Full wwPDB EM Validation Report (i)

Aug 25, 2026 – 02:56 pm BST

PDB ID	:	9FNO / pdb_00009fno
EMDB ID	:	EMD-50600
Title	:	Cryo-EM structure of human CD163 SRCR1-9 in complex with haptoglobin-hemoglobin
Authors	:	Andersen, C.B.F.; Kollman, J.M.
Deposited on	:	2024-06-10
Resolution	:	5.20 Å(reported)

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

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

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

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

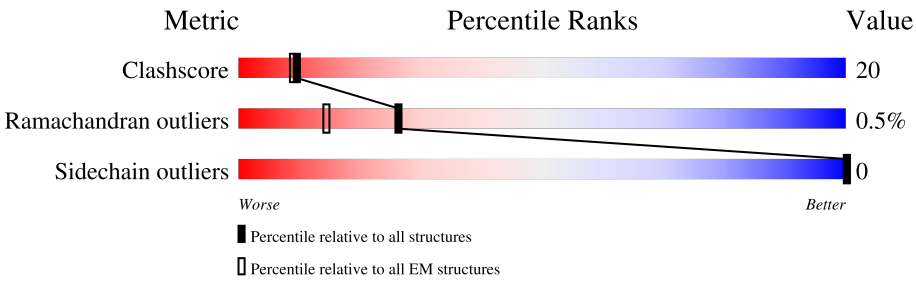
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

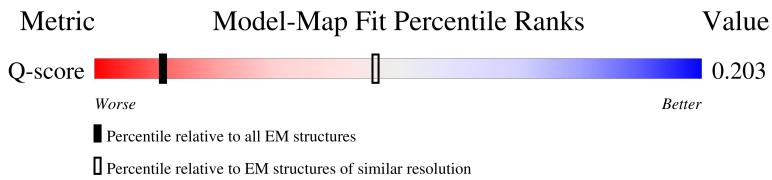
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	712 (4.70 - 5.70)

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	142	54% 45%
2	B	147	59% 41%
3	C	83	8% 88%
4	D	245	43% 56%

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Mol	Chain	Length	Quality of chain
5	E	1156	49% 25% 26%
5	F	1156	44% 21% 35%
5	G	1156	41% 24% 35%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 22254 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 Hemopressin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	141	1069	685	187	194	3	0	0

- Molecule 2 is a protein called Spinorphin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	146	1123	724	195	201	3	0	0

- Molecule 3 is a protein called Isoform 2 of Haptoglobin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	10	70	43	14	12	1	0	0

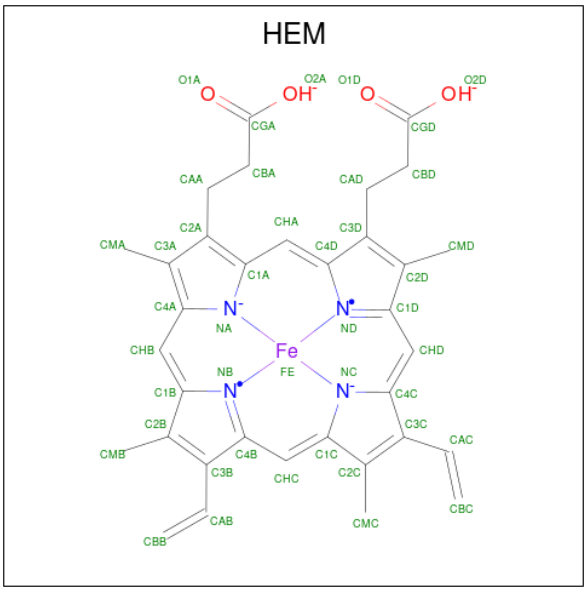
- Molecule 4 is a protein called Haptoglobin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	244	1912	1222	320	361	9	0	0

- Molecule 5 is a protein called Scavenger receptor cysteine-rich type 1 protein M130.

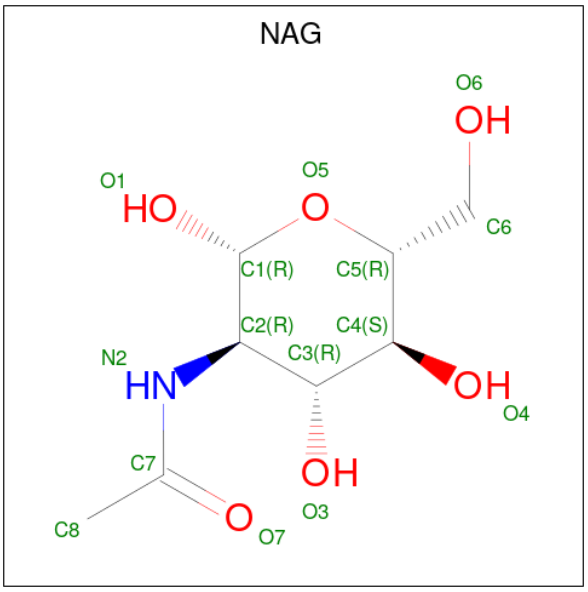
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	857	6484	3975	1178	1258	73	0	0
5	F	749	5669	3480	1027	1099	63	0	0
5	G	749	5669	3480	1027	1099	63	0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
6	A	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
6	B	1	43	34	1	4	4	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	D	1	14	8	1	5	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	D	1	14	8	1	5	0
7	D	1	14	8	1	5	0
7	E	1	14	8	1	5	0
7	E	1	14	8	1	5	0
7	E	1	14	8	1	5	0
7	F	1	14	8	1	5	0
7	F	1	14	8	1	5	0
7	F	1	14	8	1	5	0
7	G	1	14	8	1	5	0
7	G	1	14	8	1	5	0
7	G	1	14	8	1	5	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

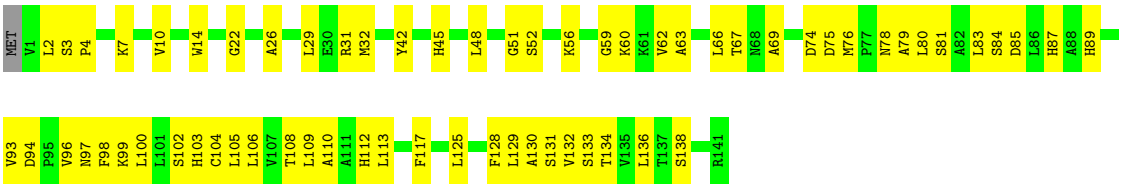
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
8	E	2	2	2	0
8	F	1	1	1	0
8	G	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

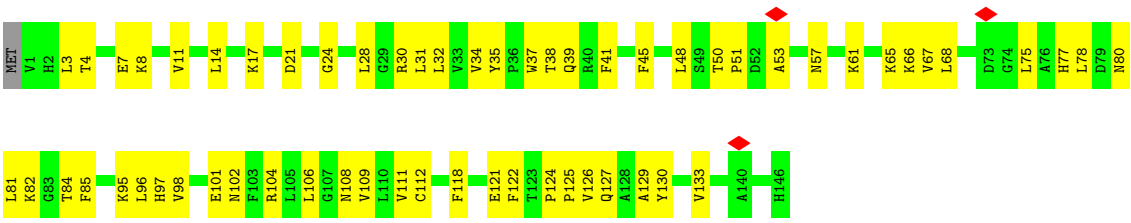
- Molecule 1: Hemopressin

Chain A:



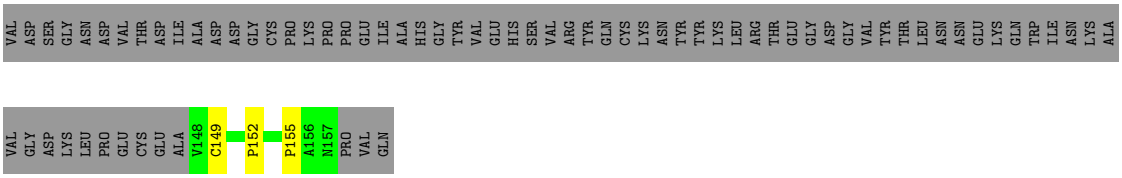
- Molecule 2: Spinorphin

Chain B:



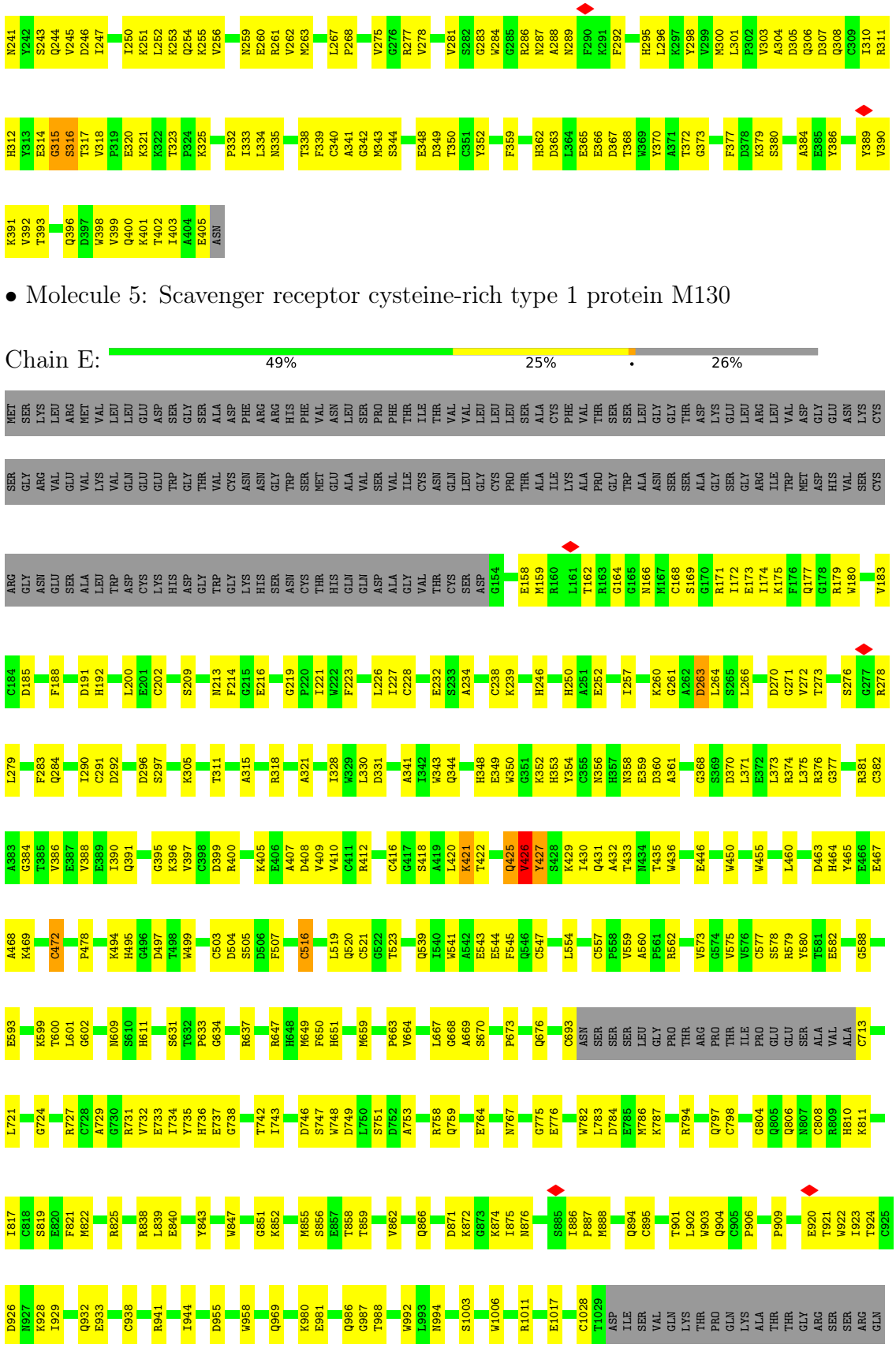
- Molecule 3: Isoform 2 of Haptoglobin alpha chain

Chain C:

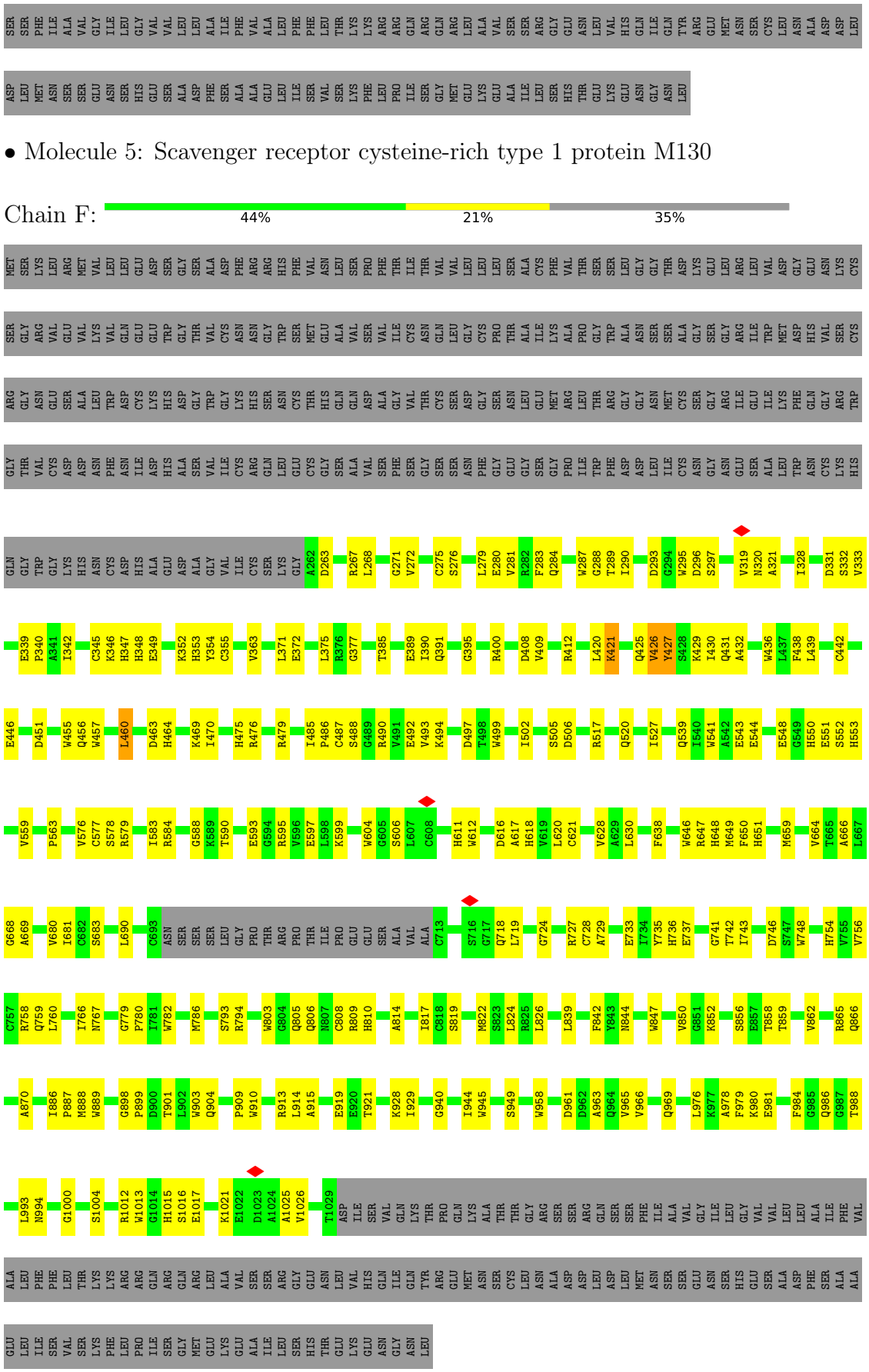


- Molecule 4: Haptoglobin beta chain

Chain D:



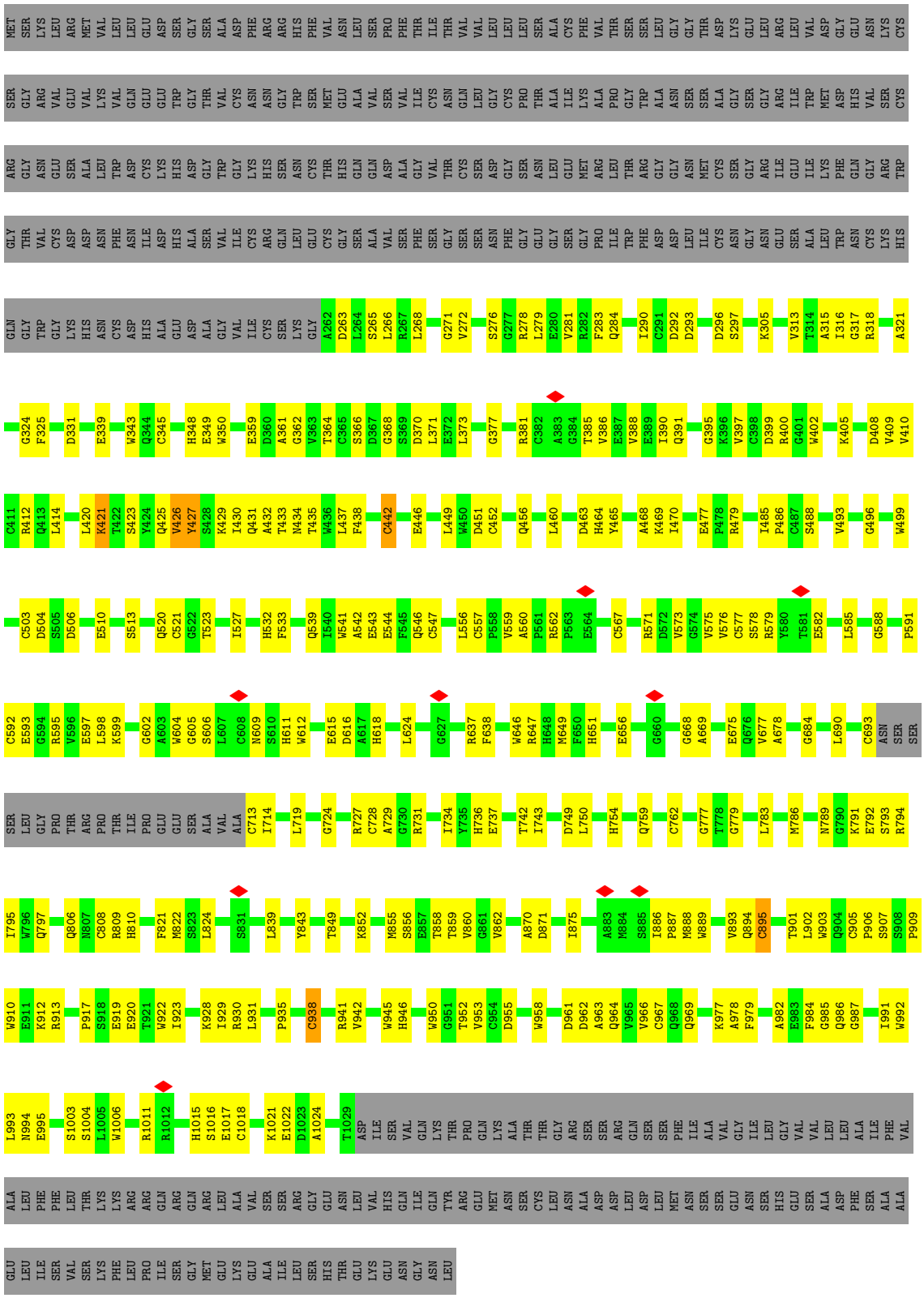
• Molecule 5: Scavenger receptor cysteine-rich type 1 protein M130



• Molecule 5: Scavenger receptor cysteine-rich type 1 protein M130

- Molecule 5: Scavenger receptor cysteine-rich type 1 protein M130

Chain G: 41% 24% 35%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	90	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	35.157	Depositor
Minimum map value	-25.318	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.24	0/1097	0.72	0/1491
2	B	0.24	0/1153	0.70	0/1566
3	C	0.29	0/71	1.13	0/95
4	D	0.24	0/1958	0.72	0/2661
5	E	0.21	0/6633	0.66	4/8980 (0.0%)
5	F	0.23	0/5800	0.67	3/7859 (0.0%)
5	G	0.26	0/5800	0.73	4/7859 (0.1%)
All	All	0.23	0/22512	0.69	11/30511 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
5	E	0	3
5	F	0	3
5	G	0	3
All	All	0	11

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	516	CYS	CA-CB-SG	7.43	131.50	114.40
5	F	578	SER	N-CA-C	7.01	125.74	110.80
5	G	895	CYS	CA-CB-SG	6.75	129.91	114.40
5	F	442	CYS	CA-CB-SG	6.30	128.90	114.40
5	G	442	CYS	CA-CB-SG	6.18	128.61	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	967	CYS	CA-CB-SG	5.36	126.74	114.40
5	F	767	ASN	N-CA-CB	-5.35	101.82	110.71
5	E	578	SER	CA-C-N	-5.26	113.32	122.37
5	E	578	SER	C-N-CA	-5.26	113.32	122.37
5	G	938	CYS	CA-CB-SG	5.07	126.05	114.40
5	E	472	CYS	CA-CB-SG	5.06	126.03	114.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	315	GLY	Peptide
4	D	316	SER	Peptide
5	E	425	GLN	Peptide
5	E	426	VAL	Peptide
5	E	460	LEU	Peptide
5	F	425	GLN	Peptide
5	F	426	VAL	Peptide
5	F	460	LEU	Peptide
5	G	425	GLN	Peptide
5	G	426	VAL	Peptide
5	G	460	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1073	56	0
2	B	1123	0	1118	50	0
3	C	70	0	72	2	0
4	D	1912	0	1882	123	0
5	E	6484	0	6026	230	0
5	F	5669	0	5287	210	0
5	G	5669	0	5287	216	0
6	A	43	0	30	1	0
6	B	43	0	30	4	0
7	D	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	42	0	39	0	0
7	F	42	0	39	2	0
7	G	42	0	39	0	0
8	E	2	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
All	All	22254	0	20961	861	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 20.

All (861) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:668:GLY:HA2	5:E:909:PRO:HA	1.49	0.94
5:G:433:THR:HG22	5:G:435:THR:H	1.31	0.94
5:E:374:ARG:HH22	5:E:376:ARG:HH21	1.13	0.92
5:E:433:THR:HG22	5:E:435:THR:H	1.34	0.92
5:E:177:GLN:OE1	5:E:179:ARG:NH1	2.04	0.90
4:D:393:THR:HA	4:D:396:GLN:HG2	1.56	0.88
5:F:420:LEU:HG	5:F:421:LYS:HE3	1.53	0.88
5:E:520:GLN:O	5:E:579:ARG:NH1	2.07	0.87
5:E:811:LYS:HE2	5:F:1017:GLU:OE1	1.76	0.86
4:D:234:GLU:HG3	4:D:253:LYS:HA	1.56	0.86
5:G:750:LEU:O	5:G:754:HIS:ND1	2.09	0.85
5:E:399:ASP:HB3	5:E:468:ALA:HB2	1.59	0.85
4:D:277:ARG:HE	4:D:278:VAL:H	1.24	0.85
5:G:822:MET:HE1	5:G:843:TYR:CD1	2.12	0.85
5:G:278:ARG:HE	5:G:362:GLY:HA3	1.40	0.83
1:A:89:HIS:CE1	5:F:354:TYR:CE2	2.67	0.83
5:F:279:LEU:HD21	5:F:363:VAL:HG13	1.62	0.81
5:G:266:LEU:HB2	5:G:343:TRP:HH2	1.45	0.81
5:E:633:PRO:HB2	5:E:637:ARG:NH1	1.97	0.79
5:E:776:GLU:OE2	5:E:810:HIS:ND1	2.14	0.79
5:E:634:GLY:O	5:E:637:ARG:NH2	2.15	0.79
5:F:490:ARG:NH2	5:F:492:GLU:OE2	2.16	0.78
5:G:743:ILE:HD12	5:G:783:LEU:HB2	1.64	0.78
5:G:395:GLY:HA2	5:G:433:THR:HG21	1.66	0.77
5:E:227:ILE:HD11	5:E:239:LYS:HD2	1.64	0.77
4:D:323:THR:HB	4:D:325:LYS:HE2	1.66	0.77
5:F:281:VAL:HG23	5:F:290:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:339:PHE:HD2	4:D:391:LYS:HG2	1.51	0.76
5:G:368:GLY:HA2	5:G:371:LEU:HD13	1.68	0.76
4:D:398:TRP:O	4:D:401:LYS:HG2	1.86	0.76
5:G:994:ASN:ND2	5:G:1018:CYS:SG	2.59	0.75
5:F:421:LYS:NZ	5:F:552:SER:OG	2.18	0.75
5:E:767:ASN:HB3	5:E:817:ILE:HG12	1.68	0.75
5:F:742:THR:O	5:F:782:TRP:N	2.19	0.75
5:F:803:TRP:O	5:F:805:GLN:NE2	2.20	0.75
5:G:727:ARG:NH1	5:G:762:CYS:SG	2.60	0.75
5:G:438:PHE:HB2	5:G:456:GLN:HB3	1.69	0.74
5:G:822:MET:HE1	5:G:843:TYR:HD1	1.49	0.74
5:G:953:VAL:HG23	5:G:1024:ALA:HB3	1.69	0.74
1:A:109:LEU:HG	1:A:117:PHE:HZ	1.53	0.73
5:F:913:ARG:NH1	5:F:919:GLU:OE2	2.21	0.73
5:G:668:GLY:HA3	5:G:910:TRP:CD1	2.24	0.73
5:F:736:HIS:ND1	5:F:737:GLU:OE1	2.22	0.73
5:F:727:ARG:NH1	5:F:728:CYS:SG	2.62	0.72
5:E:746:ASP:OD2	5:F:1021:LYS:HE3	1.88	0.72
2:B:45:PHE:HB3	2:B:57:ASN:HD21	1.54	0.72
4:D:235:LYS:NZ	4:D:236:VAL:O	2.22	0.72
5:E:746:ASP:CG	5:F:1021:LYS:HE3	2.15	0.72
5:F:520:GLN:O	5:F:579:ARG:NH1	2.23	0.72
5:F:487:CYS:HB3	5:F:577:CYS:HB2	1.70	0.72
5:E:724:GLY:HA3	5:E:729:ALA:O	1.90	0.71
5:G:913:ARG:NH2	5:G:919:GLU:OE2	2.23	0.71
5:G:520:GLN:O	5:G:579:ARG:NH1	2.24	0.70
2:B:101:GLU:OE1	2:B:104:ARG:NH1	2.24	0.70
5:E:257:ILE:HG21	5:E:350:TRP:HZ3	1.56	0.69
5:G:281:VAL:HG23	5:G:290:ILE:HD11	1.73	0.69
1:A:29:LEU:O	1:A:32:MET:HG2	1.93	0.69
5:G:385:THR:HG23	5:G:469:LYS:HE3	1.75	0.69
5:F:590:THR:OG1	5:F:593:GLU:OE1	2.08	0.69
5:G:612:TRP:CZ3	5:G:616:ASP:HB3	2.28	0.69
4:D:349:ASP:OD1	4:D:350:THR:N	2.23	0.69
5:G:797:GLN:N	5:G:797:GLN:OE1	2.26	0.69
5:G:856:SER:O	5:G:859:THR:OG1	2.09	0.69
4:D:194:GLU:HB2	4:D:255:LYS:HE2	1.74	0.69
5:E:356:ASN:ND2	5:E:358:ASN:OD1	2.26	0.69
5:F:980:LYS:HG3	5:F:981:GLU:OE1	1.92	0.69
5:G:649:MET:HE2	5:G:651:HIS:HE1	1.58	0.69
1:A:75:ASP:OD2	1:A:78:ASN:ND2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:724:GLY:HA3	5:F:729:ALA:O	1.94	0.68
2:B:95:LYS:HD2	2:B:96:LEU:HD22	1.75	0.68
5:E:266:LEU:HD11	5:E:279:LEU:HD22	1.76	0.68
5:E:901:THR:HB	5:E:903:TRP:HE3	1.59	0.67
5:E:928:LYS:HD3	5:E:1006:TRP:HE1	1.60	0.67
5:E:633:PRO:HB2	5:E:637:ARG:CZ	2.24	0.67
2:B:4:THR:N	2:B:7:GLU:OE2	2.28	0.67
4:D:400:GLN:O	4:D:403:ILE:HG22	1.95	0.67
4:D:275:VAL:HA	4:D:303:VAL:HG13	1.76	0.67
4:D:176:GLN:CD	4:D:296:LEU:HD21	2.20	0.67
4:D:310:ILE:HD13	4:D:334:LEU:HD23	1.77	0.66
5:F:647:ARG:HH12	5:F:909:PRO:HG3	1.59	0.66
5:F:268:LEU:HD21	5:F:279:LEU:HD13	1.76	0.66
5:F:741:GLY:HA3	5:F:782:TRP:HD1	1.59	0.66
1:A:99:LYS:NZ	4:D:288:ALA:O	2.28	0.66
5:G:532:HIS:HD2	5:G:533:PHE:CE1	2.14	0.66
5:E:822:MET:HE1	5:E:843:TYR:HD1	1.58	0.66
1:A:128:PHE:HD2	1:A:129:LEU:HD12	1.61	0.66
5:E:192:HIS:HE1	5:E:228:CYS:H	1.43	0.66
1:A:132:VAL:O	1:A:136:LEU:HD12	1.95	0.66
5:F:668:GLY:HA3	5:F:910:TRP:CD1	2.30	0.66
5:E:647:ARG:NH2	5:E:669:ALA:O	2.28	0.65
5:E:743:ILE:HD12	5:E:783:LEU:HB3	1.77	0.65
4:D:247:ILE:HD11	4:D:390:VAL:HG11	1.77	0.65
5:E:185:ASP:OD1	5:E:252:GLU:HG2	1.96	0.65
5:E:894:GLN:NE2	5:E:906:PRO:HB2	2.12	0.65
5:F:505:SER:HB3	5:F:988:THR:HG22	1.77	0.65
5:G:779:GLY:O	5:G:810:HIS:NE2	2.27	0.65
5:E:874:LYS:NZ	5:E:926:ASP:OD1	2.28	0.65
4:D:352:TYR:HE1	4:D:379:LYS:HA	1.61	0.65
5:F:743:ILE:HD11	5:F:786:MET:HG3	1.77	0.65
4:D:235:LYS:HB3	4:D:251:LYS:HD3	1.78	0.65
5:E:395:GLY:HA2	5:E:433:THR:HG21	1.79	0.65
5:E:188:PHE:HA	5:E:192:HIS:HD2	1.61	0.65
5:E:649:MET:HE2	5:E:651:HIS:HE1	1.61	0.65
2:B:50:THR:HG23	2:B:53:ALA:H	1.61	0.64
5:E:875:ILE:HA	5:E:923:ILE:HD13	1.78	0.64
5:F:439:LEU:HD13	5:F:455:TRP:HB3	1.77	0.64
2:B:118:PHE:O	2:B:121:GLU:HG3	1.97	0.64
5:E:732:VAL:HG21	5:E:748:TRP:HH2	1.63	0.64
5:G:504:ASP:HA	5:G:573:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:856:SER:O	5:E:859:THR:OG1	2.12	0.64
5:G:647:ARG:NH1	5:G:669:ALA:O	2.31	0.64
5:F:856:SER:O	5:F:859:THR:OG1	2.15	0.64
5:G:668:GLY:HA2	5:G:909:PRO:HA	1.80	0.64
5:G:266:LEU:HD11	5:G:279:LEU:HD12	1.79	0.63
1:A:2:LEU:O	1:A:7:LYS:NZ	2.32	0.63
4:D:343:MET:HE1	4:D:349:ASP:HB2	1.80	0.63
5:E:928:LYS:HZ3	5:E:1006:TRP:HZ2	1.46	0.63
5:E:852:LYS:HA	5:E:855:MET:HE2	1.79	0.63
4:D:245:VAL:HG12	4:D:247:ILE:HD13	1.80	0.63
5:F:395:GLY:HA3	5:F:457:TRP:HH2	1.64	0.63
5:F:901:THR:OG1	5:F:904:GLN:OE1	2.15	0.63
4:D:231:VAL:HG21	4:D:252:LEU:HD13	1.79	0.63
5:G:373:LEU:HD21	5:G:410:VAL:HG13	1.80	0.62
5:G:582:GLU:HG2	5:G:582:GLU:O	1.98	0.62
4:D:349:ASP:CG	4:D:350:THR:H	2.08	0.62
5:E:412:ARG:NH2	5:E:446:GLU:O	2.33	0.62
5:G:611:HIS:CD2	5:G:649:MET:HE3	2.35	0.62
5:G:961:ASP:O	5:G:964:GLN:HG2	2.00	0.62
5:E:328:ILE:HB	5:E:353:HIS:CD2	2.35	0.61
5:E:929:ILE:HG12	5:E:944:ILE:HG22	1.80	0.61
5:E:932:GLN:HG2	5:E:933:GLU:HG2	1.81	0.61
4:D:380:SER:HB2	4:D:384:ALA:HB3	1.81	0.61
5:G:595:ARG:HD2	5:G:677:VAL:HG21	1.81	0.61
2:B:97:HIS:HB3	4:D:167:LEU:HD23	1.81	0.61
4:D:342:GLY:HA2	4:D:386:TYR:HD1	1.64	0.61
5:E:721:LEU:H	5:E:727:ARG:HH21	1.48	0.61
5:F:779:GLY:O	5:F:810:HIS:NE2	2.32	0.61
2:B:8:LYS:HE3	2:B:78:LEU:HD12	1.83	0.61
5:E:429:LYS:HE2	5:E:431:GLN:OE1	1.99	0.61
5:G:928:LYS:NZ	5:G:1006:TRP:HD1	1.98	0.61
5:G:724:GLY:HA3	5:G:729:ALA:O	2.01	0.61
2:B:77:HIS:CE1	2:B:84:THR:HB	2.36	0.61
5:F:993:LEU:HD21	5:F:1013:TRP:CD1	2.36	0.61
5:E:368:GLY:HA2	5:E:371:LEU:HD13	1.82	0.61
5:E:421:LYS:HD2	5:E:422:THR:H	1.66	0.61
5:G:599:LYS:HD3	5:G:604:TRP:CE2	2.36	0.61
5:G:1011:ARG:NH1	5:G:1015:HIS:O	2.33	0.61
1:A:89:HIS:CE1	5:F:354:TYR:HE2	2.15	0.60
5:E:969:GLN:NE2	5:E:1003:SER:O	2.33	0.60
5:G:278:ARG:HH11	5:G:321:ALA:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:727:ARG:HD2	5:F:728:CYS:SG	2.41	0.60
5:G:399:ASP:HB3	5:G:468:ALA:HB2	1.83	0.60
2:B:106:LEU:HA	2:B:109:VAL:HG12	1.83	0.60
5:E:183:VAL:HG23	5:E:223:PHE:HB2	1.84	0.60
5:E:822:MET:HE1	5:E:843:TYR:CD1	2.37	0.60
5:E:866:GLN:NE2	5:E:902:LEU:N	2.50	0.60
5:E:219:GLY:O	5:E:250:HIS:NE2	2.34	0.60
2:B:77:HIS:HE1	2:B:84:THR:HB	1.67	0.59
5:G:822:MET:HB3	5:G:903:TRP:HE1	1.67	0.59
5:G:855:MET:HE2	5:G:860:VAL:HG22	1.83	0.59
4:D:260:GLU:OE2	4:D:261:ARG:NH2	2.35	0.59
5:E:463:ASP:HB3	5:E:465:TYR:CE1	2.37	0.59
5:F:782:TRP:HZ3	5:F:803:TRP:HB3	1.67	0.59
5:G:615:GLU:OE2	5:G:615:GLU:N	2.35	0.59
5:G:675:GLU:OE1	5:G:675:GLU:N	2.35	0.59
1:A:97:ASN:HA	1:A:100:LEU:HD12	1.85	0.59
3:C:152:PRO:HG2	3:C:155:PRO:HB3	1.85	0.59
1:A:80:LEU:HD13	1:A:83:LEU:HD13	1.84	0.59
5:E:226:LEU:HD11	5:E:238:CYS:HB2	1.84	0.59
5:F:620:LEU:HD11	5:F:680:VAL:HG11	1.84	0.59
5:E:290:ILE:HD12	5:E:330:LEU:H	1.68	0.59
5:E:693:CYS:N	5:E:713:CYS:SG	2.76	0.59
5:E:852:LYS:HA	5:E:855:MET:CE	2.33	0.58
5:E:783:LEU:HD23	5:E:784:ASP:N	2.17	0.58
5:F:331:ASP:OD1	5:F:348:HIS:HB3	2.02	0.58
5:G:637:ARG:HG3	5:G:638:PHE:CD1	2.38	0.58
5:E:886:ILE:HG13	5:E:887:PRO:HD2	1.85	0.58
5:G:585:LEU:HD11	5:G:591:PRO:O	2.03	0.58
1:A:85:ASP:CG	5:F:354:TYR:CE1	2.82	0.58
2:B:45:PHE:HB3	2:B:57:ASN:ND2	2.16	0.58
5:E:504:ASP:HA	5:E:573:VAL:HB	1.85	0.58
5:F:782:TRP:CE3	5:F:803:TRP:HE3	2.22	0.58
5:G:339:GLU:OE2	5:G:345:CYS:N	2.37	0.58
2:B:31:LEU:HD21	2:B:38:THR:HG21	1.85	0.58
2:B:39:GLN:NE2	2:B:48:LEU:O	2.36	0.58
4:D:344:SER:HB2	4:D:348:GLU:H	1.67	0.58
5:E:386:VAL:HB	5:E:397:VAL:HG12	1.86	0.58
1:A:85:ASP:CG	5:F:354:TYR:HE1	2.10	0.57
5:F:593:GLU:HG3	5:F:681:ILE:HA	1.85	0.57
1:A:31:ARG:NH1	1:A:104:CYS:SG	2.77	0.57
4:D:284:TRP:CD1	4:D:296:LEU:HD13	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:319:VAL:HG12	5:F:457:TRP:CD1	2.38	0.57
4:D:362:HIS:NE2	4:D:367:ASP:OD1	2.34	0.57
5:F:377:GLY:O	5:F:427:TYR:HD2	1.86	0.57
5:G:870:ALA:HA	5:G:945:TRP:CD1	2.39	0.57
5:E:278:ARG:HB2	5:E:321:ALA:HB1	1.86	0.57
5:G:929:ILE:HD11	5:G:942:VAL:HG13	1.86	0.57
5:F:595:ARG:NH1	5:F:638:PHE:O	2.37	0.57
5:E:748:TRP:CD1	5:E:748:TRP:C	2.83	0.57
5:E:331:ASP:OD1	5:E:348:HIS:HB3	2.04	0.57
5:E:582:GLU:OE2	5:E:582:GLU:N	2.30	0.57
5:E:747:SER:HB3	5:E:787:LYS:HE3	1.84	0.57
5:F:420:LEU:O	5:F:421:LYS:HG3	2.05	0.57
5:G:386:VAL:HB	5:G:397:VAL:HG12	1.86	0.57
1:A:98:PHE:HE2	1:A:136:LEU:HD22	1.68	0.57
5:E:408:ASP:OD1	5:E:409:VAL:N	2.37	0.57
5:F:319:VAL:HG12	5:F:457:TRP:HD1	1.69	0.56
1:A:45:HIS:CD2	5:F:400:ARG:HH21	2.23	0.56
4:D:332:PRO:HG2	4:D:334:LEU:HD11	1.87	0.56
5:E:164:GLY:O	5:E:169:SER:OG	2.23	0.56
5:G:278:ARG:HH11	5:G:321:ALA:CB	2.17	0.56
4:D:318:VAL:HG22	4:D:320:GLU:OE1	2.05	0.56
5:E:305:LYS:HG2	5:E:311:THR:HG21	1.86	0.56
5:E:503:CYS:HB2	5:E:562:ARG:HH22	1.71	0.56
5:G:324:GLY:O	5:G:325:PHE:HD1	1.89	0.56
5:G:421:LYS:HD3	5:G:423:SER:HB3	1.87	0.56
5:E:721:LEU:H	5:E:727:ARG:NH2	2.02	0.56
5:E:866:GLN:NE2	5:E:902:LEU:H	2.03	0.56
5:F:371:LEU:HG	5:F:390:ILE:HD12	1.87	0.56
5:G:272:VAL:HG21	5:G:391:GLN:HB3	1.87	0.56
5:G:824:LEU:HD11	5:G:839:LEU:HD11	1.87	0.56
2:B:61:LYS:O	2:B:65:LYS:HG2	2.05	0.56
5:F:866:GLN:NE2	5:F:903:TRP:CZ3	2.74	0.56
5:G:377:GLY:O	5:G:427:TYR:HD2	1.89	0.56
5:F:289:THR:HG23	5:F:328:ILE:HG22	1.86	0.56
1:A:87:HIS:NE2	6:A:201:HEM:NA	2.53	0.56
4:D:177:ALA:HB1	4:D:223:LEU:HD11	1.88	0.56
5:E:159:MET:CE	5:E:174:ILE:HG13	2.36	0.56
5:F:296:ASP:CG	5:F:297:SER:H	2.14	0.56
5:F:915:ALA:HA	5:F:919:GLU:OE2	2.05	0.56
5:G:420:LEU:O	5:G:421:LYS:HB2	2.06	0.56
5:G:542:ALA:O	5:G:562:ARG:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ALA:O	2:B:133:VAL:HG23	2.06	0.55
5:E:862:VAL:O	5:E:866:GLN:HG3	2.05	0.55
5:G:278:ARG:CZ	5:G:318:ARG:HA	2.36	0.55
5:G:612:TRP:CD1	5:G:678:ALA:HB1	2.41	0.55
1:A:63:ALA:O	1:A:67:THR:HG23	2.06	0.55
1:A:129:LEU:HA	1:A:132:VAL:HG12	1.87	0.55
5:G:585:LEU:HD12	5:G:593:GLU:C	2.30	0.55
5:F:408:ASP:OD1	5:F:409:VAL:N	2.39	0.55
5:G:719:LEU:HD13	5:G:734:ILE:CD1	2.36	0.55
5:G:969:GLN:NE2	5:G:1003:SER:O	2.39	0.55
2:B:3:LEU:CB	2:B:8:LYS:HD3	2.37	0.55
4:D:208:HIS:HE1	4:D:217:ILE:HA	1.71	0.55
5:F:328:ILE:HD11	5:F:353:HIS:CD2	2.41	0.55
5:E:384:GLY:C	5:E:469:LYS:HG3	2.32	0.55
5:E:759:GLN:HG3	5:E:794:ARG:HH11	1.70	0.55
5:G:941:ARG:NH1	5:G:987:GLY:HA2	2.21	0.55
5:E:647:ARG:HH22	5:E:909:PRO:HG3	1.72	0.55
1:A:45:HIS:CD2	5:F:400:ARG:NH2	2.75	0.55
5:E:543:GLU:HG2	5:E:559:VAL:HB	1.89	0.55
5:G:429:LYS:HG2	5:G:430:ILE:N	2.21	0.55
4:D:342:GLY:HA2	4:D:386:TYR:CD1	2.41	0.55
5:F:741:GLY:HA3	5:F:782:TRP:CD1	2.40	0.55
5:E:821:PHE:O	5:E:822:MET:HE2	2.07	0.55
5:G:331:ASP:OD1	5:G:348:HIS:HB3	2.07	0.55
4:D:333:ILE:C	4:D:334:LEU:HD12	2.32	0.54
5:E:158:GLU:HB3	5:E:175:LYS:HB3	1.89	0.54
4:D:163:LEU:HB2	4:D:288:ALA:HB2	1.88	0.54
5:G:928:LYS:NZ	5:G:1004:SER:OG	2.40	0.54
1:A:94:ASP:OD2	1:A:96:VAL:HG22	2.07	0.54
2:B:14:LEU:HD23	2:B:130:TYR:HE2	1.73	0.54
5:F:743:ILE:HG23	5:F:814:ALA:HB3	1.89	0.54
4:D:183:HIS:O	4:D:183:HIS:ND1	2.40	0.54
5:G:485:ILE:HG13	5:G:486:PRO:HD2	1.90	0.54
1:A:48:LEU:H	1:A:48:LEU:HD23	1.73	0.54
5:F:429:LYS:HG2	5:F:430:ILE:N	2.23	0.54
4:D:243:SER:OG	4:D:244:GLN:OE1	2.26	0.54
5:E:171:ARG:NH2	5:E:214:PHE:O	2.33	0.54
5:F:272:VAL:HG21	5:F:391:GLN:HB3	1.88	0.54
4:D:246:ASP:C	4:D:247:ILE:HD12	2.33	0.54
5:E:611:HIS:CD2	5:E:649:MET:HE3	2.43	0.54
5:G:582:GLU:HG3	5:G:599:LYS:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:901:THR:HB	5:G:903:TRP:HE3	1.71	0.54
5:F:913:ARG:NH1	5:F:914:LEU:O	2.41	0.54
5:G:296:ASP:CG	5:G:297:SER:H	2.15	0.54
5:G:599:LYS:HB2	5:G:604:TRP:CE3	2.43	0.54
4:D:207:ASN:O	4:D:208:HIS:HD2	1.91	0.54
4:D:234:GLU:CG	4:D:253:LYS:HA	2.35	0.54
5:E:547:CYS:N	5:E:557:CYS:SG	2.81	0.54
1:A:26:ALA:HB1	1:A:56:LYS:HE2	1.89	0.54
4:D:259:ASN:OD1	4:D:261:ARG:HG2	2.08	0.53
5:E:283:PHE:O	5:E:284:GLN:HG3	2.07	0.53
5:G:977:LYS:HG2	5:G:979:PHE:CE1	2.43	0.53
5:F:965:VAL:CG1	5:F:969:GLN:HE22	2.21	0.53
2:B:108:ASN:O	2:B:111:VAL:HG12	2.07	0.53
5:F:280:GLU:OE1	5:F:287:TRP:HB3	2.07	0.53
5:F:647:ARG:HG3	5:F:669:ALA:HB3	1.89	0.53
5:F:766:ILE:HG22	5:F:817:ILE:O	2.08	0.53
5:F:822:MET:HA	5:F:842:PHE:O	2.07	0.53
2:B:50:THR:OG1	2:B:51:PRO:HD2	2.09	0.53
5:E:782:TRP:O	5:E:804:GLY:N	2.37	0.53
5:F:395:GLY:HA3	5:F:457:TRP:CH2	2.43	0.53
5:F:493:VAL:HG22	5:F:502:ILE:HD11	1.91	0.53
5:F:806:GLN:OE1	5:F:808:CYS:N	2.40	0.53
5:G:649:MET:HE2	5:G:651:HIS:CE1	2.40	0.53
5:E:400:ARG:HB2	5:E:465:TYR:HE2	1.73	0.53
5:E:748:TRP:HD1	5:E:749:ASP:N	2.07	0.53
5:G:961:ASP:HA	5:G:964:GLN:HG2	1.89	0.53
1:A:98:PHE:HB3	1:A:133:SER:HB3	1.91	0.53
5:E:399:ASP:CB	5:E:468:ALA:HB2	2.35	0.53
5:F:289:THR:CG2	5:F:328:ILE:HG22	2.39	0.53
5:F:438:PHE:HB3	5:F:456:GLN:HB3	1.90	0.53
1:A:110:ALA:HA	1:A:117:PHE:CE2	2.44	0.53
5:F:527:ILE:HD11	5:F:949:SER:HB3	1.90	0.53
1:A:29:LEU:HA	1:A:32:MET:HE3	1.91	0.53
4:D:239:HIS:CD2	4:D:241:ASN:H	2.26	0.53
5:E:748:TRP:HE1	5:E:753:ALA:HB2	1.74	0.53
5:F:348:HIS:CD2	5:F:352:LYS:HB3	2.44	0.53
5:G:920:GLU:HG3	5:G:922:TRP:HE1	1.74	0.53
5:E:272:VAL:HG13	5:E:273:THR:HG23	1.91	0.53
5:G:504:ASP:OD2	5:G:571:ARG:HB2	2.09	0.52
5:G:994:ASN:OD1	5:G:995:GLU:N	2.42	0.52
5:E:649:MET:HE2	5:E:651:HIS:CE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:475:HIS:ND1	5:F:476:ARG:HG3	2.24	0.52
5:F:958:TRP:NE1	5:F:978:ALA:HB1	2.24	0.52
5:G:895:CYS:HB3	5:G:905:CYS:HA	1.91	0.52
5:E:162:THR:HB	5:E:171:ARG:HG2	1.90	0.52
5:E:341:ALA:HB3	5:E:344:GLN:OE1	2.10	0.52
5:E:651:HIS:HB2	5:E:663:PRO:HG2	1.91	0.52
5:F:929:ILE:HD11	5:F:966:VAL:HG13	1.92	0.52
4:D:239:HIS:HD2	4:D:241:ASN:H	1.57	0.52
5:E:994:ASN:OD1	5:E:1011:ARG:HB2	2.10	0.52
5:F:746:ASP:OD2	5:G:1021:LYS:NZ	2.26	0.52
5:F:958:TRP:CD1	5:F:978:ALA:HB1	2.44	0.52
1:A:131:SER:O	1:A:134:THR:OG1	2.27	0.52
4:D:202:LYS:N	4:D:246:ASP:OD1	2.35	0.52
4:D:255:LYS:NZ	4:D:256:VAL:O	2.42	0.52
5:E:296:ASP:CG	5:E:297:SER:H	2.18	0.52
5:G:510:GLU:O	5:G:513:SER:OG	2.24	0.52
4:D:344:SER:HB2	4:D:348:GLU:N	2.24	0.52
5:F:333:VAL:HG11	5:F:342:ILE:HD11	1.91	0.52
5:F:339:GLU:OE2	5:F:345:CYS:N	2.42	0.52
5:F:593:GLU:HG2	5:F:681:ILE:HG23	1.92	0.52
5:G:875:ILE:HA	5:G:923:ILE:HD13	1.90	0.52
4:D:332:PRO:HG2	4:D:334:LEU:CD1	2.40	0.52
4:D:352:TYR:CE1	4:D:379:LYS:HA	2.45	0.52
5:E:862:VAL:HG12	5:E:866:GLN:NE2	2.25	0.52
5:F:599:LYS:HD2	5:F:604:TRP:CE2	2.45	0.52
5:G:585:LEU:HD22	5:G:624:LEU:HD13	1.92	0.52
5:G:582:GLU:O	5:G:598:LEU:HD12	2.09	0.51
5:G:952:THR:OG1	5:G:991:ILE:HG22	2.10	0.51
4:D:236:VAL:HG22	4:D:250:ILE:HD12	1.92	0.51
5:E:519:LEU:HD23	5:E:519:LEU:O	2.11	0.51
5:F:963:ALA:HB1	5:F:1026:VAL:HG23	1.93	0.51
1:A:14:TRP:CE2	1:A:66:LEU:HD22	2.45	0.51
2:B:41:PHE:CE2	2:B:98:VAL:HG22	2.45	0.51
4:D:163:LEU:HD23	4:D:348:GLU:OE2	2.11	0.51
4:D:200:THR:HA	4:D:247:ILE:HA	1.92	0.51
5:E:396:LYS:HZ1	5:E:467:GLU:HG3	1.74	0.51
5:F:606:SER:O	5:F:646:TRP:N	2.42	0.51
5:F:1012:ARG:HD3	5:F:1013:TRP:O	2.10	0.51
1:A:85:ASP:OD1	5:F:354:TYR:HE1	1.93	0.51
5:E:377:GLY:O	5:E:427:TYR:HD2	1.93	0.51
5:F:617:ALA:HA	5:F:620:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:809:ARG:HH12	5:G:1017:GLU:HA	1.75	0.51
5:G:953:VAL:HG12	5:G:993:LEU:HB2	1.92	0.51
5:E:582:GLU:HG3	5:E:599:LYS:HB3	1.92	0.51
5:F:733:GLU:OE1	5:F:742:THR:HG22	2.11	0.51
5:G:806:GLN:OE1	5:G:808:CYS:N	2.42	0.51
4:D:209:SER:OG	5:F:346:LYS:HE2	2.10	0.51
5:E:371:LEU:HG	5:E:390:ILE:HD12	1.93	0.51
5:E:667:LEU:HD21	5:E:903:TRP:CD1	2.45	0.51
5:E:894:GLN:HE22	5:E:906:PRO:HB2	1.75	0.51
5:G:963:ALA:HA	5:G:966:VAL:HG22	1.92	0.51
4:D:268:PRO:HB3	4:D:370:TYR:HB3	1.93	0.51
5:E:271:GLY:HA3	5:E:276:SER:O	2.11	0.51
5:E:667:LEU:CD2	5:E:903:TRP:HA	2.41	0.51
5:F:475:HIS:HE1	5:F:476:ARG:HE	1.59	0.51
4:D:178:LYS:HB2	4:D:284:TRP:CD1	2.46	0.51
4:D:179:MET:SD	4:D:221:LEU:HD22	2.51	0.50
5:G:388:VAL:HG12	5:G:390:ILE:HG12	1.93	0.50
1:A:7:LYS:O	1:A:10:VAL:HG12	2.11	0.50
2:B:24:GLY:H	2:B:68:LEU:HD22	1.77	0.50
5:E:463:ASP:OD1	5:E:464:HIS:N	2.42	0.50
5:G:894:GLN:O	5:G:894:GLN:HG2	2.10	0.50
4:D:318:VAL:HG13	4:D:321:LYS:HG3	1.94	0.50
5:F:741:GLY:HA3	5:F:780:PRO:HG2	1.92	0.50
4:D:339:PHE:CD2	4:D:391:LYS:HG2	2.40	0.50
5:E:1017:GLU:O	5:G:809:ARG:NH1	2.45	0.50
5:F:822:MET:SD	5:F:910:TRP:HZ2	2.35	0.50
5:G:585:LEU:HD23	5:G:585:LEU:H	1.77	0.50
5:G:849:THR:O	5:G:888:MET:HG3	2.12	0.50
2:B:14:LEU:O	2:B:17:LYS:HG2	2.11	0.50
2:B:98:VAL:HG13	2:B:102:ASN:HD21	1.77	0.50
4:D:164:GLY:H	4:D:348:GLU:CD	2.19	0.50
5:F:842:PHE:HD1	5:F:847:TRP:CD1	2.29	0.50
5:E:188:PHE:HA	5:E:192:HIS:CD2	2.45	0.50
5:E:647:ARG:HH21	5:E:670:SER:C	2.20	0.50
5:F:446:GLU:HB3	5:F:451:ASP:HB2	1.93	0.50
5:F:543:GLU:HB3	5:F:559:VAL:CG2	2.42	0.50
5:F:793:SER:C	5:F:794:ARG:HD2	2.37	0.50
5:F:824:LEU:HD21	5:F:839:LEU:HD11	1.93	0.50
5:F:889:TRP:HB3	5:F:910:TRP:CZ3	2.47	0.50
5:G:567:CYS:SG	5:G:571:ARG:NE	2.82	0.50
5:G:871:ASP:HB3	5:G:945:TRP:CH2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:866:GLN:HE22	5:E:902:LEU:HB2	1.77	0.50
5:F:719:LEU:HD21	5:F:756:VAL:HG13	1.93	0.50
5:F:889:TRP:HB3	5:F:910:TRP:HZ3	1.77	0.50
5:E:425:GLN:NE2	5:E:469:LYS:HE3	2.27	0.50
5:F:866:GLN:NE2	5:F:903:TRP:HZ3	2.09	0.50
5:E:168:CYS:HB2	5:E:261:GLY:HA3	1.94	0.50
5:E:631:SER:C	5:E:633:PRO:HD3	2.36	0.50
5:F:850:VAL:O	5:F:921:THR:HG23	2.11	0.50
5:F:372:GLU:HG3	5:F:389:GLU:HB3	1.94	0.49
5:F:563:PRO:HB2	5:F:986:GLN:HE22	1.77	0.49
4:D:236:VAL:HG22	4:D:250:ILE:CD1	2.43	0.49
4:D:284:TRP:NE1	4:D:296:LEU:HD13	2.27	0.49
5:E:429:LYS:HG2	5:E:430:ILE:N	2.27	0.49
5:F:965:VAL:HG13	5:F:969:GLN:HE22	1.76	0.49
5:E:202:CYS:HA	5:E:260:LYS:HE3	1.94	0.49
5:E:731:ARG:NE	5:E:733:GLU:OE2	2.44	0.49
5:F:719:LEU:HD23	5:F:760:LEU:HG	1.94	0.49
5:E:539:GLN:HE22	5:E:541:TRP:HA	1.77	0.49
5:E:748:TRP:C	5:E:748:TRP:HD1	2.20	0.49
5:G:409:VAL:O	5:G:412:ARG:HG2	2.12	0.49
2:B:28:LEU:O	2:B:32:LEU:HD23	2.12	0.49
5:E:407:ALA:HA	5:E:410:VAL:HG12	1.95	0.49
5:F:759:GLN:NE2	5:F:794:ARG:HG3	2.27	0.49
5:G:506:ASP:HA	5:G:544:GLU:OE1	2.13	0.49
1:A:85:ASP:HB3	5:F:354:TYR:CD1	2.48	0.49
5:E:582:GLU:O	5:E:582:GLU:HG2	2.13	0.49
5:F:295:TRP:HH2	5:F:363:VAL:HG12	1.78	0.49
5:G:941:ARG:NH1	5:G:986:GLN:O	2.45	0.49
5:E:667:LEU:HD23	5:E:903:TRP:HA	1.95	0.49
5:E:840:GLU:CD	5:E:847:TRP:HB3	2.38	0.49
5:F:328:ILE:CD1	5:F:355:CYS:HB2	2.43	0.49
5:F:612:TRP:HH2	5:F:620:LEU:HD23	1.78	0.49
4:D:314:GLU:CD	4:D:316:SER:H	2.21	0.49
5:G:991:ILE:HG13	5:G:1016:SER:HB3	1.95	0.49
5:G:266:LEU:HB2	5:G:343:TRP:CH2	2.35	0.49
5:F:476:ARG:HA	5:F:494:LYS:O	2.13	0.48
5:G:278:ARG:NE	5:G:362:GLY:HA3	2.17	0.48
5:G:405:LYS:O	5:G:408:ASP:OD1	2.31	0.48
4:D:217:ILE:O	4:D:220:THR:OG1	2.31	0.48
5:E:742:THR:HG22	5:E:743:ILE:H	1.79	0.48
5:F:965:VAL:O	5:F:969:GLN:OE1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:539:GLN:HE22	5:G:541:TRP:HA	1.78	0.48
5:E:209:SER:HB2	5:E:213:ASN:ND2	2.28	0.48
5:E:650:PHE:CZ	5:E:659:MET:HE2	2.48	0.48
5:E:928:LYS:O	5:E:944:ILE:HA	2.13	0.48
5:F:870:ALA:HA	5:F:945:TRP:NE1	2.29	0.48
5:E:370:ASP:OD2	5:E:391:GLN:HA	2.13	0.48
5:F:328:ILE:HD11	5:F:353:HIS:CG	2.48	0.48
5:G:893:VAL:HG13	5:G:907:SER:OG	2.13	0.48
4:D:208:HIS:ND1	4:D:217:ILE:HG12	2.29	0.48
5:E:177:GLN:O	5:E:179:ARG:NH1	2.47	0.48
5:E:396:LYS:NZ	5:E:467:GLU:HG3	2.29	0.48
5:F:385:THR:HG22	5:F:469:LYS:HG2	1.96	0.48
4:D:310:ILE:CD1	4:D:334:LEU:HD23	2.41	0.48
5:E:371:LEU:HD23	5:E:450:TRP:CE2	2.49	0.48
5:E:941:ARG:NH1	5:E:986:GLN:O	2.46	0.48
5:F:494:LYS:HZ2	5:F:497:ASP:C	2.22	0.48
5:F:280:GLU:OE1	5:F:288:GLY:N	2.46	0.48
5:G:348:HIS:CD2	5:G:349:GLU:N	2.81	0.48
5:G:463:ASP:HB3	5:G:465:TYR:CE2	2.47	0.48
1:A:125:LEU:O	1:A:129:LEU:HD13	2.14	0.48
4:D:162:ILE:N	4:D:286:ARG:O	2.46	0.48
5:E:794:ARG:HB2	5:E:797:GLN:HG3	1.95	0.48
5:G:794:ARG:HB2	5:G:797:GLN:NE2	2.28	0.48
1:A:81:SER:O	1:A:84:SER:HB2	2.13	0.48
1:A:89:HIS:ND1	5:F:354:TYR:CD2	2.82	0.48
5:F:295:TRP:CH2	5:F:363:VAL:HG12	2.49	0.48
5:G:931:LEU:HD22	5:G:938:CYS:C	2.38	0.48
4:D:208:HIS:CE1	4:D:217:ILE:HA	2.49	0.48
5:E:396:LYS:HG3	5:E:436:TRP:CD1	2.49	0.48
5:E:731:ARG:NH1	5:E:775:GLY:O	2.47	0.48
5:F:506:ASP:HB3	5:F:544:GLU:HA	1.95	0.48
5:F:888:MET:HE3	5:F:913:ARG:HD3	1.96	0.48
4:D:234:GLU:HG3	4:D:253:LYS:CA	2.36	0.47
4:D:275:VAL:HG21	4:D:305:ASP:HA	1.96	0.47
5:E:400:ARG:HB2	5:E:465:TYR:CE2	2.49	0.47
5:F:958:TRP:HE1	5:F:978:ALA:HB1	1.78	0.47
5:G:821:PHE:O	5:G:822:MET:HE2	2.13	0.47
4:D:261:ARG:HG3	4:D:262:VAL:HG23	1.96	0.47
4:D:402:THR:HA	4:D:405:GLU:OE1	2.14	0.47
5:E:421:LYS:HD2	5:E:422:THR:N	2.28	0.47
4:D:192:ILE:HG12	4:D:198:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:388:VAL:HG12	5:E:390:ILE:HG12	1.96	0.47
5:G:373:LEU:HD22	5:G:449:LEU:HD22	1.94	0.47
1:A:103:HIS:O	1:A:106:LEU:HG	2.14	0.47
5:E:806:GLN:OE1	5:E:808:CYS:N	2.46	0.47
5:F:597:GLU:OE2	5:F:597:GLU:N	2.47	0.47
5:G:547:CYS:N	5:G:557:CYS:SG	2.87	0.47
2:B:34:VAL:HG23	2:B:35:TYR:CD2	2.50	0.47
4:D:195:GLN:HB3	4:D:196:TRP:CD1	2.50	0.47
4:D:207:ASN:O	4:D:208:HIS:CD2	2.67	0.47
5:E:169:SER:HB2	5:E:257:ILE:CD1	2.45	0.47
5:E:736:HIS:CE1	5:E:737:GLU:HG3	2.50	0.47
5:F:339:GLU:HG3	5:F:340:PRO:HD2	1.96	0.47
5:G:279:LEU:HB3	5:G:290:ILE:HD13	1.95	0.47
4:D:380:SER:CB	4:D:384:ALA:HB3	2.44	0.47
5:E:516:CYS:O	5:E:521:CYS:N	2.32	0.47
5:F:375:LEU:HD21	5:F:470:ILE:HB	1.97	0.47
5:G:278:ARG:NH1	5:G:318:ARG:HA	2.29	0.47
2:B:14:LEU:HD11	2:B:118:PHE:CD2	2.50	0.47
5:E:742:THR:HG22	5:E:743:ILE:N	2.29	0.47
5:F:488:SER:OG	5:F:576:VAL:HG22	2.15	0.47
5:F:595:ARG:NE	5:F:597:GLU:OE1	2.47	0.47
5:G:292:ASP:HA	5:G:361:ALA:HB2	1.97	0.47
5:G:477:GLU:O	5:G:493:VAL:HA	2.14	0.47
5:G:592:CYS:SG	5:G:684:GLY:HA2	2.55	0.47
5:G:875:ILE:HD12	5:G:922:TRP:O	2.14	0.47
5:G:955:ASP:N	5:G:1022:GLU:O	2.44	0.47
4:D:359:PHE:HD2	4:D:372:THR:OG1	1.97	0.47
5:E:822:MET:HB3	5:E:903:TRP:NE1	2.30	0.47
5:E:941:ARG:NH1	5:E:987:GLY:HA2	2.30	0.47
5:F:737:GLU:OE2	5:F:782:TRP:CZ2	2.68	0.47
5:F:993:LEU:HD23	5:F:993:LEU:HA	1.74	0.47
5:G:946:HIS:HB3	5:G:992:TRP:CE2	2.49	0.47
2:B:101:GLU:HG3	4:D:287:ASN:ND2	2.30	0.47
5:E:776:GLU:OE1	5:E:811:LYS:HA	2.15	0.47
5:E:858:THR:O	5:E:862:VAL:HG23	2.15	0.47
5:E:875:ILE:HD12	5:E:922:TRP:O	2.14	0.47
5:F:420:LEU:HD21	5:F:553:HIS:CE1	2.50	0.47
2:B:24:GLY:HA3	2:B:68:LEU:HB2	1.96	0.47
2:B:67:VAL:HG13	6:B:201:HEM:C2B	2.50	0.47
5:E:399:ASP:OD1	5:E:465:TYR:HD2	1.97	0.47
5:F:438:PHE:O	5:F:456:GLN:N	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:612:TRP:CZ3	5:F:616:ASP:HB3	2.50	0.47
5:F:858:THR:O	5:F:862:VAL:HG23	2.15	0.47
5:F:271:GLY:HA3	5:F:276:SER:O	2.16	0.46
5:G:479:ARG:HD3	5:G:499:TRP:CH2	2.50	0.46
5:E:221:ILE:HD12	5:E:246:HIS:CE1	2.50	0.46
5:F:347:HIS:HD2	5:F:348:HIS:O	1.98	0.46
5:F:463:ASP:OD1	5:F:464:HIS:N	2.46	0.46
5:G:402:TRP:HH2	5:G:410:VAL:HG21	1.80	0.46
1:A:52:SER:O	1:A:56:LYS:HG2	2.14	0.46
1:A:103:HIS:HA	1:A:106:LEU:HG	1.97	0.46
5:E:839:LEU:HD13	5:E:921:THR:HG22	1.97	0.46
5:F:819:SER:HB2	5:F:844:ASN:HA	1.97	0.46
4:D:253:LYS:HG2	4:D:254:GLN:NE2	2.30	0.46
5:F:584:ARG:HG2	5:F:604:TRP:CZ3	2.50	0.46
5:G:822:MET:HB3	5:G:903:TRP:NE1	2.29	0.46
6:B:201:HEM:HBC2	6:B:201:HEM:HMC1	1.96	0.46
4:D:190:THR:O	4:D:197:LEU:HB2	2.15	0.46
5:F:517:ARG:NH2	5:F:551:GLU:O	2.33	0.46
5:G:271:GLY:HA3	5:G:276:SER:O	2.15	0.46
3:C:149:CYS:HB3	4:D:368:THR:HB	1.98	0.46
4:D:187:THR:HB	4:D:203:ASN:ND2	2.31	0.46
4:D:363:ASP:O	4:D:367:ASP:HA	2.15	0.46
5:G:731:ARG:NH1	5:G:777:GLY:HA2	2.31	0.46
4:D:210:GLU:HG3	5:F:349:GLU:OE2	2.16	0.46
5:E:478:PRO:HD3	5:E:554:LEU:HD21	1.97	0.46
5:F:505:SER:HA	5:F:988:THR:HB	1.98	0.46
5:F:620:LEU:HD12	5:F:621:CYS:N	2.30	0.46
5:F:782:TRP:CZ3	5:F:803:TRP:HB3	2.48	0.46
5:G:402:TRP:CZ2	5:G:470:ILE:HD11	2.51	0.46
5:G:544:GLU:O	5:G:546:GLN:NE2	2.49	0.46
5:G:901:THR:HB	5:G:903:TRP:CE3	2.49	0.46
1:A:69:ALA:HB2	1:A:80:LEU:HD21	1.98	0.46
2:B:4:THR:HB	2:B:7:GLU:OE1	2.15	0.46
2:B:78:LEU:HA	2:B:81:LEU:HD21	1.97	0.46
5:E:876:ASN:HD21	5:E:924:THR:HG22	1.79	0.46
5:F:852:LYS:HA	5:F:921:THR:HG22	1.98	0.46
5:G:370:ASP:OD2	5:G:391:GLN:HA	2.16	0.46
1:A:22:GLY:HA3	1:A:60:LYS:HE2	1.98	0.46
2:B:104:ARG:HD2	4:D:289:ASN:HD21	1.81	0.46
5:E:264:LEU:HD13	5:E:343:TRP:CG	2.50	0.46
5:E:507:PHE:HE2	5:E:575:VAL:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:737:GLU:OE2	5:F:782:TRP:HZ2	1.99	0.46
4:D:316:SER:HB2	4:D:318:VAL:O	2.15	0.46
5:E:172:ILE:HB	5:E:183:VAL:HG12	1.98	0.46
5:G:597:GLU:OE1	5:G:604:TRP:HE3	1.99	0.46
2:B:14:LEU:HD11	2:B:118:PHE:HD2	1.81	0.45
5:E:734:ILE:HD12	5:E:743:ILE:HD11	1.98	0.45
5:E:859:THR:HG22	5:E:895:CYS:H	1.80	0.45
5:F:599:LYS:HG3	5:F:604:TRP:CD2	2.51	0.45
5:G:567:CYS:HA	5:G:571:ARG:HH21	1.80	0.45
5:G:656:GLU:OE2	5:G:656:GLU:N	2.36	0.45
2:B:3:LEU:HB3	2:B:8:LYS:HD3	1.98	0.45
2:B:30:ARG:O	2:B:34:VAL:HG22	2.15	0.45
4:D:277:ARG:O	4:D:303:VAL:HG12	2.16	0.45
5:E:544:GLU:OE2	5:E:560:ALA:HB3	2.17	0.45
5:F:409:VAL:O	5:F:412:ARG:HG2	2.16	0.45
5:F:455:TRP:HZ3	5:F:457:TRP:HB2	1.81	0.45
5:F:479:ARG:HD3	5:F:499:TRP:CH2	2.52	0.45
1:A:138:SER:HA	4:D:352:TYR:OH	2.16	0.45
5:F:648:HIS:CD2	5:F:666:ALA:HB2	2.52	0.45
5:F:980:LYS:HG3	5:F:981:GLU:CD	2.41	0.45
5:G:894:GLN:N	5:G:906:PRO:O	2.47	0.45
4:D:267:LEU:HD21	4:D:399:VAL:HG21	1.99	0.45
5:F:628:VAL:HG22	5:F:683:SER:HB3	1.98	0.45
5:F:928:LYS:O	5:F:944:ILE:HA	2.16	0.45
5:G:789:ASN:HB3	5:G:791:LYS:NZ	2.32	0.45
4:D:166:HIS:HB2	4:D:298:TYR:O	2.16	0.45
4:D:174:PRO:HB2	4:D:263:MET:HG3	1.98	0.45
4:D:405:GLU:N	4:D:405:GLU:OE2	2.50	0.45
5:G:588:GLY:HA3	5:G:593:GLU:O	2.16	0.45
1:A:85:ASP:OD1	5:F:354:TYR:CE1	2.69	0.45
2:B:82:LYS:NZ	5:G:293:ASP:OD1	2.50	0.45
2:B:122:PHE:CE2	2:B:127:GLN:HG2	2.51	0.45
4:D:343:MET:CE	4:D:349:ASP:HB2	2.46	0.45
5:F:748:TRP:HH2	5:F:756:VAL:HG21	1.81	0.45
5:G:278:ARG:HE	5:G:362:GLY:CA	2.22	0.45
5:G:305:LYS:O	5:G:305:LYS:HD3	2.17	0.45
5:G:599:LYS:HD3	5:G:604:TRP:CD2	2.52	0.45
5:E:932:GLN:HB3	5:E:941:ARG:HG2	1.98	0.45
5:G:296:ASP:CG	5:G:297:SER:N	2.75	0.45
5:G:727:ARG:HD2	5:G:728:CYS:SG	2.57	0.45
2:B:80:ASN:OD1	5:G:400:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:PHE:O	4:D:176:GLN:HG2	2.17	0.45
4:D:300:MET:O	4:D:301:LEU:HD22	2.17	0.45
5:G:292:ASP:N	5:G:359:GLU:O	2.48	0.45
5:G:935:PRO:HD3	5:G:984:PHE:HE2	1.82	0.45
5:G:961:ASP:OD1	5:G:962:ASP:N	2.50	0.45
1:A:14:TRP:CZ2	1:A:66:LEU:HD22	2.52	0.44
5:E:980:LYS:O	5:E:981:GLU:HG3	2.17	0.44
5:G:278:ARG:NH2	5:G:317:GLY:O	2.50	0.44
5:G:902:LEU:HA	5:G:905:CYS:SG	2.57	0.44
4:D:162:ILE:HD11	4:D:283:GLY:HA3	1.98	0.44
5:G:442:CYS:HB3	5:G:452:CYS:HB3	1.65	0.44
5:G:618:HIS:NE2	5:G:690:LEU:HG	2.32	0.44
5:G:955:ASP:HA	5:G:958:TRP:HB2	2.00	0.44
5:E:724:GLY:HA3	5:E:729:ALA:C	2.42	0.44
5:E:822:MET:HG3	5:E:903:TRP:CD1	2.52	0.44
5:E:944:ILE:HD11	5:E:992:TRP:HB2	1.99	0.44
5:F:319:VAL:C	5:F:321:ALA:H	2.26	0.44
5:G:408:ASP:OD1	5:G:409:VAL:N	2.50	0.44
5:G:437:LEU:HA	5:G:456:GLN:O	2.17	0.44
5:G:792:GLU:OE1	5:G:792:GLU:N	2.42	0.44
1:A:78:ASN:OD1	1:A:79:ALA:N	2.48	0.44
1:A:134:THR:O	1:A:138:SER:N	2.49	0.44
4:D:314:GLU:OE1	4:D:315:GLY:N	2.51	0.44
5:F:494:LYS:NZ	5:F:497:ASP:O	2.49	0.44
1:A:105:LEU:HA	1:A:108:THR:HG22	1.98	0.44
4:D:202:LYS:HA	4:D:202:LYS:HD2	1.82	0.44
5:E:315:ALA:HB2	5:E:455:TRP:CH2	2.52	0.44
5:E:318:ARG:HB2	5:E:321:ALA:HB3	2.00	0.44
5:E:664:VAL:HG13	5:E:904:GLN:HG2	2.00	0.44
5:F:993:LEU:HD21	5:F:1013:TRP:HD1	1.81	0.44
5:G:521:CYS:HB3	5:G:577:CYS:HB2	1.99	0.44
5:G:794:ARG:HG2	5:G:794:ARG:HH11	1.83	0.44
5:G:446:GLU:HB3	5:G:451:ASP:HB2	1.98	0.44
5:G:941:ARG:CZ	5:G:987:GLY:HA2	2.48	0.44
5:G:958:TRP:CD1	5:G:978:ALA:HB1	2.53	0.44
1:A:59:GLY:HA2	1:A:62:VAL:HG22	1.99	0.44
4:D:335:ASN:O	4:D:338:THR:HG22	2.17	0.44
5:E:416:CYS:HB3	5:E:472:CYS:SG	2.58	0.44
5:E:767:ASN:HB3	5:E:817:ILE:CG1	2.44	0.44
5:E:851:GLY:HA2	5:E:888:MET:HE2	2.00	0.44
5:F:431:GLN:HA	5:F:432:ALA:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:548:GLU:CD	5:F:550:HIS:H	2.26	0.44
5:F:976:LEU:HD13	7:F:1204:NAG:H82	1.98	0.44
5:G:470:ILE:N	5:G:470:ILE:HD12	2.33	0.44
5:E:839:LEU:HD11	5:E:923:ILE:HB	2.00	0.44
5:F:965:VAL:HG23	5:F:1000:GLY:HA2	2.00	0.44
5:G:313:VAL:HG12	5:G:366:SER:O	2.18	0.44
5:G:597:GLU:OE1	5:G:604:TRP:CE3	2.71	0.44
5:G:886:ILE:HG23	5:G:887:PRO:HD2	2.00	0.44
2:B:66:LYS:HB3	6:B:201:HEM:HMA1	2.00	0.44
5:E:429:LYS:HG2	5:E:430:ILE:H	1.82	0.44
5:E:599:LYS:HE2	5:E:602:GLY:HA2	2.00	0.44
4:D:373:GLY:HA2	4:D:392:VAL:HG23	2.00	0.43
5:E:400:ARG:NE	5:E:465:TYR:OH	2.45	0.43
5:E:758:ARG:NH1	5:E:758:ARG:HA	2.33	0.43
5:E:764:GLU:O	5:E:819:SER:N	2.45	0.43
5:G:546:GLN:NE2	5:G:560:ALA:HB3	2.33	0.43
2:B:75:LEU:HA	2:B:78:LEU:HD21	2.01	0.43
4:D:365:GLU:HG2	4:D:366:GLU:N	2.33	0.43
5:E:296:ASP:CG	5:E:297:SER:N	2.76	0.43
5:E:825:ARG:NH2	5:E:840:GLU:OE1	2.50	0.43
5:F:650:PHE:CD1	5:F:650:PHE:N	2.86	0.43
4:D:163:LEU:HA	4:D:287:ASN:HA	2.00	0.43
5:F:940:GLY:HA2	5:F:984:PHE:HD2	1.83	0.43
5:G:794:ARG:HB2	5:G:797:GLN:CD	2.43	0.43
4:D:295:HIS:CE1	4:D:296:LEU:O	2.71	0.43
5:E:523:THR:O	5:E:577:CYS:HB3	2.18	0.43
5:F:862:VAL:HG22	5:F:865:ARG:NH2	2.33	0.43
5:G:858:THR:O	5:G:862:VAL:HG23	2.18	0.43
4:D:178:LYS:HD2	4:D:284:TRP:CD2	2.54	0.43
5:F:296:ASP:CG	5:F:297:SER:N	2.75	0.43
5:G:889:TRP:CZ3	5:G:912:LYS:HB2	2.54	0.43
4:D:307:ASP:OD1	4:D:308:GLN:N	2.47	0.43
5:E:418:SER:O	5:E:472:CYS:HB2	2.18	0.43
5:E:855:MET:HE1	5:E:921:THR:CG2	2.48	0.43
5:F:976:LEU:CD1	7:F:1204:NAG:H82	2.49	0.43
5:G:543:GLU:OE2	5:G:559:VAL:HB	2.19	0.43
5:G:585:LEU:HD12	5:G:593:GLU:O	2.19	0.43
2:B:57:ASN:O	2:B:61:LYS:NZ	2.46	0.43
5:E:263:ASP:O	5:E:283:PHE:HA	2.18	0.43
5:F:348:HIS:CD2	5:F:349:GLU:N	2.87	0.43
5:F:420:LEU:HD21	5:F:553:HIS:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:494:LYS:HZ3	5:F:499:TRP:CD1	2.37	0.43
5:G:786:MET:HE2	5:G:795:ILE:HG23	2.01	0.43
4:D:306:GLN:O	4:D:310:ILE:HG12	2.17	0.43
5:E:290:ILE:HD12	5:E:330:LEU:HB2	1.99	0.43
5:E:611:HIS:O	5:E:611:HIS:ND1	2.51	0.43
5:F:293:ASP:O	5:F:332:SER:HA	2.18	0.43
5:F:612:TRP:CH2	5:F:620:LEU:HD23	2.53	0.43
5:F:649:MET:HG2	5:F:651:HIS:NE2	2.33	0.43
2:B:35:TYR:HB3	2:B:37:TRP:CZ2	2.54	0.43
2:B:84:THR:HG23	2:B:85:PHE:CD2	2.54	0.43
4:D:173:PHE:HB2	4:D:176:GLN:NE2	2.33	0.43
5:E:749:ASP:OD1	5:E:751:SER:N	2.52	0.43
5:F:754:HIS:CE1	5:F:758:ARG:HG3	2.54	0.43
5:G:343:TRP:HD1	5:G:350:TRP:CZ2	2.36	0.43
5:G:609:ASN:HB3	5:G:677:VAL:C	2.44	0.43
1:A:99:LYS:O	1:A:102:SER:OG	2.29	0.43
4:D:187:THR:HB	4:D:203:ASN:HD21	1.84	0.43
4:D:396:GLN:O	4:D:399:VAL:HG22	2.19	0.43
5:E:159:MET:HE2	5:E:159:MET:HA	2.01	0.43
5:G:463:ASP:OD1	5:G:464:HIS:N	2.48	0.43
5:G:611:HIS:O	5:G:611:HIS:ND1	2.52	0.43
5:G:693:CYS:N	5:G:713:CYS:SG	2.91	0.43
2:B:11:VAL:HG13	2:B:130:TYR:CZ	2.54	0.42
2:B:122:PHE:CD1	2:B:126:VAL:HG13	2.53	0.42
2:B:124:PRO:HB2	2:B:125:PRO:HD3	2.01	0.42
5:E:264:LEU:HD13	5:E:343:TRP:CD2	2.54	0.42
5:E:516:CYS:HB2	5:E:521:CYS:HB2	2.01	0.42
5:E:545:PHE:CD1	5:E:559:VAL:HG12	2.54	0.42
5:F:548:GLU:HG3	5:F:551:GLU:OE2	2.18	0.42
5:G:268:LEU:HA	5:G:268:LEU:HD23	1.76	0.42
5:G:503:CYS:HB3	5:G:506:ASP:OD2	2.19	0.42
2:B:78:LEU:HD23	2:B:81:LEU:HD21	2.00	0.42
5:E:505:SER:CB	5:E:988:THR:HB	2.49	0.42
5:E:588:GLY:HA3	5:E:593:GLU:O	2.19	0.42
5:G:316:ILE:HG13	5:G:456:GLN:OE1	2.19	0.42
5:G:930:ARG:HD3	5:G:950:TRP:CZ2	2.54	0.42
1:A:112:HIS:O	1:A:113:LEU:HD22	2.19	0.42
5:F:267:ARG:HE	5:F:280:GLU:HG2	1.85	0.42
5:F:994:ASN:ND2	5:F:1015:HIS:O	2.52	0.42
5:G:485:ILE:HD11	5:G:582:GLU:OE1	2.19	0.42
5:G:606:SER:O	5:G:646:TRP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:928:LYS:HE3	5:G:1006:TRP:CD1	2.54	0.42
5:G:930:ARG:C	5:G:931:LEU:HD12	2.45	0.42
1:A:51:GLY:HA2	1:A:56:LYS:HE3	2.01	0.42
5:E:582:GLU:CG	5:E:599:LYS:HB3	2.49	0.42
5:F:460:LEU:HD23	5:F:460:LEU:HA	1.81	0.42
5:G:982:ALA:HB1	5:G:985:GLY:C	2.44	0.42
4:D:245:VAL:CG1	4:D:247:ILE:HD13	2.46	0.42
4:D:316:SER:OG	4:D:317:THR:N	2.52	0.42
5:E:381:ARG:NH2	5:E:497:ASP:OD2	2.53	0.42
5:F:969:GLN:HE21	5:F:1004:SER:HA	1.85	0.42
5:G:431:GLN:HA	5:G:432:ALA:HA	1.86	0.42
5:G:567:CYS:SG	5:G:571:ARG:HG3	2.60	0.42
5:G:852:LYS:NZ	5:G:919:GLU:HA	2.34	0.42
5:G:991:ILE:HG13	5:G:991:ILE:O	2.20	0.42
1:A:42:TYR:CE2	1:A:93:VAL:HA	2.55	0.42
5:F:758:ARG:NH1	5:F:758:ARG:HB3	2.35	0.42
5:G:265:SER:O	5:G:281:VAL:HA	2.19	0.42
5:G:556:LEU:HD23	5:G:556:LEU:O	2.18	0.42
2:B:21:ASP:HA	2:B:65:LYS:HD2	2.00	0.42
4:D:185:LEU:HD13	4:D:292:PHE:HZ	1.85	0.42
4:D:223:LEU:O	4:D:230:LEU:HD12	2.19	0.42
4:D:312:HIS:ND1	4:D:386:TYR:HD2	2.17	0.42
5:E:431:GLN:HA	5:E:432:ALA:HA	1.90	0.42
5:G:719:LEU:HG	5:G:759:GLN:CD	2.44	0.42
5:F:328:ILE:HD13	5:F:328:ILE:HG21	1.72	0.42
5:F:826:LEU:HD23	5:F:839:LEU:HA	2.02	0.42
5:F:979:PHE:HB2	5:F:1025:ALA:HB3	2.00	0.42
5:G:821:PHE:C	5:G:822:MET:HE2	2.44	0.42
5:E:270:ASP:HB2	5:E:321:ALA:HA	2.01	0.42
5:E:786:MET:HE3	5:E:798:CYS:HB2	2.02	0.42
5:G:433:THR:HG22	5:G:434:ASN:N	2.35	0.42
5:G:731:ARG:HE	5:G:731:ARG:HB2	1.65	0.42
5:G:793:SER:OG	5:G:794:ARG:HD2	2.20	0.42
4:D:311:ARG:NH2	5:E:216:GLU:OE2	2.53	0.42
5:E:191:ASP:OD1	5:E:191:ASP:N	2.51	0.42
5:E:348:HIS:CG	5:E:349:GLU:N	2.88	0.42
5:G:272:VAL:HG11	5:G:391:GLN:HG3	2.01	0.42
4:D:283:GLY:O	4:D:296:LEU:HD12	2.20	0.41
5:E:735:TYR:HE1	5:E:738:GLY:C	2.28	0.41
5:F:475:HIS:CE1	5:F:476:ARG:HE	2.38	0.41
5:F:479:ARG:NH2	5:F:492:GLU:OE1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:611:HIS:CG	5:F:649:MET:HG3	2.54	0.41
5:F:630:LEU:HD11	5:F:683:SER:HA	2.02	0.41
5:G:605:GLY:HA3	5:G:646:TRP:CD1	2.55	0.41
4:D:341:ALA:HB3	4:D:389:TYR:HE1	1.85	0.41
5:E:159:MET:HG3	5:E:200:LEU:HD21	2.01	0.41
5:E:495:HIS:HB3	5:E:541:TRP:CZ2	2.54	0.41
5:E:955:ASP:HA	5:E:958:TRP:HB2	2.03	0.41
5:F:268:LEU:HD23	5:F:268:LEU:HA	1.76	0.41
5:F:268:LEU:HD12	5:F:275:CYS:HA	2.01	0.41
5:F:886:ILE:HG23	5:F:887:PRO:HD2	2.02	0.41
5:G:931:LEU:HD12	5:G:931:LEU:N	2.34	0.41
1:A:3:SER:HB2	1:A:4:PRO:HD2	2.03	0.41
4:D:179:MET:HG2	4:D:222:THR:O	2.20	0.41
4:D:281:VAL:HG21	4:D:389:TYR:OH	2.20	0.41
4:D:304:ALA:HB3	4:D:340:CYS:SG	2.61	0.41
5:E:494:LYS:HB2	5:E:499:TRP:CE2	2.55	0.41
5:E:543:GLU:CG	5:E:559:VAL:HB	2.49	0.41
5:E:871:ASP:OD1	5:E:872:LYS:HG2	2.20	0.41
5:E:941:ARG:HH11	5:E:987:GLY:HA2	1.85	0.41
5:G:283:PHE:O	5:G:284:GLN:HG2	2.20	0.41
5:G:736:HIS:CE1	5:G:737:GLU:HG3	2.55	0.41
5:E:166:ASN:ND2	5:E:261:GLY:O	2.48	0.41
5:E:375:LEU:HD22	5:E:382:CYS:C	2.44	0.41
5:E:609:ASN:OD1	5:E:676:GLN:HB3	2.20	0.41
5:F:898:GLY:N	5:F:899:PRO:HD2	2.35	0.41
5:G:315:ALA:HB3	5:G:364:THR:CG2	2.50	0.41
5:G:414:LEU:HG	5:G:414:LEU:O	2.21	0.41
5:F:588:GLY:HA3	5:F:593:GLU:O	2.21	0.41
5:F:618:HIS:NE2	5:F:690:LEU:HG	2.35	0.41
5:E:292:ASP:N	5:E:359:GLU:O	2.38	0.41
1:A:74:ASP:OD2	5:E:354:TYR:OH	2.34	0.41
5:E:673:PRO:HB2	5:E:676:GLN:HE22	1.85	0.41
5:F:429:LYS:HG2	5:F:430:ILE:H	1.84	0.41
5:F:646:TRP:HA	5:F:646:TRP:CE3	2.55	0.41
5:F:994:ASN:ND2	5:F:1016:SER:HA	2.36	0.41
5:G:381:ARG:NH2	5:G:496:GLY:HA3	2.36	0.41
5:G:928:LYS:HZ2	5:G:1006:TRP:HD1	1.68	0.41
5:G:952:THR:HG21	5:G:987:GLY:HA3	2.03	0.41
1:A:130:ALA:O	1:A:134:THR:HG23	2.20	0.41
4:D:233:ILE:O	4:D:233:ILE:HG13	2.21	0.41
5:E:173:GLU:OE1	5:E:180:TRP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:373:LEU:HD21	5:E:450:TRP:CH2	2.55	0.41
5:F:485:ILE:HG23	5:F:486:PRO:HD2	2.03	0.41
5:G:585:LEU:HD11	5:G:591:PRO:C	2.45	0.41
5:G:675:GLU:H	5:G:675:GLU:CD	2.26	0.41
5:G:749:ASP:OD1	5:G:749:ASP:C	2.63	0.41
5:G:794:ARG:HB2	5:G:797:GLN:OE1	2.21	0.41
5:G:917:PRO:HA	5:G:920:GLU:OE2	2.21	0.41
1:A:83:LEU:HD12	1:A:83:LEU:H	1.86	0.41
1:A:109:LEU:HG	1:A:117:PHE:CZ	2.44	0.41
4:D:213:THR:O	4:D:217:ILE:HG13	2.21	0.41
4:D:316:SER:HG	4:D:317:THR:N	2.19	0.41
4:D:332:PRO:HB3	4:D:377:PHE:CD1	2.56	0.41
5:E:221:ILE:HB	5:E:246:HIS:CD2	2.56	0.41
5:E:290:ILE:O	5:E:361:ALA:N	2.48	0.41
5:E:291:CYS:HA	5:E:360:ASP:HA	2.03	0.41
5:E:405:LYS:O	5:E:409:VAL:HG23	2.21	0.41
5:E:420:LEU:O	5:E:421:LYS:HB2	2.20	0.41
5:E:426:VAL:HG23	5:E:427:TYR:N	2.36	0.41
5:E:749:ASP:OD1	5:E:749:ASP:C	2.63	0.41
5:E:851:GLY:O	5:E:855:MET:HE2	2.20	0.41
5:F:664:VAL:HG13	5:F:904:GLN:HG3	2.02	0.41
5:G:523:THR:O	5:G:578:SER:N	2.54	0.41
5:G:714:ILE:HG13	5:G:714:ILE:O	2.21	0.41
5:E:732:VAL:HG21	5:E:748:TRP:CH2	2.51	0.41
5:F:539:GLN:HE22	5:F:541:TRP:HA	1.86	0.41
5:F:583:ILE:HD11	5:F:659:MET:HE3	2.03	0.41
5:G:527:ILE:CD1	5:G:575:VAL:HG22	2.51	0.41
2:B:109:VAL:O	2:B:112:CYS:HB2	2.21	0.40
5:E:232:GLU:HG3	5:E:234:ALA:H	1.85	0.40
5:E:600:THR:O	5:E:601:LEU:HG	2.20	0.40
5:E:838:ARG:NH2	5:E:922:TRP:HZ2	2.18	0.40
5:F:718:GLN:H	5:F:735:TYR:HB3	1.85	0.40
5:E:352:LYS:HD2	5:E:352:LYS:HA	1.84	0.40
5:E:673:PRO:HB2	5:E:676:GLN:OE1	2.21	0.40
5:F:283:PHE:O	5:F:284:GLN:HG2	2.22	0.40
5:F:436:TRP:HZ2	5:F:460:LEU:N	2.20	0.40
5:F:822:MET:SD	5:F:903:TRP:NE1	2.94	0.40
5:F:961:ASP:O	5:F:965:VAL:HG23	2.21	0.40
5:E:580:TYR:CD1	5:E:580:TYR:N	2.90	0.40
6:B:201:HEM:HHC	6:B:201:HEM:HBB2	2.04	0.40
5:E:786:MET:CE	5:E:798:CYS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:838:ARG:NH2	5:E:920:GLU:OE1	2.53	0.40
5:F:431:GLN:N	5:F:431:GLN:OE1	2.54	0.40
5:F:494:LYS:HE2	5:F:499:TRP:CD1	2.57	0.40
5:F:550:HIS:O	5:F:550:HIS:CG	2.74	0.40
5:F:647:ARG:HG3	5:F:647:ARG:O	2.21	0.40
5:G:429:LYS:HG2	5:G:430:ILE:H	1.85	0.40
5:G:742:THR:O	5:G:743:ILE:HD13	2.21	0.40
1:A:76:MET:HG2	1:A:80:LEU:HD23	2.03	0.40
4:D:379:LYS:HD3	4:D:379:LYS:N	2.36	0.40
5:E:938:CYS:HB3	5:E:1028:CYS:HB2	2.03	0.40
5:F:940:GLY:HA2	5:F:984:PHE:CD2	2.57	0.40
5:G:488:SER:OG	5:G:576:VAL:HG22	2.22	0.40
5:G:599:LYS:NZ	5:G:602:GLY:O	2.34	0.40
5:G:618:HIS:CE1	5:G:690:LEU:HG	2.56	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	139/142 (98%)	128 (92%)	11 (8%)	0	100	100
2	B	144/147 (98%)	142 (99%)	2 (1%)	0	100	100
3	C	8/83 (10%)	8 (100%)	0	0	100	100
4	D	242/245 (99%)	224 (93%)	18 (7%)	0	100	100
5	E	853/1156 (74%)	824 (97%)	25 (3%)	4 (0%)	24	63
5	F	745/1156 (64%)	719 (96%)	21 (3%)	5 (1%)	18	55
5	G	745/1156 (64%)	720 (97%)	21 (3%)	4 (0%)	24	63
All	All	2876/4085 (70%)	2765 (96%)	98 (3%)	13 (0%)	26	63

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	421	LYS
5	E	426	VAL
5	E	427	TYR
5	F	421	LYS
5	F	426	VAL
5	F	427	TYR
5	G	421	LYS
5	G	426	VAL
5	G	427	TYR
5	E	263	ASP
5	F	320	ASN
5	F	263	ASP
5	G	263	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/114 (99%)	113 (100%)	0	100	100
2	B	118/119 (99%)	118 (100%)	0	100	100
3	C	8/71 (11%)	8 (100%)	0	100	100
4	D	209/210 (100%)	209 (100%)	0	100	100
5	E	697/953 (73%)	697 (100%)	0	100	100
5	F	610/953 (64%)	610 (100%)	0	100	100
5	G	610/953 (64%)	610 (100%)	0	100	100
All	All	2365/3373 (70%)	2365 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

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Mol	Chain	Res	Type
1	A	45	HIS
1	A	103	HIS
4	D	208	HIS
4	D	239	HIS
4	D	289	ASN
4	D	312	HIS
5	E	353	HIS
5	E	356	ASN
5	E	358	ASN
5	E	539	GLN
5	E	622	GLN
5	E	651	HIS
5	E	754	HIS
5	E	866	GLN
5	E	876	ASN
5	E	892	ASN
5	E	946	HIS
5	F	358	ASN
5	F	658	HIS
5	F	773	HIS
5	F	969	GLN
5	G	348	HIS
5	G	456	GLN
5	G	539	GLN
5	G	651	HIS
5	G	964	GLN
5	G	969	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
7	NAG	D	1001	4	14,14,15	0.75	0	17,19,21	0.82	0
7	NAG	F	1204	5	14,14,15	0.84	0	17,19,21	1.70	4 (23%)
7	NAG	D	1003	4	14,14,15	0.76	0	17,19,21	0.97	1 (5%)
7	NAG	E	2005	5	14,14,15	0.75	0	17,19,21	0.81	0
7	NAG	F	1203	5	14,14,15	0.79	0	17,19,21	1.43	1 (5%)
7	NAG	E	2003	5	14,14,15	0.69	0	17,19,21	1.89	3 (17%)
7	NAG	F	1202	5	14,14,15	0.74	0	17,19,21	0.77	0
7	NAG	D	1002	4	14,14,15	0.76	0	17,19,21	1.34	2 (11%)
6	HEM	B	201	2	50,50,50	1.46	7 (14%)	66,82,82	1.16	6 (9%)
7	NAG	G	1202	5	14,14,15	0.67	0	17,19,21	1.83	2 (11%)
7	NAG	G	1203	5	14,14,15	0.78	0	17,19,21	1.46	2 (11%)
7	NAG	G	1204	5	14,14,15	0.84	0	17,19,21	1.61	4 (23%)
6	HEM	A	201	1	50,50,50	1.33	6 (12%)	66,82,82	1.08	4 (6%)
7	NAG	E	2004	5	14,14,15	0.74	0	17,19,21	1.40	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	1001	4	-	0/6/23/26	0/1/1/1
7	NAG	F	1204	5	-	4/6/23/26	0/1/1/1
7	NAG	D	1003	4	-	0/6/23/26	0/1/1/1
7	NAG	E	2005	5	-	1/6/23/26	0/1/1/1
7	NAG	F	1203	5	-	2/6/23/26	0/1/1/1
7	NAG	E	2003	5	-	3/6/23/26	0/1/1/1
7	NAG	F	1202	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	1002	4	-	3/6/23/26	0/1/1/1
6	HEM	B	201	2	-	4/14/54/54	-
7	NAG	G	1202	5	-	3/6/23/26	0/1/1/1
7	NAG	G	1203	5	-	1/6/23/26	0/1/1/1
7	NAG	G	1204	5	-	4/6/23/26	0/1/1/1
6	HEM	A	201	1	-	2/14/54/54	-
7	NAG	E	2004	5	-	1/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	201	HEM	FE-ND	3.56	2.05	1.94
6	B	201	HEM	FE-NB	3.38	2.05	1.94
6	B	201	HEM	FE-NA	3.36	2.06	1.95
6	B	201	HEM	FE-NC	3.26	2.06	1.95
6	B	201	HEM	CAC-C3C	2.99	1.55	1.47
6	A	201	HEM	CAC-C3C	2.91	1.55	1.47
6	A	201	HEM	CAB-C3B	2.88	1.55	1.47
6	A	201	HEM	FE-NA	2.84	2.04	1.95
6	B	201	HEM	CAB-C3B	2.73	1.54	1.47
6	A	201	HEM	FE-NB	2.63	2.03	1.94
6	A	201	HEM	FE-ND	2.62	2.03	1.94
6	A	201	HEM	FE-NC	2.35	2.03	1.95
6	B	201	HEM	CMC-C2C	2.05	1.55	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	2003	NAG	C1-O5-C5	5.85	120.12	112.19
7	G	1202	NAG	C1-O5-C5	5.51	119.66	112.19
7	F	1203	NAG	C1-O5-C5	4.86	118.77	112.19
7	E	2004	NAG	C1-O5-C5	4.55	118.36	112.19
7	G	1203	NAG	C1-O5-C5	4.12	117.77	112.19
7	F	1204	NAG	C1-O5-C5	3.77	117.31	112.19
7	G	1204	NAG	C1-O5-C5	3.32	116.69	112.19
7	F	1204	NAG	C4-C3-C2	3.27	115.81	111.02
7	E	2003	NAG	C2-N2-C7	3.20	127.46	122.90
7	G	1202	NAG	C2-N2-C7	3.12	127.34	122.90
7	G	1204	NAG	C2-N2-C7	3.06	127.27	122.90
7	D	1002	NAG	C1-O5-C5	3.03	116.30	112.19
6	B	201	HEM	C1B-NB-C4B	2.76	107.92	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1002	NAG	C2-N2-C7	2.74	126.80	122.90
7	G	1203	NAG	C4-C3-C2	-2.69	107.07	111.02
7	G	1204	NAG	C4-C3-C2	2.60	114.83	111.02
6	B	201	HEM	C3B-C2B-C1B	2.59	108.41	106.49
7	D	1003	NAG	O5-C1-C2	-2.52	107.31	111.29
6	A	201	HEM	C4D-ND-C1D	2.47	107.63	105.07
6	A	201	HEM	C1B-NB-C4B	2.47	107.63	105.07
7	F	1204	NAG	C2-N2-C7	2.41	126.34	122.90
6	B	201	HEM	C4D-ND-C1D	2.41	107.56	105.07
6	B	201	HEM	C4A-NA-C1A	2.32	107.62	105.35
6	A	201	HEM	C4C-NC-C1C	2.30	107.60	105.35
6	A	201	HEM	C4A-NA-C1A	2.16	107.47	105.35
7	F	1204	NAG	O5-C5-C4	-2.15	105.60	110.83
7	E	2003	NAG	C3-C4-C5	-2.15	106.41	110.24
7	G	1204	NAG	O5-C5-C4	-2.12	105.68	110.83
6	B	201	HEM	CAD-CBD-CGD	-2.04	109.21	113.60
6	B	201	HEM	C4C-NC-C1C	2.01	107.32	105.35

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	2003	NAG	C1-C2-N2-C7
7	F	1204	NAG	O5-C5-C6-O6
7	F	1204	NAG	C4-C5-C6-O6
7	F	1204	NAG	C1-C2-N2-C7
7	G	1202	NAG	C1-C2-N2-C7
7	G	1204	NAG	C1-C2-N2-C7
7	G	1204	NAG	O5-C5-C6-O6
7	F	1203	NAG	O5-C5-C6-O6
7	G	1203	NAG	O5-C5-C6-O6
7	G	1204	NAG	C4-C5-C6-O6
7	E	2005	NAG	O5-C5-C6-O6
7	E	2004	NAG	O5-C5-C6-O6
7	D	1002	NAG	C4-C5-C6-O6
7	G	1202	NAG	O5-C5-C6-O6
7	E	2003	NAG	O5-C5-C6-O6
7	E	2003	NAG	C3-C2-N2-C7
7	G	1202	NAG	C3-C2-N2-C7
7	G	1204	NAG	C3-C2-N2-C7
6	B	201	HEM	CAD-CBD-CGD-O1D
6	A	201	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	A	201	HEM	CAD-CBD-CGD-O2D
6	B	201	HEM	CAD-CBD-CGD-O2D
7	D	1002	NAG	O5-C5-C6-O6
6	B	201	HEM	CAA-CBA-CGA-O1A
7	F	1203	NAG	C1-C2-N2-C7
7	D	1002	NAG	C3-C2-N2-C7
7	F	1204	NAG	C3-C2-N2-C7
6	B	201	HEM	CAA-CBA-CGA-O2A

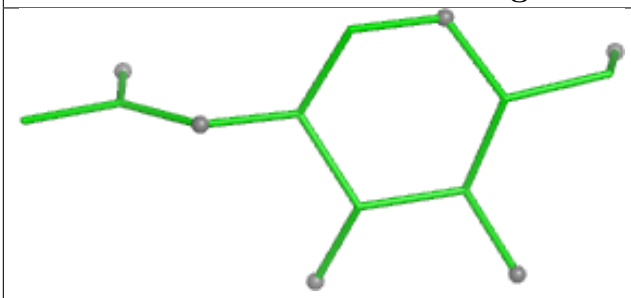
There are no ring outliers.

3 monomers are involved in 7 short contacts:

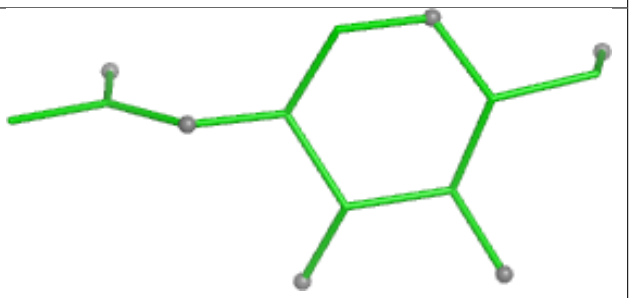
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1204	NAG	2	0
6	B	201	HEM	4	0
6	A	201	HEM	1	0

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

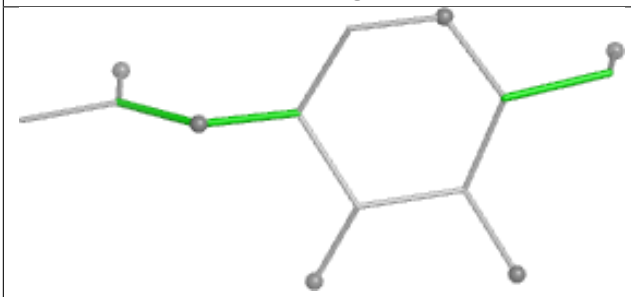
Ligand NAG D 1001



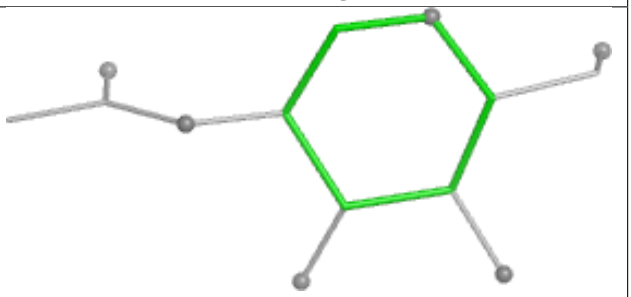
Bond lengths



Bond angles



Torsions



Rings

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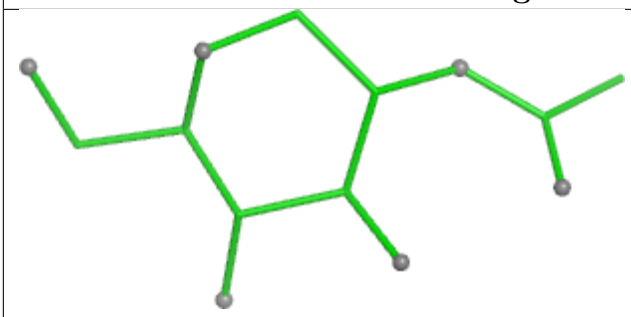
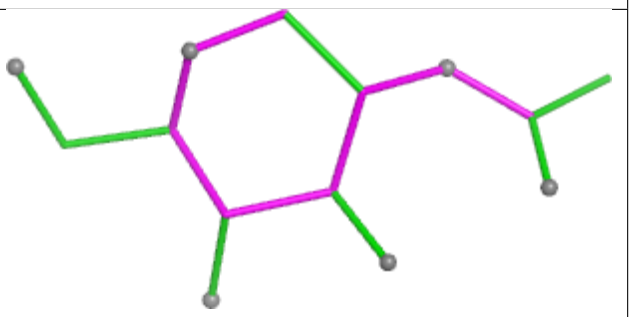
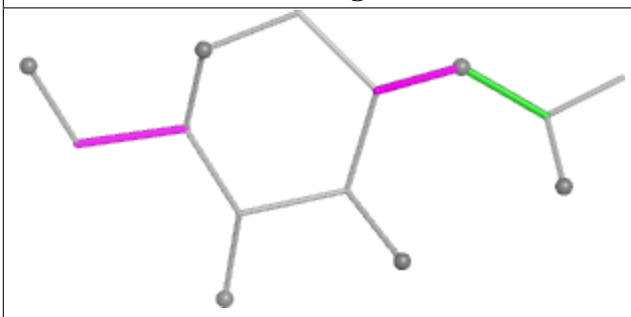


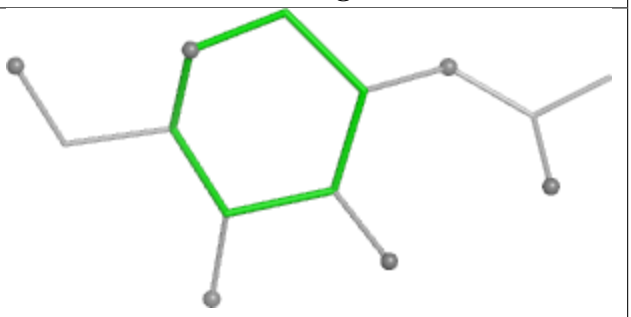
Bond lengths



Bond angles

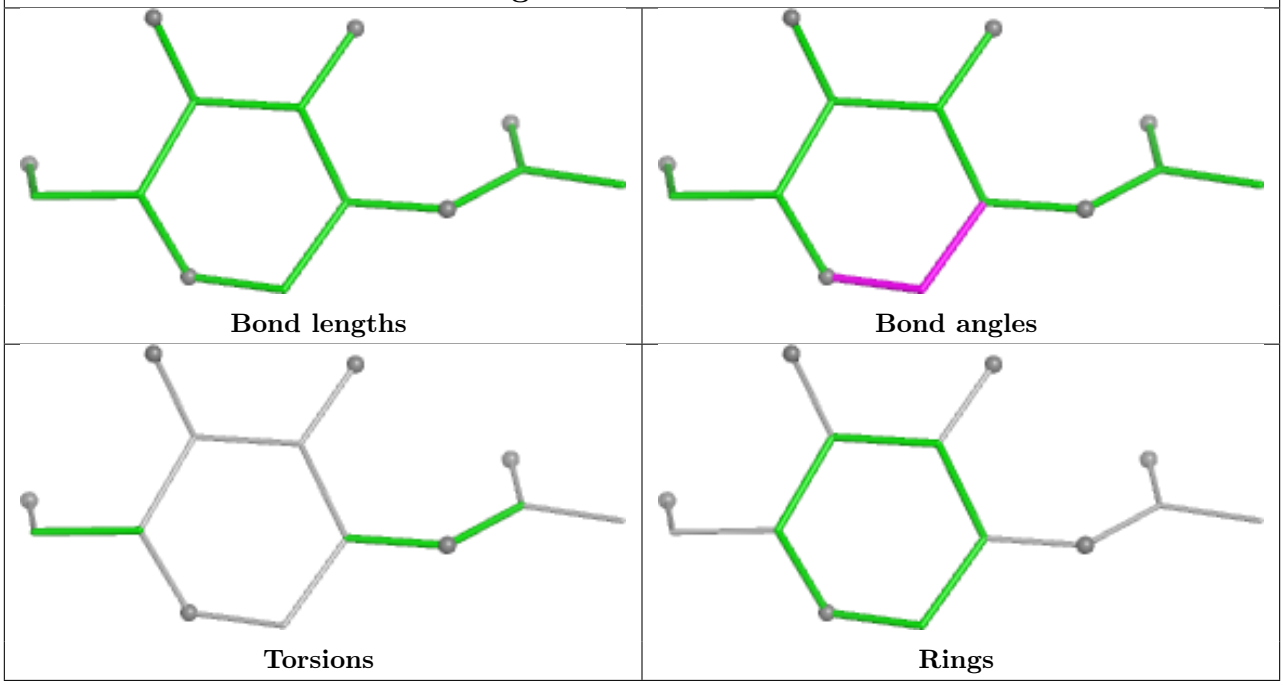


Torsions

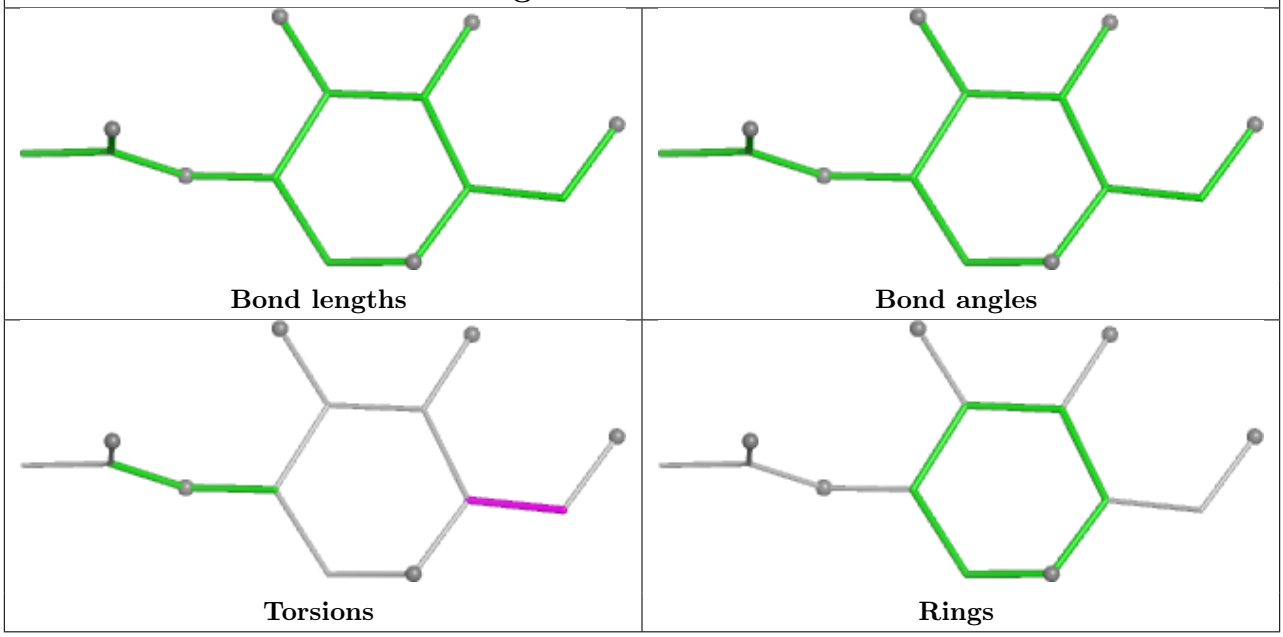


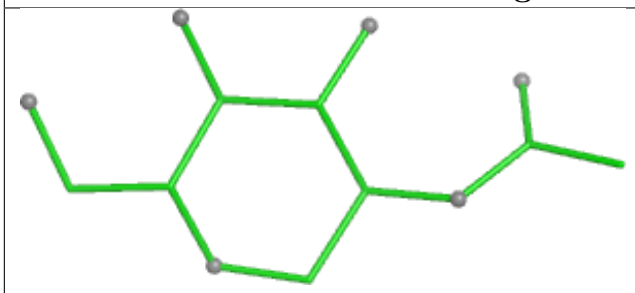
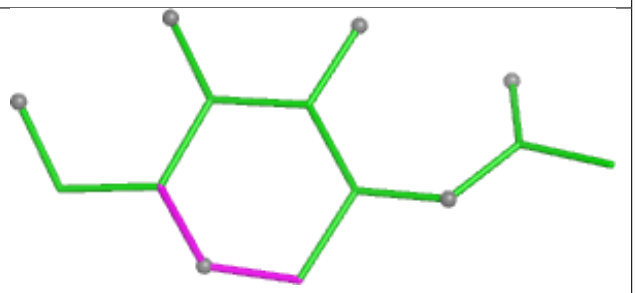
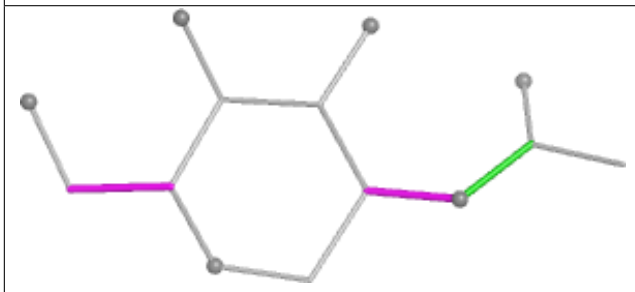
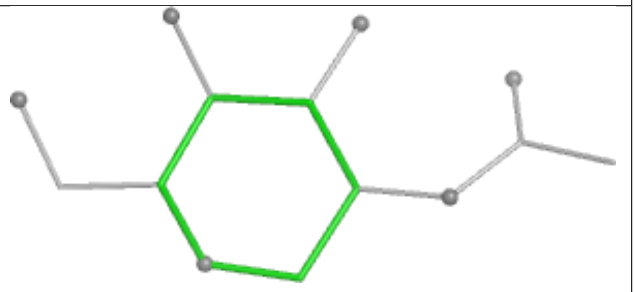
Rings

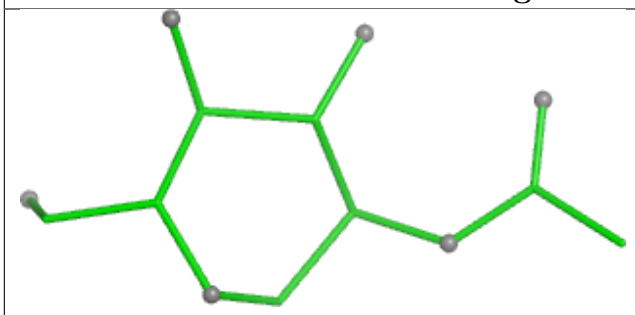
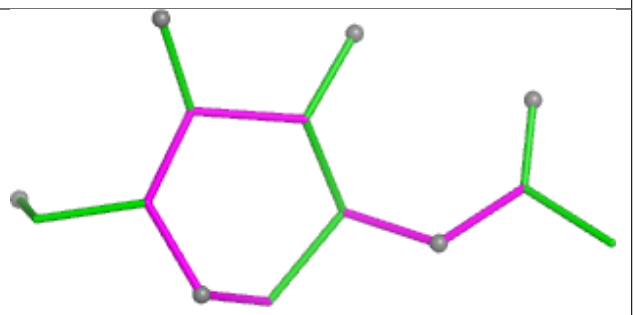
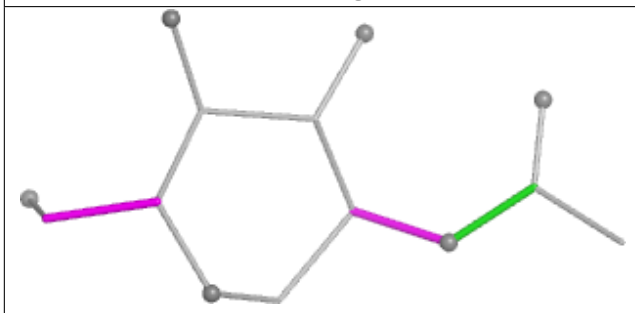
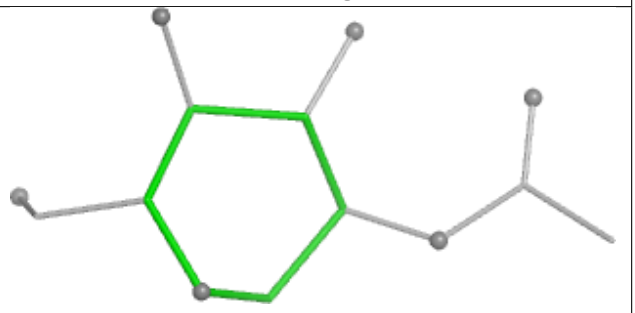
Ligand NAG D 1003



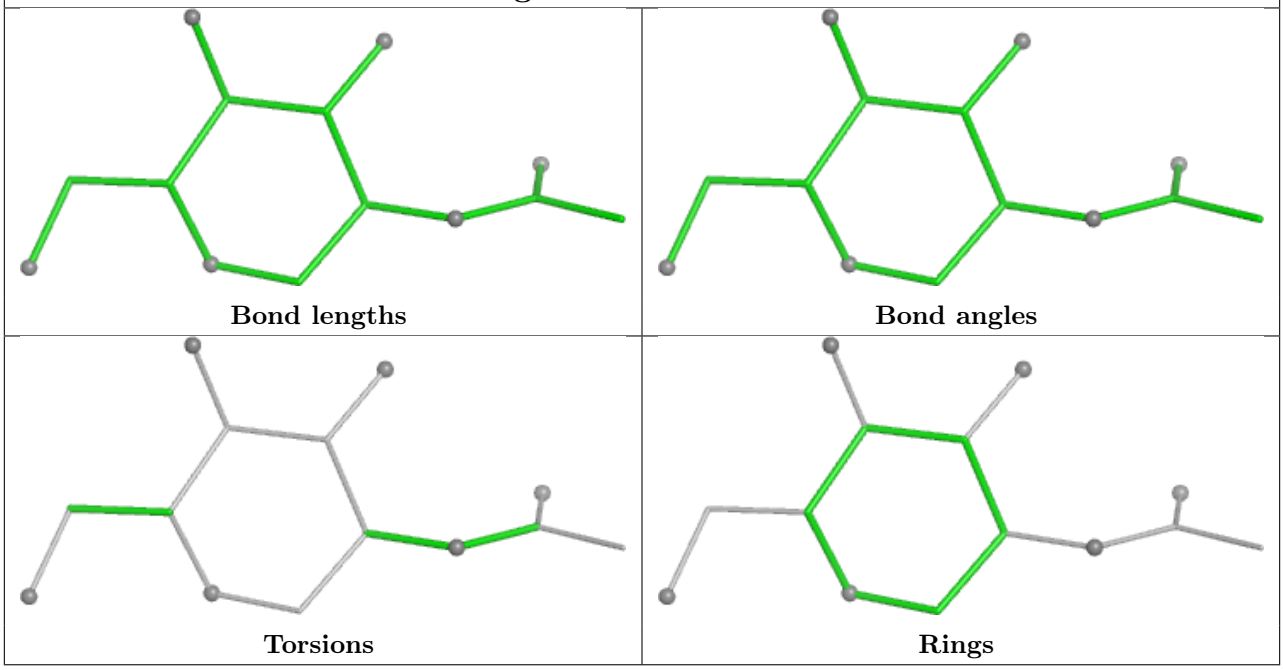
Ligand NAG E 2005



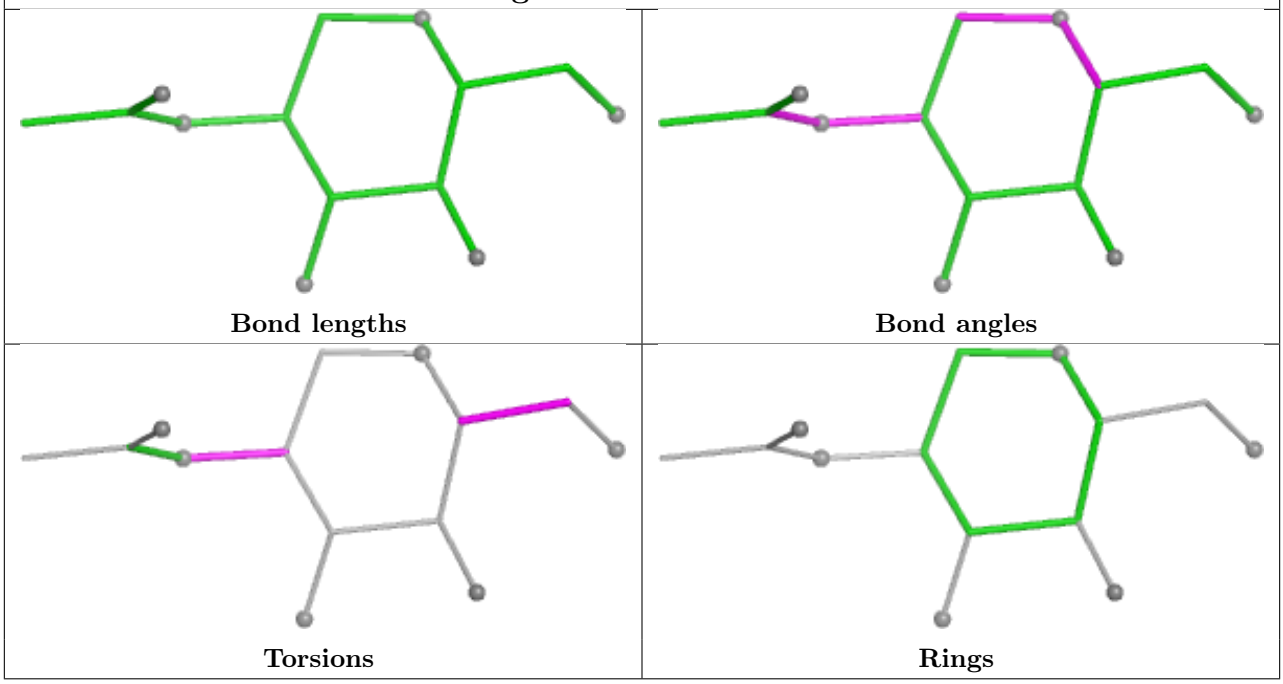
Ligand NAG F 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG E 2003	
 Bond lengths	 Bond angles
 Torsions	 Rings

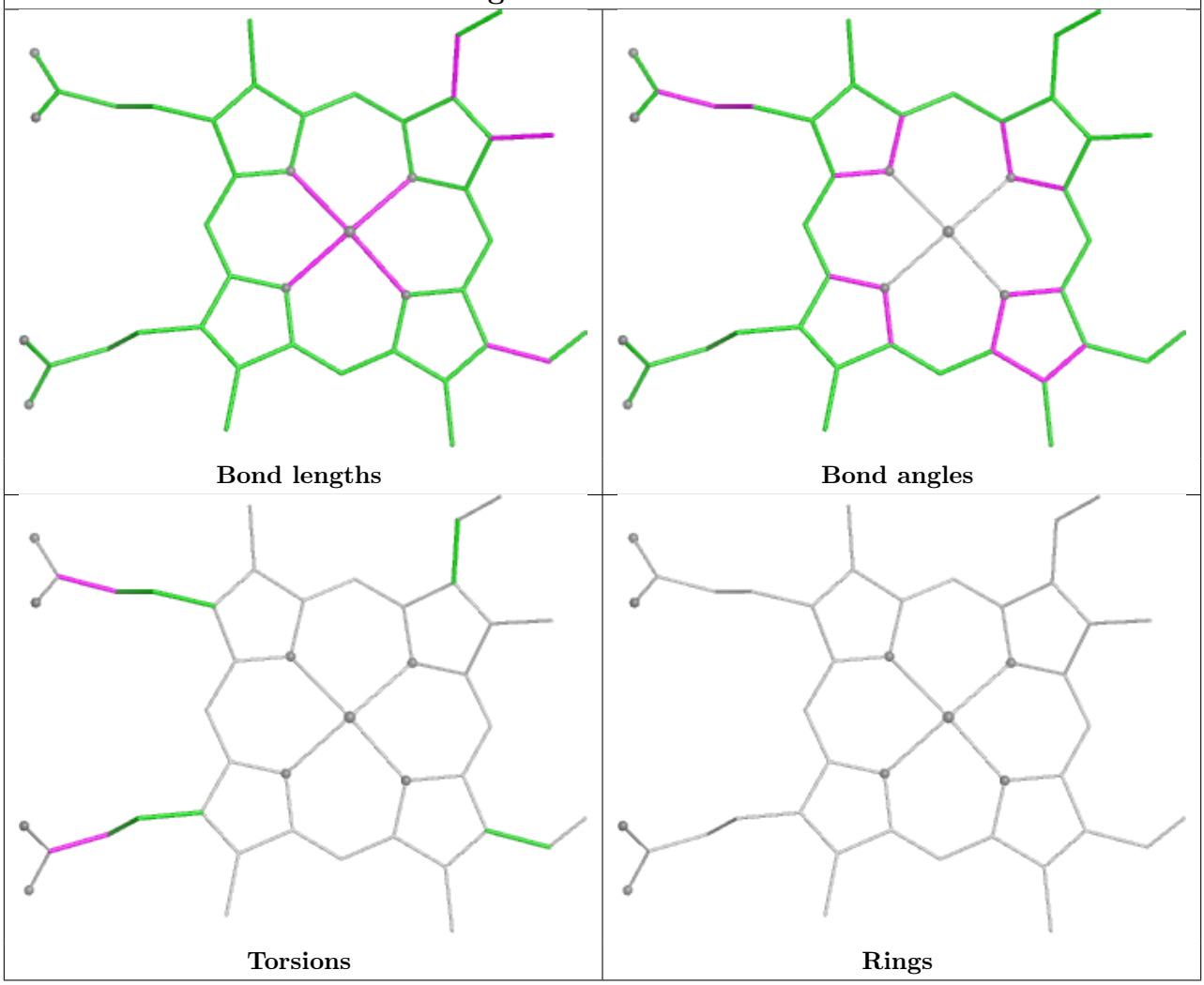
Ligand NAG F 1202

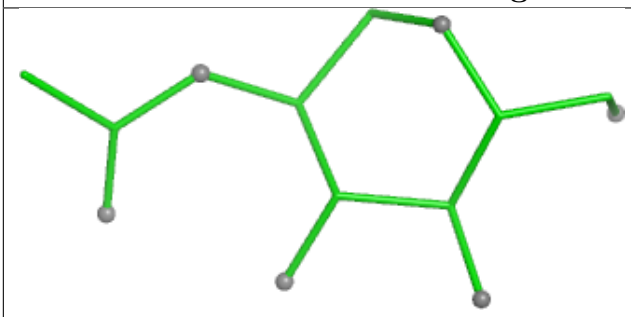
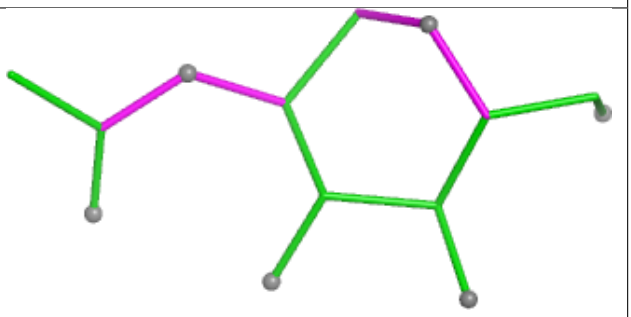
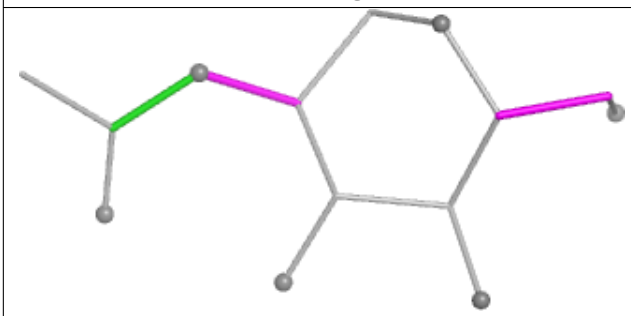
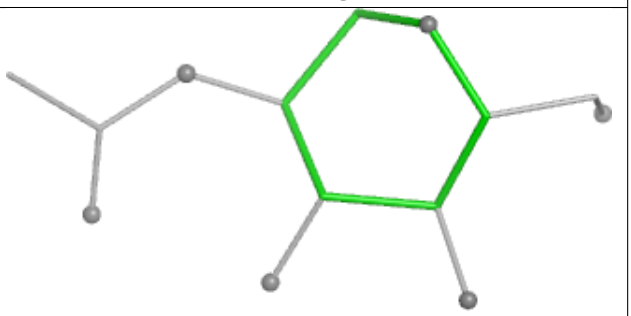


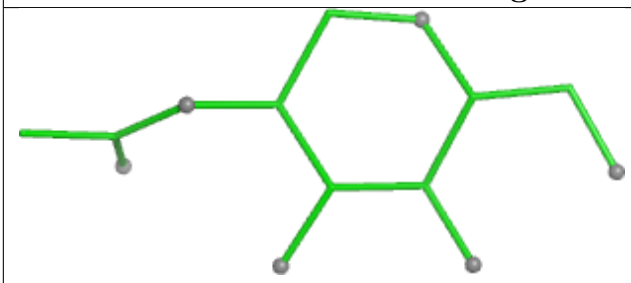
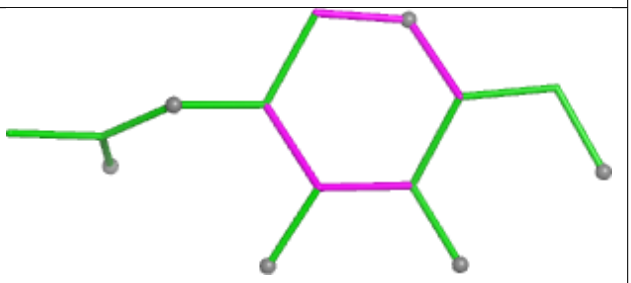
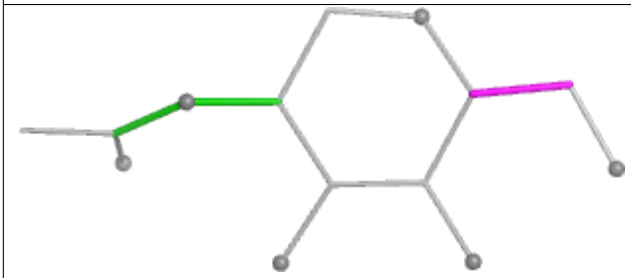
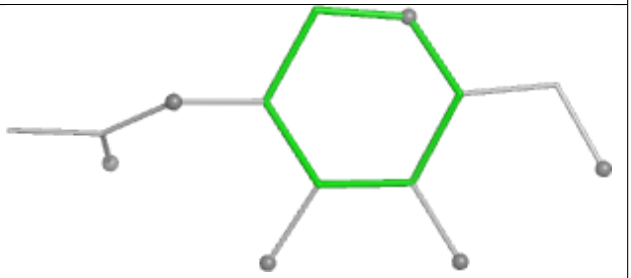
Ligand NAG D 1002

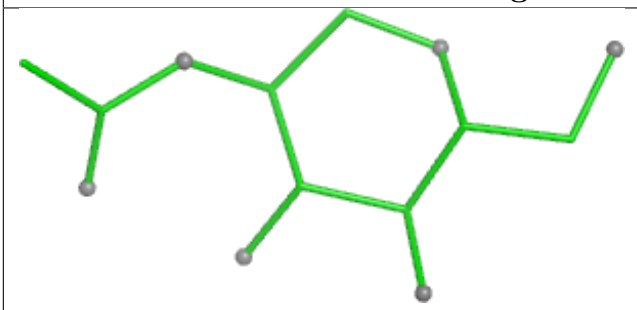
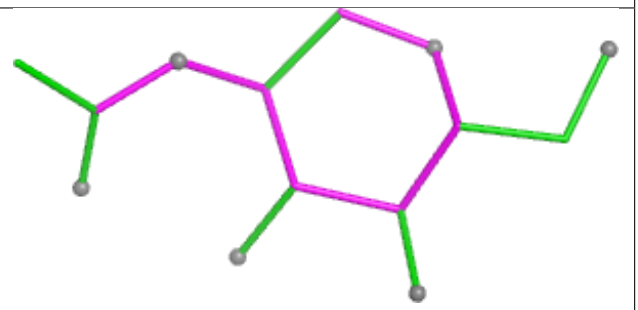
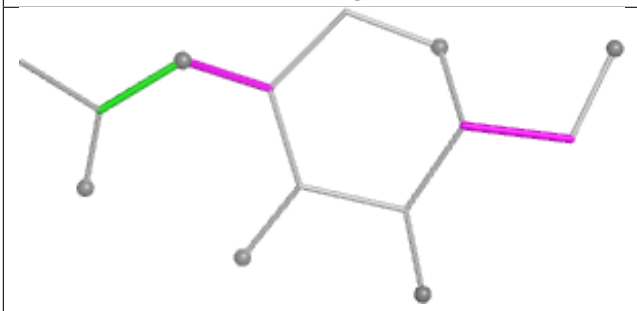
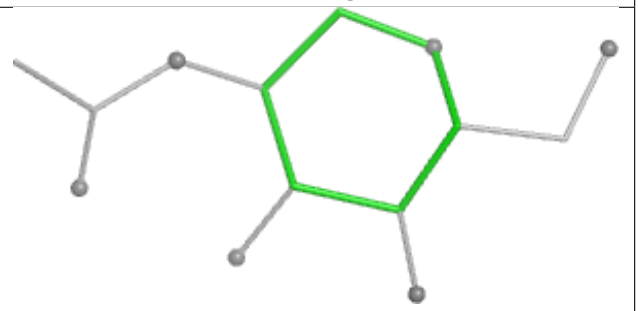


Ligand HEM B 201

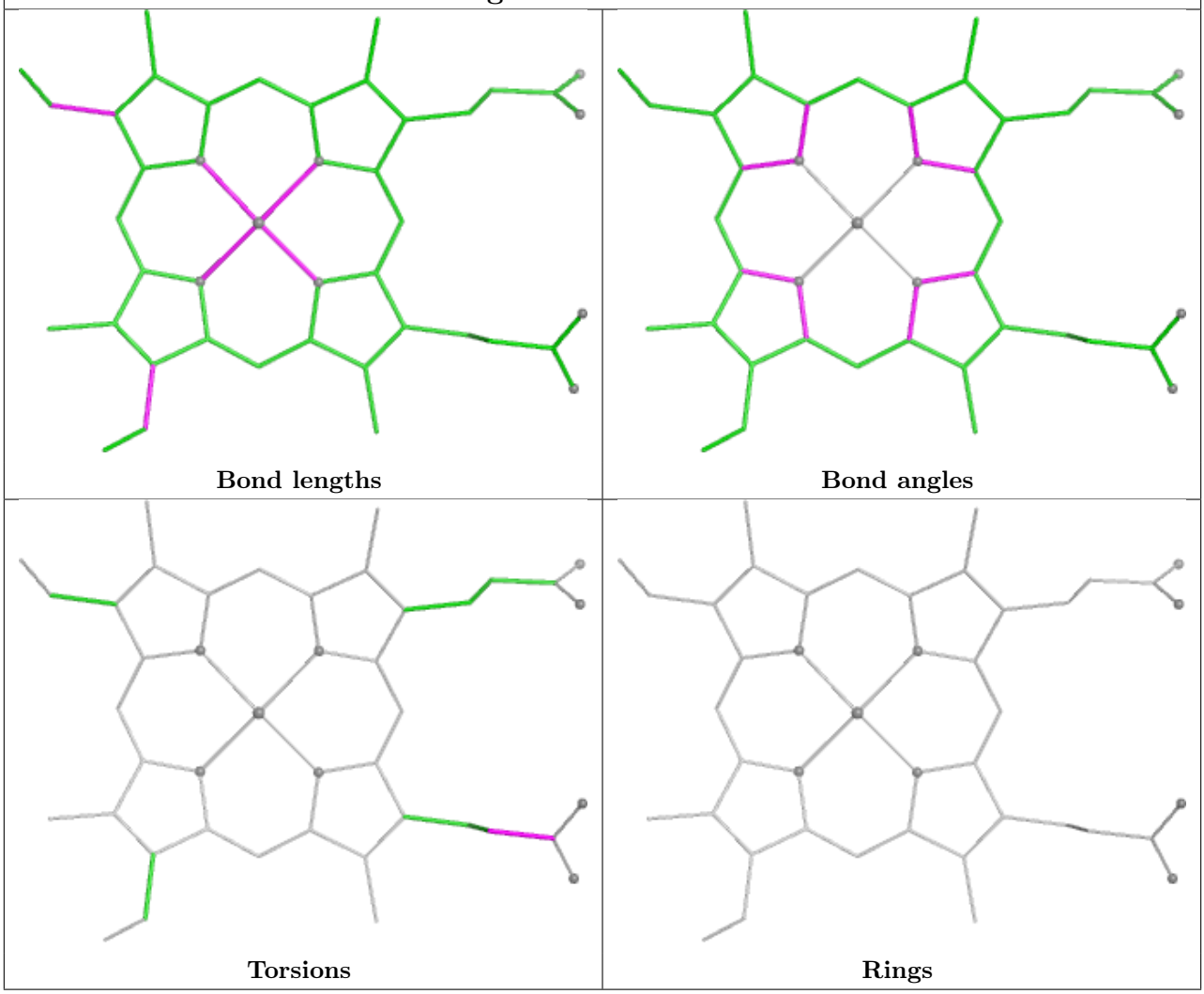


Ligand NAG G 1202	
 Bond lengths	 Bond angles
 Torsions	 Rings

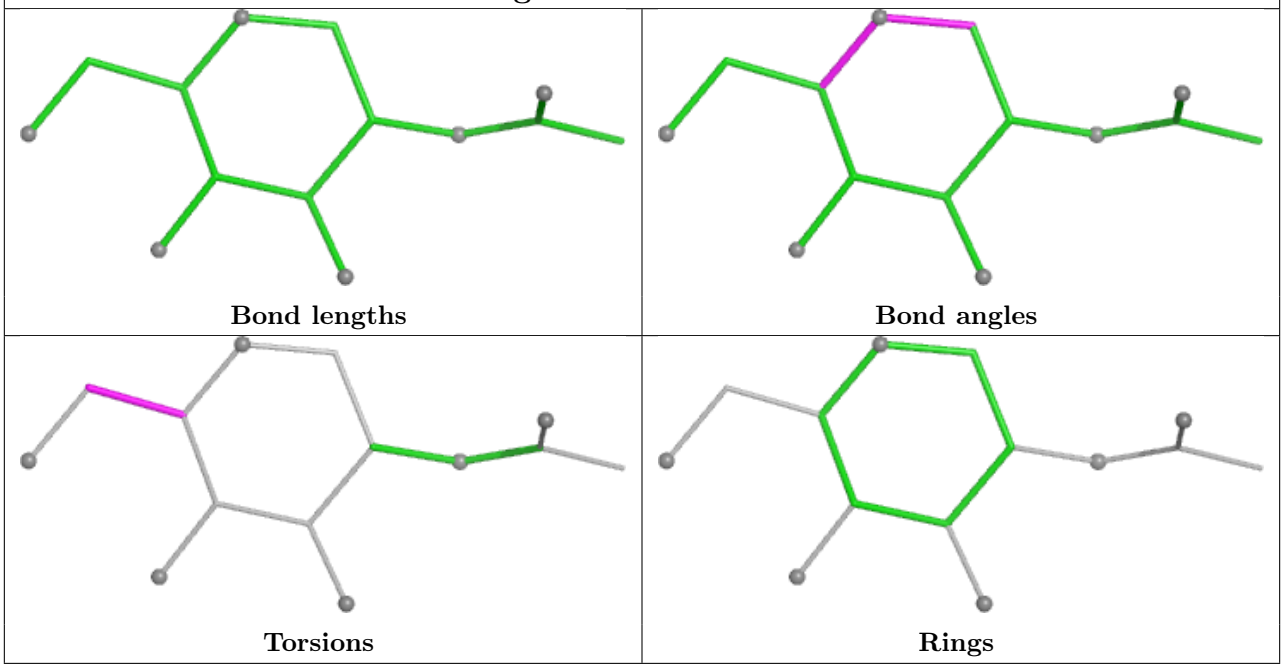
Ligand NAG G 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG G 1204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM A 201



Ligand NAG E 2004



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

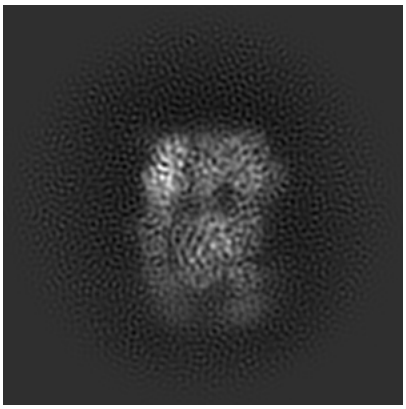
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-50600. These allow visual inspection of the internal detail of the map and identification of artifacts.

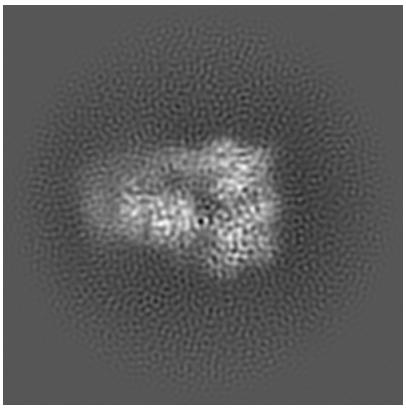
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

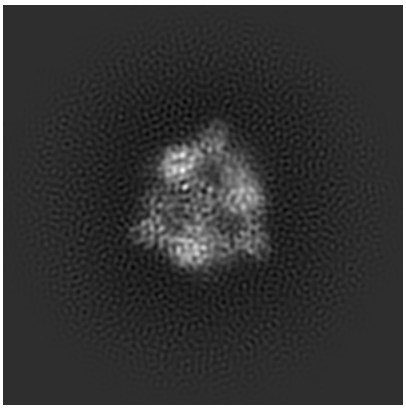
6.1.1 Primary map



X

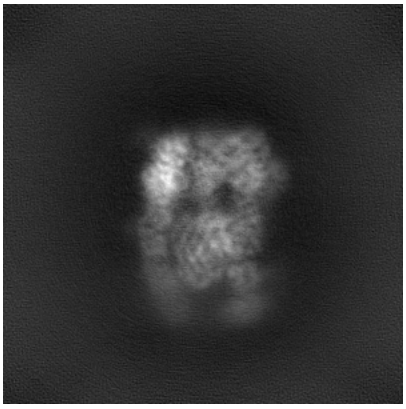


Y

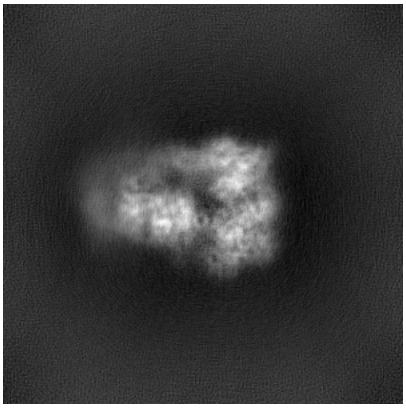


Z

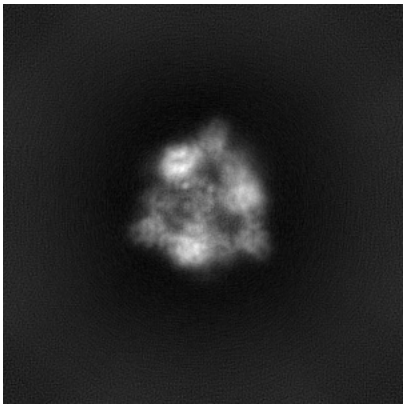
6.1.2 Raw map



X



Y

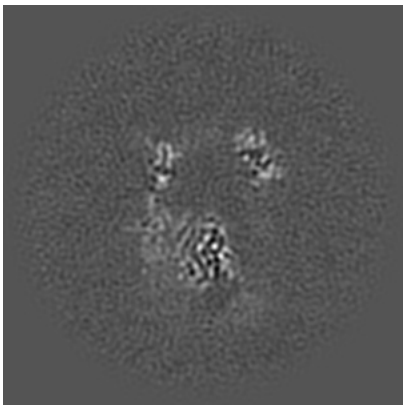


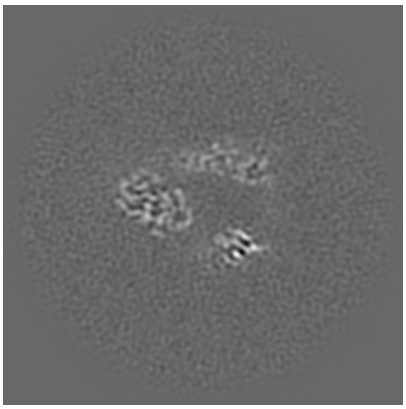
Z

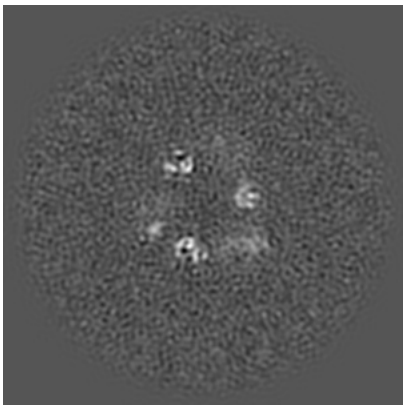
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

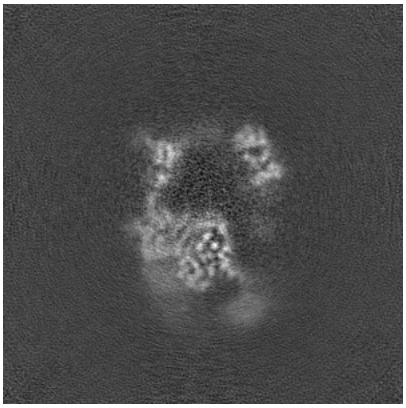
6.2.1 Primary map

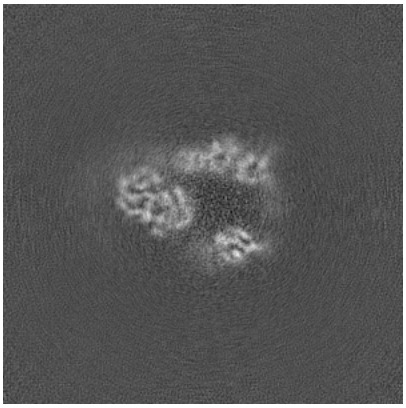

X Index: 160

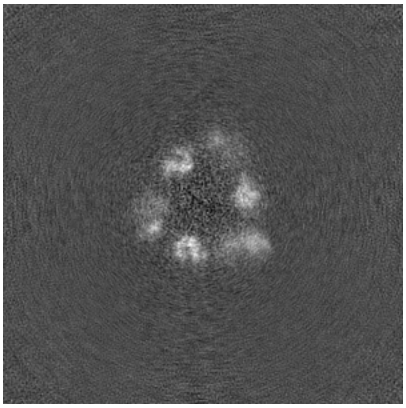

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

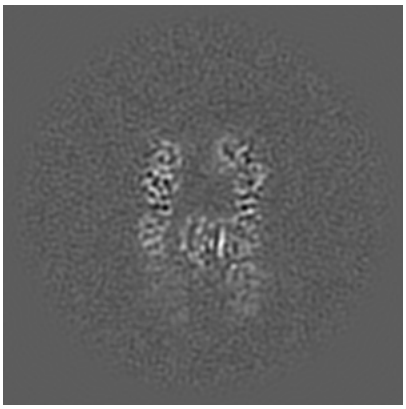

Y Index: 160

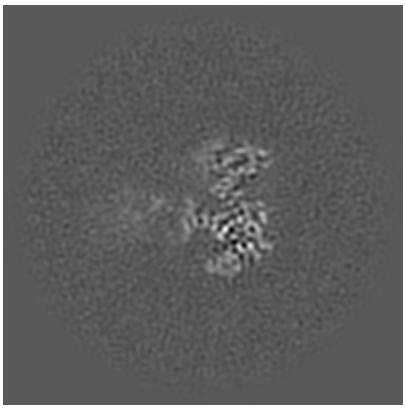

Z Index: 160

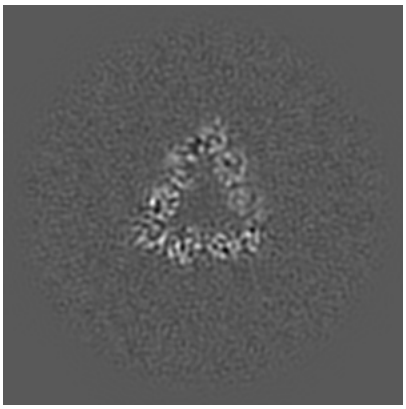
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

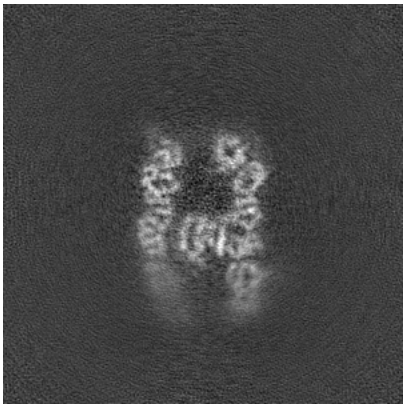
6.3.1 Primary map

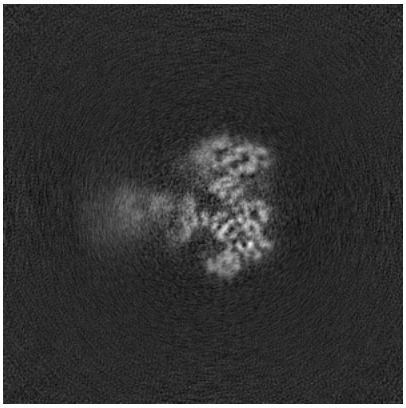

X Index: 146

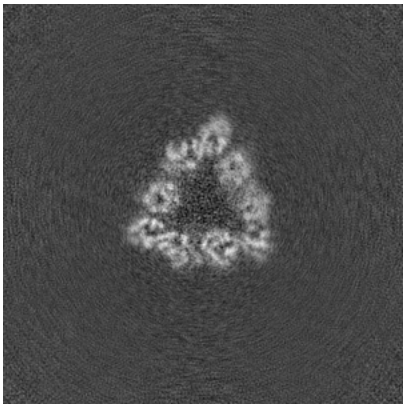

Y Index: 131


Z Index: 188

6.3.2 Raw map


X Index: 145

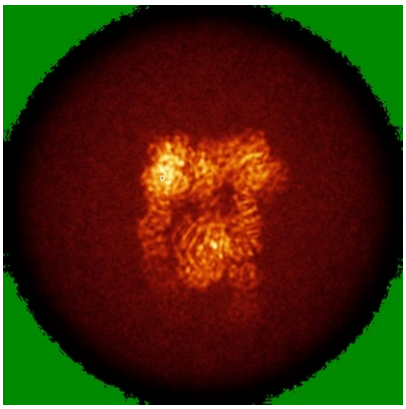

Y Index: 131

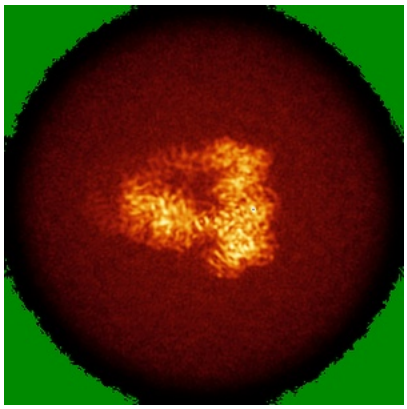

Z Index: 181

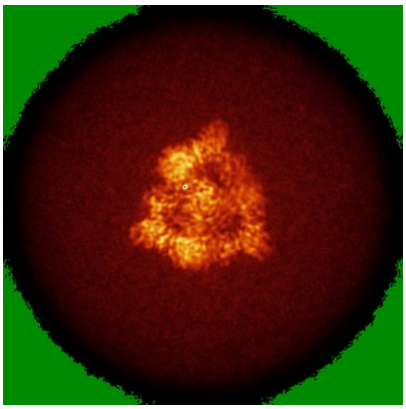
The images above show the largest variance slices of the map in three orthogonal directions.

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

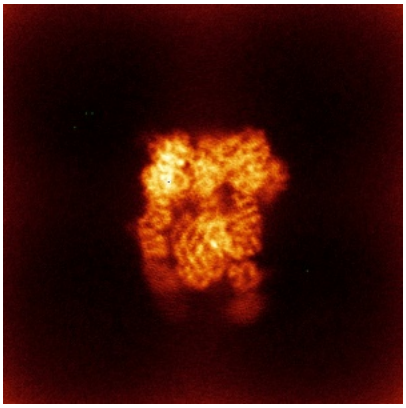
6.4.1 Primary map

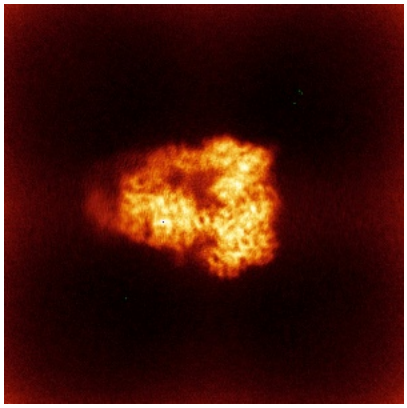

X

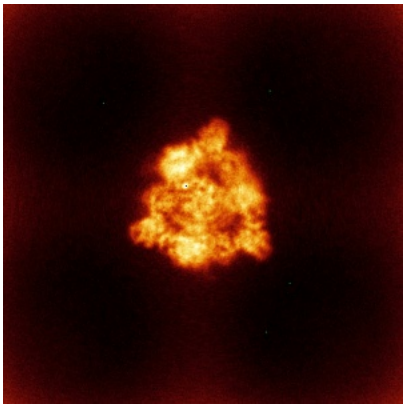

Y


Z

6.4.2 Raw 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.

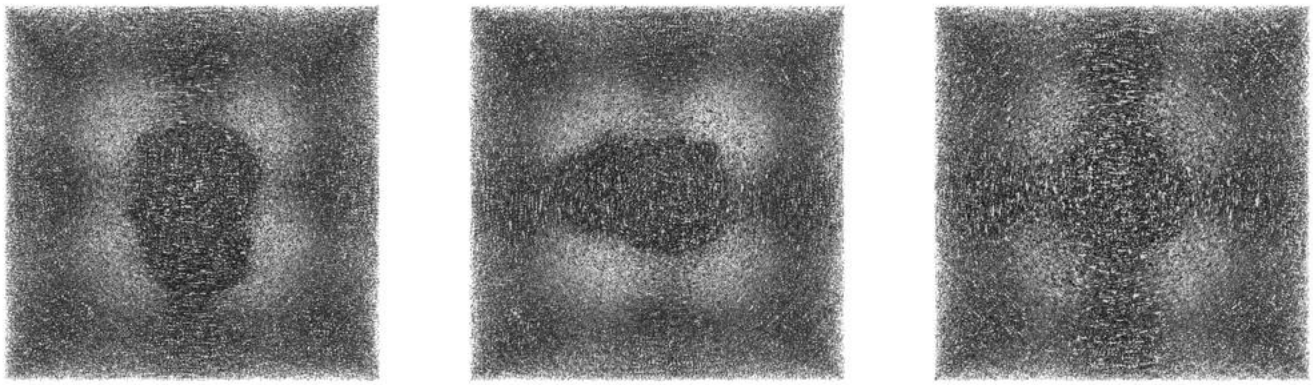
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

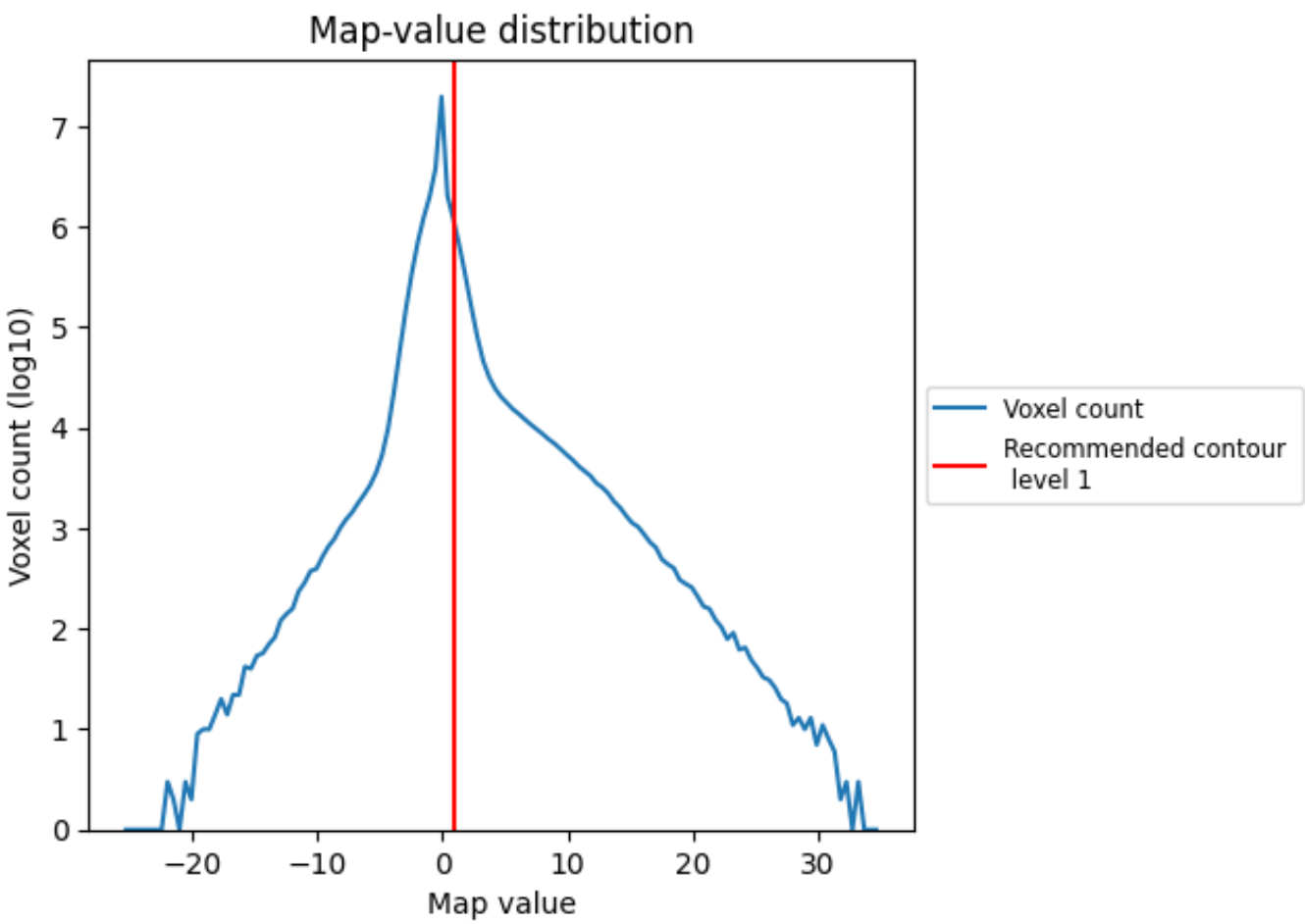
6.6 Mask visualisation (i)

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

7 Map analysis (i)

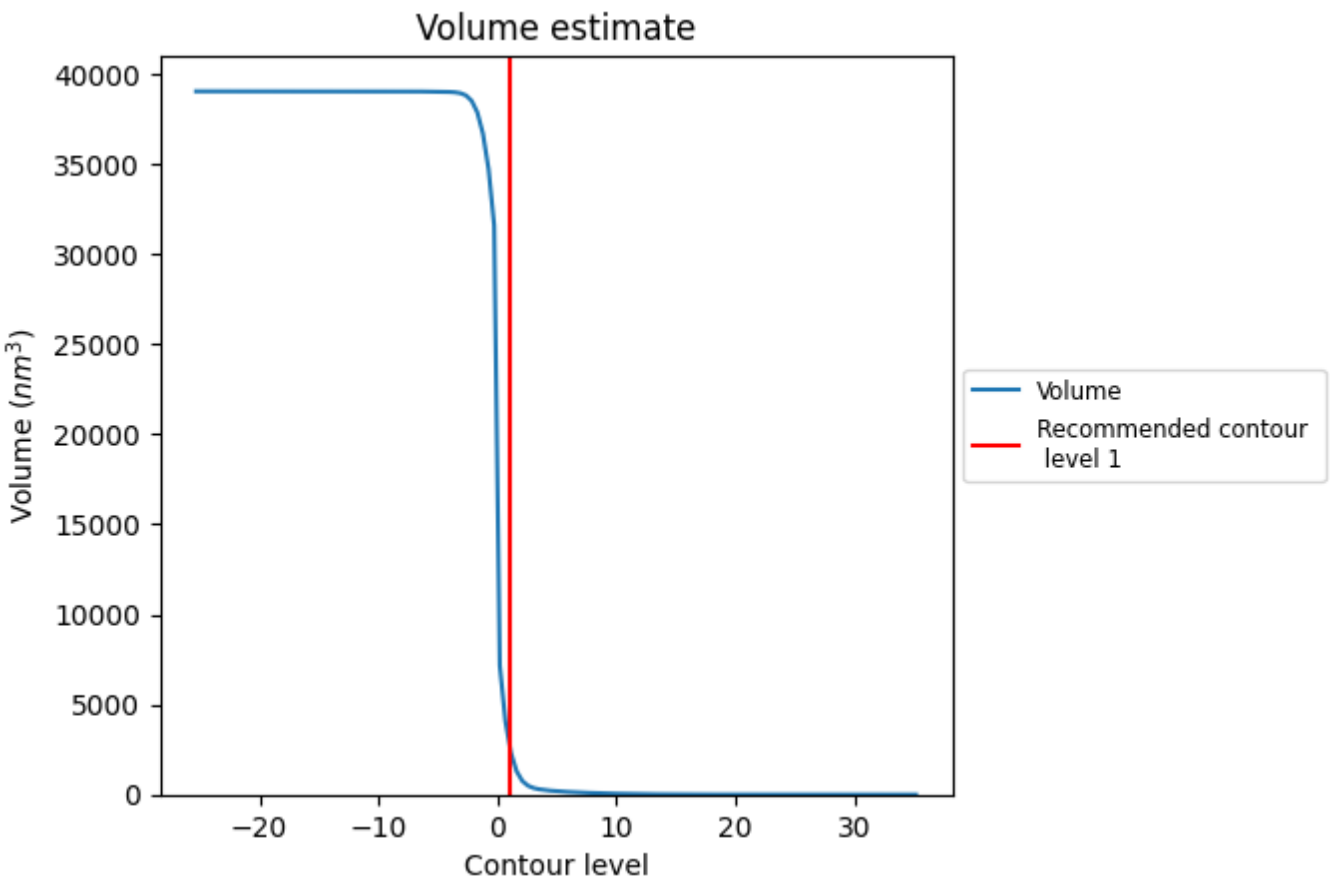
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

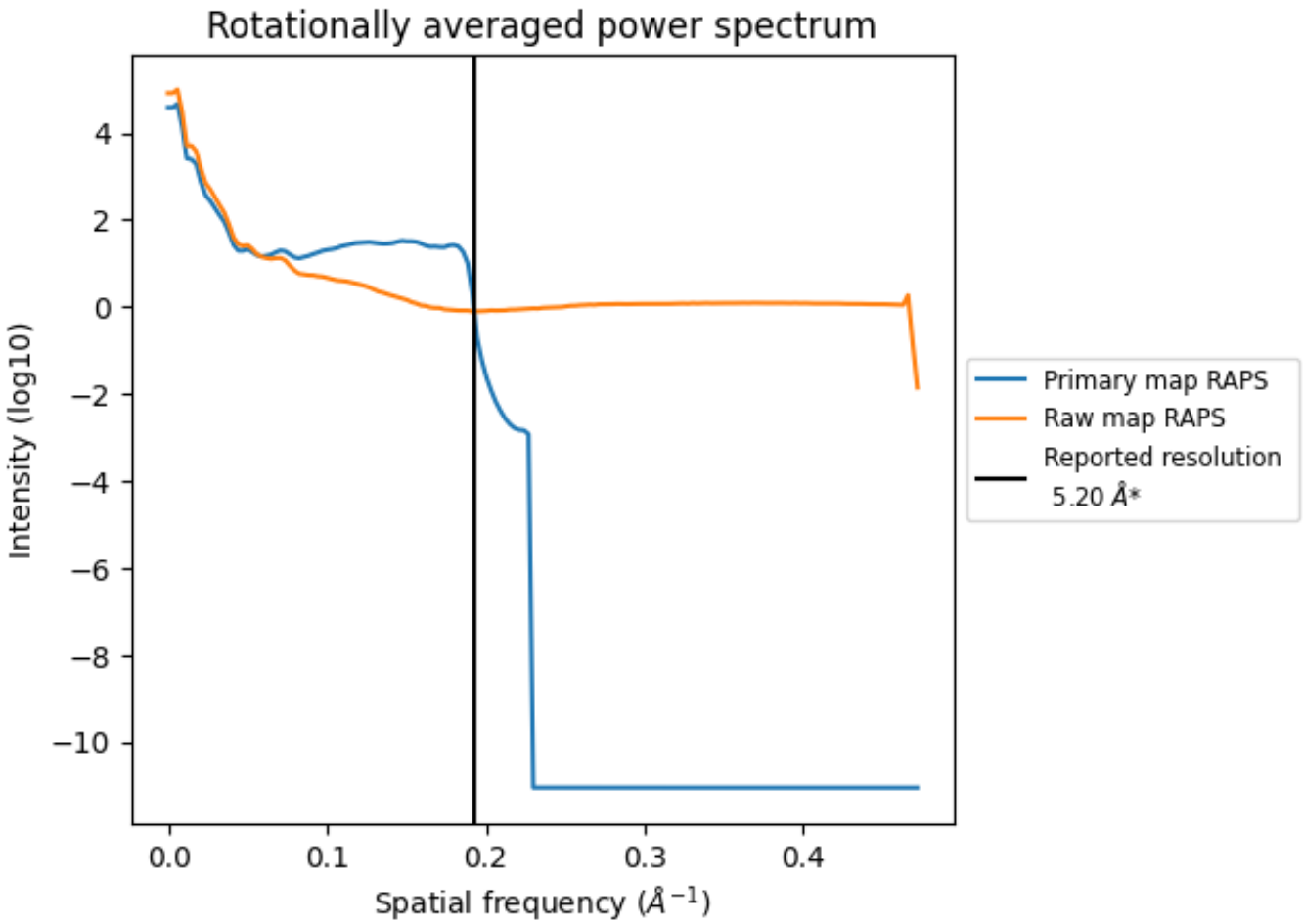
7.2 Volume estimate (i)



The volume at the recommended contour level is 2820 nm^3; this corresponds to an approximate mass of 2548 kDa.

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

7.3 Rotationally averaged power spectrum (i)

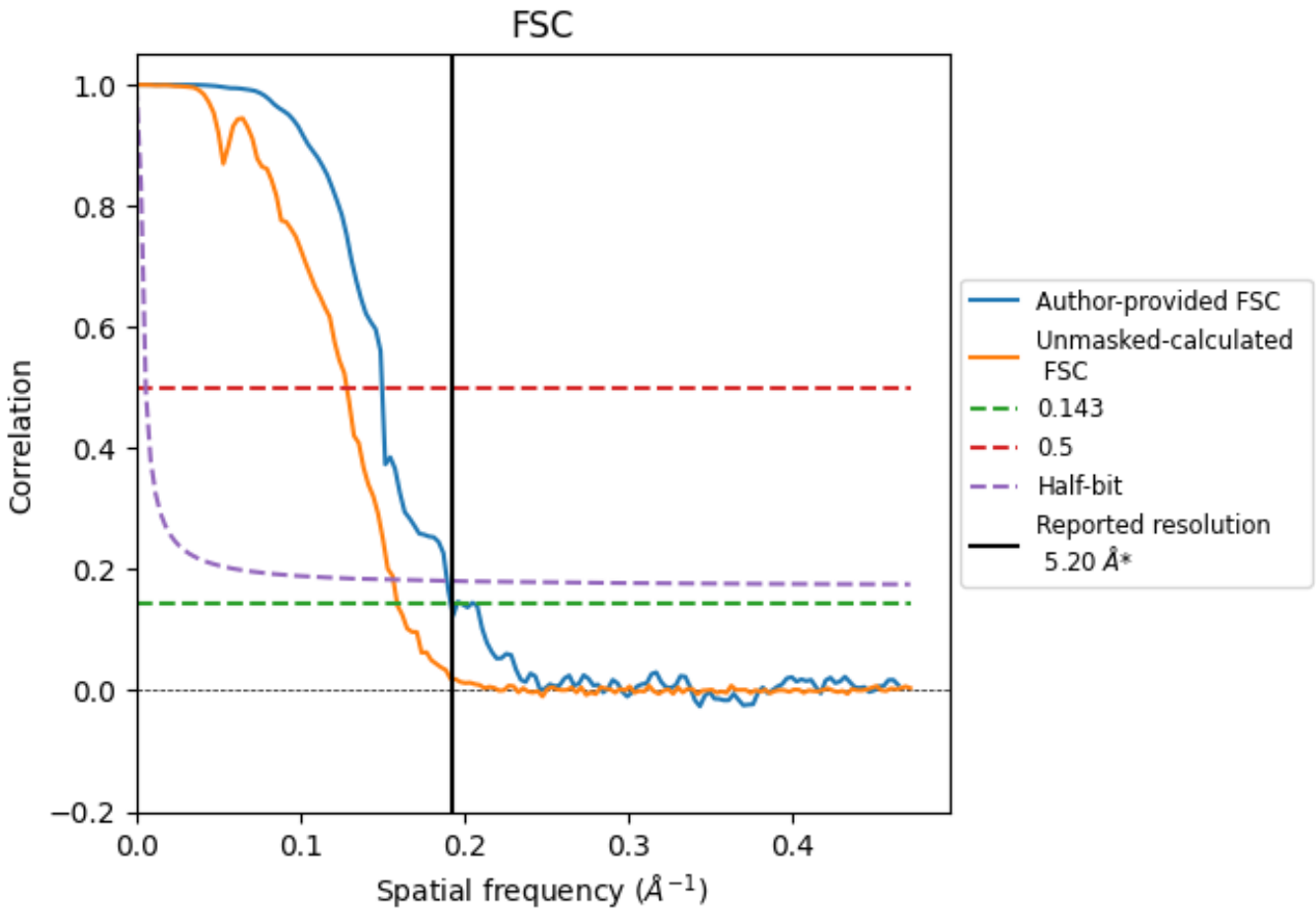


*Reported resolution corresponds to spatial frequency of 0.192 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.192 Å^{-1}

8.2 Resolution estimates (i)

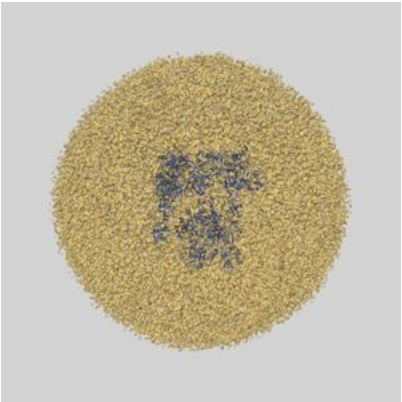
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	5.22	6.68	5.28
Unmasked-calculated*	6.29	7.79	6.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.29 differs from the reported value 5.2 by more than 10 %

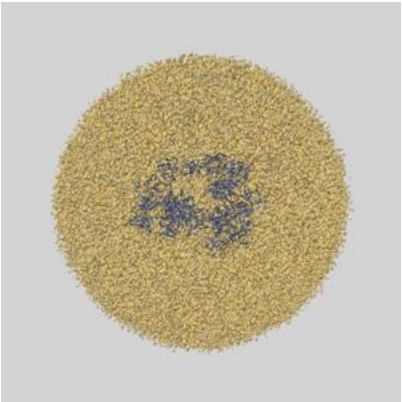
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-50600 and PDB model 9FNO. Per-residue inclusion information can be found in section 3 on page 7.

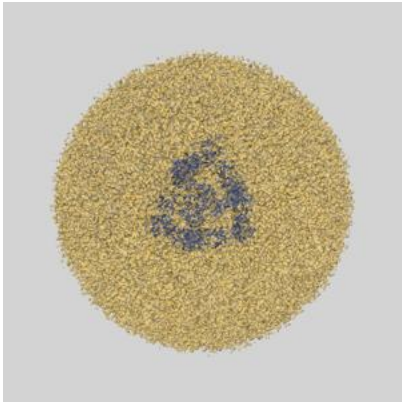
9.1 Map-model overlay (i)



X



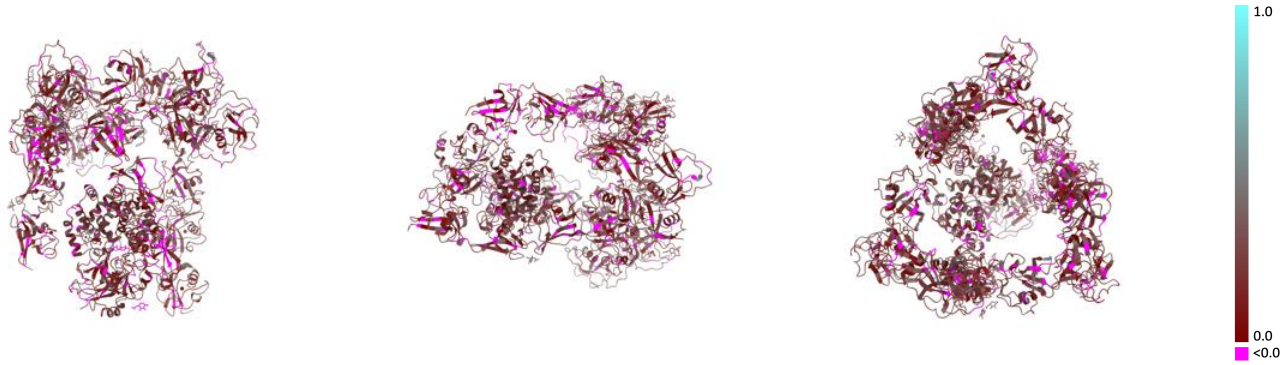
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

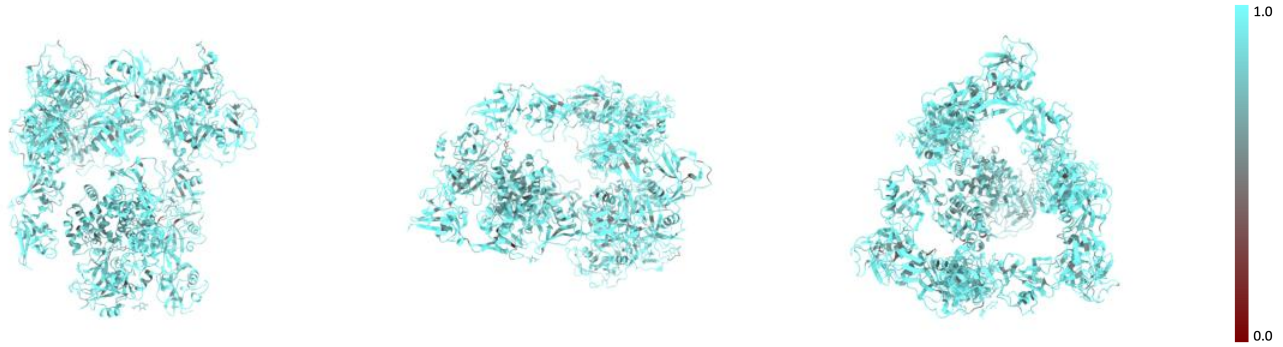
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

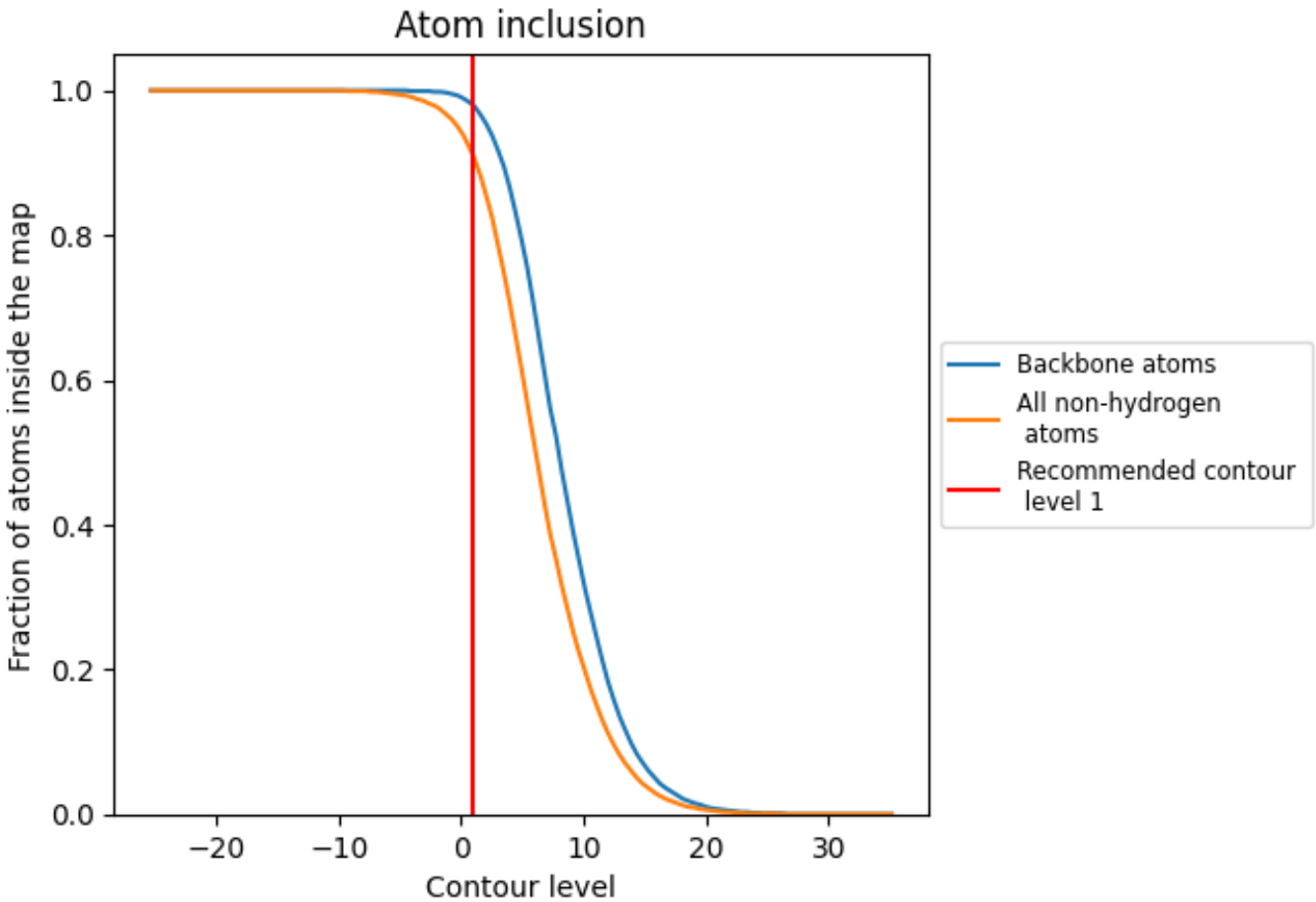
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.2030
A	0.8920	0.2200
B	0.8940	0.1810
C	0.8860	0.1580
D	0.8840	0.1840
E	0.9120	0.2100
F	0.9230	0.1810
G	0.9090	0.2240