CB	2.81	0.63
1:A:1223:VAL:HG13	1:A:1283:LEU:O	1.99	0.63
4:B:1598:TYR:CE2	4:B:1621:LEU:HG	2.34	0.63
1:A:1208:TYR:CD1	1:A:1273:PHE:CE2	2.87	0.63
1:A:1212:LEU:HD13	1:A:1273:PHE:CG	2.34	0.63
2:C:391:GLN:CA	4:B:2596:THR:HG22	2.28	0.63
11:E:531:ARG:O	11:E:535:LYS:N	2.31	0.63
12:D:167:ASN:O	12:D:168:TYR:CD2	2.51	0.63
1:A:1926:PHE:HB3	1:A:1974:ILE:HG23	1.80	0.63
4:B:764:GLN:O	4:B:765:PHE:O	2.17	0.63
1:A:3128:THR:HG22	1:A:3422:LEU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1880:VAL:HA	2:C:1883:ILE:HD12	1.79	0.63
4:B:898:PRO:HB3	4:B:1076:LEU:C	2.18	0.63
1:A:3212:VAL:HG13	1:A:3335:TRP:CD1	2.34	0.63
4:B:1531:ILE:HG23	4:B:1622:SER:CB	2.29	0.63
4:B:3878:ILE:HD11	4:B:3887:ALA:HB2	1.81	0.63
12:D:397:ASP:CB	12:D:398:PRO:HD3	2.29	0.62
2:C:903:PRO:HB3	2:C:3080:GLY:HA2	1.82	0.62
4:B:1599:LEU:HD22	4:B:1617:LEU:HD12	1.81	0.62
1:A:1219:PHE:CZ	1:A:1263:TYR:CB	2.82	0.62
2:C:1135:ALA:HB1	2:C:1212:GLU:CD	2.20	0.62
4:B:1538:ILE:CB	4:B:1622:SER:O	2.40	0.62
5:I:51:ALA:HB1	5:I:52:PRO:CD	2.30	0.62
8:F:80:ARG:NH2	8:F:103:CYS:SG	2.73	0.62
1:A:1276:GLN:OE1	12:D:153:HIS:ND1	2.31	0.62
1:A:1219:PHE:CZ	1:A:1263:TYR:CA	2.80	0.62
1:A:1392:ASN:O	1:A:1396:PRO:N	2.33	0.62
4:B:1599:LEU:HD21	4:B:1618:LEU:HA	1.81	0.62
4:B:3525:ILE:HG22	4:B:3644:ILE:HD13	1.82	0.62
7:G:107:THR:HG21	7:G:137:VAL:HG11	1.81	0.62
4:B:898:PRO:CG	4:B:1077:ARG:CB	2.78	0.61
4:B:898:PRO:CD	4:B:1073:ILE:HG12	2.29	0.61
4:B:3314:ILE:CD1	4:B:3344:VAL:HG21	2.30	0.61
4:B:1599:LEU:HD11	4:B:1618:LEU:CG	2.31	0.61
4:B:2984:VAL:HG13	4:B:3004:LEU:HD12	1.81	0.61
2:C:1081:ILE:HD11	2:C:1117:GLN:CB	2.29	0.61
1:A:1458:MET:SD	1:A:1549:MET:HA	2.39	0.61
1:A:2171:THR:O	1:A:2175:THR:HG23	1.99	0.61
4:B:764:GLN:C	4:B:766:ILE:N	2.51	0.61
4:B:900:PHE:O	4:B:1077:ARG:N	2.33	0.61
2:C:2722:VAL:HG12	2:C:2813:ILE:HD13	1.82	0.61
4:B:1230:MET:HE1	4:B:1267:TYR:HA	1.81	0.61
4:B:1602:LYS:O	4:B:1683:GLU:HB2	2.01	0.61
2:C:2738:ILE:HG22	2:C:2746:PRO:HD3	1.83	0.61
4:B:765:PHE:O	4:B:766:ILE:O	2.19	0.61
11:E:423:GLY:HA2	11:E:505:ILE:HD12	1.82	0.61
1:A:4287:THR:HG22	1:A:4549:ILE:HD12	1.82	0.61
1:A:91:LYS:CB	4:B:136:PRO:CB	2.79	0.60
2:C:1132:LYS:CD	2:C:1151:LEU:HD21	2.31	0.60
4:B:829:VAL:HG11	4:B:940:ILE:HG23	1.83	0.60
4:B:1102:LEU:HA	4:B:1105:GLN:HB2	1.84	0.60
4:B:3327:ALA:O	4:B:3329:GLN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:24:ILE:HD11	12:D:207:ALA:HB1	1.82	0.60
1:A:1212:LEU:CD2	1:A:1275:LEU:CD1	2.79	0.60
1:A:1396:PRO:O	1:A:1400:TYR:N	2.34	0.60
1:A:1806:PHE:CD1	1:A:4194:VAL:HG22	2.36	0.60
2:C:2790:ASN:HB2	2:C:2821:VAL:HG22	1.82	0.60
4:B:723:ASN:O	4:B:726:LYS:N	2.34	0.60
1:A:3533:PRO:HD3	1:A:3648:THR:HG22	1.83	0.60
2:C:1718:VAL:HG21	2:C:1737:LEU:HD21	1.82	0.60
4:B:3153:LEU:HD13	4:B:3707:LEU:HD11	1.83	0.60
5:I:51:ALA:HB1	5:I:52:PRO:HD2	1.83	0.60
1:A:1539:LYS:HE2	4:B:3859:VAL:CG2	2.32	0.60
1:A:1789:VAL:HG21	1:A:2010:VAL:HG22	1.83	0.60
4:B:3326:MET:O	4:B:3327:ALA:C	2.40	0.60
4:B:1598:TYR:HD2	4:B:1621:LEU:CD2	2.13	0.60
4:B:1603:LYS:HG3	4:B:1609:PHE:CD2	2.37	0.60
2:C:359:GLY:O	2:C:386:GLY:O	2.19	0.60
4:B:1598:TYR:CD2	4:B:1621:LEU:CD2	2.84	0.60
10:O:102:LEU:HD12	12:D:75:LEU:HD12	1.84	0.60
1:A:4056:ILE:HD11	1:A:4072:LEU:HD21	1.82	0.60
1:A:1031:ILE:HG21	1:A:1095:GLN:HG3	1.84	0.59
1:A:2042:ARG:HG3	1:A:2278:ASN:HA	1.84	0.59
1:A:3895:GLU:O	1:A:3899:LEU:HD13	2.02	0.59
4:B:1490:GLN:HB2	4:B:3614:ILE:HG23	1.84	0.59
4:B:3327:ALA:HA	4:B:3334:SER:HB2	1.84	0.59
1:A:3914:ASN:O	1:A:3950:ARG:NH1	2.34	0.59
4:B:898:PRO:CA	4:B:1073:ILE:HG23	2.32	0.59
4:B:1061:GLN:HE21	4:B:1091:VAL:HG12	1.67	0.59
4:B:4206:ARG:NH2	4:B:4573:ILE:HD13	2.17	0.59
4:B:886:ILE:HA	4:B:1075:TRP:NE1	2.18	0.59
4:B:898:PRO:CB	4:B:1076:LEU:C	2.71	0.59
1:A:1632:ASP:HB2	1:A:1892:PHE:CD1	2.37	0.59
2:C:1132:LYS:HE3	2:C:1151:LEU:HD21	1.60	0.59
1:A:1445:PHE:CZ	1:A:1508:LEU:HD21	2.36	0.59
4:B:1492:LYS:HZ2	4:B:3606:GLN:HB2	1.67	0.59
4:B:1599:LEU:HD13	4:B:1617:LEU:CA	2.32	0.59
4:B:1603:LYS:CE	4:B:1609:PHE:C	2.51	0.59
12:D:352:CYS:SG	12:D:402:VAL:N	2.74	0.59
4:B:899:LEU:N	4:B:1076:LEU:HA	2.05	0.59
4:B:1606:PHE:CZ	4:B:1690:GLU:HG2	2.37	0.59
4:B:3472:LEU:O	4:B:3476:THR:OG1	2.21	0.59
1:A:539:PHE:HA	1:A:544:TYR:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2217:ASN:HD22	2:C:2247:THR:HG23	1.68	0.59
4:B:900:PHE:O	4:B:1077:ARG:O	2.21	0.59
1:A:1227:ARG:CB	1:A:1286:THR:HA	2.33	0.58
2:C:1067:VAL:HA	2:C:1152:SER:O	2.03	0.58
4:B:898:PRO:CB	4:B:1077:ARG:HB2	2.32	0.58
4:B:1603:LYS:CG	4:B:1609:PHE:CG	2.81	0.58
4:B:1603:LYS:HG3	4:B:1609:PHE:CG	2.37	0.58
4:B:898:PRO:HB3	4:B:1073:ILE:HG23	1.84	0.58
4:B:2174:LEU:HD11	4:B:2302:ILE:HD11	1.85	0.58
4:B:1537:ASP:HB3	4:B:1624:GLY:HA3	1.84	0.58
4:B:1603:LYS:HD2	4:B:1617:LEU:HD22	1.85	0.58
2:C:2722:VAL:CG1	2:C:2813:ILE:HD13	2.33	0.58
4:B:3324:LYS:O	4:B:3327:ALA:N	2.37	0.58
4:B:3528:CYS:SG	4:B:3642:THR:HG21	2.42	0.58
11:E:306:ILE:HG23	11:E:343:LEU:HD12	1.85	0.58
1:A:2033:LEU:CD2	1:A:4498:LEU:HD23	2.34	0.58
2:C:2821:VAL:O	2:C:2825:ASP:N	2.36	0.58
2:C:3732:HIS:CG	2:C:3757:LEU:HD12	2.39	0.58
4:B:898:PRO:N	4:B:1073:ILE:CG2	2.67	0.58
4:B:2740:ASN:O	4:B:2742:ARG:N	2.37	0.58
1:A:1066:VAL:HB	1:A:1069:TYR:CE1	2.38	0.58
1:A:1216:ILE:HG23	1:A:1279:LYS:CB	2.33	0.58
2:C:2534:VAL:HG21	2:C:2586:THR:HG22	1.86	0.58
1:A:936:GLN:HA	1:A:1081:ILE:CB	2.34	0.58
1:A:3223:LEU:HD11	1:A:3332:ILE:CD1	2.34	0.58
2:C:1186:THR:O	2:C:1188:LEU:N	2.36	0.58
4:B:3764:LEU:HD11	4:B:3816:LEU:HD21	1.84	0.58
2:C:2555:LEU:HD22	2:C:2953:ASN:HD22	1.68	0.57
1:A:4599:CYS:O	1:A:4599:CYS:SG	2.63	0.57
4:B:1110:GLN:O	4:B:1114:LEU:HG	2.04	0.57
4:B:3081:ASN:HD21	4:B:3484:LYS:HD3	1.69	0.57
10:O:102:LEU:CD1	12:D:75:LEU:HD12	2.34	0.57
2:C:1559:LEU:HD23	2:C:1607:LEU:HD21	1.86	0.57
12:D:571:LEU:HB3	12:D:647:TYR:CE2	2.40	0.57
4:B:1237:ARG:HH21	4:B:1263:THR:N	1.97	0.57
1:A:2030:LEU:HB2	1:A:2101:ILE:HD13	1.87	0.57
2:C:1081:ILE:HD11	2:C:1117:GLN:HB3	1.86	0.57
4:B:1603:LYS:CE	4:B:1617:LEU:HD22	2.34	0.57
2:C:1136:PHE:HB3	2:C:1139:PHE:CD2	2.40	0.57
1:A:1209:LEU:HB2	1:A:1273:PHE:CE1	2.35	0.57
1:A:2786:CYS:HB3	1:A:2850:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3829:VAL:HG11	4:B:3946:ILE:HD13	1.86	0.57
10:O:98:ALA:HA	12:D:107:VAL:HA	1.86	0.57
2:C:1333:VAL:HG12	2:C:1340:GLN:HE21	1.68	0.57
2:C:2631:ALA:HB1	2:C:2886:ALA:HB1	1.85	0.57
1:A:1013:VAL:HG12	1:A:1017:LEU:HD12	1.86	0.56
1:A:3223:LEU:HD21	1:A:3332:ILE:CD1	2.35	0.56
2:C:136:ALA:HB2	2:C:168:ASN:HA	1.87	0.56
4:B:1209:ALA:CB	4:B:1286:LYS:CB	2.83	0.56
4:B:2264:ASP:O	4:B:2625:ARG:NH2	2.38	0.56
4:B:3984:PHE:CD2	4:B:4076:LEU:HD11	2.40	0.56
2:C:1900:TYR:O	2:C:1903:VAL:N	2.38	0.56
4:B:4370:ILE:HD13	4:B:4384:MET:HB3	1.87	0.56
1:A:1525:PHE:HB2	1:A:1541:PHE:HD2	1.70	0.56
1:A:1631:PHE:CZ	1:A:1687:LEU:HD22	2.41	0.56
4:B:1535:SER:HB3	4:B:1623:ASN:CG	2.25	0.56
4:B:3984:PHE:CE2	4:B:4076:LEU:HD11	2.40	0.56
1:A:1544:ILE:HG12	1:A:1580:LYS:HG2	1.88	0.56
2:C:1132:LYS:CG	2:C:1151:LEU:CD2	2.73	0.56
4:B:1603:LYS:CA	4:B:1609:PHE:CD2	2.89	0.56
4:B:3267:ILE:HD12	4:B:3279:LYS:CD	2.36	0.56
1:A:1220:THR:HG22	1:A:1279:LYS:HA	1.87	0.56
4:B:1606:PHE:CA	4:B:1607:PRO:HD3	2.35	0.56
4:B:773:VAL:O	4:B:777:PHE:HB2	2.05	0.56
2:C:1541:LEU:HD13	2:C:1584:LEU:HD22	1.88	0.56
1:A:1065:ILE:HG21	1:A:1082:CYS:SG	2.46	0.56
4:B:1603:LYS:HE3	4:B:1617:LEU:HD22	1.86	0.56
1:A:3220:ILE:HD11	1:A:3290:LEU:HD12	1.89	0.56
1:A:3709:ASP:HB3	1:A:3712:LEU:HD12	1.87	0.56
2:C:34:ILE:HD12	2:C:116:THR:HG22	1.88	0.56
4:B:319:PRO:CB	11:E:552:ILE:HG22	2.36	0.56
12:D:294:GLN:HE21	12:D:297:LYS:HE2	1.71	0.55
17:M:65:ILE:HD13	17:M:85:TRP:CH2	2.40	0.55
4:B:1599:LEU:HD21	4:B:1618:LEU:CA	2.35	0.55
4:B:3267:ILE:HG23	4:B:3271:ASP:HB2	1.88	0.55
4:B:3586:ILE:HG21	4:B:3594:LEU:HD11	1.88	0.55
1:A:3018:LEU:O	1:A:3022:CYS:SG	2.64	0.55
2:C:913:MET:CE	2:C:959:THR:HG22	2.37	0.55
4:B:2703:ALA:HB2	4:B:2763:ASP:HB2	1.87	0.55
9:N:38:TYR:O	9:N:75:GLN:NE2	2.39	0.55
2:C:1069:ARG:CG	2:C:1155:ASN:ND2	2.69	0.55
2:C:1128:PHE:CE2	2:C:1151:LEU:HD13	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2008:LEU:HD23	2:C:2150:ILE:HD11	1.89	0.55
2:C:2790:ASN:HB3	2:C:2821:VAL:HG22	1.88	0.55
4:B:1535:SER:CB	4:B:1622:SER:C	2.65	0.55
4:B:2040:LEU:CD1	4:B:2083:LEU:HD22	2.35	0.55
4:B:1531:ILE:HG23	4:B:1618:LEU:O	2.07	0.55
1:A:1500:THR:O	1:A:1504:VAL:HG23	2.06	0.55
4:B:3020:LEU:HD13	4:B:3022:PHE:CZ	2.42	0.55
2:C:2128:MET:HE1	2:C:2137:VAL:HG21	1.88	0.55
4:B:900:PHE:H	4:B:1076:LEU:CB	2.19	0.55
4:B:1937:ALA:HB2	4:B:1969:GLN:HE22	1.72	0.55
4:B:1490:GLN:OE1	4:B:3568:THR:O	2.24	0.55
12:D:75:LEU:HD23	12:D:75:LEU:N	2.22	0.55
1:A:942:VAL:HG21	1:A:1021:THR:HG22	1.89	0.54
4:B:2122:PHE:CE2	4:B:2126:ILE:HD11	2.42	0.54
4:B:3314:ILE:HD12	4:B:3344:VAL:HG21	1.90	0.54
14:L:42:ILE:HD12	14:L:98:LEU:HD12	1.89	0.54
4:B:898:PRO:CB	4:B:1077:ARG:CB	2.84	0.54
1:A:1016:PHE:CE2	1:A:1069:TYR:HB2	2.43	0.54
1:A:1129:ILE:HD11	1:A:1211:GLU:HB3	1.89	0.54
1:A:3235:TYR:OH	1:A:3258:PHE:CD1	2.60	0.54
2:C:2822:LYS:O	2:C:2826:VAL:HG23	2.07	0.54
1:A:2216:TRP:O	1:A:2220:ASN:ND2	2.38	0.54
2:C:955:ILE:O	2:C:959:THR:HG23	2.07	0.54
2:C:2066:GLN:HE21	2:C:2066:GLN:CA	2.17	0.54
4:B:162:TYR:CB	4:B:176:LEU:CB	2.85	0.54
4:B:1234:GLU:HB2	4:B:1308:LEU:CB	2.37	0.54
4:B:3085:VAL:HG21	4:B:3456:ALA:HB1	1.89	0.54
1:A:3099:TYR:HA	1:A:3451:THR:HG21	1.88	0.54
2:C:539:LYS:CB	2:C:702:PHE:CB	2.84	0.54
2:C:3460:ASN:N	2:C:3460:ASN:HD22	2.05	0.54
2:C:4077:LEU:HD13	2:C:4105:MET:HG2	1.90	0.54
12:D:174:GLN:HA	17:M:62:GLY:HA2	1.89	0.54
1:A:4125:ASN:HD21	1:A:4187:LEU:HG	1.73	0.54
4:B:1602:LYS:HA	4:B:1683:GLU:HG3	1.87	0.54
4:B:3902:TYR:O	4:B:3934:ARG:NH1	2.40	0.54
1:A:1504:VAL:HG22	1:A:1565:CYS:HB3	1.89	0.54
4:B:904:LEU:O	4:B:1083:MET:HB2	2.08	0.54
4:B:3658:ILE:HD11	4:B:3748:ARG:HE	1.72	0.54
2:C:881:ILE:O	2:C:881:ILE:HG22	2.07	0.54
1:A:3500:ILE:HD12	1:A:3515:ILE:HG23	1.89	0.54
2:C:1067:VAL:CA	2:C:1152:SER:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:744:MET:HE1	4:B:773:VAL:HG23	1.90	0.54
5:I:90:GLN:HB2	5:I:93:THR:HG21	1.90	0.54
1:A:1536:LEU:HD21	4:B:3888:HIS:CB	2.37	0.54
1:A:3124:ILE:O	1:A:3128:THR:HG23	2.07	0.54
1:A:3449:LEU:HD21	1:A:3474:VAL:HG22	1.90	0.54
4:B:3085:VAL:HG23	4:B:3477:TRP:CE2	2.43	0.54
12:D:120:SER:OG	12:D:123:TYR:N	2.38	0.54
1:A:2418:ILE:CG2	1:A:2428:VAL:HG22	2.38	0.53
2:C:214:LEU:C	2:C:214:LEU:HD22	2.29	0.53
4:B:898:PRO:CB	4:B:1077:ARG:HA	2.35	0.53
12:D:66:LEU:HB2	12:D:70:MET:HB2	1.91	0.53
4:B:716:ASP:O	4:B:719:VAL:N	2.41	0.53
4:B:769:SER:O	4:B:773:VAL:N	2.41	0.53
4:B:1527:ILE:HG23	4:B:1615:GLN:OE1	2.07	0.53
1:A:2745:LEU:HD11	1:A:2754:VAL:HG21	1.89	0.53
4:B:1117:ILE:HG12	4:B:1190:ILE:HD11	1.91	0.53
4:B:1484:LEU:HD12	4:B:1508:LEU:HD12	1.90	0.53
1:A:1609:THR:HG21	1:A:1629:LYS:HE3	1.91	0.53
4:B:1477:LEU:HD22	4:B:1508:LEU:HD22	1.89	0.53
2:C:912:SER:HA	2:C:966:LEU:HD22	1.91	0.53
2:C:2693:GLN:O	2:C:2696:SER:OG	2.20	0.53
1:A:1445:PHE:CE1	1:A:1561:VAL:HG13	2.43	0.53
1:A:1487:VAL:HA	1:A:1490:PHE:CZ	2.44	0.53
1:A:1536:LEU:CD2	4:B:3888:HIS:CB	2.80	0.53
2:C:972:LEU:HD21	2:C:1017:MET:SD	2.48	0.53
4:B:718:ILE:HD11	4:B:773:VAL:HG21	1.90	0.53
12:D:364:ALA:HB2	12:D:404:TRP:NE1	2.23	0.53
1:A:3170:GLY:HA3	1:A:3380:ILE:HG21	1.91	0.53
1:A:3702:SER:HB3	1:A:3712:LEU:HD11	1.91	0.53
1:A:4505:THR:HG22	1:A:4558:VAL:HG12	1.90	0.53
2:C:1136:PHE:CE2	2:C:1138:ARG:C	2.53	0.53
2:C:2659:ALA:CB	2:C:2858:VAL:HG22	2.35	0.53
4:B:1212:ILE:HG22	4:B:1213:PRO:HD3	1.91	0.53
4:B:3257:ARG:O	4:B:3258:VAL:C	2.45	0.53
1:A:2567:VAL:HG22	1:A:2573:GLN:HG3	1.90	0.53
1:A:3913:LYS:O	1:A:3947:ARG:NH1	2.40	0.53
2:C:1135:ALA:O	2:C:1137:PRO:HD3	2.08	0.53
2:C:2755:LEU:O	2:C:2758:MET:N	2.41	0.53
4:B:2846:LEU:HD11	4:B:2872:VAL:HG11	1.90	0.53
1:A:1634:ILE:HD13	1:A:1656:ILE:CG2	2.39	0.53
4:B:2711:VAL:HA	4:B:2714:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:38:ILE:HG22	10:O:67:LEU:HD11	1.91	0.53
11:E:384:LEU:HD23	11:E:417:TRP:CE2	2.43	0.53
14:L:80:LYS:HB2	17:M:60:ASN:HD21	1.73	0.53
1:A:2411:LEU:HD12	1:A:2428:VAL:HG21	1.90	0.53
1:A:4234:PHE:O	1:A:4236:TYR:N	2.42	0.53
2:C:2128:MET:HE1	2:C:2137:VAL:CG2	2.39	0.53
4:B:533:ARG:HB3	4:B:534:PRO:CD	2.39	0.53
1:A:3229:PRO:HB2	1:A:3233:ILE:HG23	1.92	0.52
4:B:2696:LEU:HD23	4:B:2699:ILE:HD12	1.91	0.52
7:G:99:ILE:HG23	7:G:103:ILE:HD12	1.91	0.52
5:I:12:ILE:HG23	7:G:120:THR:HG23	1.90	0.52
9:N:88:TYR:HA	11:E:23:THR:HG22	1.91	0.52
10:O:76:VAL:N	10:O:77:PRO:CD	2.73	0.52
12:D:89:TYR:CD1	15:K:56:PRO:HB3	2.44	0.52
12:D:519:ALA:HB1	12:D:545:VAL:CG1	2.39	0.52
2:C:90:ILE:HD11	2:C:96:LEU:HD23	1.90	0.52
2:C:4017:LEU:HD21	2:C:4022:LEU:HD11	1.91	0.52
4:B:569:VAL:HG13	4:B:578:LEU:HD11	1.91	0.52
4:B:765:PHE:O	4:B:767:SER:N	2.43	0.52
4:B:1102:LEU:HD23	4:B:1105:GLN:CB	2.39	0.52
2:C:1207:LEU:HD13	2:C:1214:TYR:CE1	2.44	0.52
2:C:4051:THR:HG21	2:C:4143:ASN:HD22	1.74	0.52
4:B:3331:TYR:O	4:B:3332:ALA:C	2.47	0.52
4:B:3332:ALA:O	4:B:3333:ALA:C	2.48	0.52
1:A:2676:TRP:CD2	1:A:2699:LEU:HD21	2.45	0.52
2:C:2896:ALA:O	2:C:2900:VAL:HG23	2.10	0.52
2:C:4084:ILE:HD11	2:C:4106:PRO:HG3	1.91	0.52
4:B:721:ASN:OD1	4:B:777:PHE:CE2	2.63	0.52
4:B:1102:LEU:O	4:B:1106:PHE:N	2.35	0.52
1:A:1422:SER:HB2	1:A:1486:HIS:CE1	2.45	0.52
2:C:2617:VAL:CG2	2:C:3183:ILE:HD13	2.40	0.52
2:C:3227:ALA:HA	2:C:3393:ILE:HG22	1.91	0.52
4:B:361:LYS:HA	4:B:477:ILE:HG23	1.90	0.52
4:B:2863:VAL:HG21	4:B:3059:VAL:HA	1.91	0.52
4:B:3020:LEU:HD13	4:B:3022:PHE:CE2	2.45	0.52
1:A:2676:TRP:CE2	1:A:2699:LEU:HD21	2.45	0.52
2:C:2096:ILE:HD11	2:C:2141:TYR:CD2	2.45	0.52
4:B:591:TRP:CD1	11:E:411:TYR:OH	2.63	0.52
4:B:716:ASP:O	4:B:718:ILE:N	2.43	0.52
4:B:1149:ASP:O	4:B:1153:VAL:N	2.43	0.52
4:B:1205:PHE:HE2	4:B:1286:LYS:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:LEU:HB3	1:A:1166:TYR:CE2	2.45	0.52
2:C:403:GLU:O	4:B:2988:ARG:CZ	2.54	0.52
2:C:1017:MET:HE2	2:C:1030:VAL:HB	1.91	0.52
7:G:71:LYS:HG3	7:G:72:THR:HG23	1.91	0.52
17:M:65:ILE:HG21	17:M:85:TRP:CE2	2.45	0.52
1:A:1208:TYR:CD1	1:A:1273:PHE:HE2	2.27	0.52
1:A:3163:SER:HA	1:A:3387:LEU:HD13	1.91	0.52
1:A:3220:ILE:CD1	1:A:3290:LEU:HD12	2.40	0.52
4:B:825:LYS:O	4:B:829:VAL:HG23	2.10	0.52
4:B:898:PRO:CG	4:B:1073:ILE:CG1	2.77	0.52
4:B:1599:LEU:HD13	4:B:1617:LEU:C	2.30	0.52
4:B:1599:LEU:CD1	4:B:1617:LEU:CB	2.61	0.52
7:G:149:GLN:HE22	12:D:252:VAL:HA	1.74	0.52
1:A:1276:GLN:CD	12:D:153:HIS:ND1	2.63	0.51
1:A:1825:ILE:HD12	1:A:1889:LEU:HA	1.91	0.51
4:B:885:GLN:O	4:B:1075:TRP:HD1	1.93	0.51
4:B:1212:ILE:HG21	4:B:1285:GLU:O	2.10	0.51
4:B:1599:LEU:HB2	4:B:1617:LEU:HD23	1.75	0.51
4:B:2608:ASN:ND2	4:B:2655:ASN:O	2.42	0.51
4:B:3085:VAL:HG23	4:B:3477:TRP:CZ2	2.45	0.51
1:A:1276:GLN:CG	12:D:153:HIS:HE1	2.05	0.51
2:C:1856:TYR:HA	2:C:1934:TRP:HH2	1.75	0.51
2:C:2751:TRP:O	2:C:2754:SER:HB3	2.10	0.51
4:B:1109:THR:O	4:B:1113:LEU:HG	2.10	0.51
4:B:2150:THR:HG22	4:B:2203:ASN:HD22	1.75	0.51
4:B:2695:HIS:CG	4:B:2695:HIS:O	2.63	0.51
10:O:19:LEU:HA	10:O:22:LEU:HD21	1.91	0.51
1:A:1135:VAL:HG13	1:A:1201:TYR:OH	2.11	0.51
1:A:3170:GLY:HA2	1:A:3380:ILE:HD13	1.91	0.51
4:B:1595:LEU:HD13	4:B:1618:LEU:HD22	1.89	0.51
1:A:3132:ASN:N	1:A:3419:ILE:HD11	2.25	0.51
2:C:1864:ILE:HD11	2:C:1910:ILE:HG23	1.91	0.51
4:B:4545:CYS:SG	4:B:4579:ILE:HD13	2.50	0.51
8:F:26:PHE:CE2	8:F:52:VAL:HG11	2.46	0.51
1:A:2490:LEU:HD11	1:A:2611:MET:HG2	1.93	0.51
1:A:2935:LEU:HD12	1:A:2938:ILE:HD11	1.91	0.51
2:C:4138:PHE:CE1	2:C:4141:THR:HA	2.46	0.51
4:B:1605:SER:O	4:B:1687:LEU:HD22	2.11	0.51
4:B:3694:LEU:HD22	4:B:3715:ASN:HD22	1.76	0.51
12:D:509:ASN:HD21	12:D:512:HIS:HB3	1.74	0.51
1:A:1634:ILE:HD11	1:A:1637:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1603:LYS:O	4:B:1607:PRO:N	2.43	0.51
4:B:1603:LYS:HA	4:B:1609:PHE:CD2	2.45	0.51
1:A:1108:LEU:O	1:A:1112:THR:N	2.42	0.51
4:B:1069:THR:HB	4:B:1070:PRO:HD2	1.92	0.51
12:D:603:LEU:HD22	12:D:611:VAL:HG12	1.91	0.51
1:A:1126:VAL:HG21	1:A:1135:VAL:HG11	1.92	0.51
1:A:1868:GLY:O	1:A:1973:PHE:HA	2.11	0.51
1:A:935:VAL:HG22	1:A:1017:LEU:HD21	1.92	0.51
1:A:2564:MET:N	1:A:2565:PRO:HD2	2.26	0.51
2:C:834:VAL:CG2	2:C:881:ILE:HD11	2.40	0.51
2:C:2007:LEU:HD11	2:C:2128:MET:HE2	1.93	0.51
4:B:1641:LEU:HD13	4:B:1662:MET:HB2	1.93	0.51
2:C:2177:ILE:CG2	2:C:2233:PRO:HA	2.39	0.50
4:B:804:ARG:NH1	4:B:898:PRO:O	2.44	0.50
4:B:3789:THR:HG22	4:B:3803:ASN:HD22	1.75	0.50
1:A:4583:TYR:HB3	1:A:4584:PRO:HD2	1.94	0.50
4:B:1596:ASN:N	4:B:1618:LEU:HD21	2.26	0.50
4:B:1599:LEU:HD12	4:B:1618:LEU:HG	1.92	0.50
1:A:1482:ASN:HA	1:A:1487:VAL:HG11	1.92	0.50
4:B:1490:GLN:OE1	4:B:3614:ILE:CB	2.57	0.50
11:E:42:GLN:HE22	14:L:91:ASN:ND2	2.09	0.50
2:C:1132:LYS:HG2	2:C:1151:LEU:CG	2.40	0.50
4:B:1599:LEU:CB	4:B:1617:LEU:CD1	2.83	0.50
13:P:53:LEU:O	13:P:57:ILE:N	2.44	0.50
14:L:86:LEU:HD12	17:M:54:ASN:HB3	1.93	0.50
4:B:1212:ILE:HB	4:B:1213:PRO:HD2	1.94	0.50
1:A:1209:LEU:CA	1:A:1273:PHE:HE1	2.23	0.50
2:C:3064:ILE:HG13	2:C:3115:ILE:HD12	1.94	0.50
4:B:1602:LYS:CB	4:B:1609:PHE:CE2	2.92	0.50
4:B:2621:ILE:HG23	4:B:2667:LEU:HD13	1.90	0.50
1:A:1276:GLN:OE1	12:D:153:HIS:CG	2.64	0.50
1:A:2117:GLU:HG2	1:A:2141:ILE:HD11	1.94	0.50
1:A:4240:VAL:HG11	1:A:4270:PRO:HG2	1.93	0.50
2:C:1296:ILE:HD11	2:C:1542:MET:SD	2.52	0.50
4:B:871:ILE:HG21	4:B:959:ILE:HD11	1.93	0.50
4:B:2005:ASN:N	4:B:2005:ASN:HD22	2.09	0.50
1:A:1915:VAL:HA	1:A:1970:VAL:HG21	1.94	0.50
2:C:2659:ALA:HB1	2:C:2858:VAL:HG13	1.94	0.50
1:A:1183:LEU:C	1:A:1183:LEU:HD23	2.32	0.50
2:C:1069:ARG:HH21	2:C:1155:ASN:ND2	2.10	0.50
4:B:898:PRO:N	4:B:1073:ILE:HG21	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2704:GLN:O	4:B:2707:ALA:N	2.31	0.50
2:C:403:GLU:O	4:B:2999:ASN:OD1	2.22	0.49
2:C:972:LEU:HD13	2:C:1029:GLU:HG2	1.94	0.49
4:B:1238:LYS:HG2	4:B:1311:MET:CB	2.42	0.49
4:B:1527:ILE:HG23	4:B:1615:GLN:CD	2.32	0.49
1:A:675:ILE:HG22	1:A:686:VAL:HA	1.94	0.49
1:A:3131:ILE:HD12	1:A:3422:LEU:HD11	1.93	0.49
4:B:2099:ASP:HB2	4:B:2100:PRO:HD3	1.94	0.49
12:D:519:ALA:HB1	12:D:545:VAL:HG12	1.94	0.49
1:A:1209:LEU:CB	1:A:1273:PHE:CE1	2.92	0.49
1:A:3322:ALA:HB2	1:A:3333:LEU:HD12	1.94	0.49
4:B:1602:LYS:C	4:B:1609:PHE:CD2	2.86	0.49
1:A:3223:LEU:HD11	1:A:3332:ILE:HD11	1.94	0.49
2:C:1069:ARG:HH21	2:C:1155:ASN:HD22	1.60	0.49
4:B:1527:ILE:HG23	4:B:1615:GLN:NE2	2.27	0.49
4:B:1602:LYS:HB3	4:B:1683:GLU:CB	2.24	0.49
11:E:133:PHE:HZ	12:D:360:ALA:HB3	1.77	0.49
12:D:545:VAL:HA	12:D:562:THR:HG22	1.94	0.49
2:C:1989:THR:HG23	2:C:2019:LEU:HD22	1.94	0.49
4:B:898:PRO:HG3	4:B:1077:ARG:HG3	1.94	0.49
4:B:2619:SER:N	4:B:2620:PRO:HD2	2.27	0.49
2:C:1221:THR:O	2:C:1225:THR:HG23	2.12	0.49
2:C:2002:VAL:HG12	2:C:2002:VAL:O	2.13	0.49
2:C:2719:VAL:HG13	2:C:2720:PRO:HD3	1.94	0.49
9:N:90:ASP:O	9:N:93:THR:OG1	2.25	0.49
11:E:41:VAL:HG22	11:E:42:GLN:HG3	1.95	0.49
1:A:1563:PRO:O	1:A:1567:ASN:N	2.44	0.49
2:C:2212:LEU:HD11	18:C:4203:ADP:H8	1.77	0.49
4:B:3446:SER:HB2	4:B:3489:THR:HG23	1.94	0.49
1:A:883:THR:HA	1:A:886:ILE:HD12	1.94	0.49
1:A:2840:VAL:HG22	18:A:4703:ADP:HN62	1.78	0.49
1:A:3533:PRO:CD	1:A:3648:THR:HG22	2.41	0.49
4:B:715:LEU:O	4:B:717:MET:N	2.45	0.49
4:B:898:PRO:HG2	4:B:1077:ARG:HD2	1.95	0.49
4:B:4359:LEU:HD22	4:B:4404:ALA:CB	2.43	0.49
4:B:4359:LEU:HD22	4:B:4404:ALA:HB2	1.94	0.49
1:A:1522:GLU:HG3	1:A:1523:PRO:HD3	1.95	0.49
1:A:2793:VAL:HG23	1:A:2804:ALA:HB2	1.95	0.49
1:A:3691:LEU:HB3	1:A:3719:THR:HG22	1.95	0.49
4:B:1603:LYS:CD	4:B:1617:LEU:HD22	2.43	0.49
4:B:1708:ALA:HA	4:B:1711:TRP:NE1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2769:ARG:CD	4:B:2836:GLN:HE22	2.26	0.49
4:B:3676:LEU:HD21	4:B:3733:ALA:HB2	1.95	0.49
1:A:1230:TYR:CB	1:A:1290:ILE:N	2.76	0.48
1:A:2938:ILE:HD12	1:A:2999:LEU:HD21	1.95	0.48
4:B:1058:LYS:HG3	4:B:1166:GLU:O	2.12	0.48
4:B:1128:PRO:HG2	4:B:1131:HIS:CG	2.48	0.48
1:A:1889:LEU:HD12	1:A:1920:TRP:CZ2	2.48	0.48
2:C:1188:LEU:HD21	2:C:1218:VAL:HG22	1.95	0.48
2:C:2740:ILE:HG22	2:C:2741:ASP:H	1.78	0.48
4:B:938:PHE:HB3	4:B:956:LEU:HD13	1.95	0.48
4:B:2267:ILE:HG22	4:B:2271:TRP:HZ3	1.78	0.48
4:B:3850:LEU:O	4:B:3931:ARG:NH2	2.43	0.48
6:H:70:THR:HG23	11:E:68:THR:HB	1.95	0.48
1:A:2418:ILE:HG22	1:A:2419:PRO:CD	2.43	0.48
1:A:4461:LEU:HD21	1:A:4516:ILE:HG21	1.95	0.48
2:C:3938:LEU:HD12	2:C:3982:LYS:HD3	1.94	0.48
4:B:696:THR:HG22	4:B:697:THR:HG23	1.95	0.48
4:B:883:ASN:HA	4:B:886:ILE:HG22	1.95	0.48
9:N:76:THR:CG2	11:E:39:GLN:HE22	2.23	0.48
12:D:299:VAL:HG11	12:D:605:GLY:HA3	1.94	0.48
1:A:3303:ILE:HD11	1:A:3340:TYR:CE2	2.48	0.48
2:C:2709:ALA:HA	2:C:2758:MET:SD	2.53	0.48
4:B:1602:LYS:HB3	4:B:1609:PHE:CE2	2.40	0.48
9:N:89:GLN:HG2	9:N:94:ASP:HB2	1.94	0.48
1:A:1634:ILE:CD1	1:A:1656:ILE:HG23	2.44	0.48
1:A:3248:LEU:HB2	3:Q:104:TYR:CE1	2.48	0.48
1:A:3331:GLY:O	1:A:3335:TRP:N	2.45	0.48
2:C:29:VAL:CG1	2:C:116:THR:HG21	2.43	0.48
2:C:913:MET:HE1	2:C:959:THR:HG22	1.96	0.48
2:C:1047:LEU:HG	2:C:1111:LEU:HD11	1.94	0.48
2:C:1132:LYS:HG3	2:C:1151:LEU:HD21	1.89	0.48
4:B:558:VAL:HG11	4:B:599:ILE:HD11	1.94	0.48
2:C:1385:ILE:HA	2:C:1388:THR:HG22	1.96	0.48
4:B:669:ILE:CD1	4:B:752:ILE:HD11	2.43	0.48
4:B:898:PRO:N	4:B:1073:ILE:HG23	2.29	0.48
6:H:67:SER:O	11:E:72:GLY:HA2	2.14	0.48
4:B:720:ASP:O	4:B:721:ASN:C	2.52	0.48
4:B:1599:LEU:CD1	4:B:1617:LEU:HB3	2.19	0.48
4:B:2758:GLN:HE22	4:B:2834:TYR:H	1.62	0.48
12:D:87:THR:HG22	12:D:98:THR:HA	1.95	0.48
1:A:2697:ARG:NH1	18:A:4701:ADP:O3B	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1270:PHE:CG	2:C:1336:ALA:HB2	2.49	0.48
2:C:1856:TYR:CE2	2:C:1903:VAL:HG22	2.49	0.48
4:B:3223:ALA:HB1	4:B:3349:ILE:HD13	1.94	0.48
8:F:87:TYR:HB3	8:F:98:LEU:HD11	1.94	0.48
1:A:3748:ARG:HB3	1:A:3749:PRO:HD3	1.95	0.48
2:C:2734:PHE:CE2	2:C:2767:LYS:HG3	2.49	0.48
4:B:1535:SER:HB3	4:B:1623:ASN:OD1	2.14	0.48
11:E:423:GLY:N	11:E:501:GLU:OE1	2.47	0.48
2:C:968:MET:HB2	2:C:1026:PHE:CZ	2.48	0.48
2:C:2758:MET:O	2:C:2759:LYS:C	2.52	0.48
4:B:447:THR:OG1	4:B:513:ASP:HB3	2.14	0.48
4:B:1819:SER:HA	4:B:1857:VAL:HG13	1.96	0.48
4:B:2308:LEU:HD23	4:B:2316:VAL:HG22	1.96	0.48
1:A:1687:LEU:C	1:A:1687:LEU:HD23	2.35	0.47
2:C:2826:VAL:O	2:C:2828:GLN:N	2.47	0.47
4:B:1114:LEU:HA	4:B:1117:ILE:HD12	1.96	0.47
4:B:1531:ILE:CG2	4:B:1622:SER:CB	2.85	0.47
4:B:2987:VAL:HG12	4:B:2987:VAL:O	2.14	0.47
4:B:3350:PHE:HA	4:B:3353:VAL:HG12	1.95	0.47
10:O:30:TYR:N	10:O:31:PRO:CD	2.78	0.47
1:A:1634:ILE:HD11	1:A:1637:VAL:CG2	2.44	0.47
2:C:10:LEU:HD11	2:C:67:CYS:HB3	1.96	0.47
2:C:306:LEU:HD11	2:C:317:LYS:HG2	1.95	0.47
2:C:1081:ILE:HD11	2:C:1117:GLN:HB2	1.96	0.47
2:C:1262:TRP:CE2	2:C:1321:SER:HB2	2.49	0.47
4:B:898:PRO:CG	4:B:1073:ILE:CG2	2.85	0.47
4:B:1205:PHE:HE2	4:B:1286:LYS:CA	2.27	0.47
4:B:2210:TYR:HA	4:B:2260:TRP:O	2.14	0.47
4:B:3245:LEU:O	4:B:3247:SER:N	2.46	0.47
4:B:3863:LEU:N	4:B:3863:LEU:HD22	2.29	0.47
9:N:84:GLN:HB2	10:O:64:VAL:HG21	1.95	0.47
1:A:1539:LYS:HE2	4:B:3859:VAL:HG21	1.95	0.47
2:C:2659:ALA:HB1	2:C:2858:VAL:CG2	2.39	0.47
2:C:2800:PRO:HG3	2:C:2818:VAL:HG21	1.96	0.47
4:B:1483:ASP:O	4:B:1487:MET:N	2.47	0.47
4:B:1490:GLN:CG	4:B:3614:ILE:HG21	2.38	0.47
4:B:2769:ARG:HD2	4:B:2836:GLN:HE22	1.79	0.47
1:A:3577:THR:HG22	1:A:3622:LYS:HB2	1.95	0.47
2:C:214:LEU:O	2:C:231:ILE:HA	2.14	0.47
2:C:1047:LEU:O	2:C:1051:GLN:HG3	2.14	0.47
2:C:2687:ALA:HB1	2:C:2830:VAL:CG2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2795:MET:N	2:C:2796:PRO:CD	2.78	0.47
4:B:2804:ILE:O	4:B:2806:GLU:N	2.47	0.47
4:B:3657:PHE:O	4:B:3661:VAL:HG23	2.14	0.47
8:F:33:LEU:HD11	11:E:99:ILE:HG21	1.96	0.47
2:C:4128:THR:HA	2:C:4163:MET:O	2.14	0.47
4:B:736:LEU:HD12	4:B:859:TYR:HB2	1.96	0.47
4:B:1075:TRP:CE3	4:B:1076:LEU:HB3	2.48	0.47
4:B:4348:VAL:HG21	4:B:4453:ALA:HB2	1.96	0.47
1:A:1118:LEU:HD12	1:A:1142:ILE:HG13	1.96	0.47
1:A:1760:HIS:O	1:A:1764:LEU:HG	2.15	0.47
1:A:2866:VAL:HG11	1:A:3026:TRP:CZ3	2.50	0.47
2:C:29:VAL:HG11	2:C:116:THR:HG21	1.97	0.47
2:C:2617:VAL:HG22	2:C:3183:ILE:HG21	1.96	0.47
2:C:2738:ILE:HD12	2:C:2740:ILE:O	2.14	0.47
4:B:591:TRP:HD1	11:E:411:TYR:OH	1.97	0.47
4:B:915:PRO:HA	4:B:925:THR:HA	1.95	0.47
4:B:2040:LEU:HD13	4:B:2083:LEU:HD22	1.96	0.47
4:B:2936:ILE:HG22	4:B:3012:ILE:HD13	1.95	0.47
5:I:75:TRP:CE3	5:I:109:LYS:HB2	2.49	0.47
17:M:3:HIS:CE1	17:M:78:ASN:HD22	2.33	0.47
1:A:1149:ILE:HG21	1:A:1187:TRP:CZ2	2.50	0.47
1:A:2511:ASP:HB2	1:A:2514:LYS:HB2	1.96	0.47
4:B:447:THR:OG1	4:B:448:LYS:N	2.47	0.47
4:B:1897:GLY:O	4:B:2001:PHE:HA	2.14	0.47
2:C:2082:LEU:HD11	2:C:2096:ILE:CD1	2.44	0.47
2:C:2730:LEU:HD23	2:C:2738:ILE:HD13	1.97	0.47
4:B:1666:ASP:HB2	4:B:1870:ASN:HD21	1.79	0.47
4:B:3236:LYS:N	4:B:3237:PRO:HD2	2.28	0.47
4:B:3878:ILE:CD1	4:B:3887:ALA:HB2	2.43	0.47
1:A:4422:ASP:HB2	1:A:4423:PRO:HD2	1.96	0.47
2:C:39:LEU:HD23	2:C:83:CYS:SG	2.55	0.47
2:C:2688:GLN:N	2:C:2689:PRO:CD	2.78	0.47
2:C:2734:PHE:HE2	2:C:2767:LYS:HG3	1.79	0.47
4:B:721:ASN:OD1	4:B:777:PHE:CD2	2.68	0.47
4:B:898:PRO:HG2	4:B:1077:ARG:CB	2.40	0.47
4:B:2115:VAL:HG12	4:B:2323:PHE:CE2	2.50	0.47
4:B:2200:SER:O	4:B:2204:SER:N	2.48	0.47
4:B:3887:ALA:O	4:B:3890:LEU:N	2.48	0.47
6:H:20:MET:O	6:H:24:VAL:HG23	2.15	0.47
1:A:61:GLU:CB	1:A:98:ILE:O	2.63	0.47
1:A:766:GLY:HA3	1:A:780:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1487:VAL:HG23	1:A:1490:PHE:CE1	2.50	0.47
1:A:3286:PHE:CE2	1:A:3290:LEU:HD11	2.50	0.47
1:A:3897:PRO:HA	1:A:3900:ILE:HG22	1.97	0.47
2:C:2740:ILE:HG13	2:C:2744:LYS:HB3	1.97	0.47
4:B:521:PHE:CE2	4:B:605:LYS:HB3	2.49	0.47
4:B:898:PRO:HB3	4:B:1077:ARG:CA	2.43	0.47
4:B:3826:THR:HG22	4:B:3942:LEU:HD22	1.97	0.47
11:E:75:HIS:CG	11:E:75:HIS:O	2.68	0.47
1:A:3242:VAL:HA	1:A:3248:LEU:HD11	1.95	0.46
2:C:1128:PHE:CZ	2:C:1151:LEU:HB3	2.40	0.46
2:C:3483:LEU:HD12	2:C:3490:TRP:CD1	2.50	0.46
4:B:1599:LEU:N	4:B:1621:LEU:CD2	2.77	0.46
4:B:1944:SER:HA	4:B:1998:VAL:HG11	1.96	0.46
4:B:2971:ILE:HG23	4:B:2974:LEU:HB2	1.97	0.46
1:A:4562:ASN:CG	1:A:4562:ASN:O	2.54	0.46
2:C:884:ARG:HA	2:C:889:ILE:HD11	1.97	0.46
4:B:459:ILE:HG23	4:B:499:LEU:HD11	1.97	0.46
4:B:3284:MET:SD	4:B:3290:PHE:CD1	3.08	0.46
5:I:97:MET:O	5:I:105:VAL:HB	2.15	0.46
1:A:3307:GLU:N	1:A:3308:PRO:HD2	2.30	0.46
2:C:169:TYR:HB3	4:B:865:VAL:HG21	1.97	0.46
2:C:1864:ILE:HD11	2:C:1910:ILE:CG2	2.44	0.46
2:C:3072:ILE:HD12	2:C:3102:LEU:HD11	1.97	0.46
3:Q:43:GLY:HA3	3:Q:67:SER:CB	2.45	0.46
4:B:885:GLN:O	4:B:1075:TRP:CD1	2.69	0.46
4:B:3255:THR:CB	4:B:3337:CYS:SG	3.02	0.46
5:I:95:LEU:HD23	5:I:107:ILE:HD11	1.97	0.46
7:G:145:LEU:HD22	12:D:248:MET:HG3	1.96	0.46
11:E:224:ASN:HD21	11:E:277:SER:CB	2.27	0.46
12:D:75:LEU:HD23	12:D:75:LEU:H	1.81	0.46
1:A:1667:ILE:HD12	1:A:1838:PHE:CD1	2.51	0.46
2:C:2698:LEU:HD21	2:C:2820:ILE:CA	2.46	0.46
2:C:4113:VAL:HG12	2:C:4114:PRO:HD2	1.96	0.46
2:C:3151:LYS:CE	2:C:3217:ILE:HD11	2.45	0.46
4:B:1595:LEU:C	4:B:1618:LEU:HD21	2.36	0.46
4:B:3290:PHE:O	4:B:3293:LYS:N	2.48	0.46
4:B:3481:ILE:HG21	4:B:3488:ILE:CD1	2.46	0.46
11:E:261:HIS:CE1	11:E:283:SER:HB3	2.51	0.46
16:J:68:MET:HB3	16:J:76:TRP:CD1	2.50	0.46
1:A:2515:MET:HA	1:A:2553:LYS:O	2.16	0.46
2:C:58:PHE:CD2	2:C:71:GLN:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:TYR:O	2:C:106:LEU:HB2	2.16	0.46
2:C:859:ILE:CB	2:C:864:MET:SD	3.04	0.46
2:C:2705:ASP:O	2:C:2708:GLN:N	2.49	0.46
4:B:1238:LYS:HE2	4:B:1308:LEU:N	2.26	0.46
4:B:1603:LYS:HG2	4:B:1609:PHE:C	2.36	0.46
4:B:2890:GLY:HA3	4:B:3048:PHE:HB2	1.97	0.46
8:F:74:ILE:HD12	8:F:77:ILE:HD11	1.98	0.46
2:C:3412:HIS:HA	2:C:3415:ILE:HD12	1.96	0.46
4:B:3154:GLN:CB	4:B:3419:ALA:HB1	2.46	0.46
11:E:566:ASN:HB2	11:E:567:PRO:HD2	1.98	0.46
1:A:2704:LYS:O	1:A:2708:THR:HG23	2.16	0.46
1:A:2723:ILE:HG21	1:A:2776:LYS:HE2	1.98	0.46
4:B:3343:ILE:O	4:B:3346:PHE:HB3	2.16	0.46
1:A:3268:PHE:CD1	3:Q:35:ILE:CB	2.99	0.46
1:A:4139:ILE:HD13	1:A:4223:TYR:OH	2.16	0.46
1:A:4477:MET:HG3	1:A:4524:VAL:HG23	1.98	0.46
2:C:2708:GLN:HE21	2:C:2809:ALA:HA	1.80	0.46
4:B:1602:LYS:HA	4:B:1683:GLU:CB	2.46	0.46
4:B:3258:VAL:HG11	4:B:3321:PHE:CZ	2.51	0.46
11:E:152:LEU:HD22	11:E:486:THR:HG22	1.97	0.46
12:D:367:LEU:HD12	12:D:368:TYR:O	2.16	0.46
1:A:870:PRO:C	1:A:871:LEU:HD13	2.37	0.46
1:A:1009:THR:HB	1:A:1074:MET:SD	2.56	0.46
2:C:2708:GLN:CD	2:C:2813:ILE:HD11	2.37	0.46
4:B:1620:ILE:HG23	4:B:1630:VAL:HG13	1.97	0.46
1:A:5:LYS:CB	1:A:48:GLU:HA	2.46	0.45
1:A:92:ALA:O	1:A:124:THR:CB	2.63	0.45
1:A:1113:GLU:O	1:A:1116:LYS:N	2.49	0.45
1:A:2116:VAL:HG23	1:A:2173:VAL:HG11	1.98	0.45
4:B:1127:ASN:CB	4:B:1128:PRO:CD	2.94	0.45
4:B:1538:ILE:HG21	4:B:1622:SER:OG	2.16	0.45
4:B:2904:THR:HG21	4:B:2911:ILE:HB	1.98	0.45
4:B:3268:THR:HG22	4:B:3269:LEU:HD12	1.97	0.45
5:I:12:ILE:HG21	7:G:119:PRO:HG2	1.98	0.45
2:C:106:LEU:N	2:C:106:LEU:HD12	2.31	0.45
2:C:973:LYS:HA	2:C:976:ILE:HD12	1.98	0.45
2:C:2218:VAL:HG23	2:C:2247:THR:HG21	1.99	0.45
2:C:3611:ALA:O	2:C:3615:CYS:SG	2.71	0.45
4:B:1606:PHE:CB	4:B:1687:LEU:HB2	2.41	0.45
7:G:103:ILE:N	7:G:104:PRO:HD2	2.31	0.45
12:D:66:LEU:HD21	12:D:73:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:372:VAL:HG13	12:D:414:PHE:CZ	2.51	0.45
2:C:1728:LEU:HD12	2:C:1728:LEU:O	2.17	0.45
4:B:2897:GLN:HA	4:B:2947:MET:CE	2.46	0.45
4:B:4017:LEU:HD12	4:B:4044:ILE:HD13	1.97	0.45
1:A:1522:GLU:N	1:A:1523:PRO:CD	2.80	0.45
1:A:4534:CYS:SG	1:A:4535:LYS:N	2.90	0.45
2:C:1142:VAL:HG21	2:C:1167:ILE:HD13	1.97	0.45
4:B:3264:ASN:HB2	4:B:3306:ILE:HD11	1.98	0.45
4:B:4475:ILE:HD13	4:B:4525:THR:HG23	1.98	0.45
1:A:1013:VAL:HG13	1:A:1076:LEU:CD1	2.45	0.45
1:A:2727:LEU:HD22	1:A:2772:GLU:HG2	1.99	0.45
1:A:3120:GLY:HA2	1:A:3696:LEU:HD13	1.98	0.45
2:C:2792:TYR:O	2:C:2796:PRO:HG3	2.17	0.45
4:B:1599:LEU:HA	4:B:1617:LEU:HD11	1.99	0.45
4:B:2839:ILE:N	4:B:2840:PRO:HD2	2.32	0.45
4:B:3339:TRP:CZ2	4:B:3343:ILE:HD12	2.51	0.45
4:B:3914:LEU:O	4:B:3914:LEU:HG	2.17	0.45
5:I:10:MET:HB3	5:I:15:LEU:HD21	1.98	0.45
1:A:1171:ILE:HD13	1:A:1171:ILE:H	1.82	0.45
1:A:2027:PHE:CE2	1:A:2051:ILE:HG23	2.50	0.45
1:A:2866:VAL:HG11	1:A:3026:TRP:CH2	2.52	0.45
2:C:1174:LEU:CD1	2:C:1191:ILE:HG22	2.47	0.45
2:C:3276:THR:HG23	2:C:3656:ASN:HA	1.98	0.45
4:B:3241:GLU:O	4:B:3244:ASN:N	2.49	0.45
4:B:4543:TYR:CE2	4:B:4545:CYS:HB3	2.52	0.45
11:E:153:PHE:HB3	11:E:200:TRP:CE2	2.52	0.45
12:D:364:ALA:HB1	12:D:414:PHE:CE1	2.52	0.45
1:A:2877:THR:HG21	1:A:2923:LEU:HD13	1.98	0.45
2:C:221:SER:O	2:C:282:ARG:NH1	2.49	0.45
2:C:1612:ILE:N	2:C:1613:PRO:HD2	2.32	0.45
2:C:1674:LEU:HD21	2:C:1797:LEU:HD11	1.98	0.45
2:C:2365:GLY:HA2	18:C:4206:ADP:O3'	2.16	0.45
2:C:2532:GLU:N	2:C:2533:PRO:HD2	2.31	0.45
4:B:24:ILE:O	4:B:25:GLN:CB	2.64	0.45
4:B:436:PHE:CZ	4:B:499:LEU:HD23	2.52	0.45
4:B:3481:ILE:HG21	4:B:3488:ILE:HD12	1.99	0.45
4:B:4322:GLU:HB3	4:B:4325:ASN:HB3	1.98	0.45
12:D:162:LEU:O	12:D:162:LEU:HD23	2.16	0.45
12:D:564:ASP:HA	12:D:590:LEU:HD13	1.98	0.45
1:A:1601:ARG:NE	1:A:1688:GLU:OE1	2.49	0.45
1:A:1825:ILE:HG21	1:A:1889:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3252:GLN:HE22	3:Q:36:PRO:HA	1.82	0.45
1:A:4562:ASN:O	1:A:4562:ASN:ND2	2.50	0.45
2:C:537:GLU:O	2:C:698:GLU:O	2.34	0.45
2:C:1524:ARG:HH22	2:C:3759:ILE:HG21	1.81	0.45
1:A:1638:THR:HG21	1:A:1655:GLN:HE21	1.81	0.45
1:A:2340:GLN:NE2	1:A:2399:TYR:OH	2.50	0.45
2:C:972:LEU:HD21	2:C:1017:MET:HE1	1.96	0.45
2:C:2770:ASN:O	2:C:2771:PHE:C	2.55	0.45
4:B:4510:LEU:HD22	4:B:4563:LEU:HD11	1.99	0.45
1:A:1790:HIS:CE1	1:A:1794:ILE:HD11	2.52	0.45
2:C:972:LEU:HD11	2:C:1017:MET:HE3	1.98	0.45
2:C:2332:LEU:HD13	18:C:4206:ADP:O2'	2.17	0.45
2:C:2705:ASP:O	2:C:2706:PHE:C	2.55	0.45
4:B:1700:ILE:CG2	4:B:1729:ILE:HD13	2.47	0.45
4:B:2889:VAL:HG11	4:B:3047:TRP:CZ3	2.52	0.45
4:B:3740:ILE:O	4:B:3744:ARG:N	2.48	0.45
5:I:98:PHE:HB3	5:I:104:ALA:HA	1.99	0.45
1:A:1087:THR:O	1:A:1087:THR:HG22	2.17	0.44
1:A:2033:LEU:HD23	1:A:2097:LEU:HD22	1.99	0.44
1:A:4252:PRO:HG3	1:A:4265:TYR:CG	2.52	0.44
2:C:1382:THR:HA	2:C:1385:ILE:HG22	1.99	0.44
2:C:3244:VAL:HB	2:C:3878:VAL:HG22	2.00	0.44
2:C:4082:TRP:CZ2	2:C:4091:GLY:HA3	2.52	0.44
4:B:1209:ALA:HB2	4:B:1286:LYS:CB	2.47	0.44
4:B:1230:MET:HE2	4:B:1267:TYR:HA	1.98	0.44
11:E:164:VAL:HG22	11:E:181:TYR:CE1	2.52	0.44
12:D:397:ASP:CB	12:D:398:PRO:CD	2.96	0.44
12:D:517:ILE:HG12	12:D:550:TRP:CE2	2.51	0.44
1:A:3102:LEU:HD23	1:A:3451:THR:HG23	1.97	0.44
1:A:4347:LEU:CD1	1:A:4368:LEU:HD23	2.47	0.44
4:B:473:VAL:O	4:B:473:VAL:HG13	2.18	0.44
4:B:1237:ARG:CZ	4:B:1263:THR:H	2.28	0.44
4:B:1943:LEU:HD11	4:B:1950:GLY:HA3	1.98	0.44
4:B:2959:LEU:O	4:B:2959:LEU:HD13	2.17	0.44
1:A:753:LEU:N	1:A:754:PRO:HD2	2.32	0.44
1:A:1696:LYS:HA	1:A:1836:TYR:CE1	2.52	0.44
1:A:4143:ARG:NH1	1:A:4610:LEU:O	2.50	0.44
2:C:928:VAL:HA	2:C:951:TYR:CE1	2.52	0.44
4:B:808:PRO:CD	4:B:1077:ARG:HH11	2.26	0.44
4:B:1230:MET:HE1	4:B:1267:TYR:CA	2.47	0.44
4:B:1602:LYS:HD2	4:B:1683:GLU:HG3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1606:PHE:CA	4:B:1687:LEU:HD13	2.38	0.44
4:B:1708:ALA:HA	4:B:1711:TRP:CD1	2.51	0.44
4:B:2897:GLN:HA	4:B:2947:MET:HE2	1.99	0.44
6:H:85:ALA:HB2	11:E:75:HIS:CD2	2.53	0.44
14:L:99:LEU:N	14:L:100:PRO:HD2	2.33	0.44
1:A:1790:HIS:NE2	1:A:1794:ILE:HD11	2.32	0.44
1:A:3877:ILE:HD11	1:A:3900:ILE:HD13	1.98	0.44
2:C:1132:LYS:CG	2:C:1151:LEU:CD1	2.79	0.44
2:C:1927:SER:CB	2:C:1946:ILE:HG21	2.47	0.44
4:B:3081:ASN:HD21	4:B:3484:LYS:CD	2.30	0.44
4:B:3252:VAL:HG22	4:B:3333:ALA:HB2	2.00	0.44
1:A:3709:ASP:CB	1:A:3712:LEU:HD12	2.47	0.44
2:C:870:LYS:HE2	2:C:2325:ASP:O	2.18	0.44
2:C:2096:ILE:HD13	2:C:2137:VAL:HG11	2.00	0.44
2:C:2621:GLU:HG3	2:C:2900:VAL:HG21	1.98	0.44
2:C:3054:SER:OG	2:C:3055:ALA:N	2.50	0.44
4:B:1189:GLN:HA	4:B:1192:ASN:ND2	2.32	0.44
4:B:1599:LEU:CA	4:B:1617:LEU:HD11	2.48	0.44
4:B:1603:LYS:CA	4:B:1609:PHE:HB2	2.47	0.44
11:E:49:ASP:HA	14:L:85:SER:HA	1.99	0.44
11:E:140:HIS:CE1	12:D:362:LEU:HD21	2.53	0.44
1:A:470:PHE:CB	1:A:485:THR:CB	2.95	0.44
1:A:1525:PHE:HB2	1:A:1541:PHE:CD2	2.51	0.44
1:A:2548:ALA:HB2	1:A:2603:LYS:HG2	1.99	0.44
1:A:2602:MET:SD	1:A:2602:MET:N	2.90	0.44
1:A:2840:VAL:HG11	1:A:3041:THR:HG21	2.00	0.44
1:A:3240:VAL:HG22	1:A:3335:TRP:CE3	2.52	0.44
2:C:870:LYS:CE	2:C:2325:ASP:O	2.65	0.44
4:B:1537:ASP:N	4:B:1625:GLN:HG3	2.31	0.44
4:B:1606:PHE:CG	4:B:1687:LEU:HD13	2.49	0.44
4:B:3264:ASN:CB	4:B:3306:ILE:HD11	2.47	0.44
12:D:162:LEU:HD23	12:D:162:LEU:C	2.38	0.44
17:M:84:LEU:HD12	17:M:84:LEU:C	2.38	0.44
1:A:3257:VAL:HG21	1:A:3266:VAL:HG13	1.98	0.44
2:C:2357:LEU:HD12	2:C:2512:ILE:HG22	1.99	0.44
4:B:737:VAL:HG13	4:B:737:VAL:O	2.17	0.44
4:B:744:MET:CE	4:B:773:VAL:HG23	2.48	0.44
4:B:1596:ASN:OD1	4:B:1618:LEU:HD11	2.17	0.44
4:B:3223:ALA:HB1	4:B:3349:ILE:CD1	2.47	0.44
4:B:3326:MET:O	4:B:3327:ALA:O	2.34	0.44
1:A:3877:ILE:HG13	1:A:3946:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1819:SER:HA	4:B:1857:VAL:CG1	2.48	0.44
4:B:3823:ILE:HG23	4:B:4286:LEU:HD12	1.99	0.44
4:B:4206:ARG:CZ	4:B:4573:ILE:HD13	2.46	0.44
12:D:183:ARG:HB2	15:K:72:TYR:HE2	1.83	0.44
1:A:1143:ARG:CZ	12:D:169:ASN:ND2	2.81	0.44
4:B:898:PRO:CG	4:B:1077:ARG:CG	2.96	0.44
14:L:69:ILE:HG22	14:L:69:ILE:O	2.18	0.44
1:A:3746:GLN:O	1:A:3799:VAL:HG21	2.18	0.43
2:C:336:ILE:HG22	2:C:349:LEU:HD11	1.99	0.43
2:C:830:ASP:O	2:C:834:VAL:HG23	2.18	0.43
2:C:1839:PHE:CE1	2:C:1891:LEU:HD11	2.53	0.43
4:B:2299:MET:HE3	4:B:2300:ARG:O	2.17	0.43
1:A:1205:GLN:HA	1:A:1208:TYR:HB3	1.99	0.43
1:A:2656:TYR:CG	1:A:2711:LYS:HD2	2.53	0.43
1:A:3224:LYS:HA	1:A:3281:LEU:HD11	2.00	0.43
1:A:3298:ILE:HG22	1:A:3300:GLU:HG3	1.99	0.43
1:A:4287:THR:HG22	1:A:4549:ILE:CD1	2.47	0.43
2:C:2357:LEU:C	2:C:2357:LEU:HD13	2.38	0.43
2:C:2691:VAL:HG22	2:C:2827:ILE:HG13	2.00	0.43
2:C:2800:PRO:HA	2:C:2814:CYS:HB3	1.99	0.43
2:C:3381:SER:N	2:C:3382:PRO:HD2	2.33	0.43
4:B:3494:PRO:HA	4:B:3497:ILE:HG22	2.00	0.43
11:E:62:ASN:HB2	15:K:40:ASN:HB2	2.00	0.43
1:A:944:LEU:HD23	1:A:944:LEU:N	2.33	0.43
4:B:745:GLU:HA	4:B:748:VAL:HG12	1.99	0.43
4:B:1142:SER:O	4:B:1146:VAL:HG23	2.18	0.43
4:B:1490:GLN:HB2	4:B:3614:ILE:CG2	2.46	0.43
4:B:1599:LEU:HD11	4:B:1618:LEU:CB	2.47	0.43
1:A:1219:PHE:CE2	1:A:1263:TYR:CE2	3.05	0.43
2:C:1702:ASP:OD1	2:C:1703:LYS:N	2.51	0.43
4:B:951:MET:N	4:B:952:PRO:HD2	2.33	0.43
4:B:1602:LYS:CA	4:B:1683:GLU:CB	2.96	0.43
4:B:1728:GLN:HE21	4:B:1868:ILE:HD12	1.83	0.43
12:D:509:ASN:HA	12:D:550:TRP:CD1	2.54	0.43
1:A:966:SER:HB3	1:A:989:ILE:HD12	1.99	0.43
1:A:1162:LEU:C	1:A:1162:LEU:HD23	2.39	0.43
2:C:3528:LEU:N	2:C:3529:PRO:CD	2.82	0.43
4:B:429:LEU:HD22	4:B:496:ILE:HD12	2.00	0.43
4:B:1238:LYS:HE3	4:B:1308:LEU:N	2.18	0.43
4:B:1490:GLN:HE22	4:B:3572:SER:HB3	1.69	0.43
12:D:174:GLN:HE22	14:L:49:LEU:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:304:TRP:CZ2	12:D:603:LEU:HD12	2.54	0.43
1:A:1596:ARG:HD3	1:A:1603:TYR:CD1	2.54	0.43
2:C:1040:VAL:HA	2:C:1102:CYS:SG	2.59	0.43
2:C:2708:GLN:CG	2:C:2809:ALA:HB1	2.49	0.43
2:C:2771:PHE:O	2:C:2774:VAL:N	2.51	0.43
2:C:3438:HIS:ND1	2:C:3443:LYS:HB2	2.34	0.43
2:C:4084:ILE:HG22	2:C:4085:GLY:N	2.34	0.43
4:B:1936:MET:HG2	4:B:1966:VAL:HG22	2.01	0.43
4:B:3654:GLU:O	4:B:3658:ILE:HG13	2.18	0.43
1:A:3131:ILE:HG21	1:A:3418:LEU:HB3	2.00	0.43
1:A:3199:GLU:O	1:A:3203:PRO:HD2	2.19	0.43
1:A:3587:VAL:HG11	1:A:3638:LEU:HD13	2.00	0.43
1:A:4046:CYS:SG	1:A:4074:ILE:HG23	2.59	0.43
2:C:321:ARG:HA	2:C:342:ALA:HB2	2.01	0.43
2:C:364:ILE:C	2:C:383:GLU:CB	2.87	0.43
2:C:2728:TYR:CG	2:C:2728:TYR:O	2.71	0.43
4:B:1599:LEU:HD21	4:B:1618:LEU:N	2.34	0.43
12:D:92:TYR:CG	17:M:29:LYS:HB3	2.53	0.43
1:A:3223:LEU:HD21	1:A:3332:ILE:HD11	2.01	0.43
2:C:164:HIS:CE1	4:B:957:GLN:HG3	2.53	0.43
2:C:2242:HIS:HB2	2:C:2289:LEU:CD1	2.48	0.43
2:C:3010:LEU:HA	2:C:3102:LEU:HB2	2.00	0.43
4:B:751:GLY:O	4:B:752:ILE:C	2.56	0.43
4:B:1051:ASP:HB3	4:B:1162:THR:HG21	1.99	0.43
4:B:1602:LYS:CA	4:B:1683:GLU:HB3	2.48	0.43
12:D:624:GLY:N	12:D:625:PRO:CD	2.82	0.43
1:A:1653:ILE:HB	1:A:1674:VAL:HB	2.00	0.43
1:A:2821:CYS:HB3	1:A:2841:LEU:HD13	2.01	0.43
1:A:4172:TYR:CD2	1:A:4195:ARG:NH2	2.86	0.43
1:A:4541:LEU:HD21	1:A:4597:LEU:HD13	2.00	0.43
2:C:261:ILE:N	2:C:262:PRO:HD2	2.34	0.43
2:C:3460:ASN:N	2:C:3460:ASN:ND2	2.67	0.43
4:B:1212:ILE:HG22	4:B:1213:PRO:CD	2.49	0.43
4:B:3267:ILE:HD12	4:B:3279:LYS:HD3	2.00	0.43
4:B:4119:ILE:HD12	4:B:4130:LEU:HD13	2.01	0.43
2:C:2212:LEU:C	2:C:2212:LEU:HD13	2.39	0.43
4:B:669:ILE:HD13	4:B:752:ILE:HD11	2.01	0.43
4:B:724:HIS:O	4:B:724:HIS:CD2	2.72	0.43
4:B:1075:TRP:CZ3	4:B:1076:LEU:HD13	2.53	0.43
4:B:1602:LYS:HA	4:B:1683:GLU:CG	2.49	0.43
4:B:1602:LYS:HE2	4:B:1683:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3269:LEU:O	4:B:3269:LEU:HD22	2.19	0.43
12:D:353:LEU:HG	12:D:363:LEU:HD21	2.01	0.43
1:A:994:GLU:O	1:A:998:VAL:HG23	2.19	0.42
2:C:2079:ILE:HG21	2:C:2082:LEU:HD13	2.00	0.42
2:C:2943:LYS:HB3	2:C:2994:VAL:HG11	2.01	0.42
4:B:1096:ARG:O	4:B:1100:ASP:N	2.46	0.42
4:B:1858:ASP:O	4:B:1892:ASN:ND2	2.52	0.42
1:A:3251:ILE:HG22	1:A:3252:GLN:N	2.34	0.42
2:C:287:PHE:HB3	2:C:320:PRO:HB2	2.01	0.42
2:C:2093:GLN:HB2	2:C:2096:ILE:HG22	2.00	0.42
2:C:4072:ILE:HD12	2:C:4110:ALA:HB2	2.00	0.42
4:B:3223:ALA:O	4:B:3226:SER:OG	2.37	0.42
5:I:35:LEU:HD22	5:I:95:LEU:HD13	2.01	0.42
1:A:2455:GLN:HB2	1:A:2458:GLN:HE21	1.85	0.42
1:A:3305:LEU:CD2	3:Q:81:ARG:CB	2.97	0.42
1:A:3816:ARG:HA	1:A:3973:TYR:CE1	2.54	0.42
2:C:259:PRO:HD2	2:C:328:TYR:CE2	2.53	0.42
2:C:1742:LEU:HD12	2:C:1780:LEU:HD22	1.99	0.42
2:C:2708:GLN:HG2	2:C:2809:ALA:HB1	2.00	0.42
2:C:2727:ILE:HD13	2:C:2745:LYS:HD3	2.01	0.42
2:C:4049:ILE:HD11	2:C:4110:ALA:HB1	2.01	0.42
4:B:439:LEU:HD21	4:B:456:ILE:HG23	2.01	0.42
4:B:1761:GLN:HE22	4:B:1798:ARG:HG3	1.84	0.42
4:B:2692:LEU:O	4:B:2695:HIS:N	2.52	0.42
5:I:12:ILE:HG23	7:G:120:THR:CG2	2.49	0.42
7:G:126:LEU:HD13	8:F:79:LEU:HD23	2.02	0.42
10:O:19:LEU:O	10:O:19:LEU:HD23	2.19	0.42
1:A:3131:ILE:HD12	1:A:3422:LEU:CD1	2.48	0.42
1:A:4123:HIS:NE2	1:A:4188:PRO:HD3	2.34	0.42
1:A:4448:GLN:HE21	1:A:4448:GLN:HB3	1.68	0.42
2:C:2687:ALA:CB	2:C:2830:VAL:HG22	2.44	0.42
2:C:2803:MET:HB3	2:C:2814:CYS:SG	2.60	0.42
2:C:3276:THR:OG1	2:C:3658:ARG:NH2	2.53	0.42
4:B:790:ILE:HG12	4:B:836:ILE:HG23	2.00	0.42
4:B:2609:MET:N	4:B:2610:PRO:HD2	2.35	0.42
6:H:11:ILE:HG22	6:H:79:LEU:HB3	2.01	0.42
12:D:314:VAL:HG21	12:D:611:VAL:HG21	2.01	0.42
1:A:3568:LEU:C	1:A:3568:LEU:HD23	2.40	0.42
2:C:2715:PRO:HG2	2:C:2719:VAL:HB	2.02	0.42
2:C:3711:LEU:HD21	2:C:3725:LEU:HD23	2.02	0.42
4:B:1886:THR:HA	4:B:4193:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2040:LEU:HD12	4:B:2040:LEU:HA	1.90	0.42
11:E:121:TYR:HB3	12:D:266:TYR:OH	2.19	0.42
11:E:367:LEU:N	11:E:388:ASP:OD2	2.53	0.42
1:A:1539:LYS:HE2	4:B:3859:VAL:HG22	2.00	0.42
1:A:1782:GLU:O	1:A:1786:THR:HG23	2.19	0.42
1:A:1926:PHE:CE2	1:A:1934:LEU:HD22	2.54	0.42
1:A:4126:TRP:CZ2	1:A:4130:ILE:HD11	2.55	0.42
2:C:2246:ARG:CD	2:C:2344:ARG:HG2	2.50	0.42
2:C:2719:VAL:CG1	2:C:2720:PRO:HD3	2.50	0.42
4:B:719:VAL:O	4:B:722:TYR:HB3	2.19	0.42
4:B:3122:LEU:HD11	4:B:3448:ILE:HG12	2.01	0.42
12:D:439:ILE:HD13	12:D:484:CYS:HB3	2.02	0.42
1:A:3884:THR:HA	1:A:3891:PRO:HA	2.01	0.42
2:C:1191:ILE:HG23	2:C:1201:PHE:CE2	2.54	0.42
2:C:4081:ALA:N	2:C:4094:ILE:O	2.51	0.42
4:B:58:SER:H	4:B:71:CYS:CB	2.32	0.42
4:B:898:PRO:HB3	4:B:1077:ARG:HA	2.01	0.42
4:B:1626:ASN:ND2	4:B:1655:THR:HG21	2.35	0.42
4:B:2267:ILE:HG22	4:B:2271:TRP:CZ3	2.53	0.42
4:B:2531:ARG:C	4:B:2649:LEU:HD21	2.40	0.42
4:B:2560:VAL:HG13	4:B:2601:ILE:HD13	2.02	0.42
4:B:2667:LEU:O	4:B:2670:ASN:N	2.53	0.42
4:B:3885:ASN:O	4:B:3889:GLN:HG2	2.19	0.42
1:A:1220:THR:HG22	1:A:1279:LYS:CA	2.50	0.42
2:C:2082:LEU:HG	2:C:2137:VAL:HG21	2.00	0.42
2:C:2792:TYR:O	2:C:2796:PRO:HD3	2.19	0.42
4:B:1192:ASN:OD1	4:B:1193:ALA:N	2.52	0.42
5:I:93:THR:HB	5:I:109:LYS:HB3	2.00	0.42
12:D:422:ARG:NH2	12:D:424:MET:SD	2.92	0.42
1:A:1143:ARG:NH1	12:D:169:ASN:ND2	2.67	0.42
1:A:1227:ARG:H	1:A:1286:THR:CB	2.33	0.42
2:C:908:LEU:CD1	2:C:948:LEU:HD13	2.50	0.42
2:C:1128:PHE:CZ	2:C:1151:LEU:HD13	2.54	0.42
4:B:1163:ARG:O	4:B:1167:MET:N	2.53	0.42
4:B:2776:LYS:NZ	4:B:2814:ILE:HG23	2.35	0.42
9:N:68:CYS:HA	10:O:101:CYS:HA	2.01	0.42
12:D:526:ARG:HB2	12:D:528:TRP:CH2	2.54	0.42
1:A:598:ARG:HD3	12:D:319:TYR:CE1	2.55	0.42
1:A:1027:CYS:O	1:A:1027:CYS:SG	2.78	0.42
1:A:2159:THR:HG22	1:A:2624:ARG:HD2	2.01	0.42
1:A:3638:LEU:HA	1:A:3641:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4113:ILE:HD11	1:A:4134:CYS:SG	2.59	0.42
2:C:997:LEU:HB2	2:C:1051:GLN:HE22	1.84	0.42
2:C:2082:LEU:HD11	2:C:2096:ILE:HD13	2.02	0.42
2:C:2711:SER:HB2	2:C:2755:LEU:HD23	2.02	0.42
2:C:3034:LEU:HB3	2:C:3041:ILE:HG22	2.02	0.42
4:B:1536:GLU:C	4:B:1625:GLN:NE2	2.73	0.42
4:B:3767:MET:HG3	4:B:3768:ASP:N	2.35	0.42
5:I:19:MET:HB2	5:I:22:LYS:HG2	2.01	0.42
9:N:76:THR:HG21	11:E:39:GLN:NE2	2.26	0.42
9:N:86:THR:HG22	11:E:25:THR:HG22	2.01	0.42
1:A:4056:ILE:CD1	1:A:4072:LEU:HD21	2.47	0.41
2:C:868:ILE:O	2:C:872:ARG:N	2.46	0.41
4:B:2192:CYS:O	4:B:2196:THR:HG23	2.19	0.41
4:B:3582:ILE:HG23	4:B:3582:ILE:O	2.19	0.41
4:B:4227:PHE:CD1	4:B:4263:ALA:HA	2.55	0.41
4:B:4287:LEU:HD11	4:B:4393:LEU:HG	2.01	0.41
12:D:66:LEU:N	12:D:66:LEU:HD22	2.35	0.41
1:A:1918:GLY:HA3	1:A:1967:ILE:HG21	2.02	0.41
2:C:162:GLY:HA2	2:C:203:HIS:CE1	2.55	0.41
2:C:2066:GLN:CA	2:C:2066:GLN:NE2	2.83	0.41
2:C:2826:VAL:C	2:C:2828:GLN:N	2.73	0.41
4:B:1068:LYS:CB	4:B:1084:LYS:HE2	2.50	0.41
5:I:15:LEU:HD22	12:D:212:ILE:HD13	2.01	0.41
11:E:492:ASP:HA	11:E:495:TYR:CE2	2.54	0.41
11:E:517:LYS:O	11:E:521:THR:HG23	2.20	0.41
1:A:1620:PRO:HB2	1:A:1639:PHE:CE1	2.54	0.41
1:A:3308:PRO:HB3	3:Q:33:PHE:CB	2.50	0.41
1:A:3951:THR:OG1	1:A:4293:SER:HB2	2.21	0.41
2:C:115:LYS:O	2:C:119:TYR:N	2.53	0.41
2:C:3408:LEU:HD23	2:C:3413:LYS:HA	2.01	0.41
2:C:3927:VAL:HG21	2:C:4031:ALA:HB2	2.02	0.41
4:B:2026:ALA:HB1	4:B:4200:VAL:HG12	2.02	0.41
1:A:3758:TYR:CE2	1:A:3762:ILE:HD11	2.55	0.41
4:B:1933:LYS:HG3	4:B:1965:VAL:HG11	2.01	0.41
2:C:2742:LYS:HG3	2:C:2743:ASN:HD22	1.85	0.41
4:B:441:LYS:O	11:E:518:ASN:ND2	2.53	0.41
4:B:679:ARG:HB2	11:E:186:PHE:HE2	1.85	0.41
4:B:984:ASN:HA	4:B:987:ARG:HD3	2.03	0.41
4:B:1061:GLN:HG2	4:B:1091:VAL:CG1	2.50	0.41
4:B:3571:ILE:HD11	4:B:3593:LEU:HD22	2.03	0.41
4:B:3877:LEU:HD13	4:B:3928:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:68:PHE:HA	11:E:71:ARG:O	2.20	0.41
14:L:92:VAL:HG12	14:L:92:VAL:O	2.20	0.41
17:M:57:VAL:HG22	17:M:82:LEU:HG	2.01	0.41
1:A:8:LYS:CB	1:A:109:SER:HA	2.50	0.41
1:A:151:ILE:O	1:A:153:PHE:N	2.53	0.41
2:C:2005:PRO:HB2	2:C:2145:PHE:CD1	2.55	0.41
2:C:2007:LEU:HD13	2:C:2126:ALA:HB3	2.02	0.41
2:C:2770:ASN:O	2:C:2773:ASP:N	2.45	0.41
4:B:447:THR:HG21	4:B:513:ASP:C	2.41	0.41
4:B:1237:ARG:HH21	4:B:1263:THR:CA	2.34	0.41
4:B:3268:THR:HG23	4:B:3309:GLN:OE1	2.20	0.41
4:B:3582:ILE:HG23	4:B:3626:THR:HG22	2.02	0.41
4:B:3594:LEU:HD22	4:B:3641:CYS:SG	2.61	0.41
1:A:1205:GLN:HG2	12:D:166:PHE:CD1	2.56	0.41
1:A:1638:THR:HB	1:A:1655:GLN:HG2	2.03	0.41
2:C:1328:LEU:HG	2:C:1333:VAL:HG21	2.02	0.41
2:C:1383:ASP:O	2:C:1387:VAL:HG23	2.20	0.41
2:C:2812:GLY:O	2:C:2815:SER:CB	2.68	0.41
4:B:459:ILE:HG23	4:B:499:LEU:CD1	2.50	0.41
4:B:2417:LEU:N	4:B:2418:PRO:HD2	2.35	0.41
4:B:2771:TRP:O	4:B:2772:ALA:C	2.59	0.41
9:N:88:TYR:N	10:O:81:ILE:O	2.54	0.41
1:A:1642:ALA:HB2	1:A:1652:GLN:HB3	2.03	0.41
1:A:3132:ASN:CA	1:A:3419:ILE:HD11	2.51	0.41
2:C:3136:LEU:HD21	2:C:3221:SER:HB2	2.02	0.41
2:C:3588:VAL:HG11	2:C:3621:TRP:CD2	2.56	0.41
4:B:1109:THR:C	4:B:1113:LEU:HG	2.41	0.41
4:B:2157:LEU:HD21	4:B:2196:THR:CG2	2.51	0.41
4:B:2715:TYR:O	4:B:2718:PHE:N	2.54	0.41
4:B:3321:PHE:CE1	4:B:3337:CYS:SG	3.14	0.41
4:B:3907:PRO:HG3	4:B:3934:ARG:HD3	2.03	0.41
8:F:11:LEU:HB3	8:F:23:TYR:OH	2.21	0.41
2:C:841:ILE:HG13	2:C:891:ILE:HD13	2.02	0.41
2:C:895:LEU:C	2:C:895:LEU:HD23	2.41	0.41
2:C:2717:ALA:CB	2:C:2803:MET:SD	3.06	0.41
2:C:3622:ILE:HD11	2:C:3624:LEU:HD21	2.03	0.41
4:B:1536:GLU:O	4:B:1625:GLN:NE2	2.54	0.41
4:B:1599:LEU:CD2	4:B:1621:LEU:HB2	2.51	0.41
4:B:1602:LYS:CB	4:B:1683:GLU:CB	2.87	0.41
4:B:1603:LYS:HA	4:B:1609:PHE:HB2	2.03	0.41
4:B:2609:MET:N	4:B:2610:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2900:CYS:SG	4:B:3019:VAL:HG11	2.60	0.41
4:B:3255:THR:HG23	4:B:3337:CYS:SG	2.61	0.41
4:B:4106:ASN:HD21	4:B:4141:ILE:HB	1.85	0.41
1:A:1698:ILE:HG21	1:A:1722:ILE:HD13	2.03	0.41
1:A:1967:ILE:O	1:A:1970:VAL:HG23	2.21	0.41
1:A:2963:ILE:HD13	1:A:2987:PHE:HB2	2.03	0.41
1:A:3131:ILE:HG21	1:A:3418:LEU:CB	2.51	0.41
4:B:898:PRO:HG2	4:B:1077:ARG:CG	2.51	0.41
4:B:1119:LYS:HB3	4:B:1138:LYS:HD3	2.02	0.41
4:B:2180:CYS:SG	4:B:2181:PHE:N	2.94	0.41
4:B:2695:HIS:O	4:B:2695:HIS:CD2	2.74	0.41
4:B:3271:ASP:CG	4:B:3272:PRO:HD2	2.41	0.41
4:B:3826:THR:HG22	4:B:3942:LEU:CD2	2.51	0.41
2:C:22:SER:HB3	2:C:341:TRP:HB2	2.03	0.40
4:B:55:GLN:O	4:B:85:LYS:HA	2.22	0.40
4:B:137:LEU:O	4:B:138:ASN:CB	2.69	0.40
4:B:1480:HIS:O	4:B:1484:LEU:HG	2.21	0.40
4:B:1598:TYR:CD2	4:B:1621:LEU:CG	3.04	0.40
4:B:2537:ILE:HA	4:B:2654:LEU:O	2.21	0.40
4:B:4040:MET:HG2	4:B:4075:PHE:HB2	2.03	0.40
4:B:4220:LEU:O	4:B:4220:LEU:HD23	2.21	0.40
4:B:4480:ILE:O	4:B:4480:ILE:HG22	2.21	0.40
6:H:24:VAL:HG22	6:H:49:PHE:HZ	1.86	0.40
13:P:27:ASN:HA	13:P:95:GLU:HA	2.03	0.40
1:A:1698:ILE:CG2	1:A:1722:ILE:HD13	2.51	0.40
1:A:3322:ALA:CB	1:A:3333:LEU:HD12	2.51	0.40
1:A:4347:LEU:HD11	1:A:4368:LEU:HD23	2.02	0.40
2:C:225:GLN:OE1	2:C:225:GLN:N	2.54	0.40
2:C:1328:LEU:HG	2:C:1333:VAL:HG11	2.02	0.40
4:B:937:PHE:CD1	4:B:937:PHE:N	2.88	0.40
4:B:1071:GLU:HG2	4:B:1079:ASN:HD22	1.86	0.40
1:A:1161:SER:O	1:A:1164:ASP:N	2.54	0.40
1:A:1631:PHE:HB2	1:A:1634:ILE:HG21	2.01	0.40
2:C:1305:LYS:N	2:C:1306:PRO:CD	2.84	0.40
4:B:722:TYR:O	4:B:723:ASN:O	2.39	0.40
4:B:4187:ILE:O	4:B:4212:LEU:HD21	2.21	0.40
16:J:44:THR:HG22	16:J:64:LEU:HD22	2.03	0.40
1:A:1562:ILE:HB	1:A:1563:PRO:HD3	2.04	0.40
1:A:1857:THR:HG21	1:A:1997:VAL:HG22	2.04	0.40
1:A:2576:LEU:HD13	1:A:2621:ILE:HG13	2.04	0.40
1:A:2789:LEU:HD21	1:A:2811:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1048:LEU:HD13	2:C:1048:LEU:C	2.42	0.40
2:C:1559:LEU:CD2	2:C:1607:LEU:HD21	2.50	0.40
2:C:2555:LEU:HD12	2:C:2555:LEU:C	2.42	0.40
2:C:2775:VAL:HG22	2:C:2824:TYR:CE1	2.56	0.40
2:C:3460:ASN:HB3	2:C:3466:ALA:HB1	2.03	0.40
4:B:808:PRO:CG	4:B:1077:ARG:HB2	2.52	0.40
4:B:1602:LYS:HD2	4:B:1683:GLU:CB	2.48	0.40
4:B:1627:ALA:HB3	4:B:1628:PRO:HD3	2.03	0.40
4:B:2055:PHE:CE1	4:B:2106:LEU:HD21	2.56	0.40
4:B:3080:LEU:HD12	4:B:3484:LYS:HE2	2.03	0.40
4:B:4548:TYR:CD2	4:B:4553:ARG:HD2	2.57	0.40
11:E:37:ILE:HG23	11:E:39:GLN:HG3	2.04	0.40
1:A:1118:LEU:HD13	1:A:1118:LEU:HA	1.99	0.40
1:A:1541:PHE:HA	1:A:1544:ILE:HB	2.03	0.40
1:A:1787:ILE:HD13	1:A:1847:ILE:HD11	2.04	0.40
2:C:1839:PHE:HE1	2:C:1891:LEU:HD11	1.86	0.40
2:C:3151:LYS:HE3	2:C:3217:ILE:HD11	2.03	0.40
4:B:801:ILE:HG22	4:B:802:ILE:N	2.36	0.40
4:B:2146:ILE:O	4:B:2150:THR:HG23	2.22	0.40
4:B:2150:THR:CG2	4:B:2203:ASN:HD22	2.35	0.40
4:B:4129:ILE:HG23	4:B:4169:MET:SD	2.61	0.40
8:F:11:LEU:HD22	8:F:23:TYR:CE1	2.56	0.40
8:F:97:MET:HG3	8:F:98:LEU:N	2.35	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	4381/4620 (95%)	4081 (93%)	258 (6%)	42 (1%)	15 55
2	C	3914/4168 (94%)	3582 (92%)	283 (7%)	49 (1%)	12 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	190/202 (94%)	163 (86%)	24 (13%)	3 (2%)	9	44
4	B	4488/4595 (98%)	4017 (90%)	383 (8%)	88 (2%)	7	38
5	I	104/110 (94%)	95 (91%)	8 (8%)	1 (1%)	15	55
6	H	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
7	G	92/159 (58%)	87 (95%)	5 (5%)	0	100	100
8	F	108/133 (81%)	96 (89%)	11 (10%)	1 (1%)	17	57
9	N	112/117 (96%)	92 (82%)	17 (15%)	3 (3%)	5	31
10	O	118/132 (89%)	103 (87%)	10 (8%)	5 (4%)	3	22
11	E	551/670 (82%)	496 (90%)	51 (9%)	4 (1%)	22	63
12	D	569/667 (85%)	510 (90%)	51 (9%)	8 (1%)	11	46
13	P	103/122 (84%)	86 (84%)	11 (11%)	6 (6%)	1	18
14	L	96/111 (86%)	91 (95%)	4 (4%)	1 (1%)	15	55
15	K	88/93 (95%)	79 (90%)	9 (10%)	0	100	100
16	J	93/111 (84%)	84 (90%)	8 (9%)	1 (1%)	14	52
17	M	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	6	33
All	All	15181/16189 (94%)	13817 (91%)	1150 (8%)	214 (1%)	15	46

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	197	ILE
1	A	871	LEU
1	A	973	ASP
1	A	3251	ILE
1	A	4235	PHE
2	C	435	MET
2	C	529	GLU
2	C	2733	TYR
2	C	2744	LYS
2	C	3054	SER
2	C	3443	LYS
3	Q	19	PRO
3	Q	39	GLU
4	B	6	GLN
4	B	37	GLN
4	B	533	ARG

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Mol	Chain	Res	Type
4	B	692	LEU
4	B	750	PRO
4	B	765	PHE
4	B	1127	ASN
4	B	1607	PRO
4	B	2249	GLU
4	B	2741	PHE
4	B	2760	SER
4	B	3248	PRO
4	B	3267	ILE
4	B	3329	GLN
4	B	3331	TYR
4	B	3333	ALA
9	N	7	GLU
10	O	29	PHE
11	E	37	ILE
12	D	397	ASP
13	P	37	PRO
13	P	107	ILE
13	P	119	PRO
17	M	51	TYR
1	A	27	ILE
1	A	28	VAL
1	A	158	GLU
1	A	282	ARG
1	A	720	GLU
1	A	1670	THR
1	A	4430	TRP
1	A	4563	LYS
2	C	140	ILE
2	C	155	GLU
2	C	322	GLU
2	C	400	GLY
2	C	861	SER
2	C	1170	ALA
2	C	1901	LEU
2	C	2718	GLY
2	C	2759	LYS
2	C	2771	PHE
2	C	3619	GLY
2	C	4106	PRO
3	Q	49	LEU

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Mol	Chain	Res	Type
4	B	18	LEU
4	B	19	SER
4	B	24	ILE
4	B	27	GLU
4	B	74	TYR
4	B	136	PRO
4	B	138	ASN
4	B	307	PRO
4	B	720	ASP
4	B	723	ASN
4	B	751	GLY
4	B	752	ILE
4	B	799	VAL
4	B	801	ILE
4	B	1124	ILE
4	B	1947	GLY
4	B	1990	GLY
4	B	2353	MET
4	B	3323	GLU
4	B	3327	ALA
4	B	3328	GLY
4	B	3332	ALA
4	B	4152	ASN
4	B	4228	PRO
4	B	4484	GLU
4	B	4489	GLU
4	B	4527	CYS
5	I	51	ALA
10	O	31	PRO
11	E	19	ASN
11	E	350	LYS
12	D	168	TYR
12	D	563	MET
13	P	36	TYR
17	M	50	GLY
1	A	18	CYS
1	A	103	ASP
1	A	149	GLU
1	A	283	PRO
1	A	818	LEU
1	A	970	TYR
1	A	1172	THR

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Mol	Chain	Res	Type
1	A	1347	TRP
1	A	1396	PRO
2	C	223	THR
2	C	237	ASP
2	C	390	THR
2	C	1214	TYR
2	C	2362	GLY
2	C	2716	PRO
2	C	2732	GLY
2	C	2735	ASN
2	C	2746	PRO
2	C	2750	SER
2	C	2770	ASN
2	C	2805	SER
2	C	4092	TYR
4	B	361	LYS
4	B	764	GLN
4	B	774	ASP
4	B	806	ASN
4	B	898	PRO
4	B	2252	TYR
4	B	2969	GLY
4	B	3246	GLY
4	B	4225	GLU
9	N	25	PHE
11	E	275	THR
12	D	236	MET
16	J	101	GLU
1	A	26	MET
1	A	127	THR
1	A	152	GLN
1	A	591	LYS
1	A	1030	SER
1	A	1897	ASN
1	A	3585	ASN
1	A	4562	ASN
1	A	4599	CYS
2	C	84	TYR
2	C	1897	ASN
2	C	2247	THR
2	C	2756	LYS
2	C	3983	ALA

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Mol	Chain	Res	Type
4	B	169	LYS
4	B	334	TYR
4	B	1333	ILE
4	B	1489	SER
4	B	1856	ILE
4	B	2469	ALA
4	B	2491	TRP
4	B	2571	THR
4	B	3223	ALA
4	B	3237	PRO
4	B	3268	THR
4	B	3273	ASP
12	D	231	LYS
12	D	523	TRP
13	P	68	LEU
13	P	71	GLN
14	L	71	ASP
1	A	101	PRO
1	A	106	LYS
1	A	3972	SER
2	C	392	ASN
2	C	881	ILE
2	C	1082	ASP
2	C	2066	GLN
2	C	4090	ASP
4	B	89	ILE
4	B	99	LEU
4	B	306	GLN
4	B	719	VAL
4	B	1626	ASN
4	B	1641	LEU
4	B	2207	ASP
4	B	3302	ILE
4	B	3306	ILE
4	B	3466	ALA
4	B	4144	ARG
4	B	4182	PRO
10	O	77	PRO
12	D	321	PHE
12	D	398	PRO
1	A	772	TRP
1	A	878	VAL

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Mol	Chain	Res	Type
1	A	1745	ASN
2	C	438	GLY
4	B	407	LEU
4	B	2702	LYS
4	B	3221	LEU
8	F	29	SER
1	A	817	VAL
1	A	1171	ILE
1	A	1401	ILE
4	B	2	GLY
9	N	80	GLY
10	O	53	PRO
1	A	3535	GLY
2	C	442	ILE
2	C	2813	ILE
4	B	1212	ILE
4	B	1213	PRO
4	B	4150	GLY
2	C	99	GLY
2	C	1401	PRO
4	B	3258	VAL
2	C	2826	VAL
4	B	88	GLY
4	B	2186	PRO
4	B	3261	ILE
4	B	4147	GLY
10	O	25	ILE
2	C	1717	VAL
2	C	2715	PRO

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	3420/4197 (82%)	3338 (98%)	82 (2%)	49 69
2	C	3149/3691 (85%)	3095 (98%)	54 (2%)	60 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	10/186 (5%)	10 (100%)	0	100	100
4	B	3497/4145 (84%)	3399 (97%)	98 (3%)	43	65
5	I	91/95 (96%)	87 (96%)	4 (4%)	28	53
6	H	82/83 (99%)	80 (98%)	2 (2%)	49	69
7	G	86/149 (58%)	85 (99%)	1 (1%)	71	83
8	F	93/109 (85%)	86 (92%)	7 (8%)	13	38
9	N	85/104 (82%)	84 (99%)	1 (1%)	71	83
10	O	106/119 (89%)	99 (93%)	7 (7%)	16	41
11	E	484/597 (81%)	467 (96%)	17 (4%)	36	59
12	D	507/609 (83%)	482 (95%)	25 (5%)	25	50
14	L	87/99 (88%)	83 (95%)	4 (5%)	27	52
15	K	80/82 (98%)	79 (99%)	1 (1%)	69	81
16	J	81/97 (84%)	79 (98%)	2 (2%)	47	68
17	M	78/78 (100%)	74 (95%)	4 (5%)	24	48
All	All	11936/14440 (83%)	11627 (97%)	309 (3%)	49	66

All (309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	581	ASP
1	A	582	THR
1	A	616	LYS
1	A	674	LEU
1	A	751	LEU
1	A	758	ASP
1	A	763	LEU
1	A	810	LEU
1	A	818	LEU
1	A	861	ASP
1	A	871	LEU
1	A	1016	PHE
1	A	1020	PHE
1	A	1023	PHE
1	A	1069	TYR
1	A	1086	SER
1	A	1132	LEU
1	A	1136	MET

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Mol	Chain	Res	Type
1	A	1153	PHE
1	A	1171	ILE
1	A	1201	TYR
1	A	1205	GLN
1	A	1559	LYS
1	A	1567	ASN
1	A	1573	PHE
1	A	1581	LEU
1	A	1609	THR
1	A	1631	PHE
1	A	1634	ILE
1	A	1644	ASP
1	A	1711	LEU
1	A	1778	ARG
1	A	1922	CYS
1	A	2034	CYS
1	A	2075	MET
1	A	2098	LEU
1	A	2228	THR
1	A	2267	ASN
1	A	2320	SER
1	A	2418	ILE
1	A	2426	GLU
1	A	2434	SER
1	A	2443	CYS
1	A	2470	GLU
1	A	2471	MET
1	A	2487	ASN
1	A	2729	LEU
1	A	2844	ASP
1	A	2901	ASP
1	A	3046	PHE
1	A	3122	ASN
1	A	3125	GLN
1	A	3203	PRO
1	A	3283	ASP
1	A	3308	PRO
1	A	3315	ASP
1	A	3345	LYS
1	A	3449	LEU
1	A	3578	LEU
1	A	3588	ASP

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Mol	Chain	Res	Type
1	A	3647	PHE
1	A	3881	SER
1	A	3951	THR
1	A	3952	LEU
1	A	3973	TYR
1	A	4046	CYS
1	A	4130	ILE
1	A	4143	ARG
1	A	4155	TYR
1	A	4216	PHE
1	A	4287	THR
1	A	4288	PHE
1	A	4448	GLN
1	A	4465	THR
1	A	4497	SER
1	A	4504	SER
1	A	4506	THR
1	A	4542	ASP
1	A	4562	ASN
1	A	4578	CYS
1	A	4588	ASP
1	A	4593	PHE
2	C	36	PHE
2	C	39	LEU
2	C	110	ASP
2	C	111	THR
2	C	214	LEU
2	C	220	TRP
2	C	239	TRP
2	C	329	ASP
2	C	346	LEU
2	C	352	LEU
2	C	950	ASP
2	C	1113	ASN
2	C	1249	ASP
2	C	1453	CYS
2	C	1499	CYS
2	C	1650	ASP
2	C	1660	ASP
2	C	1702	ASP
2	C	1722	ASP
2	C	1868	CYS

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Mol	Chain	Res	Type
2	C	1884	CYS
2	C	1953	GLN
2	C	2043	ASN
2	C	2066	GLN
2	C	2121	ASN
2	C	2122	THR
2	C	2224	LEU
2	C	2225	SER
2	C	2292	CYS
2	C	2432	ASN
2	C	2483	ASN
2	C	2488	ILE
2	C	2696	SER
2	C	2711	SER
2	C	2712	PHE
2	C	2728	TYR
2	C	2748	ASP
2	C	2757	LEU
2	C	2771	PHE
2	C	2776	ASP
2	C	3059	ASN
2	C	3460	ASN
2	C	3602	GLN
2	C	3704	ASN
2	C	3793	THR
2	C	3824	PHE
2	C	3877	GLU
2	C	3883	SER
2	C	3908	ASP
2	C	3918	VAL
2	C	4050	GLN
2	C	4092	TYR
2	C	4113	VAL
2	C	4146	MET
4	B	423	CYS
4	B	440	GLU
4	B	480	ILE
4	B	485	PHE
4	B	489	PHE
4	B	581	ASN
4	B	609	LEU
4	B	693	GLU

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Mol	Chain	Res	Type
4	B	706	GLU
4	B	766	ILE
4	B	769	SER
4	B	801	ILE
4	B	802	ILE
4	B	804	ARG
4	B	810	SER
4	B	813	ASP
4	B	850	ASP
4	B	937	PHE
4	B	1067	ILE
4	B	1183	THR
4	B	1186	PRO
4	B	1208	LYS
4	B	1213	PRO
4	B	1518	TRP
4	B	1537	ASP
4	B	1559	MET
4	B	1607	PRO
4	B	1734	THR
4	B	1929	ASP
4	B	2103	MET
4	B	2139	GLN
4	B	2206	GLU
4	B	2258	HIS
4	B	2419	LYS
4	B	2425	GLU
4	B	2454	ASP
4	B	2607	PHE
4	B	2610	PRO
4	B	2647	ASP
4	B	2653	CYS
4	B	2752	CYS
4	B	2846	LEU
4	B	2873	SER
4	B	2874	ARG
4	B	2931	GLU
4	B	2949	THR
4	B	2959	LEU
4	B	2963	ASN
4	B	2971	ILE
4	B	2982	SER

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Mol	Chain	Res	Type
4	B	3004	LEU
4	B	3032	ARG
4	B	3080	LEU
4	B	3222	PRO
4	B	3231	VAL
4	B	3269	LEU
4	B	3288	GLN
4	B	3298	ASP
4	B	3330	SER
4	B	3343	ILE
4	B	3349	ILE
4	B	3350	PHE
4	B	3355	PRO
4	B	3407	GLN
4	B	3450	ASP
4	B	3469	ARG
4	B	3489	THR
4	B	3521	ASN
4	B	3614	ILE
4	B	3708	ASP
4	B	3756	MET
4	B	3757	LEU
4	B	3800	LEU
4	B	3842	TYR
4	B	3920	ASP
4	B	3942	LEU
4	B	3945	PHE
4	B	3976	ASP
4	B	4012	PHE
4	B	4104	LYS
4	B	4125	LYS
4	B	4151	TRP
4	B	4176	ASN
4	B	4182	PRO
4	B	4255	SER
4	B	4279	CYS
4	B	4304	LYS
4	B	4352	GLU
4	B	4365	LYS
4	B	4369	GLU
4	B	4443	ARG
4	B	4476	THR

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Mol	Chain	Res	Type
4	B	4482	GLU
4	B	4503	TRP
4	B	4520	SER
4	B	4540	LYS
4	B	4547	VAL
4	B	4553	ARG
5	I	19	MET
5	I	60	CYS
5	I	81	GLU
5	I	97	MET
6	H	8	GLN
6	H	68	PHE
7	G	140	ASP
8	F	9	ASP
8	F	13	GLN
8	F	35	ARG
8	F	51	LEU
8	F	84	SER
8	F	96	THR
8	F	97	MET
9	N	18	ASP
10	O	22	LEU
10	O	32	SER
10	O	77	PRO
10	O	99	SER
10	O	103	TRP
10	O	104	ASP
10	O	122	CYS
11	E	37	ILE
11	E	44	ASN
11	E	47	PHE
11	E	49	ASP
11	E	127	ASP
11	E	193	MET
11	E	225	GLN
11	E	261	HIS
11	E	262	TYR
11	E	266	THR
11	E	353	VAL
11	E	361	LEU
11	E	385	SER
11	E	402	ILE

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Mol	Chain	Res	Type
11	E	422	SER
11	E	515	LYS
11	E	560	HIS
12	D	62	THR
12	D	69	ASP
12	D	75	LEU
12	D	90	ASP
12	D	99	ASP
12	D	104	GLN
12	D	115	TYR
12	D	169	ASN
12	D	172	GLU
12	D	177	ASN
12	D	266	TYR
12	D	289	PHE
12	D	320	ASP
12	D	371	THR
12	D	392	ASN
12	D	395	HIS
12	D	399	VAL
12	D	414	PHE
12	D	477	GLU
12	D	488	TYR
12	D	509	ASN
12	D	518	SER
12	D	523	TRP
12	D	570	ASP
12	D	595	PHE
14	L	50	GLU
14	L	51	LYS
14	L	71	ASP
14	L	86	LEU
15	K	18	MET
16	J	21	PHE
16	J	86	CYS
17	M	10	THR
17	M	15	ASP
17	M	60	ASN
17	M	64	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	599	ASN
1	A	687	ASN
1	A	804	ASN
1	A	837	GLN
1	A	1114	GLN
1	A	1205	GLN
1	A	1566	GLN
1	A	1567	ASN
1	A	1585	GLN
1	A	1624	GLN
1	A	1666	ASN
1	A	1690	ASN
1	A	1718	GLN
1	A	1728	GLN
1	A	1940	GLN
1	A	2095	ASN
1	A	2251	ASN
1	A	2279	ASN
1	A	2340	GLN
1	A	2369	GLN
1	A	2373	GLN
1	A	2458	GLN
1	A	2479	GLN
1	A	2487	ASN
1	A	2508	ASN
1	A	2628	GLN
1	A	2889	GLN
1	A	3113	GLN
1	A	3122	ASN
1	A	3252	GLN
1	A	3311	ASN
1	A	3343	HIS
1	A	3606	GLN
1	A	3746	GLN
1	A	3888	GLN
1	A	4088	GLN
1	A	4137	HIS
1	A	4330	ASN
1	A	4479	GLN
1	A	4574	ASN
2	C	17	GLN
2	C	168	ASN
2	C	1051	GLN

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Mol	Chain	Res	Type
2	C	1113	ASN
2	C	1155	ASN
2	C	1238	GLN
2	C	1300	GLN
2	C	1428	ASN
2	C	1888	GLN
2	C	1981	ASN
2	C	2066	GLN
2	C	2142	GLN
2	C	2207	HIS
2	C	2217	ASN
2	C	2483	ASN
2	C	2778	ASN
2	C	2784	ASN
2	C	2819	ASN
2	C	2951	ASN
2	C	2953	ASN
2	C	3004	ASN
2	C	3460	ASN
2	C	3654	HIS
2	C	3674	GLN
2	C	3791	HIS
2	C	3870	GLN
2	C	3958	ASN
2	C	4050	GLN
2	C	4068	ASN
2	C	4143	ASN
4	B	672	ASN
4	B	721	ASN
4	B	724	HIS
4	B	764	GLN
4	B	775	GLN
4	B	832	ASN
4	B	883	ASN
4	B	923	GLN
4	B	957	GLN
4	B	975	ASN
4	B	1079	ASN
4	B	1081	GLN
4	B	1625	GLN
4	B	1728	GLN
4	B	1761	GLN

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Mol	Chain	Res	Type
4	B	1807	GLN
4	B	1870	ASN
4	B	1956	ASN
4	B	1969	GLN
4	B	2005	ASN
4	B	2038	ASN
4	B	2148	GLN
4	B	2203	ASN
4	B	2325	ASN
4	B	2462	ASN
4	B	2476	GLN
4	B	2591	ASN
4	B	2608	ASN
4	B	2656	GLN
4	B	2836	GLN
4	B	2897	GLN
4	B	2940	ASN
4	B	3042	ASN
4	B	3081	ASN
4	B	3093	ASN
4	B	3288	GLN
4	B	3407	GLN
4	B	3521	ASN
4	B	3715	ASN
4	B	3772	GLN
4	B	3803	ASN
4	B	3879	ASN
4	B	4097	ASN
4	B	4106	ASN
4	B	4176	ASN
4	B	4177	GLN
5	I	100	ASN
6	H	36	ASN
7	G	129	GLN
7	G	149	GLN
9	N	75	GLN
11	E	31	GLN
11	E	39	GLN
11	E	42	GLN
11	E	52	ASN
11	E	122	GLN
11	E	144	ASN

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Mol	Chain	Res	Type
11	E	224	ASN
11	E	237	ASN
11	E	379	ASN
11	E	481	GLN
12	D	64	GLN
12	D	153	HIS
12	D	167	ASN
12	D	177	ASN
12	D	294	GLN
12	D	298	ASN
12	D	324	GLN
12	D	413	ASN
12	D	431	ASN
14	L	28	GLN
14	L	64	GLN
16	J	87	GLN
17	M	3	HIS
17	M	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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$
19	ATP	C	4201	20	26,33,33	0.68	0	31,52,52	0.94	2 (6%)
19	ATP	B	4701	20	26,33,33	0.66	0	31,52,52	0.91	1 (3%)
18	ADP	B	4706	20	24,29,29	0.66	0	29,45,45	0.72	1 (3%)
18	ADP	C	4203	20	24,29,29	0.69	1 (4%)	29,45,45	1.04	1 (3%)
18	ADP	C	4206	20	24,29,29	0.66	0	29,45,45	0.87	2 (6%)
19	ATP	A	4702	20	26,33,33	0.65	0	31,52,52	0.86	1 (3%)
18	ADP	A	4701	20	24,29,29	0.70	0	29,45,45	0.78	1 (3%)
18	ADP	A	4703	-	24,29,29	0.65	0	29,45,45	0.80	1 (3%)
18	ADP	B	4705	20	24,29,29	0.72	0	29,45,45	0.83	1 (3%)

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
19	ATP	C	4201	20	-	4/18/38/38	0/3/3/3
19	ATP	B	4701	20	-	2/18/38/38	0/3/3/3
18	ADP	B	4706	20	-	3/12/32/32	0/3/3/3
18	ADP	C	4203	20	-	5/12/32/32	0/3/3/3
18	ADP	C	4206	20	-	3/12/32/32	0/3/3/3
19	ATP	A	4702	20	-	5/18/38/38	0/3/3/3
18	ADP	A	4701	20	-	5/12/32/32	0/3/3/3
18	ADP	A	4703	-	-	1/12/32/32	0/3/3/3
18	ADP	B	4705	20	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	4203	ADP	C8-N7	-2.07	1.31	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	4203	ADP	C1'-N9-C4	2.70	131.39	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4201	ATP	PA-O3A-PB	-2.44	124.46	132.83
19	B	4701	ATP	C5-C6-N6	2.38	123.97	120.35
18	C	4206	ADP	C5-C6-N6	2.23	123.74	120.35
19	A	4702	ATP	C5-C6-N6	2.18	123.67	120.35
18	B	4706	ADP	C5-C6-N6	2.16	123.64	120.35
19	C	4201	ATP	C5-C6-N6	2.14	123.61	120.35
18	B	4705	ADP	C5-C6-N6	2.06	123.48	120.35
18	C	4206	ADP	C3'-C2'-C1'	2.05	104.06	100.98
18	A	4701	ADP	C5-C6-N6	2.04	123.45	120.35
18	A	4703	ADP	C5-C6-N6	2.02	123.43	120.35

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	4701	ADP	PA-O3A-PB-O3B
18	C	4203	ADP	C5'-O5'-PA-O1A
18	C	4203	ADP	C5'-O5'-PA-O2A
18	C	4206	ADP	O4'-C4'-C5'-O5'
18	B	4705	ADP	PB-O3A-PA-O5'
18	B	4705	ADP	C5'-O5'-PA-O1A
19	C	4201	ATP	C5'-O5'-PA-O1A
19	C	4201	ATP	C5'-O5'-PA-O3A
18	C	4203	ADP	C3'-C4'-C5'-O5'
18	C	4206	ADP	C3'-C4'-C5'-O5'
19	A	4702	ATP	O4'-C4'-C5'-O5'
18	C	4203	ADP	O4'-C4'-C5'-O5'
18	B	4706	ADP	PA-O3A-PB-O2B
18	A	4701	ADP	O4'-C4'-C5'-O5'
19	A	4702	ATP	PB-O3A-PA-O2A
18	B	4705	ADP	C4'-C5'-O5'-PA
18	B	4705	ADP	C5'-O5'-PA-O2A
19	A	4702	ATP	C3'-C4'-C5'-O5'
18	B	4706	ADP	C4'-C5'-O5'-PA
18	A	4703	ADP	C4'-C5'-O5'-PA
19	C	4201	ATP	O4'-C4'-C5'-O5'
18	C	4206	ADP	PB-O3A-PA-O1A
19	B	4701	ATP	O4'-C4'-C5'-O5'
18	A	4701	ADP	PA-O3A-PB-O1B
18	A	4701	ADP	PA-O3A-PB-O2B
19	A	4702	ATP	PB-O3B-PG-O2G
18	C	4203	ADP	C5'-O5'-PA-O3A

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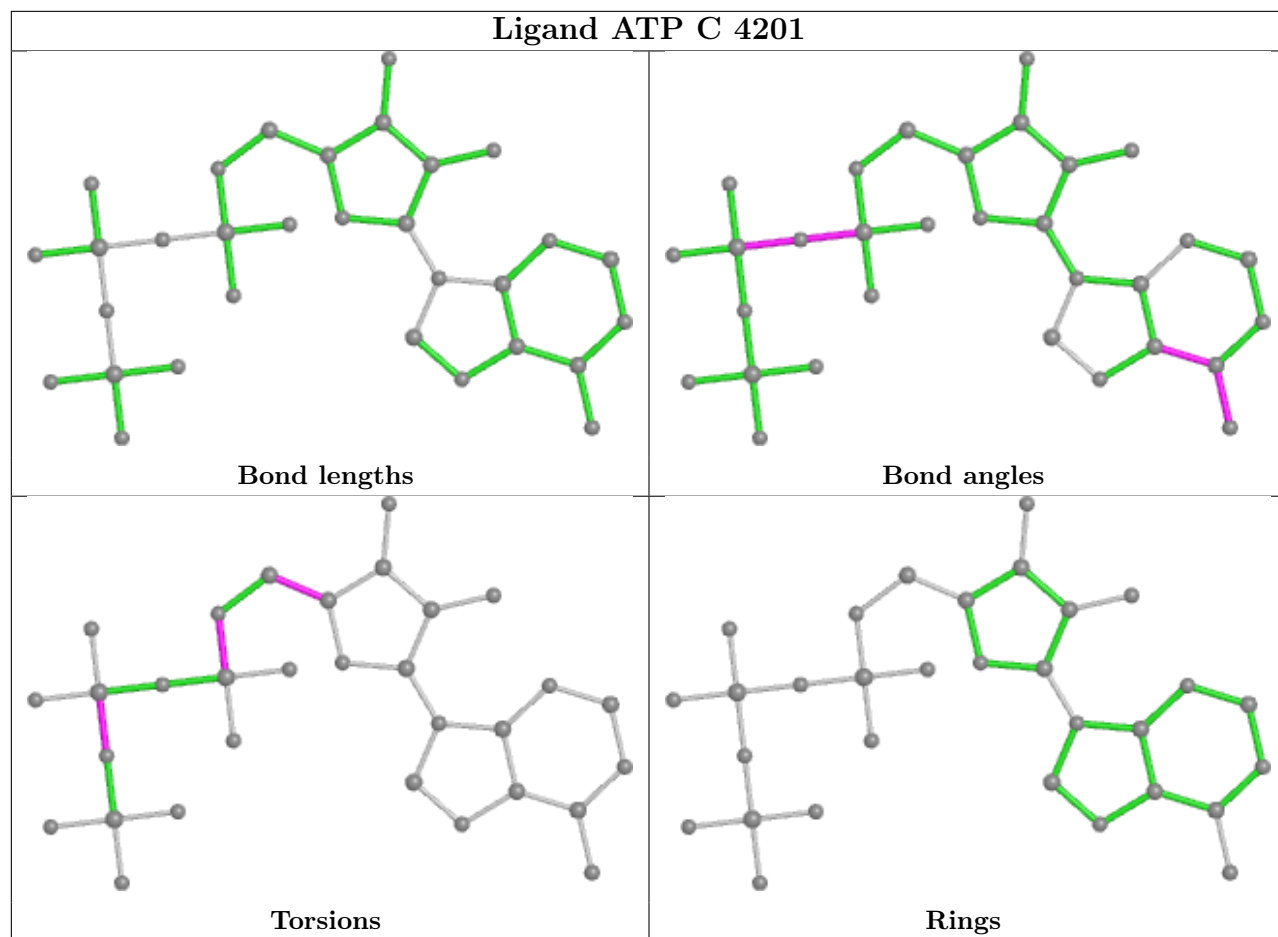
Mol	Chain	Res	Type	Atoms
18	B	4705	ADP	C5'-O5'-PA-O3A
19	B	4701	ATP	C5'-O5'-PA-O3A
18	B	4706	ADP	O4'-C4'-C5'-O5'
19	A	4702	ATP	PB-O3A-PA-O1A
19	C	4201	ATP	PG-O3B-PB-O2B
18	A	4701	ADP	C4'-C5'-O5'-PA

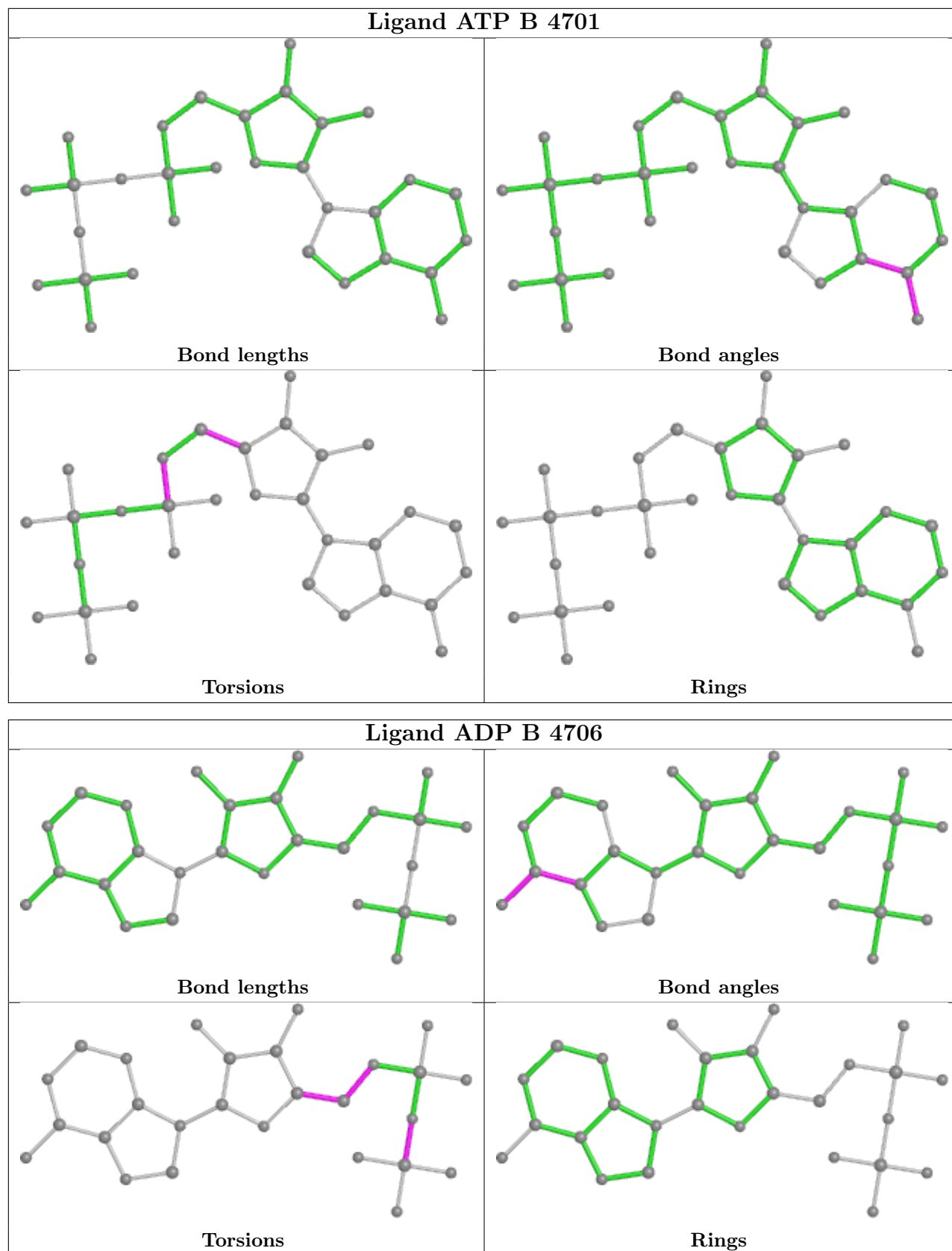
There are no ring outliers.

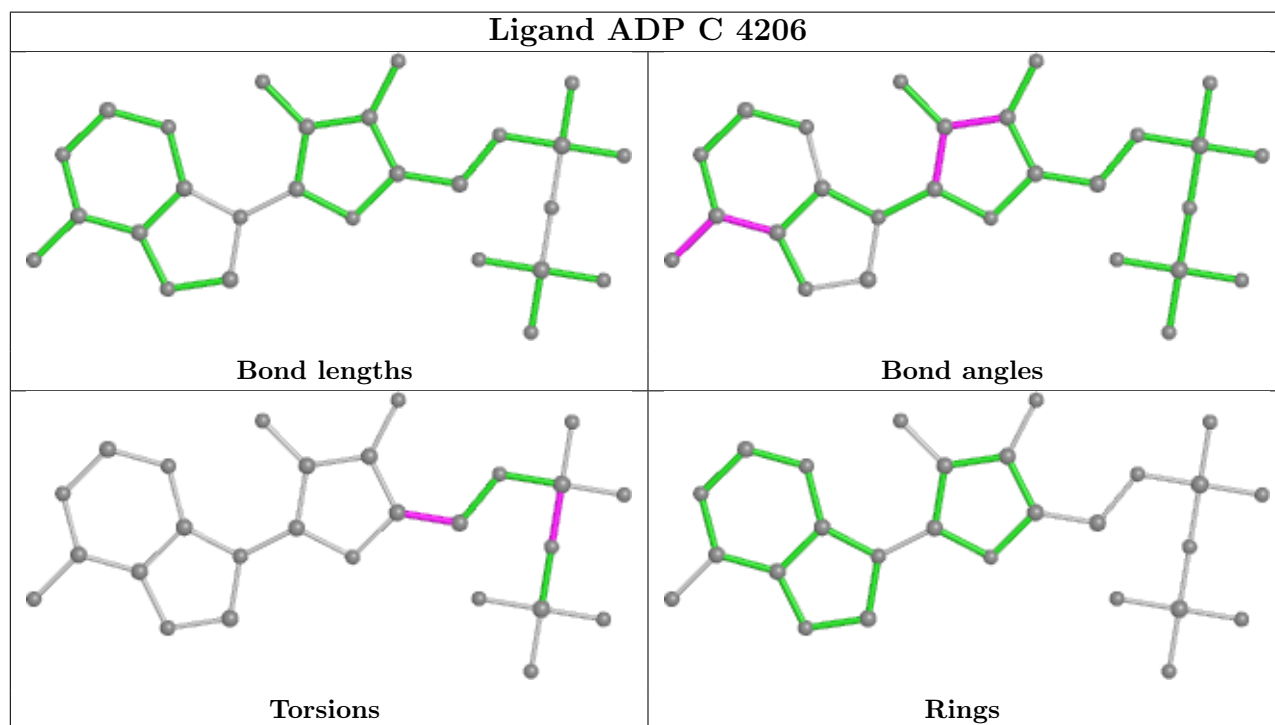
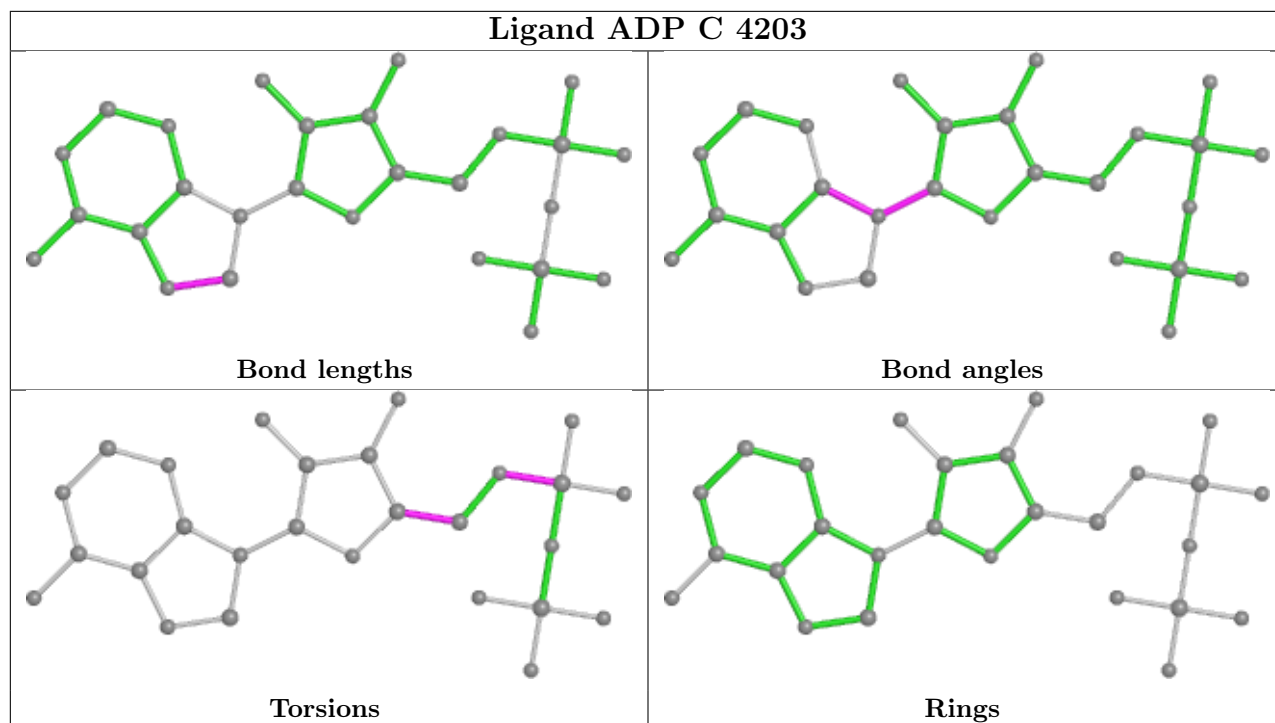
5 monomers are involved in 6 short contacts:

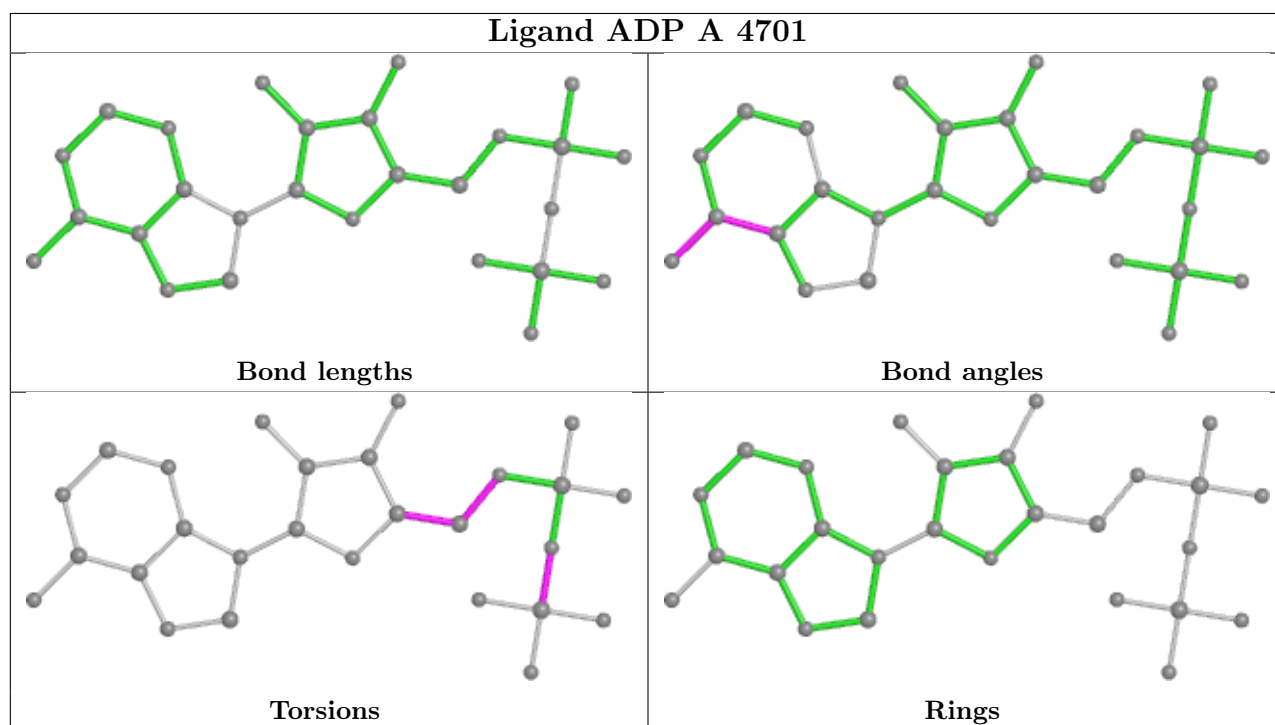
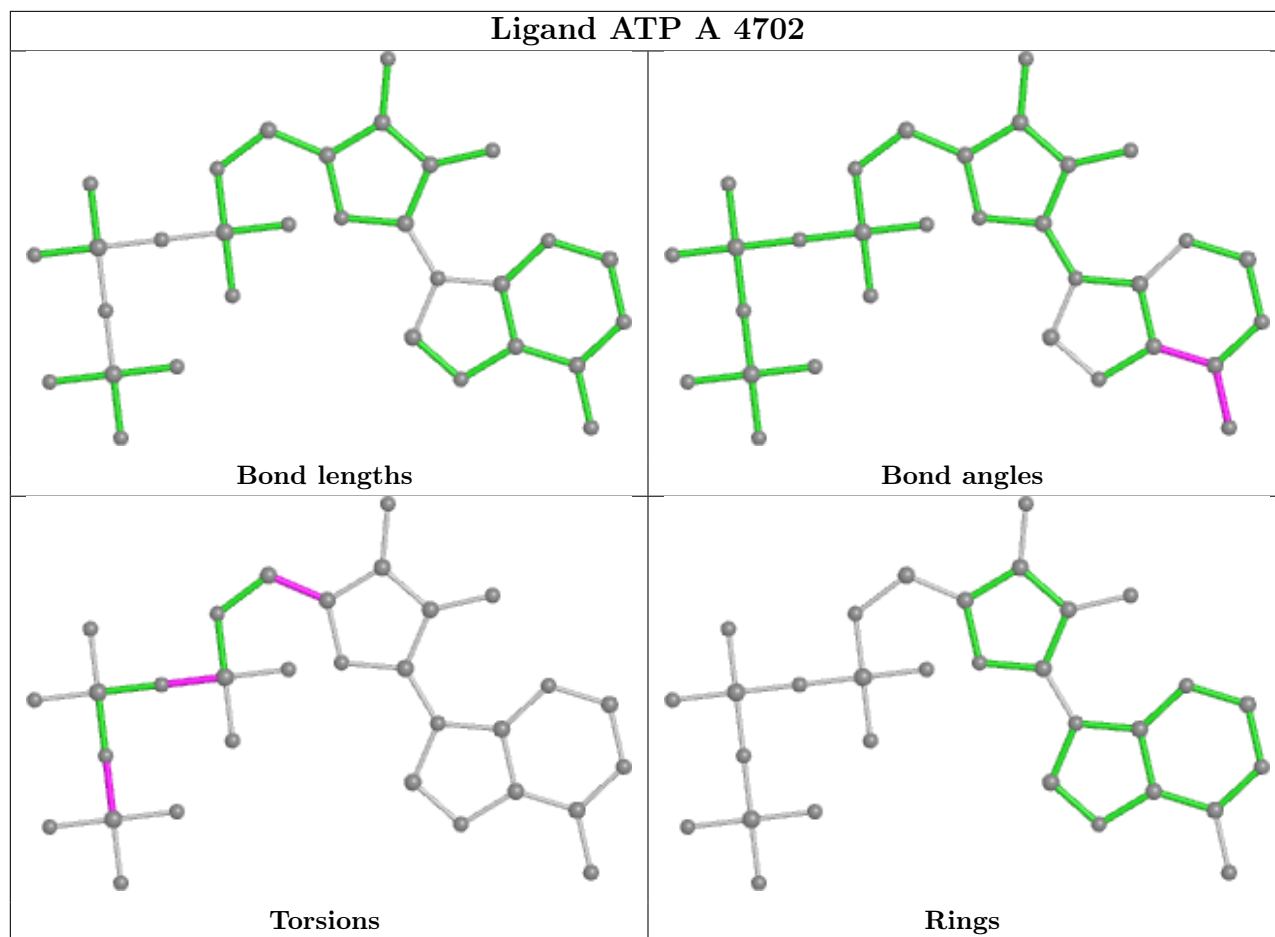
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	4701	ATP	1	0
18	C	4203	ADP	1	0
18	C	4206	ADP	2	0
18	A	4701	ADP	1	0
18	A	4703	ADP	1	0

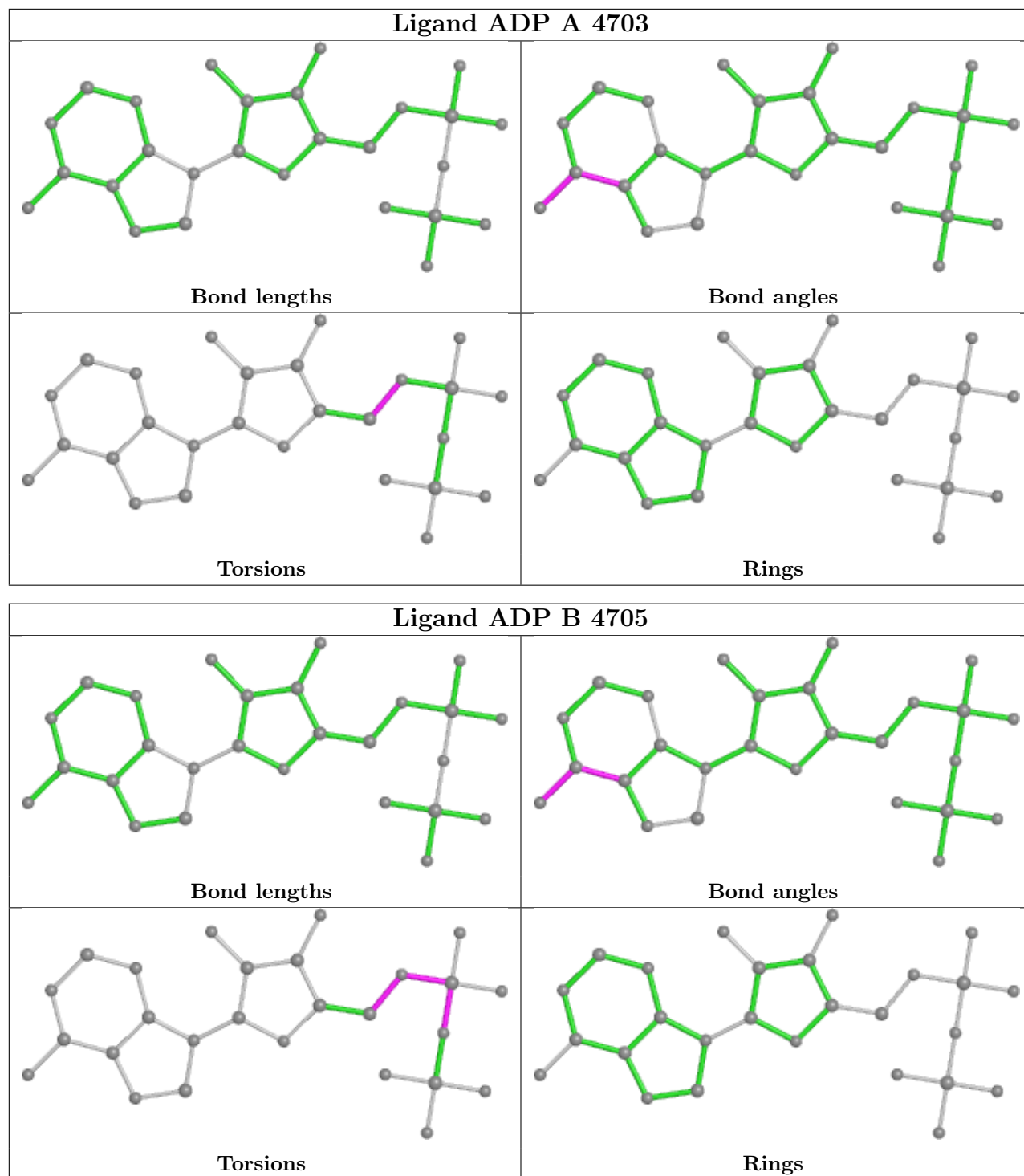
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
2	C	3
4	B	3
12	D	2
13	P	1
7	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	364:ILE	C	365:PHE	N	4.18
1	B	25:GLN	C	26:LYS	N	3.78
1	D	216:HIS	C	217:GLN	N	3.67
1	A	53:ILE	C	54:PHE	N	3.57
1	A	115:ASP	C	116:ASN	N	3.46
1	A	40:LEU	C	41:LEU	N	3.38
1	A	24:LYS	C	25:ASP	N	3.36
1	P	15:SER	C	16:GLU	N	3.31
1	C	305:ASN	C	306:LEU	N	3.20
1	G	58:SER	C	59:GLU	N	3.19
1	D	238:SER	C	239:THR	N	3.15
1	B	994:SER	C	995:TYR	N	2.89
1	B	1606:PHE	C	1607:PRO	N	1.73
1	C	1136:PHE	C	1137:PRO	N	1.65

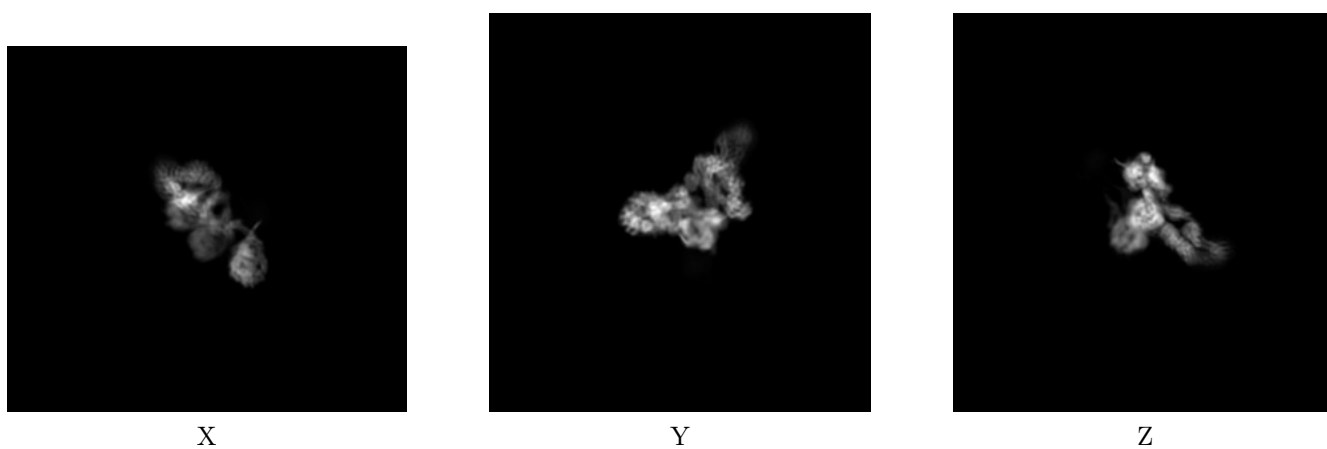
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22840. 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](#)

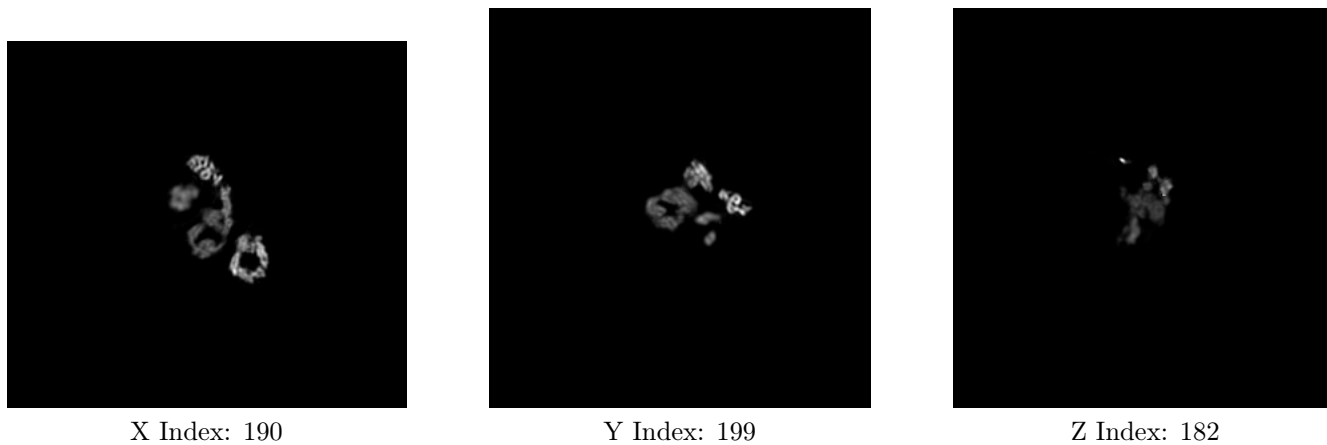
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



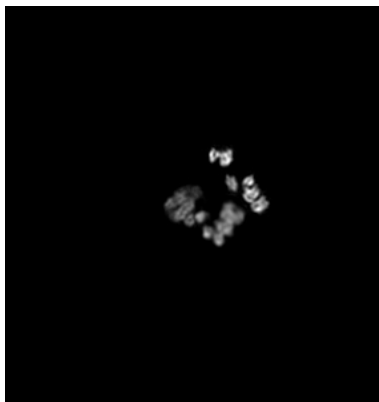
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 186

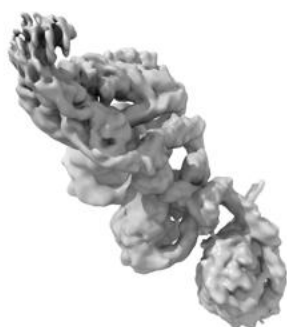


Z Index: 209

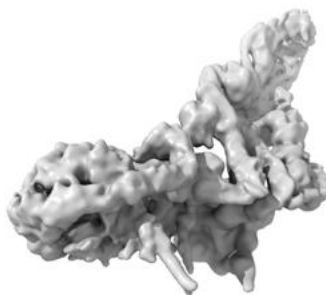
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

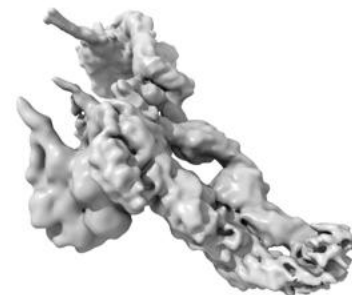
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

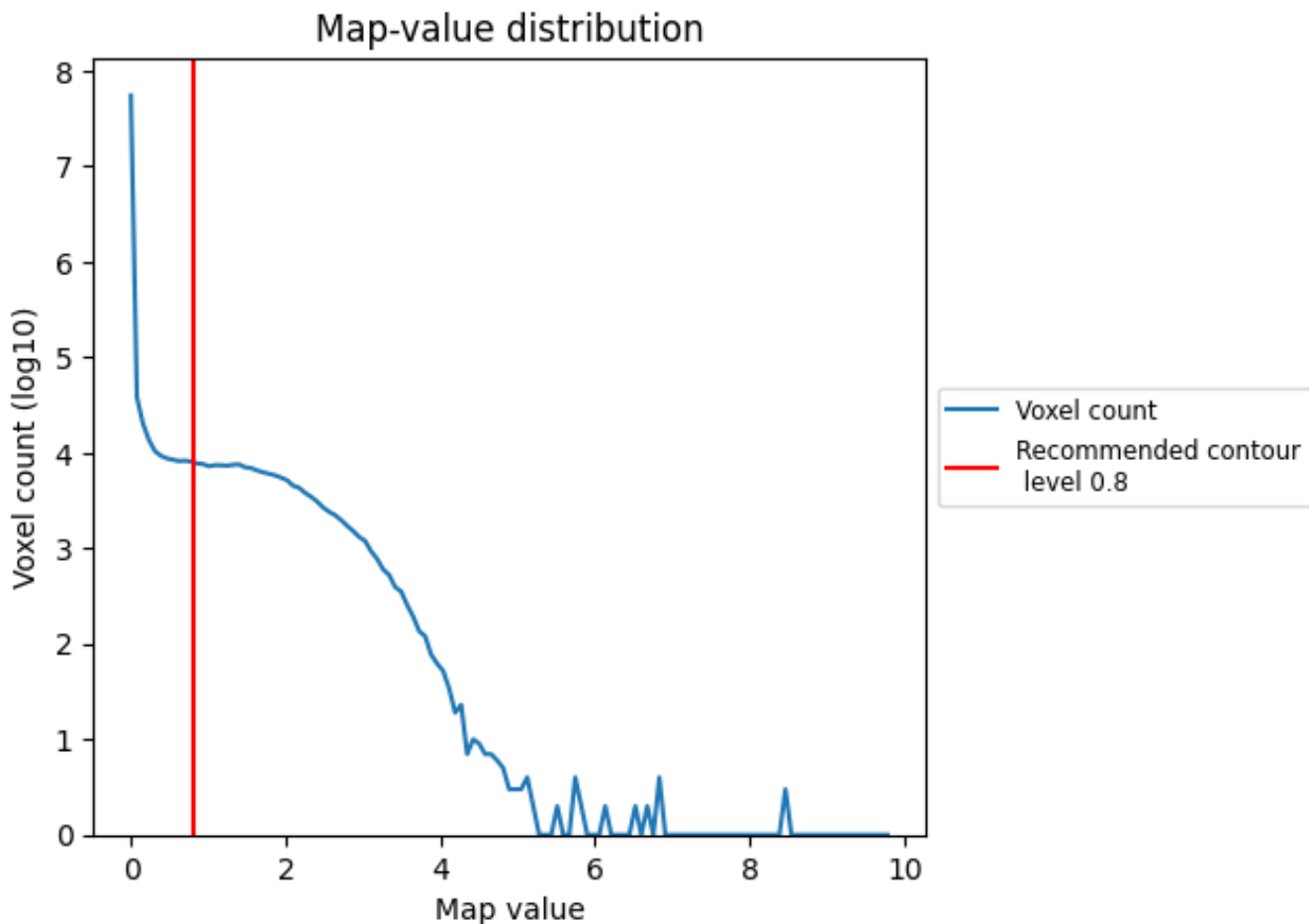
6.5 Mask visualisation

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

7 Map analysis [i](#)

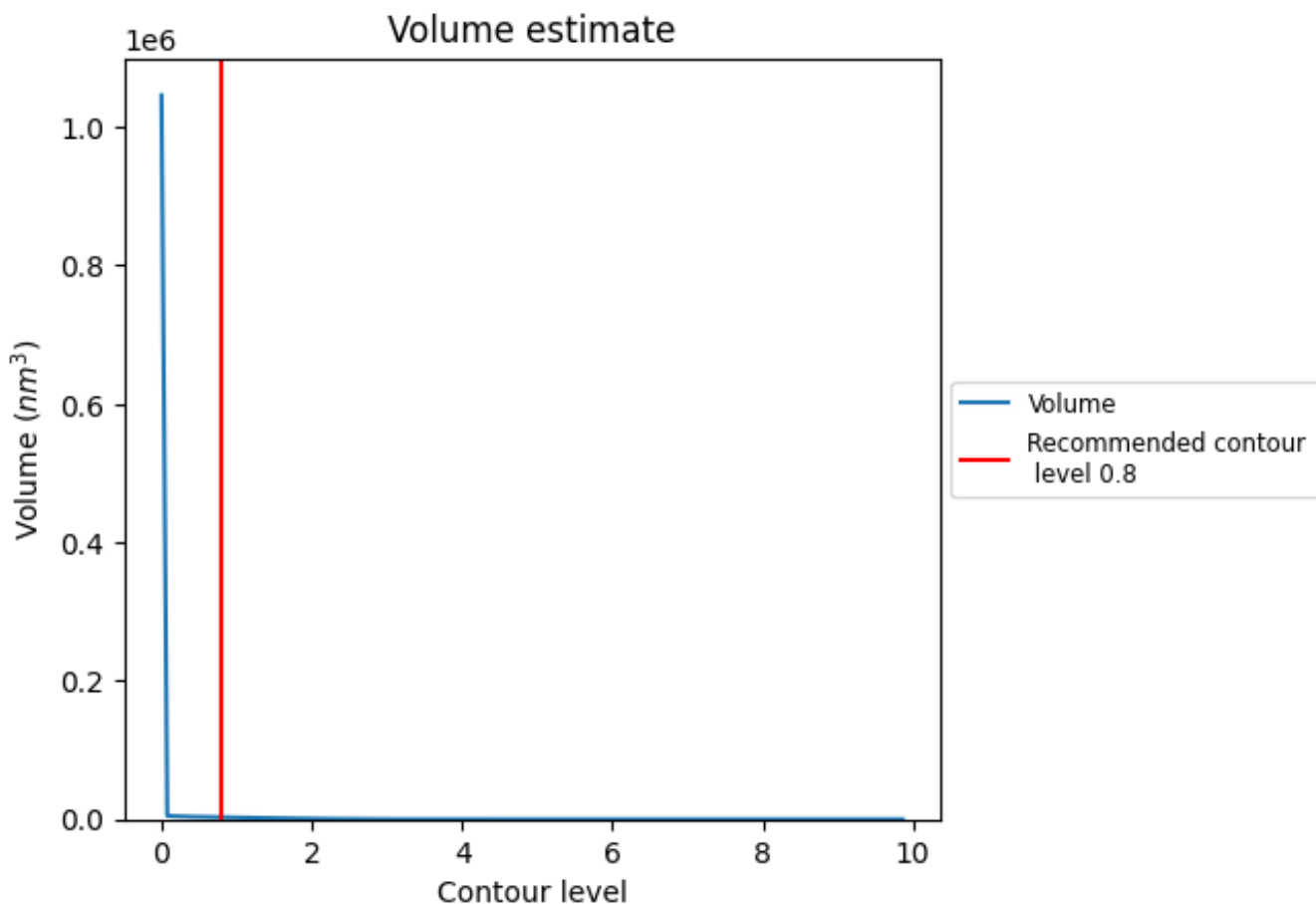
This section contains the results of statistical analysis of the map.

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 2909 nm^3 ; this corresponds to an approximate mass of 2628 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

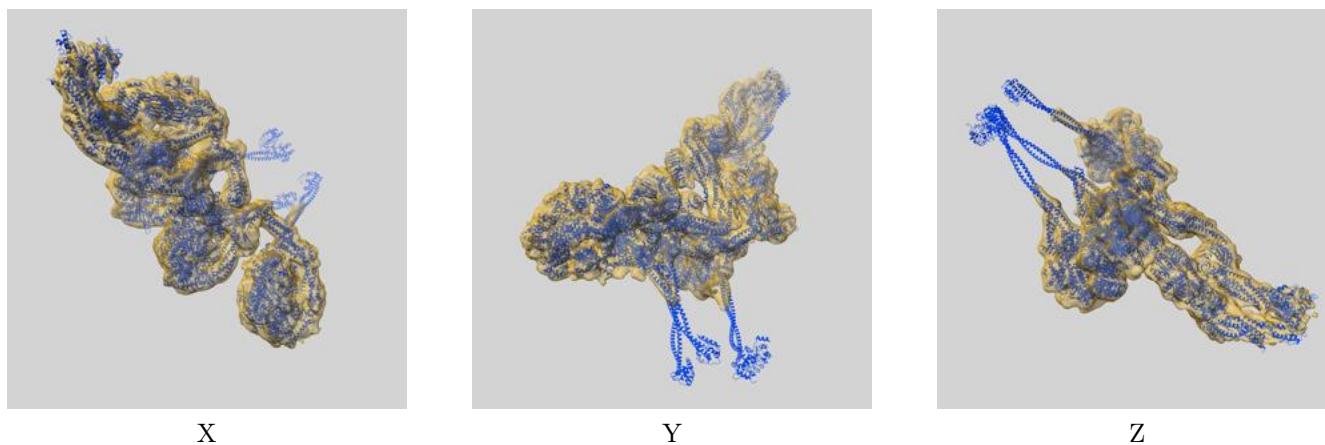
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

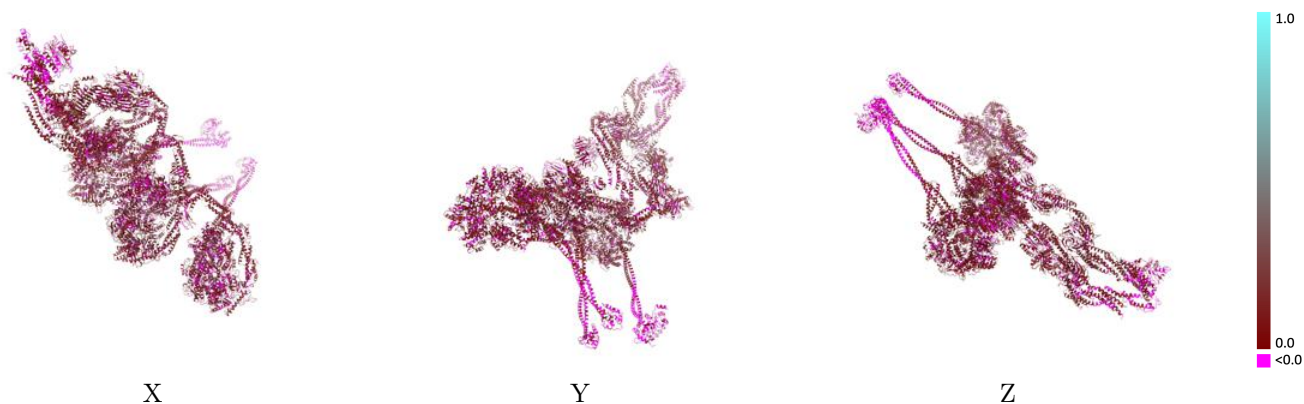
This section contains information regarding the fit between EMDB map EMD-22840 and PDB model 7KEK. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



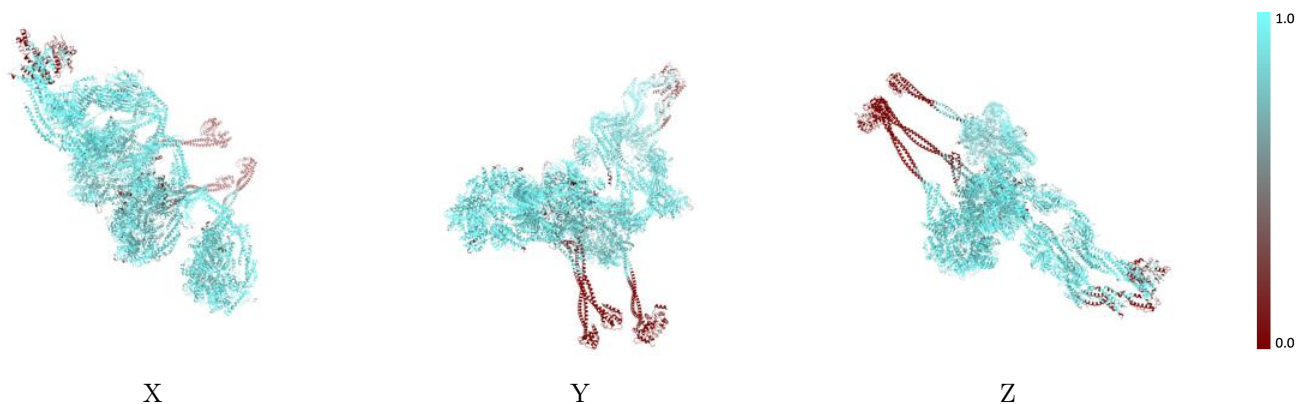
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



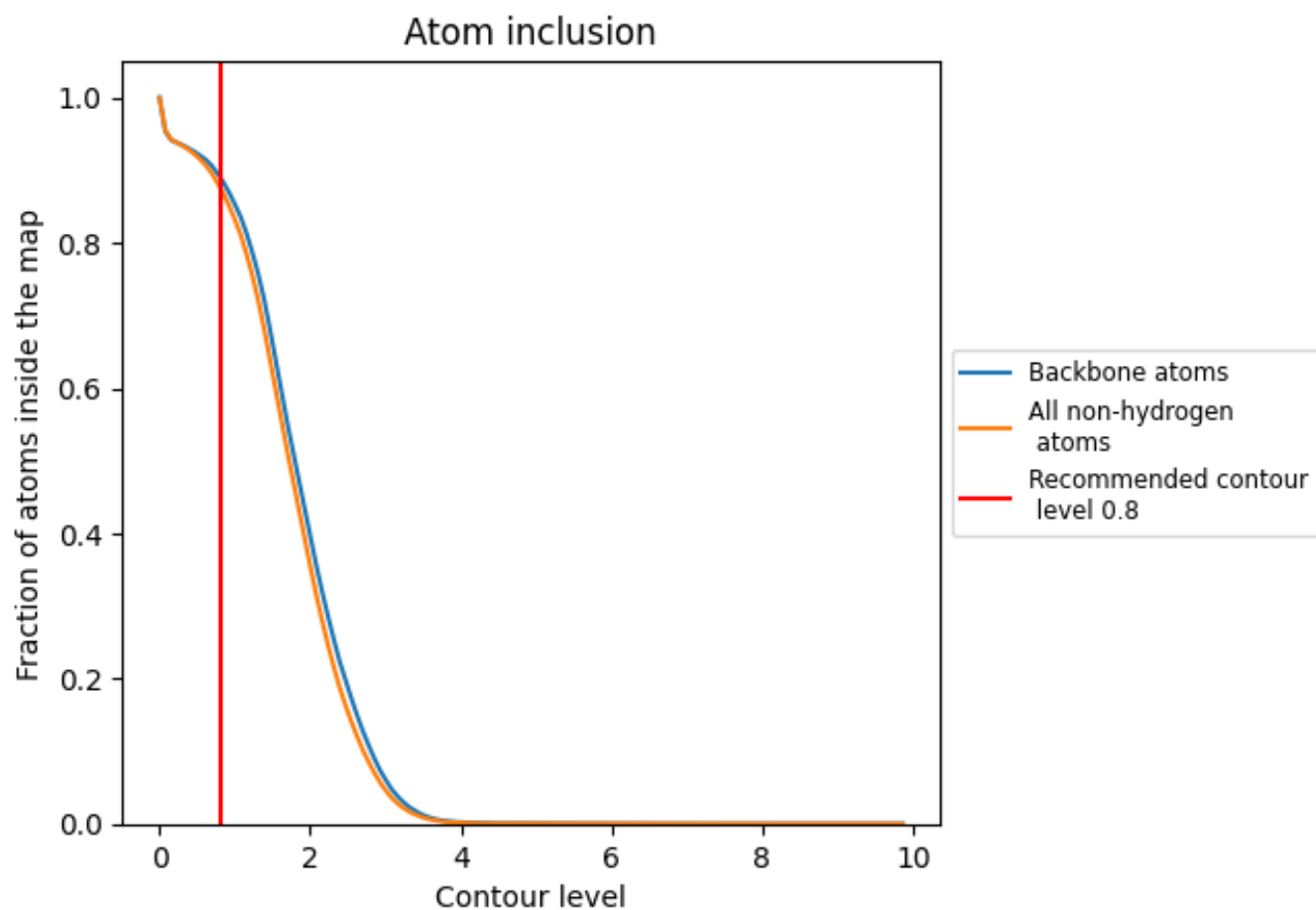
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [\(i\)](#)



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 (0.8).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8775	 0.0820
A	 0.8686	 0.0750
B	 0.8442	 0.0940
C	 0.8997	 0.0720
D	 0.9769	 0.0930
E	 0.9657	 0.0980
F	 0.9941	 0.1140
G	 0.9729	 0.1140
H	 0.9878	 0.1000
I	 0.9671	 0.1140
J	 0.9861	 0.0810
K	 0.9852	 0.0970
L	 0.9871	 0.1020
M	 0.9724	 0.0830
N	 0.9113	 0.0660
O	 0.9666	 0.0780
P	 0.9760	 0.1150
Q	 0.0000	 -0.0550

