Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:47 PM BST

PDB ID	:	1PGG
Title	:	PROSTAGLANDIN H2 SYNTHASE-1 COMPLEXED WITH 1-(4-IODOBENZOYL)-5-METHOXY-2-METHYLINDOLE-3-ACETIC ACID (IODOINDOMETHACIN), TRANS MODEL
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Deposited on	:	1995-12-02
Resolution	:	4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

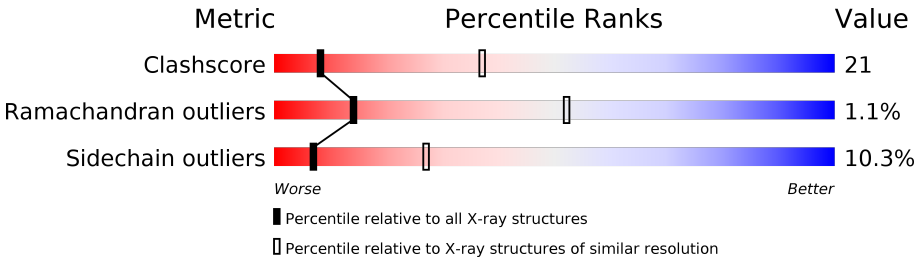
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	576	56% 33% 6% ·
1	B	576	56% 34% 6% ·
2	C	2	50% 50%
2	D	2	50% 50%

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
5	IMM	A	1	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IMM	B	1	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9202 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

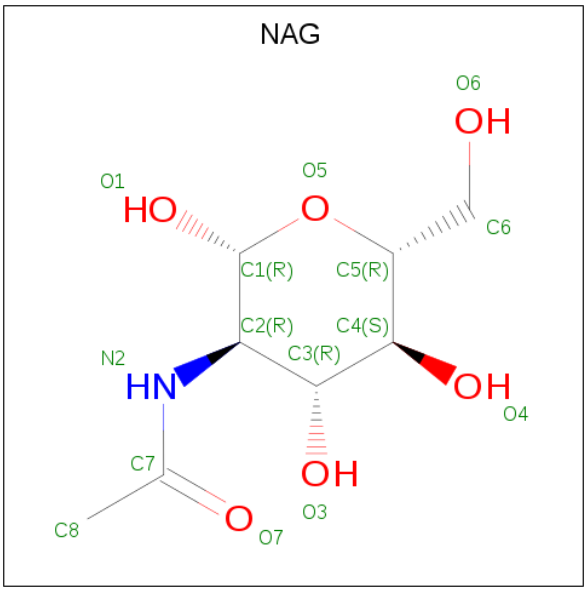
- Molecule 1 is a protein called PROSTAGLANDIN H2 SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			
1	B	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

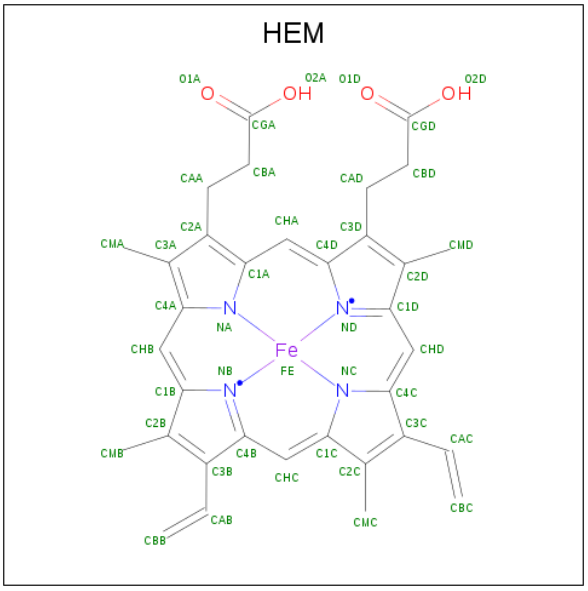
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



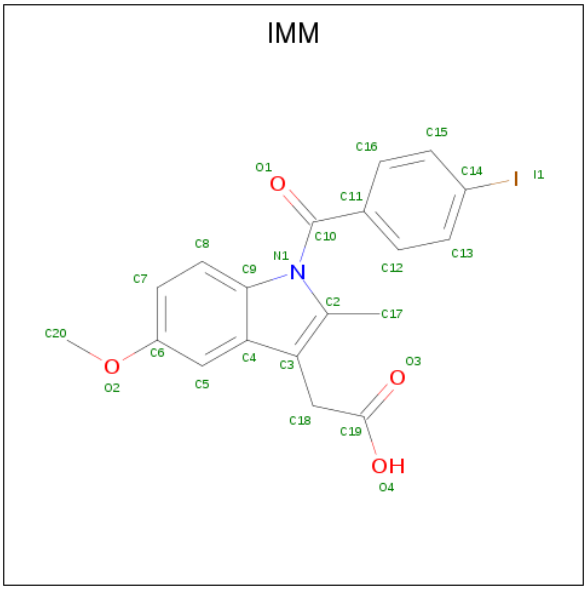
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 1-(4-IODOBENZOYL)-5-METHOXY-2-METHYL INDOLE-3-ACETIC ACID (three-letter code: IMM) (formula: $C_{19}H_{16}INO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
5	B	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

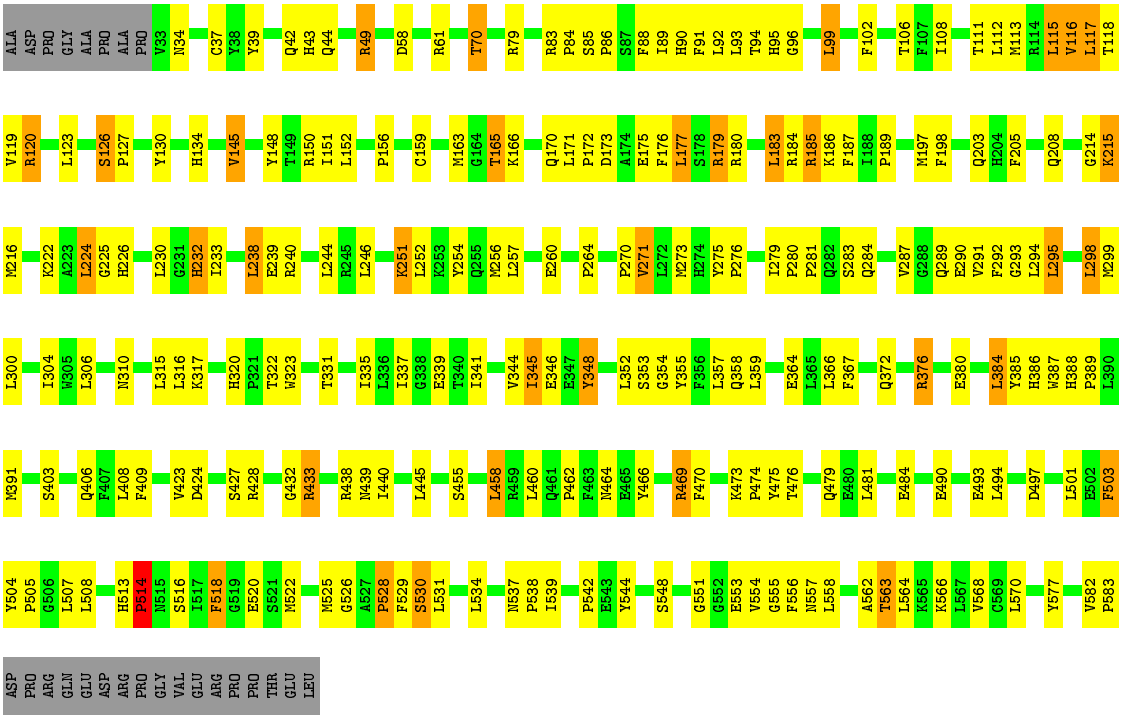
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

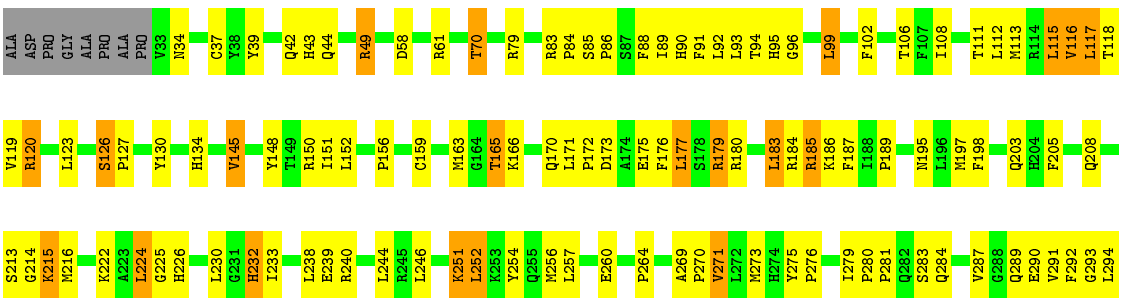
- Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1

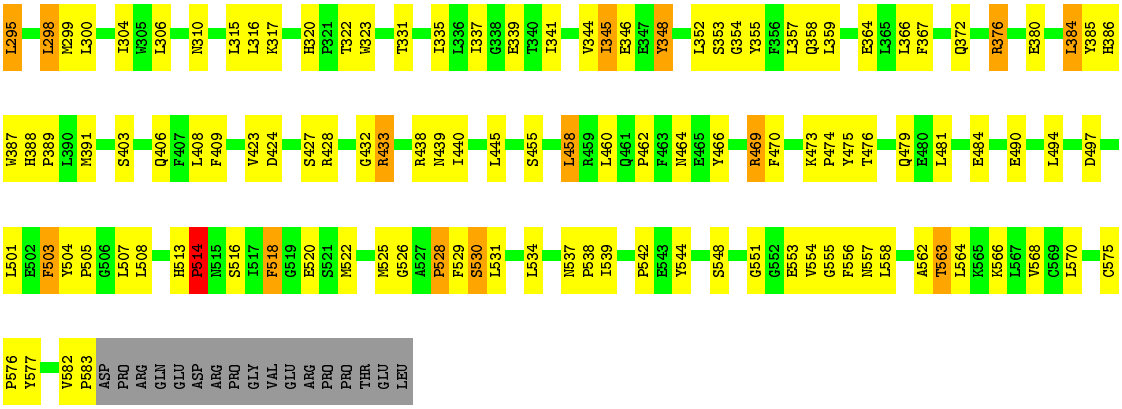
Chain A:



- Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1

Chain B:





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	99.22Å 208.99Å 232.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.50	Depositor
% Data completeness (in resolution range)	79.2 (8.00-4.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.254 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, IMM, 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	0.70	0/4615	0.86	8/6264 (0.1%)
1	B	0.70	0/4615	0.86	8/6264 (0.1%)
All	All	0.70	0/9230	0.86	16/12528 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	433	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	433	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	408	LEU	N-CA-C	6.29	127.97	111.00
1	B	408	LEU	N-CA-C	6.28	127.96	111.00
1	A	148	TYR	N-CA-C	-5.82	95.30	111.00
1	B	148	TYR	N-CA-C	-5.80	95.34	111.00
1	A	225	GLY	N-CA-C	-5.51	99.32	113.10
1	B	225	GLY	N-CA-C	-5.51	99.33	113.10
1	A	224	LEU	N-CA-C	-5.47	96.23	111.00
1	B	224	LEU	N-CA-C	-5.46	96.25	111.00
1	B	460	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	460	LEU	CA-CB-CG	5.17	127.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	177	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	177	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	99	LEU	CA-CB-CG	-5.03	103.73	115.30
1	A	99	LEU	CA-CB-CG	-5.03	103.74	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	TYR	Sidechain
1	B	39	TYR	Sidechain

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	4477	0	4383	188	0
1	B	4477	0	4383	197	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	43	0	30	7	0
4	B	43	0	30	7	0
5	A	25	0	15	15	0
5	B	25	0	15	16	0
All	All	9202	0	8958	383	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 21.

All (383) 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:A:391:MET:HG3	4:A:601:HEM:HAB	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.41	0.98
5:B:1:IMM:H172	5:B:1:IMM:H16	1.52	0.90
5:A:1:IMM:H16	5:A:1:IMM:H172	1.52	0.89
1:A:91:PHE:HD1	1:A:92:LEU:HD12	1.38	0.89
1:B:91:PHE:HD1	1:B:92:LEU:HD12	1.38	0.88
1:A:359:LEU:HD13	5:A:1:IMM:H203	1.56	0.87
1:B:359:LEU:HD13	5:B:1:IMM:H203	1.56	0.85
1:B:172:PRO:HB2	1:B:177:LEU:HD22	1.60	0.84
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.14	0.83
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.60	0.83
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.14	0.83
1:A:530:SER:CB	5:A:1:IMM:H12	2.10	0.82
1:B:530:SER:CB	5:B:1:IMM:H12	2.10	0.82
1:A:344:VAL:O	1:A:348:TYR:HB3	1.84	0.78
1:A:563:THR:HG22	1:A:566:LYS:H	1.50	0.77
1:B:344:VAL:O	1:B:348:TYR:HB3	1.84	0.77
1:B:563:THR:HG22	1:B:566:LYS:H	1.49	0.77
1:B:352:LEU:HD11	1:B:387:TRP:CH2	2.21	0.76
1:A:352:LEU:HD11	1:A:387:TRP:CH2	2.21	0.76
1:B:150:ARG:HD3	1:B:152:LEU:O	1.87	0.75
1:B:294:LEU:HD22	1:B:409:PHE:CD1	2.22	0.75
1:A:150:ARG:HD3	1:A:152:LEU:O	1.87	0.75
1:A:294:LEU:HD22	1:A:409:PHE:CD1	2.22	0.74
1:A:88:PHE:O	1:A:92:LEU:HD13	1.88	0.74
1:B:352:LEU:HD11	1:B:387:TRP:HH2	1.51	0.74
1:B:88:PHE:O	1:B:92:LEU:HD13	1.88	0.73
1:A:352:LEU:HD11	1:A:387:TRP:HH2	1.51	0.73
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.70	0.73
1:B:102:PHE:O	1:B:106:THR:HG23	1.89	0.73
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.70	0.72
1:A:294:LEU:HD22	1:A:409:PHE:HD1	1.54	0.72
1:B:152:LEU:HD21	1:B:469:ARG:HG2	1.70	0.72
1:A:152:LEU:HD21	1:A:469:ARG:HG2	1.70	0.71
1:B:294:LEU:HD22	1:B:409:PHE:HD1	1.54	0.71
5:A:1:IMM:C16	5:A:1:IMM:H172	2.21	0.71
1:A:102:PHE:O	1:A:106:THR:HG23	1.89	0.71
1:B:359:LEU:HD22	5:B:1:IMM:C20	2.21	0.70
1:B:294:LEU:O	1:B:295:LEU:HG	1.91	0.70
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.26	0.70
1:B:84:PRO:CG	1:B:89:ILE:HD11	2.22	0.70
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:O	1:A:295:LEU:HG	1.91	0.69
1:A:359:LEU:HD22	5:A:1:IMM:C20	2.21	0.69
1:A:84:PRO:CG	1:A:89:ILE:HD11	2.22	0.69
5:B:1:IMM:H172	5:B:1:IMM:C16	2.21	0.69
1:B:530:SER:HB3	5:B:1:IMM:H12	1.75	0.68
1:B:91:PHE:CD1	1:B:92:LEU:HD12	2.26	0.68
1:A:530:SER:HB3	5:A:1:IMM:H12	1.75	0.68
1:A:91:PHE:CD1	1:A:92:LEU:HD12	2.26	0.67
1:A:79:ARG:O	1:A:83:ARG:HG3	1.94	0.67
1:B:79:ARG:O	1:B:83:ARG:HG3	1.94	0.66
1:A:187:PHE:HE1	1:A:189:PRO:HB3	1.60	0.66
1:B:187:PHE:HE1	1:B:189:PRO:HB3	1.60	0.66
1:B:386:HIS:HD2	1:B:388:HIS:HE1	1.43	0.66
1:A:386:HIS:HD2	1:A:388:HIS:HE1	1.43	0.66
1:A:88:PHE:CD2	1:A:89:ILE:HD13	2.33	0.63
1:B:88:PHE:CD2	1:B:89:ILE:HD13	2.33	0.63
1:B:88:PHE:HD2	1:B:89:ILE:HD13	1.64	0.63
1:A:88:PHE:HD2	1:A:89:ILE:HD13	1.64	0.63
1:B:116:VAL:O	1:B:120:ARG:HB2	1.98	0.62
1:A:116:VAL:O	1:A:120:ARG:HB2	1.98	0.62
1:B:123:LEU:O	1:B:469:ARG:NH2	2.32	0.62
1:B:359:LEU:HD22	5:B:1:IMM:H203	1.82	0.62
1:A:123:LEU:O	1:A:469:ARG:NH2	2.32	0.62
1:A:470:PHE:CZ	1:A:529:PHE:CE2	2.87	0.62
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.39	0.62
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.39	0.62
1:B:553:GLU:HG3	1:B:557:ASN:HD21	1.65	0.62
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.35	0.62
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.35	0.61
1:B:470:PHE:CZ	1:B:529:PHE:CE2	2.87	0.61
1:B:126:SER:HA	1:B:127:PRO:C	2.20	0.61
5:A:1:IMM:C17	5:A:1:IMM:H16	2.26	0.61
1:A:359:LEU:HD22	5:A:1:IMM:H203	1.82	0.61
5:B:1:IMM:C17	5:B:1:IMM:H16	2.26	0.61
1:A:553:GLU:HG3	1:A:557:ASN:HD21	1.65	0.61
1:A:126:SER:HA	1:A:127:PRO:C	2.20	0.60
5:B:1:IMM:C19	5:B:1:IMM:H5	2.31	0.60
1:B:85:SER:O	1:B:89:ILE:HG12	2.01	0.60
1:A:85:SER:O	1:A:89:ILE:HG12	2.01	0.60
1:A:49:ARG:O	1:B:320:HIS:HD2	1.85	0.60
1:A:117:LEU:HD12	1:A:531:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD12	1:B:531:LEU:HD13	1.84	0.59
1:B:208:GLN:NE2	1:B:230:LEU:H	2.00	0.59
5:A:1:IMM:H5	5:A:1:IMM:C19	2.31	0.59
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.38	0.59
1:B:337:ILE:O	1:B:341:ILE:HG13	2.02	0.59
1:A:290:GLU:H	1:A:290:GLU:CD	2.06	0.59
1:A:531:LEU:HD21	5:A:1:IMM:H7	1.85	0.58
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.38	0.58
1:B:145:VAL:HG12	1:B:224:LEU:HD22	1.85	0.58
1:A:208:GLN:NE2	1:A:230:LEU:H	2.00	0.58
1:A:337:ILE:O	1:A:341:ILE:HG13	2.02	0.58
1:B:348:TYR:C	1:B:348:TYR:CD1	2.77	0.58
1:A:320:HIS:HD2	1:B:49:ARG:O	1.86	0.58
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.39	0.58
1:A:348:TYR:CD1	1:A:348:TYR:C	2.77	0.58
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.85	0.57
1:A:203:GLN:HA	4:A:601:HEM:HBC2	1.86	0.57
1:A:185:ARG:HH21	1:A:438:ARG:HG2	1.69	0.57
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.39	0.57
1:B:290:GLU:CD	1:B:290:GLU:H	2.06	0.57
1:B:424:ASP:O	1:B:428:ARG:HG3	2.05	0.57
1:B:531:LEU:HD21	5:B:1:IMM:H7	1.85	0.57
1:B:306:LEU:HD23	1:B:306:LEU:C	2.25	0.57
1:B:203:GLN:HA	4:B:601:HEM:HBC2	1.86	0.57
1:A:306:LEU:HD23	1:A:306:LEU:C	2.25	0.57
1:A:424:ASP:O	1:A:428:ARG:HG3	2.05	0.56
1:B:185:ARG:HH21	1:B:438:ARG:HG2	1.69	0.56
1:A:346:GLU:HG2	1:A:359:LEU:O	2.06	0.56
1:A:518:PHE:CE2	1:A:522:MET:HG2	2.40	0.56
1:B:346:GLU:HG2	1:B:359:LEU:O	2.06	0.56
1:B:518:PHE:CE2	1:B:522:MET:HG2	2.40	0.56
1:B:173:ASP:OD2	1:B:175:GLU:HB3	2.06	0.55
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.41	0.55
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.47	0.55
1:A:79:ARG:HH11	1:A:83:ARG:HH21	1.55	0.55
1:A:173:ASP:OD2	1:A:175:GLU:HB3	2.06	0.55
1:B:176:PHE:HE2	1:B:494:LEU:HD11	1.72	0.55
1:B:289:GLN:HG3	1:B:292:PHE:CZ	2.41	0.55
1:B:113:MET:SD	5:B:1:IMM:H201	2.47	0.54
1:B:386:HIS:HD2	1:B:388:HIS:CE1	2.25	0.54
1:A:113:MET:SD	5:A:1:IMM:H201	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:HE2	1:A:494:LEU:HD11	1.72	0.54
1:A:180:ARG:NH1	1:A:490:GLU:OE1	2.40	0.54
1:A:503:PHE:CE2	1:A:507:LEU:HD11	2.42	0.54
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.47	0.54
1:B:180:ARG:NH1	1:B:490:GLU:OE1	2.40	0.54
1:B:503:PHE:CE2	1:B:507:LEU:HD11	2.42	0.54
1:B:79:ARG:HH11	1:B:83:ARG:HH21	1.55	0.54
1:A:215:LYS:H	1:A:215:LYS:CD	2.21	0.53
1:B:554:VAL:HG23	1:B:555:GLY:N	2.23	0.53
1:B:513:HIS:HB2	1:B:516:SER:OG	2.08	0.53
1:A:151:ILE:HG13	1:A:529:PHE:CZ	2.43	0.53
1:B:151:ILE:HG13	1:B:529:PHE:CZ	2.43	0.53
1:B:215:LYS:H	1:B:215:LYS:CD	2.21	0.53
1:B:367:PHE:CD1	1:B:542:PRO:HG3	2.44	0.53
1:A:388:HIS:N	1:A:389:PRO:CD	2.71	0.53
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.91	0.53
1:B:388:HIS:N	1:B:389:PRO:CD	2.71	0.53
1:A:513:HIS:HB2	1:A:516:SER:OG	2.08	0.53
1:B:403:SER:OG	1:B:406:GLN:HG3	2.09	0.53
1:A:554:VAL:HG23	1:A:555:GLY:N	2.23	0.52
1:A:150:ARG:NH2	1:A:458:LEU:O	2.41	0.52
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.44	0.52
1:A:403:SER:OG	1:A:406:GLN:HG3	2.09	0.52
1:B:537:ASN:OD1	1:B:538:PRO:HD2	2.10	0.52
1:A:537:ASN:OD1	1:A:538:PRO:HD2	2.10	0.52
1:B:353:SER:OG	1:B:354:GLY:N	2.42	0.52
1:A:294:LEU:CD2	1:A:409:PHE:HD1	2.23	0.52
1:B:150:ARG:NH2	1:B:458:LEU:O	2.42	0.52
1:A:88:PHE:CZ	1:A:92:LEU:HD21	2.45	0.51
1:A:353:SER:OG	1:A:354:GLY:N	2.42	0.51
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.91	0.51
5:A:1:IMM:C5	5:A:1:IMM:C19	2.89	0.51
1:A:386:HIS:HD2	1:A:388:HIS:CE1	2.25	0.51
1:B:391:MET:HG3	4:B:601:HEM:CAB	2.29	0.51
1:B:464:ASN:ND2	1:B:474:PRO:HB2	2.25	0.51
1:A:42:GLN:HG3	1:A:70:THR:CG2	2.41	0.51
1:B:187:PHE:CE1	1:B:189:PRO:HB3	2.43	0.51
1:B:391:MET:CG	4:B:601:HEM:HAB	2.29	0.51
1:A:58:ASP:HB2	1:B:548:SER:HB3	1.92	0.51
1:A:464:ASN:ND2	1:A:474:PRO:HB2	2.25	0.51
1:A:88:PHE:O	1:A:91:PHE:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:O	1:A:95:HIS:ND1	2.44	0.50
1:B:42:GLN:HG3	1:B:70:THR:CG2	2.41	0.50
1:B:294:LEU:CD2	1:B:409:PHE:HD1	2.23	0.50
1:B:94:THR:O	1:B:95:HIS:ND1	2.44	0.50
1:B:427:SER:HB3	1:B:577:TYR:CD2	2.46	0.50
1:A:187:PHE:CE1	1:A:189:PRO:HB3	2.43	0.50
1:B:175:GLU:O	1:B:179:ARG:HG3	2.11	0.50
1:A:175:GLU:O	1:A:179:ARG:HG3	2.11	0.50
1:A:427:SER:HB3	1:A:577:TYR:CD2	2.46	0.50
1:B:359:LEU:CD1	5:B:1:IMM:H203	2.36	0.50
1:B:88:PHE:CZ	1:B:92:LEU:HD21	2.45	0.50
1:B:88:PHE:O	1:B:91:PHE:HB3	2.11	0.50
1:B:115:LEU:HD23	1:B:119:VAL:HG21	1.94	0.50
5:B:1:IMM:C19	5:B:1:IMM:C5	2.89	0.49
1:A:359:LEU:CD1	5:A:1:IMM:H203	2.36	0.49
1:B:184:ARG:HA	1:B:438:ARG:O	2.12	0.49
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.48	0.49
1:A:184:ARG:HA	1:A:438:ARG:O	2.12	0.49
1:A:522:MET:O	1:A:526:GLY:N	2.46	0.49
1:B:525:MET:O	1:B:529:PHE:HD2	1.95	0.49
1:B:522:MET:O	1:B:526:GLY:N	2.46	0.49
1:A:525:MET:O	1:A:529:PHE:HD2	1.95	0.49
1:A:118:THR:OG1	1:A:119:VAL:N	2.46	0.48
1:A:203:GLN:HG3	4:A:601:HEM:C1C	2.48	0.48
1:B:445:LEU:O	1:B:445:LEU:HG	2.12	0.48
1:A:256:MET:O	1:A:257:LEU:HD23	2.13	0.48
1:A:280:PRO:HG2	1:A:283:SER:OG	2.13	0.48
1:A:93:LEU:HD13	1:A:355:TYR:CE2	2.48	0.48
1:A:445:LEU:HG	1:A:445:LEU:O	2.12	0.48
1:A:528:PRO:O	1:A:529:PHE:C	2.49	0.48
1:B:118:THR:OG1	1:B:119:VAL:N	2.46	0.48
1:B:280:PRO:HG2	1:B:283:SER:OG	2.13	0.48
1:B:203:GLN:HG3	4:B:601:HEM:C1C	2.48	0.48
1:B:528:PRO:O	1:B:529:PHE:C	2.49	0.48
1:B:388:HIS:N	1:B:389:PRO:HD3	2.29	0.48
1:B:93:LEU:HD13	1:B:355:TYR:CE2	2.48	0.48
1:B:304:ILE:HD13	1:B:568:VAL:HG22	1.96	0.48
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.48	0.48
1:A:388:HIS:N	1:A:389:PRO:HD3	2.29	0.47
1:B:348:TYR:C	1:B:348:TYR:HD1	2.17	0.47
1:B:582:VAL:HG22	1:B:583:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD23	1:A:119:VAL:HG21	1.94	0.47
1:A:320:HIS:CD2	1:B:49:ARG:O	2.68	0.47
1:A:276:PRO:HG2	1:A:279:ILE:HD12	1.97	0.47
1:B:208:GLN:HB3	1:B:232:HIS:CD2	2.49	0.47
1:B:320:HIS:HE1	1:B:551:GLY:O	1.98	0.47
1:B:320:HIS:CE1	1:B:551:GLY:O	2.67	0.47
1:A:254:TYR:HA	1:A:264:PRO:HD3	1.96	0.47
1:A:320:HIS:CE1	1:A:551:GLY:O	2.67	0.47
1:B:256:MET:O	1:B:257:LEU:HD23	2.13	0.47
1:A:90:HIS:O	1:A:90:HIS:CD2	2.68	0.47
1:B:273:MET:HE2	1:B:287:VAL:HG22	1.96	0.47
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.49	0.47
1:A:475:TYR:CE2	1:A:481:LEU:HD12	2.50	0.47
1:B:90:HIS:CD2	1:B:90:HIS:O	2.68	0.47
1:A:130:TYR:HB3	1:A:134:HIS:O	2.15	0.47
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.96	0.47
1:A:348:TYR:C	1:A:348:TYR:HD1	2.17	0.47
1:A:548:SER:HB3	1:B:58:ASP:HB2	1.96	0.46
1:B:179:ARG:HH11	1:B:179:ARG:HB3	1.80	0.46
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.79	0.46
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.51	0.46
1:B:205:PHE:O	1:B:208:GLN:HG2	2.14	0.46
1:B:254:TYR:HA	1:B:264:PRO:HD3	1.96	0.46
1:B:293:GLY:HA2	1:B:299:MET:HE3	1.97	0.46
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.79	0.46
1:A:582:VAL:HG22	1:A:583:PRO:HD2	1.97	0.46
1:B:130:TYR:HB3	1:B:134:HIS:O	2.15	0.46
1:B:276:PRO:HG2	1:B:279:ILE:CD1	2.46	0.46
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.80	0.46
1:A:276:PRO:HG2	1:A:279:ILE:CD1	2.46	0.46
1:B:475:TYR:CE2	1:B:481:LEU:HD12	2.50	0.46
1:A:205:PHE:O	1:A:208:GLN:HG2	2.14	0.46
1:A:304:ILE:HD13	1:A:568:VAL:HG22	1.96	0.46
1:B:275:TYR:CE2	1:B:284:GLN:HB3	2.51	0.46
1:B:470:PHE:HZ	1:B:529:PHE:CE2	2.32	0.46
1:A:214:GLY:N	1:A:215:LYS:HE2	2.31	0.45
1:A:553:GLU:HG3	1:A:557:ASN:ND2	2.30	0.45
1:B:276:PRO:HG2	1:B:279:ILE:HD12	1.97	0.45
1:A:320:HIS:HE1	1:A:551:GLY:O	1.98	0.45
1:A:388:HIS:CD2	4:A:601:HEM:NB	2.85	0.45
1:A:185:ARG:NE	1:A:438:ARG:HH11	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.87	0.45
1:A:61:ARG:NH1	1:B:542:PRO:O	2.50	0.45
1:B:469:ARG:HA	1:B:469:ARG:HD2	1.52	0.45
1:B:256:MET:HA	1:B:260:GLU:O	2.16	0.45
1:B:185:ARG:NE	1:B:438:ARG:HH11	2.14	0.45
1:B:214:GLY:N	1:B:215:LYS:HE2	2.31	0.45
1:A:389:PRO:HG3	1:A:440:ILE:CG1	2.47	0.45
1:B:289:GLN:HG3	1:B:292:PHE:CE1	2.52	0.45
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.76	0.44
1:B:470:PHE:HZ	1:B:529:PHE:CZ	2.35	0.44
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.52	0.44
1:A:49:ARG:O	1:B:320:HIS:CD2	2.67	0.44
1:A:470:PHE:HZ	1:A:529:PHE:CE2	2.32	0.44
1:B:298:LEU:HD12	1:B:298:LEU:HA	1.72	0.44
1:A:115:LEU:O	1:A:119:VAL:HG23	2.18	0.44
1:A:289:GLN:HG3	1:A:292:PHE:CE1	2.52	0.44
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.82	0.44
1:A:256:MET:HA	1:A:260:GLU:O	2.17	0.44
1:A:88:PHE:CE2	1:A:92:LEU:HD21	2.53	0.44
1:B:315:LEU:HD12	1:B:558:LEU:HD11	1.99	0.44
1:A:216:MET:HG2	2:C:2:NAG:H83	1.99	0.44
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.99	0.44
1:A:387:TRP:HZ2	5:A:1:IMM:I1	2.71	0.44
1:A:315:LEU:HD12	1:A:558:LEU:HD11	1.99	0.44
1:B:387:TRP:NE1	1:B:522:MET:HE3	2.33	0.44
1:A:357:LEU:HD12	1:A:358:GLN:N	2.33	0.44
1:B:251:LYS:HG3	1:B:310:ASN:CG	2.38	0.44
1:B:88:PHE:CE2	1:B:92:LEU:HD21	2.53	0.44
1:B:216:MET:HG2	2:D:2:NAG:H83	1.99	0.44
1:B:115:LEU:O	1:B:119:VAL:HG23	2.18	0.44
1:B:357:LEU:HD12	1:B:358:GLN:N	2.33	0.44
1:A:344:VAL:CG1	1:A:534:LEU:HD21	2.48	0.44
1:B:331:THR:O	1:B:335:ILE:HG13	2.18	0.44
1:B:344:VAL:CG1	1:B:534:LEU:HD21	2.48	0.44
1:A:331:THR:O	1:A:335:ILE:HG13	2.18	0.43
1:A:387:TRP:NE1	1:A:522:MET:CE	2.81	0.43
1:A:88:PHE:CE1	1:A:92:LEU:HD11	2.53	0.43
1:A:341:ILE:HD12	1:A:539:ILE:HD11	2.01	0.43
1:B:387:TRP:NE1	1:B:522:MET:CE	2.81	0.43
1:B:388:HIS:CD2	4:B:601:HEM:NB	2.85	0.43
1:B:163:MET:HB3	1:B:462:PRO:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:GLU:HG3	1:B:557:ASN:ND2	2.31	0.43
1:A:251:LYS:HG3	1:A:310:ASN:CG	2.38	0.43
1:A:391:MET:CG	4:A:601:HEM:HAB	2.30	0.43
1:B:387:TRP:HZ2	5:B:1:IMM:I1	2.71	0.43
1:B:389:PRO:HG3	1:B:440:ILE:CG1	2.47	0.43
1:B:503:PHE:CZ	1:B:507:LEU:HD11	2.53	0.43
1:B:88:PHE:CE1	1:B:92:LEU:HD11	2.53	0.43
1:B:345:ILE:HG12	1:B:534:LEU:HD23	2.01	0.43
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.52	0.43
1:A:189:PRO:HA	1:A:432:GLY:HA2	2.00	0.43
1:A:273:MET:HE2	1:A:287:VAL:HG22	2.01	0.43
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.88	0.43
1:A:470:PHE:HZ	1:A:529:PHE:CZ	2.35	0.43
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.87	0.43
1:A:127:PRO:HG2	1:B:544:TYR:CE1	2.53	0.43
1:A:503:PHE:CZ	1:A:507:LEU:HD11	2.53	0.43
1:B:215:LYS:HE3	1:B:222:LYS:NZ	2.34	0.43
1:B:189:PRO:HA	1:B:432:GLY:HA2	2.00	0.43
1:B:85:SER:HA	1:B:86:PRO:HD3	1.78	0.43
1:A:165:THR:HG22	1:A:166:LYS:HG2	2.01	0.43
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.72	0.43
1:B:43:HIS:O	1:B:44:GLN:HB2	2.19	0.43
1:A:239:GLU:CD	1:A:239:GLU:H	2.22	0.43
1:B:165:THR:HG22	1:B:166:LYS:HG2	2.01	0.43
1:B:384:LEU:HG	5:B:1:IMM:I1	2.89	0.43
1:B:295:LEU:HD21	4:B:601:HEM:HBB2	2.01	0.43
1:A:391:MET:HG3	4:A:601:HEM:CAB	2.29	0.42
1:B:341:ILE:HD12	1:B:539:ILE:HD11	2.01	0.42
1:A:555:GLY:O	1:A:558:LEU:HB2	2.19	0.42
1:B:366:LEU:HA	1:B:366:LEU:HD23	1.76	0.42
1:B:575:CYS:HA	1:B:576:PRO:HD2	1.93	0.42
1:A:215:LYS:HE3	1:A:222:LYS:NZ	2.34	0.42
1:A:198:PHE:C	1:A:198:PHE:CD1	2.93	0.42
1:A:387:TRP:NE1	1:A:522:MET:HE3	2.34	0.42
1:A:372:GLN:HE22	1:B:372:GLN:HA	1.83	0.42
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.50	0.42
1:A:345:ILE:HG12	1:A:534:LEU:HD23	2.01	0.42
1:B:198:PHE:CD1	1:B:198:PHE:C	2.93	0.42
1:B:252:LEU:HA	1:B:252:LEU:HD12	1.92	0.42
1:A:43:HIS:O	1:A:44:GLN:HB2	2.19	0.42
1:A:544:TYR:CE1	1:B:127:PRO:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLU:H	1:B:239:GLU:CD	2.22	0.42
1:A:384:LEU:HG	5:A:1:IMM:I1	2.89	0.42
1:A:355:TYR:CD1	1:A:355:TYR:N	2.88	0.42
1:A:42:GLN:HG3	1:A:70:THR:HG23	2.02	0.42
1:A:481:LEU:HD22	1:A:501:LEU:CD2	2.50	0.42
1:B:240:ARG:HG3	1:B:271:VAL:CG2	2.50	0.42
1:A:339:GLU:HG2	1:A:562:ALA:HB2	2.02	0.42
1:A:513:HIS:HB3	1:A:514:PRO:HD2	2.02	0.41
1:A:566:LYS:O	1:A:570:LEU:HB2	2.20	0.41
1:A:88:PHE:HD2	1:A:89:ILE:CD1	2.32	0.41
1:B:513:HIS:HB3	1:B:514:PRO:HD2	2.02	0.41
1:B:339:GLU:HG2	1:B:562:ALA:HB2	2.02	0.41
1:B:88:PHE:HD2	1:B:89:ILE:CD1	2.32	0.41
1:A:183:LEU:HD23	1:A:184:ARG:N	2.35	0.41
1:B:294:LEU:HD22	1:B:409:PHE:CE1	2.55	0.41
1:B:555:GLY:O	1:B:558:LEU:HB2	2.19	0.41
1:B:566:LYS:O	1:B:570:LEU:HB2	2.20	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.76	0.41
1:A:230:LEU:HG	1:A:233:ILE:HD12	2.03	0.41
1:A:295:LEU:HD21	4:A:601:HEM:HBB2	2.01	0.41
1:A:389:PRO:HG3	1:A:440:ILE:HG13	2.02	0.41
1:B:108:ILE:O	1:B:112:LEU:HG	2.21	0.41
1:B:481:LEU:HD22	1:B:501:LEU:CD2	2.50	0.41
1:A:240:ARG:HG3	1:A:271:VAL:HG22	2.03	0.41
1:B:355:TYR:N	1:B:355:TYR:CD1	2.88	0.41
1:A:372:GLN:HA	1:B:372:GLN:HE22	1.85	0.41
1:B:96:GLY:O	1:B:99:LEU:N	2.54	0.41
1:A:469:ARG:HD2	1:A:469:ARG:HA	1.51	0.41
1:B:42:GLN:HG3	1:B:70:THR:HG23	2.02	0.41
1:A:108:ILE:O	1:A:112:LEU:HG	2.21	0.41
1:B:389:PRO:HG3	1:B:440:ILE:HG13	2.02	0.41
1:B:494:LEU:HD23	1:B:494:LEU:HA	1.87	0.41
1:B:522:MET:O	1:B:526:GLY:HA3	2.21	0.41
1:B:208:GLN:HE22	1:B:230:LEU:HD12	1.86	0.41
1:B:386:HIS:CD2	1:B:388:HIS:HE1	2.32	0.41
1:A:197:MET:CE	1:A:423:VAL:HG13	2.51	0.41
1:A:96:GLY:O	1:A:99:LEU:N	2.54	0.41
1:A:294:LEU:HD22	1:A:409:PHE:CE1	2.55	0.40
1:A:490:GLU:HA	1:A:493:GLU:HG2	2.03	0.40
1:A:85:SER:HA	1:A:86:PRO:HD3	1.78	0.40
1:B:195:ASN:ND2	1:B:427:SER:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLN:NE2	1:B:358:GLN:HA	2.36	0.40
1:B:108:ILE:HG13	1:B:108:ILE:H	1.67	0.40
1:B:269:ALA:O	1:B:271:VAL:N	2.54	0.40
1:B:197:MET:CE	1:B:423:VAL:HG13	2.51	0.40
1:B:84:PRO:HB2	1:B:88:PHE:CD2	2.57	0.40
1:A:184:ARG:HB2	1:A:439:ASN:C	2.42	0.40
1:B:183:LEU:HD23	1:B:184:ARG:N	2.35	0.40
1:B:184:ARG:HB2	1:B:439:ASN:C	2.42	0.40
1:B:531:LEU:HG	5:B:1:IMM:C7	2.52	0.40
1:B:213:SER:OG	1:B:215:LYS:HG2	2.21	0.40
1:B:230:LEU:HG	1:B:233:ILE:HD12	2.03	0.40
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.35	0.40
1:A:542:PRO:O	1:B:61:ARG:NH1	2.54	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/576 (95%)	496 (90%)	47 (9%)	6 (1%)	14	52
1	B	549/576 (95%)	496 (90%)	47 (9%)	6 (1%)	14	52
All	All	1098/1152 (95%)	992 (90%)	94 (9%)	12 (1%)	14	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PRO
1	B	514	PRO
1	A	520	GLU
1	A	528	PRO
1	B	520	GLU

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Mol	Chain	Res	Type
1	B	528	PRO
1	A	503	PHE
1	B	503	PHE
1	A	270	PRO
1	A	295	LEU
1	B	270	PRO
1	B	295	LEU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	486/506 (96%)	436 (90%)	50 (10%)	7 27
1	B	486/506 (96%)	436 (90%)	50 (10%)	7 27
All	All	972/1012 (96%)	872 (90%)	100 (10%)	7 27

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	70	THR
1	A	111	THR
1	A	115	LEU
1	A	116	VAL
1	A	117	LEU
1	A	120	ARG
1	A	126	SER
1	A	145	VAL
1	A	165	THR
1	A	170	GLN
1	A	171	LEU
1	A	179	ARG
1	A	183	LEU
1	A	185	ARG
1	A	186	LYS

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Mol	Chain	Res	Type
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	251	LYS
1	A	252	LEU
1	A	271	VAL
1	A	291	VAL
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU
1	A	317	LYS
1	A	322	THR
1	A	345	ILE
1	A	348	TYR
1	A	376	ARG
1	A	384	LEU
1	A	385	TYR
1	A	433	ARG
1	A	455	SER
1	A	458	LEU
1	A	469	ARG
1	A	473	LYS
1	A	476	THR
1	A	479	GLN
1	A	484	GLU
1	A	497	ASP
1	A	514	PRO
1	A	518	PHE
1	A	530	SER
1	A	556	PHE
1	A	563	THR
1	A	564	LEU
1	B	49	ARG
1	B	70	THR
1	B	111	THR
1	B	115	LEU
1	B	116	VAL
1	B	117	LEU
1	B	120	ARG
1	B	126	SER

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Mol	Chain	Res	Type
1	B	145	VAL
1	B	165	THR
1	B	170	GLN
1	B	171	LEU
1	B	179	ARG
1	B	183	LEU
1	B	185	ARG
1	B	186	LYS
1	B	215	LYS
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	251	LYS
1	B	252	LEU
1	B	271	VAL
1	B	291	VAL
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	317	LYS
1	B	322	THR
1	B	345	ILE
1	B	348	TYR
1	B	376	ARG
1	B	384	LEU
1	B	385	TYR
1	B	433	ARG
1	B	455	SER
1	B	458	LEU
1	B	469	ARG
1	B	473	LYS
1	B	476	THR
1	B	479	GLN
1	B	484	GLU
1	B	497	ASP
1	B	514	PRO
1	B	518	PHE
1	B	530	SER
1	B	556	PHE
1	B	563	THR
1	B	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	170	GLN
1	A	203	GLN
1	A	207	HIS
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	320	HIS
1	A	358	GLN
1	A	372	GLN
1	A	375	ASN
1	A	443	HIS
1	A	513	HIS
1	A	557	ASN
1	B	134	HIS
1	B	170	GLN
1	B	203	GLN
1	B	207	HIS
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	320	HIS
1	B	358	GLN
1	B	375	ASN
1	B	443	HIS
1	B	513	HIS
1	B	557	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.53	0	17,19,21	1.06	1 (5%)
2	NAG	C	2	2	14,14,15	1.12	2 (14%)	17,19,21	1.29	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
2	NAG	D	2	2	14,14,15	1.13	2 (14%)	17,19,21	1.28	2 (11%)

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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C4-C5	2.35	1.58	1.53
2	C	2	NAG	C4-C5	2.34	1.58	1.53
2	D	2	NAG	O5-C5	2.02	1.47	1.43
2	C	2	NAG	O5-C5	2.02	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C4-C3-C2	-3.14	106.42	111.02
2	D	2	NAG	C4-C3-C2	-3.12	106.44	111.02
2	D	1	NAG	C6-C5-C4	-2.45	107.25	113.00
2	C	1	NAG	C6-C5-C4	-2.45	107.26	113.00
2	C	2	NAG	O5-C1-C2	-2.21	107.80	111.29
2	D	2	NAG	O5-C1-C2	-2.16	107.88	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7

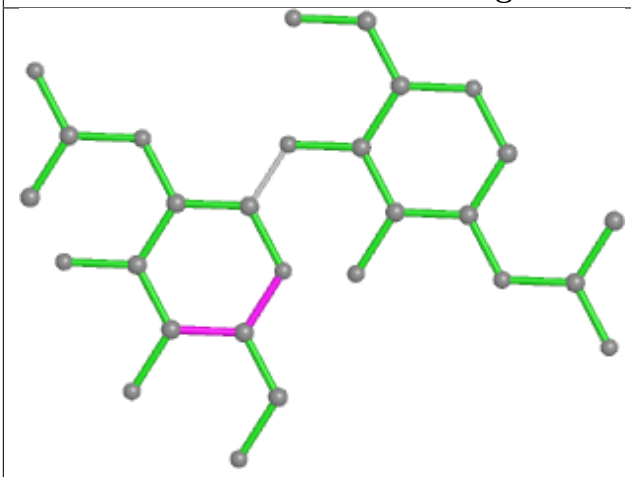
There are no ring outliers.

2 monomers are involved in 2 short contacts:

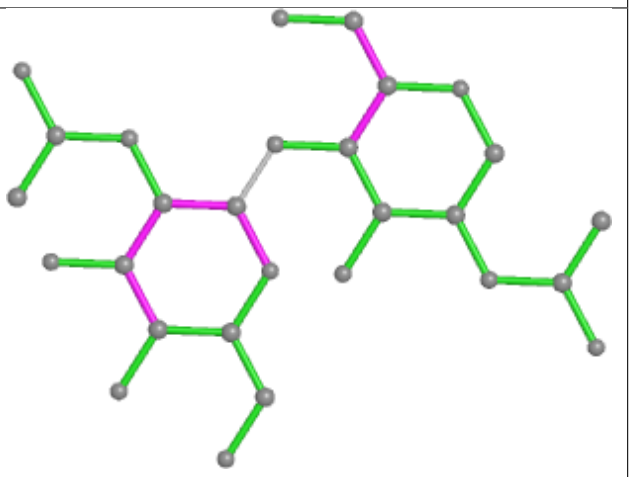
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	D	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

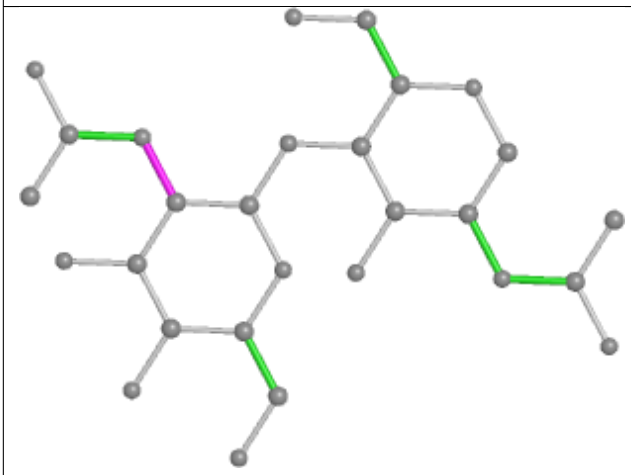
Oligosaccharide Chain C



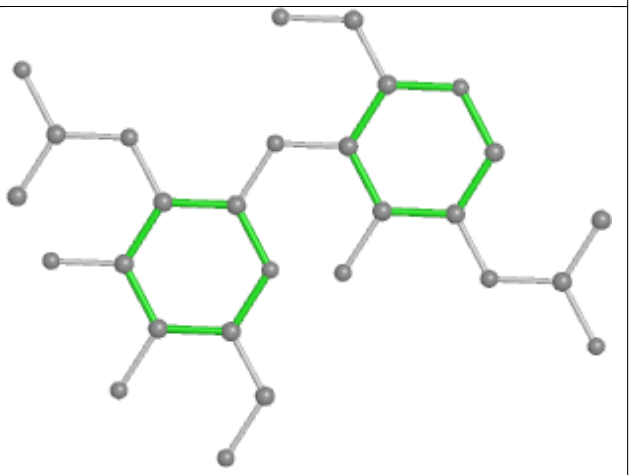
Bond lengths



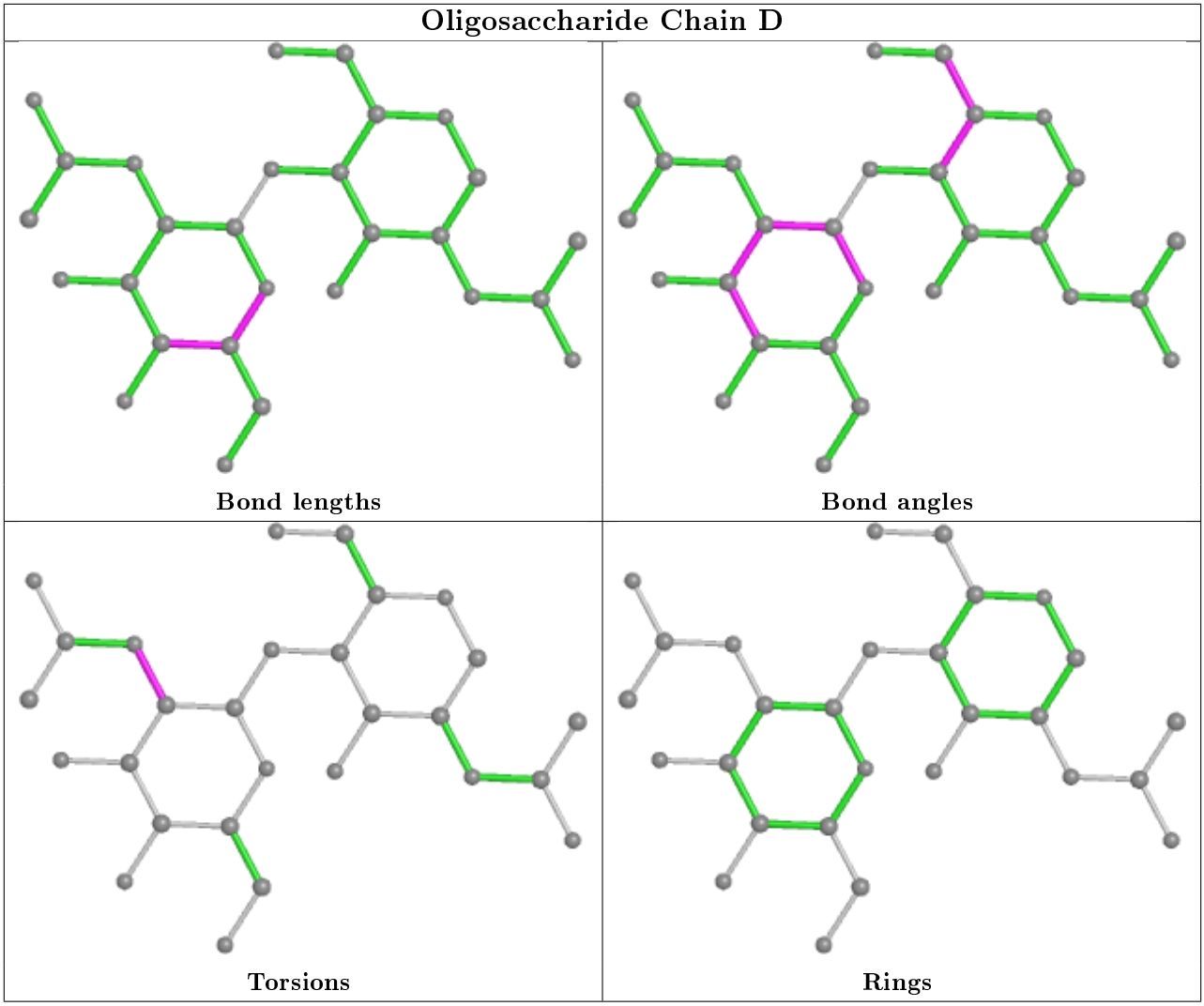
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HEM	B	601	1	27,50,50	2.76	9 (33%)	17,82,82	2.09	4 (23%)
3	NAG	B	661	1	14,14,15	0.79	0	17,19,21	1.21	1 (5%)
5	IMM	B	1	-	21,27,27	1.39	2 (9%)	26,39,39	1.14	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HEM	A	601	1	27,50,50	2.75	9 (33%)	17,82,82	2.10	4 (23%)
3	NAG	A	681	1	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	A	661	1	14,14,15	0.78	0	17,19,21	1.21	1 (5%)
5	IMM	A	1	-	21,27,27	1.38	2 (9%)	26,39,39	1.14	2 (7%)
3	NAG	B	681	1	14,14,15	0.75	0	17,19,21	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	601	1	-	1/6/54/54	-
3	NAG	B	661	1	-	0/6/23/26	0/1/1/1
5	IMM	B	1	-	-	4/8/14/14	0/3/3/3
4	HEM	A	601	1	-	1/6/54/54	-
3	NAG	A	681	1	-	1/6/23/26	0/1/1/1
3	NAG	A	661	1	-	0/6/23/26	0/1/1/1
5	IMM	A	1	-	-	4/8/14/14	0/3/3/3
3	NAG	B	681	1	-	1/6/23/26	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C3B-C2B	-7.43	1.30	1.40
4	A	601	HEM	C3B-C2B	-7.40	1.30	1.40
4	A	601	HEM	C3C-CAC	-6.12	1.35	1.47
4	B	601	HEM	C3C-CAC	-6.11	1.35	1.47
4	B	601	HEM	C3C-C2C	-5.21	1.33	1.40
4	A	601	HEM	C3C-C2C	-5.20	1.33	1.40
4	B	601	HEM	C1B-C2B	4.30	1.52	1.42
4	A	601	HEM	C1B-C2B	4.29	1.52	1.42
5	B	1	IMM	C2-N1	3.85	1.43	1.36
5	A	1	IMM	C2-N1	3.82	1.43	1.36
4	A	601	HEM	C3B-CAB	-3.73	1.40	1.47
4	B	601	HEM	C3B-CAB	-3.71	1.40	1.47
4	B	601	HEM	C1A-CHA	-2.81	1.33	1.41
4	A	601	HEM	C1A-CHA	-2.80	1.33	1.41
4	B	601	HEM	CAA-C2A	2.78	1.56	1.52
4	A	601	HEM	CAA-C2A	2.77	1.56	1.52
4	B	601	HEM	CBB-CAB	2.68	1.47	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEM	CBB-CAB	2.67	1.47	1.29
4	A	601	HEM	C1D-ND	2.47	1.41	1.36
4	B	601	HEM	C1D-ND	2.45	1.41	1.36
5	B	1	IMM	C8-C9	-2.07	1.36	1.41
5	A	1	IMM	C8-C9	-2.05	1.37	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	HEM	CBA-CAA-C2A	4.75	121.24	112.49
4	A	601	HEM	CBA-CAA-C2A	4.74	121.22	112.49
4	A	601	HEM	C4A-C3A-C2A	4.66	110.24	107.00
4	B	601	HEM	C4A-C3A-C2A	4.62	110.21	107.00
3	B	661	NAG	C2-N2-C7	-4.31	116.76	122.90
3	A	661	NAG	C2-N2-C7	-4.29	116.80	122.90
5	B	1	IMM	C11-C10-N1	3.69	122.26	117.95
5	A	1	IMM	C11-C10-N1	3.69	122.26	117.95
4	A	601	HEM	C3B-C4B-NB	3.51	113.75	109.21
4	B	601	HEM	C3B-C4B-NB	3.47	113.70	109.21
5	A	1	IMM	C17-C2-C3	-2.35	124.16	129.24
5	B	1	IMM	C17-C2-C3	-2.34	124.18	129.24
4	B	601	HEM	C4C-C3C-C2C	2.11	108.37	106.90
4	A	601	HEM	C4C-C3C-C2C	2.08	108.35	106.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	IMM	C7-C6-O2-C20
5	A	1	IMM	C7-C6-O2-C20
5	B	1	IMM	C5-C6-O2-C20
5	A	1	IMM	C5-C6-O2-C20
3	B	681	NAG	C4-C5-C6-O6
3	A	681	NAG	C4-C5-C6-O6
5	B	1	IMM	C19-C18-C3-C4
5	A	1	IMM	C19-C18-C3-C4
4	B	601	HEM	C2A-CAA-CBA-CGA
4	A	601	HEM	C2A-CAA-CBA-CGA
5	B	1	IMM	C19-C18-C3-C2
5	A	1	IMM	C19-C18-C3-C2

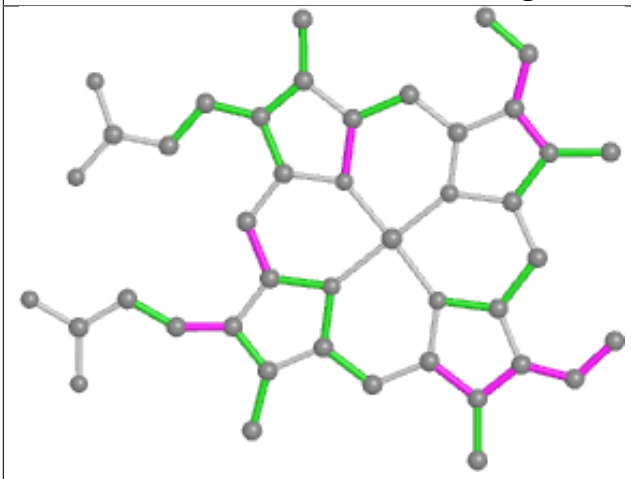
There are no ring outliers.

4 monomers are involved in 45 short contacts:

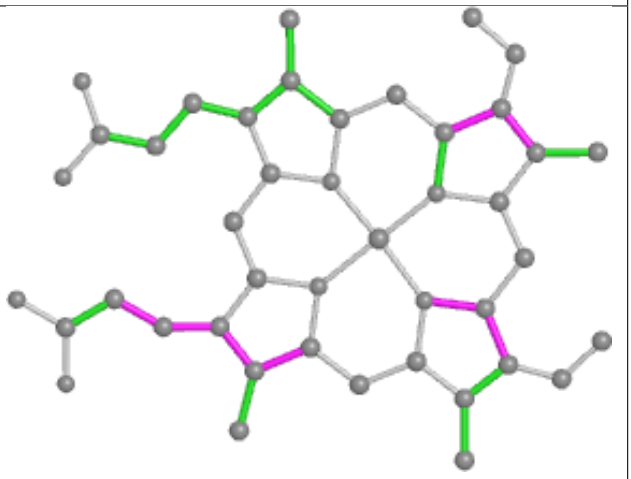
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	HEM	7	0
5	B	1	IMM	16	0
4	A	601	HEM	7	0
5	A	1	IMM	15	0

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.

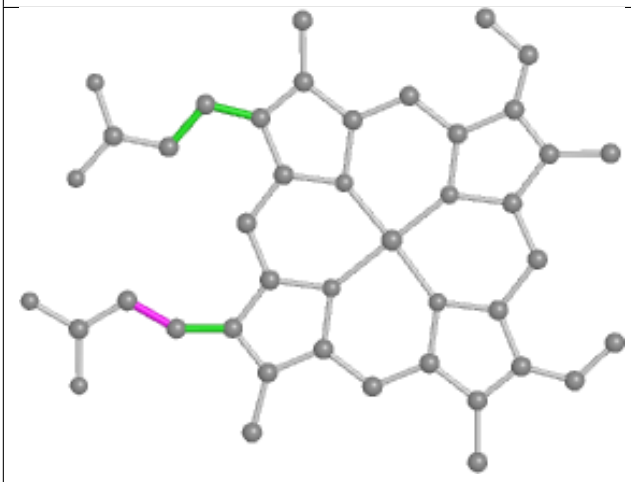
Ligand HEM B 601



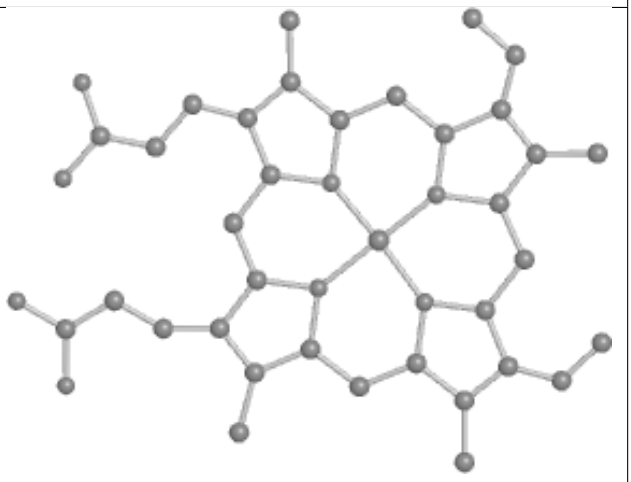
Bond lengths



Bond angles

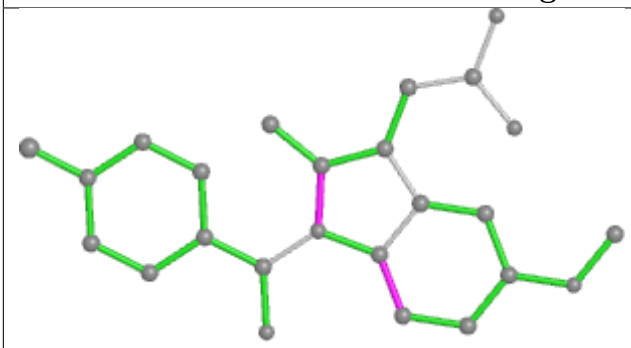


Torsions

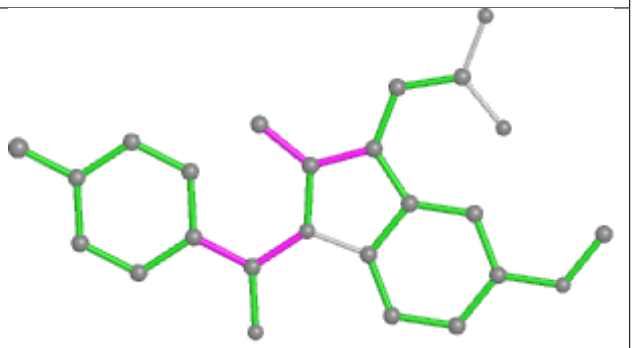


Rings

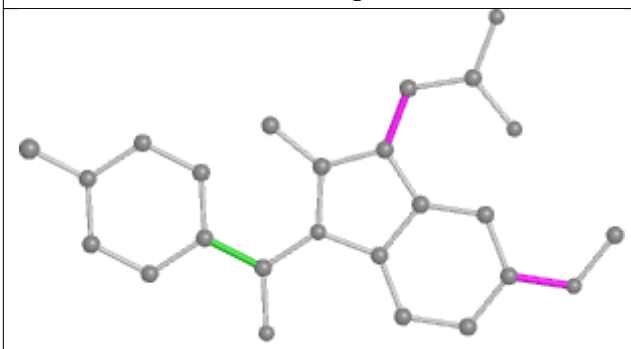
Ligand IMM B 1



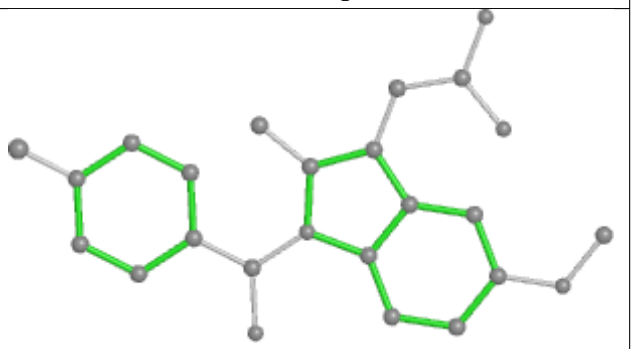
Bond lengths



Bond angles

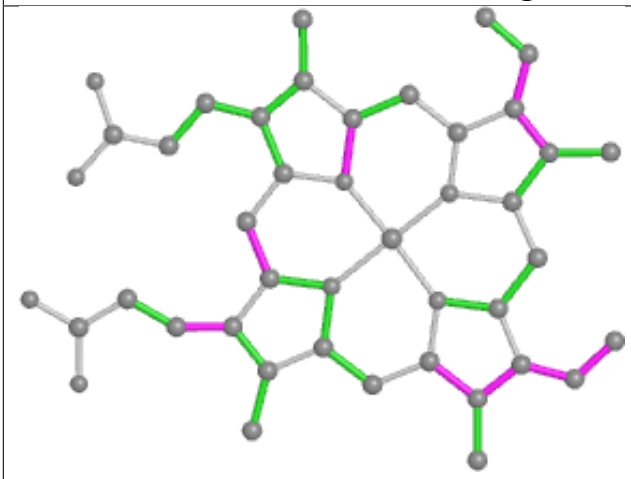


Torsions

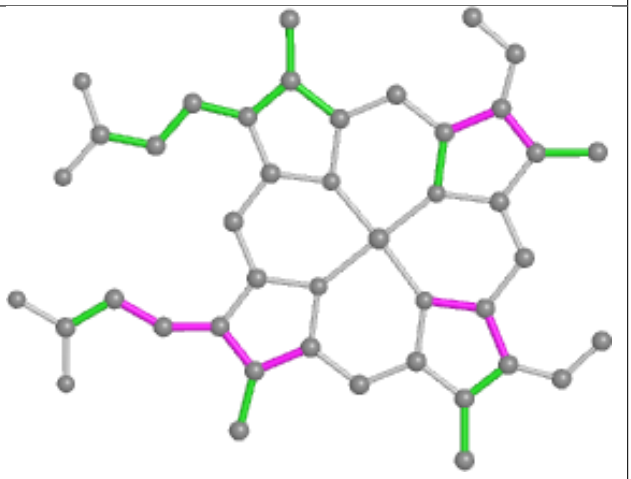


Rings

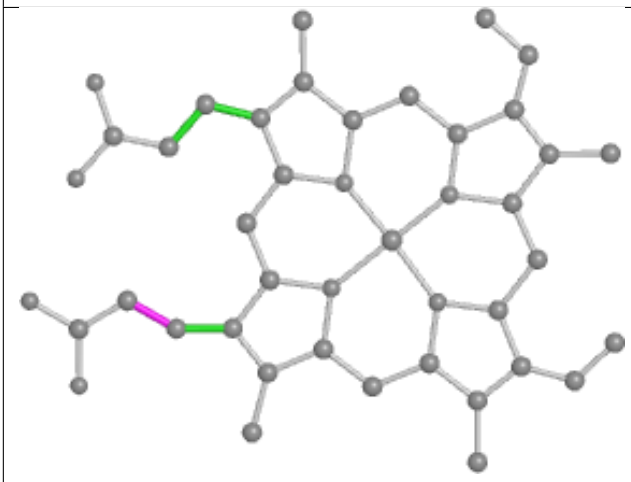
Ligand HEM A 601



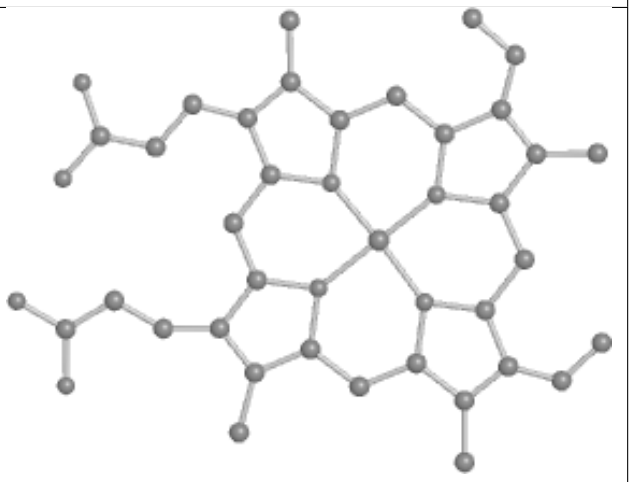
Bond lengths



Bond angles

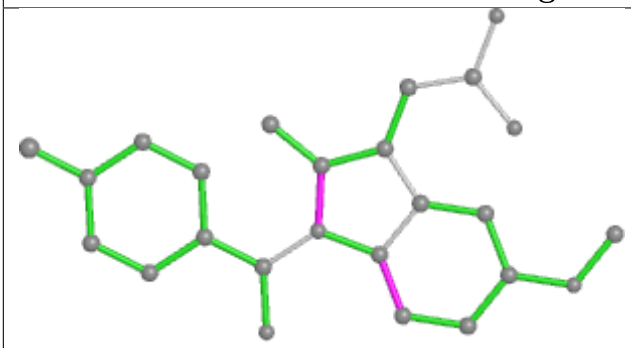


Torsions

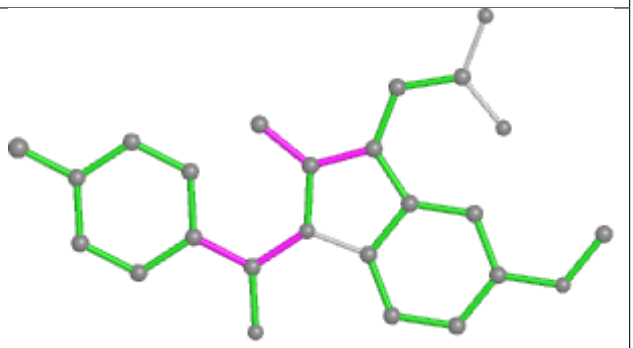


Rings

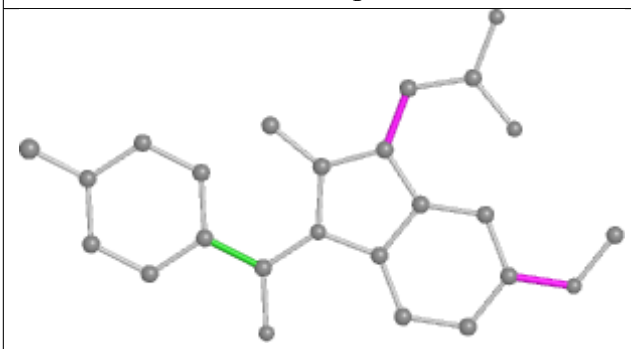
Ligand IMM A 1



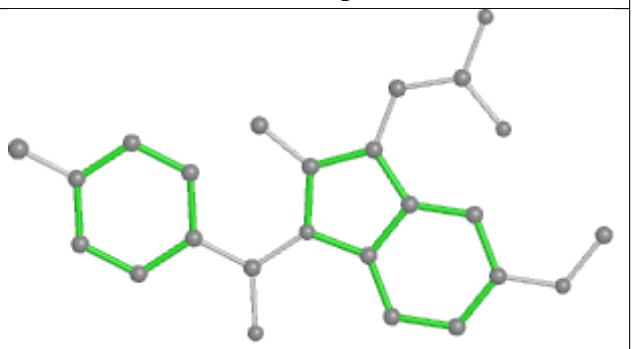
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.