Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:40 AM UTC

PDB ID	:	7JZ2 / pdb_00007jz2
EMDB ID	:	EMD-22528
Title	:	Succinate: quinone oxidoreductase SQR from E.coli K12
Authors	:	Lyu, M.; Su, C.-C.; Morgan, C.E.; Bolla, J.R.; Robinson, C.V.; Yu, E.W.
Deposited on	:	2020-09-01
Resolution	:	2.50 Å(reported)

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

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

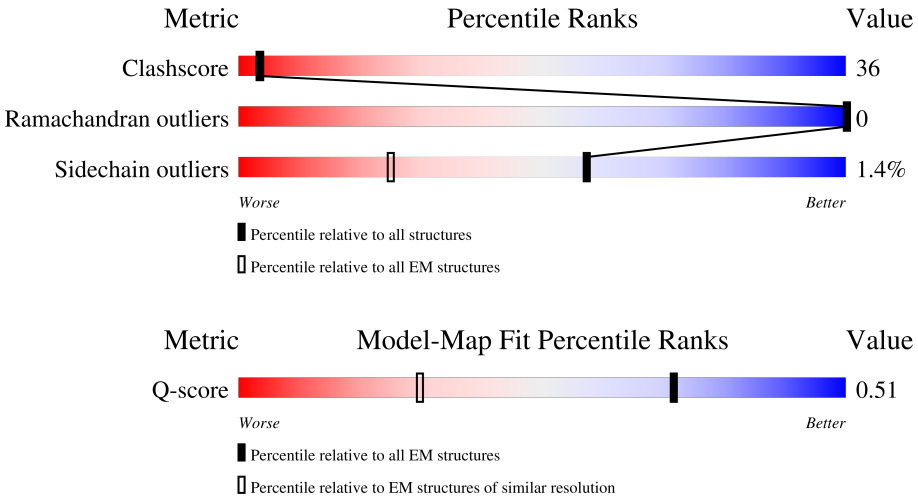
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	A	588	35% 47% 18%
1	E	588	34% 47% 18%
1	I	588	35% 46% 18%
2	B	238	50% 48%

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Mol	Chain	Length	Quality of chain
2	F	238	51% 47%
2	J	238	51% 48%
3	C	129	5% 44% 52%
3	G	129	5% 43% 53%
3	K	129	44% 52%
4	D	115	32% 63%
4	H	115	33% 63%
4	L	115	32% 63%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SF4	B	302	-	-	X	-
8	SF4	F	302	-	-	X	-
8	SF4	J	302	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 22866 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	481	Total 3707	C 2299	N 670	O 714	S 24	0	0
1	E	481	Total 3707	C 2299	N 670	O 714	S 24	0	0
1	I	481	Total 3707	C 2299	N 670	O 714	S 24	0	0

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	238	Total 1869	C 1172	N 329	O 348	S 20	0	0
2	F	238	Total 1869	C 1172	N 329	O 348	S 20	0	0
2	J	238	Total 1869	C 1172	N 329	O 348	S 20	0	0

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b556 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	125	Total 972	C 647	N 158	O 162	S 5	0	0
3	G	125	Total 972	C 647	N 158	O 162	S 5	0	0
3	K	125	Total 972	C 647	N 158	O 162	S 5	0	0

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	113	Total 898	C 615	N 136	O 144	S 3	0	0

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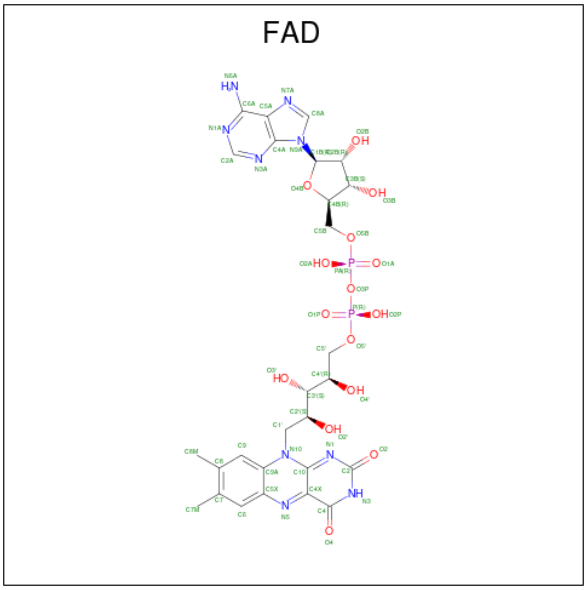
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	113	Total	C	N	O	S	0	0
			898	615	136	144	3		
4	L	113	Total	C	N	O	S	0	0
			898	615	136	144	3		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

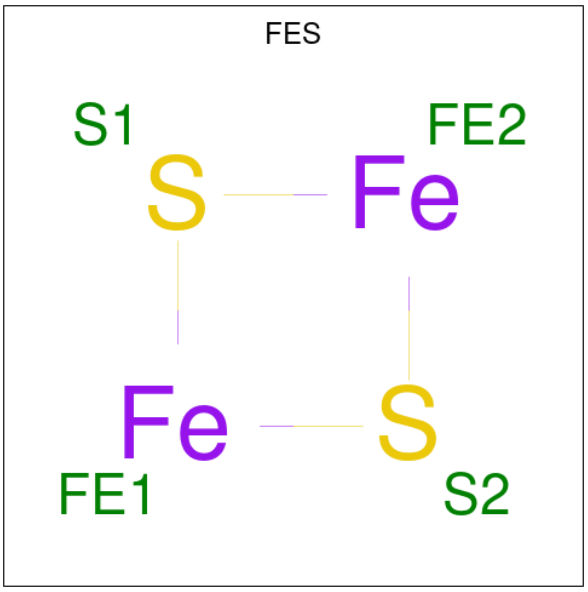


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
5	E	1	Total	C	N	O	P	0
			53	27	9	15	2	
5	I	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

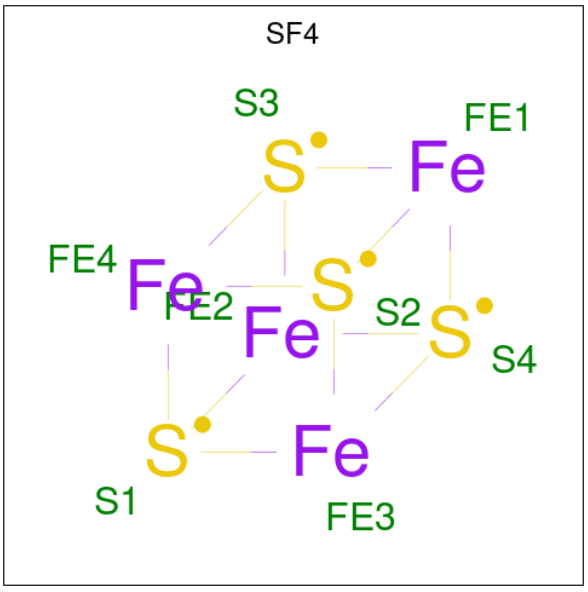
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Na	0
			1	1	
6	E	1	Total	Na	0
			1	1	
6	I	1	Total	Na	0
			1	1	

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	Fe	S	0
			4	2	2	
7	F	1	Total	Fe	S	0
			4	2	2	
7	J	1	Total	Fe	S	0
			4	2	2	

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	Fe	S	0
			8	4	4	

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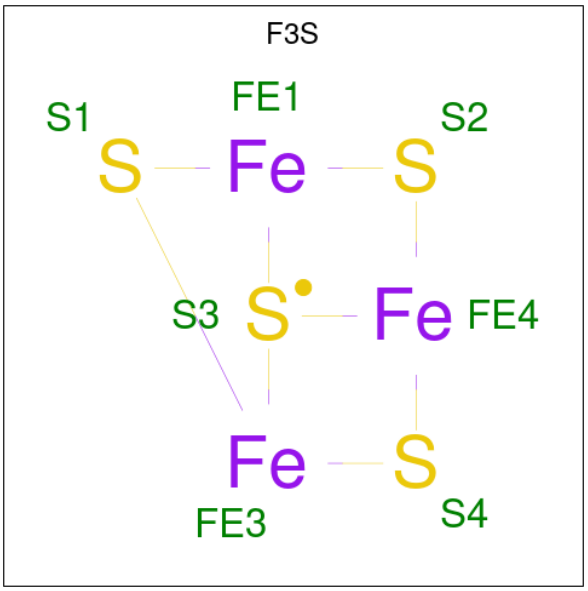
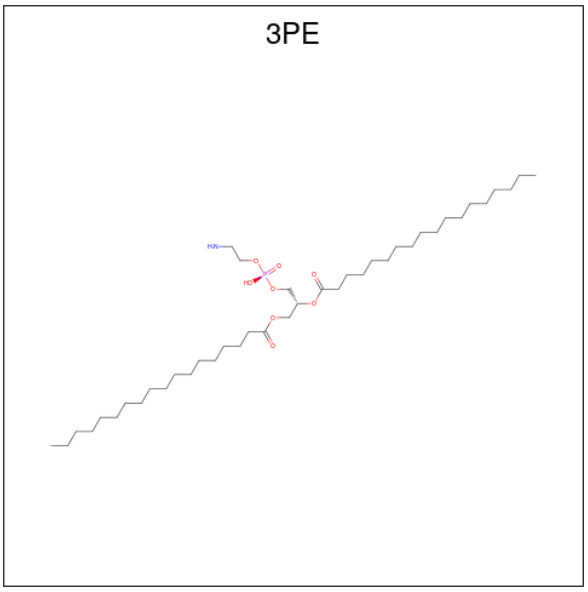
Mol	Chain	Residues	Atoms	AltConf
8	F	1	Total Fe S 8 4 4	0
8	J	1	Total Fe S 8 4 4	0

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



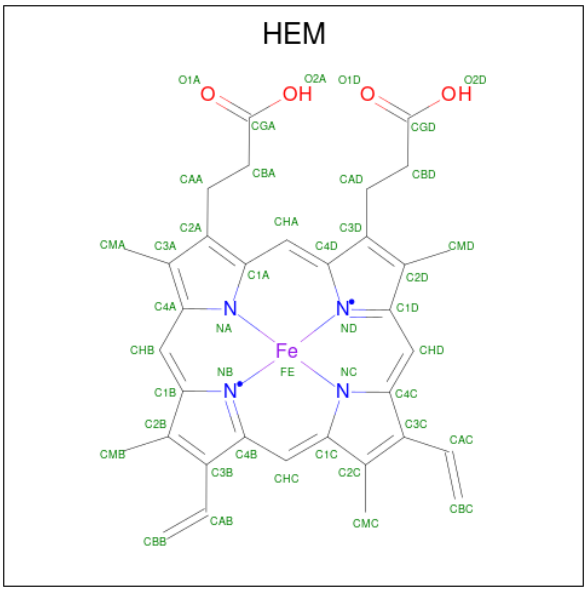
Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total Fe S 7 3 4	0
9	F	1	Total Fe S 7 3 4	0
9	J	1	Total Fe S 7 3 4	0

- Molecule 10 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



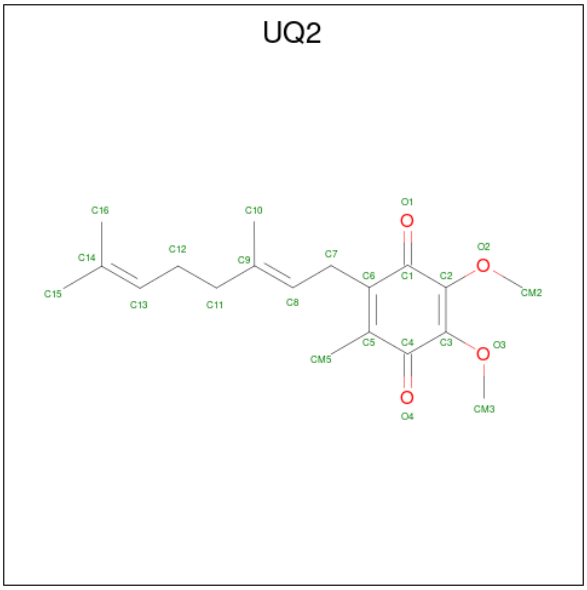
Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
10	G	1	Total	C	N	O	P	0
			37	27	1	8	1	
10	K	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



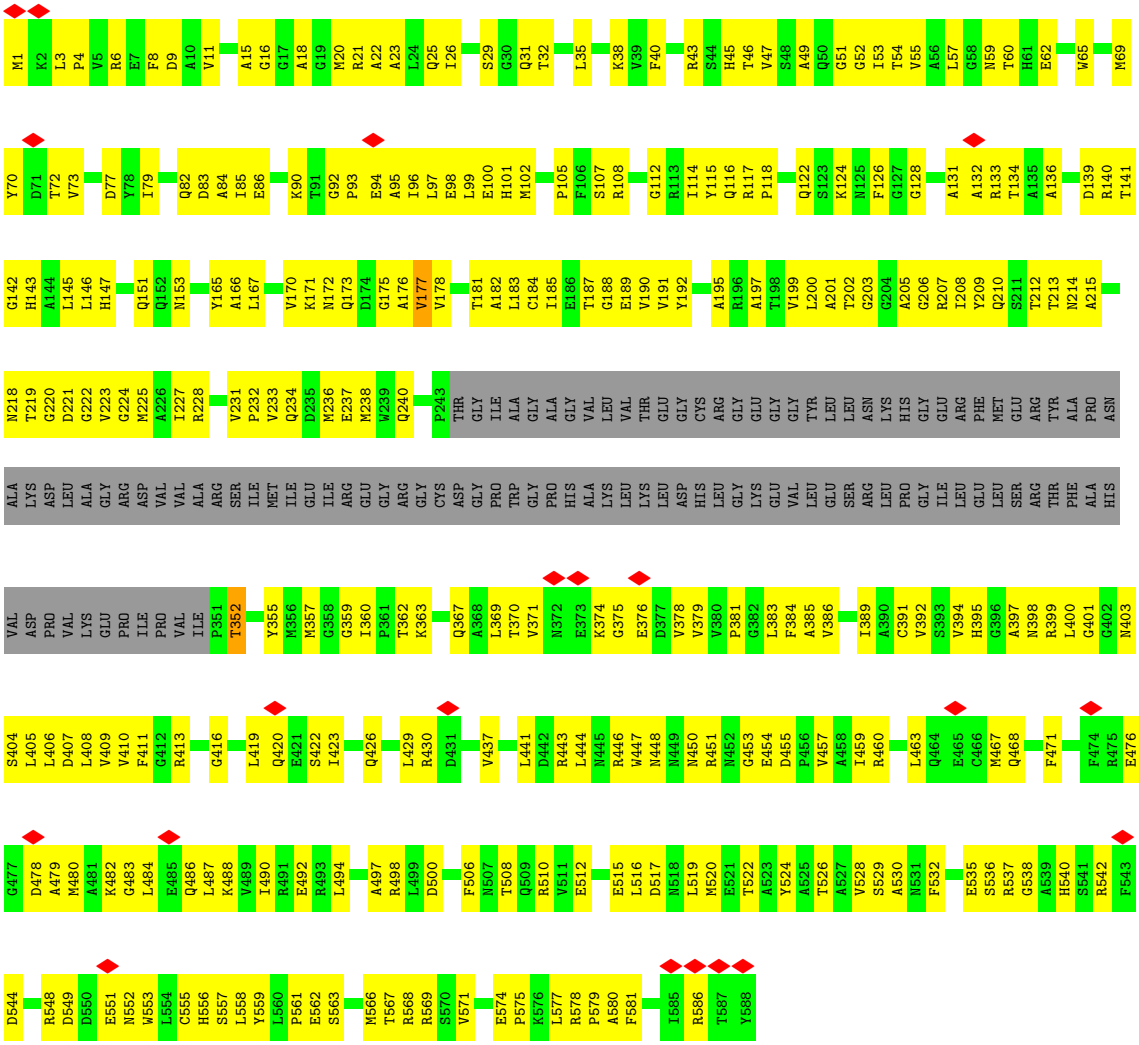
Mol	Chain	Residues	Atoms			AltConf
12	D	1	Total	C	O	0
			23	19	4	
12	H	1	Total	C	O	0
			23	19	4	
12	L	1	Total	C	O	0
			23	19	4	

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.

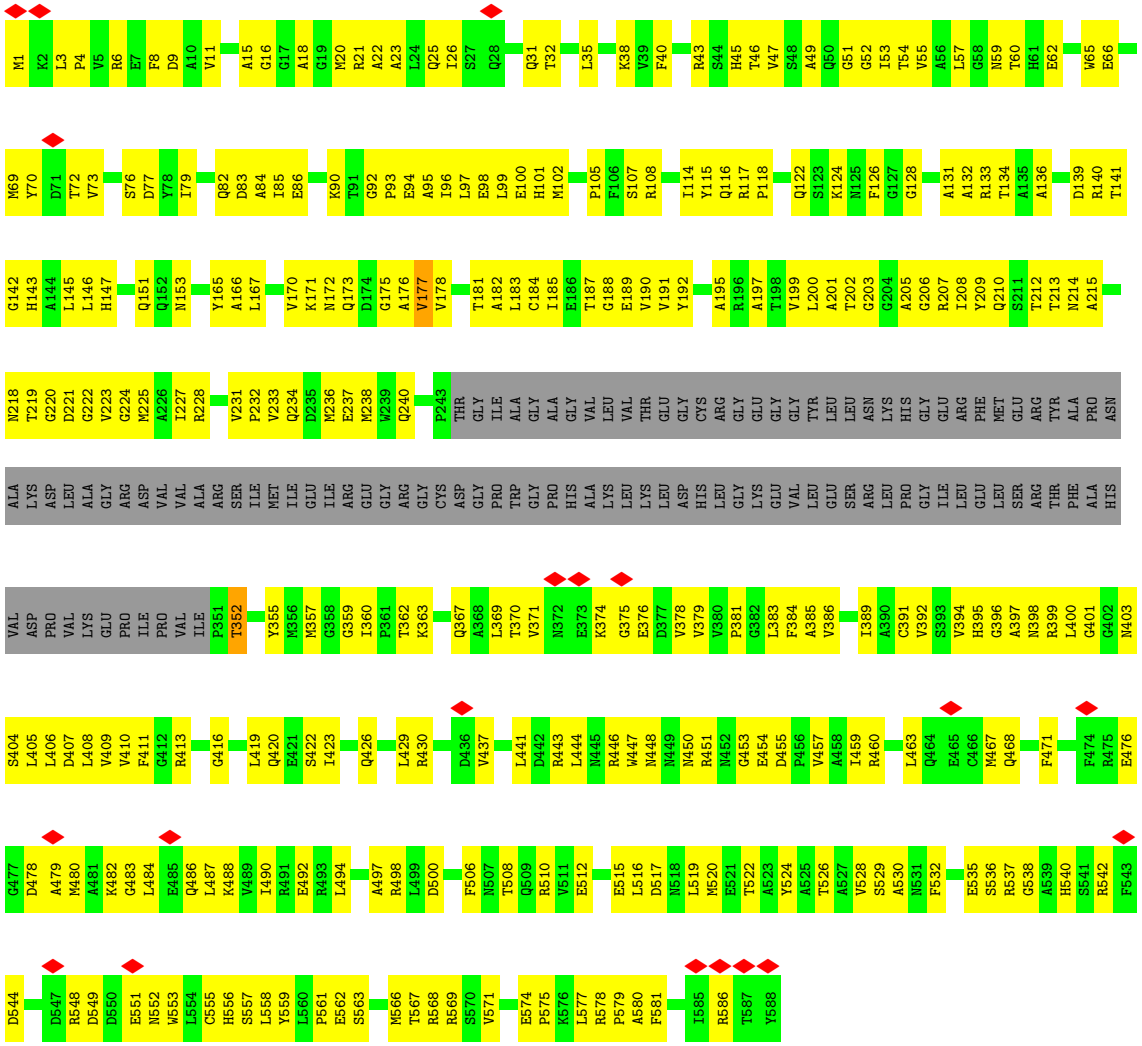
• Molecule 1: Succinate dehydrogenase flavoprotein subunit

Chain A:



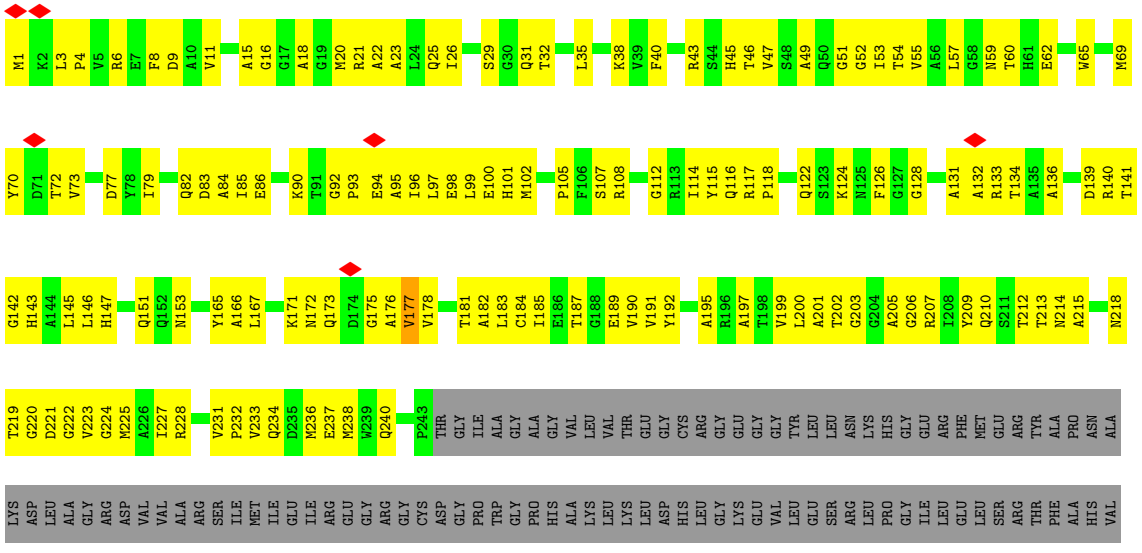
• Molecule 1: Succinate dehydrogenase flavoprotein subunit

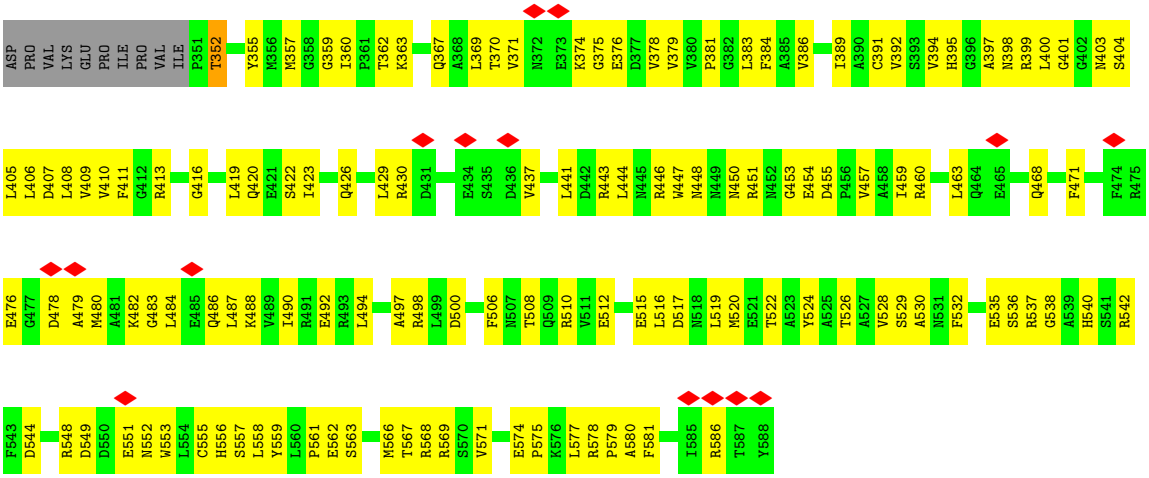
Chain E:



• Molecule 1: Succinate dehydrogenase flavoprotein subunit

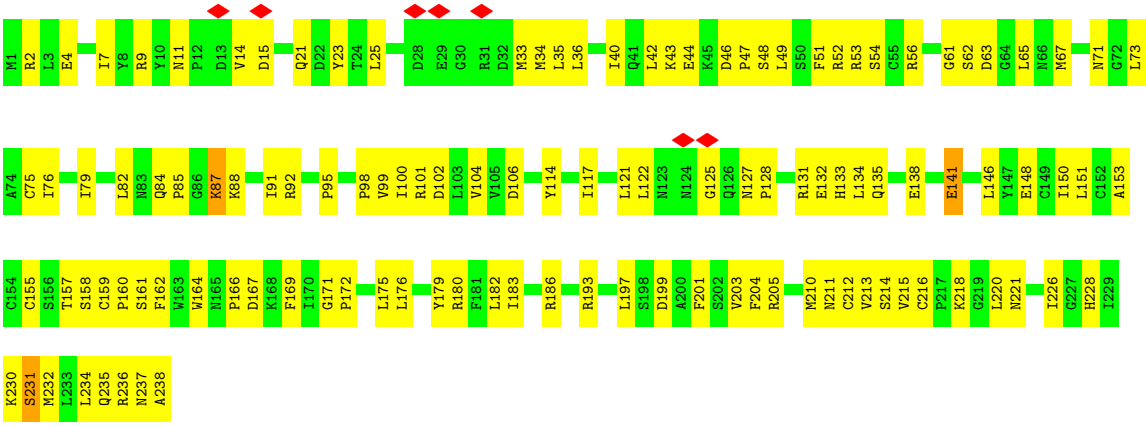
Chain I:





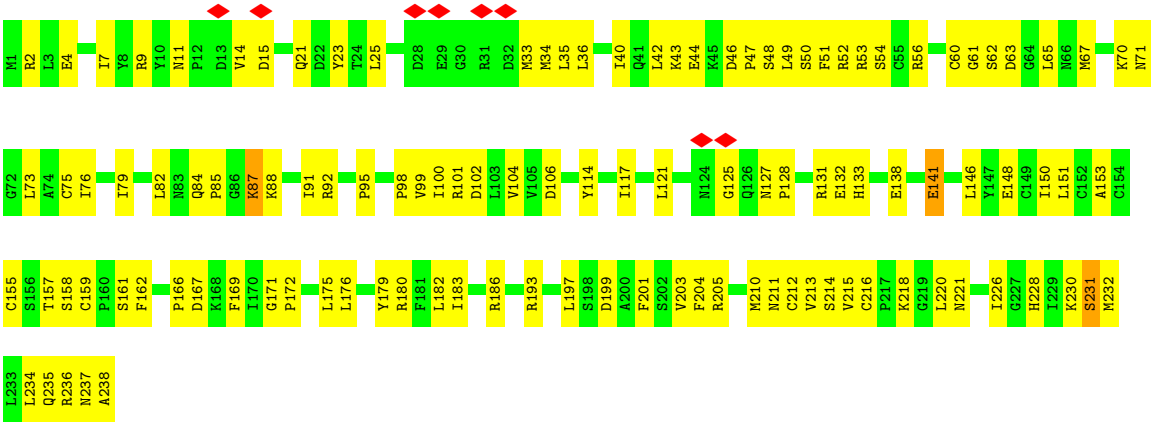
• Molecule 2: Succinate dehydrogenase iron-sulfur subunit

Chain B:

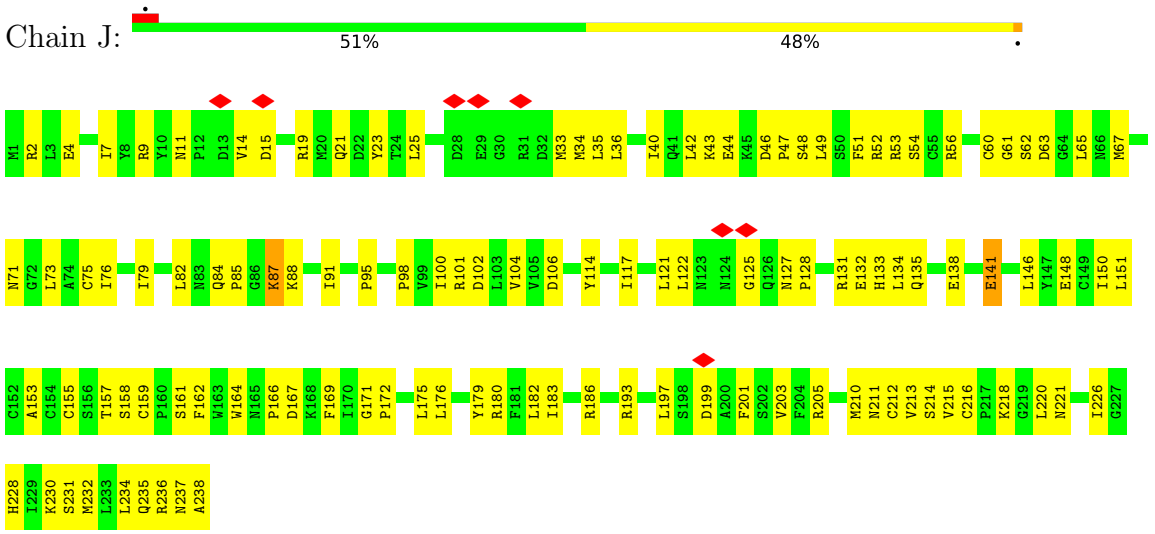


• Molecule 2: Succinate dehydrogenase iron-sulfur subunit

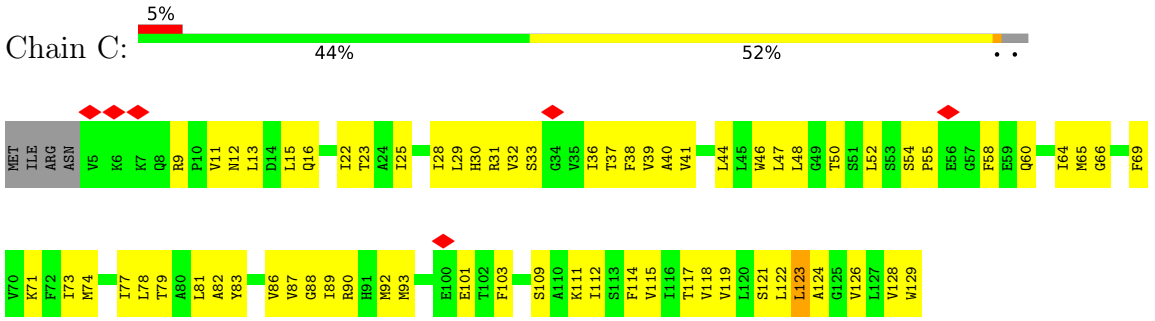
Chain F:



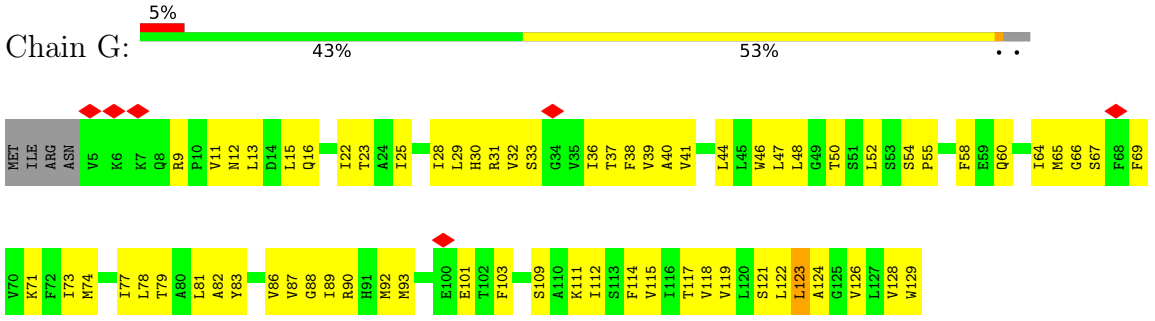
• Molecule 2: Succinate dehydrogenase iron-sulfur subunit



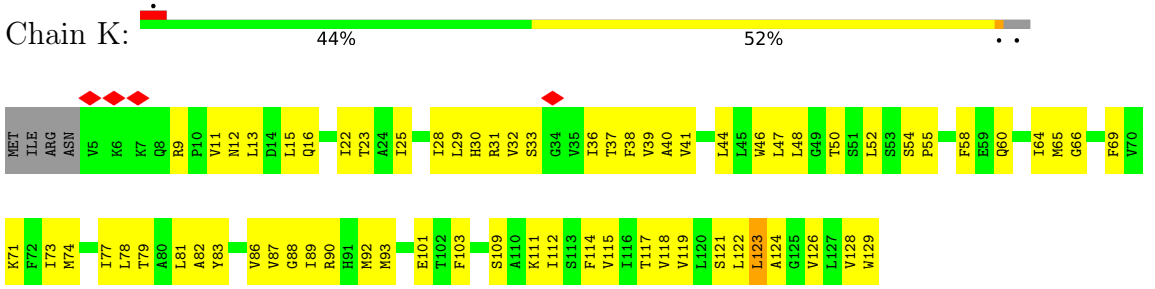
• Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



• Molecule 3: Succinate dehydrogenase cytochrome b556 subunit

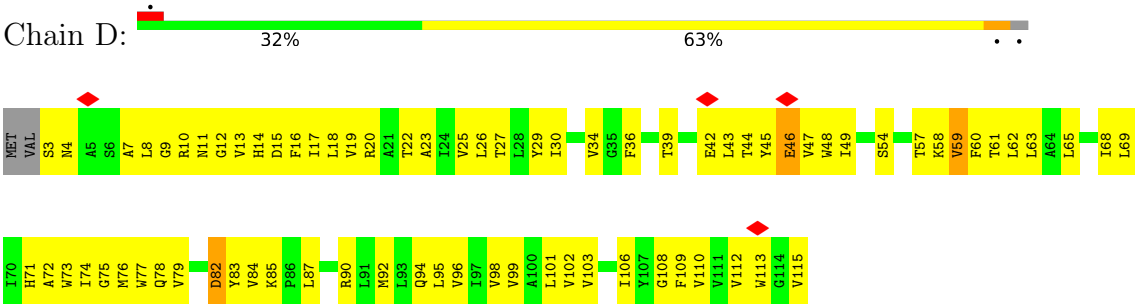


• Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



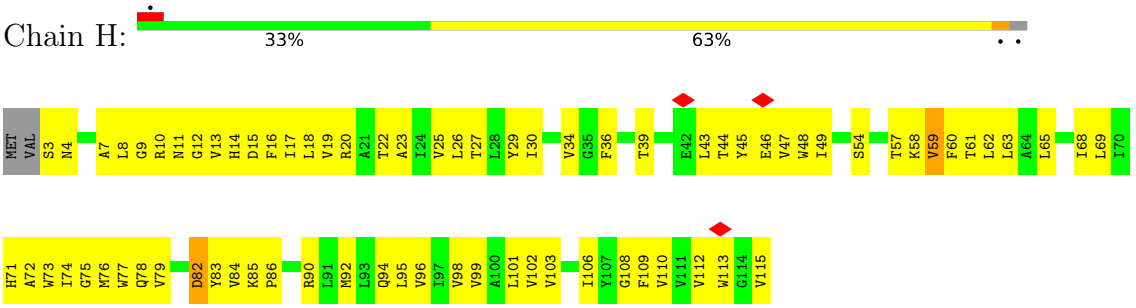
• Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor subunit

Chain D:



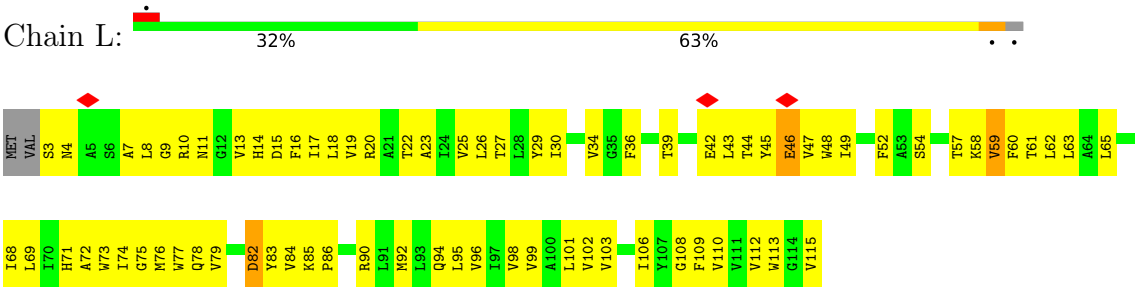
• Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor subunit

Chain H:



• Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor subunit

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.666	Depositor
Minimum map value	-1.544	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.172	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	151.20001, 151.20001, 147.96	wwPDB
Map dimensions	137, 140, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, FAD, 3PE, SF4, HEM, NA, UQ2, FES

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	0.10	0/3778	0.30	0/5110
1	E	0.10	0/3778	0.30	0/5110
1	I	0.10	0/3778	0.30	0/5110
2	B	0.10	0/1908	0.31	0/2578
2	F	0.10	0/1908	0.31	0/2578
2	J	0.10	0/1908	0.31	0/2578
3	C	0.10	0/994	0.24	0/1348
3	G	0.11	0/994	0.24	0/1348
3	K	0.11	0/994	0.24	0/1348
4	D	0.11	0/923	0.26	0/1262
4	H	0.11	0/923	0.26	0/1262
4	L	0.11	0/923	0.26	0/1262
All	All	0.10	0/22809	0.29	0/30894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3707	0	3597	307	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3707	0	3597	309	0
1	I	3707	0	3597	306	0
2	B	1869	0	1859	119	0
2	F	1869	0	1859	120	0
2	J	1869	0	1859	117	0
3	C	972	0	1024	65	0
3	G	972	0	1024	66	0
3	K	972	0	1024	63	0
4	D	898	0	936	82	0
4	H	898	0	936	81	0
4	L	898	0	936	78	0
5	A	53	0	29	5	0
5	E	53	0	29	7	0
5	I	53	0	29	6	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
6	I	1	0	0	0	0
7	B	4	0	0	1	0
7	F	4	0	0	1	0
7	J	4	0	0	1	0
8	B	8	0	0	3	0
8	F	8	0	0	3	0
8	J	8	0	0	3	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
9	J	7	0	0	0	0
10	C	37	0	48	4	0
10	G	37	0	48	4	0
10	K	37	0	48	4	0
11	D	43	0	30	11	0
11	G	43	0	30	9	0
11	K	43	0	30	10	0
12	D	23	0	26	4	0
12	H	23	0	26	2	0
12	L	23	0	26	3	0
All	All	22866	0	22647	1617	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 36.

All (1617) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:VAL:HG21	1:E:383:LEU:HB2	1.50	0.93
1:I:177:VAL:HG21	1:I:383:LEU:HB2	1.50	0.93
1:A:177:VAL:HG21	1:A:383:LEU:HB2	1.50	0.92
11:D:201:HEM:HBB2	11:D:201:HEM:HHC	1.53	0.91
11:D:201:HEM:HHD	11:D:201:HEM:HBC2	1.55	0.89
11:G:201:HEM:HHC	11:G:201:HEM:HBB2	1.53	0.88
11:K:201:HEM:HBB2	11:K:201:HEM:HHC	1.53	0.88
1:A:46:THR:HG23	1:A:146:LEU:HD22	1.56	0.88
11:G:201:HEM:HHD	11:G:201:HEM:HBC2	1.55	0.88
1:I:46:THR:HG23	1:I:146:LEU:HD22	1.56	0.87
1:A:114:ILE:HG13	2:B:132:GLU:HG3	1.56	0.87
11:K:201:HEM:HBC2	11:K:201:HEM:HHD	1.55	0.87
1:E:46:THR:HG23	1:E:146:LEU:HD22	1.56	0.86
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.58	0.85
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.58	0.85
1:I:49:ALA:HB3	1:I:142:GLY:HA3	1.58	0.85
1:A:236:MET:HE2	1:A:236:MET:HA	1.60	0.84
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.59	0.84
3:G:37:THR:O	3:G:41:VAL:HG23	1.77	0.84
3:C:37:THR:O	3:C:41:VAL:HG23	1.77	0.83
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.59	0.83
2:J:205:ARG:NH1	4:L:82:ASP:OD1	2.11	0.83
3:K:37:THR:O	3:K:41:VAL:HG23	1.78	0.83
1:I:94:GLU:OE1	1:I:413:ARG:NH1	2.12	0.83
1:A:52:GLY:HA3	1:A:136:ALA:HB2	1.61	0.83
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.59	0.82
2:F:146:LEU:HB3	2:F:180:ARG:HB2	1.61	0.82
1:E:94:GLU:OE1	1:E:413:ARG:NH1	2.12	0.82
4:L:23:ALA:O	4:L:27:THR:HG23	1.80	0.82
1:A:94:GLU:OE1	1:A:413:ARG:NH1	2.12	0.82
1:E:236:MET:HA	1:E:236:MET:HE2	1.59	0.81
2:B:146:LEU:HB3	2:B:180:ARG:HB2	1.61	0.81
1:E:52:GLY:HA3	1:E:136:ALA:HB2	1.61	0.81
3:K:81:LEU:HD21	4:L:30:ILE:HD13	1.61	0.81
4:D:23:ALA:O	4:D:27:THR:HG23	1.80	0.81
2:J:146:LEU:HB3	2:J:180:ARG:HB2	1.61	0.81
1:I:236:MET:HE2	1:I:236:MET:HA	1.60	0.81
1:A:124:LYS:O	1:A:128:GLY:N	2.14	0.81
1:I:97:LEU:HD21	2:J:131:ARG:HE	1.44	0.81
4:H:23:ALA:O	4:H:27:THR:HG23	1.80	0.80
1:I:52:GLY:HA3	1:I:136:ALA:HB2	1.61	0.80
1:A:79:ILE:O	1:A:556:HIS:NE2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:490:ILE:HG13	1:I:520:MET:HE1	1.64	0.80
1:E:79:ILE:O	1:E:556:HIS:NE2	2.14	0.80
3:C:81:LEU:HD21	4:D:30:ILE:HD13	1.63	0.80
1:I:124:LYS:O	1:I:128:GLY:N	2.14	0.79
2:F:205:ARG:NH1	4:H:82:ASP:OD1	2.15	0.79
1:E:490:ILE:HG13	1:E:520:MET:HE1	1.64	0.79
1:I:532:PHE:HB2	1:I:566:MET:HG3	1.65	0.79
2:F:62:SER:N	7:F:301:FES:S1	2.54	0.79
1:I:79:ILE:O	1:I:556:HIS:NE2	2.14	0.79
1:A:490:ILE:HG13	1:A:520:MET:HE1	1.64	0.79
1:A:532:PHE:HB2	1:A:566:MET:HG3	1.65	0.78
3:C:82:ALA:O	3:C:86:VAL:HG23	1.84	0.78
1:E:532:PHE:HB2	1:E:566:MET:HG3	1.65	0.78
3:K:46:TRP:O	3:K:50:THR:HG23	1.83	0.78
3:G:46:TRP:O	3:G:50:THR:HG23	1.84	0.78
2:J:213:VAL:HG22	2:J:221:ASN:HA	1.66	0.78
1:E:124:LYS:O	1:E:128:GLY:N	2.14	0.78
2:J:100:ILE:HD11	2:J:106:ASP:HA	1.66	0.78
3:K:82:ALA:O	3:K:86:VAL:HG23	1.84	0.78
4:L:4:ASN:HD22	4:L:77:TRP:HZ2	1.32	0.77
1:A:108:ARG:NH1	2:B:133:HIS:O	2.17	0.77
1:I:367:GLN:HB3	1:I:379:VAL:HG13	1.67	0.77
4:D:4:ASN:HD22	4:D:77:TRP:HZ2	1.32	0.77
1:A:367:GLN:HB3	1:A:379:VAL:HG13	1.67	0.77
2:F:213:VAL:HG22	2:F:221:ASN:HA	1.66	0.77
1:I:455:ASP:OD1	1:I:457:VAL:HG22	1.85	0.77
3:C:46:TRP:O	3:C:50:THR:HG23	1.83	0.77
2:B:213:VAL:HG22	2:B:221:ASN:HA	1.66	0.77
1:E:558:LEU:HB3	1:E:567:THR:HG23	1.67	0.77
1:A:455:ASP:OD1	1:A:457:VAL:HG22	1.85	0.76
4:H:29:TYR:HA	4:H:60:PHE:CE2	2.20	0.76
1:E:455:ASP:OD1	1:E:457:VAL:HG22	1.85	0.76
2:B:100:ILE:HD11	2:B:106:ASP:HA	1.66	0.76
4:D:29:TYR:HA	4:D:60:PHE:CE2	2.21	0.76
3:G:82:ALA:O	3:G:86:VAL:HG23	1.84	0.76
2:F:100:ILE:HD11	2:F:106:ASP:HA	1.66	0.76
1:I:558:LEU:HB3	1:I:567:THR:HG23	1.67	0.76
1:E:97:LEU:HD21	2:F:131:ARG:HE	1.50	0.75
4:H:4:ASN:HD22	4:H:77:TRP:HZ2	1.32	0.75
1:E:367:GLN:HB3	1:E:379:VAL:HG13	1.67	0.75
4:L:29:TYR:HA	4:L:60:PHE:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:SER:N	7:B:301:FES:S1	2.54	0.75
3:C:60:GLN:O	3:C:64:ILE:HG12	1.86	0.75
3:K:60:GLN:O	3:K:64:ILE:HG12	1.86	0.75
1:I:114:ILE:HG13	2:J:132:GLU:HG3	1.67	0.75
1:A:107:SER:HB2	1:A:115:TYR:HB3	1.69	0.75
1:E:578:ARG:HG2	1:E:579:PRO:HD2	1.68	0.75
3:G:60:GLN:O	3:G:64:ILE:HG12	1.86	0.75
1:A:578:ARG:HG2	1:A:579:PRO:HD2	1.68	0.74
1:A:219:THR:HG21	1:A:515:GLU:HB3	1.68	0.74
1:I:219:THR:HG21	1:I:515:GLU:HB3	1.68	0.74
1:E:107:SER:HB2	1:E:115:TYR:HB3	1.69	0.74
1:A:535:GLU:HG2	1:A:536:SER:H	1.52	0.74
1:E:404:SER:O	1:E:408:LEU:HG	1.88	0.74
1:A:558:LEU:HB3	1:A:567:THR:HG23	1.67	0.74
1:E:21:ARG:NH2	1:E:98:GLU:OE2	2.18	0.74
2:B:205:ARG:NH1	4:D:82:ASP:OD1	2.20	0.74
1:E:219:THR:HG21	1:E:515:GLU:HB3	1.68	0.74
3:G:81:LEU:HD21	4:H:30:ILE:HD13	1.69	0.73
1:I:107:SER:HB2	1:I:115:TYR:HB3	1.69	0.73
2:J:62:SER:N	7:J:301:FES:S1	2.54	0.73
1:I:404:SER:O	1:I:408:LEU:HG	1.88	0.73
1:A:3:LEU:HD22	1:A:441:LEU:HD11	1.70	0.73
1:E:99:LEU:HD21	1:E:145:LEU:HD13	1.71	0.73
1:I:535:GLU:HG2	1:I:536:SER:H	1.52	0.73
1:A:237:GLU:HB3	1:A:529:SER:HB3	1.71	0.73
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.71	0.73
1:A:21:ARG:NH2	1:A:98:GLU:OE2	2.18	0.73
1:E:3:LEU:HD22	1:E:441:LEU:HD11	1.70	0.73
1:E:97:LEU:O	1:E:101:HIS:ND1	2.21	0.73
1:I:237:GLU:HB3	1:I:529:SER:HB3	1.71	0.73
1:A:99:LEU:HD21	1:A:145:LEU:HD13	1.71	0.73
4:D:27:THR:CG2	11:D:201:HEM:HAC	2.19	0.73
1:I:578:ARG:HG2	1:I:579:PRO:HD2	1.68	0.73
1:A:363:LYS:HG3	1:A:369:LEU:HD21	1.71	0.72
1:A:219:THR:HA	1:A:519:LEU:HD21	1.70	0.72
1:A:404:SER:O	1:A:408:LEU:HG	1.88	0.72
1:E:535:GLU:HG2	1:E:536:SER:H	1.52	0.72
1:I:99:LEU:HD21	1:I:145:LEU:HD13	1.71	0.72
3:K:28:ILE:O	3:K:32:VAL:HG23	1.90	0.72
1:I:97:LEU:O	1:I:101:HIS:ND1	2.21	0.72
1:E:219:THR:HA	1:E:519:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:ASP:OD1	2:F:48:SER:OG	2.07	0.72
1:I:219:THR:HA	1:I:519:LEU:HD21	1.70	0.72
2:B:9:ARG:NE	2:B:102:ASP:OD2	2.23	0.71
2:B:234:LEU:HD23	4:D:13:VAL:HG13	1.70	0.71
1:E:363:LYS:HG3	1:E:369:LEU:HD21	1.71	0.71
3:G:28:ILE:O	3:G:32:VAL:HG23	1.90	0.71
1:I:3:LEU:HD22	1:I:441:LEU:HD11	1.70	0.71
1:A:97:LEU:O	1:A:101:HIS:ND1	2.21	0.71
1:E:494:LEU:HD21	1:E:517:ASP:OD1	1.90	0.71
3:C:28:ILE:O	3:C:32:VAL:HG23	1.90	0.71
2:F:121:LEU:HD11	2:F:186:ARG:HB3	1.73	0.71
2:F:9:ARG:NE	2:F:102:ASP:OD2	2.23	0.71
1:I:136:ALA:HB1	1:I:141:THR:OG1	1.91	0.71
1:I:363:LYS:HG3	1:I:369:LEU:HD21	1.71	0.71
2:B:121:LEU:HD11	2:B:186:ARG:HB3	1.73	0.71
2:J:121:LEU:HD11	2:J:186:ARG:HB3	1.73	0.71
1:A:136:ALA:HB1	1:A:141:THR:OG1	1.91	0.71
1:E:237:GLU:HB3	1:E:529:SER:HB3	1.71	0.71
3:G:52:LEU:HD22	4:H:115:VAL:HG21	1.72	0.71
2:J:101:ARG:HB3	2:J:104:VAL:HG22	1.73	0.71
2:J:9:ARG:NE	2:J:102:ASP:OD2	2.23	0.71
11:G:201:HEM:HAC	4:H:27:THR:CG2	2.21	0.70
1:I:494:LEU:HD21	1:I:517:ASP:OD1	1.90	0.70
2:J:9:ARG:NH1	2:J:23:TYR:OH	2.25	0.70
2:J:46:ASP:OD1	2:J:48:SER:OG	2.07	0.70
1:A:494:LEU:HD21	1:A:517:ASP:OD1	1.90	0.70
1:A:77:ASP:OD2	1:A:586:ARG:NH1	2.24	0.70
2:F:9:ARG:NH1	2:F:23:TYR:OH	2.25	0.70
1:E:118:PRO:HG3	1:E:132:ALA:HB2	1.73	0.70
2:F:101:ARG:HG3	2:F:102:ASP:H	1.57	0.70
1:E:136:ALA:HB1	1:E:141:THR:OG1	1.91	0.70
2:J:148:GLU:N	2:J:148:GLU:OE2	2.24	0.70
2:B:101:ARG:HB3	2:B:104:VAL:HG22	1.73	0.70
3:K:83:TYR:HB2	3:K:117:THR:HG21	1.74	0.70
2:F:148:GLU:N	2:F:148:GLU:OE2	2.24	0.70
11:K:201:HEM:HAC	4:L:27:THR:CG2	2.21	0.70
1:A:118:PRO:HG3	1:A:132:ALA:HB2	1.73	0.69
3:C:83:TYR:HB2	3:C:117:THR:HG21	1.74	0.69
1:I:21:ARG:NH2	1:I:98:GLU:OE2	2.18	0.69
2:B:101:ARG:HG3	2:B:102:ASP:H	1.57	0.69
1:E:92:GLY:O	1:E:96:ILE:HG12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:GLU:N	2:B:148:GLU:OE2	2.24	0.69
4:H:110:VAL:HA	4:H:113:TRP:NE1	2.08	0.69
1:I:55:VAL:HG13	1:I:57:LEU:HG	1.74	0.69
2:B:9:ARG:NH1	2:B:23:TYR:OH	2.24	0.69
4:D:110:VAL:HA	4:D:113:TRP:NE1	2.08	0.69
1:I:118:PRO:HG3	1:I:132:ALA:HB2	1.73	0.69
2:F:101:ARG:HB3	2:F:104:VAL:HG22	1.73	0.69
1:E:77:ASP:OD2	1:E:586:ARG:NH1	2.24	0.69
1:I:92:GLY:O	1:I:96:ILE:HG12	1.92	0.69
1:I:187:THR:CG2	1:I:189:GLU:HG2	2.23	0.69
3:G:83:TYR:HB2	3:G:117:THR:HG21	1.74	0.69
1:A:92:GLY:O	1:A:96:ILE:HG12	1.92	0.69
1:I:538:GLY:HA2	1:I:586:ARG:HH22	1.57	0.69
1:I:555:CYS:HB2	1:I:569:ARG:O	1.93	0.69
1:A:187:THR:CG2	1:A:189:GLU:HG2	2.23	0.69
1:E:555:CYS:HB2	1:E:569:ARG:O	1.93	0.69
1:A:538:GLY:HA2	1:A:586:ARG:HH22	1.57	0.69
1:E:55:VAL:HG13	1:E:57:LEU:HG	1.74	0.69
1:E:488:LYS:O	1:E:492:GLU:HG2	1.93	0.69
1:I:77:ASP:OD2	1:I:586:ARG:NH1	2.24	0.69
2:J:101:ARG:HG3	2:J:102:ASP:H	1.57	0.69
3:C:28:ILE:HG23	3:C:29:LEU:HD22	1.76	0.68
4:L:110:VAL:HA	4:L:113:TRP:NE1	2.07	0.68
1:E:122:GLN:HB3	1:E:131:ALA:HB3	1.76	0.68
1:I:15:ALA:O	1:I:20:MET:HE3	1.94	0.68
2:B:25:LEU:HB2	2:B:42:LEU:HD21	1.75	0.68
1:A:488:LYS:O	1:A:492:GLU:HG2	1.93	0.68
4:H:84:VAL:O	4:H:90:ARG:NH2	2.27	0.68
2:B:211:ASN:O	2:B:215:VAL:HG22	1.94	0.68
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.74	0.68
1:A:15:ALA:O	1:A:20:MET:HE3	1.94	0.68
1:A:555:CYS:HB2	1:A:569:ARG:O	1.93	0.68
1:E:187:THR:CG2	1:E:189:GLU:HG2	2.22	0.68
1:E:15:ALA:O	1:E:20:MET:HE3	1.93	0.68
1:E:506:PHE:CZ	2:F:104:VAL:HG11	2.28	0.68
1:A:122:GLN:HB3	1:A:131:ALA:HB3	1.76	0.67
3:C:52:LEU:HD22	4:D:115:VAL:HG21	1.74	0.67
3:K:28:ILE:HG23	3:K:29:LEU:HD22	1.76	0.67
1:A:97:LEU:HD21	2:B:131:ARG:HE	1.59	0.67
1:A:444:LEU:HD11	1:A:510:ARG:HD3	1.77	0.67
1:E:16:GLY:O	1:E:20:MET:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:GLY:HA2	1:E:586:ARG:HH22	1.57	0.67
1:I:16:GLY:O	1:I:20:MET:HG2	1.94	0.67
1:I:444:LEU:HD11	1:I:510:ARG:HD3	1.77	0.67
1:I:488:LYS:O	1:I:492:GLU:HG2	1.93	0.67
1:I:18:ALA:HB2	1:I:408:LEU:HB3	1.77	0.67
1:A:484:LEU:O	1:A:488:LYS:HG2	1.94	0.67
2:B:46:ASP:OD1	2:B:48:SER:OG	2.07	0.67
1:E:231:VAL:HG21	1:E:383:LEU:CD2	2.25	0.67
1:E:476:GLU:HB2	1:E:479:ALA:HB3	1.76	0.67
1:E:575:PRO:HD2	1:E:580:ALA:HB2	1.76	0.67
2:F:4:GLU:OE1	2:F:88:LYS:NZ	2.28	0.67
1:A:16:GLY:O	1:A:20:MET:HG2	1.94	0.67
2:F:25:LEU:HB2	2:F:42:LEU:HD21	1.75	0.67
3:G:28:ILE:HG23	3:G:29:LEU:HD22	1.76	0.67
1:A:18:ALA:HB2	1:A:408:LEU:HB3	1.77	0.67
2:F:211:ASN:O	2:F:215:VAL:HG22	1.94	0.67
1:I:575:PRO:HD2	1:I:580:ALA:HB2	1.76	0.67
2:J:25:LEU:HB2	2:J:42:LEU:HD21	1.75	0.67
1:A:231:VAL:HG21	1:A:383:LEU:CD2	2.25	0.67
1:E:215:ALA:HB1	2:F:54:SER:O	1.94	0.67
1:E:484:LEU:O	1:E:488:LYS:HG2	1.94	0.67
2:F:11:ASN:O	2:F:15:ASP:HB2	1.95	0.67
1:I:484:LEU:O	1:I:488:LYS:HG2	1.94	0.67
4:L:84:VAL:O	4:L:90:ARG:NH2	2.27	0.67
1:A:23:ALA:CB	1:A:35:LEU:HD12	2.25	0.67
2:B:141:GLU:HA	2:B:141:GLU:OE2	1.95	0.67
1:E:23:ALA:CB	1:E:35:LEU:HD12	2.25	0.67
2:J:11:ASN:O	2:J:15:ASP:HB2	1.95	0.67
2:J:211:ASN:O	2:J:215:VAL:HG22	1.94	0.67
4:H:10:ARG:HH21	4:L:3:SER:HB3	1.60	0.66
1:I:231:VAL:HG21	1:I:383:LEU:CD2	2.25	0.66
1:E:18:ALA:HB2	1:E:408:LEU:HB3	1.77	0.66
2:B:4:GLU:OE1	2:B:88:LYS:NZ	2.28	0.66
4:D:10:ARG:HH21	4:H:3:SER:HB3	1.59	0.66
1:A:476:GLU:HB2	1:A:479:ALA:HB3	1.76	0.66
1:I:60:THR:OG1	1:I:116:GLN:HB2	1.96	0.66
1:I:444:LEU:CD1	1:I:510:ARG:HD3	2.26	0.66
1:A:190:VAL:HG11	1:A:441:LEU:HD21	1.78	0.66
1:A:444:LEU:CD1	1:A:510:ARG:HD3	2.26	0.66
1:A:575:PRO:HD2	1:A:580:ALA:HB2	1.76	0.66
1:I:23:ALA:CB	1:I:35:LEU:HD12	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:GLN:HB3	1:I:131:ALA:HB3	1.76	0.66
1:A:60:THR:OG1	1:A:116:GLN:HB2	1.96	0.66
1:E:444:LEU:CD1	1:E:510:ARG:HD3	2.26	0.66
1:I:476:GLU:HB2	1:I:479:ALA:HB3	1.76	0.66
1:A:454:GLU:O	1:A:498:ARG:HG2	1.95	0.66
2:J:4:GLU:OE1	2:J:88:LYS:NZ	2.28	0.66
1:E:190:VAL:HG11	1:E:441:LEU:HD21	1.78	0.66
1:I:108:ARG:NH1	2:J:133:HIS:O	2.28	0.66
2:J:141:GLU:HA	2:J:141:GLU:OE2	1.95	0.66
2:B:11:ASN:O	2:B:15:ASP:HB2	1.95	0.65
1:I:454:GLU:O	1:I:498:ARG:HG2	1.95	0.65
1:E:95:ALA:O	1:E:98:GLU:HG2	1.96	0.65
1:E:444:LEU:HD11	1:E:510:ARG:HD3	1.77	0.65
1:I:95:ALA:O	1:I:98:GLU:HG2	1.96	0.65
1:I:460:ARG:HB2	1:I:516:LEU:CD1	2.26	0.65
1:I:552:ASN:O	1:I:568:ARG:NH1	2.29	0.65
3:K:69:PHE:O	3:K:73:ILE:HD12	1.96	0.65
1:A:95:ALA:O	1:A:98:GLU:HG2	1.96	0.65
1:A:460:ARG:HB2	1:A:516:LEU:CD1	2.27	0.65
2:F:141:GLU:HA	2:F:141:GLU:OE2	1.95	0.65
1:E:552:ASN:O	1:E:568:ARG:NH1	2.29	0.65
3:C:69:PHE:O	3:C:73:ILE:HD12	1.96	0.65
4:D:84:VAL:O	4:D:90:ARG:NH2	2.27	0.65
2:F:175:LEU:CD1	2:F:226:ILE:HG12	2.27	0.65
4:D:110:VAL:HA	4:D:113:TRP:CE2	2.32	0.65
1:E:214:ASN:HB3	1:E:218:ASN:OD1	1.97	0.65
1:E:454:GLU:O	1:E:498:ARG:HG2	1.95	0.65
2:J:175:LEU:CD1	2:J:226:ILE:HG12	2.27	0.65
1:A:448:ASN:O	1:A:451:ARG:NH1	2.30	0.65
1:A:552:ASN:O	1:A:568:ARG:NH1	2.29	0.65
1:E:60:THR:OG1	1:E:116:GLN:HB2	1.96	0.65
1:E:478:ASP:O	1:E:482:LYS:HG2	1.97	0.65
1:I:82:GLN:HE22	1:I:581:PHE:H	1.45	0.65
1:I:190:VAL:HG11	1:I:441:LEU:HD21	1.78	0.65
1:I:453:GLY:CA	1:I:498:ARG:HB3	2.27	0.65
2:J:234:LEU:HD23	4:L:13:VAL:HG13	1.78	0.65
1:A:478:ASP:O	1:A:482:LYS:HG2	1.97	0.64
1:E:114:ILE:HG13	2:F:132:GLU:HG3	1.78	0.64
1:E:448:ASN:O	1:E:451:ARG:NH1	2.30	0.64
4:H:110:VAL:HA	4:H:113:TRP:CE2	2.32	0.64
1:I:214:ASN:HB3	1:I:218:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:506:PHE:CZ	2:J:104:VAL:HG11	2.31	0.64
1:A:167:LEU:O	1:A:443:ARG:NH2	2.30	0.64
1:A:453:GLY:CA	1:A:498:ARG:HB3	2.27	0.64
2:B:175:LEU:CD1	2:B:226:ILE:HG12	2.27	0.64
1:E:82:GLN:HE22	1:E:581:PHE:H	1.45	0.64
1:E:453:GLY:CA	1:E:498:ARG:HB3	2.27	0.64
3:C:30:HIS:CD2	3:C:87:VAL:HB	2.32	0.64
4:D:23:ALA:HB2	4:D:71:HIS:HE1	1.62	0.64
3:G:69:PHE:O	3:G:73:ILE:HD12	1.96	0.64
1:I:448:ASN:O	1:I:451:ARG:NH1	2.30	0.64
2:J:220:LEU:HD12	8:J:302:SF4:S4	2.38	0.64
3:C:86:VAL:O	3:C:89:ILE:HG22	1.97	0.64
3:K:30:HIS:CD2	3:K:87:VAL:HB	2.33	0.64
1:A:40:PHE:HB3	1:A:43:ARG:HD3	1.80	0.64
2:F:220:LEU:HD12	8:F:302:SF4:S4	2.38	0.64
1:I:117:ARG:O	1:I:134:THR:HB	1.98	0.64
3:K:86:VAL:O	3:K:89:ILE:HG22	1.97	0.64
1:A:117:ARG:O	1:A:134:THR:HB	1.98	0.64
2:B:220:LEU:HD12	8:B:302:SF4:S4	2.38	0.64
1:E:460:ARG:HB2	1:E:516:LEU:CD1	2.27	0.64
3:G:86:VAL:O	3:G:89:ILE:HG22	1.97	0.64
4:H:23:ALA:HB2	4:H:71:HIS:HE1	1.61	0.64
4:L:23:ALA:HB2	4:L:71:HIS:HE1	1.61	0.64
1:A:82:GLN:HE22	1:A:581:PHE:H	1.45	0.64
1:A:214:ASN:HB3	1:A:218:ASN:OD1	1.97	0.64
1:I:40:PHE:HB3	1:I:43:ARG:HD3	1.80	0.64
1:I:215:ALA:HB1	2:J:54:SER:O	1.98	0.64
1:I:367:GLN:HB3	1:I:379:VAL:CG1	2.28	0.64
1:A:367:GLN:HB3	1:A:379:VAL:CG1	2.28	0.63
1:A:453:GLY:N	1:A:498:ARG:HB3	2.14	0.63
1:E:234:GLN:NE2	1:E:569:ARG:HD3	2.13	0.63
1:A:551:GLU:OE1	1:A:551:GLU:N	2.30	0.63
4:D:57:THR:O	4:D:61:THR:HG23	1.98	0.63
1:E:117:ARG:O	1:E:134:THR:HB	1.98	0.63
3:G:30:HIS:CD2	3:G:87:VAL:HB	2.33	0.63
1:I:167:LEU:O	1:I:443:ARG:NH2	2.30	0.63
1:I:234:GLN:NE2	1:I:569:ARG:HD3	2.13	0.63
4:L:110:VAL:HA	4:L:113:TRP:CE2	2.32	0.63
2:F:234:LEU:O	2:F:238:ALA:HB3	1.99	0.63
1:I:478:ASP:O	1:I:482:LYS:HG2	1.97	0.63
3:K:36:ILE:O	3:K:39:VAL:HG12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:O	2:B:134:LEU:HA	1.99	0.63
2:B:234:LEU:O	2:B:238:ALA:HB3	1.99	0.63
1:E:31:GLN:NE2	1:E:420:GLN:OE1	2.32	0.63
1:E:551:GLU:OE1	1:E:551:GLU:N	2.30	0.63
1:I:227:ILE:HG23	1:I:561:PRO:HB3	1.81	0.63
1:I:453:GLY:N	1:I:498:ARG:HB3	2.13	0.63
2:J:234:LEU:O	2:J:238:ALA:HB3	1.99	0.63
1:A:234:GLN:NE2	1:A:569:ARG:HD3	2.13	0.63
3:G:36:ILE:O	3:G:39:VAL:HG12	1.99	0.63
4:L:57:THR:O	4:L:61:THR:HG23	1.99	0.63
1:E:167:LEU:O	1:E:443:ARG:NH2	2.30	0.63
2:F:43:LYS:NZ	2:F:49:LEU:O	2.23	0.63
3:K:52:LEU:HD22	4:L:115:VAL:HG21	1.79	0.63
1:A:506:PHE:CZ	2:B:104:VAL:HG11	2.34	0.63
2:F:182:LEU:HD21	2:F:193:ARG:HB3	1.81	0.63
1:I:199:VAL:HG22	1:I:384:PHE:HB2	1.81	0.63
3:C:36:ILE:O	3:C:39:VAL:HG12	1.99	0.63
1:E:227:ILE:HG23	1:E:561:PRO:HB3	1.81	0.63
1:I:31:GLN:NE2	1:I:420:GLN:OE1	2.32	0.63
1:E:100:GLU:OE1	2:F:132:GLU:HB2	1.99	0.62
1:I:201:ALA:O	5:I:601:FAD:H52A	1.99	0.62
1:E:367:GLN:HB3	1:E:379:VAL:CG1	2.28	0.62
3:G:90:ARG:HE	3:G:109:SER:HB2	1.64	0.62
4:H:57:THR:O	4:H:61:THR:HG23	1.99	0.62
1:A:237:GLU:HB2	1:A:530:ALA:HA	1.81	0.62
4:D:23:ALA:HB2	4:D:71:HIS:CE1	2.34	0.62
1:E:237:GLU:HB2	1:E:530:ALA:HA	1.81	0.62
1:E:453:GLY:N	1:E:498:ARG:HB3	2.14	0.62
1:I:237:GLU:HB2	1:I:530:ALA:HA	1.81	0.62
4:L:23:ALA:HB2	4:L:71:HIS:CE1	2.34	0.62
1:E:199:VAL:HG22	1:E:384:PHE:HB2	1.81	0.62
3:G:89:ILE:O	3:G:93:MET:HG3	1.99	0.62
4:L:75:GLY:O	4:L:79:VAL:HG23	2.00	0.62
1:A:201:ALA:O	5:A:601:FAD:H52A	2.00	0.62
1:E:40:PHE:HB3	1:E:43:ARG:HD3	1.80	0.62
2:J:182:LEU:HD21	2:J:193:ARG:HB3	1.81	0.62
4:H:23:ALA:HB2	4:H:71:HIS:CE1	2.34	0.62
1:A:31:GLN:NE2	1:A:420:GLN:OE1	2.32	0.62
4:H:75:GLY:O	4:H:79:VAL:HG23	2.00	0.62
3:K:89:ILE:O	3:K:93:MET:HG3	1.99	0.62
3:K:90:ARG:HE	3:K:109:SER:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HB2	1:A:490:ILE:HD12	1.81	0.62
1:E:92:GLY:HA2	1:E:406:LEU:HD11	1.82	0.62
1:E:201:ALA:O	5:E:601:FAD:H52A	2.00	0.62
2:F:75:CYS:SG	2:F:76:ILE:HG23	2.40	0.62
1:A:227:ILE:HG23	1:A:561:PRO:HB3	1.81	0.61
1:A:494:LEU:O	1:A:494:LEU:HD23	2.00	0.61
2:B:75:CYS:SG	2:B:76:ILE:HG23	2.40	0.61
1:E:234:GLN:HE22	1:E:569:ARG:HD3	1.65	0.61
1:I:234:GLN:HE22	1:I:569:ARG:HD3	1.65	0.61
1:I:463:LEU:HB2	1:I:490:ILE:HD12	1.81	0.61
4:D:75:GLY:O	4:D:79:VAL:HG23	2.00	0.61
2:F:125:GLY:O	2:F:128:PRO:HG3	2.00	0.61
1:E:52:GLY:CA	1:E:136:ALA:HB2	2.30	0.61
1:I:52:GLY:CA	1:I:136:ALA:HB2	2.30	0.61
1:I:224:GLY:O	1:I:228:ARG:HG3	2.00	0.61
1:I:69:MET:CE	1:I:86:GLU:HB2	2.30	0.61
2:J:73:LEU:HB2	2:J:76:ILE:HG12	1.82	0.61
2:B:182:LEU:HD21	2:B:193:ARG:HB3	1.81	0.61
2:J:75:CYS:SG	2:J:76:ILE:HG23	2.40	0.61
1:A:199:VAL:HG22	1:A:384:PHE:HB2	1.81	0.61
3:C:89:ILE:O	3:C:93:MET:HG3	1.99	0.61
3:C:90:ARG:HE	3:C:109:SER:HB2	1.64	0.61
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.83	0.61
1:E:69:MET:CE	1:E:86:GLU:HB2	2.30	0.61
1:E:463:LEU:HB2	1:E:490:ILE:HD12	1.81	0.61
2:F:33:MET:O	2:F:79:ILE:HG12	2.01	0.61
2:J:33:MET:O	2:J:79:ILE:HG12	2.01	0.61
2:B:125:GLY:O	2:B:128:PRO:HG3	2.00	0.61
1:I:92:GLY:HA2	1:I:406:LEU:HD11	1.82	0.61
1:I:494:LEU:O	1:I:494:LEU:HD23	2.00	0.61
1:A:234:GLN:HE22	1:A:569:ARG:HD3	1.65	0.60
1:A:69:MET:CE	1:A:86:GLU:HB2	2.30	0.60
3:K:112:ILE:O	3:K:115:VAL:HG22	2.02	0.60
1:A:92:GLY:HA2	1:A:406:LEU:HD11	1.82	0.60
2:B:73:LEU:HB2	2:B:76:ILE:HG12	1.82	0.60
1:E:224:GLY:O	1:E:228:ARG:HG3	2.01	0.60
2:F:73:LEU:HB2	2:F:76:ILE:HG12	1.82	0.60
3:G:112:ILE:O	3:G:115:VAL:HG22	2.02	0.60
1:I:54:THR:O	1:I:406:LEU:HD22	2.01	0.60
1:E:54:THR:O	1:E:406:LEU:HD22	2.01	0.60
1:E:494:LEU:HD23	1:E:494:LEU:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:ILE:HG23	3:G:9:ARG:NH2	2.17	0.60
1:I:359:GLY:N	1:I:391:CYS:HB2	2.16	0.60
1:I:551:GLU:OE1	1:I:551:GLU:N	2.30	0.60
1:A:224:GLY:O	1:A:228:ARG:HG3	2.00	0.60
1:I:363:LYS:CG	1:I:369:LEU:HD21	2.32	0.60
2:J:125:GLY:O	2:J:128:PRO:HG3	2.00	0.60
1:E:363:LYS:CG	1:E:369:LEU:HD21	2.32	0.60
1:I:100:GLU:OE1	2:J:132:GLU:HB2	2.01	0.60
1:A:52:GLY:CA	1:A:136:ALA:HB2	2.30	0.60
1:A:359:GLY:N	1:A:391:CYS:HB2	2.16	0.60
2:B:33:MET:O	2:B:79:ILE:HG12	2.01	0.60
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.83	0.60
1:A:54:THR:O	1:A:406:LEU:HD22	2.01	0.60
1:A:400:LEU:HB2	1:A:403:ASN:OD1	2.02	0.60
1:A:575:PRO:HG2	1:A:578:ARG:O	2.02	0.60
3:C:112:ILE:O	3:C:115:VAL:HG22	2.02	0.60
4:H:83:TYR:OH	12:H:1201:UQ2:O1	2.16	0.60
3:K:115:VAL:O	3:K:119:VAL:HG23	2.02	0.60
1:A:105:PRO:HG3	2:B:180:ARG:NH2	2.17	0.59
1:A:363:LYS:CG	1:A:369:LEU:HD21	2.32	0.59
3:C:115:VAL:O	3:C:119:VAL:HG23	2.02	0.59
2:J:98:PRO:HA	3:K:11:VAL:HG22	1.83	0.59
2:B:100:ILE:HG23	3:C:9:ARG:NH2	2.16	0.59
1:E:369:LEU:HD12	1:E:569:ARG:HH22	1.68	0.59
1:E:575:PRO:HG2	1:E:578:ARG:O	2.02	0.59
3:G:111:LYS:O	3:G:115:VAL:HG13	2.02	0.59
3:K:111:LYS:O	3:K:115:VAL:HG13	2.02	0.59
1:I:45:HIS:CE1	1:I:214:ASN:HA	2.37	0.59
3:K:66:GLY:HA2	3:K:71:LYS:NZ	2.17	0.59
1:A:578:ARG:HG2	1:A:579:PRO:CD	2.33	0.59
3:C:123:LEU:O	3:C:126:VAL:HG22	2.03	0.59
3:G:115:VAL:O	3:G:119:VAL:HG23	2.02	0.59
3:G:123:LEU:O	3:G:126:VAL:HG22	2.03	0.59
3:C:66:GLY:HA2	3:C:71:LYS:NZ	2.17	0.59
1:E:578:ARG:HG2	1:E:579:PRO:CD	2.33	0.59
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.83	0.59
1:A:176:ALA:CB	1:A:381:PRO:HB2	2.33	0.59
1:E:359:GLY:N	1:E:391:CYS:HB2	2.16	0.59
1:A:558:LEU:HB3	1:A:567:THR:CG2	2.33	0.59
2:B:34:MET:HG3	2:B:75:CYS:O	2.03	0.59
2:B:98:PRO:HA	3:C:11:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:VAL:HG23	4:H:106:ILE:HG22	1.82	0.59
2:F:236:ARG:HH11	2:F:237:ASN:HD21	1.51	0.59
1:A:53:ILE:HG12	1:A:405:LEU:HB3	1.85	0.59
1:E:494:LEU:HD11	1:E:516:LEU:HD23	1.84	0.59
3:G:66:GLY:HA2	3:G:71:LYS:NZ	2.17	0.59
1:E:558:LEU:HB3	1:E:567:THR:CG2	2.33	0.59
3:C:111:LYS:O	3:C:115:VAL:HG13	2.02	0.58
2:F:34:MET:HG3	2:F:75:CYS:O	2.03	0.58
3:C:16:GLN:OE1	3:C:16:GLN:N	2.36	0.58
1:E:45:HIS:CE1	1:E:214:ASN:HA	2.37	0.58
1:E:400:LEU:HB2	1:E:403:ASN:OD1	2.02	0.58
1:I:494:LEU:HD11	1:I:516:LEU:HD23	1.84	0.58
1:E:176:ALA:CB	1:E:381:PRO:HB2	2.33	0.58
3:G:16:GLN:OE1	3:G:16:GLN:N	2.36	0.58
3:G:48:LEU:HB2	10:G:202:3PE:H281	1.85	0.58
1:I:369:LEU:HD12	1:I:569:ARG:HH22	1.68	0.58
1:I:578:ARG:HG2	1:I:579:PRO:CD	2.33	0.58
3:K:16:GLN:OE1	3:K:16:GLN:N	2.36	0.58
3:K:48:LEU:HB2	10:K:202:3PE:H281	1.85	0.58
2:F:49:LEU:HD12	2:F:102:ASP:OD2	2.03	0.58
1:I:176:ALA:CB	1:I:381:PRO:HB2	2.33	0.58
1:I:575:PRO:HG2	1:I:578:ARG:O	2.02	0.58
1:A:45:HIS:CE1	1:A:214:ASN:HA	2.37	0.58
1:A:392:VAL:HG13	1:A:394:VAL:HG22	1.85	0.58
1:E:406:LEU:O	1:E:410:VAL:HG23	2.04	0.58
2:J:34:MET:HG3	2:J:75:CYS:O	2.03	0.58
3:K:123:LEU:O	3:K:126:VAL:HG22	2.03	0.58
1:A:369:LEU:HD12	1:A:569:ARG:HH22	1.68	0.58
1:E:487:LEU:HA	1:E:490:ILE:HG12	1.86	0.58
1:I:488:LYS:HE2	1:I:524:TYR:OH	2.04	0.58
1:I:53:ILE:HG12	1:I:405:LEU:HB3	1.85	0.58
1:I:558:LEU:HB3	1:I:567:THR:CG2	2.33	0.58
1:A:165:TYR:HD1	1:A:167:LEU:HD22	1.69	0.58
1:A:357:MET:HE1	1:A:399:ARG:HB2	1.85	0.58
1:A:406:LEU:O	1:A:410:VAL:HG23	2.04	0.58
2:B:49:LEU:HD12	2:B:102:ASP:OD2	2.03	0.58
2:B:236:ARG:HH11	2:B:237:ASN:HD21	1.51	0.58
1:E:165:TYR:HD1	1:E:167:LEU:HD22	1.68	0.58
2:J:100:ILE:HD11	2:J:106:ASP:CA	2.34	0.58
1:A:215:ALA:HB1	2:B:54:SER:O	2.04	0.57
1:E:357:MET:HE1	1:E:399:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:VAL:HG13	1:E:394:VAL:HG22	1.85	0.57
2:F:153:ALA:O	2:F:157:THR:HG23	2.04	0.57
2:J:155:CYS:SG	2:J:172:PRO:HG2	2.44	0.57
1:A:220:GLY:O	1:A:223:VAL:HG12	2.04	0.57
1:E:53:ILE:HG12	1:E:405:LEU:HB3	1.85	0.57
2:F:100:ILE:HD11	2:F:106:ASP:CA	2.34	0.57
2:J:49:LEU:HD12	2:J:102:ASP:OD2	2.03	0.57
11:K:201:HEM:CBB	4:L:26:LEU:HD13	2.33	0.57
4:L:19:VAL:HG13	4:L:71:HIS:CE1	2.40	0.57
2:B:65:LEU:HD23	2:B:91:ILE:CG2	2.34	0.57
2:B:100:ILE:HD11	2:B:106:ASP:CA	2.34	0.57
4:D:27:THR:HG22	11:D:201:HEM:HAC	1.86	0.57
1:E:220:GLY:O	1:E:223:VAL:HG12	2.04	0.57
2:F:65:LEU:HD23	2:F:91:ILE:CG2	2.34	0.57
11:G:201:HEM:HAC	4:H:27:THR:HG22	1.86	0.57
1:A:487:LEU:HA	1:A:490:ILE:HG12	1.85	0.57
4:D:19:VAL:HG13	4:D:71:HIS:CE1	2.40	0.57
2:F:155:CYS:SG	2:F:172:PRO:HG2	2.44	0.57
1:A:46:THR:CG2	1:A:146:LEU:HD22	2.33	0.57
1:A:488:LYS:HE2	1:A:524:TYR:OH	2.04	0.57
2:B:193:ARG:O	2:B:197:LEU:HD23	2.04	0.57
1:E:65:TRP:CE2	1:E:90:LYS:HD3	2.40	0.57
4:H:19:VAL:HG13	4:H:71:HIS:CE1	2.39	0.57
1:I:392:VAL:HG13	1:I:394:VAL:HG22	1.85	0.57
1:I:406:LEU:O	1:I:410:VAL:HG23	2.04	0.57
4:H:59:VAL:HG23	4:L:106:ILE:HG22	1.86	0.57
1:I:400:LEU:HB2	1:I:403:ASN:OD1	2.02	0.57
2:B:155:CYS:SG	2:B:172:PRO:HG2	2.44	0.57
3:C:48:LEU:HB2	10:C:1301:3PE:H281	1.85	0.57
4:D:3:SER:HB3	4:L:10:ARG:HH21	1.69	0.57
1:E:487:LEU:HD23	1:E:490:ILE:HD11	1.87	0.57
1:E:488:LYS:HE2	1:E:524:TYR:OH	2.04	0.57
1:I:487:LEU:HA	1:I:490:ILE:HG12	1.85	0.57
1:A:65:TRP:CE2	1:A:90:LYS:HD3	2.39	0.57
1:E:232:PRO:HB2	1:E:558:LEU:HD11	1.87	0.57
1:I:187:THR:HG23	1:I:189:GLU:HG2	1.87	0.57
1:I:487:LEU:HD23	1:I:490:ILE:HD11	1.87	0.57
2:J:100:ILE:HG23	3:K:9:ARG:NH2	2.20	0.57
2:J:236:ARG:HH11	2:J:237:ASN:HD21	1.51	0.57
1:A:487:LEU:HD23	1:A:490:ILE:HD11	1.87	0.57
1:I:65:TRP:CE2	1:I:90:LYS:HD3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:TYR:HD1	1:I:167:LEU:HD22	1.69	0.57
2:J:65:LEU:HD23	2:J:91:ILE:CG2	2.34	0.57
1:A:494:LEU:HD11	1:A:516:LEU:HD23	1.85	0.57
2:B:127:ASN:N	2:B:128:PRO:HD3	2.20	0.57
4:D:92:MET:O	4:D:96:VAL:HG23	2.05	0.57
1:E:419:LEU:O	1:E:423:ILE:HG13	2.05	0.57
2:F:114:TYR:O	2:F:117:ILE:HG12	2.05	0.57
4:H:62:LEU:HD21	4:H:112:VAL:HG21	1.86	0.57
1:I:357:MET:HE1	1:I:399:ARG:HB2	1.85	0.57
1:I:363:LYS:HE3	1:I:369:LEU:HD21	1.87	0.57
4:L:62:LEU:HD21	4:L:112:VAL:HG21	1.86	0.57
1:A:419:LEU:O	1:A:423:ILE:HG13	2.05	0.56
1:E:187:THR:HG23	1:E:189:GLU:HG2	1.87	0.56
1:E:487:LEU:CD2	1:E:490:ILE:HD11	2.35	0.56
2:F:193:ARG:O	2:F:197:LEU:HD23	2.04	0.56
1:A:528:VAL:HG11	1:A:559:TYR:HE1	1.71	0.56
1:A:555:CYS:HA	1:A:571:VAL:CG2	2.33	0.56
2:B:114:TYR:O	2:B:117:ILE:HG12	2.04	0.56
1:E:99:LEU:HD21	1:E:145:LEU:CD1	2.35	0.56
1:I:487:LEU:CD2	1:I:490:ILE:HD11	2.35	0.56
4:D:16:PHE:O	4:D:20:ARG:HD3	2.05	0.56
4:D:83:TYR:OH	12:D:202:UQ2:O1	2.14	0.56
1:E:528:VAL:HG11	1:E:559:TYR:HE1	1.71	0.56
2:J:193:ARG:O	2:J:197:LEU:HD23	2.04	0.56
4:L:16:PHE:O	4:L:20:ARG:HD3	2.05	0.56
4:D:26:LEU:HD13	11:D:201:HEM:CBB	2.35	0.56
4:D:106:ILE:HG22	4:L:59:VAL:HG23	1.86	0.56
4:H:92:MET:O	4:H:96:VAL:HG23	2.05	0.56
1:I:220:GLY:O	1:I:223:VAL:HG12	2.04	0.56
4:L:92:MET:O	4:L:96:VAL:HG23	2.05	0.56
1:A:99:LEU:HD21	1:A:145:LEU:CD1	2.35	0.56
1:I:232:PRO:HB2	1:I:558:LEU:HD11	1.87	0.56
2:J:153:ALA:O	2:J:157:THR:HG23	2.04	0.56
2:B:56:ARG:O	2:B:56:ARG:HG2	2.05	0.56
2:B:153:ALA:O	2:B:157:THR:HG23	2.04	0.56
4:D:62:LEU:HD21	4:D:112:VAL:HG21	1.86	0.56
1:E:79:ILE:CG1	1:E:537:ARG:HD3	2.36	0.56
1:E:363:LYS:HE3	1:E:369:LEU:HD21	1.87	0.56
4:H:16:PHE:O	4:H:20:ARG:HD3	2.05	0.56
1:I:79:ILE:CG1	1:I:537:ARG:HD3	2.36	0.56
1:I:528:VAL:HG11	1:I:559:TYR:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:555:CYS:HA	1:I:571:VAL:CG2	2.33	0.56
2:J:114:TYR:O	2:J:117:ILE:HG12	2.05	0.56
1:A:171:LYS:HE3	1:A:175:GLY:O	2.06	0.56
2:B:67:MET:HB3	2:B:82:LEU:HD21	1.88	0.56
1:E:43:ARG:NH2	2:F:61:GLY:O	2.39	0.56
1:I:399:ARG:HH11	1:I:401:GLY:HA2	1.70	0.56
1:I:419:LEU:O	1:I:423:ILE:HG13	2.05	0.56
1:A:79:ILE:CG1	1:A:537:ARG:HD3	2.36	0.56
1:A:232:PRO:HB2	1:A:558:LEU:HD11	1.87	0.56
2:F:56:ARG:HG2	2:F:56:ARG:O	2.05	0.56
2:F:98:PRO:HA	3:G:11:VAL:HG22	1.88	0.56
1:A:82:GLN:HE22	1:A:581:PHE:N	2.04	0.56
4:D:29:TYR:HA	4:D:60:PHE:HE2	1.69	0.56
1:I:82:GLN:HE22	1:I:581:PHE:N	2.04	0.56
1:I:171:LYS:HE3	1:I:175:GLY:O	2.06	0.56
2:J:127:ASN:N	2:J:128:PRO:HD3	2.20	0.56
1:A:538:GLY:HA2	1:A:586:ARG:NH2	2.21	0.55
1:A:487:LEU:CD2	1:A:490:ILE:HD11	2.35	0.55
1:E:46:THR:CG2	1:E:146:LEU:HD22	2.33	0.55
1:E:171:LYS:HE3	1:E:175:GLY:O	2.06	0.55
2:F:127:ASN:N	2:F:128:PRO:HD3	2.20	0.55
1:E:460:ARG:HB2	1:E:516:LEU:HD11	1.88	0.55
1:E:538:GLY:HA2	1:E:586:ARG:NH2	2.21	0.55
1:I:370:THR:O	1:I:378:VAL:HG12	2.07	0.55
1:I:506:PHE:CE2	2:J:104:VAL:HG11	2.41	0.55
1:A:363:LYS:HE3	1:A:369:LEU:HD21	1.87	0.55
1:A:460:ARG:HB2	1:A:516:LEU:HD11	1.88	0.55
2:F:67:MET:HB3	2:F:82:LEU:HD21	1.88	0.55
3:G:48:LEU:HD12	3:G:48:LEU:O	2.06	0.55
1:I:145:LEU:CD2	1:I:405:LEU:HD22	2.37	0.55
2:J:67:MET:HB3	2:J:82:LEU:HD21	1.88	0.55
1:A:202:THR:HG21	1:A:222:GLY:CA	2.37	0.55
1:A:370:THR:O	1:A:378:VAL:HG12	2.07	0.55
1:I:99:LEU:HD21	1:I:145:LEU:CD1	2.35	0.55
2:J:56:ARG:O	2:J:56:ARG:HG2	2.05	0.55
2:B:95:PRO:HA	3:C:12:ASN:O	2.07	0.55
1:E:145:LEU:CD2	1:E:405:LEU:HD22	2.37	0.55
4:L:43:LEU:HD12	4:L:47:VAL:HG23	1.88	0.55
1:A:187:THR:HG23	1:A:189:GLU:HG2	1.87	0.55
1:E:399:ARG:HH11	1:E:401:GLY:HA2	1.70	0.55
1:I:202:THR:HG21	1:I:222:GLY:CA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:LEU:HD12	3:C:48:LEU:O	2.06	0.55
1:E:352:THR:O	1:E:352:THR:HG22	2.07	0.55
4:H:113:TRP:HA	4:L:113:TRP:CH2	2.42	0.55
1:I:538:GLY:HA2	1:I:586:ARG:NH2	2.21	0.55
1:A:190:VAL:HG11	1:A:441:LEU:CD2	2.37	0.55
2:B:210:MET:HB2	3:C:23:THR:HG21	1.87	0.55
1:E:202:THR:HG21	1:E:222:GLY:CA	2.37	0.55
1:E:223:VAL:CG2	1:E:233:VAL:HG11	2.37	0.55
1:I:46:THR:CG2	1:I:146:LEU:HD22	2.33	0.55
1:I:460:ARG:HB2	1:I:516:LEU:HD11	1.88	0.55
2:J:95:PRO:HA	3:K:12:ASN:O	2.07	0.55
1:A:399:ARG:HH11	1:A:401:GLY:HA2	1.70	0.54
3:G:40:ALA:O	3:G:44:LEU:HG	2.07	0.54
4:L:108:GLY:O	4:L:112:VAL:HG13	2.07	0.54
3:C:78:LEU:HD13	3:C:124:ALA:HB1	1.90	0.54
1:E:82:GLN:HE22	1:E:581:PHE:N	2.04	0.54
1:I:223:VAL:HG23	1:I:233:VAL:HG11	1.89	0.54
3:K:48:LEU:HD12	3:K:48:LEU:O	2.06	0.54
1:A:490:ILE:CG1	1:A:520:MET:HE1	2.36	0.54
3:C:40:ALA:O	3:C:44:LEU:HG	2.07	0.54
4:D:108:GLY:O	4:D:112:VAL:HG13	2.07	0.54
2:F:210:MET:HB2	3:G:23:THR:HG21	1.89	0.54
1:I:223:VAL:CG2	1:I:233:VAL:HG11	2.37	0.54
1:A:223:VAL:HG23	1:A:233:VAL:HG11	1.89	0.54
1:A:535:GLU:HG2	1:A:536:SER:N	2.22	0.54
4:D:43:LEU:HD12	4:D:47:VAL:HG23	1.89	0.54
1:E:190:VAL:HG11	1:E:441:LEU:CD2	2.37	0.54
1:E:506:PHE:CE2	2:F:104:VAL:HG11	2.43	0.54
1:E:555:CYS:HA	1:E:571:VAL:CG2	2.33	0.54
2:F:150:ILE:HG12	8:F:302:SF4:S1	2.48	0.54
2:F:176:LEU:HD21	2:F:220:LEU:HD13	1.90	0.54
1:I:207:ARG:HB2	1:I:218:ASN:O	2.08	0.54
3:K:78:LEU:HD13	3:K:124:ALA:HB1	1.90	0.54
1:A:69:MET:O	1:A:73:VAL:HG23	2.08	0.54
1:E:69:MET:O	1:E:73:VAL:HG23	2.08	0.54
1:I:69:MET:O	1:I:73:VAL:HG23	2.08	0.54
1:I:190:VAL:HG11	1:I:441:LEU:CD2	2.37	0.54
3:K:40:ALA:O	3:K:44:LEU:HG	2.07	0.54
1:A:145:LEU:CD2	1:A:405:LEU:HD22	2.37	0.54
2:B:150:ILE:HG12	8:B:302:SF4:S1	2.48	0.54
1:E:490:ILE:CG1	1:E:520:MET:HE1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:108:GLY:O	4:H:112:VAL:HG13	2.07	0.54
1:A:53:ILE:HG12	1:A:405:LEU:CB	2.38	0.54
1:A:118:PRO:HA	1:A:132:ALA:HA	1.90	0.54
1:A:223:VAL:CG2	1:A:233:VAL:HG11	2.37	0.54
1:E:223:VAL:HG23	1:E:233:VAL:HG11	1.89	0.54
1:E:367:GLN:OE1	1:E:422:SER:OG	2.15	0.54
11:G:201:HEM:CBB	4:H:26:LEU:HD13	2.38	0.54
4:H:43:LEU:HD12	4:H:47:VAL:HG23	1.89	0.54
1:I:21:ARG:NH2	1:I:413:ARG:HG3	2.24	0.54
2:J:176:LEU:HD21	2:J:220:LEU:HD13	1.90	0.54
1:A:352:THR:HG22	1:A:352:THR:O	2.07	0.53
1:A:363:LYS:HE3	1:A:369:LEU:CD2	2.38	0.53
1:E:363:LYS:HE3	1:E:369:LEU:CD2	2.38	0.53
2:F:175:LEU:HD13	2:F:226:ILE:HG12	1.90	0.53
4:H:29:TYR:HA	4:H:60:PHE:HE2	1.69	0.53
1:I:43:ARG:NH2	2:J:151:LEU:O	2.42	0.53
1:I:363:LYS:HE3	1:I:369:LEU:CD2	2.38	0.53
1:E:21:ARG:NH2	1:E:413:ARG:HG3	2.23	0.53
1:E:108:ARG:NH1	2:F:133:HIS:O	2.41	0.53
1:E:370:THR:O	1:E:378:VAL:HG12	2.07	0.53
4:H:65:LEU:CD1	4:H:108:GLY:HA3	2.39	0.53
1:E:53:ILE:HG12	1:E:405:LEU:CB	2.38	0.53
1:E:147:HIS:O	1:E:151:GLN:HG3	2.09	0.53
3:C:65:MET:HE2	10:C:1301:3PE:H31	1.90	0.53
4:D:65:LEU:CD1	4:D:108:GLY:HA3	2.39	0.53
1:E:535:GLU:HG2	1:E:536:SER:N	2.22	0.53
1:A:147:HIS:O	1:A:151:GLN:HG3	2.09	0.53
1:E:219:THR:HG22	1:E:519:LEU:HD11	1.91	0.53
1:I:53:ILE:HG12	1:I:405:LEU:CB	2.38	0.53
1:I:352:THR:O	1:I:352:THR:HG22	2.07	0.53
2:J:150:ILE:HG12	8:J:302:SF4:S1	2.48	0.53
2:J:210:MET:HB2	3:K:23:THR:HG21	1.90	0.53
4:L:65:LEU:CD1	4:L:108:GLY:HA3	2.39	0.53
2:J:175:LEU:HD13	2:J:226:ILE:HG12	1.90	0.53
4:L:9:GLY:HA3	4:L:15:ASP:OD1	2.09	0.53
4:L:29:TYR:HA	4:L:60:PHE:HE2	1.69	0.53
1:A:167:LEU:H	1:A:182:ALA:HA	1.74	0.53
1:E:118:PRO:HA	1:E:132:ALA:HA	1.90	0.53
1:E:200:LEU:HD13	1:E:383:LEU:HD11	1.91	0.53
4:H:106:ILE:O	4:H:110:VAL:HG23	2.09	0.53
1:I:147:HIS:O	1:I:151:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:574:GLU:HG3	1:I:574:GLU:O	2.09	0.53
2:J:171:GLY:O	2:J:175:LEU:HG	2.09	0.53
11:K:201:HEM:HAC	4:L:27:THR:HG22	1.91	0.53
1:A:21:ARG:NH2	1:A:413:ARG:HG3	2.23	0.53
1:A:108:ARG:HG3	2:B:135:GLN:HG3	1.90	0.53
4:D:9:GLY:HA3	4:D:15:ASP:OD1	2.09	0.53
1:E:207:ARG:HB2	1:E:218:ASN:O	2.08	0.53
3:G:78:LEU:HD13	3:G:124:ALA:HB1	1.89	0.53
1:A:221:ASP:O	1:A:225:MET:HG3	2.09	0.53
4:D:8:LEU:HG	4:D:8:LEU:O	2.09	0.53
1:E:143:HIS:CE1	2:F:150:ILE:HG22	2.44	0.53
1:I:51:GLY:N	5:I:601:FAD:O4	2.37	0.53
1:I:118:PRO:HA	1:I:132:ALA:HA	1.90	0.53
1:I:219:THR:HG22	1:I:519:LEU:HD11	1.91	0.53
2:J:9:ARG:NH1	2:J:21:GLN:OE1	2.42	0.53
2:B:176:LEU:HD21	2:B:220:LEU:HD13	1.90	0.53
4:D:106:ILE:O	4:D:110:VAL:HG23	2.09	0.53
2:F:9:ARG:NH1	2:F:21:GLN:OE1	2.42	0.53
1:I:3:LEU:CD2	1:I:441:LEU:HD11	2.39	0.53
1:I:200:LEU:HD13	1:I:383:LEU:HD11	1.91	0.53
1:I:363:LYS:HG2	1:I:369:LEU:HD11	1.91	0.53
2:B:84:GLN:HB2	2:B:87:LYS:HE3	1.92	0.52
2:F:95:PRO:HA	3:G:12:ASN:O	2.09	0.52
1:A:207:ARG:HB2	1:A:218:ASN:O	2.08	0.52
2:B:101:ARG:CG	2:B:102:ASP:H	2.22	0.52
3:G:65:MET:HE2	10:G:202:3PE:H31	1.90	0.52
4:H:9:GLY:HA3	4:H:15:ASP:OD1	2.09	0.52
1:I:221:ASP:O	1:I:225:MET:HG3	2.09	0.52
2:J:14:VAL:HG23	2:J:14:VAL:O	2.10	0.52
2:J:49:LEU:HD23	2:J:51:PHE:HE2	1.75	0.52
2:B:14:VAL:HG23	2:B:14:VAL:O	2.10	0.52
2:J:84:GLN:HG3	2:J:87:LYS:NZ	2.25	0.52
4:L:8:LEU:HG	4:L:8:LEU:O	2.09	0.52
1:A:184:CYS:SG	1:A:187:THR:HG22	2.50	0.52
1:A:200:LEU:HD13	1:A:383:LEU:HD11	1.91	0.52
2:F:171:GLY:O	2:F:175:LEU:HG	2.09	0.52
1:I:105:PRO:HG3	2:J:180:ARG:NH2	2.24	0.52
2:J:175:LEU:HD12	2:J:226:ILE:HG12	1.92	0.52
2:B:84:GLN:HG3	2:B:87:LYS:NZ	2.25	0.52
1:E:55:VAL:O	1:E:133:ARG:HB2	2.10	0.52
1:E:167:LEU:H	1:E:182:ALA:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:8:LEU:HG	4:H:8:LEU:O	2.09	0.52
1:E:363:LYS:HG2	1:E:369:LEU:HD11	1.91	0.52
1:I:184:CYS:SG	1:I:187:THR:HG22	2.50	0.52
1:E:221:ASP:O	1:E:225:MET:HG3	2.09	0.52
1:I:52:GLY:HA2	1:I:141:THR:HG21	1.92	0.52
3:K:65:MET:HE2	10:K:202:3PE:H31	1.90	0.52
4:L:8:LEU:HB2	4:L:73:TRP:CD2	2.45	0.52
1:A:360:ILE:O	1:A:362:THR:HG23	2.10	0.52
1:A:363:LYS:HG2	1:A:369:LEU:HD11	1.91	0.52
1:A:574:GLU:HG3	1:A:574:GLU:O	2.09	0.52
1:I:206:GLY:HA3	1:I:214:ASN:HD22	1.75	0.52
4:L:106:ILE:O	4:L:110:VAL:HG23	2.09	0.52
1:A:535:GLU:HG3	1:A:549:ASP:H	1.75	0.52
1:E:227:ILE:HG23	1:E:561:PRO:CB	2.40	0.52
2:F:49:LEU:HD23	2:F:51:PHE:HE2	1.75	0.52
1:I:55:VAL:O	1:I:133:ARG:HB2	2.10	0.52
1:I:167:LEU:H	1:I:182:ALA:HA	1.74	0.52
1:A:219:THR:HG22	1:A:519:LEU:HD11	1.91	0.51
2:B:171:GLY:O	2:B:175:LEU:HG	2.09	0.51
4:D:8:LEU:HB2	4:D:73:TRP:CD2	2.45	0.51
1:E:8:PHE:HD1	1:E:32:THR:HG22	1.75	0.51
1:E:183:LEU:HG	1:E:189:GLU:O	2.11	0.51
1:A:55:VAL:O	1:A:133:ARG:HB2	2.10	0.51
2:B:9:ARG:NH1	2:B:21:GLN:OE1	2.42	0.51
2:B:175:LEU:HD13	2:B:226:ILE:HG12	1.90	0.51
1:E:22:ALA:O	1:E:26:ILE:HG13	2.10	0.51
1:E:52:GLY:HA2	1:E:141:THR:HG21	1.92	0.51
1:I:535:GLU:HG3	1:I:549:ASP:H	1.75	0.51
3:C:30:HIS:HD2	3:C:87:VAL:HB	1.75	0.51
1:E:11:VAL:HG23	1:E:195:ALA:CB	2.40	0.51
1:E:184:CYS:SG	1:E:187:THR:HG22	2.50	0.51
1:E:535:GLU:HG3	1:E:549:ASP:H	1.75	0.51
1:I:183:LEU:HG	1:I:189:GLU:O	2.11	0.51
1:I:227:ILE:HG23	1:I:561:PRO:CB	2.40	0.51
11:D:201:HEM:HBA2	11:D:201:HEM:CHA	2.41	0.51
1:E:202:THR:HG21	1:E:222:GLY:N	2.26	0.51
1:E:206:GLY:HA3	1:E:214:ASN:HD22	1.75	0.51
2:F:14:VAL:O	2:F:14:VAL:HG23	2.10	0.51
2:F:84:GLN:HG3	2:F:87:LYS:NZ	2.25	0.51
2:F:175:LEU:HD12	2:F:226:ILE:HG12	1.91	0.51
1:I:22:ALA:O	1:I:26:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:360:ILE:O	1:I:362:THR:HG23	2.10	0.51
3:K:83:TYR:HB2	3:K:117:THR:CG2	2.40	0.51
1:A:202:THR:HG21	1:A:222:GLY:N	2.25	0.51
4:H:99:VAL:HA	4:H:102:VAL:HG22	1.93	0.51
1:I:11:VAL:HG23	1:I:195:ALA:CB	2.40	0.51
4:L:7:ALA:HB2	4:L:77:TRP:CD1	2.46	0.51
1:A:206:GLY:HA3	1:A:214:ASN:HD22	1.75	0.51
1:A:506:PHE:CE2	2:B:104:VAL:HG11	2.46	0.51
3:C:25:ILE:O	3:C:29:LEU:HD23	2.11	0.51
1:I:8:PHE:HD1	1:I:32:THR:HG22	1.75	0.51
1:I:202:THR:HG21	1:I:222:GLY:N	2.25	0.51
1:I:240:GLN:NE2	1:I:398:ASN:OD1	2.42	0.51
1:I:490:ILE:CG1	1:I:520:MET:HE1	2.36	0.51
1:I:508:THR:O	1:I:512:GLU:HG3	2.10	0.51
2:J:84:GLN:HB2	2:J:87:LYS:HE3	1.92	0.51
3:K:25:ILE:O	3:K:29:LEU:HD23	2.11	0.51
1:A:3:LEU:CD2	1:A:441:LEU:HD11	2.39	0.51
1:A:6:ARG:HG3	1:A:191:VAL:HG11	1.92	0.51
1:A:8:PHE:HD1	1:A:32:THR:HG22	1.75	0.51
1:A:11:VAL:HG23	1:A:195:ALA:CB	2.40	0.51
1:A:227:ILE:HG23	1:A:561:PRO:CB	2.41	0.51
1:E:360:ILE:O	1:E:362:THR:HG23	2.10	0.51
1:E:574:GLU:HG3	1:E:574:GLU:O	2.09	0.51
3:G:83:TYR:HB2	3:G:117:THR:CG2	2.40	0.51
4:L:99:VAL:O	4:L:103:VAL:HG23	2.11	0.51
1:A:508:THR:O	1:A:512:GLU:HG3	2.10	0.51
3:C:33:SER:O	3:C:37:THR:HG22	2.11	0.51
1:E:178:VAL:HG12	1:E:192:TYR:OH	2.11	0.51
3:G:25:ILE:O	3:G:29:LEU:HD23	2.11	0.51
1:I:178:VAL:HG12	1:I:192:TYR:OH	2.11	0.51
1:I:535:GLU:HG2	1:I:536:SER:N	2.22	0.51
2:J:25:LEU:HB2	2:J:42:LEU:CD2	2.41	0.51
2:B:49:LEU:HD23	2:B:51:PHE:HE2	1.75	0.51
3:C:83:TYR:HB2	3:C:117:THR:CG2	2.40	0.51
2:F:40:ILE:O	2:F:44:GLU:HG3	2.11	0.51
1:A:409:VAL:HG13	1:A:410:VAL:N	2.26	0.51
4:D:94:GLN:O	4:D:98:VAL:HG13	2.11	0.51
1:E:508:THR:O	1:E:512:GLU:HG3	2.10	0.51
4:H:7:ALA:HB2	4:H:77:TRP:CD1	2.46	0.51
1:I:20:MET:HB2	1:I:153:ASN:ND2	2.26	0.51
1:I:409:VAL:HG13	1:I:410:VAL:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:LEU:HB2	2:B:42:LEU:CD2	2.41	0.50
2:F:101:ARG:HB3	2:F:104:VAL:CG2	2.40	0.50
3:G:54:SER:HB2	3:G:55:PRO:HD2	1.93	0.50
3:G:128:VAL:HG13	3:G:129:TRP:HD1	1.76	0.50
2:J:40:ILE:O	2:J:44:GLU:HG3	2.11	0.50
1:A:22:ALA:O	1:A:26:ILE:HG13	2.10	0.50
1:A:52:GLY:HA2	1:A:141:THR:HG21	1.92	0.50
4:D:99:VAL:HA	4:D:102:VAL:HG22	1.93	0.50
1:E:6:ARG:HG3	1:E:191:VAL:HG11	1.92	0.50
3:G:47:LEU:HD22	10:G:202:3PE:H262	1.93	0.50
11:G:201:HEM:HBA2	11:G:201:HEM:CHA	2.41	0.50
1:I:62:GLU:O	1:I:62:GLU:HG2	2.11	0.50
1:A:176:ALA:CB	1:A:429:LEU:HD22	2.42	0.50
1:A:178:VAL:HG12	1:A:192:TYR:OH	2.11	0.50
4:D:7:ALA:HB2	4:D:77:TRP:CD1	2.46	0.50
1:E:139:ASP:O	1:E:140:ARG:HD3	2.11	0.50
1:E:386:VAL:O	1:E:389:ILE:HG22	2.12	0.50
1:E:460:ARG:HB2	1:E:516:LEU:HD12	1.93	0.50
1:I:176:ALA:CB	1:I:429:LEU:HD22	2.42	0.50
2:J:101:ARG:HB3	2:J:104:VAL:CG2	2.40	0.50
2:B:228:HIS:O	2:B:232:MET:HG3	2.12	0.50
1:E:4:PRO:HB2	1:E:191:VAL:HG22	1.93	0.50
1:E:20:MET:HB2	1:E:153:ASN:ND2	2.26	0.50
2:F:182:LEU:CD2	2:F:193:ARG:HD2	2.41	0.50
2:F:228:HIS:O	2:F:232:MET:HG3	2.12	0.50
4:H:8:LEU:HB2	4:H:73:TRP:CD2	2.45	0.50
4:H:94:GLN:O	4:H:98:VAL:HG13	2.11	0.50
3:K:31:ARG:HE	11:K:201:HEM:CGA	2.24	0.50
4:L:94:GLN:O	4:L:98:VAL:HG13	2.11	0.50
3:C:128:VAL:HG13	3:C:129:TRP:HD1	1.76	0.50
1:E:43:ARG:NH2	2:F:151:LEU:O	2.44	0.50
1:I:6:ARG:HG3	1:I:191:VAL:HG11	1.92	0.50
1:I:47:VAL:HG12	1:I:146:LEU:HD23	1.94	0.50
2:J:84:GLN:OE1	2:J:84:GLN:HA	2.12	0.50
1:A:4:PRO:HB2	1:A:191:VAL:HG22	1.93	0.50
1:A:221:ASP:CB	5:A:601:FAD:H61A	2.25	0.50
1:A:369:LEU:HD12	1:A:569:ARG:NH2	2.27	0.50
1:E:409:VAL:HG13	1:E:410:VAL:N	2.27	0.50
2:J:101:ARG:CG	2:J:102:ASP:H	2.22	0.50
1:A:140:ARG:HB3	1:A:143:HIS:HB3	1.94	0.50
1:A:231:VAL:HG21	1:A:383:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:LEU:HD12	2:B:226:ILE:HG12	1.91	0.50
2:B:182:LEU:CD2	2:B:193:ARG:HD2	2.41	0.50
1:E:47:VAL:HG12	1:E:146:LEU:HD23	1.94	0.50
1:E:116:GLN:HA	1:E:134:THR:O	2.12	0.50
1:E:176:ALA:CB	1:E:429:LEU:HD22	2.42	0.50
2:F:84:GLN:HB2	2:F:87:LYS:HE3	1.92	0.50
3:G:31:ARG:HE	11:G:201:HEM:CGA	2.24	0.50
3:G:33:SER:O	3:G:37:THR:HG22	2.11	0.50
3:K:54:SER:HB2	3:K:55:PRO:HD2	1.93	0.50
3:K:128:VAL:HG13	3:K:129:TRP:HD1	1.76	0.50
1:A:20:MET:HB2	1:A:153:ASN:ND2	2.26	0.50
3:C:47:LEU:HD22	10:C:1301:3PE:H262	1.93	0.50
3:C:54:SER:HB2	3:C:55:PRO:HD2	1.93	0.50
2:F:71:ASN:HD22	2:F:158:SER:HB2	1.77	0.50
2:F:159:CYS:SG	2:F:161:SER:HB2	2.52	0.50
4:H:99:VAL:O	4:H:103:VAL:HG23	2.11	0.50
2:J:159:CYS:SG	2:J:161:SER:HB2	2.52	0.50
11:K:201:HEM:HBA2	11:K:201:HEM:CHA	2.41	0.50
1:A:139:ASP:O	1:A:140:ARG:HD3	2.11	0.50
2:B:71:ASN:HD22	2:B:158:SER:HB2	1.77	0.50
2:B:204:PHE:CD2	4:D:12:GLY:HA3	2.47	0.50
1:E:77:ASP:OD2	1:E:537:ARG:HG3	2.12	0.50
1:E:231:VAL:HG21	1:E:383:LEU:HD23	1.94	0.50
2:F:101:ARG:CG	2:F:102:ASP:H	2.22	0.50
3:G:118:VAL:O	3:G:122:LEU:HD13	2.12	0.50
4:H:26:LEU:CD2	4:H:68:ILE:HG13	2.42	0.50
1:I:112:GLY:O	2:J:134:LEU:HA	2.12	0.50
1:I:139:ASP:O	1:I:140:ARG:HD3	2.11	0.50
1:I:221:ASP:CB	5:I:601:FAD:H61A	2.25	0.50
1:I:369:LEU:HD12	1:I:569:ARG:NH2	2.27	0.50
1:A:460:ARG:HB2	1:A:516:LEU:HD12	1.93	0.49
3:C:118:VAL:O	3:C:122:LEU:HD13	2.12	0.49
1:I:4:PRO:HB2	1:I:191:VAL:HG22	1.93	0.49
3:K:47:LEU:HD22	10:K:202:3PE:H262	1.93	0.49
4:L:99:VAL:HA	4:L:102:VAL:HG22	1.93	0.49
1:A:6:ARG:HB3	1:A:8:PHE:HE2	1.77	0.49
1:A:47:VAL:HG12	1:A:146:LEU:HD23	1.94	0.49
1:A:183:LEU:HG	1:A:189:GLU:O	2.10	0.49
2:B:216:CYS:SG	2:B:220:LEU:HB2	2.52	0.49
4:D:99:VAL:O	4:D:103:VAL:HG23	2.11	0.49
1:E:369:LEU:HD12	1:E:569:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:GLN:OE1	2:F:84:GLN:HA	2.12	0.49
2:F:155:CYS:HB3	8:F:302:SF4:S3	2.52	0.49
2:J:71:ASN:HD22	2:J:158:SER:HB2	1.77	0.49
2:J:197:LEU:HD12	2:J:203:VAL:HG22	1.94	0.49
4:L:26:LEU:CD2	4:L:68:ILE:HG13	2.42	0.49
1:A:62:GLU:O	1:A:62:GLU:HG2	2.11	0.49
1:A:116:GLN:HA	1:A:134:THR:O	2.12	0.49
2:B:40:ILE:O	2:B:44:GLU:HG3	2.11	0.49
2:B:159:CYS:SG	2:B:161:SER:HB2	2.52	0.49
2:B:234:LEU:HD22	4:D:17:ILE:HD11	1.94	0.49
1:E:6:ARG:HB3	1:E:8:PHE:HE2	1.78	0.49
2:F:197:LEU:HD12	2:F:203:VAL:CG2	2.43	0.49
1:I:43:ARG:NH2	2:J:61:GLY:O	2.45	0.49
1:A:46:THR:HG21	1:A:146:LEU:HD13	1.95	0.49
1:A:386:VAL:O	1:A:389:ILE:HG22	2.12	0.49
2:B:155:CYS:HB3	8:B:302:SF4:S3	2.52	0.49
2:B:197:LEU:HD12	2:B:203:VAL:HG22	1.94	0.49
2:F:216:CYS:SG	2:F:220:LEU:HB2	2.52	0.49
4:H:20:ARG:N	4:H:20:ARG:HD2	2.28	0.49
1:I:140:ARG:HB3	1:I:143:HIS:HB3	1.94	0.49
1:I:455:ASP:O	1:I:459:ILE:HG13	2.12	0.49
2:J:182:LEU:CD2	2:J:193:ARG:HD2	2.41	0.49
1:A:100:GLU:OE1	2:B:132:GLU:HB2	2.13	0.49
1:E:236:MET:O	1:E:526:THR:HG23	2.13	0.49
3:G:30:HIS:HD2	3:G:87:VAL:HB	1.75	0.49
2:B:84:GLN:OE1	2:B:84:GLN:HA	2.12	0.49
1:E:46:THR:HG21	1:E:146:LEU:HD13	1.95	0.49
1:E:167:LEU:HD21	1:E:183:LEU:HB2	1.95	0.49
1:E:455:ASP:O	1:E:459:ILE:HG13	2.12	0.49
2:F:167:ASP:OD1	2:F:167:ASP:N	2.46	0.49
1:I:116:GLN:HA	1:I:134:THR:O	2.12	0.49
3:K:33:SER:O	3:K:37:THR:HG22	2.11	0.49
1:A:77:ASP:OD2	1:A:537:ARG:HG3	2.12	0.49
1:E:107:SER:O	1:E:115:TYR:N	2.44	0.49
1:I:386:VAL:O	1:I:389:ILE:HG22	2.12	0.49
1:A:43:ARG:NH2	2:B:151:LEU:O	2.46	0.49
2:B:101:ARG:HB3	2:B:104:VAL:CG2	2.40	0.49
1:E:221:ASP:CB	5:E:601:FAD:H61A	2.25	0.49
1:E:528:VAL:HG12	1:E:566:MET:SD	2.52	0.49
1:I:528:VAL:HG12	1:I:566:MET:SD	2.52	0.49
1:I:532:PHE:CB	1:I:566:MET:HG3	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:155:CYS:HB3	8:J:302:SF4:S3	2.52	0.49
2:J:197:LEU:HD12	2:J:203:VAL:CG2	2.43	0.49
3:K:30:HIS:HD2	3:K:87:VAL:HB	1.75	0.49
1:A:236:MET:O	1:A:526:THR:HG23	2.12	0.49
1:A:57:LEU:HB2	1:A:116:GLN:NE2	2.28	0.49
1:A:167:LEU:HD21	1:A:183:LEU:HB2	1.95	0.49
1:A:528:VAL:HG12	1:A:566:MET:SD	2.52	0.49
3:C:31:ARG:HE	11:D:201:HEM:CGA	2.24	0.49
1:I:57:LEU:HB2	1:I:116:GLN:NE2	2.28	0.49
1:I:231:VAL:HG21	1:I:383:LEU:HD23	1.94	0.49
2:J:43:LYS:NZ	2:J:49:LEU:O	2.23	0.49
1:A:51:GLY:N	5:A:601:FAD:O4	2.37	0.48
1:A:165:TYR:O	1:A:182:ALA:HB1	2.13	0.48
1:E:57:LEU:HB2	1:E:116:GLN:NE2	2.28	0.48
1:E:532:PHE:CB	1:E:566:MET:HG3	2.40	0.48
2:F:197:LEU:HD12	2:F:203:VAL:HG22	1.94	0.48
1:I:167:LEU:HD21	1:I:183:LEU:HB2	1.95	0.48
1:I:367:GLN:OE1	1:I:422:SER:OG	2.15	0.48
2:B:210:MET:HE1	3:C:101:GLU:HA	1.95	0.48
3:C:128:VAL:HG13	3:C:129:TRP:CD1	2.48	0.48
1:E:62:GLU:HG2	1:E:62:GLU:O	2.11	0.48
1:E:140:ARG:HB3	1:E:143:HIS:HB3	1.94	0.48
1:E:187:THR:HG23	1:E:189:GLU:H	1.78	0.48
2:F:210:MET:HE1	3:G:101:GLU:HA	1.95	0.48
3:G:128:VAL:HG13	3:G:129:TRP:CD1	2.48	0.48
1:I:16:GLY:H	5:I:601:FAD:H4B	1.78	0.48
1:I:236:MET:O	1:I:526:THR:HG23	2.12	0.48
1:A:455:ASP:O	1:A:459:ILE:HG13	2.12	0.48
2:B:167:ASP:OD1	2:B:167:ASP:N	2.46	0.48
4:D:26:LEU:CD2	4:D:68:ILE:HG13	2.43	0.48
1:I:77:ASP:OD2	1:I:537:ARG:HG3	2.12	0.48
2:J:25:LEU:CB	2:J:42:LEU:HD21	2.43	0.48
1:A:187:THR:HG23	1:A:189:GLU:H	1.78	0.48
2:J:216:CYS:SG	2:J:220:LEU:HB2	2.53	0.48
4:D:14:HIS:NE2	4:D:18:LEU:HD11	2.29	0.48
1:I:46:THR:HG21	1:I:146:LEU:HD13	1.95	0.48
3:K:118:VAL:O	3:K:122:LEU:HD13	2.12	0.48
2:B:197:LEU:HD12	2:B:203:VAL:CG2	2.43	0.48
1:E:54:THR:HG23	1:E:122:GLN:NE2	2.29	0.48
1:I:6:ARG:HB3	1:I:8:PHE:HE2	1.77	0.48
1:I:86:GLU:OE2	1:I:577:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:7:ALA:HB2	4:L:77:TRP:CE2	2.49	0.48
1:A:16:GLY:H	5:A:601:FAD:H4B	1.78	0.48
1:A:542:ARG:NH2	1:A:544:ASP:OD2	2.47	0.48
1:E:51:GLY:N	5:E:601:FAD:O4	2.37	0.48
1:E:173:GLN:HE21	1:E:430:ARG:HH11	1.61	0.48
4:H:14:HIS:NE2	4:H:18:LEU:HD11	2.29	0.48
4:H:95:LEU:O	4:H:98:VAL:HG22	2.13	0.48
1:I:460:ARG:HB2	1:I:516:LEU:HD12	1.93	0.48
2:J:228:HIS:O	2:J:232:MET:HG3	2.12	0.48
4:L:20:ARG:HD2	4:L:20:ARG:N	2.28	0.48
1:A:8:PHE:O	1:A:195:ALA:HA	2.13	0.48
4:D:20:ARG:N	4:D:20:ARG:HD2	2.28	0.48
2:F:25:LEU:HB2	2:F:42:LEU:CD2	2.41	0.48
1:I:187:THR:HG23	1:I:189:GLU:H	1.79	0.48
2:J:167:ASP:OD1	2:J:167:ASP:N	2.46	0.48
4:L:95:LEU:O	4:L:98:VAL:HG22	2.13	0.48
1:A:26:ILE:HG12	1:A:416:GLY:HA2	1.95	0.48
1:A:54:THR:HG23	1:A:122:GLN:NE2	2.28	0.48
1:A:173:GLN:HE21	1:A:430:ARG:HH11	1.61	0.48
1:E:223:VAL:HG23	1:E:233:VAL:CG1	2.44	0.48
1:I:8:PHE:O	1:I:195:ALA:HA	2.13	0.48
4:L:83:TYR:OH	12:L:1201:UQ2:O1	2.18	0.48
3:C:90:ARG:HE	3:C:109:SER:CB	2.26	0.48
1:E:8:PHE:O	1:E:195:ALA:HA	2.13	0.48
1:E:165:TYR:O	1:E:182:ALA:HB1	2.13	0.48
2:F:234:LEU:HD22	4:H:17:ILE:HD11	1.94	0.48
1:I:185:ILE:O	1:I:506:PHE:HA	2.14	0.48
2:B:35:LEU:HD13	2:B:82:LEU:HD22	1.96	0.47
2:B:201:PHE:HE2	4:D:4:ASN:HD21	1.61	0.47
4:D:113:TRP:CH2	4:L:113:TRP:HA	2.48	0.47
1:I:70:TYR:CD2	1:I:126:PHE:HA	2.49	0.47
1:I:165:TYR:O	1:I:182:ALA:HB1	2.13	0.47
2:J:35:LEU:HD13	2:J:82:LEU:HD22	1.96	0.47
3:K:65:MET:SD	3:K:74:MET:HE3	2.54	0.47
3:C:65:MET:SD	3:C:74:MET:HE3	2.54	0.47
3:G:83:TYR:CB	3:G:117:THR:HG21	2.43	0.47
1:I:26:ILE:HG12	1:I:416:GLY:HA2	1.95	0.47
4:L:14:HIS:NE2	4:L:18:LEU:HD11	2.29	0.47
2:B:43:LYS:NZ	2:B:49:LEU:O	2.23	0.47
4:D:7:ALA:HB2	4:D:77:TRP:CE2	2.49	0.47
4:D:29:TYR:HA	4:D:60:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:54:SER:O	4:H:58:LYS:HE3	2.15	0.47
1:I:54:THR:HG23	1:I:122:GLN:NE2	2.29	0.47
1:I:542:ARG:NH2	1:I:544:ASP:OD2	2.47	0.47
4:L:29:TYR:HA	4:L:60:PHE:CZ	2.49	0.47
4:L:54:SER:O	4:L:58:LYS:HE3	2.15	0.47
1:A:43:ARG:NH2	2:B:61:GLY:O	2.46	0.47
3:C:88:GLY:O	3:C:92:MET:HG3	2.15	0.47
4:D:95:LEU:O	4:D:98:VAL:HG22	2.13	0.47
1:E:3:LEU:CD2	1:E:441:LEU:HD11	2.39	0.47
2:F:204:PHE:CD2	4:H:12:GLY:HA3	2.49	0.47
3:G:90:ARG:HE	3:G:109:SER:CB	2.26	0.47
4:H:102:VAL:O	4:H:106:ILE:HG13	2.15	0.47
1:I:107:SER:O	1:I:115:TYR:N	2.44	0.47
1:I:173:GLN:HE21	1:I:430:ARG:HH11	1.61	0.47
1:I:223:VAL:HG23	1:I:233:VAL:CG1	2.44	0.47
1:A:107:SER:O	1:A:115:TYR:N	2.44	0.47
2:F:35:LEU:HD13	2:F:82:LEU:HD22	1.96	0.47
2:F:121:LEU:CD1	2:F:186:ARG:HB3	2.44	0.47
3:K:128:VAL:HG13	3:K:129:TRP:CD1	2.48	0.47
1:A:86:GLU:OE2	1:A:577:LEU:HB2	2.14	0.47
1:A:206:GLY:HA3	1:A:214:ASN:ND2	2.30	0.47
1:A:223:VAL:HG23	1:A:233:VAL:CG1	2.44	0.47
1:E:16:GLY:H	5:E:601:FAD:H4B	1.78	0.47
1:I:357:MET:HE1	1:I:395:HIS:HB3	1.97	0.47
2:J:197:LEU:HG	2:J:197:LEU:O	2.14	0.47
2:B:218:LYS:HE2	2:B:218:LYS:HA	1.96	0.47
1:E:26:ILE:HG12	1:E:416:GLY:HA2	1.95	0.47
1:E:542:ARG:NH2	1:E:544:ASP:OD2	2.47	0.47
2:F:53:ARG:O	2:F:53:ARG:HG2	2.15	0.47
2:F:218:LYS:HA	2:F:218:LYS:HE2	1.96	0.47
3:G:88:GLY:O	3:G:92:MET:HG3	2.15	0.47
4:H:7:ALA:HB2	4:H:77:TRP:CE2	2.49	0.47
2:J:53:ARG:O	2:J:53:ARG:HG2	2.15	0.47
3:K:83:TYR:CB	3:K:117:THR:HG21	2.43	0.47
4:L:102:VAL:O	4:L:106:ILE:HG13	2.15	0.47
1:A:70:TYR:CD2	1:A:126:PHE:HA	2.49	0.47
1:A:240:GLN:HB3	1:A:355:TYR:HB3	1.97	0.47
1:A:357:MET:HE1	1:A:395:HIS:HB3	1.97	0.47
2:B:197:LEU:HG	2:B:197:LEU:O	2.14	0.47
1:E:70:TYR:CD2	1:E:126:PHE:HA	2.49	0.47
1:E:185:ILE:O	1:E:506:PHE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:MET:HE1	1:E:395:HIS:HB3	1.97	0.47
1:E:524:TYR:O	1:E:528:VAL:HG23	2.15	0.47
3:K:88:GLY:O	3:K:92:MET:HG3	2.15	0.47
1:A:185:ILE:O	1:A:506:PHE:HA	2.14	0.47
2:F:162:PHE:O	2:F:166:PRO:HG3	2.15	0.47
1:I:167:LEU:HD23	1:I:182:ALA:C	2.40	0.47
2:J:218:LYS:HE2	2:J:218:LYS:HA	1.96	0.47
11:K:201:HEM:HBC2	11:K:201:HEM:CHD	2.34	0.47
1:A:535:GLU:OE2	1:A:553:TRP:HB3	2.15	0.47
2:B:25:LEU:CB	2:B:42:LEU:HD21	2.43	0.47
4:H:29:TYR:HA	4:H:60:PHE:CZ	2.49	0.47
1:I:209:TYR:HB3	1:I:468:GLN:OE1	2.15	0.47
2:J:7:ILE:HD12	2:J:23:TYR:HD2	1.80	0.47
4:D:30:ILE:O	4:D:34:VAL:HG12	2.15	0.46
1:E:86:GLU:OE2	1:E:577:LEU:HB2	2.14	0.46
1:E:240:GLN:NE2	1:E:398:ASN:OD1	2.42	0.46
3:G:65:MET:SD	3:G:74:MET:HE3	2.54	0.46
4:L:25:VAL:HG11	4:L:63:LEU:CD2	2.45	0.46
4:L:30:ILE:O	4:L:34:VAL:HG12	2.15	0.46
1:A:167:LEU:HD21	1:A:183:LEU:CB	2.45	0.46
1:A:209:TYR:HB3	1:A:468:GLN:OE1	2.15	0.46
2:B:53:ARG:HG2	2:B:53:ARG:O	2.15	0.46
2:F:25:LEU:CB	2:F:42:LEU:HD21	2.43	0.46
4:H:25:VAL:HG11	4:H:63:LEU:CD2	2.46	0.46
1:I:240:GLN:HB3	1:I:355:TYR:HB3	1.97	0.46
2:B:7:ILE:HD12	2:B:23:TYR:HD2	1.80	0.46
2:B:162:PHE:O	2:B:166:PRO:HG3	2.15	0.46
1:E:47:VAL:HG21	2:F:60:CYS:HB3	1.96	0.46
1:E:98:GLU:O	1:E:102:MET:HG3	2.16	0.46
1:E:167:LEU:HD23	1:E:182:ALA:C	2.40	0.46
1:E:206:GLY:HA3	1:E:214:ASN:ND2	2.30	0.46
4:H:30:ILE:O	4:H:34:VAL:HG12	2.15	0.46
2:J:146:LEU:HD23	2:J:176:LEU:HD11	1.98	0.46
1:A:532:PHE:CB	1:A:566:MET:HG3	2.40	0.46
1:I:446:ARG:HD2	1:I:450:ASN:HD22	1.81	0.46
1:I:535:GLU:OE2	1:I:553:TRP:HB3	2.15	0.46
1:I:549:ASP:HB3	1:I:551:GLU:OE1	2.15	0.46
4:L:26:LEU:HD21	4:L:68:ILE:HG13	1.97	0.46
1:A:167:LEU:HD23	1:A:182:ALA:C	2.40	0.46
1:A:549:ASP:HB3	1:A:551:GLU:OE1	2.15	0.46
1:A:552:ASN:HB2	1:A:568:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:SER:O	4:D:58:LYS:HE3	2.15	0.46
1:E:240:GLN:HB3	1:E:355:TYR:HB3	1.97	0.46
1:E:446:ARG:HD2	1:E:450:ASN:HD22	1.81	0.46
2:F:197:LEU:HG	2:F:197:LEU:O	2.14	0.46
2:J:210:MET:HE1	3:K:101:GLU:HA	1.97	0.46
1:E:562:GLU:OE1	1:E:563:SER:HB3	2.16	0.46
1:I:206:GLY:HA3	1:I:214:ASN:ND2	2.30	0.46
1:I:359:GLY:HA3	1:I:389:ILE:O	2.15	0.46
1:I:562:GLU:OE1	1:I:563:SER:HB3	2.16	0.46
2:B:84:GLN:HB3	2:B:85:PRO:HD2	1.98	0.46
4:D:102:VAL:O	4:D:106:ILE:HG13	2.15	0.46
1:E:535:GLU:OE2	1:E:553:TRP:HB3	2.15	0.46
1:I:98:GLU:O	1:I:102:MET:HG3	2.16	0.46
1:E:176:ALA:HB1	1:E:381:PRO:HB2	1.98	0.46
1:E:552:ASN:HB2	1:E:568:ARG:HH12	1.81	0.46
1:I:83:ASP:OD1	1:I:84:ALA:N	2.49	0.46
1:I:167:LEU:HD21	1:I:183:LEU:CB	2.45	0.46
1:A:93:PRO:O	1:A:97:LEU:HD13	2.16	0.46
1:A:359:GLY:HA3	1:A:389:ILE:O	2.15	0.46
4:D:10:ARG:NH2	4:H:3:SER:HB3	2.29	0.46
4:D:45:TYR:CZ	4:D:49:ILE:HG13	2.51	0.46
1:E:187:THR:HG21	1:E:189:GLU:HG2	1.98	0.46
1:E:359:GLY:HA3	1:E:389:ILE:O	2.15	0.46
4:H:26:LEU:HD21	4:H:68:ILE:HG13	1.97	0.46
1:I:172:ASN:HB3	1:I:178:VAL:HG21	1.98	0.46
1:I:524:TYR:O	1:I:528:VAL:HG23	2.15	0.46
1:I:552:ASN:HB2	1:I:568:ARG:HH12	1.81	0.46
3:K:47:LEU:HD22	10:K:202:3PE:C26	2.46	0.46
2:B:121:LEU:CD1	2:B:186:ARG:HB3	2.44	0.46
4:D:26:LEU:HD21	4:D:68:ILE:HG13	1.97	0.46
4:D:115:VAL:HG22	4:D:115:VAL:OXT	2.16	0.46
1:I:79:ILE:HG23	1:I:556:HIS:HD2	1.81	0.46
1:I:108:ARG:HG3	2:J:135:GLN:HG3	1.98	0.46
1:A:47:VAL:CG1	1:A:146:LEU:HD23	2.46	0.45
1:A:446:ARG:HD2	1:A:450:ASN:HD22	1.81	0.45
3:C:58:PHE:CD2	4:D:45:TYR:HB2	2.51	0.45
4:D:25:VAL:HG11	4:D:63:LEU:CD2	2.45	0.45
2:F:7:ILE:HD12	2:F:23:TYR:HD2	1.80	0.45
3:G:13:LEU:O	3:G:15:LEU:HD12	2.16	0.45
1:I:392:VAL:O	1:I:392:VAL:HG22	2.17	0.45
3:K:52:LEU:HD11	4:L:52:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:90:ARG:HE	3:K:109:SER:CB	2.26	0.45
4:L:74:ILE:O	4:L:78:GLN:HG3	2.17	0.45
1:A:79:ILE:HG23	1:A:556:HIS:HD2	1.81	0.45
1:A:82:GLN:NE2	1:A:581:PHE:HD1	2.15	0.45
1:A:234:GLN:HG3	1:A:557:SER:O	2.17	0.45
1:A:488:LYS:HD3	1:A:524:TYR:HE1	1.81	0.45
1:A:562:GLU:OE1	1:A:563:SER:HB3	2.16	0.45
3:C:47:LEU:HD22	10:C:1301:3PE:C26	2.46	0.45
4:D:85:LYS:HD3	4:D:85:LYS:HA	1.79	0.45
1:E:167:LEU:HD21	1:E:183:LEU:CB	2.45	0.45
1:E:209:TYR:HB3	1:E:468:GLN:OE1	2.15	0.45
4:H:45:TYR:CZ	4:H:49:ILE:HG13	2.51	0.45
4:H:62:LEU:HD22	4:H:109:PHE:CD1	2.52	0.45
1:I:82:GLN:NE2	1:I:581:PHE:HD1	2.15	0.45
1:I:93:PRO:O	1:I:97:LEU:HD13	2.16	0.45
3:K:13:LEU:O	3:K:15:LEU:HD12	2.16	0.45
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.52	0.45
1:E:549:ASP:HB3	1:E:551:GLU:OE1	2.15	0.45
2:F:146:LEU:HD23	2:F:176:LEU:HD11	1.98	0.45
3:G:47:LEU:HD22	10:G:202:3PE:C26	2.46	0.45
2:J:65:LEU:HD23	2:J:91:ILE:HG23	1.98	0.45
2:J:162:PHE:O	2:J:166:PRO:HG3	2.16	0.45
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.52	0.45
3:K:40:ALA:HB1	3:K:77:ILE:CG2	2.47	0.45
1:A:524:TYR:O	1:A:528:VAL:HG23	2.15	0.45
2:B:2:ARG:O	2:B:2:ARG:HG3	2.17	0.45
3:C:40:ALA:HB1	3:C:77:ILE:CG2	2.47	0.45
1:E:234:GLN:HG3	1:E:557:SER:O	2.17	0.45
4:H:109:PHE:HA	4:H:112:VAL:HG22	1.98	0.45
4:L:45:TYR:CZ	4:L:49:ILE:HG13	2.51	0.45
4:L:85:LYS:HD3	4:L:85:LYS:HA	1.79	0.45
4:L:95:LEU:O	4:L:99:VAL:HG23	2.17	0.45
1:A:83:ASP:OD1	1:A:84:ALA:N	2.48	0.45
1:A:98:GLU:O	1:A:102:MET:HG3	2.16	0.45
1:A:536:SER:O	1:A:548:ARG:HB2	2.16	0.45
2:B:146:LEU:HD23	2:B:176:LEU:HD11	1.98	0.45
1:E:145:LEU:HD22	1:E:405:LEU:HD22	1.99	0.45
4:H:115:VAL:OXT	4:H:115:VAL:HG22	2.17	0.45
1:I:145:LEU:HD22	1:I:405:LEU:HD22	1.99	0.45
2:B:65:LEU:HD23	2:B:91:ILE:HG23	1.98	0.45
2:B:87:LYS:HE3	2:B:87:LYS:HB3	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:LEU:O	3:C:15:LEU:HD12	2.16	0.45
3:C:28:ILE:HD13	12:D:202:UQ2:C1	2.47	0.45
1:E:47:VAL:CG1	1:E:146:LEU:HD23	2.46	0.45
1:E:82:GLN:NE2	1:E:581:PHE:HD1	2.15	0.45
1:E:488:LYS:HD3	1:E:524:TYR:HE1	1.82	0.45
2:F:87:LYS:HE3	2:F:87:LYS:HB3	1.67	0.45
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.52	0.45
4:D:95:LEU:O	4:D:99:VAL:HG23	2.17	0.45
1:E:172:ASN:HB3	1:E:178:VAL:HG21	1.98	0.45
2:F:2:ARG:HG3	2:F:2:ARG:O	2.17	0.45
2:F:52:ARG:O	2:F:63:ASP:HB3	2.17	0.45
3:G:28:ILE:HD13	12:H:1201:UQ2:C1	2.47	0.45
1:I:460:ARG:HH11	1:I:516:LEU:HD12	1.82	0.45
4:L:115:VAL:HG22	4:L:115:VAL:OXT	2.16	0.45
4:D:22:THR:O	4:D:26:LEU:HG	2.17	0.45
1:E:79:ILE:HG23	1:E:556:HIS:HD2	1.81	0.45
1:E:105:PRO:HG3	2:F:180:ARG:NH2	2.32	0.45
2:F:201:PHE:HE2	4:H:4:ASN:HD21	1.64	0.45
4:H:10:ARG:HH21	4:L:3:SER:CB	2.26	0.45
4:H:19:VAL:CG2	4:H:74:ILE:HG21	2.47	0.45
4:L:109:PHE:HA	4:L:112:VAL:HG22	1.98	0.45
1:A:20:MET:HB2	1:A:153:ASN:HD21	1.82	0.45
1:A:171:LYS:HG3	1:A:177:VAL:HG13	1.99	0.45
1:A:172:ASN:HB3	1:A:178:VAL:HG21	1.98	0.45
4:D:10:ARG:HH21	4:H:3:SER:CB	2.26	0.45
4:D:62:LEU:HD22	4:D:109:PHE:CD1	2.52	0.45
3:G:40:ALA:HB1	3:G:77:ILE:CG2	2.47	0.45
4:H:72:ALA:O	4:H:76:MET:HG2	2.17	0.45
4:H:95:LEU:O	4:H:99:VAL:HG23	2.17	0.45
1:I:143:HIS:CE1	2:J:150:ILE:HG22	2.52	0.45
1:I:187:THR:HG21	1:I:189:GLU:HG2	1.98	0.45
2:J:52:ARG:O	2:J:63:ASP:HB3	2.17	0.45
1:A:54:THR:HG23	1:A:122:GLN:HE21	1.82	0.45
4:D:26:LEU:CB	11:D:201:HEM:HMC1	2.48	0.45
1:E:93:PRO:O	1:E:97:LEU:HD13	2.16	0.45
1:E:460:ARG:HH11	1:E:516:LEU:HD12	1.82	0.45
1:I:47:VAL:CG1	1:I:146:LEU:HD23	2.46	0.45
1:I:234:GLN:HG3	1:I:557:SER:O	2.17	0.45
2:J:84:GLN:HB3	2:J:85:PRO:HD2	1.98	0.45
2:J:164:TRP:HE1	12:L:1201:UQ2:H2M2	1.81	0.45
4:L:62:LEU:HD22	4:L:109:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD23	1:A:182:ALA:HA	1.99	0.44
1:A:176:ALA:HB1	1:A:381:PRO:HB2	1.98	0.44
2:B:164:TRP:HE1	12:D:202:UQ2:H2M2	1.82	0.44
1:E:83:ASP:OD1	1:E:84:ALA:N	2.48	0.44
1:E:167:LEU:HB2	1:E:181:THR:O	2.18	0.44
1:E:536:SER:O	1:E:548:ARG:HB2	2.16	0.44
3:G:58:PHE:CD2	4:H:45:TYR:HB2	2.51	0.44
1:I:20:MET:HB2	1:I:153:ASN:HD21	1.82	0.44
1:I:54:THR:HG23	1:I:122:GLN:HE21	1.82	0.44
4:L:22:THR:O	4:L:26:LEU:HG	2.17	0.44
2:B:100:ILE:HG23	3:C:9:ARG:CZ	2.48	0.44
4:D:19:VAL:CG2	4:D:74:ILE:HG21	2.47	0.44
4:D:87:LEU:HD22	2:J:235:GLN:HA	1.99	0.44
4:H:10:ARG:NH2	4:L:3:SER:HB3	2.29	0.44
4:H:74:ILE:O	4:H:78:GLN:HG3	2.17	0.44
1:I:167:LEU:HB2	1:I:181:THR:O	2.17	0.44
1:I:488:LYS:HD3	1:I:524:TYR:HE1	1.81	0.44
2:J:131:ARG:HB3	2:J:132:GLU:OE1	2.18	0.44
4:L:19:VAL:CG2	4:L:74:ILE:HG21	2.47	0.44
3:C:83:TYR:CB	3:C:117:THR:HG21	2.43	0.44
1:E:392:VAL:HG22	1:E:392:VAL:O	2.17	0.44
3:G:38:PHE:HE1	4:H:101:LEU:HD21	1.82	0.44
3:G:79:THR:HG23	3:G:121:SER:HB3	1.99	0.44
1:I:371:VAL:HB	1:I:375:GLY:HA2	1.99	0.44
1:A:167:LEU:HB2	1:A:181:THR:O	2.18	0.44
2:B:182:LEU:HG	2:B:193:ARG:HD2	2.00	0.44
1:E:494:LEU:HD23	1:E:494:LEU:C	2.42	0.44
1:I:176:ALA:HB1	1:I:381:PRO:HB2	1.98	0.44
1:I:494:LEU:HD23	1:I:494:LEU:C	2.42	0.44
1:I:536:SER:O	1:I:548:ARG:HB2	2.16	0.44
3:K:28:ILE:HD13	12:L:1201:UQ2:C1	2.47	0.44
4:L:44:THR:H	4:L:47:VAL:CG2	2.31	0.44
3:C:79:THR:HG23	3:C:121:SER:HB3	1.99	0.44
4:D:74:ILE:O	4:D:78:GLN:HG3	2.17	0.44
1:E:399:ARG:NH1	1:E:401:GLY:HA2	2.33	0.44
2:F:65:LEU:HD23	2:F:91:ILE:HG23	1.98	0.44
2:F:84:GLN:HB3	2:F:85:PRO:HD2	1.98	0.44
1:I:171:LYS:HG3	1:I:177:VAL:HG13	1.99	0.44
4:L:72:ALA:O	4:L:76:MET:HG2	2.17	0.44
2:B:52:ARG:O	2:B:63:ASP:HB3	2.17	0.44
4:D:109:PHE:HA	4:D:112:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:GLN:HG2	1:E:575:PRO:HD3	2.00	0.44
1:E:171:LYS:HG3	1:E:177:VAL:HG13	1.99	0.44
1:E:556:HIS:CD2	1:E:571:VAL:HG22	2.52	0.44
4:H:22:THR:O	4:H:26:LEU:HG	2.17	0.44
1:I:65:TRP:CZ3	1:I:86:GLU:HG3	2.53	0.44
1:I:167:LEU:HB2	1:I:181:THR:HG23	2.00	0.44
1:I:556:HIS:CD2	1:I:571:VAL:HG22	2.52	0.44
1:A:65:TRP:CZ3	1:A:86:GLU:HG3	2.53	0.44
1:A:82:GLN:HG2	1:A:575:PRO:HD3	2.00	0.44
4:D:44:THR:H	4:D:47:VAL:CG2	2.31	0.44
1:E:20:MET:HB2	1:E:153:ASN:HD21	1.82	0.44
1:E:167:LEU:HD23	1:E:182:ALA:HA	1.99	0.44
1:I:167:LEU:HD23	1:I:182:ALA:HA	1.99	0.44
2:J:182:LEU:HG	2:J:193:ARG:HD2	1.99	0.44
1:A:167:LEU:HB2	1:A:181:THR:HG23	2.00	0.44
1:A:392:VAL:O	1:A:392:VAL:HG22	2.17	0.44
2:B:214:SER:HB3	3:C:103:PHE:CE1	2.53	0.44
1:E:54:THR:HG23	1:E:122:GLN:HE21	1.82	0.44
1:E:232:PRO:HB2	1:E:558:LEU:CD1	2.48	0.44
1:A:187:THR:HG21	1:A:189:GLU:HG2	1.98	0.44
1:A:232:PRO:HB2	1:A:558:LEU:CD1	2.48	0.44
1:A:460:ARG:HH11	1:A:516:LEU:HD12	1.82	0.44
1:A:556:HIS:CD2	1:A:571:VAL:HG22	2.52	0.44
2:B:92:ARG:HB3	3:C:12:ASN:ND2	2.33	0.44
1:E:506:PHE:CE2	2:F:50:SER:HB3	2.53	0.44
4:H:44:THR:H	4:H:47:VAL:CG2	2.31	0.44
2:J:2:ARG:HG3	2:J:2:ARG:O	2.17	0.44
1:A:72:THR:HG22	1:A:85:ILE:HD13	2.00	0.43
2:B:36:LEU:O	2:B:40:ILE:HG13	2.18	0.43
4:D:72:ALA:O	4:D:76:MET:HG2	2.17	0.43
4:H:39:THR:O	4:H:39:THR:HG22	2.18	0.43
1:I:544:ASP:OD1	1:I:544:ASP:N	2.44	0.43
2:J:121:LEU:CD1	2:J:186:ARG:HB3	2.44	0.43
3:K:79:THR:HG23	3:K:121:SER:HB3	1.99	0.43
3:K:83:TYR:HD1	3:K:117:THR:HG21	1.84	0.43
1:A:100:GLU:HG3	1:A:114:ILE:HD11	2.00	0.43
1:A:486:GLN:O	1:A:490:ILE:HG23	2.18	0.43
2:B:131:ARG:HB3	2:B:132:GLU:OE1	2.18	0.43
1:E:486:GLN:O	1:E:490:ILE:HG23	2.18	0.43
1:E:490:ILE:CD1	1:E:520:MET:HE1	2.48	0.43
1:I:69:MET:HE3	1:I:86:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:GLN:HG2	1:I:575:PRO:HD3	2.00	0.43
1:I:488:LYS:HD3	1:I:524:TYR:CE1	2.54	0.43
1:A:55:VAL:CG1	1:A:57:LEU:HG	2.47	0.43
1:A:99:LEU:O	1:A:102:MET:HB2	2.18	0.43
1:A:374:LYS:HB3	1:A:376:GLU:OE1	2.18	0.43
4:D:113:TRP:HA	4:H:113:TRP:CH2	2.53	0.43
1:E:488:LYS:HD3	1:E:524:TYR:CE1	2.54	0.43
2:F:131:ARG:HB3	2:F:132:GLU:OE1	2.18	0.43
1:I:99:LEU:O	1:I:102:MET:HB2	2.18	0.43
1:I:212:THR:HA	1:I:352:THR:HG23	2.00	0.43
1:I:490:ILE:CD1	1:I:520:MET:HE1	2.48	0.43
1:E:65:TRP:CZ3	1:E:86:GLU:HG3	2.53	0.43
1:E:374:LYS:HB3	1:E:376:GLU:OE1	2.18	0.43
4:H:85:LYS:HD3	4:H:85:LYS:HA	1.79	0.43
1:E:176:ALA:HB2	1:E:381:PRO:HB2	2.00	0.43
1:E:200:LEU:HD13	1:E:383:LEU:CD1	2.48	0.43
1:E:490:ILE:HG13	1:E:520:MET:CE	2.44	0.43
1:I:176:ALA:HB2	1:I:381:PRO:HB2	2.00	0.43
1:I:200:LEU:HD13	1:I:383:LEU:CD1	2.48	0.43
2:J:214:SER:HB3	3:K:103:PHE:CE1	2.53	0.43
1:A:145:LEU:HD22	1:A:405:LEU:HD22	1.99	0.43
1:A:494:LEU:HD23	1:A:494:LEU:C	2.42	0.43
4:D:39:THR:O	4:D:39:THR:HG22	2.18	0.43
4:D:71:HIS:NE2	11:D:201:HEM:ND	2.67	0.43
1:E:205:ALA:HB2	1:E:220:GLY:CA	2.49	0.43
1:E:221:ASP:HB3	5:E:601:FAD:H61A	1.83	0.43
1:E:392:VAL:CG1	1:E:394:VAL:HG22	2.48	0.43
2:F:226:ILE:O	2:F:230:LYS:HG3	2.18	0.43
1:I:221:ASP:HB3	5:I:601:FAD:H61A	1.83	0.43
1:A:69:MET:HE3	1:A:86:GLU:HB2	2.00	0.43
1:A:184:CYS:O	1:A:188:GLY:N	2.48	0.43
1:A:371:VAL:HB	1:A:375:GLY:HA2	1.99	0.43
1:A:490:ILE:CD1	1:A:520:MET:HE1	2.48	0.43
2:B:226:ILE:O	2:B:230:LYS:HG3	2.18	0.43
4:D:10:ARG:HD2	4:H:3:SER:HB2	2.01	0.43
1:E:212:THR:HA	1:E:352:THR:HG23	2.01	0.43
1:E:371:VAL:HB	1:E:375:GLY:HA2	1.99	0.43
1:I:29:SER:O	1:I:29:SER:OG	2.33	0.43
1:I:59:ASN:ND2	1:I:114:ILE:HB	2.34	0.43
1:I:72:THR:HG22	1:I:85:ILE:HD13	2.00	0.43
1:I:100:GLU:HG3	1:I:114:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:486:GLN:O	1:I:490:ILE:HG23	2.19	0.43
1:A:29:SER:O	1:A:29:SER:OG	2.32	0.43
1:A:200:LEU:HD13	1:A:383:LEU:CD1	2.48	0.43
1:A:367:GLN:HG2	1:A:384:PHE:CE2	2.54	0.43
2:B:35:LEU:HD22	2:B:67:MET:SD	2.59	0.43
1:I:172:ASN:HB3	1:I:178:VAL:CG2	2.49	0.43
2:J:35:LEU:HD22	2:J:67:MET:SD	2.59	0.43
2:J:234:LEU:HD22	4:L:17:ILE:HD11	1.99	0.43
1:A:18:ALA:HB2	1:A:408:LEU:CB	2.48	0.43
1:A:488:LYS:HD3	1:A:524:TYR:CE1	2.54	0.43
4:D:69:LEU:CD1	4:D:101:LEU:HB3	2.49	0.43
1:E:99:LEU:O	1:E:102:MET:HB2	2.18	0.43
1:E:238:MET:SD	1:E:397:ALA:HA	2.59	0.43
1:E:506:PHE:HE2	2:F:50:SER:HB3	1.84	0.43
4:H:36:PHE:HE2	4:H:48:TRP:HZ3	1.67	0.43
1:I:18:ALA:HB2	1:I:408:LEU:CB	2.48	0.43
1:I:205:ALA:HB2	1:I:220:GLY:CA	2.49	0.43
1:A:238:MET:SD	1:A:397:ALA:HA	2.59	0.43
3:C:25:ILE:HA	3:C:28:ILE:HG22	2.00	0.43
2:F:36:LEU:O	2:F:40:ILE:HG13	2.18	0.43
1:I:374:LYS:HB3	1:I:376:GLU:OE1	2.18	0.43
4:L:39:THR:O	4:L:39:THR:HG22	2.17	0.43
1:A:406:LEU:HA	1:A:409:VAL:HG12	2.01	0.42
1:E:167:LEU:HB2	1:E:181:THR:HG23	2.00	0.42
1:E:210:GLN:H	1:E:468:GLN:HB2	1.84	0.42
1:E:367:GLN:HG2	1:E:384:PHE:CE2	2.54	0.42
2:F:182:LEU:HG	2:F:193:ARG:HD2	2.00	0.42
4:H:69:LEU:CD1	4:H:101:LEU:HB3	2.49	0.42
1:I:65:TRP:CH2	1:I:86:GLU:HG3	2.54	0.42
1:I:118:PRO:HG3	1:I:132:ALA:CB	2.47	0.42
2:J:87:LYS:HE3	2:J:87:LYS:HB3	1.67	0.42
1:A:82:GLN:NE2	1:A:580:ALA:HA	2.34	0.42
1:A:176:ALA:HB2	1:A:381:PRO:HB2	2.00	0.42
1:A:212:THR:HA	1:A:352:THR:HG23	2.00	0.42
2:B:226:ILE:HG22	2:B:230:LYS:NZ	2.35	0.42
3:C:29:LEU:HB3	3:C:83:TYR:CE2	2.55	0.42
3:C:83:TYR:HD1	3:C:117:THR:HG21	1.83	0.42
4:D:7:ALA:HB2	4:D:77:TRP:NE1	2.34	0.42
1:E:1:MET:O	1:E:1:MET:HE3	2.20	0.42
1:E:100:GLU:HG3	1:E:114:ILE:HD11	2.00	0.42
1:E:498:ARG:NH1	1:E:500:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:LEU:HD22	2:F:67:MET:SD	2.59	0.42
2:F:212:CYS:O	2:F:216:CYS:N	2.52	0.42
3:G:25:ILE:HA	3:G:28:ILE:HG22	2.00	0.42
1:I:210:GLN:H	1:I:468:GLN:HB2	1.85	0.42
2:J:36:LEU:O	2:J:40:ILE:HG13	2.19	0.42
2:J:226:ILE:O	2:J:230:LYS:HG3	2.19	0.42
3:K:54:SER:HB2	3:K:55:PRO:CD	2.49	0.42
4:L:11:ASN:OD1	4:L:13:VAL:N	2.53	0.42
2:F:7:ILE:HD12	2:F:23:TYR:CD2	2.54	0.42
4:H:11:ASN:OD1	4:H:13:VAL:N	2.53	0.42
1:I:15:ALA:HB2	1:I:35:LEU:HD21	2.01	0.42
1:I:232:PRO:HB2	1:I:558:LEU:CD1	2.48	0.42
1:I:367:GLN:HG2	1:I:384:PHE:CE2	2.54	0.42
1:I:406:LEU:HA	1:I:409:VAL:HG12	2.01	0.42
3:K:29:LEU:HB3	3:K:83:TYR:CE2	2.54	0.42
1:A:65:TRP:CH2	1:A:86:GLU:HG3	2.54	0.42
1:A:207:ARG:HD3	1:A:207:ARG:HA	1.88	0.42
1:A:476:GLU:O	1:A:480:MET:HG3	2.20	0.42
3:G:83:TYR:HD1	3:G:117:THR:HG21	1.83	0.42
4:H:7:ALA:HB2	4:H:77:TRP:NE1	2.34	0.42
1:I:203:GLY:H	1:I:389:ILE:HB	1.85	0.42
1:I:498:ARG:NH1	1:I:500:ASP:OD2	2.53	0.42
1:A:9:ASP:OD2	1:A:32:THR:HB	2.20	0.42
1:A:92:GLY:CA	1:A:406:LEU:HD11	2.49	0.42
1:A:172:ASN:HB3	1:A:178:VAL:CG2	2.49	0.42
1:A:205:ALA:HB2	1:A:220:GLY:CA	2.49	0.42
1:A:210:GLN:H	1:A:468:GLN:HB2	1.84	0.42
1:A:367:GLN:OE1	1:A:422:SER:OG	2.15	0.42
1:A:498:ARG:NH1	1:A:500:ASP:OD2	2.53	0.42
2:B:132:GLU:OE1	2:B:132:GLU:N	2.49	0.42
3:C:54:SER:HB2	3:C:55:PRO:CD	2.49	0.42
1:E:177:VAL:HG23	1:E:381:PRO:O	2.20	0.42
1:E:406:LEU:HA	1:E:409:VAL:HG12	2.01	0.42
1:E:409:VAL:HG13	1:E:410:VAL:HG23	2.02	0.42
1:E:447:TRP:CH2	1:E:497:ALA:HB3	2.55	0.42
1:I:82:GLN:NE2	1:I:580:ALA:HA	2.35	0.42
1:I:447:TRP:CH2	1:I:497:ALA:HB3	2.55	0.42
3:K:25:ILE:HA	3:K:28:ILE:HG22	2.00	0.42
3:K:38:PHE:HA	11:K:201:HEM:HMB3	2.01	0.42
3:K:111:LYS:HE3	3:K:111:LYS:HB3	1.94	0.42
1:A:26:ILE:HD13	1:A:419:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:O	1:A:409:VAL:HG12	2.20	0.42
1:E:405:LEU:O	1:E:409:VAL:HG12	2.20	0.42
3:G:54:SER:HB2	3:G:55:PRO:CD	2.49	0.42
1:I:9:ASP:OD2	1:I:32:THR:HB	2.20	0.42
1:A:25:GLN:HG2	1:A:413:ARG:O	2.20	0.42
1:A:167:LEU:HD23	1:A:183:LEU:N	2.35	0.42
1:A:221:ASP:HB3	5:A:601:FAD:H61A	1.83	0.42
1:A:240:GLN:NE2	1:A:398:ASN:OD1	2.42	0.42
1:E:172:ASN:HB3	1:E:178:VAL:CG2	2.49	0.42
1:E:559:TYR:HD1	1:E:566:MET:SD	2.43	0.42
1:I:183:LEU:HD23	1:I:184:CYS:C	2.45	0.42
1:I:213:THR:HG23	1:I:352:THR:CG2	2.50	0.42
1:I:476:GLU:O	1:I:480:MET:HG3	2.20	0.42
2:J:179:TYR:OH	2:J:183:ILE:HD12	2.20	0.42
1:A:15:ALA:HB2	1:A:35:LEU:HD21	2.01	0.42
1:A:392:VAL:CG1	1:A:394:VAL:HG22	2.48	0.42
1:E:15:ALA:HB2	1:E:35:LEU:HD21	2.01	0.42
1:E:57:LEU:HB2	1:E:116:GLN:HE22	1.85	0.42
1:E:65:TRP:CH2	1:E:86:GLU:HG3	2.54	0.42
1:E:72:THR:HG22	1:E:85:ILE:HD13	2.00	0.42
1:E:166:ALA:HA	1:E:182:ALA:HB2	2.02	0.42
3:G:29:LEU:HB3	3:G:83:TYR:CE2	2.54	0.42
1:I:1:MET:HE3	1:I:1:MET:O	2.19	0.42
1:I:26:ILE:HD13	1:I:419:LEU:HD22	2.01	0.42
1:I:223:VAL:HG11	1:I:522:THR:HG23	2.02	0.42
1:I:399:ARG:NH1	1:I:401:GLY:HA2	2.33	0.42
1:I:423:ILE:HA	1:I:426:GLN:HG2	2.02	0.42
2:J:7:ILE:HD12	2:J:23:TYR:CD2	2.54	0.42
1:A:183:LEU:HD23	1:A:184:CYS:C	2.45	0.42
1:A:447:TRP:CH2	1:A:497:ALA:HB3	2.55	0.42
1:A:559:TYR:HD1	1:A:566:MET:SD	2.43	0.42
3:C:38:PHE:HA	11:D:201:HEM:HMB3	2.01	0.42
1:E:26:ILE:HD13	1:E:419:LEU:HD22	2.01	0.42
3:G:38:PHE:CE1	4:H:101:LEU:HD21	2.55	0.42
1:I:166:ALA:HA	1:I:182:ALA:HB2	2.02	0.42
1:I:238:MET:HG2	1:I:540:HIS:HB2	2.02	0.42
1:I:405:LEU:O	1:I:409:VAL:HG12	2.20	0.42
1:I:446:ARG:HD2	1:I:446:ARG:O	2.20	0.42
1:A:59:ASN:ND2	1:A:114:ILE:HB	2.34	0.42
4:D:36:PHE:HE2	4:D:48:TRP:HZ3	1.67	0.42
1:E:59:ASN:ND2	1:E:114:ILE:HB	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:HIS:HE1	2:F:150:ILE:HG22	1.83	0.42
1:E:446:ARG:HD2	1:E:446:ARG:O	2.20	0.42
2:F:43:LYS:NZ	2:F:47:PRO:O	2.53	0.42
1:I:25:GLN:HG2	1:I:413:ARG:O	2.20	0.42
1:I:177:VAL:HG23	1:I:381:PRO:O	2.20	0.42
1:I:236:MET:HA	1:I:236:MET:CE	2.41	0.42
1:A:170:VAL:O	1:A:178:VAL:N	2.53	0.41
2:B:179:TYR:OH	2:B:183:ILE:HD12	2.20	0.41
1:E:9:ASP:OD2	1:E:32:THR:HB	2.20	0.41
1:E:25:GLN:HG3	1:E:416:GLY:C	2.45	0.41
1:E:69:MET:HE3	1:E:86:GLU:HB2	2.00	0.41
1:E:476:GLU:O	1:E:480:MET:HG3	2.20	0.41
2:F:226:ILE:HG22	2:F:230:LYS:NZ	2.34	0.41
3:G:38:PHE:HA	11:G:201:HEM:HMB3	2.01	0.41
1:I:55:VAL:CG1	1:I:57:LEU:HG	2.47	0.41
4:L:7:ALA:HB2	4:L:77:TRP:NE1	2.34	0.41
1:A:1:MET:HE3	1:A:1:MET:O	2.20	0.41
1:A:399:ARG:NH1	1:A:401:GLY:HA2	2.33	0.41
2:B:7:ILE:HD12	2:B:23:TYR:CD2	2.54	0.41
1:E:25:GLN:HG2	1:E:413:ARG:O	2.20	0.41
1:E:82:GLN:NE2	1:E:580:ALA:HA	2.35	0.41
1:E:167:LEU:HD23	1:E:183:LEU:N	2.35	0.41
1:E:183:LEU:HD23	1:E:184:CYS:C	2.45	0.41
1:E:223:VAL:HG11	1:E:522:THR:HG23	2.02	0.41
2:F:179:TYR:OH	2:F:183:ILE:HD12	2.20	0.41
3:G:111:LYS:HE3	3:G:111:LYS:HB3	1.94	0.41
11:G:201:HEM:HBC2	11:G:201:HEM:CHD	2.34	0.41
1:I:409:VAL:HG13	1:I:410:VAL:HG23	2.02	0.41
1:I:471:PHE:HE1	1:I:483:GLY:HA3	1.85	0.41
1:I:559:TYR:HD1	1:I:566:MET:SD	2.43	0.41
2:J:226:ILE:HG22	2:J:230:LYS:NZ	2.34	0.41
4:L:69:LEU:CD1	4:L:101:LEU:HB3	2.49	0.41
1:A:223:VAL:HG11	1:A:522:THR:HG23	2.01	0.41
1:E:92:GLY:CA	1:E:406:LEU:HD11	2.49	0.41
1:E:238:MET:HG2	1:E:540:HIS:HB2	2.02	0.41
1:I:25:GLN:HG3	1:I:416:GLY:C	2.45	0.41
1:A:177:VAL:HG23	1:A:381:PRO:O	2.19	0.41
1:A:238:MET:HG2	1:A:540:HIS:HB2	2.02	0.41
1:A:409:VAL:HG13	1:A:410:VAL:HG23	2.02	0.41
1:A:423:ILE:HA	1:A:426:GLN:HG2	2.02	0.41
1:A:446:ARG:HD2	1:A:446:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:PHE:HE1	4:D:101:LEU:HD21	1.84	0.41
1:E:203:GLY:H	1:E:389:ILE:HB	1.85	0.41
1:E:213:THR:HG23	1:E:352:THR:CG2	2.50	0.41
3:G:22:ILE:HD11	3:G:114:PHE:CE2	2.56	0.41
3:G:114:PHE:O	3:G:118:VAL:HG23	2.21	0.41
1:I:197:ALA:HB1	1:I:419:LEU:HD11	2.02	0.41
1:I:210:GLN:HB3	1:I:468:GLN:HG2	2.03	0.41
2:J:84:GLN:HG3	2:J:87:LYS:HZ1	1.86	0.41
2:J:212:CYS:O	2:J:216:CYS:N	2.52	0.41
3:K:22:ILE:HD11	3:K:114:PHE:CE2	2.56	0.41
1:A:213:THR:HG23	1:A:352:THR:CG2	2.50	0.41
1:I:238:MET:SD	1:I:397:ALA:HA	2.59	0.41
3:K:58:PHE:CD2	4:L:45:TYR:HB2	2.55	0.41
4:L:36:PHE:HE2	4:L:48:TRP:HZ3	1.67	0.41
1:A:97:LEU:C	1:A:101:HIS:HD1	2.24	0.41
1:A:143:HIS:CE1	2:B:150:ILE:HG22	2.55	0.41
1:A:236:MET:HA	1:A:236:MET:CE	2.42	0.41
1:A:471:PHE:HE1	1:A:483:GLY:HA3	1.85	0.41
4:D:11:ASN:OD1	4:D:13:VAL:N	2.53	0.41
5:E:601:FAD:H9	5:E:601:FAD:H1'1	1.87	0.41
3:K:83:TYR:CD1	3:K:117:THR:HG21	2.56	0.41
1:A:57:LEU:HB2	1:A:116:GLN:HE22	1.85	0.41
1:E:170:VAL:O	1:E:178:VAL:N	2.53	0.41
3:K:38:PHE:HE1	4:L:101:LEU:HD21	1.84	0.41
2:B:160:PRO:HB2	12:D:202:UQ2:H2M3	2.03	0.41
2:B:199:ASP:OD2	2:B:201:PHE:HB2	2.20	0.41
2:B:212:CYS:O	2:B:216:CYS:N	2.52	0.41
1:E:423:ILE:HA	1:E:426:GLN:HG2	2.02	0.41
2:F:231:SER:O	2:F:235:GLN:HG2	2.21	0.41
4:H:85:LYS:HB2	4:H:86:PRO:HD3	2.03	0.41
1:I:167:LEU:HD23	1:I:183:LEU:N	2.35	0.41
1:I:392:VAL:CG1	1:I:394:VAL:HG22	2.48	0.41
1:A:203:GLY:H	1:A:389:ILE:HB	1.85	0.41
3:C:114:PHE:O	3:C:118:VAL:HG23	2.21	0.41
4:D:42:GLU:OE2	4:D:42:GLU:HA	2.21	0.41
11:D:201:HEM:HBA2	11:D:201:HEM:HHA	2.03	0.41
1:E:197:ALA:HB1	1:E:419:LEU:HD11	2.02	0.41
1:E:236:MET:HA	1:E:236:MET:CE	2.41	0.41
1:E:471:PHE:HE1	1:E:483:GLY:HA3	1.85	0.41
2:F:70:LYS:HE3	2:F:215:VAL:HG12	2.02	0.41
2:F:101:ARG:HA	2:F:101:ARG:HD2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:ASP:OD2	2:F:201:PHE:HB2	2.20	0.41
4:H:10:ARG:HD2	4:L:3:SER:HB2	2.03	0.41
1:I:408:LEU:HD11	5:I:601:FAD:C5'	2.51	0.41
2:J:43:LYS:NZ	2:J:47:PRO:O	2.53	0.41
2:J:132:GLU:OE1	2:J:132:GLU:N	2.49	0.41
4:L:42:GLU:OE2	4:L:42:GLU:HA	2.21	0.41
1:A:25:GLN:HG3	1:A:416:GLY:C	2.45	0.41
1:A:197:ALA:HB1	1:A:419:LEU:HD11	2.02	0.41
2:B:99:VAL:O	3:C:9:ARG:HD3	2.21	0.41
4:D:106:ILE:HG22	4:L:59:VAL:CG2	2.51	0.41
2:F:92:ARG:HB3	3:G:12:ASN:ND2	2.36	0.41
1:I:38:LYS:HD3	1:I:515:GLU:OE2	2.21	0.41
1:I:219:THR:HA	1:I:519:LEU:CD2	2.47	0.41
11:K:201:HEM:HBA2	11:K:201:HEM:HHA	2.03	0.41
1:A:166:ALA:HA	1:A:182:ALA:HB2	2.02	0.40
1:A:362:THR:HG21	1:A:385:ALA:HB3	2.04	0.40
2:B:43:LYS:NZ	2:B:47:PRO:O	2.53	0.40
3:C:22:ILE:HD11	3:C:114:PHE:CE2	2.56	0.40
3:C:83:TYR:CD1	3:C:117:THR:HG21	2.56	0.40
1:E:66:GLU:HB3	1:E:578:ARG:NH1	2.36	0.40
1:E:184:CYS:O	1:E:188:GLY:N	2.48	0.40
1:I:47:VAL:HG21	2:J:60:CYS:HB3	2.03	0.40
1:I:407:ASP:OD1	1:I:411:PHE:CD2	2.75	0.40
4:L:85:LYS:HB2	4:L:86:PRO:HD3	2.03	0.40
2:B:231:SER:O	2:B:235:GLN:HG2	2.21	0.40
1:E:407:ASP:OD1	1:E:411:PHE:CD2	2.75	0.40
1:E:408:LEU:HD11	5:E:601:FAD:C5'	2.51	0.40
3:G:67:SER:O	3:G:71:LYS:HG2	2.21	0.40
1:I:57:LEU:HB2	1:I:116:GLN:HE22	1.85	0.40
2:J:121:LEU:O	2:J:122:LEU:HD23	2.22	0.40
2:J:199:ASP:OD2	2:J:201:PHE:HB2	2.21	0.40
1:A:38:LYS:HD3	1:A:515:GLU:OE2	2.21	0.40
1:A:40:PHE:CB	1:A:43:ARG:HH11	2.35	0.40
2:B:121:LEU:O	2:B:122:LEU:HD23	2.22	0.40
3:C:28:ILE:HG23	3:C:29:LEU:CD2	2.49	0.40
4:D:26:LEU:O	4:D:30:ILE:HG13	2.22	0.40
1:E:38:LYS:HD3	1:E:515:GLU:OE2	2.21	0.40
1:E:76:SER:HB2	1:E:396:GLY:HA3	2.03	0.40
1:E:118:PRO:HG3	1:E:132:ALA:CB	2.47	0.40
1:E:233:VAL:CG2	1:E:236:MET:HG3	2.51	0.40
2:F:100:ILE:HG23	3:G:9:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:26:LEU:O	4:H:30:ILE:HG13	2.22	0.40
3:K:114:PHE:O	3:K:118:VAL:HG23	2.21	0.40
1:A:15:ALA:CB	1:A:35:LEU:HD21	2.52	0.40
1:A:208:ILE:HD12	1:A:467:MET:HE2	2.04	0.40
1:E:362:THR:HG21	1:E:385:ALA:HB3	2.04	0.40
1:I:15:ALA:CB	1:I:35:LEU:HD21	2.52	0.40
2:J:19:ARG:NH2	2:J:21:GLN:HB2	2.37	0.40
2:J:71:ASN:ND2	2:J:158:SER:HB2	2.36	0.40
4:L:44:THR:HG23	4:L:46:GLU:H	1.87	0.40
1:A:407:ASP:OD1	1:A:411:PHE:CD2	2.74	0.40
4:D:44:THR:HG23	4:D:46:GLU:H	1.87	0.40
1:E:178:VAL:HG12	1:E:178:VAL:O	2.22	0.40
1:E:208:ILE:HD12	1:E:467:MET:HE2	2.04	0.40
2:F:52:ARG:HG3	2:F:104:VAL:HG12	2.04	0.40
2:F:99:VAL:O	3:G:9:ARG:HD3	2.22	0.40
2:F:214:SER:HB3	3:G:103:PHE:CE1	2.56	0.40
1:I:207:ARG:HA	1:I:207:ARG:HD3	1.88	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	477/588 (81%)	461 (97%)	16 (3%)	0	100	100
1	E	477/588 (81%)	461 (97%)	16 (3%)	0	100	100
1	I	477/588 (81%)	461 (97%)	16 (3%)	0	100	100
2	B	236/238 (99%)	224 (95%)	12 (5%)	0	100	100
2	F	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
2	J	236/238 (99%)	224 (95%)	12 (5%)	0	100	100
3	C	123/129 (95%)	123 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	123/129 (95%)	123 (100%)	0	0	100	100
3	K	123/129 (95%)	123 (100%)	0	0	100	100
4	D	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
4	H	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
4	L	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
All	All	2841/3210 (88%)	2740 (96%)	101 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	389/473 (82%)	386 (99%)	3 (1%)	73	88
1	E	389/473 (82%)	386 (99%)	3 (1%)	73	88
1	I	389/473 (82%)	386 (99%)	3 (1%)	73	88
2	B	208/208 (100%)	204 (98%)	4 (2%)	50	76
2	F	208/208 (100%)	204 (98%)	4 (2%)	50	76
2	J	208/208 (100%)	204 (98%)	4 (2%)	50	76
3	C	105/109 (96%)	104 (99%)	1 (1%)	68	86
3	G	105/109 (96%)	104 (99%)	1 (1%)	68	86
3	K	105/109 (96%)	104 (99%)	1 (1%)	68	86
4	D	94/96 (98%)	91 (97%)	3 (3%)	34	62
4	H	94/96 (98%)	91 (97%)	3 (3%)	34	62
4	L	94/96 (98%)	91 (97%)	3 (3%)	34	62
All	All	2388/2658 (90%)	2355 (99%)	33 (1%)	57	81

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	A	352	THR
1	A	437	VAL
2	B	87	LYS
2	B	138	GLU
2	B	141	GLU
2	B	231	SER
3	C	123	LEU
4	D	46	GLU
4	D	59	VAL
4	D	82	ASP
1	E	177	VAL
1	E	352	THR
1	E	437	VAL
2	F	87	LYS
2	F	138	GLU
2	F	141	GLU
2	F	231	SER
3	G	123	LEU
4	H	46	GLU
4	H	59	VAL
4	H	82	ASP
1	I	177	VAL
1	I	352	THR
1	I	437	VAL
2	J	87	LYS
2	J	138	GLU
2	J	141	GLU
2	J	231	SER
3	K	123	LEU
4	L	46	GLU
4	L	59	VAL
4	L	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	116	GLN
1	A	122	GLN
1	A	143	HIS
1	A	147	HIS
1	A	153	ASN

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Mol	Chain	Res	Type
1	A	173	GLN
1	A	234	GLN
1	A	242	HIS
1	A	354	HIS
1	A	450	ASN
1	A	452	ASN
1	A	470	ASN
1	A	572	ASN
2	B	68	ASN
2	B	133	HIS
2	B	237	ASN
3	C	91	HIS
4	D	4	ASN
1	E	82	GLN
1	E	116	GLN
1	E	122	GLN
1	E	143	HIS
1	E	147	HIS
1	E	153	ASN
1	E	173	GLN
1	E	234	GLN
1	E	242	HIS
1	E	354	HIS
1	E	450	ASN
1	E	452	ASN
1	E	470	ASN
1	E	572	ASN
2	F	68	ASN
2	F	71	ASN
2	F	207	HIS
2	F	237	ASN
3	G	91	HIS
4	H	4	ASN
1	I	82	GLN
1	I	116	GLN
1	I	122	GLN
1	I	143	HIS
1	I	147	HIS
1	I	153	ASN
1	I	173	GLN
1	I	234	GLN
1	I	242	HIS

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Mol	Chain	Res	Type
1	I	354	HIS
1	I	450	ASN
1	I	452	ASN
1	I	470	ASN
1	I	572	ASN
2	J	68	ASN
2	J	133	HIS
2	J	237	ASN
3	K	91	HIS
4	L	4	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
11	HEM	D	201	4,3	50,50,50	1.47	6 (12%)	67,82,82	1.18	4 (5%)
5	FAD	A	601	-	58,58,58	0.29	0	85,89,89	0.27	0
11	HEM	K	201	4,3	50,50,50	1.47	7 (14%)	67,82,82	1.19	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SF4	J	302	-	0,12,12	-	-	-		
8	SF4	F	302	-	0,12,12	-	-	-		
10	3PE	K	202	-	36,36,50	1.03	4 (11%)	39,41,55	1.13	2 (5%)
12	UQ2	D	202	-	23,23,23	2.75	6 (26%)	30,31,31	1.12	3 (10%)
12	UQ2	L	1201	-	23,23,23	2.74	7 (30%)	30,31,31	1.13	3 (10%)
12	UQ2	H	1201	-	23,23,23	2.75	6 (26%)	30,31,31	1.13	3 (10%)
9	F3S	B	303	2	0,9,9	-	-	-		
9	F3S	J	303	2	0,9,9	-	-	-		
5	FAD	I	601	-	58,58,58	0.29	0	85,89,89	0.27	0
8	SF4	B	302	-	0,12,12	-	-	-		
7	FES	B	301	2	0,4,4	-	-	-		
10	3PE	G	202	-	36,36,50	1.02	4 (11%)	39,41,55	1.12	2 (5%)
9	F3S	F	303	2	0,9,9	-	-	-		
5	FAD	E	601	-	58,58,58	0.29	0	85,89,89	0.27	0
11	HEM	G	201	3	50,50,50	1.47	8 (16%)	67,82,82	1.19	4 (5%)
7	FES	J	301	2	0,4,4	-	-	-		
10	3PE	C	1301	-	36,36,50	1.03	4 (11%)	39,41,55	1.12	2 (5%)
7	FES	F	301	2	0,4,4	-	-	-		

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
11	HEM	D	201	4,3	-	6/14/54/54	-
5	FAD	A	601	-	-	12/34/50/50	0/6/6/6
11	HEM	K	201	4,3	-	6/14/54/54	-
8	SF4	J	302	-	-	-	0/6/5/5
10	3PE	K	202	-	-	20/40/40/54	-
8	SF4	F	302	-	-	-	0/6/5/5
12	UQ2	D	202	-	-	5/15/39/39	0/1/1/1
12	UQ2	L	1201	-	-	5/15/39/39	0/1/1/1
12	UQ2	H	1201	-	-	5/15/39/39	0/1/1/1
9	F3S	B	303	2	-	-	0/3/3/3
9	F3S	J	303	2	-	-	0/3/3/3
5	FAD	I	601	-	-	13/34/50/50	0/6/6/6
8	SF4	B	302	-	-	-	0/6/5/5
7	FES	B	301	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	3PE	G	202	-	-	20/40/40/54	-
9	F3S	F	303	2	-	-	0/3/3/3
5	FAD	E	601	-	-	13/34/50/50	0/6/6/6
11	HEM	G	201	3	-	6/14/54/54	-
7	FES	J	301	2	-	-	0/1/1/1
10	3PE	C	1301	-	-	20/40/40/54	-
7	FES	F	301	2	-	-	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	1201	UQ2	C6-C5	10.34	1.53	1.35
12	D	202	UQ2	C6-C5	10.33	1.53	1.35
12	L	1201	UQ2	C6-C5	10.26	1.53	1.35
12	H	1201	UQ2	C3-C2	4.53	1.52	1.36
12	L	1201	UQ2	C3-C2	4.53	1.52	1.36
12	D	202	UQ2	C3-C2	4.53	1.52	1.36
11	D	201	HEM	FE-ND	3.61	2.06	1.94
11	G	201	HEM	FE-ND	3.61	2.06	1.94
11	K	201	HEM	FE-NB	3.59	2.06	1.94
11	K	201	HEM	FE-ND	3.59	2.06	1.94
11	G	201	HEM	FE-NB	3.57	2.05	1.94
11	D	201	HEM	FE-NB	3.56	2.05	1.94
11	K	201	HEM	FE-NA	3.53	2.06	1.95
11	D	201	HEM	FE-NA	3.52	2.06	1.95
11	G	201	HEM	FE-NA	3.50	2.06	1.95
11	D	201	HEM	FE-NC	3.19	2.05	1.95
11	K	201	HEM	FE-NC	3.18	2.05	1.95
11	G	201	HEM	FE-NC	3.18	2.05	1.95
11	G	201	HEM	CAB-C3B	2.89	1.55	1.47
11	D	201	HEM	CAB-C3B	2.88	1.55	1.47
11	K	201	HEM	CAB-C3B	2.88	1.55	1.47
11	D	201	HEM	CAC-C3C	2.87	1.55	1.47
11	G	201	HEM	CAC-C3C	2.86	1.55	1.47
11	K	201	HEM	CAC-C3C	2.83	1.55	1.47
10	K	202	3PE	O21-C2	-2.68	1.40	1.46
10	C	1301	3PE	O21-C2	-2.67	1.40	1.46
10	G	202	3PE	O21-C2	-2.64	1.40	1.46
10	C	1301	3PE	O31-C31	2.48	1.40	1.33
10	K	202	3PE	O31-C31	2.46	1.40	1.33
12	L	1201	UQ2	C6-C1	2.46	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	1201	UQ2	C6-C1	2.45	1.53	1.46
10	G	202	3PE	O31-C31	2.45	1.40	1.33
12	D	202	UQ2	C6-C1	2.45	1.53	1.46
12	D	202	UQ2	O3-CM3	-2.34	1.40	1.45
12	L	1201	UQ2	O3-CM3	-2.33	1.40	1.45
12	H	1201	UQ2	O3-CM3	-2.31	1.40	1.45
12	H	1201	UQ2	O2-CM2	-2.28	1.40	1.45
12	D	202	UQ2	O2-CM2	-2.25	1.40	1.45
12	L	1201	UQ2	O2-CM2	-2.25	1.40	1.45
10	C	1301	3PE	O31-C3	-2.14	1.40	1.45
10	K	202	3PE	O31-C3	-2.13	1.40	1.45
10	K	202	3PE	O21-C21	2.12	1.40	1.34
10	G	202	3PE	O31-C3	-2.12	1.40	1.45
10	C	1301	3PE	O21-C21	2.12	1.40	1.34
10	G	202	3PE	O21-C21	2.11	1.40	1.34
12	D	202	UQ2	O1-C1	-2.04	1.18	1.23
11	K	201	HEM	CMB-C2B	2.02	1.54	1.50
12	H	1201	UQ2	O1-C1	-2.02	1.18	1.23
12	L	1201	UQ2	O4-C4	-2.01	1.18	1.23
12	L	1201	UQ2	O1-C1	-2.01	1.18	1.23
11	G	201	HEM	CMC-C2C	2.01	1.54	1.50
11	G	201	HEM	CMA-C3A	2.01	1.54	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	202	3PE	O21-C21-C22	3.89	119.89	111.48
10	C	1301	3PE	O21-C21-C22	3.87	119.85	111.48
10	G	202	3PE	O21-C21-C22	3.85	119.80	111.48
10	G	202	3PE	O31-C31-C32	2.78	120.31	111.83
10	K	202	3PE	O31-C31-C32	2.77	120.29	111.83
10	C	1301	3PE	O31-C31-C32	2.77	120.28	111.83
11	G	201	HEM	C3B-C2B-C1B	2.66	108.41	106.41
11	D	201	HEM	C3B-C2B-C1B	2.65	108.40	106.41
11	K	201	HEM	C3B-C2B-C1B	2.65	108.40	106.41
11	K	201	HEM	C1B-NB-C4B	2.57	108.25	105.21
11	G	201	HEM	C1B-NB-C4B	2.56	108.24	105.21
11	G	201	HEM	C3B-C4B-NB	-2.54	107.64	109.47
11	D	201	HEM	C1B-NB-C4B	2.54	108.21	105.21
11	K	201	HEM	C3B-C4B-NB	-2.52	107.66	109.47
11	D	201	HEM	C3B-C4B-NB	-2.48	107.69	109.47
11	G	201	HEM	C4D-ND-C1D	2.31	107.94	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	1201	UQ2	C7-C6-C5	-2.30	120.95	124.89
11	K	201	HEM	C4D-ND-C1D	2.30	107.93	105.21
12	D	202	UQ2	C7-C6-C5	-2.29	120.96	124.89
12	H	1201	UQ2	C7-C6-C5	-2.28	120.98	124.89
11	D	201	HEM	C4D-ND-C1D	2.27	107.90	105.21
12	H	1201	UQ2	CM5-C5-C6	-2.23	120.78	124.45
12	L	1201	UQ2	C7-C8-C9	-2.22	123.01	126.83
12	D	202	UQ2	CM5-C5-C6	-2.21	120.82	124.45
12	H	1201	UQ2	C7-C8-C9	-2.21	123.03	126.83
12	D	202	UQ2	C7-C8-C9	-2.21	123.03	126.83
12	L	1201	UQ2	CM5-C5-C6	-2.19	120.85	124.45

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	C5B-O5B-PA-O1A
5	A	601	FAD	C5B-O5B-PA-O3P
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	C2'-C3'-C4'-O4'
5	A	601	FAD	O3'-C3'-C4'-O4'
5	A	601	FAD	O3'-C3'-C4'-C5'
5	E	601	FAD	C5B-O5B-PA-O1A
5	E	601	FAD	C5B-O5B-PA-O3P
5	E	601	FAD	N10-C1'-C2'-O2'
5	E	601	FAD	N10-C1'-C2'-C3'
5	E	601	FAD	C2'-C3'-C4'-O4'
5	E	601	FAD	O3'-C3'-C4'-O4'
5	E	601	FAD	O3'-C3'-C4'-C5'
5	I	601	FAD	C5B-O5B-PA-O1A
5	I	601	FAD	C5B-O5B-PA-O3P
5	I	601	FAD	N10-C1'-C2'-O2'
5	I	601	FAD	N10-C1'-C2'-C3'
5	I	601	FAD	C2'-C3'-C4'-O4'
5	I	601	FAD	O3'-C3'-C4'-O4'
5	I	601	FAD	O3'-C3'-C4'-C5'
10	C	1301	3PE	C1-O11-P-O12
10	C	1301	3PE	C1-O11-P-O13
10	C	1301	3PE	C1-O11-P-O14
10	C	1301	3PE	C11-O13-P-O11
10	C	1301	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
10	C	1301	3PE	C11-O13-P-O14
10	C	1301	3PE	O13-C11-C12-N
10	G	202	3PE	C1-O11-P-O12
10	G	202	3PE	C1-O11-P-O13
10	G	202	3PE	C1-O11-P-O14
10	G	202	3PE	C11-O13-P-O11
10	G	202	3PE	C11-O13-P-O12
10	G	202	3PE	C11-O13-P-O14
10	G	202	3PE	O13-C11-C12-N
10	K	202	3PE	C1-O11-P-O12
10	K	202	3PE	C1-O11-P-O13
10	K	202	3PE	C1-O11-P-O14
10	K	202	3PE	C11-O13-P-O11
10	K	202	3PE	C11-O13-P-O12
10	K	202	3PE	C11-O13-P-O14
10	K	202	3PE	O13-C11-C12-N
11	D	201	HEM	C1A-C2A-CAA-CBA
11	G	201	HEM	C1A-C2A-CAA-CBA
11	K	201	HEM	C1A-C2A-CAA-CBA
5	A	601	FAD	C2'-C3'-C4'-C5'
5	E	601	FAD	C2'-C3'-C4'-C5'
5	I	601	FAD	C2'-C3'-C4'-C5'
10	C	1301	3PE	C21-C22-C23-C24
10	G	202	3PE	C21-C22-C23-C24
10	K	202	3PE	C21-C22-C23-C24
10	C	1301	3PE	C28-C29-C2A-C2B
10	G	202	3PE	C28-C29-C2A-C2B
10	K	202	3PE	C28-C29-C2A-C2B
5	A	601	FAD	O4B-C4B-C5B-O5B
5	A	601	FAD	C3B-C4B-C5B-O5B
5	E	601	FAD	O4B-C4B-C5B-O5B
5	E	601	FAD	C3B-C4B-C5B-O5B
5	I	601	FAD	O4B-C4B-C5B-O5B
5	I	601	FAD	C3B-C4B-C5B-O5B
10	C	1301	3PE	C22-C21-O21-C2
10	G	202	3PE	C22-C21-O21-C2
10	K	202	3PE	C22-C21-O21-C2
10	C	1301	3PE	C36-C37-C38-C39
10	G	202	3PE	C36-C37-C38-C39
10	K	202	3PE	C36-C37-C38-C39
10	C	1301	3PE	O22-C21-O21-C2
10	G	202	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
10	K	202	3PE	O22-C21-O21-C2
11	D	201	HEM	C4B-C3B-CAB-CBB
11	D	201	HEM	C4C-C3C-CAC-CBC
11	G	201	HEM	C4B-C3B-CAB-CBB
11	G	201	HEM	C4C-C3C-CAC-CBC
11	K	201	HEM	C4B-C3B-CAB-CBB
11	K	201	HEM	C4C-C3C-CAC-CBC
10	C	1301	3PE	C34-C35-C36-C37
10	G	202	3PE	C34-C35-C36-C37
10	K	202	3PE	C34-C35-C36-C37
11	D	201	HEM	C3A-C2A-CAA-CBA
11	G	201	HEM	C3A-C2A-CAA-CBA
11	K	201	HEM	C3A-C2A-CAA-CBA
10	C	1301	3PE	C1-C2-C3-O31
10	G	202	3PE	C1-C2-C3-O31
10	K	202	3PE	C1-C2-C3-O31
12	D	202	UQ2	C1-C6-C7-C8
12	H	1201	UQ2	C1-C6-C7-C8
12	L	1201	UQ2	C1-C6-C7-C8
12	D	202	UQ2	C12-C11-C9-C10
12	H	1201	UQ2	C12-C11-C9-C10
12	L	1201	UQ2	C12-C11-C9-C10
10	C	1301	3PE	O21-C2-C3-O31
10	G	202	3PE	O21-C2-C3-O31
10	K	202	3PE	O21-C2-C3-O31
5	A	601	FAD	C5B-O5B-PA-O2A
5	E	601	FAD	C5B-O5B-PA-O2A
5	I	601	FAD	C5B-O5B-PA-O2A
12	D	202	UQ2	C9-C11-C12-C13
12	H	1201	UQ2	C9-C11-C12-C13
12	L	1201	UQ2	C9-C11-C12-C13
12	D	202	UQ2	C5-C6-C7-C8
12	H	1201	UQ2	C5-C6-C7-C8
12	L	1201	UQ2	C5-C6-C7-C8
12	D	202	UQ2	C12-C11-C9-C8
12	H	1201	UQ2	C12-C11-C9-C8
12	L	1201	UQ2	C12-C11-C9-C8
10	C	1301	3PE	C23-C24-C25-C26
10	K	202	3PE	C23-C24-C25-C26
10	G	202	3PE	C23-C24-C25-C26
10	C	1301	3PE	O11-C1-C2-C3
10	G	202	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	K	202	3PE	O11-C1-C2-C3
10	G	202	3PE	C35-C36-C37-C38
10	C	1301	3PE	C35-C36-C37-C38
11	G	201	HEM	CAD-CBD-CGD-O2D
10	K	202	3PE	C35-C36-C37-C38
11	D	201	HEM	CAD-CBD-CGD-O2D
11	K	201	HEM	CAD-CBD-CGD-O2D
10	C	1301	3PE	C24-C25-C26-C27
10	G	202	3PE	C24-C25-C26-C27
10	K	202	3PE	C24-C25-C26-C27
11	D	201	HEM	CAD-CBD-CGD-O1D
11	G	201	HEM	CAD-CBD-CGD-O1D
11	K	201	HEM	CAD-CBD-CGD-O1D
10	G	202	3PE	C22-C23-C24-C25
10	C	1301	3PE	C22-C23-C24-C25
10	K	202	3PE	C22-C23-C24-C25
5	E	601	FAD	C4B-C5B-O5B-PA
5	I	601	FAD	C4B-C5B-O5B-PA
5	A	601	FAD	PA-O3P-P-O2P
5	E	601	FAD	PA-O3P-P-O2P
5	I	601	FAD	PA-O3P-P-O2P

There are no ring outliers.

18 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	201	HEM	11	0
5	A	601	FAD	5	0
11	K	201	HEM	10	0
8	J	302	SF4	3	0
8	F	302	SF4	3	0
10	K	202	3PE	4	0
12	D	202	UQ2	4	0
12	L	1201	UQ2	3	0
12	H	1201	UQ2	2	0
5	I	601	FAD	6	0
8	B	302	SF4	3	0
7	B	301	FES	1	0
10	G	202	3PE	4	0
5	E	601	FAD	7	0
11	G	201	HEM	9	0
7	J	301	FES	1	0

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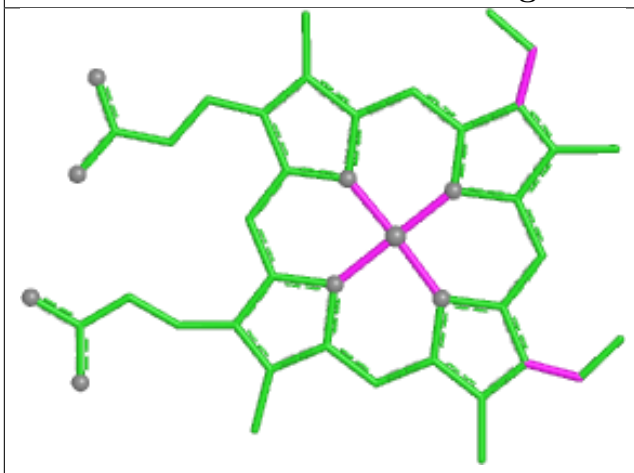
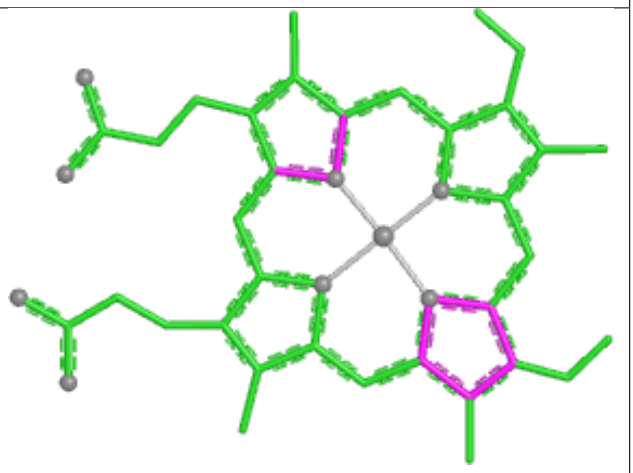
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1301	3PE	4	0
7	F	301	FES	1	0

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

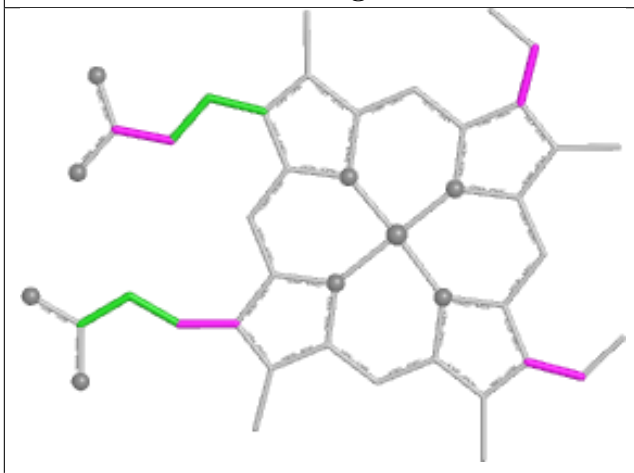
Ligand HEM D 201



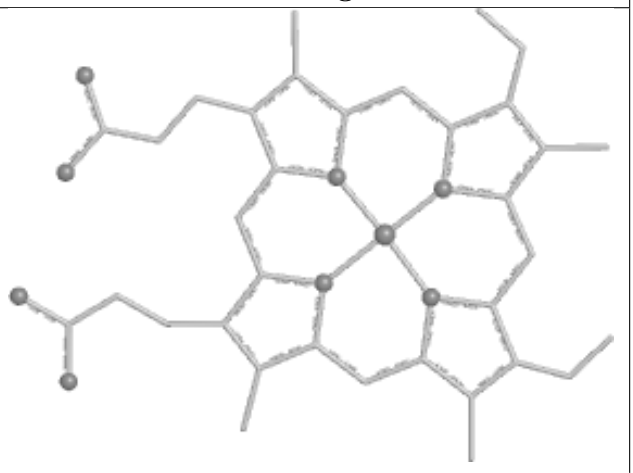
Bond lengths



Bond angles

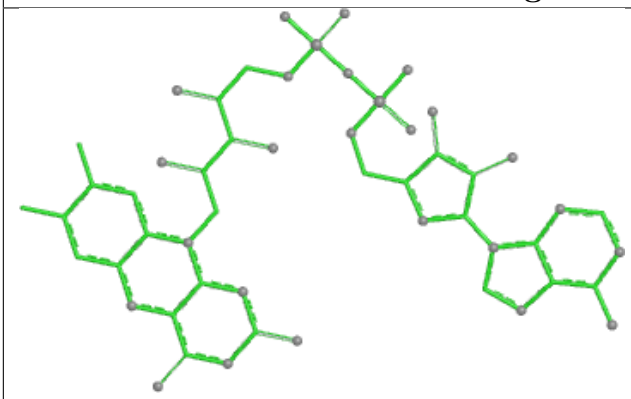


Torsions

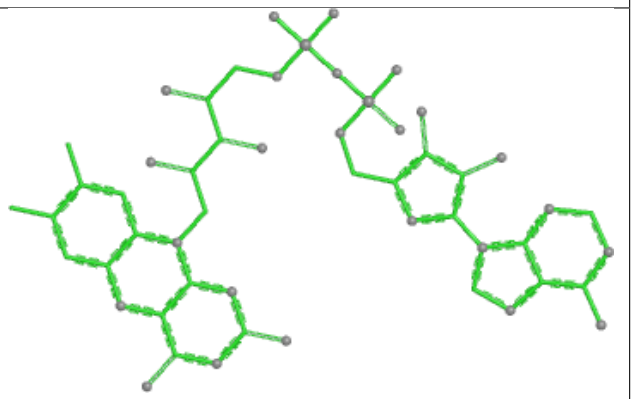


Rings

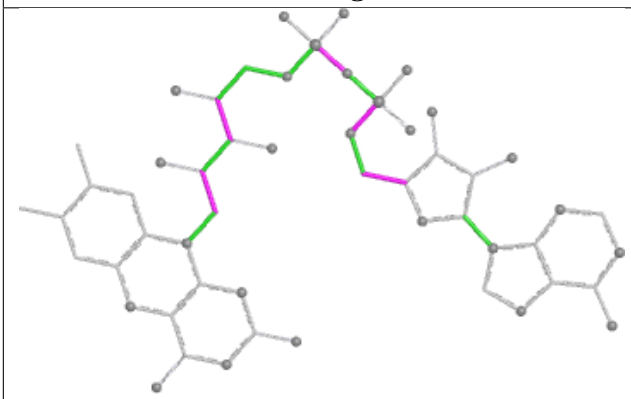
Ligand FAD A 601



Bond lengths



Bond angles



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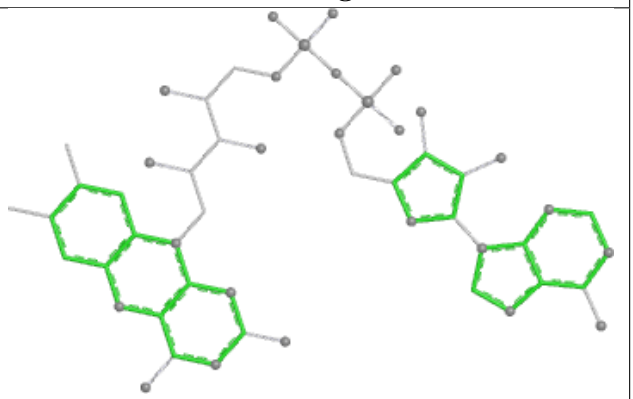
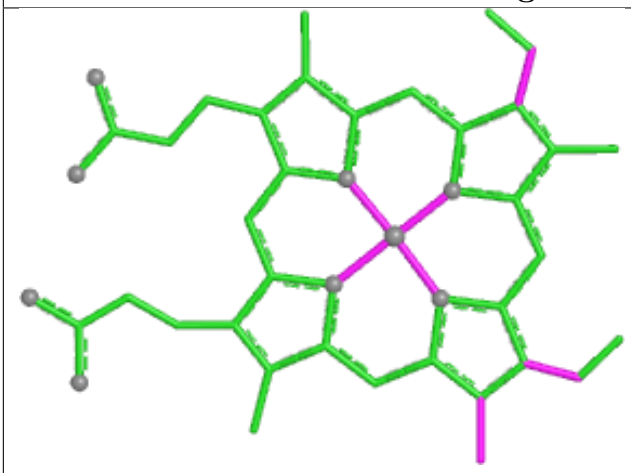
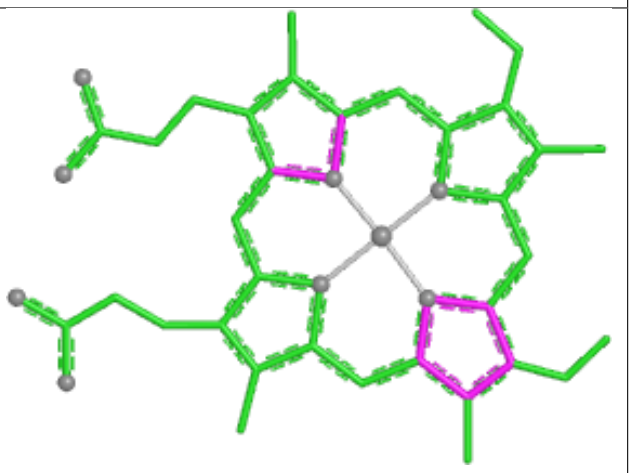


Rings

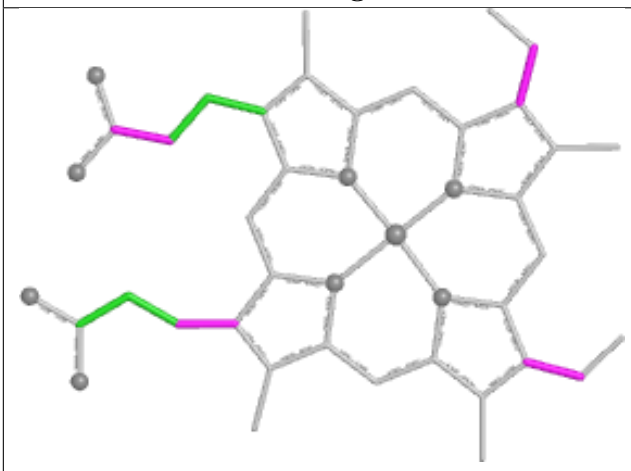
Ligand HEM K 201



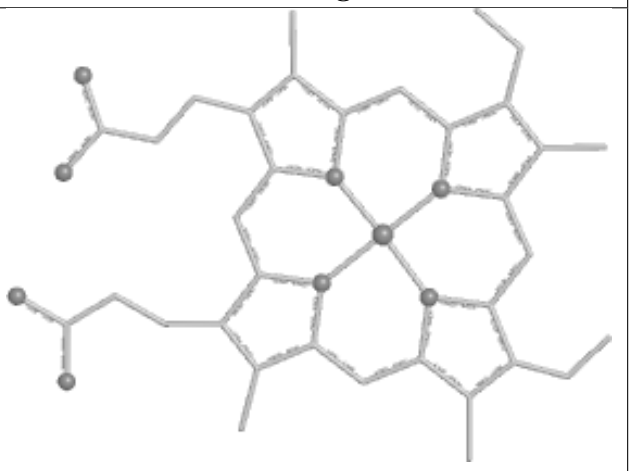
Bond lengths



Bond angles

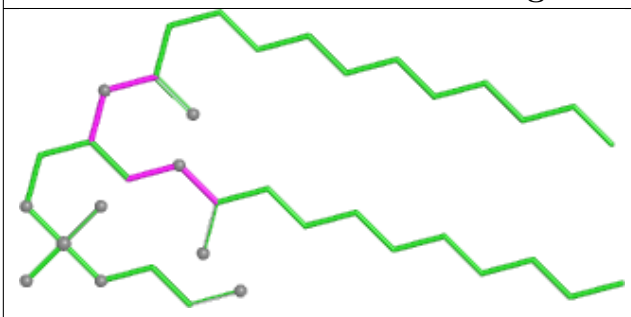


Torsions

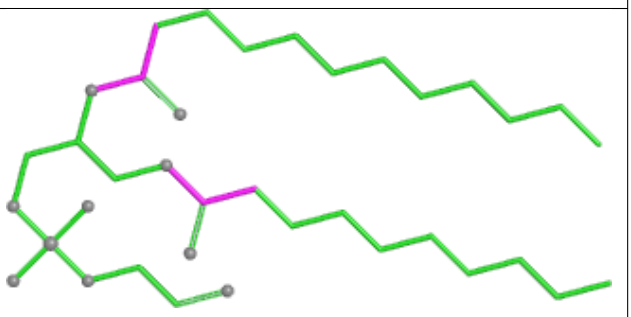


Rings

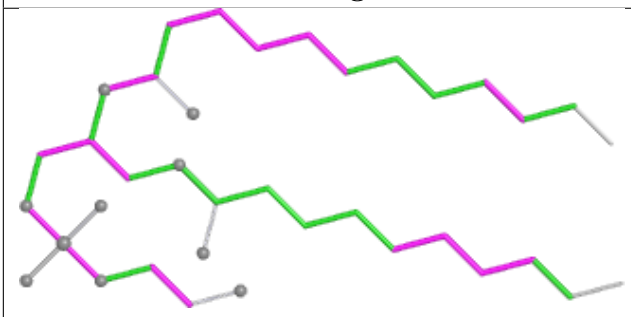
Ligand 3PE K 202



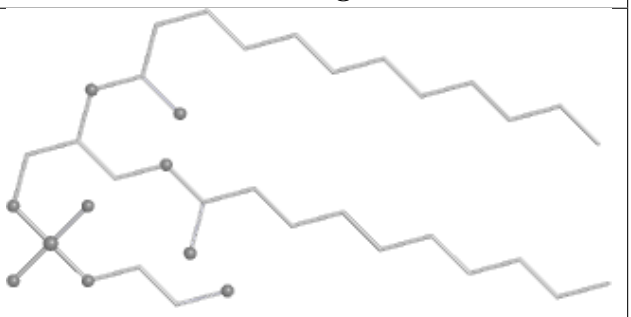
Bond lengths



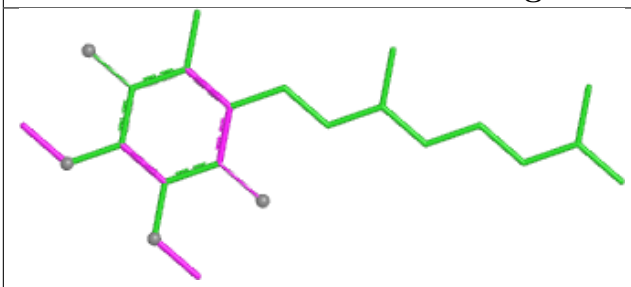
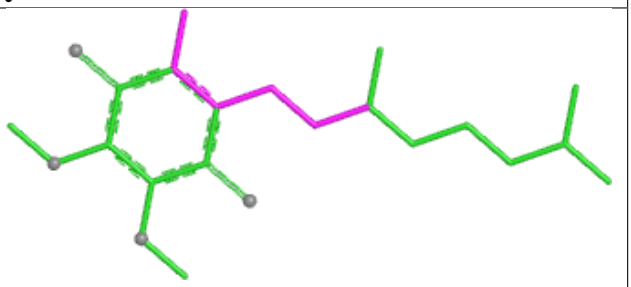
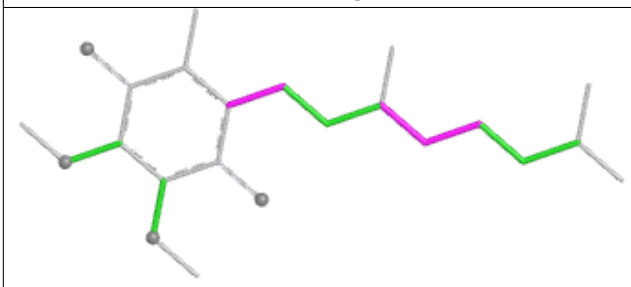
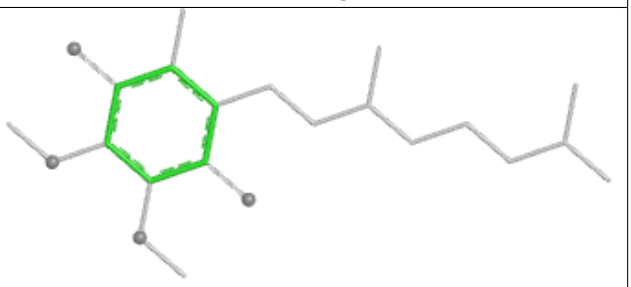
Bond angles

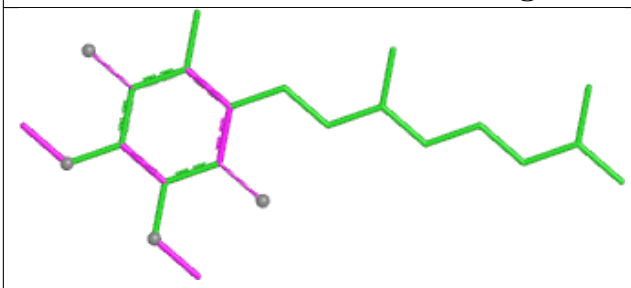
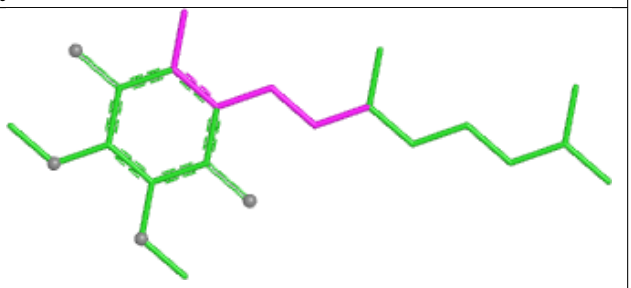
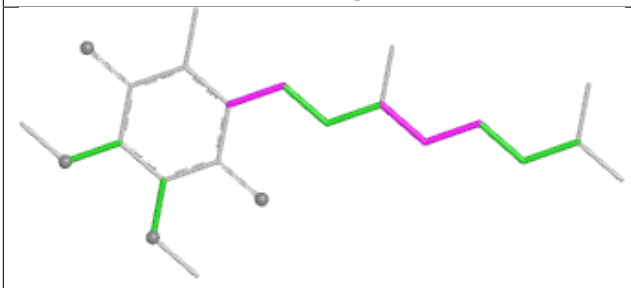
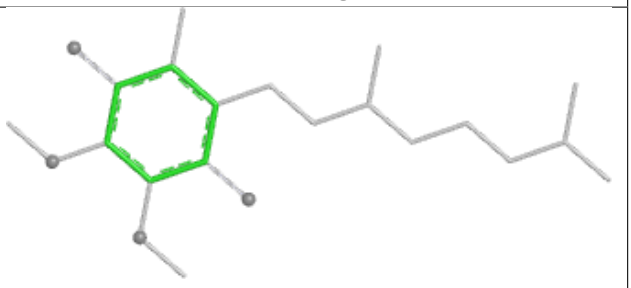


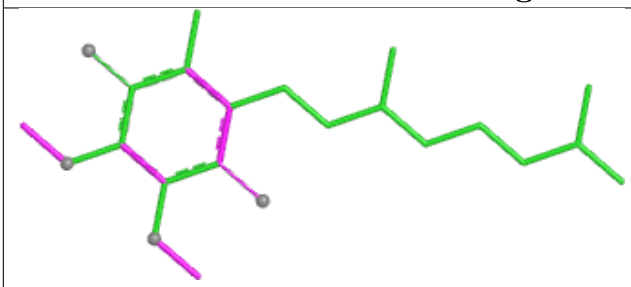
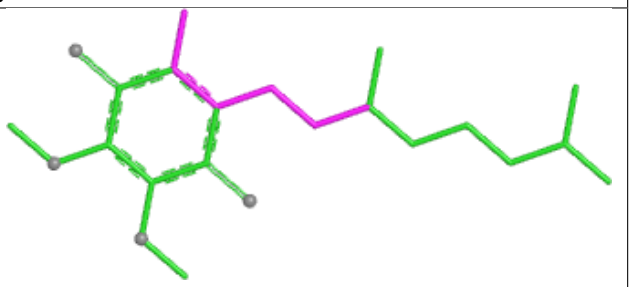
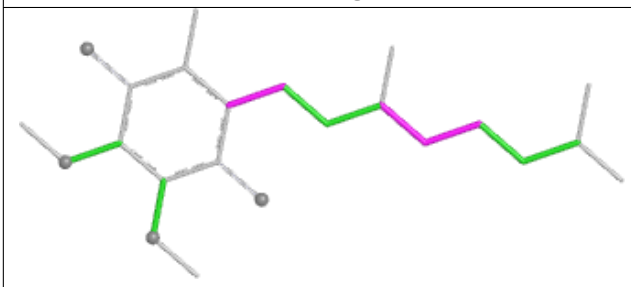
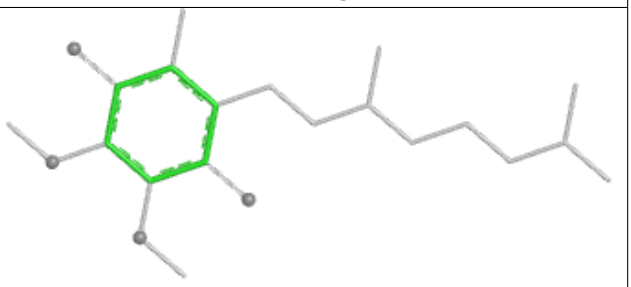
Torsions

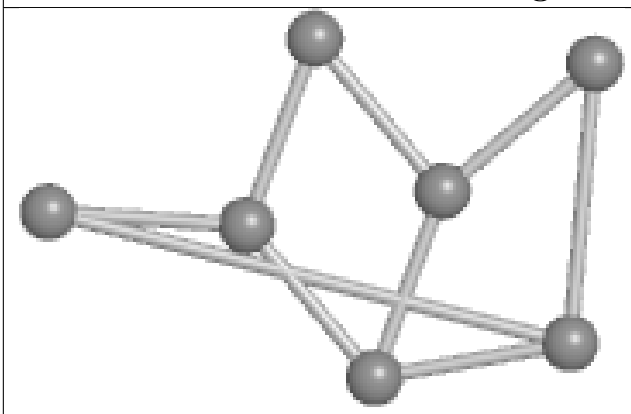
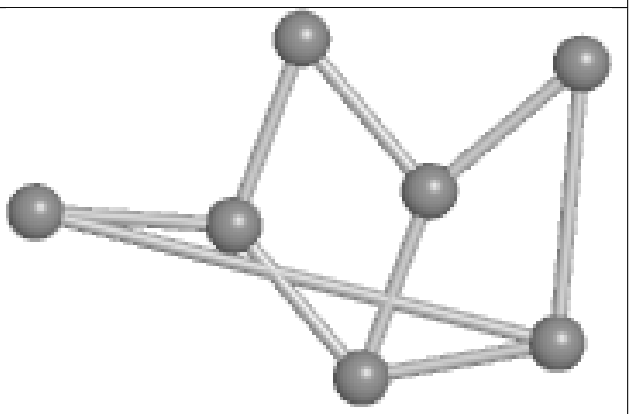
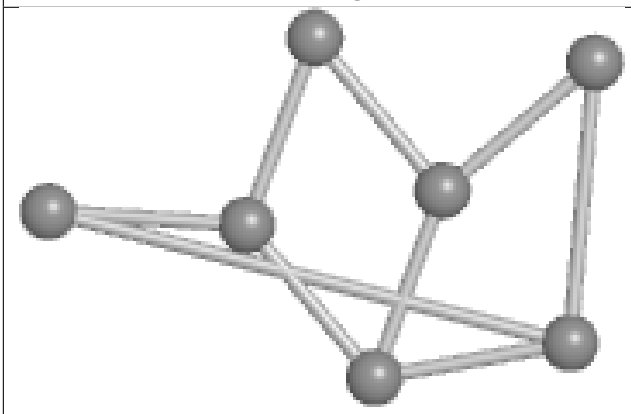
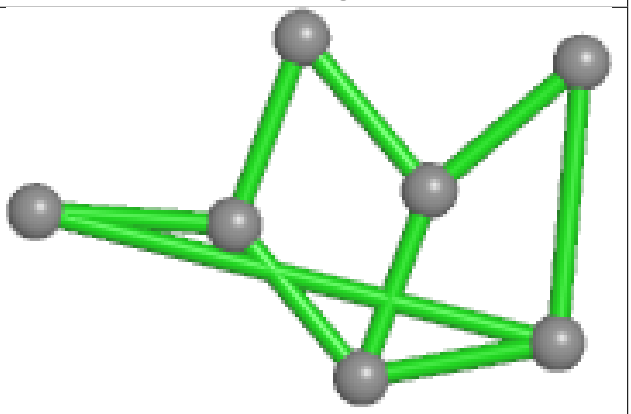


Rings

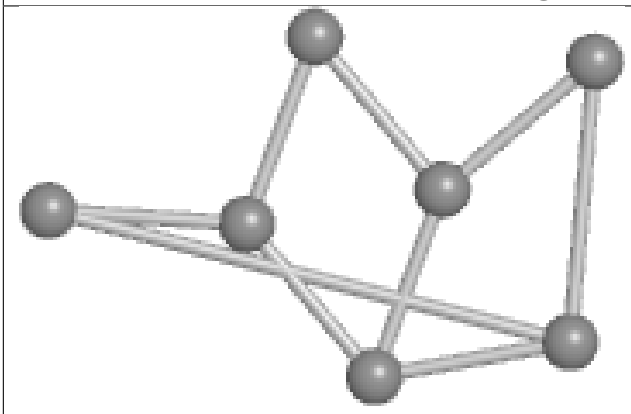
Ligand UQ2 D 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ2 L 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

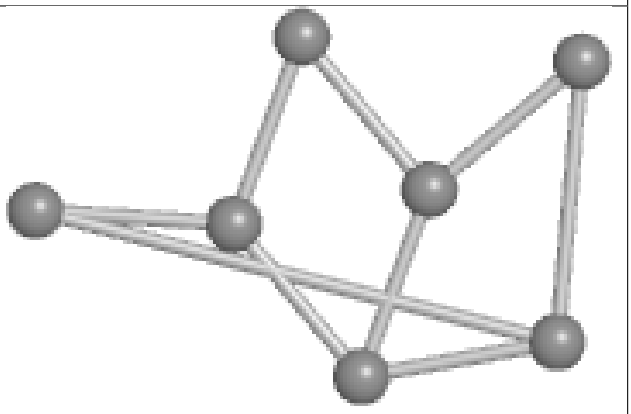
Ligand UQ2 H 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand F3S B 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

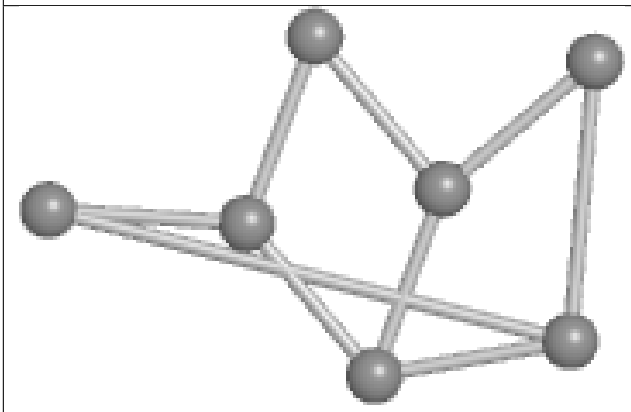
Ligand F3S J 303



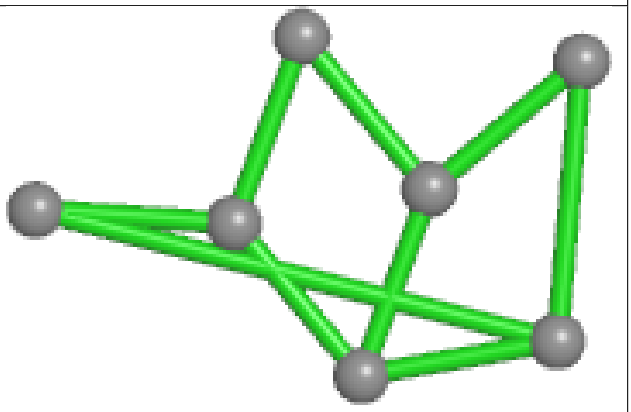
Bond lengths



Bond angles

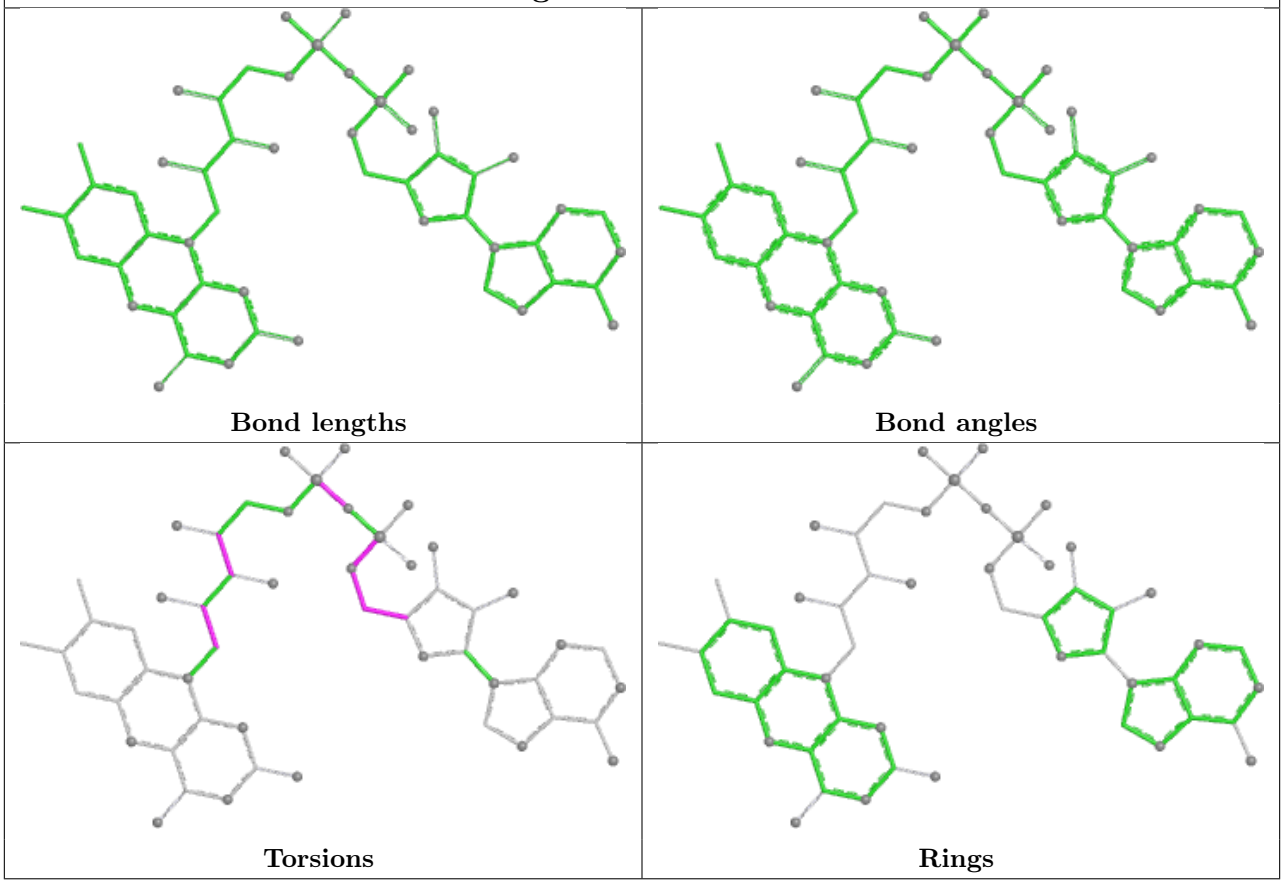


Torsions

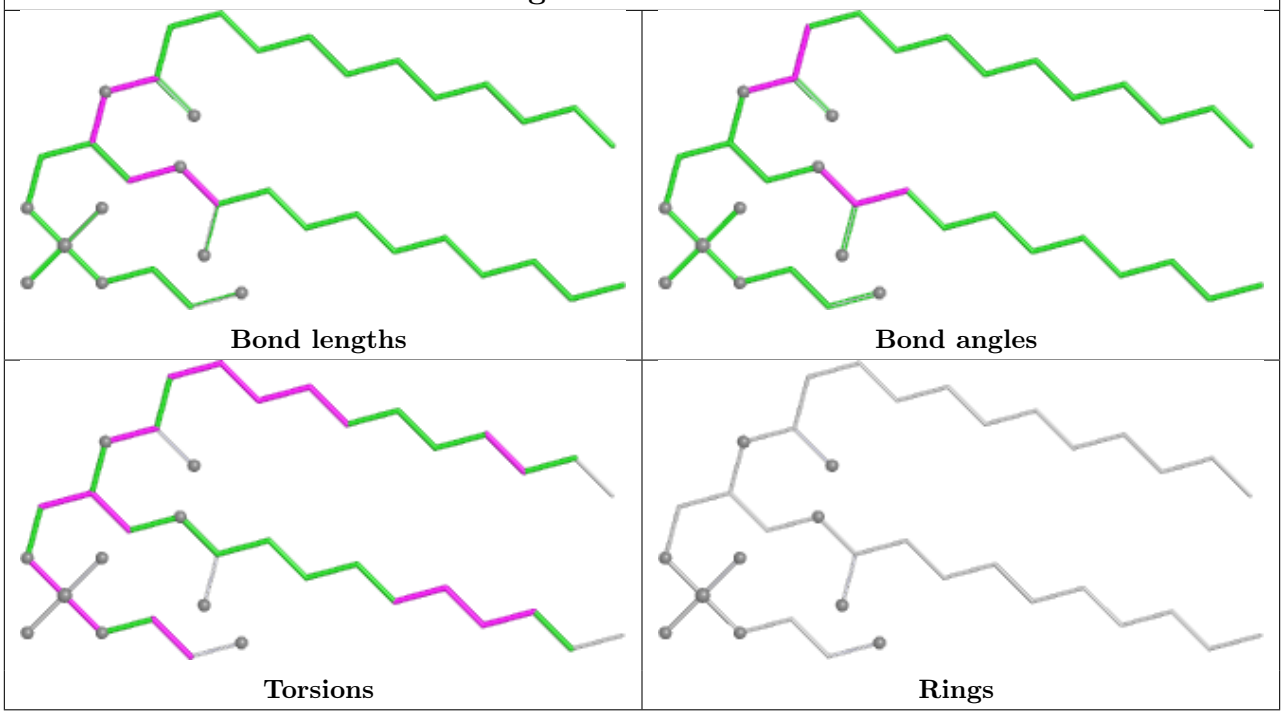


Rings

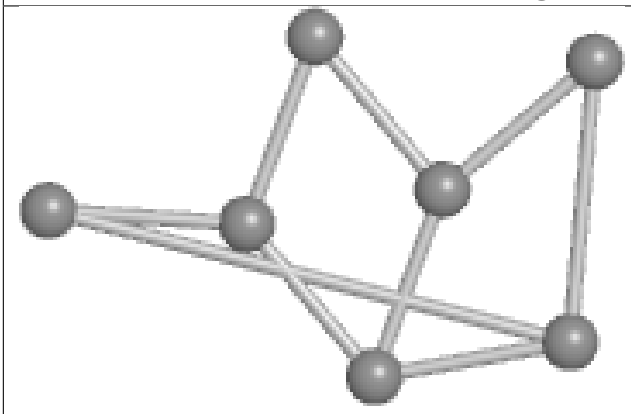
Ligand FAD I 601



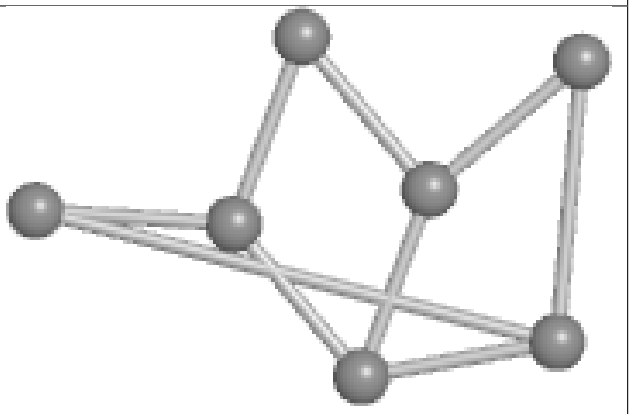
Ligand 3PE G 202



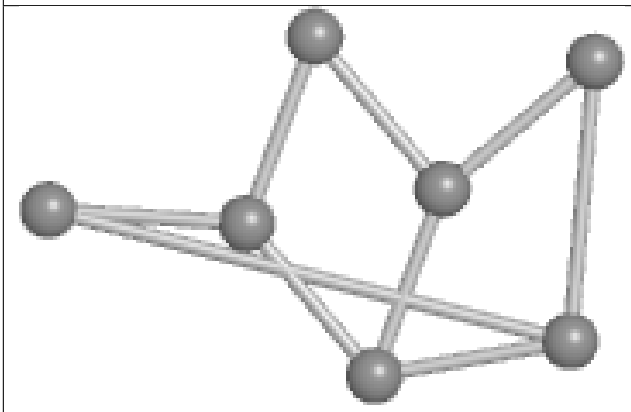
Ligand F3S F 303



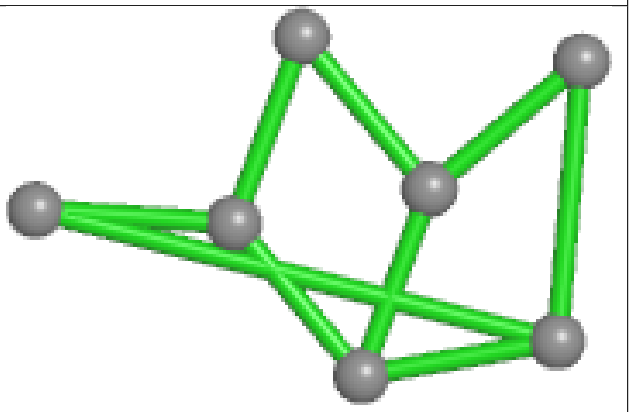
Bond lengths



Bond angles

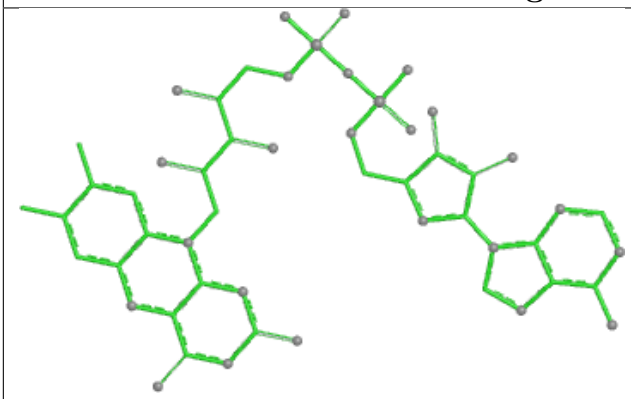


Torsions

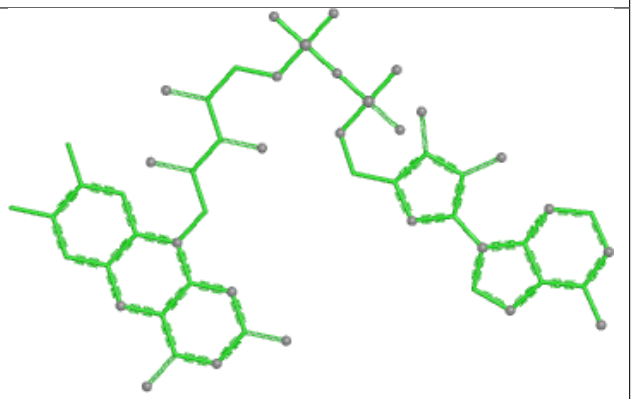


Rings

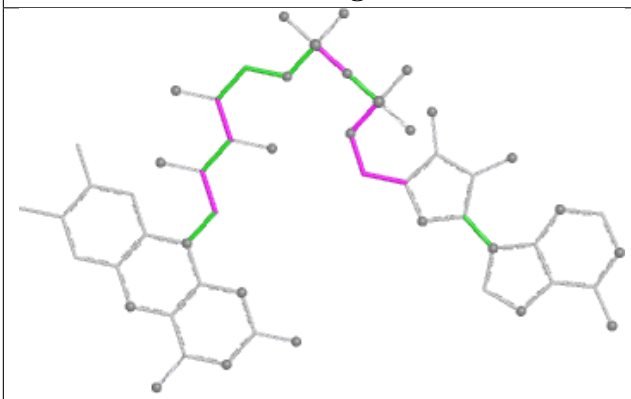
Ligand FAD E 601



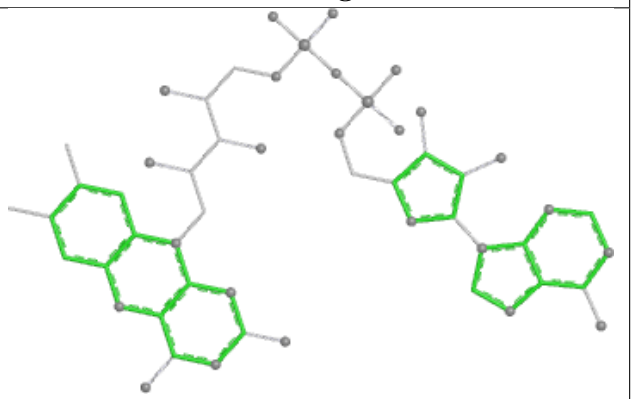
Bond lengths



Bond angles

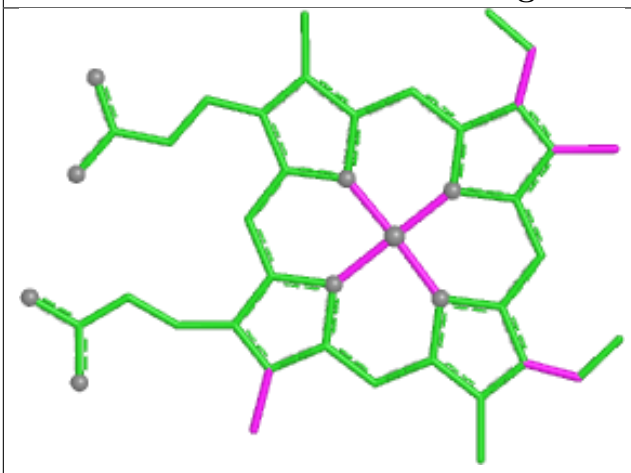


Torsions

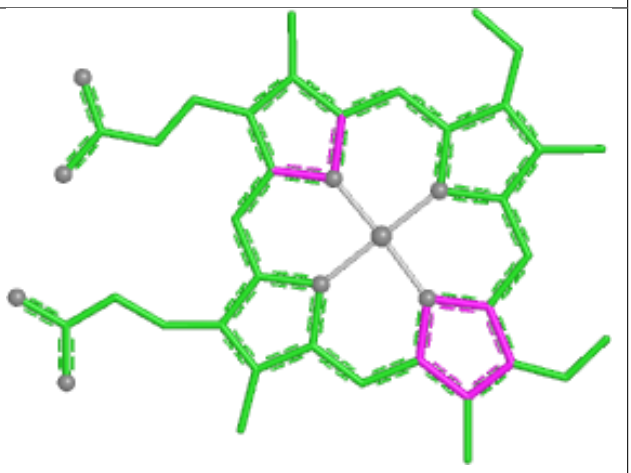


Rings

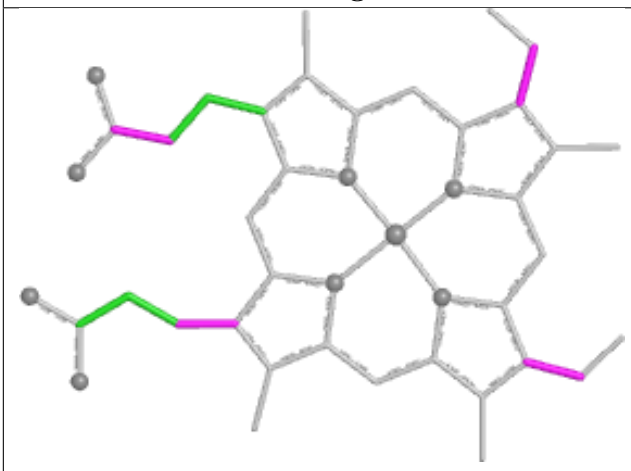
Ligand HEM G 201



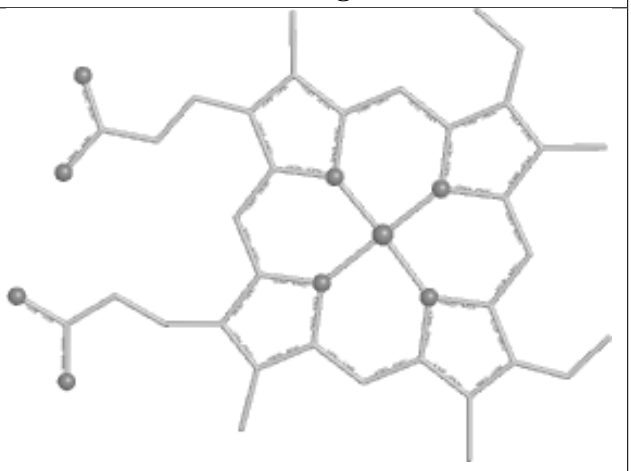
Bond lengths



Bond angles

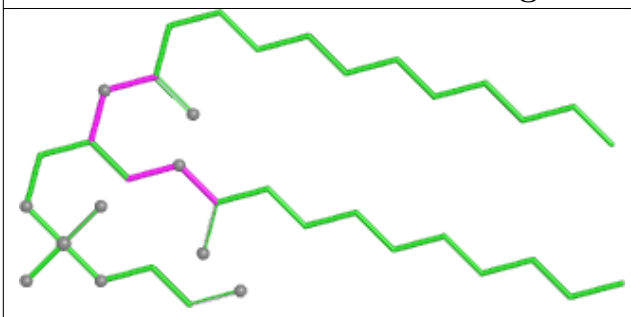


Torsions

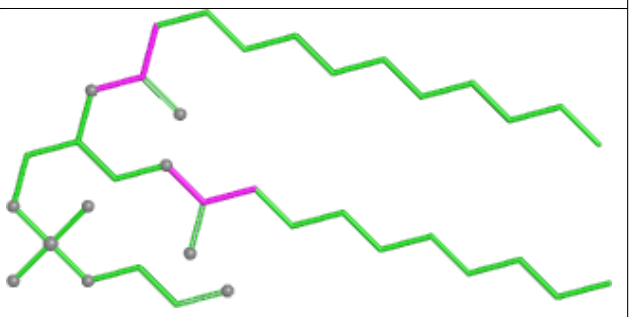


Rings

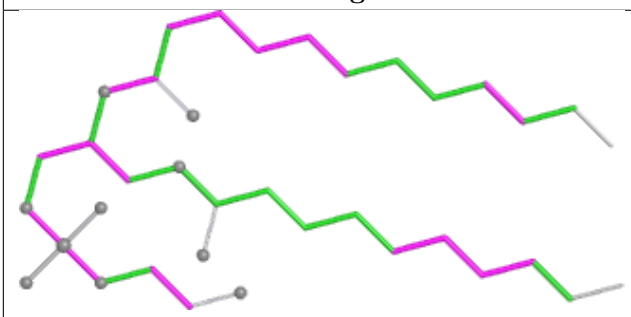
Ligand 3PE C 1301



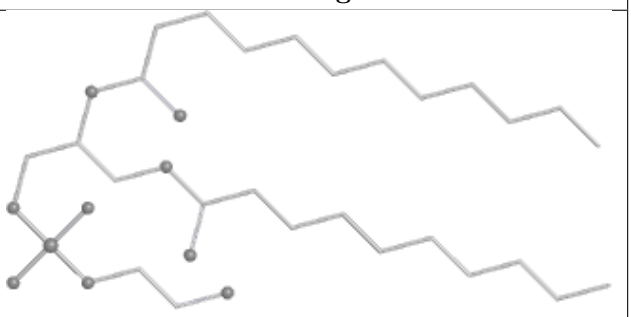
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

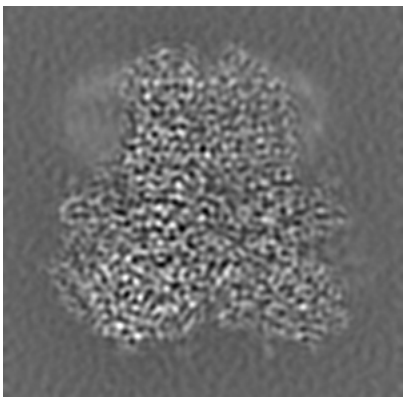
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22528. These allow visual inspection of the internal detail of the map and identification of artifacts.

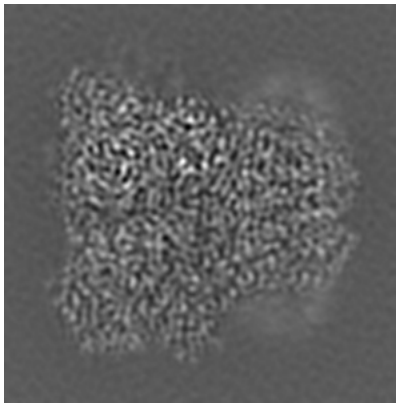
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

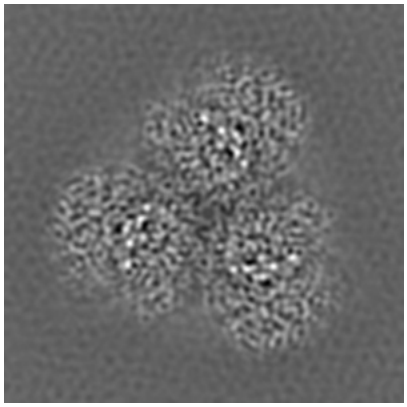
6.1.1 Primary map



X



Y

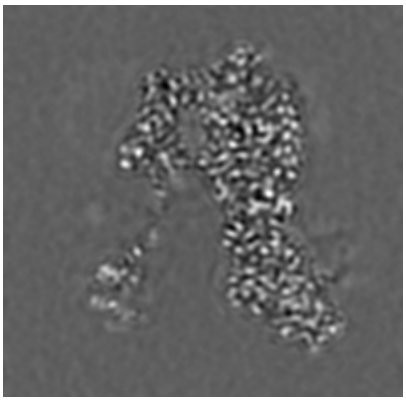


Z

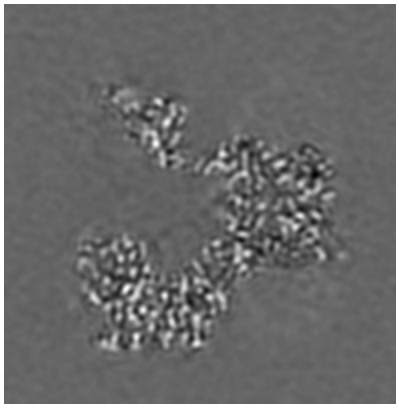
The images above show the map projected in three orthogonal directions.

6.2 Central slices

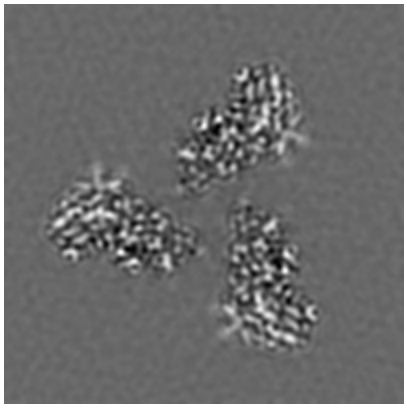
6.2.1 Primary map



X Index: 70



Y Index: 70

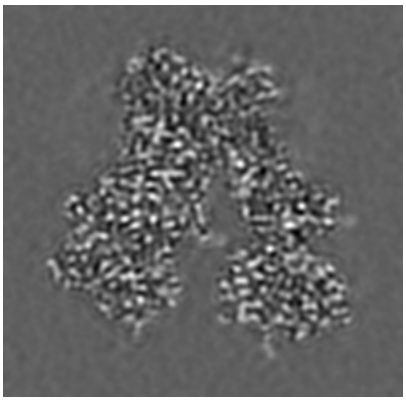


Z Index: 68

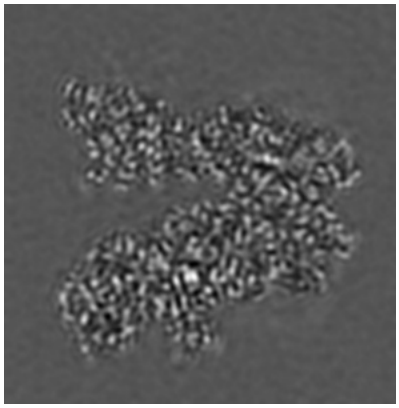
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

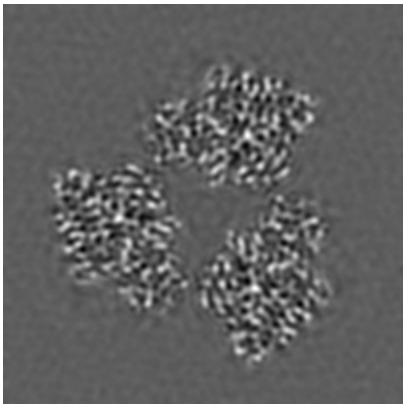
6.3.1 Primary map



X Index: 84



Y Index: 55

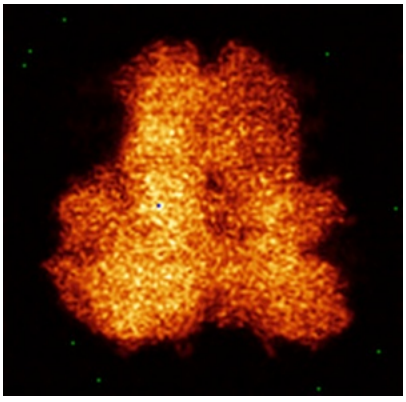


Z Index: 44

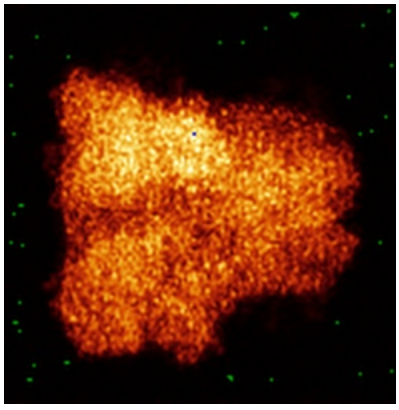
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

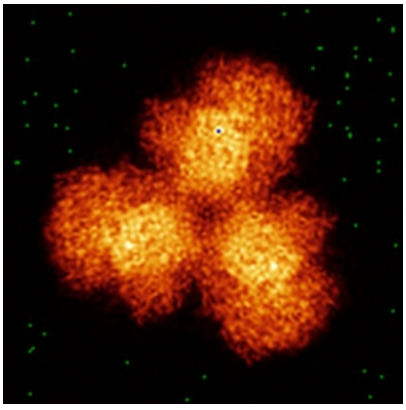
6.4.1 Primary map



X



Y

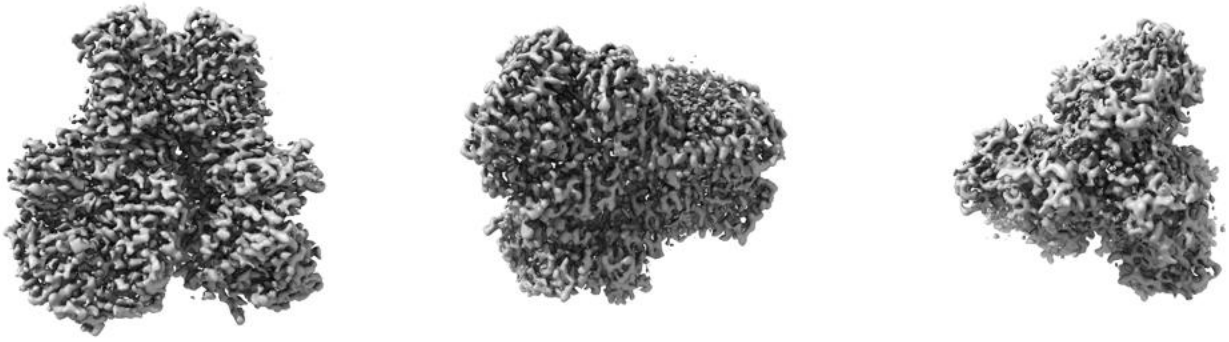


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

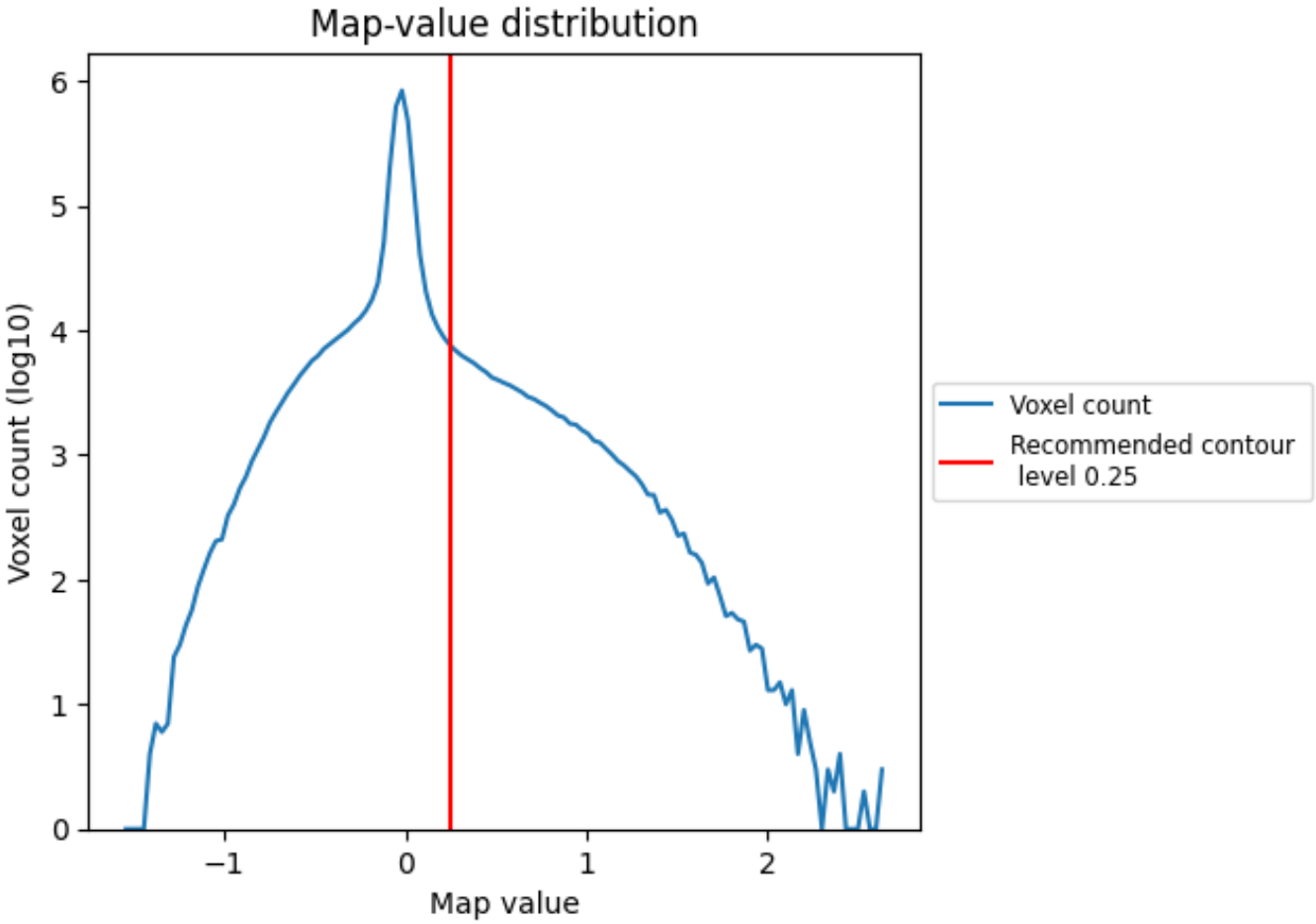
6.6 Mask visualisation (i)

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

7 Map analysis

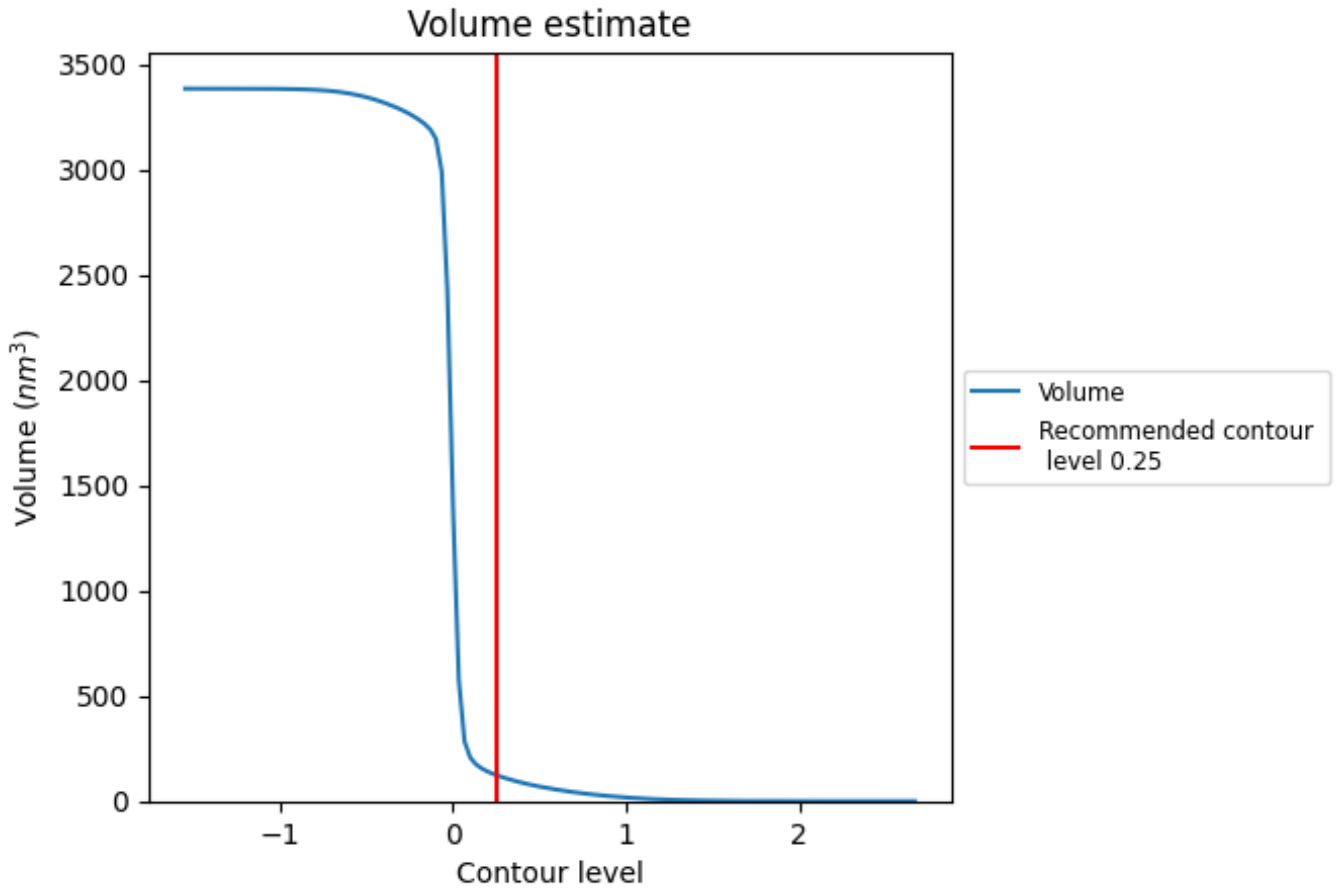
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 124 nm^3; this corresponds to an approximate mass of 112 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

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

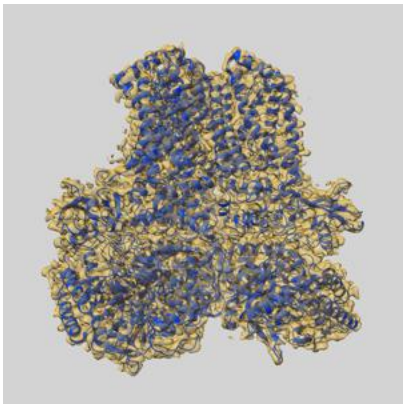
8 Fourier-Shell correlation (i)

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

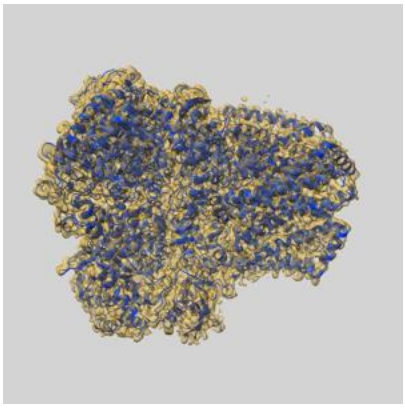
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22528 and PDB model 7JZ2. Per-residue inclusion information can be found in section 3 on page 10.

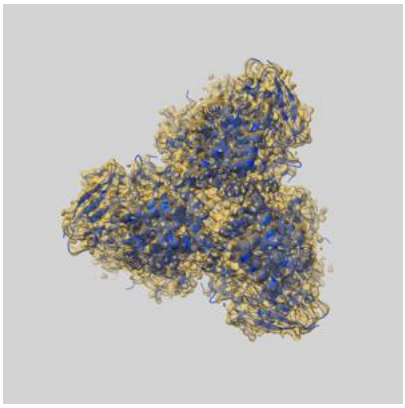
9.1 Map-model overlay



X



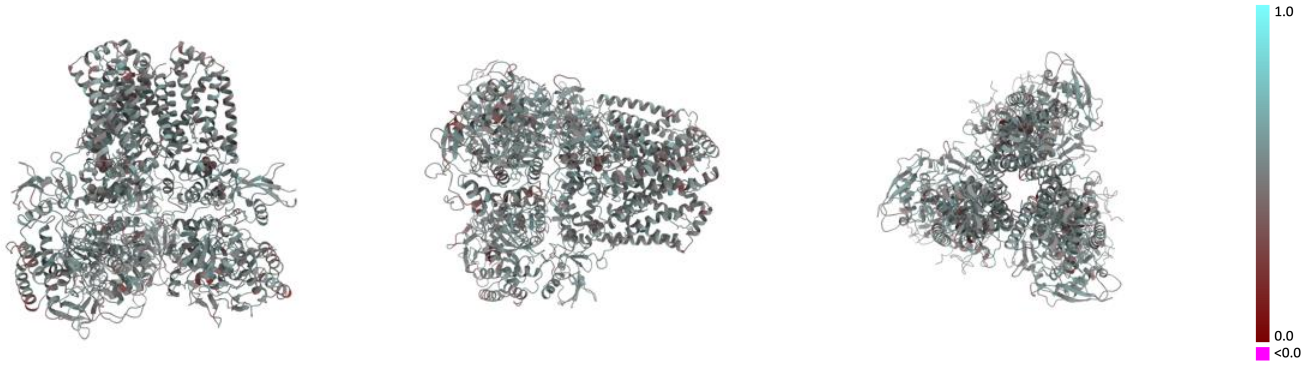
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

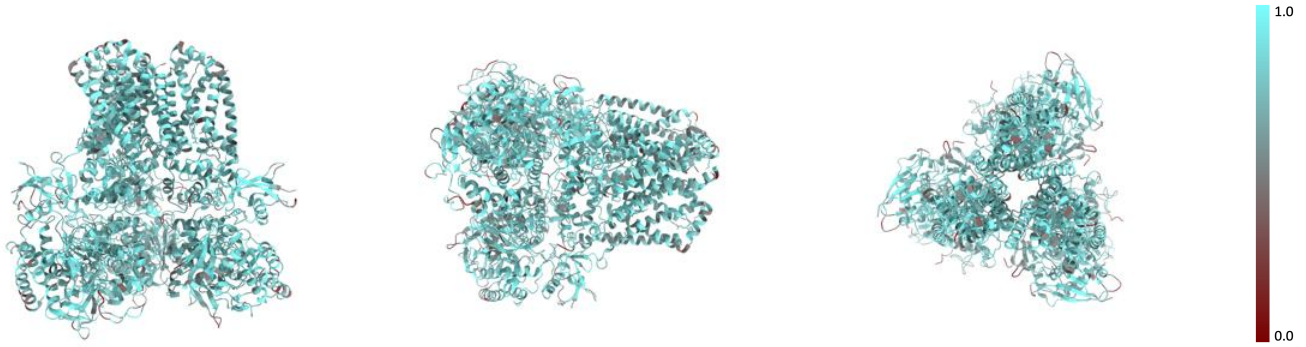
9.2 Q-score mapped to coordinate model



X Y Z

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

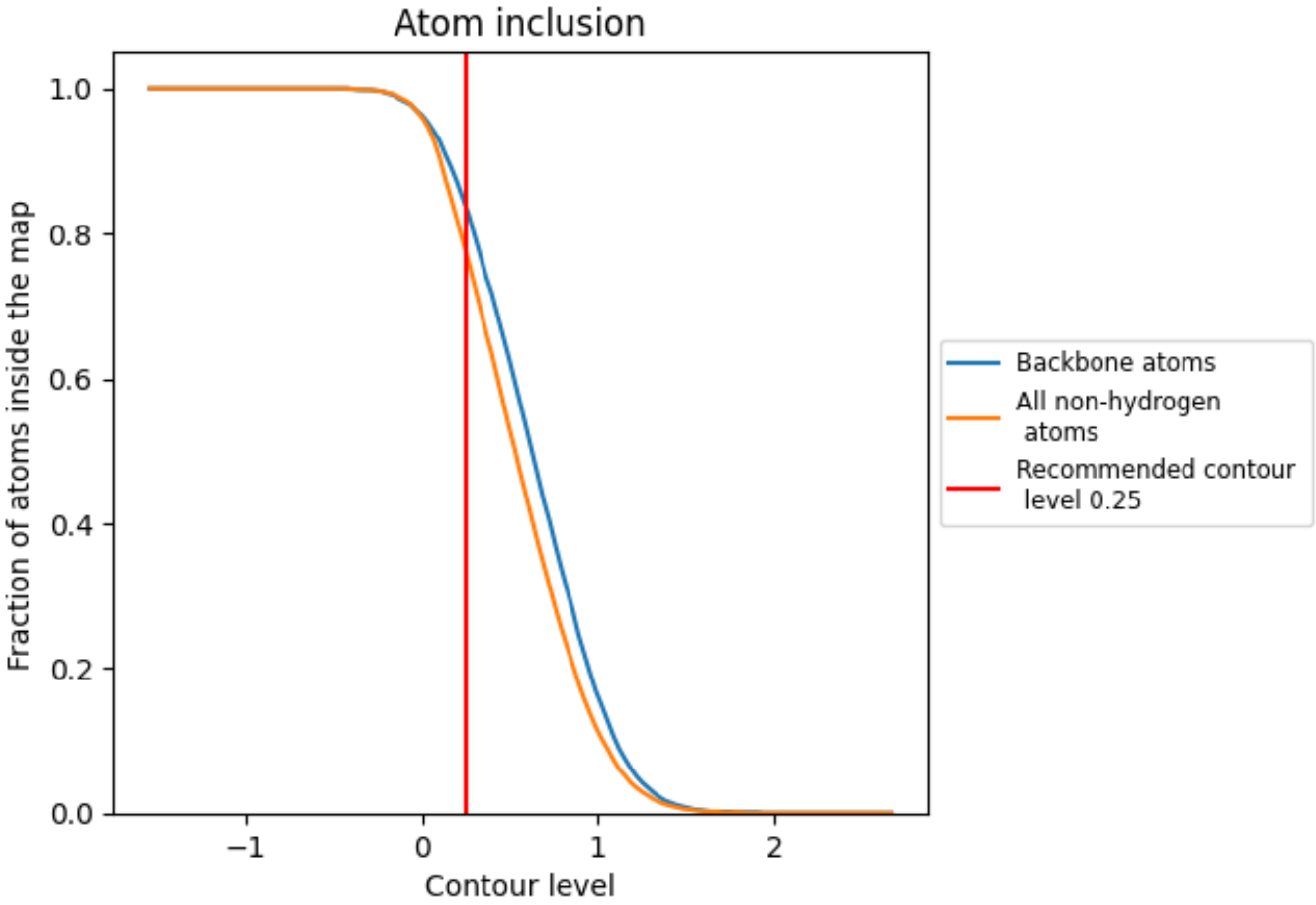
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.5100
A	0.7670	0.5040
B	0.8080	0.5280
C	0.7370	0.5070
D	0.7760	0.4980
E	0.7630	0.5030
F	0.8090	0.5300
G	0.7560	0.5120
H	0.7790	0.4970
I	0.7630	0.5030
J	0.8050	0.5300
K	0.7440	0.5110
L	0.7890	0.5000