



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:57 AM UTC

PDB ID : 1PGE / pdb_00001pge
Title : PROSTAGLANDIN H2 SYNTHASE-1 COMPLEXED WITH P-(2'-IODO-5'-THENOYL)HYDROTROPIC ACID (IODOSUPROFEN)
Authors : Loll, P.J.; Picot, D.; Garavito, R.M.
Deposited on : 1995-12-02
Resolution : 3.50 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

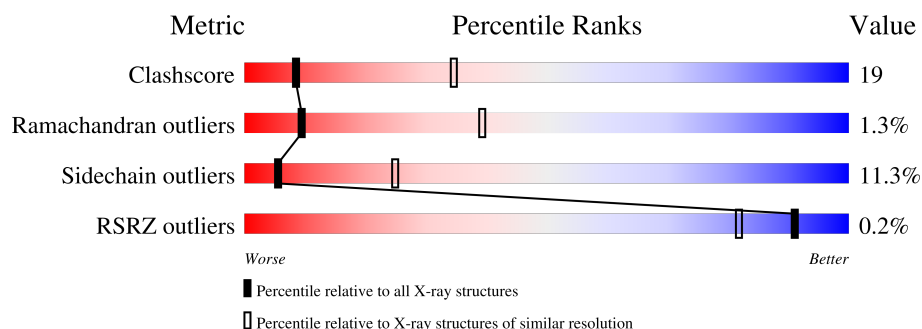
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	
2	C	2	
2	D	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9230 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.



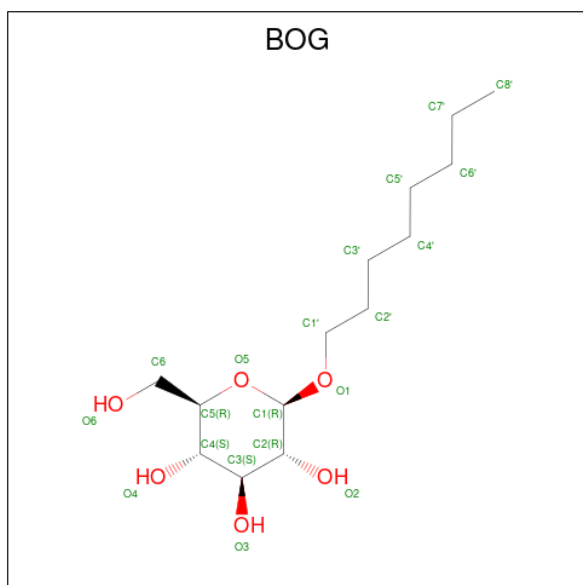
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



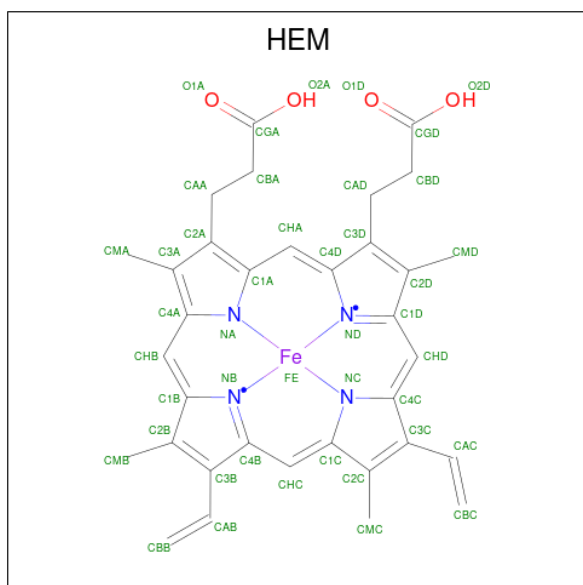
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

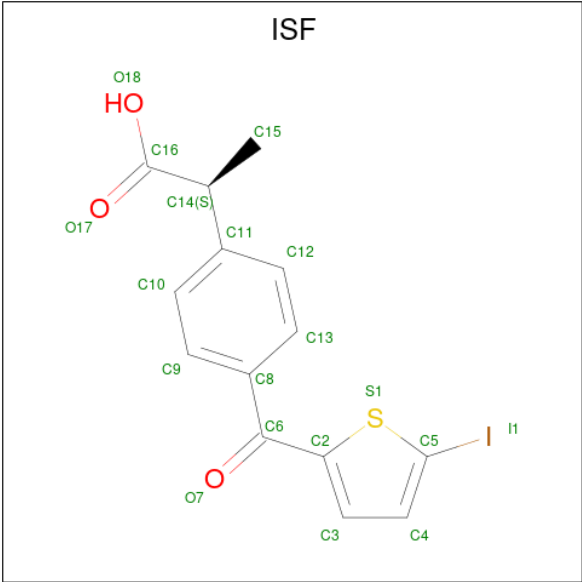
- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



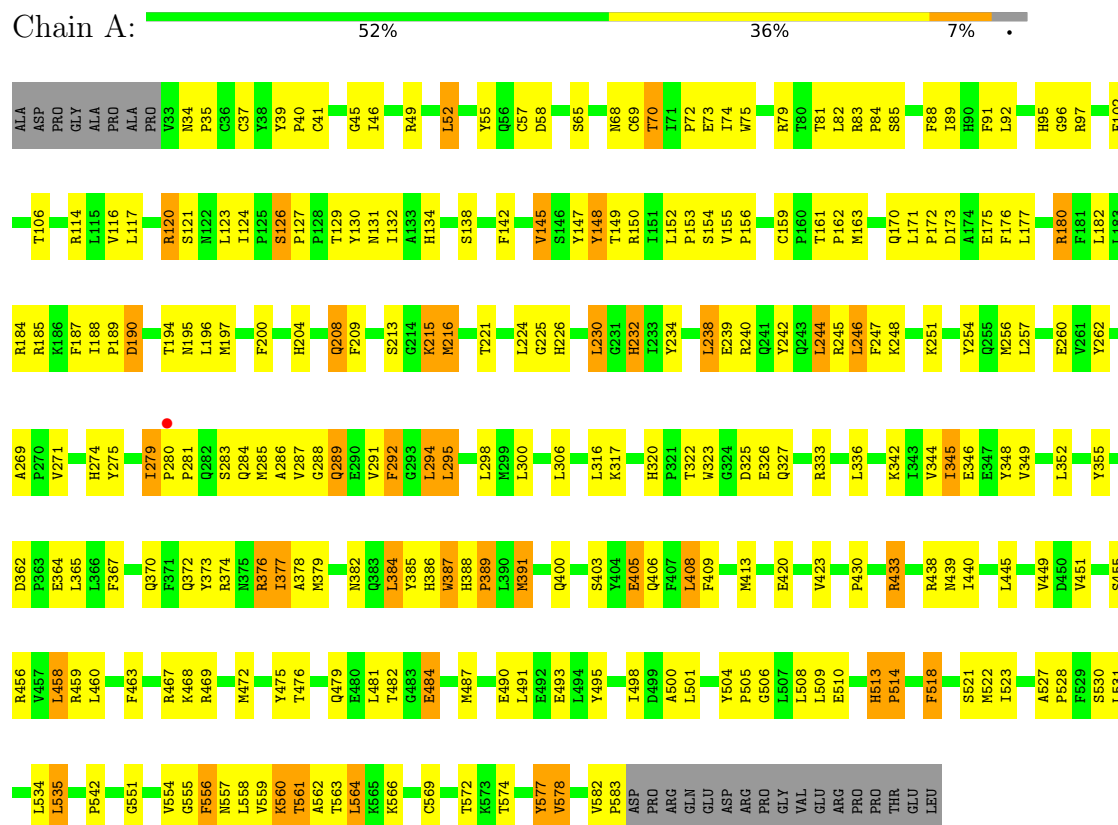


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	I	O	S	0	0
			19	14	1	3	1		
6	B	1	Total	C	I	O	S	0	0
			19	14	1	3	1		

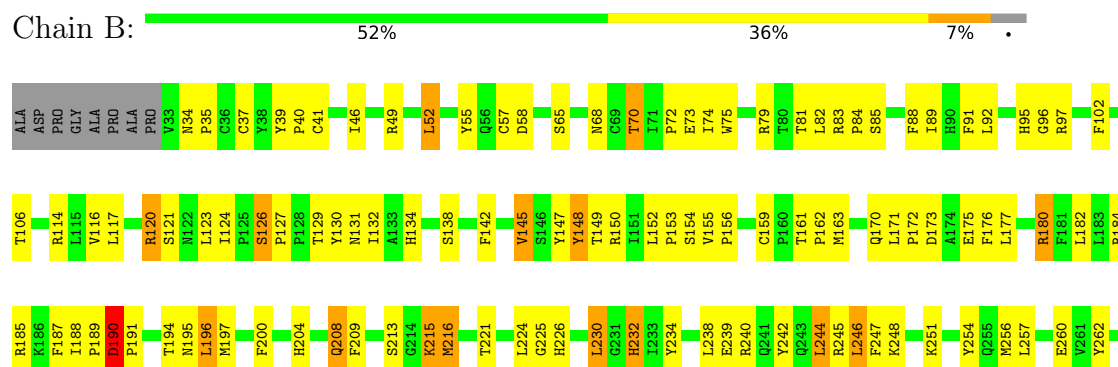
3 Residue-property plots

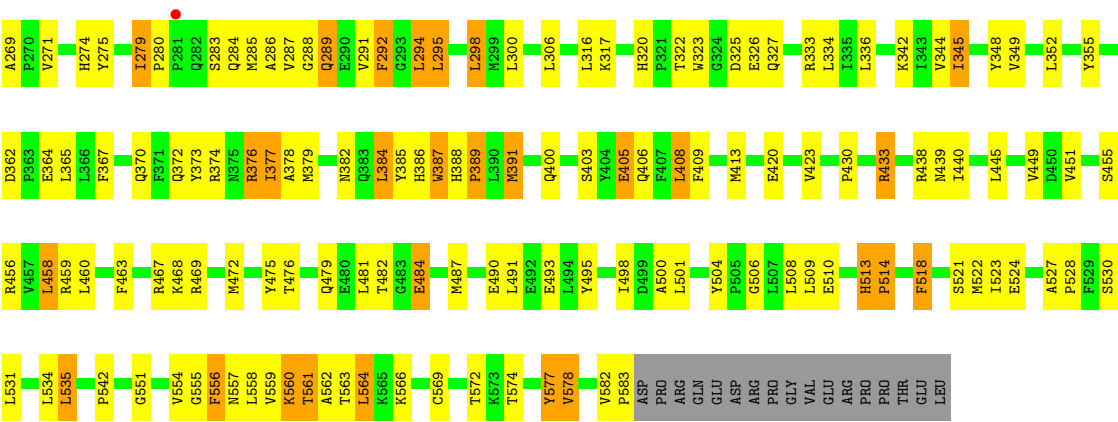
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PROSTAGLANDIN H2 SYNTHASE-1



• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1

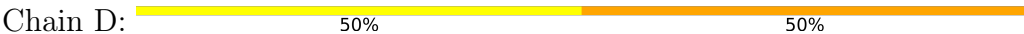




● Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.69Å 209.94Å 234.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50 15.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.9 (15.00-3.50) 89.2 (15.00-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.73 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , 0.231 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9230	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.64	0/4615	1.11	33/6264 (0.5%)
1	B	0.64	0/4615	1.11	32/6264 (0.5%)
All	All	0.64	0/9230	1.11	65/12528 (0.5%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	LEU	N-CA-C	-8.20	98.14	110.28
1	B	224	LEU	N-CA-C	-8.18	98.17	110.28
1	B	124	ILE	CA-C-N	7.81	127.57	119.76
1	B	124	ILE	C-N-CA	7.81	127.57	119.76
1	A	577	TYR	N-CA-C	-7.81	97.31	109.25
1	A	124	ILE	CA-C-N	7.79	127.55	119.76
1	A	124	ILE	C-N-CA	7.79	127.55	119.76
1	B	577	TYR	N-CA-C	-7.78	97.34	109.25
1	A	148	TYR	N-CA-C	-7.29	98.67	110.20
1	B	148	TYR	N-CA-C	-7.28	98.70	110.20
1	A	484	GLU	N-CA-C	7.19	117.51	108.45
1	B	484	GLU	N-CA-C	7.18	117.50	108.45
1	A	190	ASP	CA-C-N	7.04	127.02	119.28
1	A	190	ASP	C-N-CA	7.04	127.02	119.28
1	B	190	ASP	CA-C-N	7.03	127.01	119.28
1	B	190	ASP	C-N-CA	7.03	127.01	119.28
1	B	482	THR	N-CA-C	-6.62	100.68	110.48
1	A	482	THR	N-CA-C	-6.62	100.69	110.48
1	B	569	CYS	N-CA-C	6.51	120.69	112.87
1	A	569	CYS	N-CA-C	6.48	120.64	112.87
1	A	188	ILE	CB-CA-C	-6.46	103.80	110.71
1	B	188	ILE	CB-CA-C	-6.44	103.82	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	SER	N-CA-C	6.41	118.27	111.28
1	B	521	SER	N-CA-C	6.38	118.23	111.28
1	B	41	CYS	N-CA-C	6.21	118.93	107.99
1	A	41	CYS	N-CA-C	6.21	118.92	107.99
1	A	408	LEU	N-CA-C	6.15	123.89	110.80
1	B	408	LEU	N-CA-C	6.13	123.85	110.80
1	B	513	HIS	CA-C-N	5.78	127.06	119.84
1	B	513	HIS	C-N-CA	5.78	127.06	119.84
1	A	513	HIS	CA-C-N	5.76	127.04	119.84
1	A	513	HIS	C-N-CA	5.76	127.04	119.84
1	A	121	SER	N-CA-C	5.73	117.60	111.36
1	B	121	SER	N-CA-C	5.71	117.58	111.36
1	A	362	ASP	CA-C-N	5.70	126.08	119.47
1	A	362	ASP	C-N-CA	5.70	126.08	119.47
1	B	362	ASP	CA-C-N	5.67	126.04	119.47
1	B	362	ASP	C-N-CA	5.67	126.04	119.47
1	A	370	GLN	N-CA-C	-5.62	97.30	107.75
1	B	370	GLN	N-CA-C	-5.60	97.33	107.75
1	B	269	ALA	CA-C-N	5.59	126.83	119.84
1	B	269	ALA	C-N-CA	5.59	126.83	119.84
1	A	269	ALA	CA-C-N	5.58	126.81	119.84
1	A	269	ALA	C-N-CA	5.58	126.81	119.84
1	A	391	MET	CA-C-N	5.55	126.77	119.84
1	A	391	MET	C-N-CA	5.55	126.77	119.84
1	B	391	MET	CA-C-N	5.55	126.77	119.84
1	B	391	MET	C-N-CA	5.55	126.77	119.84
1	A	377	ILE	N-CA-C	5.51	116.37	108.93
1	B	377	ILE	N-CA-C	5.49	116.34	108.93
1	A	208	GLN	N-CA-C	-5.47	106.97	113.97
1	B	208	GLN	N-CA-C	-5.44	107.00	113.97
1	B	287	VAL	N-CA-C	5.43	120.63	109.34
1	A	287	VAL	N-CA-C	5.40	120.58	109.34
1	B	73	GLU	N-CA-C	-5.38	101.77	110.32
1	A	73	GLU	N-CA-C	-5.37	101.78	110.32
1	A	345	ILE	CB-CA-C	-5.31	104.93	111.94
1	B	345	ILE	CB-CA-C	-5.30	104.94	111.94
1	A	279	ILE	N-CA-C	-5.24	104.12	108.63
1	B	279	ILE	N-CA-C	-5.23	104.13	108.63
1	B	225	GLY	N-CA-C	-5.23	100.79	113.18
1	A	225	GLY	N-CA-C	-5.22	100.81	113.18
1	A	129	THR	N-CA-C	5.04	116.79	108.48
1	B	129	THR	N-CA-C	5.02	116.77	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	GLU	N-CA-C	5.00	118.64	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4477	0	4383	174	0
1	B	4477	0	4383	172	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	20	0	28	1	0
4	B	20	0	28	1	0
5	A	43	0	30	3	0
5	B	43	0	30	3	0
6	A	19	0	10	4	0
6	B	19	0	10	4	0
All	All	9230	0	9004	346	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 19.

All (346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.48	0.95
1:A:384:LEU:HD23	6:A:800:ISF:I1	2.39	0.93
1:B:384:LEU:HD23	6:B:800:ISF:I1	2.39	0.92
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.48	0.91
1:A:150:ARG:HB3	1:A:379:MET:HE3	1.53	0.90
1:B:150:ARG:HB3	1:B:379:MET:HE3	1.53	0.90
1:B:294:LEU:HD22	1:B:409:PHE:CE2	2.09	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.09	0.87
1:B:433:ARG:HH11	1:B:433:ARG:HB3	1.47	0.79
1:A:433:ARG:HB3	1:A:433:ARG:HH11	1.46	0.79
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.50	0.77
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.50	0.77
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.20	0.76
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.20	0.75
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.52	0.74
1:B:84:PRO:CG	1:B:89:ILE:HD11	2.18	0.74
1:A:563:THR:HG22	1:A:566:LYS:HD3	1.70	0.74
1:B:294:LEU:HD22	1:B:409:PHE:HE2	1.52	0.74
1:A:84:PRO:CG	1:A:89:ILE:HD11	2.18	0.73
1:B:563:THR:HG22	1:B:566:LYS:HD3	1.70	0.72
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.72	0.72
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.25	0.72
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.30	0.72
1:A:387:TRP:HB2	5:A:601:HEM:HAC	1.72	0.72
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.30	0.72
1:B:116:VAL:O	1:B:120:ARG:HB2	1.90	0.72
1:A:116:VAL:O	1:A:120:ARG:HB2	1.90	0.71
1:B:563:THR:HG23	1:B:566:LYS:H	1.56	0.71
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.25	0.70
1:B:172:PRO:HB2	1:B:177:LEU:HD22	1.72	0.70
1:B:384:LEU:CD2	6:B:800:ISF:I1	3.09	0.70
1:A:384:LEU:CD2	6:A:800:ISF:I1	3.09	0.70
1:A:563:THR:HG23	1:A:566:LYS:H	1.56	0.70
1:B:387:TRP:HB2	5:B:601:HEM:HAC	1.72	0.69
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.59	0.68
1:B:245:ARG:HH22	1:B:326:GLU:HG2	1.59	0.66
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.78	0.66
1:B:182:LEU:HB3	1:B:440:ILE:HD12	1.78	0.65
1:A:154:SER:HB2	1:A:459:ARG:HB2	1.78	0.65
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.32	0.65
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.32	0.64
1:A:403:SER:OG	1:A:406:GLN:HG3	1.97	0.64
1:B:403:SER:OG	1:B:406:GLN:HG3	1.97	0.64
1:B:274:HIS:O	1:B:294:LEU:HD21	1.99	0.63
1:B:154:SER:HB2	1:B:459:ARG:HB2	1.78	0.63
1:A:91:PHE:HD2	1:A:92:LEU:HD12	1.66	0.61
1:A:274:HIS:O	1:A:294:LEU:HD21	1.99	0.61
1:A:239:GLU:CD	1:A:239:GLU:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.61
1:A:213:SER:HB3	1:A:216:MET:HB2	1.83	0.61
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.83	0.61
1:B:239:GLU:CD	1:B:239:GLU:H	2.08	0.60
1:B:120:ARG:NH1	4:B:702:BOG:H1'2	2.16	0.60
1:A:197:MET:HE2	1:A:423:VAL:HG13	1.83	0.60
1:B:91:PHE:HD2	1:B:92:LEU:HD12	1.66	0.60
1:A:491:LEU:HD11	1:A:509:LEU:HD13	1.84	0.60
1:A:230:LEU:CD2	1:A:336:LEU:HB3	2.32	0.60
1:B:197:MET:HE2	1:B:423:VAL:HG13	1.83	0.60
1:A:120:ARG:NH1	4:A:702:BOG:H1'2	2.16	0.59
1:B:213:SER:HB3	1:B:216:MET:HB2	1.83	0.59
1:B:230:LEU:CD2	1:B:336:LEU:HB3	2.32	0.59
1:B:149:THR:O	1:B:378:ALA:HA	2.02	0.59
1:B:491:LEU:HD11	1:B:509:LEU:HD13	1.84	0.59
1:A:171:LEU:HD23	1:A:456:ARG:NE	2.18	0.59
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.38	0.59
1:A:149:THR:O	1:A:378:ALA:HA	2.02	0.59
1:B:171:LEU:HD23	1:B:456:ARG:NE	2.18	0.59
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.68	0.59
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.38	0.58
1:B:46:ILE:HB	1:B:58:ASP:HB3	1.85	0.58
1:A:52:LEU:HD12	1:A:52:LEU:H	1.69	0.58
1:B:52:LEU:HD12	1:B:52:LEU:H	1.69	0.58
1:B:459:ARG:HH11	1:B:459:ARG:HG2	1.68	0.58
1:A:132:ILE:HD13	1:A:458:LEU:HD12	1.86	0.57
1:B:126:SER:HA	1:B:127:PRO:C	2.29	0.57
1:A:126:SER:HA	1:A:127:PRO:C	2.29	0.57
1:A:215:LYS:HE2	1:A:215:LYS:H	1.70	0.57
1:B:132:ILE:HD13	1:B:458:LEU:HD12	1.86	0.57
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.40	0.57
1:B:176:PHE:CZ	1:B:180:ARG:HD2	2.40	0.56
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.40	0.56
1:A:433:ARG:HH11	1:A:433:ARG:CB	2.18	0.56
1:B:200:PHE:CE1	1:B:391:MET:HE1	2.40	0.56
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.41	0.56
1:A:46:ILE:HB	1:A:58:ASP:HB3	1.85	0.56
1:B:215:LYS:HE2	1:B:215:LYS:H	1.69	0.56
1:A:176:PHE:CZ	1:A:180:ARG:HD2	2.40	0.56
1:A:577:TYR:HE2	1:A:583:PRO:HD3	1.71	0.56
1:A:163:MET:HE3	1:A:171:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:MET:HE3	1:B:171:LEU:HD21	1.87	0.55
1:A:200:PHE:CE1	1:A:391:MET:HE1	2.40	0.55
1:A:102:PHE:O	1:A:106:THR:HG23	2.06	0.55
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.41	0.55
1:B:275:TYR:CE1	1:B:284:GLN:HB3	2.42	0.55
1:B:102:PHE:O	1:B:106:THR:HG23	2.06	0.55
1:A:39:TYR:OH	1:A:155:VAL:HG22	2.08	0.54
1:A:554:VAL:HG23	1:A:555:GLY:N	2.22	0.54
1:B:39:TYR:OH	1:B:155:VAL:HG22	2.08	0.54
1:B:554:VAL:HG23	1:B:555:GLY:N	2.22	0.54
1:A:130:TYR:HB3	1:A:134:HIS:O	2.08	0.54
1:B:379:MET:SD	1:B:458:LEU:HG	2.48	0.54
1:A:275:TYR:CE1	1:A:284:GLN:HB3	2.42	0.54
1:B:294:LEU:HD22	1:B:409:PHE:CD2	2.43	0.54
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.43	0.53
1:A:156:PRO:HD2	1:A:159:CYS:SG	2.48	0.53
1:A:306:LEU:HD23	1:A:306:LEU:C	2.34	0.53
1:B:156:PRO:HD2	1:B:159:CYS:SG	2.48	0.53
1:A:344:VAL:O	1:A:349:VAL:HG23	2.08	0.53
1:A:490:GLU:HA	1:A:493:GLU:HG2	1.91	0.53
1:B:344:VAL:O	1:B:349:VAL:HG23	2.08	0.53
1:B:577:TYR:HE2	1:B:583:PRO:HD3	1.71	0.53
1:A:171:LEU:HD23	1:A:456:ARG:HE	1.74	0.53
1:A:379:MET:SD	1:A:458:LEU:HG	2.48	0.53
1:B:433:ARG:HH11	1:B:433:ARG:CB	2.18	0.53
1:B:130:TYR:HB3	1:B:134:HIS:O	2.08	0.53
1:A:195:ASN:HA	1:A:430:PRO:HA	1.91	0.52
1:A:262:TYR:HB3	1:A:285:MET:HE1	1.92	0.52
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.39	0.52
1:B:187:PHE:CE2	1:B:189:PRO:HB3	2.44	0.52
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.45	0.52
1:B:582:VAL:CG2	1:B:583:PRO:HD2	2.39	0.52
1:A:342:LYS:HD2	1:A:559:VAL:O	2.09	0.52
1:B:88:PHE:CZ	1:B:92:LEU:HD11	2.45	0.52
1:B:306:LEU:C	1:B:306:LEU:HD23	2.34	0.52
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.45	0.52
1:B:342:LYS:HD2	1:B:559:VAL:O	2.09	0.52
1:A:256:MET:O	1:A:257:LEU:HD23	2.09	0.52
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.45	0.52
1:B:246:LEU:HD13	1:B:248:LYS:HB3	1.92	0.51
1:B:468:LYS:HA	1:B:472:MET:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:HD23	1:B:456:ARG:HE	1.74	0.51
1:B:490:GLU:HA	1:B:493:GLU:HG2	1.91	0.51
1:B:195:ASN:HA	1:B:430:PRO:HA	1.91	0.51
1:A:187:PHE:CE2	1:A:189:PRO:HB3	2.44	0.51
1:A:561:THR:HB	1:A:566:LYS:NZ	2.26	0.51
1:A:91:PHE:CE1	1:A:95:HIS:CD2	2.99	0.51
1:A:271:VAL:CG1	1:A:286:ALA:HB1	2.41	0.51
1:B:91:PHE:CE1	1:B:95:HIS:CD2	2.99	0.51
1:A:468:LYS:HA	1:A:472:MET:O	2.10	0.51
5:B:601:HEM:HMB1	5:B:601:HEM:HBB2	1.92	0.51
1:B:256:MET:O	1:B:257:LEU:HD23	2.09	0.51
1:B:262:TYR:HB3	1:B:285:MET:HE1	1.91	0.50
1:B:271:VAL:CG1	1:B:286:ALA:HB1	2.41	0.50
1:B:561:THR:HB	1:B:566:LYS:NZ	2.26	0.50
1:A:289:GLN:OE1	1:A:291:VAL:HG12	2.12	0.50
1:B:52:LEU:HD12	1:B:52:LEU:N	2.27	0.50
1:B:389:PRO:HG3	1:B:440:ILE:HG12	1.93	0.50
1:A:150:ARG:HD3	1:A:152:LEU:O	2.12	0.50
1:A:463:PHE:CE2	1:A:467:ARG:HD3	2.47	0.50
1:A:372:GLN:HE22	1:B:373:TYR:H	1.59	0.50
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.92	0.50
1:A:246:LEU:HD13	1:A:248:LYS:HB3	1.92	0.50
5:A:601:HEM:HMB1	5:A:601:HEM:HBB2	1.93	0.50
1:A:52:LEU:HD12	1:A:52:LEU:N	2.27	0.49
1:A:208:GLN:NE2	1:A:230:LEU:H	2.11	0.49
1:B:150:ARG:HD3	1:B:152:LEU:O	2.12	0.49
1:B:463:PHE:CE2	1:B:467:ARG:HD3	2.47	0.49
1:A:458:LEU:HB3	1:A:460:LEU:HD22	1.95	0.49
1:A:81:THR:C	1:A:82:LEU:HD12	2.38	0.49
1:B:320:HIS:HE1	1:B:551:GLY:O	1.95	0.49
1:B:262:TYR:HB3	1:B:285:MET:CE	2.43	0.49
1:A:320:HIS:HE1	1:A:551:GLY:O	1.95	0.49
1:B:123:LEU:O	1:B:469:ARG:NH2	2.46	0.49
1:B:289:GLN:OE1	1:B:291:VAL:HG12	2.12	0.49
1:B:458:LEU:HB3	1:B:460:LEU:HD22	1.95	0.49
1:A:123:LEU:O	1:A:469:ARG:NH2	2.46	0.49
1:A:522:MET:O	6:A:800:ISF:H4	2.13	0.49
1:B:81:THR:C	1:B:82:LEU:HD12	2.38	0.49
1:A:262:TYR:HB3	1:A:285:MET:CE	2.43	0.49
1:B:280:PRO:HG2	1:B:283:SER:OG	2.14	0.48
1:A:35:PRO:HB2	1:A:55:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.49	0.48
1:B:148:TYR:CZ	1:B:221:THR:HB	2.49	0.48
1:B:522:MET:O	6:B:800:ISF:H4	2.13	0.48
1:B:295:LEU:HD11	5:B:601:HEM:CAB	2.44	0.48
1:A:256:MET:HA	1:A:260:GLU:O	2.14	0.48
1:A:280:PRO:O	1:A:284:GLN:HG3	2.14	0.48
1:A:320:HIS:CE1	1:A:551:GLY:O	2.67	0.48
1:B:209:PHE:HB2	1:B:377:ILE:HG13	1.95	0.48
1:B:35:PRO:HB2	1:B:55:TYR:CD2	2.49	0.48
1:B:320:HIS:CE1	1:B:551:GLY:O	2.67	0.48
1:B:367:PHE:CD1	1:B:542:PRO:HG3	2.49	0.48
1:A:148:TYR:CZ	1:A:221:THR:HB	2.49	0.48
1:B:208:GLN:NE2	1:B:230:LEU:H	2.11	0.48
1:A:74:ILE:HG23	1:A:75:TRP:N	2.29	0.47
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.95	0.47
1:B:208:GLN:HB3	1:B:232:HIS:CD2	2.49	0.47
1:A:280:PRO:HG2	1:A:283:SER:OG	2.14	0.47
1:B:256:MET:HA	1:B:260:GLU:O	2.14	0.47
1:A:295:LEU:HD11	5:A:601:HEM:CAB	2.43	0.47
1:B:280:PRO:O	1:B:284:GLN:HG3	2.14	0.47
1:B:240:ARG:HE	1:B:288:GLY:HA2	1.80	0.47
1:B:557:ASN:O	1:B:558:LEU:C	2.58	0.47
1:A:557:ASN:O	1:A:558:LEU:C	2.58	0.47
1:B:74:ILE:HG23	1:B:75:TRP:N	2.29	0.47
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.49	0.47
1:A:81:THR:O	1:A:82:LEU:HD12	2.15	0.46
1:B:184:ARG:HB2	1:B:439:ASN:C	2.41	0.46
1:B:323:TRP:CE3	1:B:327:GLN:HG2	2.50	0.46
1:A:184:ARG:HB2	1:A:439:ASN:C	2.41	0.46
1:A:240:ARG:HE	1:A:288:GLY:HA2	1.80	0.46
1:A:323:TRP:CD2	1:A:327:GLN:HG2	2.51	0.46
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.50	0.46
1:A:531:LEU:HD11	6:A:800:ISF:H10	1.98	0.46
1:B:177:LEU:HD21	1:B:495:TYR:OH	2.16	0.46
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.69	0.46
1:A:177:LEU:HD21	1:A:495:TYR:OH	2.15	0.46
1:B:81:THR:O	1:B:82:LEU:HD12	2.15	0.46
1:B:323:TRP:CD2	1:B:327:GLN:HG2	2.51	0.46
1:A:176:PHE:CE1	1:A:180:ARG:HD2	2.51	0.46
1:A:475:TYR:CE2	1:A:481:LEU:HD12	2.52	0.45
1:A:491:LEU:HD11	1:A:509:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ARG:HE	1:B:487:MET:HE2	1.81	0.45
1:A:240:ARG:HG3	1:A:271:VAL:HG21	1.98	0.45
1:A:386:HIS:CD2	1:A:451:VAL:HG21	2.51	0.45
1:B:240:ARG:HG3	1:B:271:VAL:HG21	1.98	0.45
1:B:386:HIS:CD2	1:B:451:VAL:HG21	2.51	0.45
1:B:531:LEU:HD11	6:B:800:ISF:H10	1.98	0.45
1:A:420:GLU:HG3	1:A:572:THR:HB	1.99	0.45
1:A:438:ARG:HE	1:A:487:MET:HE2	1.82	0.45
1:B:475:TYR:CE2	1:B:481:LEU:HD12	2.51	0.45
1:A:215:LYS:H	1:A:215:LYS:CE	2.29	0.45
1:A:254:TYR:CD1	1:A:254:TYR:C	2.95	0.45
1:A:564:LEU:HD13	1:A:578:VAL:HG22	1.99	0.45
1:B:176:PHE:CE1	1:B:180:ARG:HD2	2.51	0.45
1:A:173:ASP:OD1	1:A:175:GLU:HB3	2.17	0.45
1:A:187:PHE:HE2	1:A:189:PRO:HB3	1.82	0.45
1:B:187:PHE:HE2	1:B:189:PRO:HB3	1.82	0.45
1:B:242:TYR:CD1	1:B:247:PHE:HZ	2.35	0.45
1:B:420:GLU:HG3	1:B:572:THR:HB	1.99	0.45
1:A:373:TYR:H	1:B:372:GLN:HE22	1.64	0.45
1:A:403:SER:OG	1:A:405:GLU:HG2	2.17	0.45
1:B:213:SER:CB	1:B:216:MET:HB2	2.46	0.45
1:B:215:LYS:H	1:B:215:LYS:CE	2.29	0.45
1:A:244:LEU:HD11	1:A:271:VAL:HG11	1.99	0.44
1:B:40:PRO:O	1:B:68:ASN:HB3	2.18	0.44
1:B:244:LEU:HD11	1:B:271:VAL:HG11	1.99	0.44
1:B:403:SER:OG	1:B:405:GLU:HG2	2.17	0.44
1:B:96:GLY:O	1:B:97:ARG:C	2.60	0.44
1:B:173:ASP:OD1	1:B:175:GLU:HB3	2.17	0.44
1:B:247:PHE:HD1	1:B:325:ASP:OD2	2.00	0.44
1:B:535:LEU:HD13	1:B:535:LEU:HA	1.66	0.44
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.69	0.44
1:B:491:LEU:HD11	1:B:509:LEU:CD1	2.46	0.44
1:A:184:ARG:HA	1:A:438:ARG:O	2.17	0.44
1:B:254:TYR:CD1	1:B:254:TYR:C	2.95	0.44
1:B:564:LEU:HD13	1:B:578:VAL:HG22	1.99	0.44
1:A:213:SER:CB	1:A:216:MET:HB2	2.46	0.44
1:A:70:THR:O	1:A:72:PRO:HD3	2.16	0.44
1:B:70:THR:O	1:B:72:PRO:HD3	2.16	0.44
1:B:184:ARG:HA	1:B:438:ARG:O	2.18	0.44
1:A:96:GLY:O	1:A:97:ARG:C	2.60	0.44
1:A:247:PHE:HD1	1:A:325:ASP:OD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:NE	1:B:438:ARG:HD3	2.26	0.44
1:B:114:ARG:HD3	1:B:365:LEU:O	2.18	0.44
1:B:131:ASN:ND2	1:B:147:TYR:CD2	2.86	0.44
1:A:40:PRO:O	1:A:68:ASN:HB3	2.18	0.43
1:A:242:TYR:CD1	1:A:247:PHE:HZ	2.35	0.43
1:B:563:THR:HG22	1:B:566:LYS:HB2	1.99	0.43
1:B:145:VAL:HG13	1:B:145:VAL:O	2.17	0.43
1:B:388:HIS:N	1:B:389:PRO:CD	2.81	0.43
1:B:130:TYR:CE2	1:B:153:PRO:HD3	2.54	0.43
1:A:85:SER:O	1:A:89:ILE:HG12	2.19	0.43
1:A:114:ARG:HD3	1:A:365:LEU:O	2.18	0.43
1:A:185:ARG:NE	1:A:438:ARG:HD3	2.26	0.43
1:A:145:VAL:O	1:A:145:VAL:HG13	2.17	0.43
1:A:445:LEU:O	1:A:449:VAL:HG23	2.19	0.43
1:A:130:TYR:CE2	1:A:153:PRO:HD3	2.54	0.43
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.86	0.43
1:A:481:LEU:HD11	1:A:510:GLU:HB2	2.01	0.43
1:A:563:THR:HG22	1:A:566:LYS:HB2	1.99	0.43
1:B:85:SER:O	1:B:89:ILE:HG12	2.19	0.43
1:B:240:ARG:NH1	1:B:271:VAL:HG22	2.34	0.43
1:B:382:ASN:OD1	1:B:386:HIS:HE1	2.02	0.43
1:A:498:ILE:C	1:A:500:ALA:H	2.26	0.43
1:A:535:LEU:HD13	1:A:535:LEU:HA	1.66	0.43
1:A:134:HIS:HD2	1:A:138:SER:OG	2.01	0.43
1:B:498:ILE:C	1:B:500:ALA:H	2.26	0.43
1:B:555:GLY:O	1:B:558:LEU:HB2	2.19	0.43
1:B:134:HIS:HD2	1:B:138:SER:OG	2.01	0.43
1:B:88:PHE:CE2	1:B:92:LEU:HD21	2.54	0.42
1:A:388:HIS:N	1:A:389:PRO:CD	2.81	0.42
1:B:459:ARG:HG2	1:B:459:ARG:NH1	2.34	0.42
1:B:413:MET:HE3	1:B:413:MET:HB2	1.81	0.42
1:A:555:GLY:O	1:A:558:LEU:HB2	2.19	0.42
1:B:46:ILE:O	1:B:57:CYS:HA	2.20	0.42
1:B:204:HIS:ND1	1:B:292:PHE:CE2	2.88	0.42
1:A:88:PHE:CE2	1:A:92:LEU:HD21	2.54	0.42
1:B:481:LEU:HD11	1:B:510:GLU:HB2	2.01	0.42
1:A:197:MET:CE	1:A:423:VAL:HG13	2.49	0.42
1:A:91:PHE:CD1	1:A:95:HIS:CD2	3.08	0.42
1:A:501:LEU:HD21	1:A:506:GLY:HA2	2.02	0.42
1:B:91:PHE:CD1	1:B:95:HIS:CD2	3.08	0.42
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:LEU:O	1:B:449:VAL:HG23	2.19	0.42
1:A:46:ILE:O	1:A:57:CYS:HA	2.20	0.42
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.75	0.41
1:A:355:TYR:N	1:A:355:TYR:CD1	2.88	0.41
1:A:382:ASN:OD1	1:A:386:HIS:HE1	2.02	0.41
1:A:518:PHE:CG	1:A:522:MET:HG2	2.55	0.41
1:B:226:HIS:HB3	1:B:376:ARG:HA	2.02	0.41
1:A:185:ARG:HH21	1:A:438:ARG:HG2	1.86	0.41
1:A:226:HIS:HB3	1:A:376:ARG:HA	2.02	0.41
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.93	0.41
1:B:279:ILE:O	1:B:284:GLN:NE2	2.53	0.41
1:A:142:PHE:O	1:A:142:PHE:CG	2.71	0.41
1:B:501:LEU:HD21	1:B:506:GLY:HA2	2.02	0.41
1:B:518:PHE:CG	1:B:522:MET:HG2	2.55	0.41
1:B:55:TYR:CD1	1:B:55:TYR:C	2.98	0.41
1:B:155:VAL:O	1:B:459:ARG:NE	2.53	0.41
1:B:556:PHE:CD1	1:B:560:LYS:HD2	2.56	0.41
1:A:240:ARG:NH1	1:A:271:VAL:HG22	2.34	0.41
1:A:279:ILE:O	1:A:284:GLN:NE2	2.53	0.41
1:A:238:LEU:HD13	2:D:2:NAG:H62	2.02	0.41
1:A:344:VAL:O	1:A:348:TYR:HB3	2.21	0.41
1:B:190:ASP:HA	1:B:191:PRO:HD2	1.81	0.41
1:A:161:THR:HB	1:A:162:PRO:CD	2.50	0.41
1:A:413:MET:HE3	1:A:413:MET:HB2	1.82	0.41
1:A:504:TYR:HB3	1:A:505:PRO:HD3	2.03	0.41
1:A:556:PHE:CD1	1:A:560:LYS:HD2	2.56	0.41
1:B:142:PHE:O	1:B:142:PHE:CG	2.71	0.41
1:A:88:PHE:O	1:A:91:PHE:HB3	2.21	0.41
1:A:204:HIS:ND1	1:A:292:PHE:CE2	2.88	0.41
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.34	0.41
1:A:582:VAL:HG22	1:A:583:PRO:HD2	2.02	0.41
1:B:120:ARG:NH2	1:B:524:GLU:OE1	2.54	0.41
1:B:161:THR:HB	1:B:162:PRO:CD	2.50	0.41
1:B:180:ARG:NH1	1:B:490:GLU:OE1	2.54	0.41
1:B:582:VAL:HG22	1:B:583:PRO:HD2	2.02	0.41
1:B:232:HIS:ND1	1:B:232:HIS:N	2.68	0.41
1:B:355:TYR:N	1:B:355:TYR:CD1	2.87	0.41
1:A:154:SER:HB2	1:A:459:ARG:CB	2.48	0.40
1:B:88:PHE:O	1:B:92:LEU:HD13	2.22	0.40
1:A:45:GLY:HA3	1:A:69:CYS:SG	2.61	0.40
1:A:55:TYR:CD1	1:A:55:TYR:C	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:O	1:B:348:TYR:HB3	2.21	0.40
1:A:88:PHE:O	1:A:92:LEU:HD13	2.21	0.40
1:A:325:ASP:O	1:A:326:GLU:C	2.64	0.40
1:B:79:ARG:O	1:B:83:ARG:HG3	2.22	0.40
1:B:292:PHE:HA	1:B:298:LEU:HD23	2.03	0.40
1:B:433:ARG:HH11	1:B:433:ARG:CG	2.35	0.40
1:A:79:ARG:O	1:A:83:ARG:HG3	2.22	0.40
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.62	0.40
1:A:180:ARG:NH1	1:A:490:GLU:OE1	2.54	0.40
1:B:196:LEU:HD22	1:B:196:LEU:HA	1.97	0.40
1:B:325:ASP:O	1:B:326:GLU:C	2.64	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%)	490 (89%)	52 (10%)	7 (1%)	9	39
1	B	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	9	39
All	All	1098/1152 (95%)	980 (89%)	104 (10%)	14 (1%)	9	39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	LEU
1	A	514	PRO
1	B	295	LEU
1	B	514	PRO
1	A	387	TRP
1	B	387	TRP
1	A	292	PHE

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Mol	Chain	Res	Type
1	A	408	LEU
1	A	562	ALA
1	B	292	PHE
1	B	408	LEU
1	B	562	ALA
1	A	384	LEU
1	B	384	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%)	431 (89%)	55 (11%)	5	25
1	B	486/506 (96%)	431 (89%)	55 (11%)	5	25
All	All	972/1012 (96%)	862 (89%)	110 (11%)	5	25

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	52	LEU
1	A	65	SER
1	A	70	THR
1	A	117	LEU
1	A	120	ARG
1	A	126	SER
1	A	145	VAL
1	A	170	GLN
1	A	180	ARG
1	A	190	ASP
1	A	194	THR
1	A	196	LEU
1	A	215	LYS
1	A	216	MET
1	A	230	LEU

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Mol	Chain	Res	Type
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	251	LYS
1	A	289	GLN
1	A	294	LEU
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	352	LEU
1	A	374	ARG
1	A	376	ARG
1	A	385	TYR
1	A	389	PRO
1	A	400	GLN
1	A	405	GLU
1	A	433	ARG
1	A	455	SER
1	A	458	LEU
1	A	476	THR
1	A	479	GLN
1	A	484	GLU
1	A	513	HIS
1	A	514	PRO
1	A	518	PHE
1	A	523	ILE
1	A	530	SER
1	A	534	LEU
1	A	535	LEU
1	A	556	PHE
1	A	560	LYS
1	A	561	THR
1	A	564	LEU
1	A	574	THR
1	A	578	VAL
1	B	49	ARG
1	B	52	LEU
1	B	65	SER

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Mol	Chain	Res	Type
1	B	70	THR
1	B	117	LEU
1	B	120	ARG
1	B	126	SER
1	B	145	VAL
1	B	170	GLN
1	B	180	ARG
1	B	190	ASP
1	B	194	THR
1	B	196	LEU
1	B	215	LYS
1	B	216	MET
1	B	230	LEU
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	251	LYS
1	B	289	GLN
1	B	294	LEU
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	352	LEU
1	B	374	ARG
1	B	376	ARG
1	B	385	TYR
1	B	389	PRO
1	B	400	GLN
1	B	405	GLU
1	B	433	ARG
1	B	455	SER
1	B	458	LEU
1	B	476	THR
1	B	479	GLN
1	B	484	GLU
1	B	513	HIS
1	B	514	PRO
1	B	518	PHE

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Mol	Chain	Res	Type
1	B	523	ILE
1	B	530	SER
1	B	534	LEU
1	B	535	LEU
1	B	556	PHE
1	B	560	LYS
1	B	561	THR
1	B	564	LEU
1	B	574	THR
1	B	578	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	95	HIS
1	A	134	HIS
1	A	203	GLN
1	A	208	GLN
1	A	241	GLN
1	A	320	HIS
1	A	372	GLN
1	A	375	ASN
1	A	386	HIS
1	A	443	HIS
1	A	446	HIS
1	B	56	GLN
1	B	90	HIS
1	B	95	HIS
1	B	134	HIS
1	B	170	GLN
1	B	203	GLN
1	B	208	GLN
1	B	241	GLN
1	B	320	HIS
1	B	372	GLN
1	B	375	ASN
1	B	386	HIS
1	B	443	HIS
1	B	446	HIS

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	2,1	14,14,15	0.55	0	17,19,21	1.00	1 (5%)
2	NAG	C	2	2	14,14,15	0.71	0	17,19,21	0.97	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.55	0	17,19,21	0.99	1 (5%)
2	NAG	D	2	2	14,14,15	0.71	0	17,19,21	0.96	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C4-C3-C2	-2.34	107.59	111.02
2	D	2	NAG	C4-C3-C2	-2.32	107.62	111.02
2	C	1	NAG	C2-N2-C7	-2.14	120.04	122.90
2	D	1	NAG	C2-N2-C7	-2.11	120.07	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

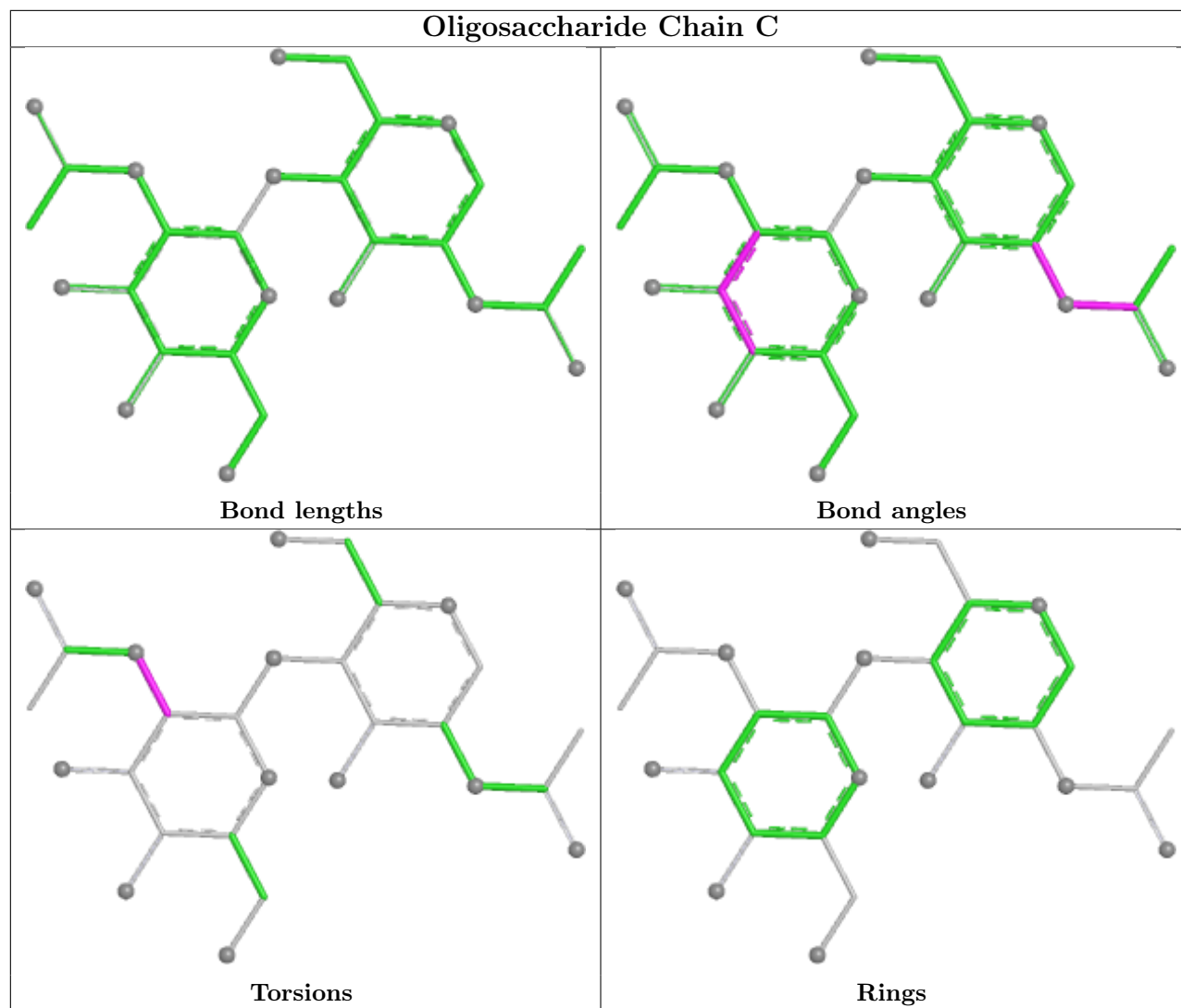
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7

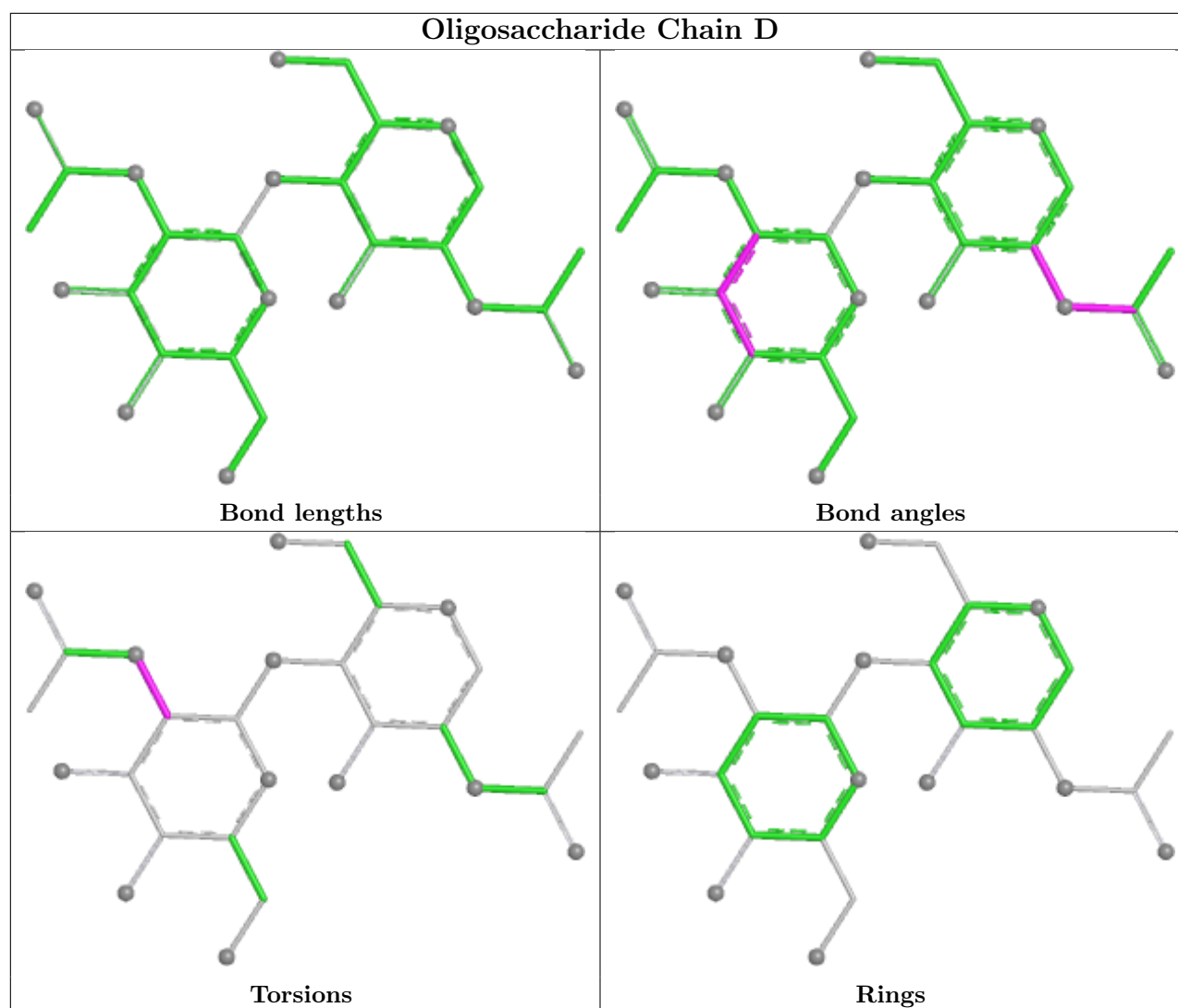
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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.





5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
5	HEM	B	601	1	50,50,50	1.51	6 (12%)	67,82,82	1.42	10 (14%)
6	ISF	B	800	-	20,20,20	1.94	6 (30%)	28,28,28	1.36	3 (10%)
6	ISF	A	800	-	20,20,20	1.95	6 (30%)	28,28,28	1.36	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	661	1	14,14,15	0.52	0	17,19,21	0.93	1 (5%)
3	NAG	B	661	1	14,14,15	0.52	0	17,19,21	0.93	1 (5%)
4	BOG	A	702	-	20,20,20	1.02	1 (5%)	25,25,25	1.28	4 (16%)
4	BOG	B	702	-	20,20,20	1.02	1 (5%)	25,25,25	1.28	4 (16%)
5	HEM	A	601	1	50,50,50	1.51	6 (12%)	67,82,82	1.42	10 (14%)
3	NAG	A	681	1	14,14,15	0.50	0	17,19,21	1.17	2 (11%)
3	NAG	B	681	1	14,14,15	0.51	0	17,19,21	1.17	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
5	HEM	B	601	1	-	5/14/54/54	-
6	ISF	B	800	-	-	0/16/16/16	0/2/2/2
6	ISF	A	800	-	-	0/16/16/16	0/2/2/2
3	NAG	A	661	1	-	0/6/23/26	0/1/1/1
3	NAG	B	661	1	-	0/6/23/26	0/1/1/1
4	BOG	A	702	-	-	3/11/31/31	0/1/1/1
4	BOG	B	702	-	-	3/11/31/31	0/1/1/1
5	HEM	A	601	1	-	5/14/54/54	-
3	NAG	A	681	1	-	0/6/23/26	0/1/1/1
3	NAG	B	681	1	-	0/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	800	ISF	C2-C6	-4.54	1.38	1.47
6	B	800	ISF	C2-C6	-4.52	1.38	1.47
6	A	800	ISF	C4-C5	3.93	1.43	1.36
6	B	800	ISF	C4-C5	3.91	1.43	1.36
5	B	601	HEM	C3B-C4B	3.65	1.52	1.44
5	A	601	HEM	C3B-C4B	3.63	1.52	1.44
5	A	601	HEM	CAC-C3C	-3.35	1.38	1.47
5	B	601	HEM	CAC-C3C	-3.33	1.38	1.47
6	A	800	ISF	C2-S1	-3.18	1.67	1.73
6	B	800	ISF	C2-S1	-3.17	1.67	1.73
5	B	601	HEM	CBB-CAB	3.17	1.45	1.30
5	A	601	HEM	CBB-CAB	3.16	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	BOG	C4-C5	3.10	1.59	1.53
4	A	702	BOG	C4-C5	3.08	1.59	1.53
5	A	601	HEM	CBC-CAC	2.81	1.43	1.30
5	B	601	HEM	CBC-CAC	2.81	1.43	1.30
5	B	601	HEM	C2A-C3A	-2.76	1.31	1.38
5	A	601	HEM	C2A-C3A	-2.74	1.31	1.38
6	A	800	ISF	C5-S1	-2.67	1.68	1.73
6	B	800	ISF	C5-S1	-2.61	1.68	1.73
5	B	601	HEM	CAB-C3B	-2.57	1.40	1.47
5	A	601	HEM	CAB-C3B	-2.56	1.40	1.47
6	B	800	ISF	C8-C6	-2.36	1.44	1.49
6	A	800	ISF	C8-C6	-2.36	1.44	1.49
6	B	800	ISF	C5-I1	-2.21	2.04	2.08
6	A	800	ISF	C5-I1	-2.19	2.04	2.08

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	800	ISF	C3-C2-S1	3.79	116.01	110.49
6	A	800	ISF	C3-C2-S1	3.76	115.96	110.49
6	B	800	ISF	C3-C2-C6	-3.22	122.94	129.60
5	A	601	HEM	CAD-C3D-C4D	3.22	130.31	124.70
5	B	601	HEM	CAD-C3D-C4D	3.22	130.31	124.70
6	A	800	ISF	C3-C2-C6	-3.21	122.97	129.60
6	B	800	ISF	C4-C3-C2	-3.08	108.16	113.37
6	A	800	ISF	C4-C3-C2	-3.06	108.18	113.37
4	A	702	BOG	O5-C5-C4	3.06	115.21	109.70
5	B	601	HEM	C2B-C1B-NB	3.06	113.36	109.84
5	A	601	HEM	C2B-C1B-NB	3.05	113.35	109.84
4	B	702	BOG	O5-C5-C4	3.05	115.19	109.70
3	B	681	NAG	C2-N2-C7	-2.97	118.92	122.90
3	A	681	NAG	C2-N2-C7	-2.97	118.92	122.90
4	A	702	BOG	C3-C4-C5	2.62	114.98	110.23
4	B	702	BOG	C3-C4-C5	2.60	114.95	110.23
5	B	601	HEM	C4D-ND-C1D	-2.56	102.18	105.21
5	A	601	HEM	CAA-C2A-C1A	2.54	129.91	124.94
5	B	601	HEM	CAA-C2A-C1A	2.54	129.90	124.94
5	B	601	HEM	C3D-C4D-ND	2.53	112.95	110.17
5	A	601	HEM	C4D-ND-C1D	-2.53	102.21	105.21
5	A	601	HEM	C3B-C4B-NB	2.53	111.28	109.47
5	A	601	HEM	C3D-C4D-ND	2.51	112.93	110.17
5	B	601	HEM	C3B-C4B-NB	2.51	111.27	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	661	NAG	C2-N2-C7	-2.50	119.55	122.90
3	A	661	NAG	C2-N2-C7	-2.48	119.58	122.90
4	A	702	BOG	C1'-O1-C1	2.41	117.79	113.68
4	B	702	BOG	C1'-O1-C1	2.40	117.78	113.68
3	B	681	NAG	C6-C5-C4	2.39	118.89	113.02
5	A	601	HEM	CHC-C4B-NB	-2.38	121.87	124.42
3	A	681	NAG	C6-C5-C4	2.37	118.85	113.02
5	B	601	HEM	CHC-C4B-NB	-2.37	121.87	124.42
5	B	601	HEM	CHA-C4D-ND	-2.26	121.57	124.37
5	A	601	HEM	CMC-C2C-C3C	-2.26	122.97	128.43
5	B	601	HEM	CMC-C2C-C3C	-2.25	122.99	128.43
5	A	601	HEM	CHA-C4D-ND	-2.24	121.60	124.37
4	B	702	BOG	C1-C2-C3	-2.23	105.33	110.01
4	A	702	BOG	C1-C2-C3	-2.22	105.35	110.01
5	B	601	HEM	C3C-C2C-C1C	2.18	109.11	107.05
5	A	601	HEM	C3C-C2C-C1C	2.18	109.11	107.05

There are no chirality outliers.

All (16) torsion outliers are listed below:

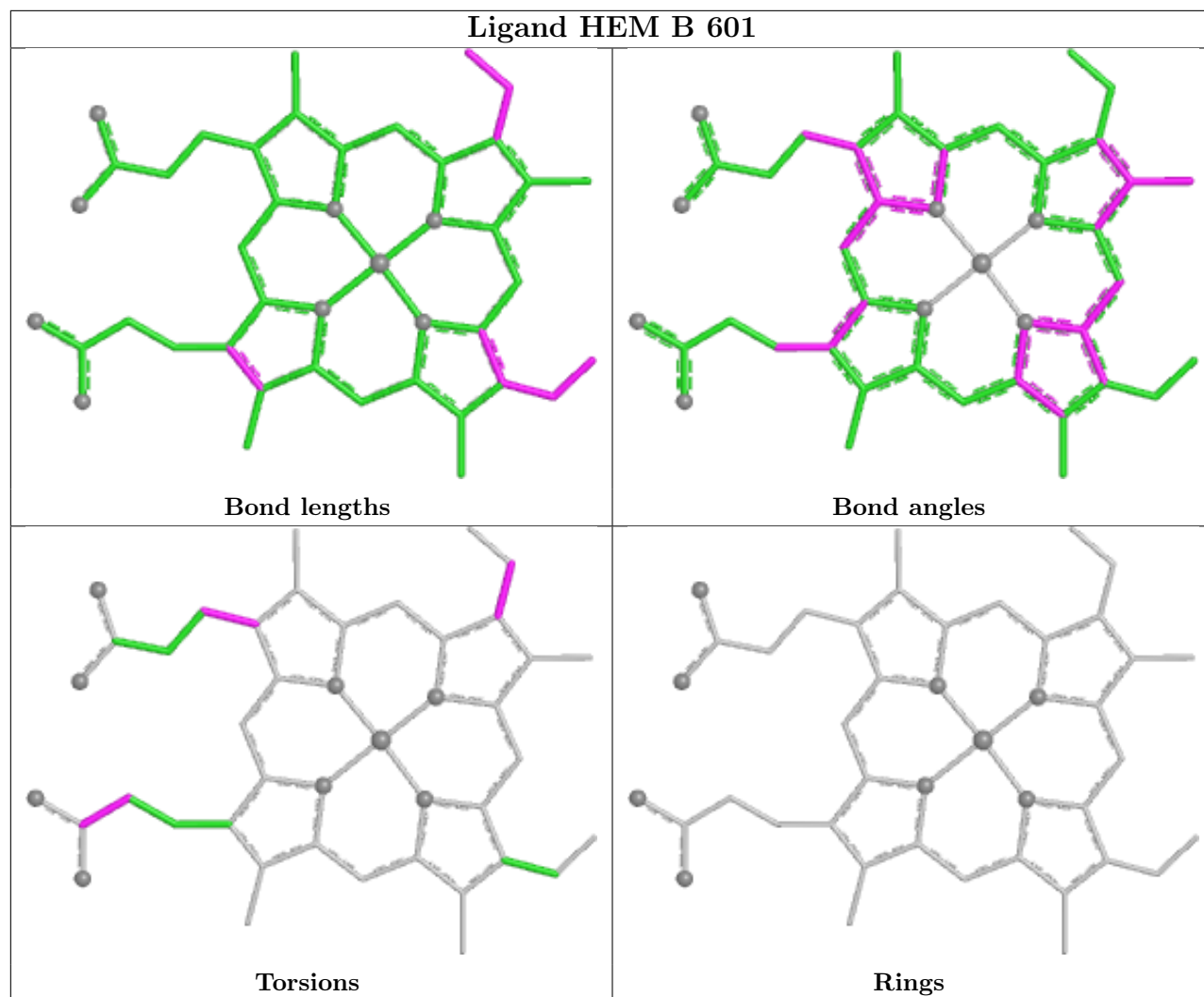
Mol	Chain	Res	Type	Atoms
5	A	601	HEM	C2C-C3C-CAC-CBC
5	A	601	HEM	C4C-C3C-CAC-CBC
5	B	601	HEM	C2C-C3C-CAC-CBC
5	B	601	HEM	C4C-C3C-CAC-CBC
4	A	702	BOG	O5-C1-O1-C1'
4	B	702	BOG	O5-C1-O1-C1'
4	A	702	BOG	C2-C1-O1-C1'
4	B	702	BOG	C2-C1-O1-C1'
4	A	702	BOG	C2'-C1'-O1-C1
4	B	702	BOG	C2'-C1'-O1-C1
5	A	601	HEM	C4D-C3D-CAD-CBD
5	B	601	HEM	C4D-C3D-CAD-CBD
5	B	601	HEM	CAA-CBA-CGA-O1A
5	A	601	HEM	CAA-CBA-CGA-O1A
5	A	601	HEM	CAA-CBA-CGA-O2A
5	B	601	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

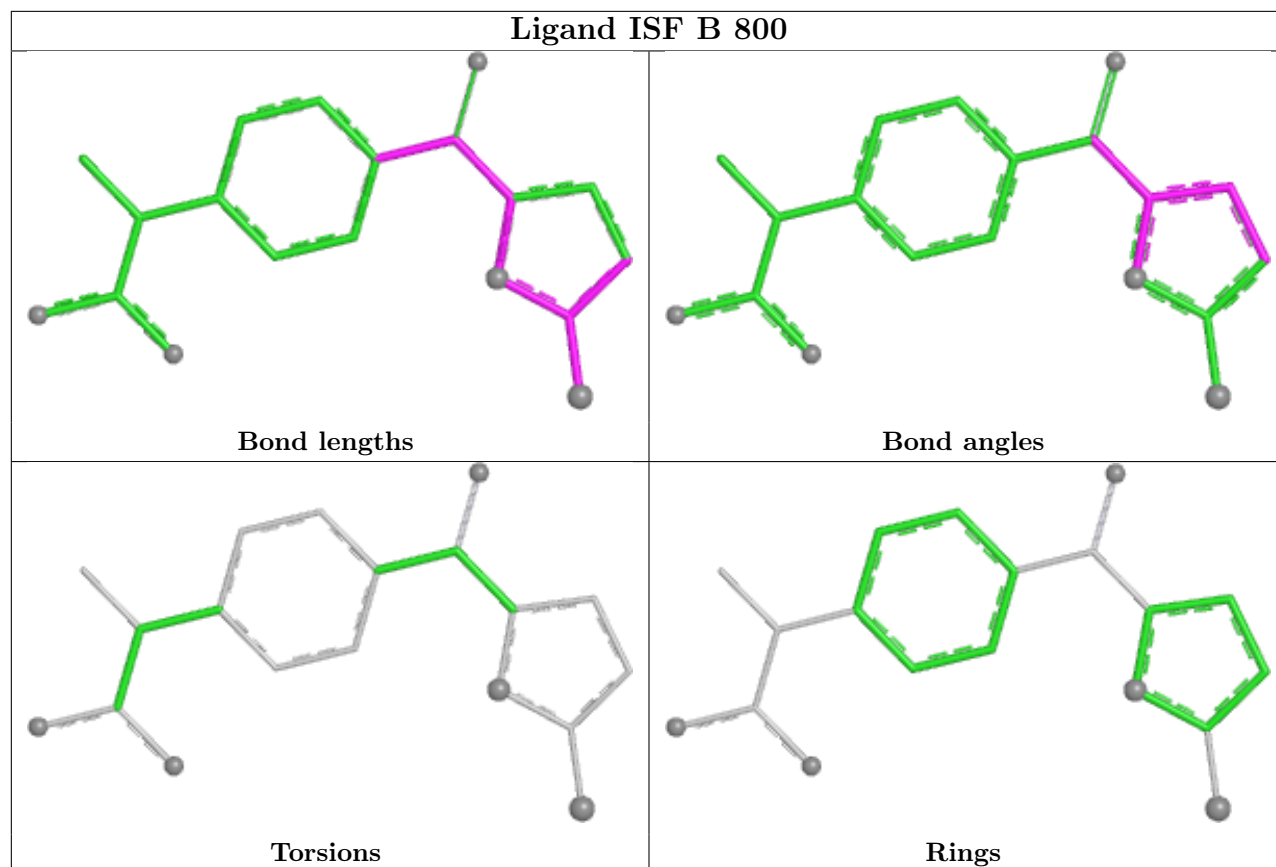
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	HEM	3	0
6	B	800	ISF	4	0
6	A	800	ISF	4	0
4	A	702	BOG	1	0
4	B	702	BOG	1	0
5	A	601	HEM	3	0

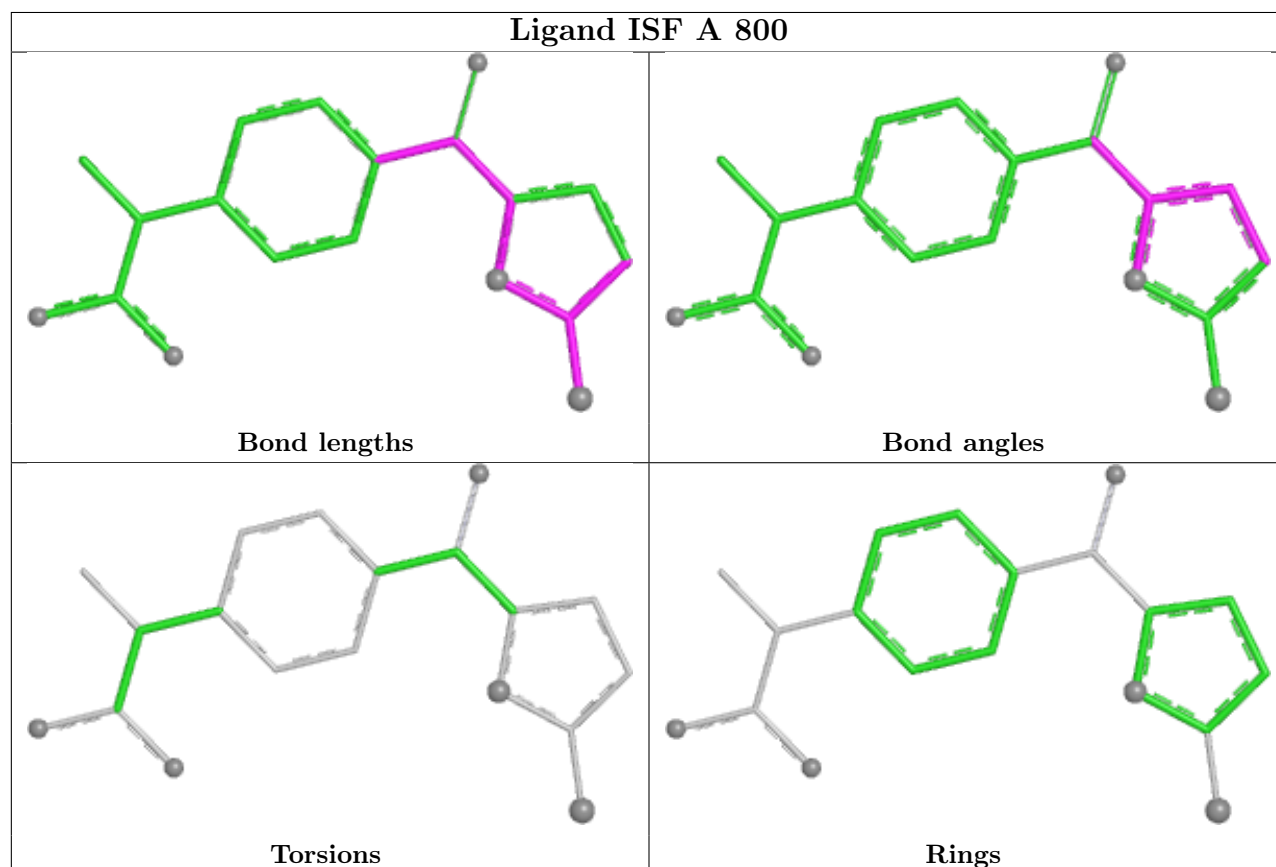
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

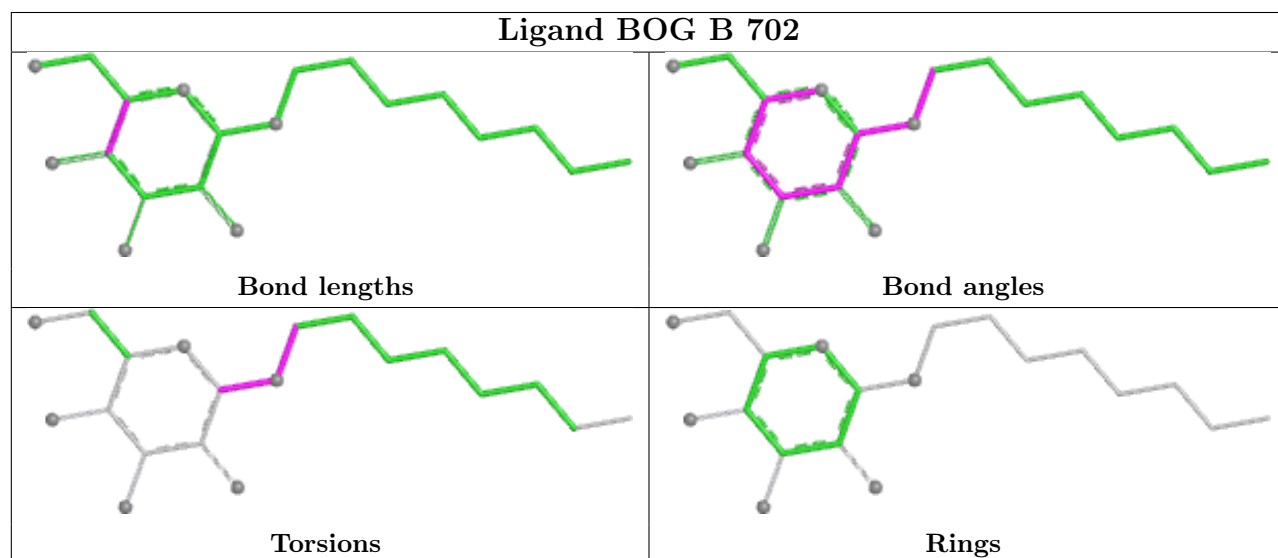
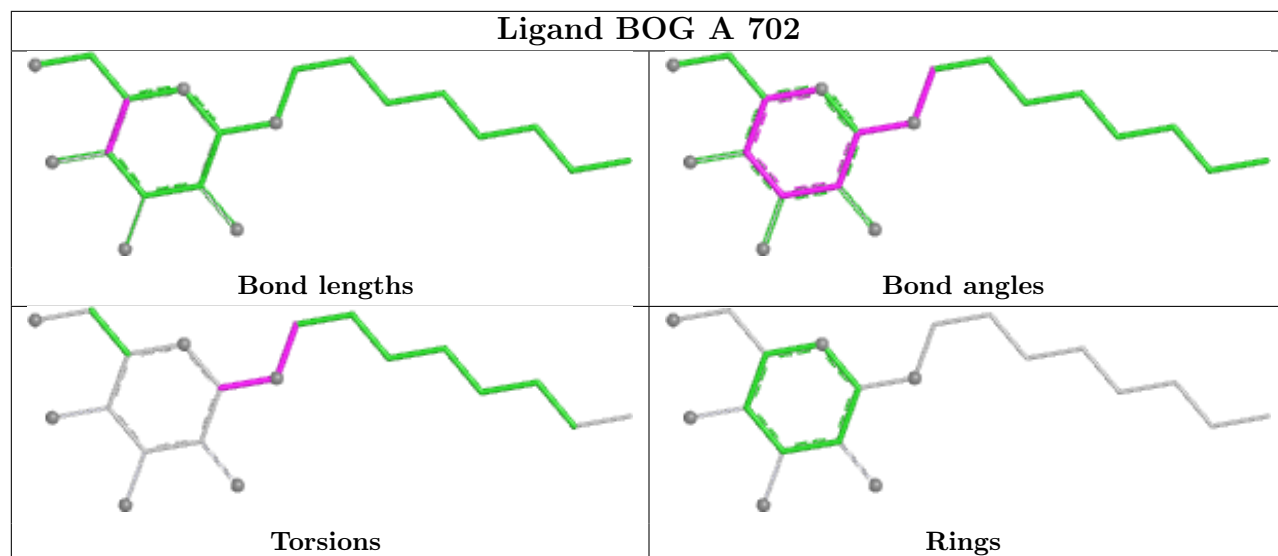


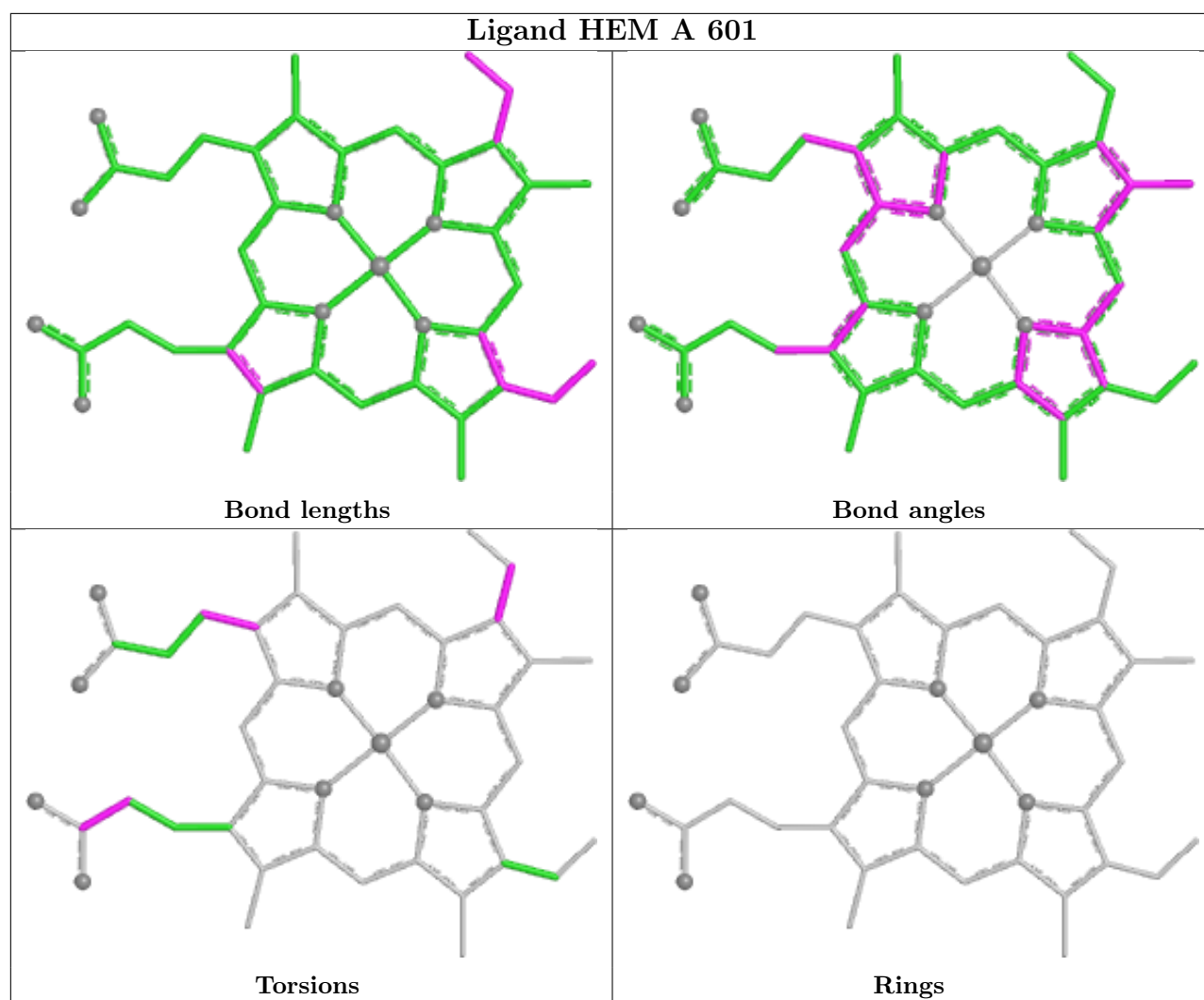
Ligand ISF B 800



Ligand ISF A 800







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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/576 (95%)	-0.34	1 (0%) 91 82	4, 18, 53, 91	0
1	B	551/576 (95%)	-0.28	1 (0%) 91 82	4, 18, 53, 91	0
All	All	1102/1152 (95%)	-0.31	2 (0%) 91 82	4, 18, 53, 91	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	PRO	2.8
1	A	280	PRO	2.7

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

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

6.3 Carbohydrates [i](#)

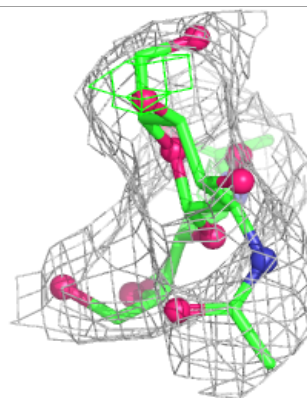
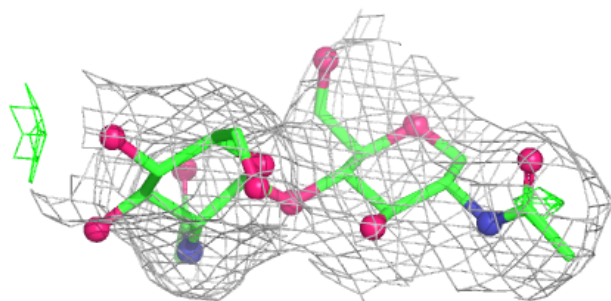
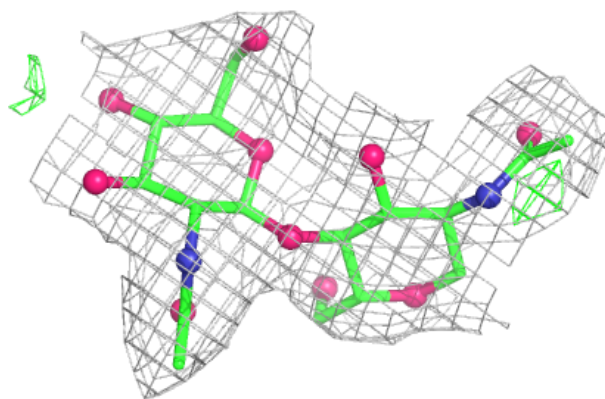
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.89	0.11	19,37,47,59	0
2	NAG	C	2	14/15	0.93	0.08	19,37,47,59	0
2	NAG	C	1	14/15	0.94	0.10	4,22,31,34	0
2	NAG	D	1	14/15	0.96	0.11	4,22,31,34	0

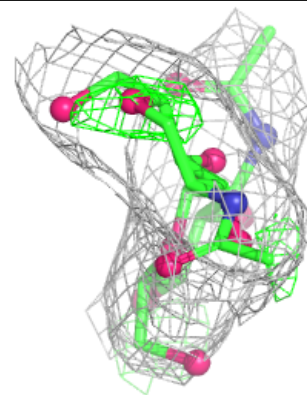
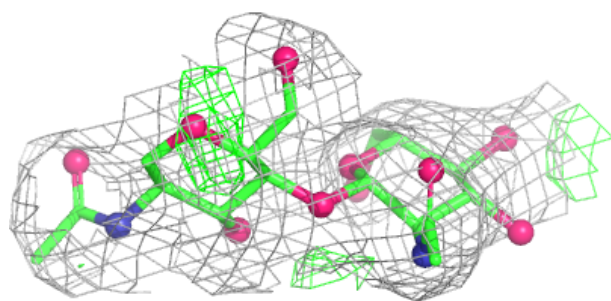
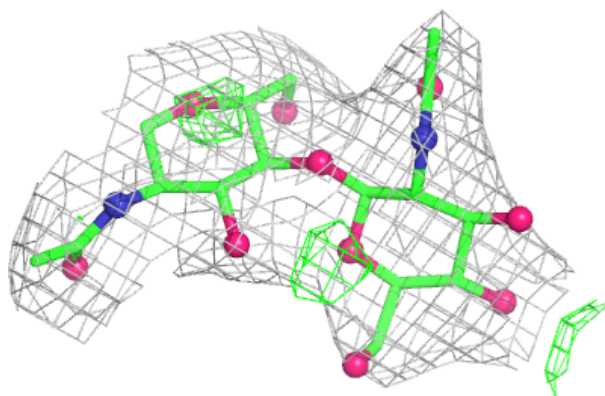
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands

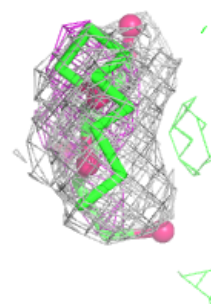
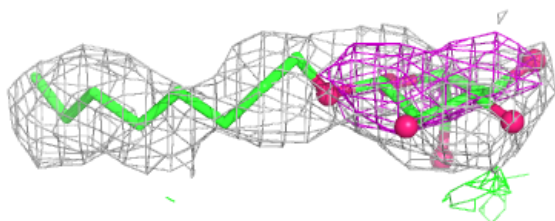
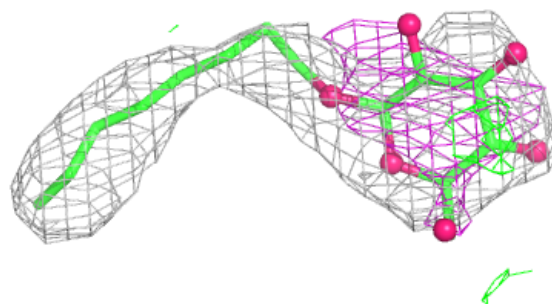
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	661	14/15	0.84	0.11	33,43,61,66	0
4	BOG	B	702	20/20	0.84	0.19	15,15,15,15	0
4	BOG	A	702	20/20	0.85	0.15	15,15,15,15	0
3	NAG	A	661	14/15	0.85	0.12	33,43,61,66	0
3	NAG	A	681	14/15	0.88	0.14	15,22,38,44	0
3	NAG	B	681	14/15	0.90	0.13	15,22,38,44	0
5	HEM	A	601	43/43	0.97	0.08	7,17,43,67	0
5	HEM	B	601	43/43	0.97	0.09	7,17,43,67	0
6	ISF	A	800	19/19	0.99	0.07	15,15,15,15	0
6	ISF	B	800	19/19	0.99	0.06	15,15,15,15	0

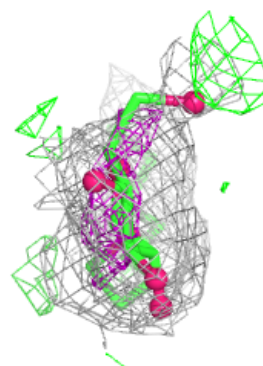
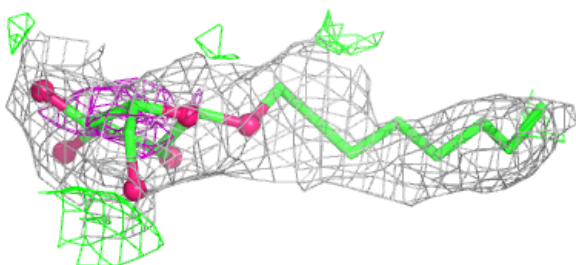
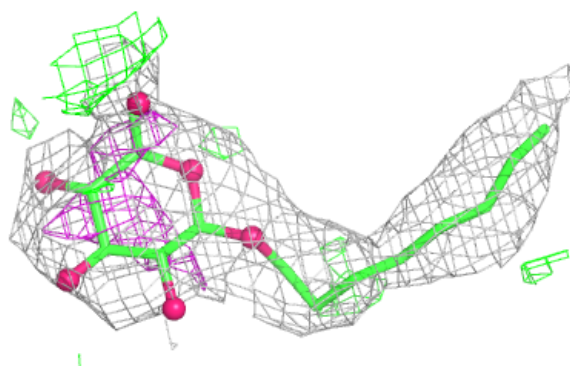
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BOG B 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

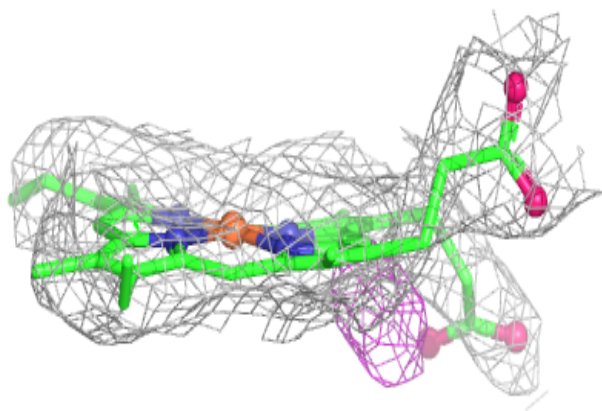
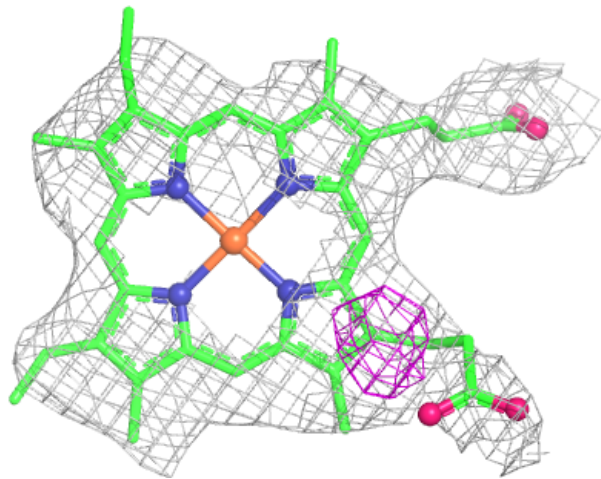
**Electron density around BOG A 702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



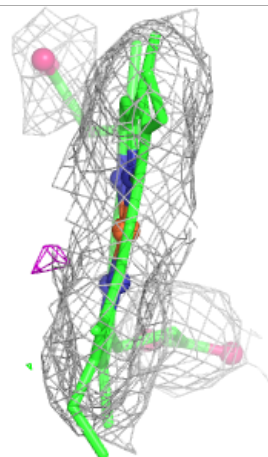
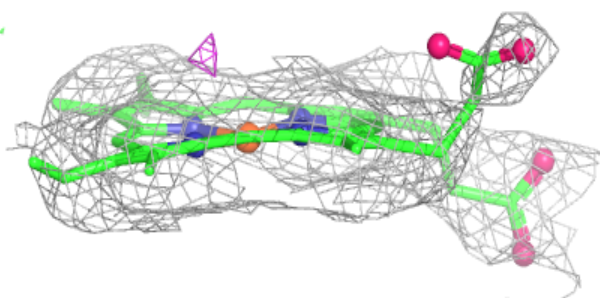
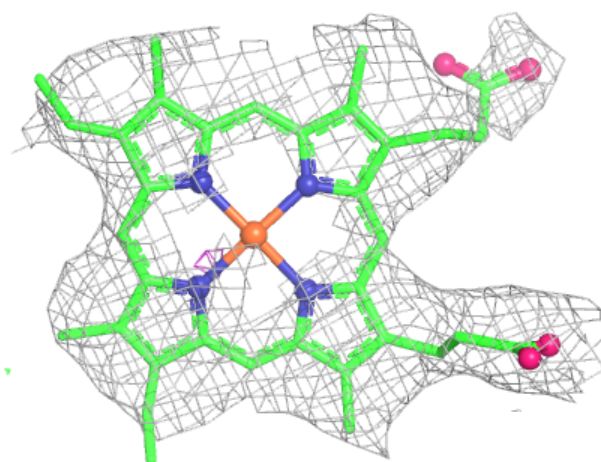
Electron density around HEM A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



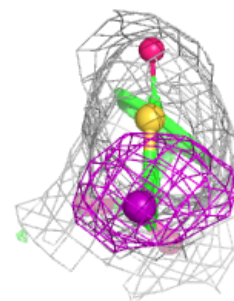
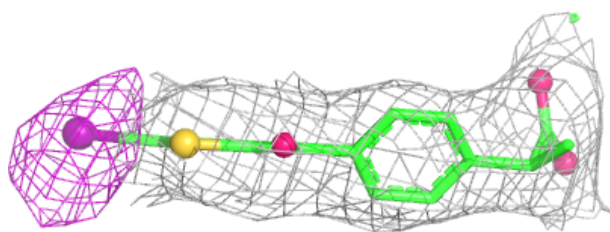
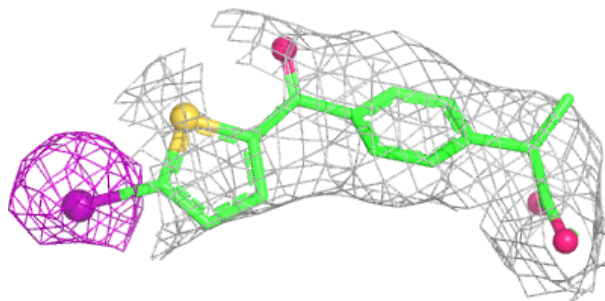
Electron density around HEM B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

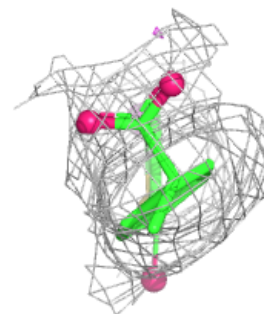
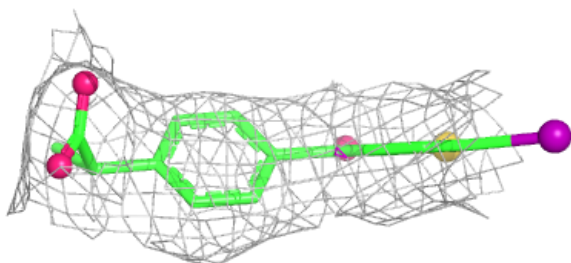
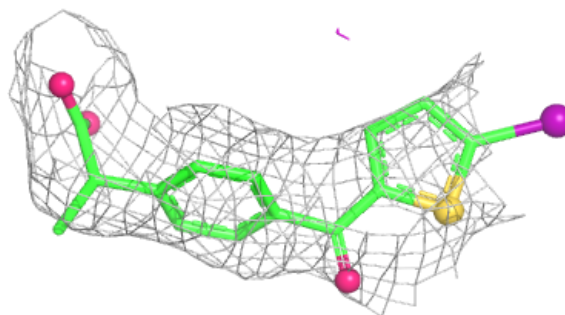


Electron density around ISF A 800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ISF B 800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.