



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:25 AM BST

PDB ID : 3Q7D
Title : Structure of (R)-naproxen bound to mCOX-2.
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Carter, B.D.; Banerjee, S.; Marnett, L.J.
Deposited on : 2011-01-04
Resolution : 2.40 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

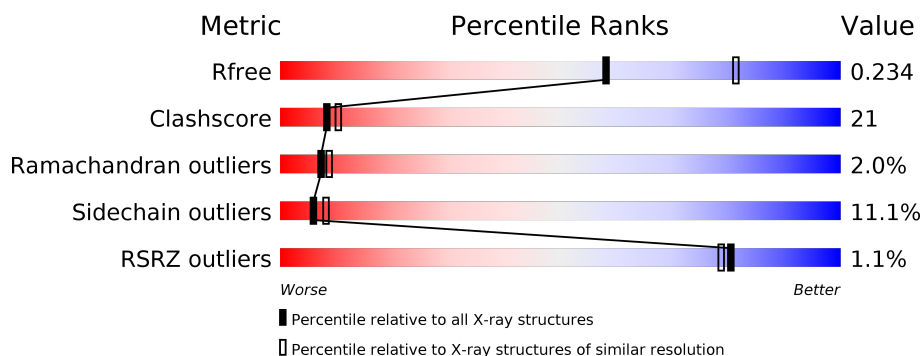
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	587	<div> <div></div> <div> <div></div> <div>65%</div> <div>23%</div> <div>5%</div> <div>6%</div> </div> </div>
1	B	587	<div> <div></div> <div> <div></div> <div>60%</div> <div>28%</div> <div>5%</div> <div>6%</div> </div> </div>

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
2	NAG	A	671	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9880 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 G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



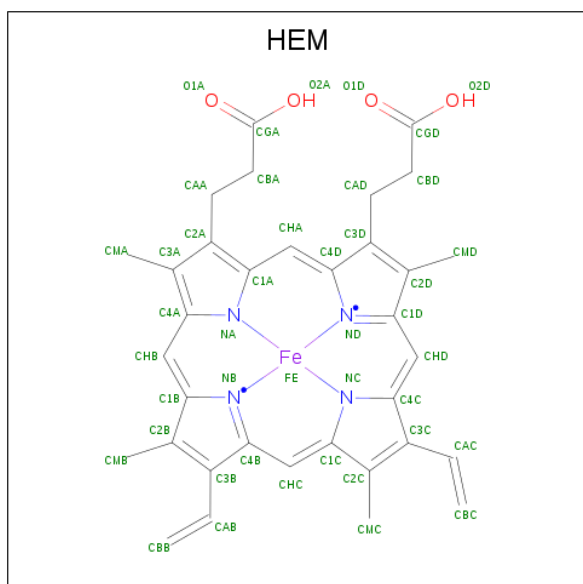
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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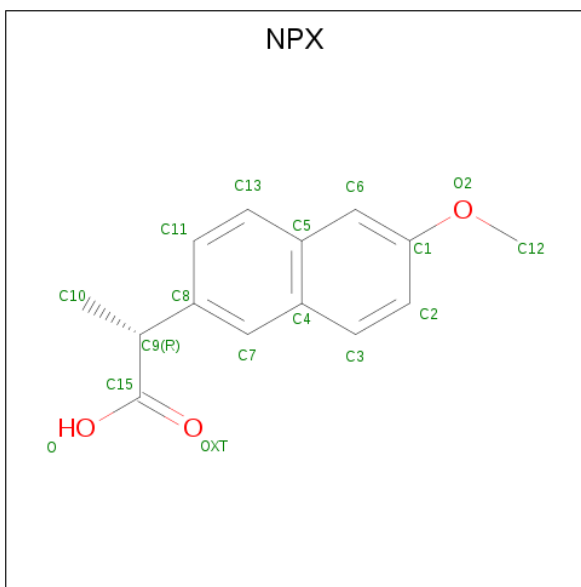
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



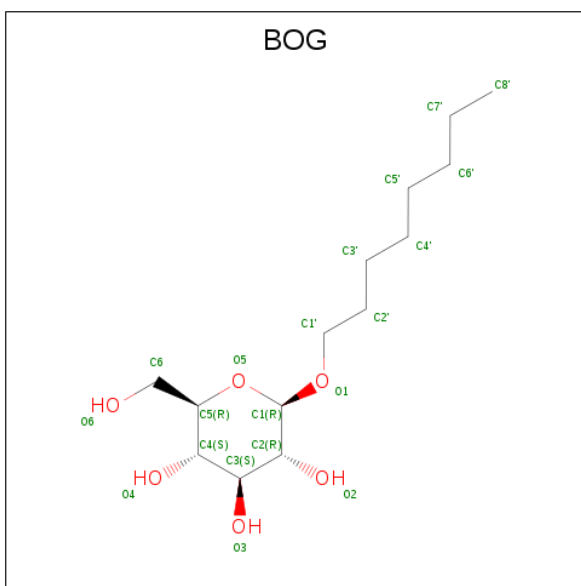
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is (2R)-2-(6-methoxynaphthalen-2-yl)propanoic acid (three-letter code: NPX) (formula: C₁₄H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	14	3		
4	B	1	Total	C	O	0	0
			17	14	3		

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

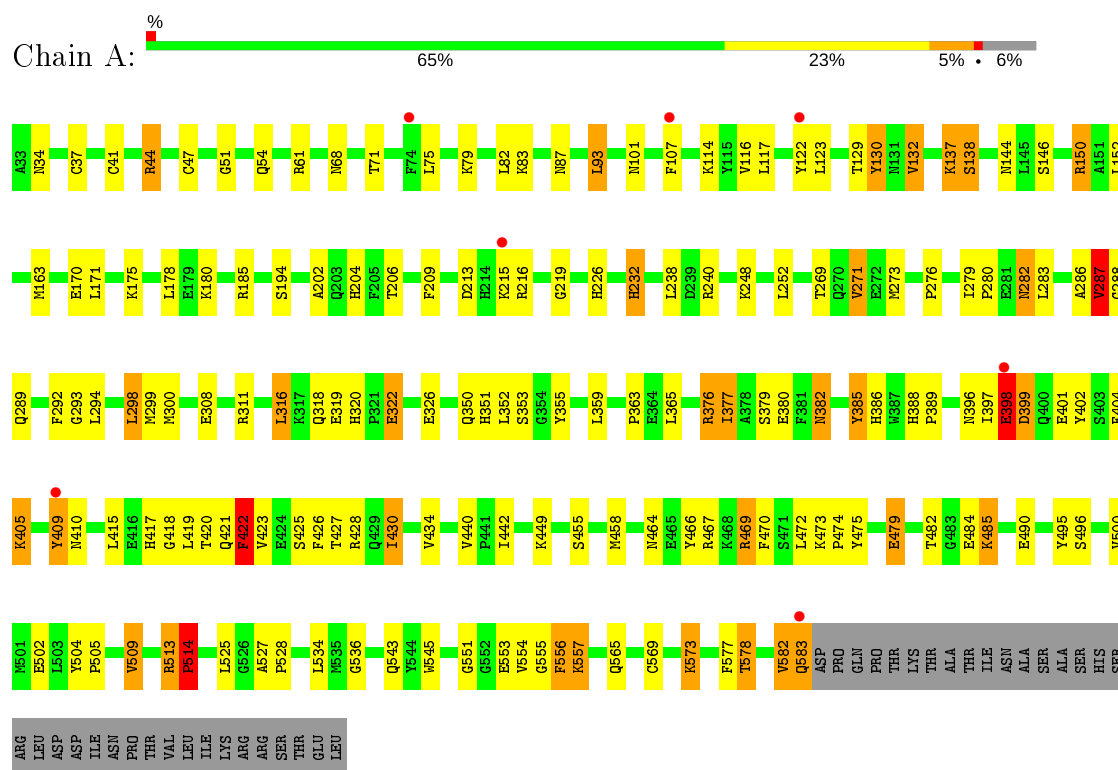
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	309	Total	O	0	0
			309	309		
7	B	289	Total	O	0	0
			289	289		

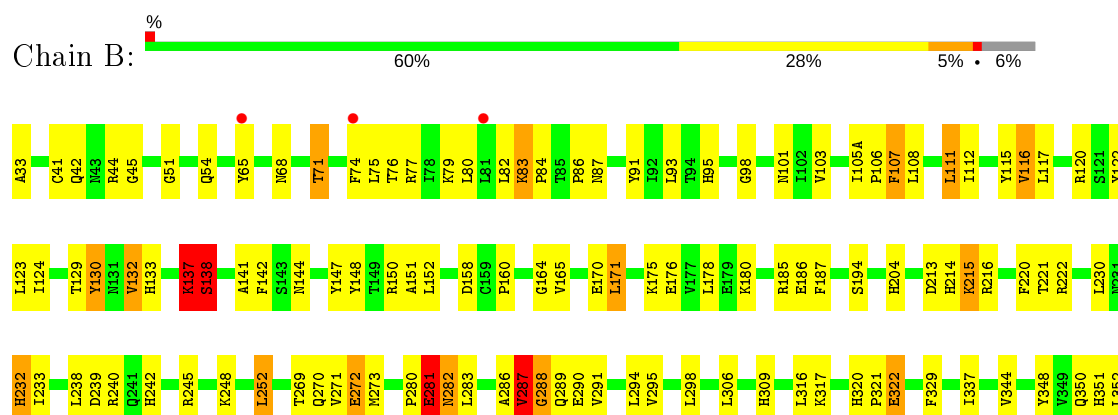
3 Residue-property plots

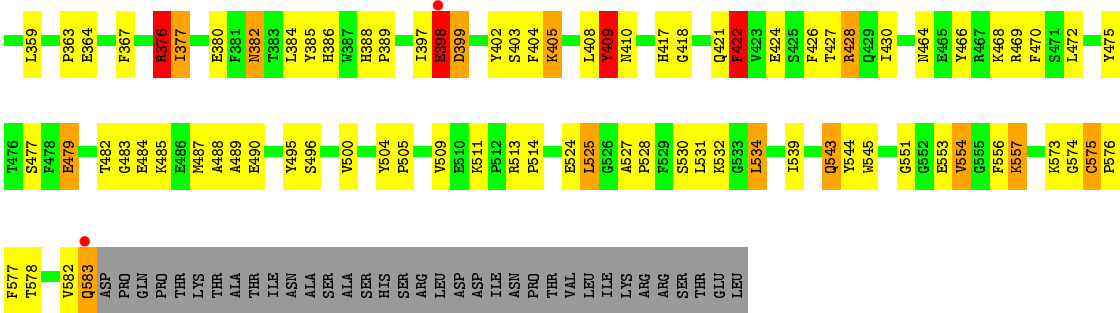
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 G/H synthase 2



• Molecule 1: Prostaglandin G/H synthase 2





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.73Å 133.03Å 181.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.40 29.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.59-2.40) 99.4 (29.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.177 , 0.233 0.179 , 0.234	Depositor DCC
R_{free} test set	3324 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9880	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: NPX, HEM, BOG, NAG, CL

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	0.42	0/4601	0.63	3/6239 (0.0%)
1	B	0.42	0/4601	0.62	2/6239 (0.0%)
All	All	0.42	0/9202	0.63	5/12478 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	376	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	287	VAL	N-CA-C	5.23	125.11	111.00
1	B	287	VAL	N-CA-C	5.03	124.59	111.00
1	A	137	LYS	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	288	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4376	171	0
1	B	4474	0	4376	209	0
2	A	56	0	52	12	0
2	B	56	0	52	10	0
3	A	43	0	30	4	0
3	B	43	0	30	5	0
4	A	17	0	13	1	0
4	B	17	0	13	0	0
5	A	60	0	84	6	0
5	B	40	0	56	5	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	309	0	0	36	0
7	B	289	0	0	51	0
All	All	9880	0	9082	386	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 (386) 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:144:ASN:HD21	2:B:671:NAG:C1	1.31	1.44
1:B:150:ARG:HB2	7:B:829:HOH:O	1.40	1.19
1:A:144:ASN:HD21	2:A:671:NAG:C1	1.57	1.16
1:B:294:LEU:HD22	1:B:409:TYR:HB3	1.26	1.11
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.12	1.11
1:A:185:ARG:HH12	5:A:3:BOG:H5'2	1.17	1.10
1:A:377:ILE:HB	7:A:677:HOH:O	1.48	1.09
1:B:144:ASN:ND2	2:B:671:NAG:C1	2.16	1.07
1:A:68:ASN:HD21	2:A:661:NAG:C1	1.68	1.06
1:B:421:GLN:O	1:B:422:PHE:HB2	1.53	1.06
1:B:322:GLU:HG3	7:B:722:HOH:O	1.52	1.06
1:A:150:ARG:HG2	1:A:150:ARG:HH11	1.20	1.05
1:A:185:ARG:NH1	5:A:3:BOG:H5'2	1.71	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLN:O	1:A:422:PHE:HB2	1.61	0.98
1:A:319:GLU:HG3	1:A:554:VAL:HG11	1.48	0.95
1:A:144:ASN:ND2	2:A:671:NAG:C1	2.30	0.94
1:A:150:ARG:HH11	1:A:150:ARG:CG	1.82	0.93
1:B:68:ASN:HD21	2:B:661:NAG:C1	1.84	0.91
1:A:350:GLN:HE22	1:A:359:LEU:H	1.18	0.91
1:B:294:LEU:CD2	1:B:409:TYR:HB3	2.01	0.90
1:B:410:ASN:HD21	2:B:681:NAG:C1	1.85	0.89
1:B:41:CYS:HB3	7:B:832:HOH:O	1.71	0.88
1:A:440:VAL:HG13	7:A:747:HOH:O	1.73	0.88
1:B:281:GLU:O	1:B:283:LEU:N	2.07	0.88
1:B:130:TYR:N	7:B:869:HOH:O	2.07	0.86
1:A:130:TYR:N	7:A:751:HOH:O	2.09	0.86
1:B:398:GLU:O	1:B:399:ASP:HB2	1.74	0.85
1:A:138:SER:N	7:A:908:HOH:O	2.10	0.84
1:B:138:SER:N	7:B:756:HOH:O	2.03	0.84
1:A:68:ASN:ND2	2:A:661:NAG:C1	2.42	0.83
1:A:294:LEU:HD22	1:A:409:TYR:HD2	1.43	0.82
1:A:185:ARG:CZ	7:A:801:HOH:O	2.27	0.82
1:B:350:GLN:HE22	1:B:359:LEU:H	1.28	0.82
1:B:87:ASN:HD22	5:B:620:BOG:H62	1.45	0.81
1:A:150:ARG:HG2	1:A:150:ARG:NH1	1.80	0.80
1:B:150:ARG:CG	1:B:152:LEU:O	2.30	0.80
1:A:479:GLU:HB3	1:A:485:LYS:HZ2	1.47	0.78
1:B:294:LEU:HD22	1:B:409:TYR:CB	2.08	0.78
3:B:682:HEM:HMB2	3:B:682:HEM:HBB2	1.66	0.78
1:A:144:ASN:HD21	2:A:671:NAG:C2	1.97	0.77
1:A:553:GLU:HG3	1:A:557:LYS:NZ	1.99	0.77
1:B:215:LYS:NZ	1:B:222:ARG:HH21	1.83	0.76
1:A:44:ARG:HG2	1:A:44:ARG:NH1	1.89	0.76
1:A:557:LYS:HE2	7:A:713:HOH:O	1.85	0.75
1:B:410:ASN:ND2	2:B:681:NAG:C1	2.48	0.75
1:B:306:LEU:HD23	1:B:306:LEU:C	2.07	0.75
1:A:194:SER:OG	1:A:351:HIS:HE1	1.69	0.75
1:A:554:VAL:HG12	7:A:849:HOH:O	1.87	0.74
1:B:245:ARG:HD2	7:B:4:HOH:O	1.87	0.74
1:B:294:LEU:HD22	1:B:409:TYR:CD2	2.23	0.74
1:A:226:HIS:HA	1:A:377:ILE:CD1	2.18	0.74
1:B:215:LYS:HD3	1:B:215:LYS:N	2.03	0.73
1:B:214:HIS:HD2	7:B:809:HOH:O	1.72	0.73
1:A:410:ASN:HD21	2:A:681:NAG:C1	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:VAL:HG13	7:B:713:HOH:O	1.89	0.72
1:A:464:ASN:HD21	1:A:475:TYR:H	1.38	0.72
1:A:180:LYS:HD3	1:A:490:GLU:HG3	1.71	0.70
1:B:83:LYS:HA	1:B:83:LYS:HE3	1.72	0.70
1:B:112:ILE:HG13	7:B:833:HOH:O	1.90	0.70
1:B:269:THR:OG1	1:B:271:VAL:HG13	1.90	0.70
1:B:288:GLY:HA3	7:B:825:HOH:O	1.90	0.70
1:A:129:THR:C	7:A:751:HOH:O	2.30	0.69
1:A:405:LYS:HE3	1:A:405:LYS:H	1.55	0.69
3:B:682:HEM:HBC2	3:B:682:HEM:HHD	1.74	0.69
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.75	0.69
1:B:215:LYS:H	1:B:215:LYS:HD3	1.58	0.68
1:A:213:ASP:OD1	1:A:215:LYS:HE2	1.92	0.68
1:A:209:PHE:HB2	1:A:377:ILE:HD12	1.75	0.68
1:B:213:ASP:OD1	1:B:215:LYS:HE2	1.93	0.68
1:A:556:PHE:HB3	1:A:557:LYS:HE3	1.76	0.68
1:A:479:GLU:HB3	1:A:485:LYS:NZ	2.09	0.68
1:B:150:ARG:HG3	1:B:152:LEU:O	1.91	0.68
1:B:294:LEU:HD22	1:B:409:TYR:HD2	1.59	0.68
1:B:294:LEU:HG	7:B:782:HOH:O	1.93	0.68
1:B:150:ARG:NE	7:B:829:HOH:O	2.26	0.68
1:B:240:ARG:HH21	1:B:288:GLY:HA2	1.59	0.68
1:A:150:ARG:NH2	1:A:458:MET:O	2.26	0.67
1:B:91:TYR:O	1:B:95:HIS:HD2	1.77	0.67
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.76	0.67
1:B:317:LYS:HD2	7:B:24:HOH:O	1.93	0.67
3:A:682:HEM:HMB2	3:A:682:HEM:HBB2	1.77	0.67
1:B:479:GLU:HB3	1:B:485:LYS:HZ3	1.59	0.67
1:B:105(A):ILE:HD12	1:B:108:LEU:HD12	1.78	0.66
1:B:479:GLU:HB3	1:B:485:LYS:NZ	2.10	0.66
1:B:288:GLY:C	7:B:825:HOH:O	2.34	0.66
1:A:382:ASN:HD21	3:A:682:HEM:HAD2	1.61	0.65
1:B:215:LYS:H	1:B:215:LYS:CD	2.10	0.65
1:B:194:SER:OG	1:B:351:HIS:HE1	1.78	0.65
1:B:115:TYR:HE2	5:B:3:BOG:H3'1	1.61	0.65
1:A:51:GLY:O	1:B:322:GLU:HG2	1.96	0.65
1:B:129:THR:C	7:B:869:HOH:O	2.34	0.65
1:B:320:HIS:HE1	1:B:551:GLY:O	1.79	0.65
1:B:150:ARG:HG2	1:B:152:LEU:O	1.97	0.65
1:A:226:HIS:HA	1:A:377:ILE:HD13	1.77	0.65
1:A:583:GLN:HB3	7:A:876:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HB2	7:A:810:HOH:O	1.96	0.64
1:B:216:ARG:HG2	1:B:220:PHE:CD1	2.32	0.64
1:B:273:MET:SD	1:B:286:ALA:O	2.54	0.64
1:A:536:GLY:C	7:A:809:HOH:O	2.35	0.64
1:B:240:ARG:NH2	1:B:288:GLY:HA2	2.12	0.64
1:B:288:GLY:CA	7:B:825:HOH:O	2.46	0.64
1:B:75:LEU:HD22	1:B:79:LYS:HE2	1.79	0.64
1:B:83:LYS:HG2	7:B:878:HOH:O	1.98	0.63
1:B:418:GLY:O	1:B:421:GLN:O	2.16	0.63
1:A:287:VAL:HA	7:A:673:HOH:O	1.98	0.63
1:B:204:HIS:HD2	7:B:2:HOH:O	1.82	0.62
1:B:295:VAL:HG13	7:B:811:HOH:O	1.98	0.62
1:A:269:THR:OG1	1:A:271:VAL:HG13	1.99	0.62
1:A:388:HIS:HB2	7:A:747:HOH:O	2.00	0.62
1:A:410:ASN:ND2	2:A:681:NAG:C1	2.63	0.62
1:B:583:GLN:HB2	7:B:859:HOH:O	1.97	0.62
1:A:219:GLY:HA2	7:A:840:HOH:O	2.00	0.62
1:B:216:ARG:HG2	1:B:220:PHE:CG	2.34	0.62
1:B:120:ARG:HG3	1:B:531:LEU:HD12	1.81	0.62
1:B:294:LEU:HD13	1:B:409:TYR:CD2	2.35	0.61
1:A:427:THR:OG1	1:A:578:THR:HG22	1.99	0.61
1:B:294:LEU:HD13	1:B:409:TYR:HD2	1.66	0.61
1:A:51:GLY:C	1:B:322:GLU:HG2	2.21	0.61
1:A:382:ASN:ND2	1:A:386:HIS:HE1	1.99	0.61
2:B:671:NAG:HO4	2:B:9:NAG:C5	2.13	0.60
1:B:306:LEU:O	1:B:306:LEU:HD23	1.99	0.60
1:A:226:HIS:HA	1:A:377:ILE:HD11	1.83	0.60
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.83	0.60
1:B:204:HIS:HE1	7:B:635:HOH:O	1.83	0.60
1:B:215:LYS:HZ1	1:B:222:ARG:HH21	1.48	0.60
1:B:295:VAL:HG22	7:B:811:HOH:O	2.02	0.60
1:B:106:PRO:HD2	1:B:107:PHE:CE2	2.37	0.60
3:A:682:HEM:HBC2	3:A:682:HEM:HHD	1.84	0.59
1:B:487:MET:HE3	7:B:844:HOH:O	2.01	0.59
3:B:682:HEM:CMB	3:B:682:HEM:HBB2	2.33	0.59
1:A:132:VAL:HG22	7:A:14:HOH:O	2.02	0.59
1:B:272:GLU:HG3	7:B:842:HOH:O	2.03	0.59
1:B:402:TYR:OH	1:B:417:HIS:HE1	1.85	0.59
1:B:322:GLU:CG	7:B:722:HOH:O	2.30	0.59
2:A:671:NAG:O4	2:A:9:NAG:C1	2.51	0.58
1:B:382:ASN:HD21	3:B:682:HEM:HAD2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:TYR:CD1	1:B:377:ILE:HD11	2.38	0.58
1:A:569:CYS:HB2	7:A:723:HOH:O	2.03	0.58
1:B:124:ILE:HD11	1:B:528:PRO:HB2	1.86	0.58
1:A:320:HIS:HE1	1:A:551:GLY:O	1.87	0.58
1:B:240:ARG:HH21	1:B:288:GLY:CA	2.16	0.58
1:B:91:TYR:O	1:B:95:HIS:CD2	2.57	0.58
1:A:554:VAL:HG13	1:A:555:GLY:N	2.19	0.57
1:B:33:ALA:HB3	1:B:158:ASP:OD2	2.04	0.57
1:B:321:PRO:HD2	7:B:722:HOH:O	2.04	0.57
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.40	0.57
1:A:107:PHE:HB3	7:A:785:HOH:O	2.04	0.57
1:A:240:ARG:HE	1:A:288:GLY:HA2	1.69	0.57
1:B:350:GLN:HE22	1:B:359:LEU:N	2.01	0.57
1:B:479:GLU:CB	1:B:485:LYS:NZ	2.67	0.57
1:B:144:ASN:HD21	2:B:671:NAG:C2	2.13	0.56
1:A:273:MET:SD	1:A:286:ALA:O	2.63	0.56
1:A:282:ASN:HB3	7:A:763:HOH:O	2.04	0.56
1:A:557:LYS:N	1:A:557:LYS:HE3	2.20	0.56
1:B:116:VAL:O	1:B:120:ARG:HG2	2.06	0.56
1:A:398:GLU:O	1:A:399:ASP:HB2	2.04	0.56
1:A:470:PHE:CD1	1:A:525:LEU:HD22	2.41	0.56
1:B:352:LEU:HD12	1:B:352:LEU:C	2.26	0.56
1:B:115:TYR:CD2	5:B:3:BOG:H4'2	2.41	0.56
1:B:543:GLN:H	1:B:543:GLN:CD	2.08	0.56
1:A:129:THR:CA	7:A:751:HOH:O	2.53	0.56
1:A:226:HIS:ND1	1:A:377:ILE:HG12	2.20	0.55
1:B:148:TYR:CE1	1:B:377:ILE:HD11	2.40	0.55
1:B:175:LYS:HD2	7:B:730:HOH:O	2.06	0.55
1:B:150:ARG:CD	1:B:380:GLU:OE2	2.54	0.55
1:B:230:LEU:HD13	1:B:233:ILE:HD12	1.89	0.55
1:B:124:ILE:HD11	1:B:528:PRO:CB	2.36	0.55
1:B:142:PHE:O	1:B:376:ARG:NH2	2.29	0.55
1:A:350:GLN:NE2	1:A:359:LEU:H	1.97	0.55
1:B:382:ASN:ND2	1:B:386:HIS:HE1	2.05	0.54
1:B:483:GLY:HA3	1:B:511:LYS:HD3	1.88	0.54
1:A:283:LEU:HD21	1:A:415:LEU:HD12	1.90	0.54
1:B:123:LEU:O	1:B:469:ARG:NH2	2.41	0.54
1:B:553:GLU:HG3	1:B:557:LYS:NZ	2.21	0.54
2:B:671:NAG:O4	2:B:9:NAG:O5	2.19	0.54
1:A:185:ARG:HH11	5:A:3:BOG:H8'3	1.73	0.54
1:A:398:GLU:O	1:A:399:ASP:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:CB	5:A:620:BOG:H62	2.38	0.54
1:B:151:ALA:O	1:B:469:ARG:NH1	2.41	0.54
1:A:398:GLU:HA	1:A:398:GLU:OE1	2.08	0.53
1:B:290:GLU:HG2	7:B:684:HOH:O	2.07	0.53
1:B:103:VAL:HG11	7:B:833:HOH:O	2.08	0.53
1:B:405:LYS:H	1:B:405:LYS:CD	2.21	0.53
1:B:107:PHE:HB3	7:B:678:HOH:O	2.08	0.53
1:B:464:ASN:HD21	1:B:475:TYR:H	1.56	0.53
1:A:352:LEU:C	1:A:352:LEU:HD12	2.28	0.53
1:A:350:GLN:HE22	1:A:359:LEU:N	1.95	0.53
1:B:150:ARG:HD3	1:B:380:GLU:OE2	2.08	0.53
2:A:671:NAG:O4	2:A:9:NAG:C2	2.57	0.53
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.89	0.53
1:B:68:ASN:ND2	2:B:661:NAG:C1	2.66	0.53
1:A:554:VAL:HG13	1:A:555:GLY:H	1.74	0.52
1:B:245:ARG:HD3	1:B:329:PHE:CD1	2.43	0.52
1:A:41:CYS:SG	1:A:47:CYS:HB2	2.48	0.52
1:A:418:GLY:O	1:A:421:GLN:O	2.27	0.52
1:B:240:ARG:HE	1:B:288:GLY:HA2	1.74	0.52
1:A:405:LYS:CE	1:A:405:LYS:H	2.22	0.52
1:B:575:CYS:H	1:B:576:PRO:CD	2.22	0.52
1:B:479:GLU:OE1	1:B:488:ALA:HB1	2.09	0.52
1:B:388:HIS:N	1:B:389:PRO:CD	2.73	0.51
1:A:294:LEU:HD22	1:A:409:TYR:CD2	2.35	0.51
1:A:404:PHE:HB2	1:A:405:LYS:HE3	1.91	0.51
1:A:405:LYS:HE3	1:A:405:LYS:N	2.24	0.51
1:B:482:THR:HB	7:B:844:HOH:O	2.11	0.51
1:A:300:MET:HG3	1:A:419:LEU:CD1	2.41	0.51
1:A:479:GLU:OE1	1:A:485:LYS:HE3	2.10	0.51
1:B:176:GLU:HG3	1:B:180:LYS:HE3	1.93	0.51
1:B:306:LEU:CD2	1:B:306:LEU:C	2.79	0.51
2:A:671:NAG:O4	2:A:9:NAG:H2	2.11	0.51
1:B:428:ARG:HD2	7:B:766:HOH:O	2.10	0.51
1:B:45:GLY:HA3	7:B:832:HOH:O	2.11	0.51
1:B:86:PRO:HG2	1:B:472:LEU:CD2	2.41	0.51
1:B:180:LYS:HD3	1:B:490:GLU:HG3	1.92	0.51
1:A:396:ASN:ND2	1:A:401:GLU:HG2	2.25	0.51
1:B:238:LEU:HD11	1:B:242:HIS:NE2	2.25	0.51
1:B:280:PRO:O	1:B:281:GLU:C	2.48	0.51
1:B:421:GLN:O	1:B:422:PHE:CB	2.37	0.51
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG22	7:B:25:HOH:O	2.11	0.51
1:B:187:PHE:HE2	1:B:430:ILE:HD13	1.75	0.51
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.93	0.50
1:B:322:GLU:OE2	7:B:722:HOH:O	2.19	0.50
1:A:536:GLY:HA3	7:A:809:HOH:O	2.11	0.50
1:A:565:GLN:NE2	7:A:723:HOH:O	2.45	0.50
1:B:294:LEU:HD22	1:B:409:TYR:CG	2.46	0.50
1:A:204:HIS:HD2	7:A:11:HOH:O	1.95	0.50
1:A:150:ARG:HD2	1:A:379:SER:HB3	1.94	0.50
1:B:294:LEU:CD2	1:B:409:TYR:HD2	2.25	0.50
1:B:574:GLY:O	7:B:758:HOH:O	2.19	0.50
1:B:479:GLU:CB	1:B:485:LYS:HZ1	2.24	0.49
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.94	0.49
1:B:65:TYR:O	1:B:71:THR:HG23	2.11	0.49
1:A:276:PRO:HD2	1:A:279:ILE:CD1	2.41	0.49
1:A:286:ALA:O	1:A:288:GLY:N	2.43	0.49
1:A:553:GLU:CG	1:A:557:LYS:NZ	2.74	0.49
1:A:322:GLU:HG2	1:B:51:GLY:O	2.12	0.49
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.94	0.49
1:B:180:LYS:HB3	1:B:490:GLU:HG2	1.94	0.49
1:A:293:GLY:HA2	1:A:299:MET:CE	2.42	0.49
1:A:137:LYS:C	7:A:908:HOH:O	2.48	0.49
1:B:133:HIS:HD2	1:B:147:TYR:OH	1.95	0.49
1:B:240:ARG:NE	1:B:288:GLY:HA2	2.26	0.49
1:A:396:ASN:HB3	7:A:860:HOH:O	2.13	0.48
1:A:556:PHE:HB3	1:A:557:LYS:CE	2.43	0.48
1:B:363:PRO:HG2	1:B:545:TRP:CD2	2.48	0.48
1:A:68:ASN:HD21	2:A:661:NAG:C2	2.25	0.48
1:B:248:LYS:HB2	1:B:248:LYS:NZ	2.29	0.48
1:A:397:ILE:O	1:A:398:GLU:C	2.50	0.48
1:A:423:VAL:CG1	1:A:578:THR:HG23	2.43	0.48
1:B:384:LEU:C	1:B:384:LEU:HD12	2.33	0.48
1:B:472:LEU:HD11	1:B:524:GLU:HB2	1.96	0.48
1:A:61:ARG:NH2	1:B:367:PHE:HE2	2.10	0.48
1:A:232:HIS:HB2	1:A:292:PHE:CE2	2.49	0.48
1:B:160:PRO:HD2	1:B:164:GLY:O	2.14	0.48
1:A:553:GLU:HG3	1:A:557:LYS:HZ3	1.77	0.47
1:B:42:GLN:HE22	1:B:468:LYS:HE2	1.79	0.47
1:A:123:LEU:O	1:A:469:ARG:NH2	2.35	0.47
1:A:294:LEU:HD22	7:A:878:HOH:O	2.14	0.47
1:B:477:SER:HB2	1:B:479:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:682:HEM:HBC2	3:B:682:HEM:CHD	2.41	0.47
1:A:175:LYS:NZ	1:A:449:LYS:HD2	2.30	0.47
1:A:388:HIS:CB	7:A:747:HOH:O	2.61	0.47
1:B:115:TYR:HD2	5:B:3:BOG:H4'2	1.79	0.47
1:B:137:LYS:O	7:B:870:HOH:O	2.20	0.47
1:B:150:ARG:HD3	1:B:380:GLU:CD	2.35	0.47
1:A:322:GLU:HG3	1:B:51:GLY:C	2.35	0.47
1:A:226:HIS:CA	1:A:377:ILE:HD13	2.43	0.47
1:B:68:ASN:HD21	2:B:661:NAG:C2	2.28	0.47
1:B:215:LYS:HZ2	1:B:222:ARG:HH21	1.60	0.47
1:A:379:SER:CB	7:A:840:HOH:O	2.63	0.47
1:A:388:HIS:N	1:A:389:PRO:CD	2.78	0.47
1:B:291:VAL:O	1:B:291:VAL:HG13	2.14	0.47
1:A:129:THR:HA	7:A:751:HOH:O	2.14	0.47
1:A:152:LEU:HG	1:A:469:ARG:HG2	1.97	0.47
1:B:485:LYS:HD3	7:B:687:HOH:O	2.15	0.47
1:A:87:ASN:HB3	5:A:620:BOG:H62	1.96	0.47
1:B:215:LYS:CD	1:B:215:LYS:N	2.71	0.47
1:A:382:ASN:C	1:A:382:ASN:HD22	2.18	0.46
1:A:75:LEU:HD22	1:A:79:LYS:HE2	1.97	0.46
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.98	0.46
1:B:574:GLY:O	1:B:575:CYS:CB	2.63	0.46
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.79	0.46
1:A:485:LYS:HD3	1:A:485:LYS:HA	1.62	0.46
1:B:151:ALA:HA	7:B:701:HOH:O	2.16	0.46
1:B:575:CYS:H	1:B:576:PRO:HD3	1.80	0.46
1:B:98:GLY:O	1:B:101:ASN:HB3	2.16	0.46
1:B:214:HIS:CD2	7:B:809:HOH:O	2.57	0.46
1:A:479:GLU:CB	1:A:485:LYS:NZ	2.79	0.45
1:B:129:THR:CA	7:B:869:HOH:O	2.62	0.45
1:B:495:TYR:O	1:B:496:SER:HB3	2.16	0.45
1:A:283:LEU:HD13	7:A:726:HOH:O	2.17	0.45
1:A:464:ASN:ND2	1:A:475:TYR:H	2.10	0.45
1:A:513:ARG:O	1:A:514:PRO:C	2.54	0.45
1:B:105(A):ILE:CD1	1:B:108:LEU:HD12	2.45	0.45
1:B:148:TYR:CZ	1:B:221:THR:HB	2.51	0.45
1:B:350:GLN:NE2	1:B:359:LEU:H	2.05	0.45
1:B:111:LEU:HD12	1:B:111:LEU:C	2.37	0.45
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.98	0.45
1:B:240:ARG:CZ	1:B:288:GLY:HA2	2.46	0.45
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:PHE:O	1:B:77:ARG:HB2	2.16	0.45
1:A:93:LEU:HB3	1:A:355:TYR:CD1	2.51	0.45
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.52	0.45
1:B:83:LYS:HA	1:B:84:PRO:HD2	1.83	0.45
1:B:230:LEU:HA	1:B:232:HIS:CD2	2.51	0.45
1:A:322:GLU:CG	1:B:51:GLY:C	2.85	0.45
1:A:430:ILE:HD12	7:A:663:HOH:O	2.17	0.45
1:B:294:LEU:CD1	1:B:409:TYR:HD2	2.29	0.45
1:A:399:ASP:HB3	7:A:797:HOH:O	2.17	0.44
1:B:252:LEU:HD22	1:B:309:HIS:CG	2.52	0.44
1:B:322:GLU:CD	7:B:722:HOH:O	2.53	0.44
1:B:530:SER:O	1:B:534:LEU:HD22	2.18	0.44
1:A:426:PHE:CD1	7:A:636:HOH:O	2.69	0.44
1:A:351:HIS:HD2	7:A:760:HOH:O	2.00	0.44
1:B:272:GLU:HG2	7:B:677:HOH:O	2.16	0.44
1:B:42:GLN:NE2	1:B:468:LYS:HE2	2.33	0.44
1:A:137:LYS:N	7:A:908:HOH:O	2.51	0.44
1:A:398:GLU:HB2	1:A:425:SER:OG	2.18	0.44
1:B:500:VAL:CG1	1:B:500:VAL:O	2.65	0.44
1:A:479:GLU:H	1:A:479:GLU:CD	2.21	0.43
1:B:364:GLU:HG3	7:B:654:HOH:O	2.19	0.43
1:B:187:PHE:CE2	1:B:430:ILE:HD13	2.53	0.43
1:B:525:LEU:O	1:B:528:PRO:HD2	2.17	0.43
1:A:420:THR:OG1	1:A:573:LYS:HB3	2.18	0.43
1:A:175:LYS:HE2	1:A:175:LYS:HB2	1.82	0.43
1:A:377:ILE:HD11	7:A:635:HOH:O	2.18	0.43
1:A:423:VAL:HG13	1:A:578:THR:CG2	2.49	0.43
3:A:682:HEM:CMB	3:A:682:HEM:HBB2	2.45	0.43
1:A:467:ARG:HB3	1:A:472:LEU:HB2	2.01	0.43
1:B:105(A):ILE:CG2	1:B:107:PHE:HD2	2.31	0.43
1:B:252:LEU:HD22	1:B:309:HIS:CD2	2.54	0.43
1:B:351:HIS:HD2	7:B:810:HOH:O	2.02	0.43
1:B:408:LEU:HB2	7:B:792:HOH:O	2.19	0.43
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.54	0.43
1:B:405:LYS:H	1:B:405:LYS:HD2	1.83	0.43
1:A:163:MET:CE	1:A:502:GLU:HG2	2.49	0.43
1:B:397:ILE:HD13	1:B:422:PHE:CE2	2.53	0.43
1:B:539:ILE:HA	1:B:544:TYR:HB3	2.01	0.43
1:A:479:GLU:CG	1:A:485:LYS:HZ1	2.32	0.42
1:B:382:ASN:HD22	1:B:382:ASN:C	2.22	0.42
1:A:202:ALA:O	1:A:206:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:HA	7:A:619:HOH:O	2.20	0.42
1:A:405:LYS:CD	1:A:405:LYS:H	2.32	0.42
1:B:137:LYS:O	1:B:141:ALA:HB3	2.19	0.42
1:B:230:LEU:HG	1:B:337:ILE:HG12	2.02	0.42
1:A:308:GLU:OE2	1:A:311:ARG:NH1	2.52	0.42
1:A:150:ARG:HG3	1:A:380:GLU:OE2	2.19	0.42
1:A:482:THR:HG22	1:A:509:VAL:HG13	2.01	0.42
1:B:75:LEU:O	1:B:79:LYS:HG3	2.20	0.42
1:A:61:ARG:HD2	7:B:805:HOH:O	2.20	0.42
1:A:185:ARG:HH12	5:A:3:BOG:C5'	2.07	0.42
1:A:352:LEU:HD12	1:A:353:SER:N	2.35	0.42
1:B:112:ILE:CG1	7:B:833:HOH:O	2.58	0.42
1:B:115:TYR:CE2	5:B:3:BOG:H3'1	2.46	0.42
1:A:114:LYS:HE2	1:A:365:LEU:O	2.20	0.41
1:A:582:VAL:O	1:A:583:GLN:CG	2.68	0.41
1:A:215:LYS:HD3	1:A:215:LYS:N	2.35	0.41
1:A:144:ASN:OD1	1:A:146:SER:HB2	2.19	0.41
1:A:495:TYR:O	1:A:496:SER:HB3	2.20	0.41
1:A:430:ILE:HG13	1:A:430:ILE:H	1.54	0.41
1:A:582:VAL:O	1:A:583:GLN:HG2	2.20	0.41
1:B:124:ILE:N	1:B:124:ILE:HD12	2.35	0.41
1:B:430:ILE:O	1:B:430:ILE:HD12	2.20	0.41
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.55	0.41
1:A:557:LYS:HD3	1:A:557:LYS:HA	1.89	0.41
1:B:427:THR:HB	1:B:428:ARG:NH2	2.35	0.41
1:B:575:CYS:O	1:B:575:CYS:SG	2.79	0.41
1:A:385:TYR:CE2	4:A:1591:NPX:H121	2.56	0.41
1:B:111:LEU:HD12	1:B:111:LEU:O	2.19	0.41
1:B:403:SER:HB2	1:B:405:LYS:NZ	2.36	0.41
1:B:404:PHE:HB2	1:B:405:LYS:HE3	2.03	0.41
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.55	0.41
1:A:543:GLN:HB2	7:B:871:HOH:O	2.20	0.41
1:B:215:LYS:CE	1:B:215:LYS:H	2.33	0.41
1:A:144:ASN:CG	2:A:671:NAG:C1	2.89	0.41
1:B:422:PHE:O	1:B:426:PHE:HB2	2.21	0.41
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.90	0.40
1:B:489:ALA:HA	7:B:820:HOH:O	2.19	0.40
1:A:232:HIS:CD2	1:A:232:HIS:H	2.39	0.40
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.86	0.40
1:B:287:VAL:HA	7:B:650:HOH:O	2.20	0.40
1:B:76:THR:O	1:B:80:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LYS:HA	1:A:474:PRO:HD2	1.88	0.40
1:B:344:VAL:O	1:B:348:TYR:HB3	2.22	0.40
1:B:424:GLU:HA	1:B:428:ARG:HH21	1.87	0.40
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	550/587 (94%)	523 (95%)	19 (4%)	8 (2%)	10	14
1	B	550/587 (94%)	516 (94%)	20 (4%)	14 (2%)	5	6
All	All	1100/1174 (94%)	1039 (94%)	39 (4%)	22 (2%)	7	9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	287	VAL
1	A	422	PHE
1	B	138	SER
1	B	282	ASN
1	B	287	VAL
1	B	422	PHE
1	B	514	PRO
1	B	575	CYS
1	A	130	TYR
1	A	399	ASP
1	B	399	ASP
1	B	573	LYS
1	A	398	GLU

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Mol	Chain	Res	Type
1	A	514	PRO
1	B	130	TYR
1	B	281	GLU
1	B	398	GLU
1	A	573	LYS
1	B	137	LYS
1	B	409	TYR
1	B	82	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	493/525 (94%)	439 (89%)	54 (11%)	6	8
1	B	493/525 (94%)	438 (89%)	55 (11%)	6	8
All	All	986/1050 (94%)	877 (89%)	109 (11%)	6	8

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	54	GLN
1	A	71	THR
1	A	82	LEU
1	A	83	LYS
1	A	93	LEU
1	A	116	VAL
1	A	117	LEU
1	A	122	TYR
1	A	132	VAL
1	A	150	ARG
1	A	170	GLU
1	A	171	LEU
1	A	178	LEU
1	A	216	ARG

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Mol	Chain	Res	Type
1	A	232	HIS
1	A	238	LEU
1	A	248	LYS
1	A	252	LEU
1	A	271	VAL
1	A	282	ASN
1	A	289	GLN
1	A	298	LEU
1	A	316	LEU
1	A	318	GLN
1	A	322	GLU
1	A	326	GLU
1	A	376	ARG
1	A	377	ILE
1	A	382	ASN
1	A	385	TYR
1	A	398	GLU
1	A	405	LYS
1	A	409	TYR
1	A	422	PHE
1	A	428	ARG
1	A	430	ILE
1	A	442	ILE
1	A	455	SER
1	A	469	ARG
1	A	479	GLU
1	A	484	GLU
1	A	485	LYS
1	A	500	VAL
1	A	509	VAL
1	A	513	ARG
1	A	514	PRO
1	A	534	LEU
1	A	556	PHE
1	A	557	LYS
1	A	577	PHE
1	A	578	THR
1	A	582	VAL
1	A	583	GLN
1	B	44	ARG
1	B	54	GLN
1	B	71	THR

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Mol	Chain	Res	Type
1	B	83	LYS
1	B	93	LEU
1	B	107	PHE
1	B	111	LEU
1	B	116	VAL
1	B	117	LEU
1	B	122	TYR
1	B	132	VAL
1	B	137	LYS
1	B	138	SER
1	B	165	VAL
1	B	170	GLU
1	B	171	LEU
1	B	178	LEU
1	B	185	ARG
1	B	186	GLU
1	B	215	LYS
1	B	232	HIS
1	B	239	ASP
1	B	252	LEU
1	B	270	GLN
1	B	272	GLU
1	B	281	GLU
1	B	282	ASN
1	B	289	GLN
1	B	298	LEU
1	B	316	LEU
1	B	322	GLU
1	B	376	ARG
1	B	377	ILE
1	B	382	ASN
1	B	385	TYR
1	B	398	GLU
1	B	405	LYS
1	B	409	TYR
1	B	422	PHE
1	B	428	ARG
1	B	479	GLU
1	B	484	GLU
1	B	509	VAL
1	B	513	ARG
1	B	525	LEU

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Mol	Chain	Res	Type
1	B	532	LYS
1	B	534	LEU
1	B	543	GLN
1	B	554	VAL
1	B	556	PHE
1	B	557	LYS
1	B	577	PHE
1	B	578	THR
1	B	582	VAL
1	B	583	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	68	ASN
1	A	95	HIS
1	A	133	HIS
1	A	203	GLN
1	A	204	HIS
1	A	214	HIS
1	A	232	HIS
1	A	242	HIS
1	A	320	HIS
1	A	350	GLN
1	A	351	HIS
1	A	370	GLN
1	A	382	ASN
1	A	386	HIS
1	A	396	ASN
1	A	417	HIS
1	A	454	GLN
1	A	464	ASN
1	A	583	GLN
1	B	42	GLN
1	B	68	ASN
1	B	95	HIS
1	B	105	ASN
1	B	133	HIS
1	B	144	ASN
1	B	203	GLN
1	B	204	HIS

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Mol	Chain	Res	Type
1	B	214	HIS
1	B	232	HIS
1	B	282	ASN
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	382	ASN
1	B	386	HIS
1	B	396	ASN
1	B	411	ASN
1	B	417	HIS
1	B	454	GLN
1	B	464	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	BOG	A	620	-	20,20,20	1.40	4 (20%)	25,25,25	1.42	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BOG	B	620	-	20,20,20	1.39	3 (15%)	25,25,25	1.26	4 (16%)
2	NAG	B	9	-	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
2	NAG	B	661	-	14,14,15	0.58	0	17,19,21	1.31	2 (11%)
3	HEM	B	682	1	27,50,50	2.14	6 (22%)	17,82,82	1.55	4 (23%)
4	NPX	B	1591	-	15,18,18	1.19	1 (6%)	21,25,25	1.05	0
5	BOG	A	6	-	20,20,20	1.45	5 (25%)	25,25,25	1.40	3 (12%)
3	HEM	A	682	1,7	27,50,50	2.13	5 (18%)	17,82,82	1.45	3 (17%)
2	NAG	B	671	-	14,14,15	0.80	1 (7%)	17,19,21	1.53	4 (23%)
2	NAG	A	671	-	14,14,15	0.86	1 (7%)	17,19,21	1.75	4 (23%)
2	NAG	B	681	-	14,14,15	0.59	0	17,19,21	1.58	3 (17%)
2	NAG	A	681	-	14,14,15	0.59	0	17,19,21	0.85	0
2	NAG	A	661	-	14,14,15	0.73	1 (7%)	17,19,21	0.90	1 (5%)
2	NAG	A	9	-	14,14,15	0.59	0	17,19,21	1.35	2 (11%)
5	BOG	B	3	-	20,20,20	1.40	2 (10%)	25,25,25	1.25	4 (16%)
5	BOG	A	3	-	20,20,20	1.36	2 (10%)	25,25,25	1.11	4 (16%)
4	NPX	A	1591	-	15,18,18	1.23	1 (6%)	21,25,25	1.07	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
5	BOG	A	620	-	-	8/11/31/31	0/1/1/1
5	BOG	B	620	-	-	6/11/31/31	0/1/1/1
2	NAG	B	9	-	-	4/6/23/26	0/1/1/1
2	NAG	B	661	-	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	0/6/54/54	-
4	NPX	B	1591	-	-	0/6/10/10	0/2/2/2
5	BOG	A	6	-	-	8/11/31/31	0/1/1/1
3	HEM	A	682	1,7	-	0/6/54/54	-
2	NAG	B	671	-	-	0/6/23/26	0/1/1/1
2	NAG	A	671	-	-	0/6/23/26	0/1/1/1
2	NAG	B	681	-	-	2/6/23/26	0/1/1/1
2	NAG	A	681	-	-	2/6/23/26	0/1/1/1
2	NAG	A	661	-	-	2/6/23/26	0/1/1/1
2	NAG	A	9	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BOG	B	3	-	-	8/11/31/31	0/1/1/1
5	BOG	A	3	-	-	4/11/31/31	0/1/1/1
4	NPX	A	1591	-	-	0/6/10/10	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C3D-C2D	5.40	1.53	1.37
3	B	682	HEM	C3D-C2D	5.11	1.52	1.37
3	B	682	HEM	C3C-C2C	-4.90	1.33	1.40
3	B	682	HEM	C3B-C2B	-4.37	1.34	1.40
5	A	6	BOG	C4-C3	-4.27	1.41	1.52
5	B	3	BOG	C4-C3	-4.23	1.41	1.52
5	B	620	BOG	C4-C3	-4.21	1.41	1.52
5	A	620	BOG	C4-C3	-4.11	1.41	1.52
3	A	682	HEM	C3B-C2B	-4.05	1.34	1.40
5	A	3	BOG	C4-C3	-4.04	1.42	1.52
3	A	682	HEM	C3C-C2C	-3.97	1.34	1.40
3	A	682	HEM	C3C-CAC	3.76	1.55	1.47
3	A	682	HEM	C3B-CAB	3.64	1.55	1.47
3	B	682	HEM	C3B-CAB	3.56	1.55	1.47
3	B	682	HEM	C3C-CAC	3.19	1.54	1.47
5	A	620	BOG	O5-C5	2.50	1.50	1.44
5	B	3	BOG	O5-C5	2.40	1.50	1.44
5	A	3	BOG	O3-C3	2.31	1.48	1.43
3	B	682	HEM	CAA-C2A	2.30	1.55	1.52
5	B	620	BOG	O5-C5	2.28	1.49	1.44
2	A	671	NAG	O5-C1	-2.27	1.40	1.43
5	A	6	BOG	O4-C4	2.23	1.48	1.43
5	A	6	BOG	C3-C2	-2.17	1.46	1.52
4	B	1591	NPX	C8-C9	-2.17	1.49	1.52
4	A	1591	NPX	C8-C9	-2.14	1.49	1.52
2	B	671	NAG	O5-C1	-2.14	1.40	1.43
5	A	620	BOG	O3-C3	2.14	1.48	1.43
2	A	661	NAG	O5-C1	-2.12	1.40	1.43
5	A	6	BOG	O5-C5	2.06	1.49	1.44
5	A	6	BOG	O3-C3	2.04	1.47	1.43
5	A	620	BOG	O4-C4	2.04	1.47	1.43
5	B	620	BOG	O3-C3	2.00	1.47	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	671	NAG	C1-O5-C5	-4.87	105.60	112.19
2	B	671	NAG	C1-O5-C5	-4.35	106.30	112.19
5	A	6	BOG	O5-C5-C4	3.98	116.92	109.69
2	B	681	NAG	C1-O5-C5	-3.85	106.98	112.19
3	B	682	HEM	CBD-CAD-C3D	-3.68	105.70	112.48
5	A	620	BOG	C1'-O1-C1	3.60	119.81	113.84
2	A	9	NAG	O5-C1-C2	-3.56	105.67	111.29
2	B	681	NAG	O5-C5-C6	3.47	112.64	107.20
2	B	661	NAG	O5-C1-C2	-3.14	106.33	111.29
2	B	661	NAG	C3-C4-C5	3.12	115.80	110.24
5	A	620	BOG	O5-C5-C4	3.07	115.27	109.69
5	A	3	BOG	C1'-O1-C1	3.00	118.81	113.84
5	B	620	BOG	C1'-O1-C1	2.95	118.73	113.84
5	B	3	BOG	C1'-O1-C1	2.93	118.70	113.84
3	A	682	HEM	CBD-CAD-C3D	-2.90	107.13	112.48
5	A	620	BOG	O6-C6-C5	2.86	121.11	111.29
3	A	682	HEM	CAA-CBA-CGA	-2.79	108.00	112.67
5	A	6	BOG	C1'-O1-C1	2.78	118.45	113.84
5	B	3	BOG	O5-C5-C4	2.72	114.64	109.69
2	A	671	NAG	O5-C1-C2	-2.54	107.28	111.29
5	B	620	BOG	O1-C1'-C2'	2.53	118.42	109.56
2	A	661	NAG	C1-O5-C5	-2.52	108.78	112.19
3	B	682	HEM	C4C-C3C-C2C	2.52	108.66	106.90
2	A	671	NAG	O5-C5-C6	2.49	111.11	107.20
5	A	6	BOG	O1-C1'-C2'	2.47	118.22	109.56
5	B	620	BOG	O6-C6-C5	2.47	119.76	111.29
5	B	3	BOG	O1-C1'-C2'	2.45	118.14	109.56
2	A	671	NAG	O4-C4-C3	-2.42	104.76	110.35
2	A	9	NAG	C3-C4-C5	2.34	114.41	110.24
5	B	3	BOG	O6-C6-C5	2.33	119.27	111.29
2	B	671	NAG	C2-N2-C7	-2.32	119.60	122.90
5	B	620	BOG	O5-C5-C4	2.27	113.82	109.69
3	B	682	HEM	CBA-CAA-C2A	-2.23	108.37	112.49
5	A	3	BOG	O6-C6-C5	2.17	118.75	111.29
2	B	671	NAG	O4-C4-C3	-2.14	105.40	110.35
2	B	671	NAG	O5-C1-C2	-2.13	107.92	111.29
3	B	682	HEM	C3C-C4C-NC	-2.13	106.92	110.94
2	B	9	NAG	C1-O5-C5	2.12	115.07	112.19
5	A	3	BOG	O1-C1'-C2'	2.08	116.86	109.56
2	B	681	NAG	O5-C5-C4	-2.07	105.79	110.83
3	A	682	HEM	C3C-C4C-NC	-2.04	107.09	110.94
5	A	3	BOG	O5-C5-C4	2.04	113.39	109.69

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	620	BOG	C2-C1-O1-C1'
5	B	620	BOG	O5-C1-O1-C1'
2	B	9	NAG	C8-C7-N2-C2
2	B	9	NAG	O7-C7-N2-C2
5	A	6	BOG	C2-C1-O1-C1'
5	B	3	BOG	C2'-C1'-O1-C1
2	A	681	NAG	C8-C7-N2-C2
5	A	620	BOG	O5-C5-C6-O6
2	A	9	NAG	O5-C5-C6-O6
2	A	681	NAG	O7-C7-N2-C2
5	A	620	BOG	C4-C5-C6-O6
2	A	661	NAG	O5-C5-C6-O6
2	B	9	NAG	O5-C5-C6-O6
5	A	620	BOG	O1-C1'-C2'-C3'
2	A	661	NAG	C4-C5-C6-O6
5	A	6	BOG	O5-C1-O1-C1'
5	A	3	BOG	O1-C1'-C2'-C3'
5	B	3	BOG	C3'-C4'-C5'-C6'
5	B	3	BOG	C2-C1-O1-C1'
5	B	620	BOG	C4'-C5'-C6'-C7'
5	A	3	BOG	C3'-C4'-C5'-C6'
5	B	3	BOG	C1'-C2'-C3'-C4'
2	A	9	NAG	C4-C5-C6-O6
5	A	6	BOG	C4-C5-C6-O6
5	B	620	BOG	O1-C1'-C2'-C3'
5	B	620	BOG	C2'-C3'-C4'-C5'
5	B	3	BOG	C2'-C3'-C4'-C5'
5	B	3	BOG	O5-C1-O1-C1'
5	A	6	BOG	O1-C1'-C2'-C3'
5	B	620	BOG	O5-C5-C6-O6
5	A	6	BOG	C3'-C4'-C5'-C6'
5	B	3	BOG	O1-C1'-C2'-C3'
5	A	6	BOG	C5'-C6'-C7'-C8'
2	B	681	NAG	C4-C5-C6-O6
5	A	620	BOG	C2'-C1'-O1-C1
5	A	620	BOG	C4'-C5'-C6'-C7'
5	B	3	BOG	C4'-C5'-C6'-C7'
2	B	681	NAG	O5-C5-C6-O6
2	B	9	NAG	C4-C5-C6-O6
5	A	3	BOG	C4'-C5'-C6'-C7'
5	A	6	BOG	O5-C5-C6-O6
5	A	620	BOG	C2-C1-O1-C1'

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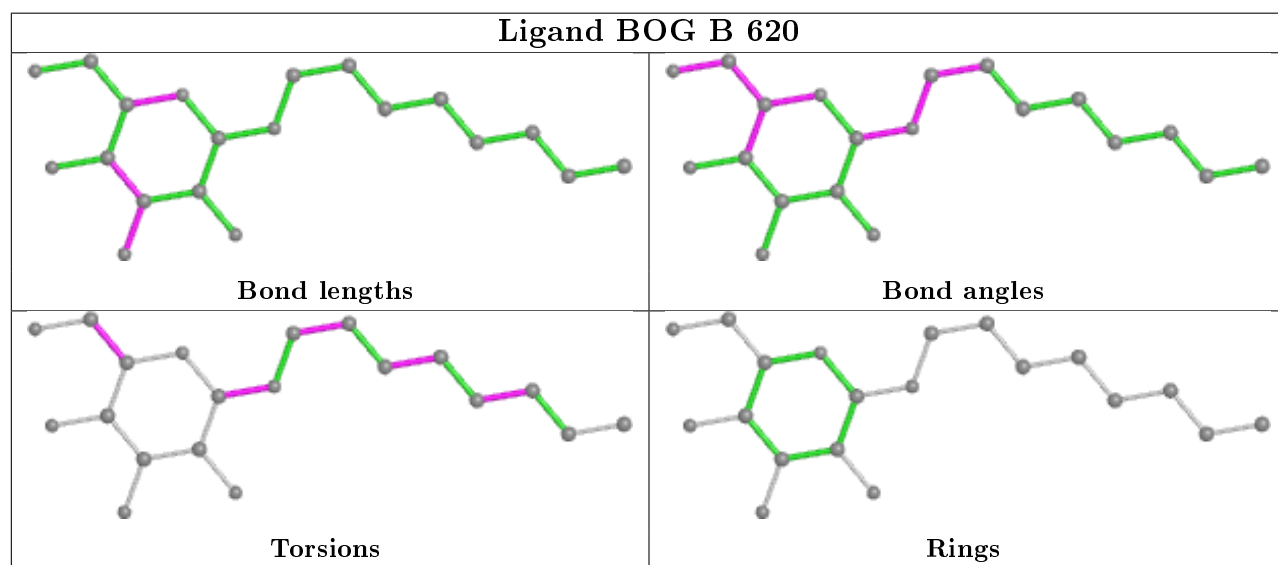
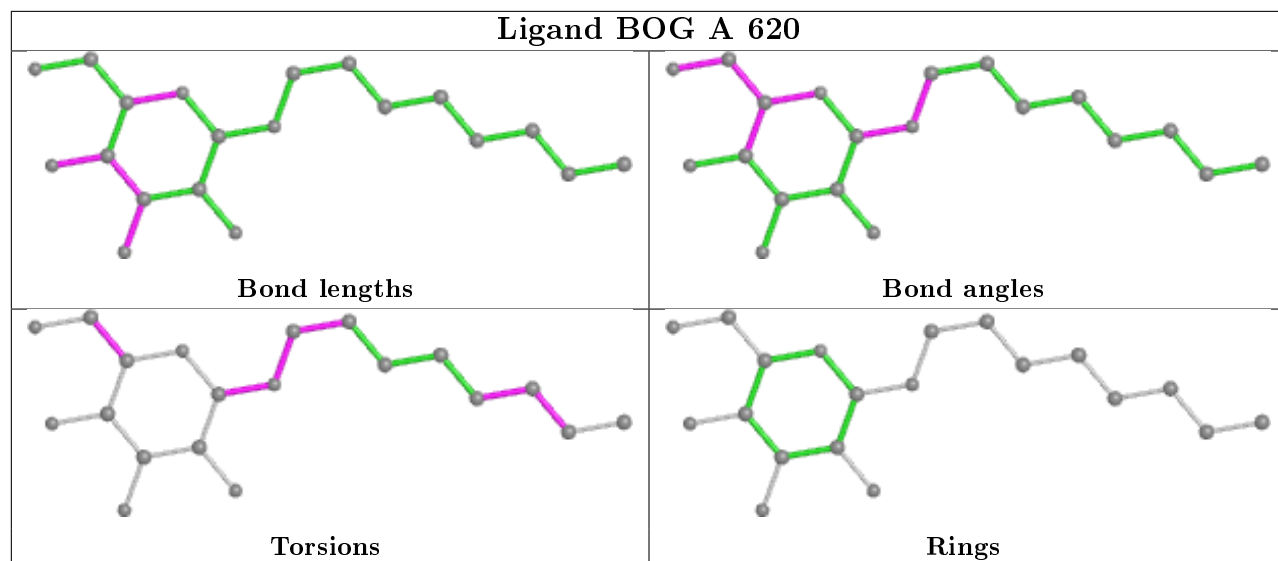
Mol	Chain	Res	Type	Atoms
5	A	620	BOG	O5-C1-O1-C1'
5	A	3	BOG	C5'-C6'-C7'-C8'
5	A	620	BOG	C5'-C6'-C7'-C8'
5	A	6	BOG	C4'-C5'-C6'-C7'

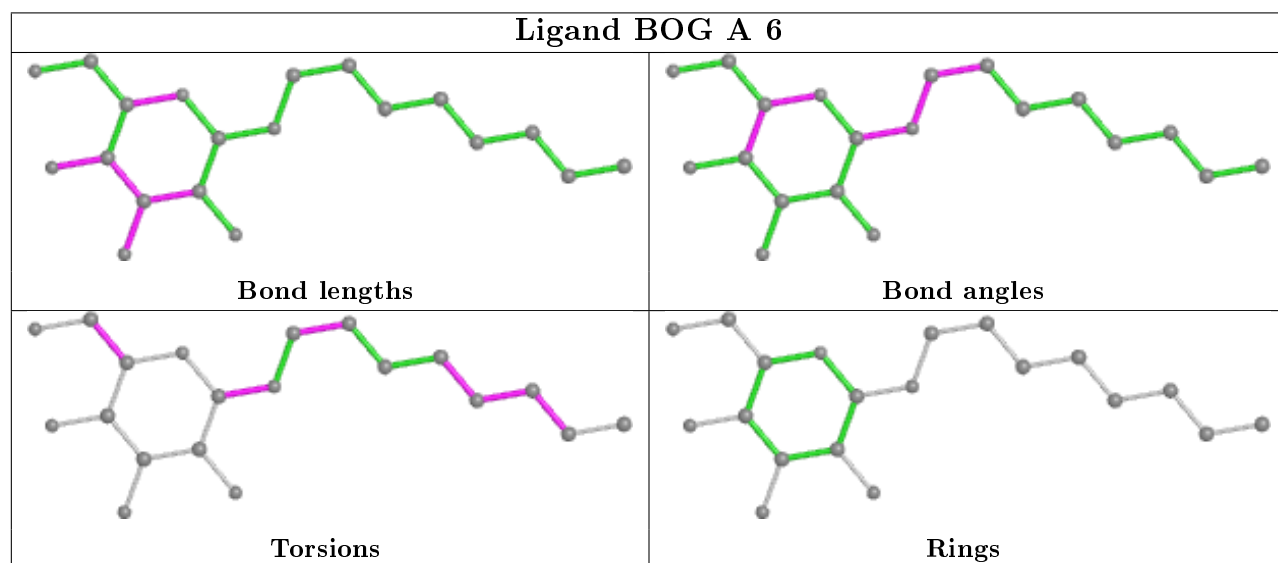
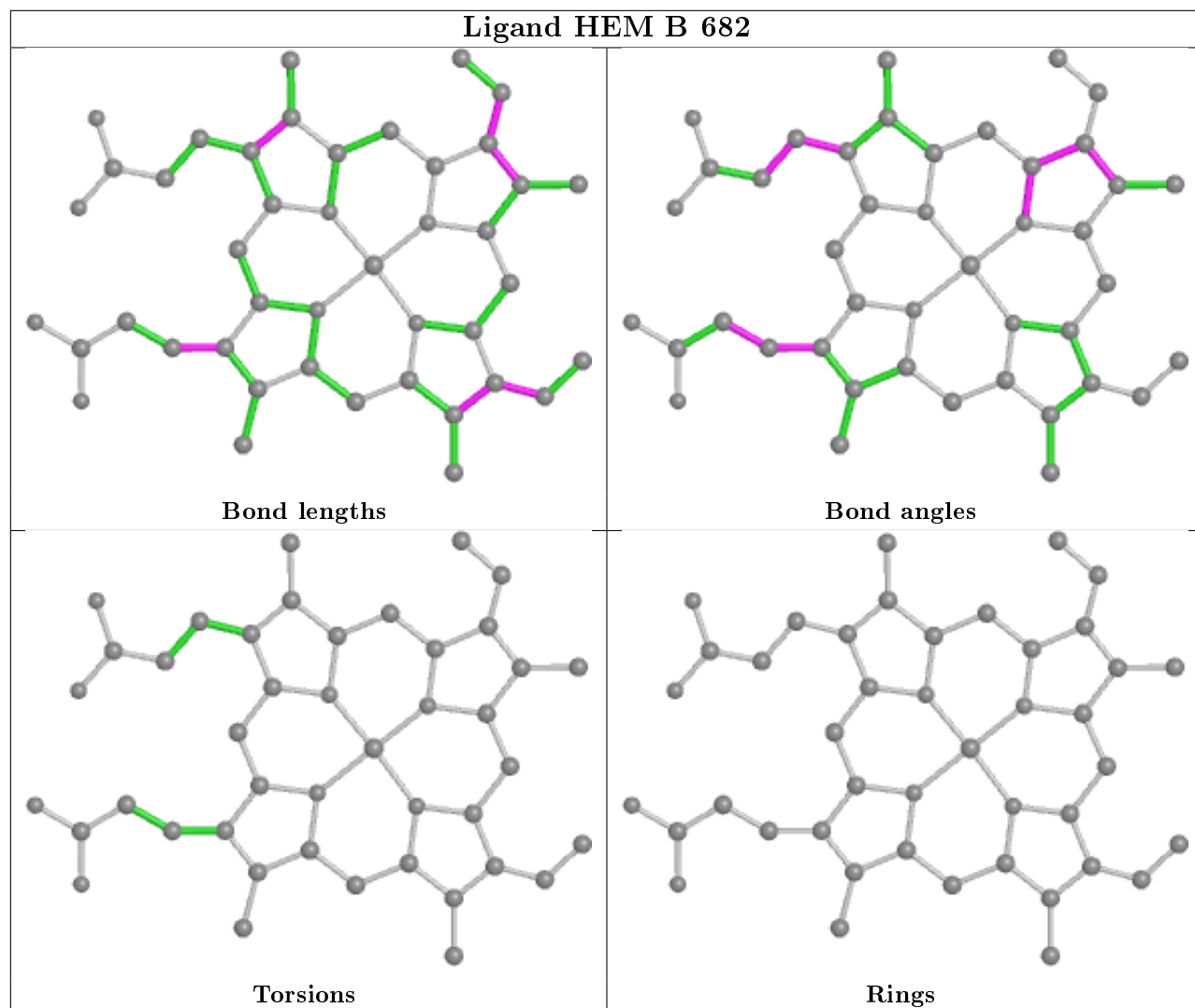
There are no ring outliers.

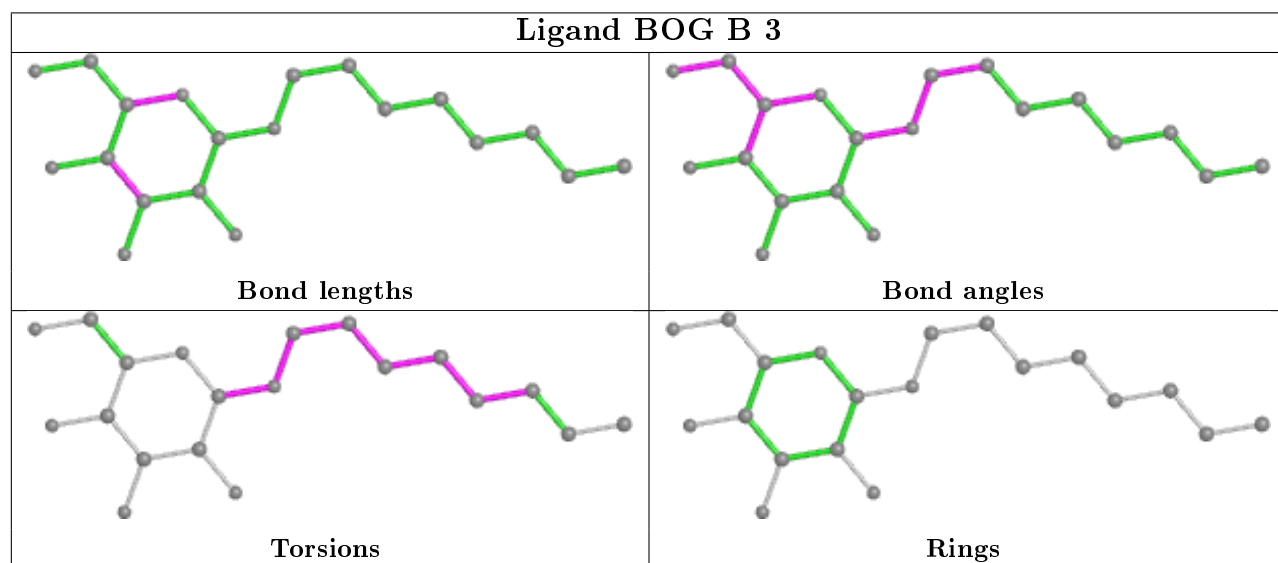
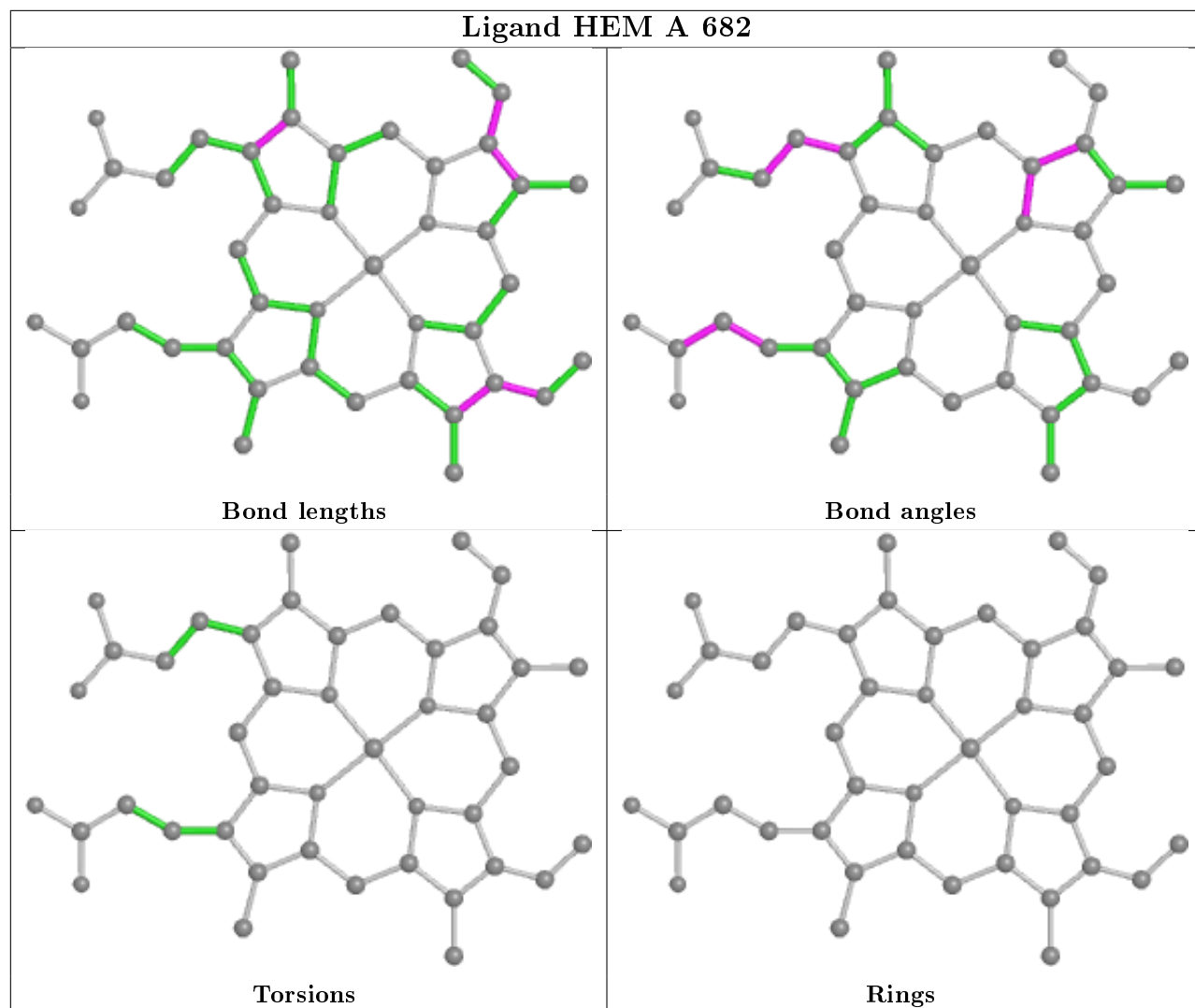
15 monomers are involved in 43 short contacts:

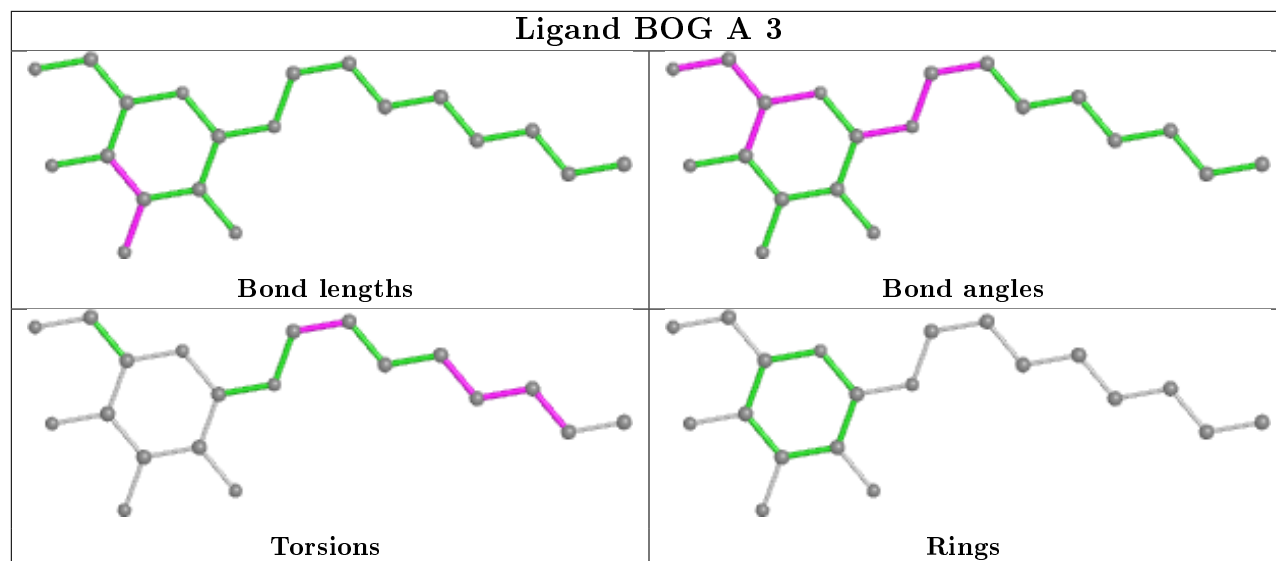
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	620	BOG	2	0
5	B	620	BOG	1	0
2	B	9	NAG	2	0
2	B	661	NAG	3	0
3	B	682	HEM	5	0
3	A	682	HEM	4	0
2	B	671	NAG	5	0
2	A	671	NAG	7	0
2	B	681	NAG	2	0
2	A	681	NAG	2	0
2	A	661	NAG	3	0
2	A	9	NAG	3	0
5	B	3	BOG	4	0
5	A	3	BOG	4	0
4	A	1591	NPX	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	552/587 (94%)	-0.57	7 (1%) 77 75	15, 26, 47, 62	0
1	B	552/587 (94%)	-0.60	5 (0%) 84 82	14, 26, 47, 70	0
All	All	1104/1174 (94%)	-0.58	12 (1%) 80 79	14, 26, 47, 70	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	PHE	3.6
1	A	583	GLN	3.4
1	A	409	TYR	3.0
1	B	583	GLN	3.0
1	A	122	TYR	2.8
1	B	74	PHE	2.8
1	B	81	LEU	2.8
1	B	398	GLU	2.7
1	A	398	GLU	2.6
1	A	107	PHE	2.3
1	B	65	TYR	2.2
1	A	215	LYS	2.0

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](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

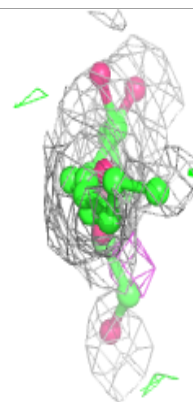
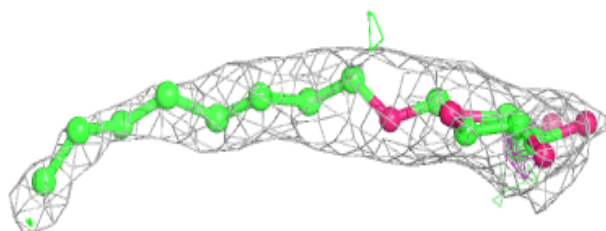
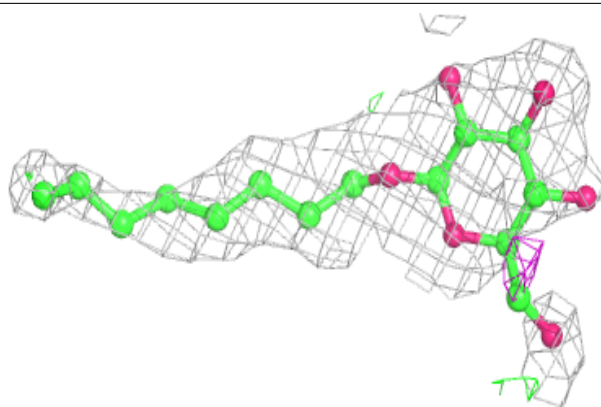
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BOG	A	620	20/20	0.77	0.27	43,58,65,65	0
5	BOG	B	620	20/20	0.79	0.27	39,63,73,75	0
2	NAG	B	661	14/15	0.82	0.28	43,54,60,62	0
2	NAG	A	681	14/15	0.85	0.19	40,48,54,55	0
2	NAG	A	9	14/15	0.87	0.23	37,54,62,63	0
2	NAG	B	9	14/15	0.88	0.36	41,54,64,66	0
2	NAG	A	661	14/15	0.88	0.24	43,55,64,64	0
5	BOG	A	6	20/20	0.88	0.17	45,51,58,59	0
5	BOG	B	3	20/20	0.89	0.17	49,55,63,64	0
2	NAG	B	681	14/15	0.90	0.20	40,46,50,57	0
2	NAG	B	671	14/15	0.94	0.11	25,30,35,38	0
4	NPX	B	1591	17/17	0.94	0.14	20,28,43,45	0
5	BOG	A	3	20/20	0.94	0.10	27,33,37,39	0
4	NPX	A	1591	17/17	0.94	0.12	21,24,34,40	0
2	NAG	A	671	14/15	0.95	0.14	21,30,36,39	0
3	HEM	A	682	43/43	0.95	0.10	17,25,44,60	0
3	HEM	B	682	43/43	0.96	0.11	20,25,40,61	0
6	CL	A	1	1/1	0.98	0.12	33,33,33,33	0
6	CL	B	1	1/1	0.99	0.07	32,32,32,32	0

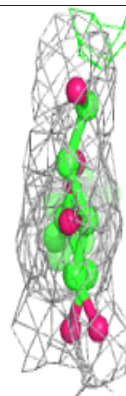
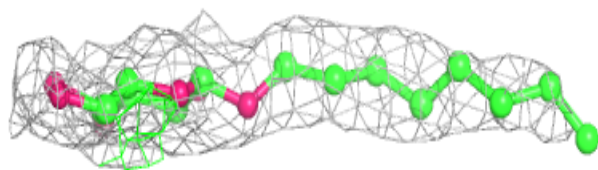
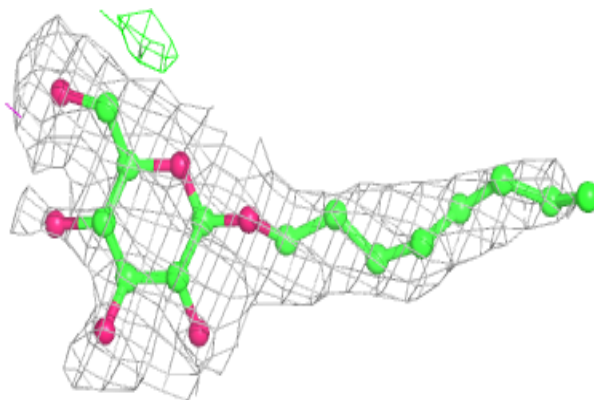
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 620:

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

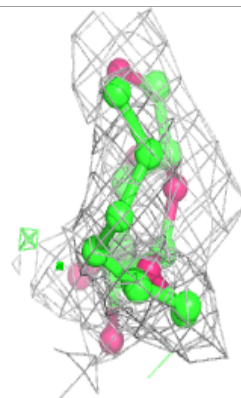
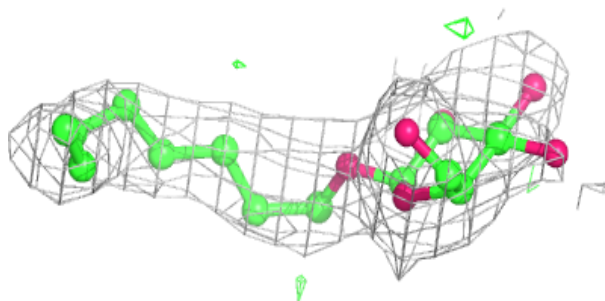
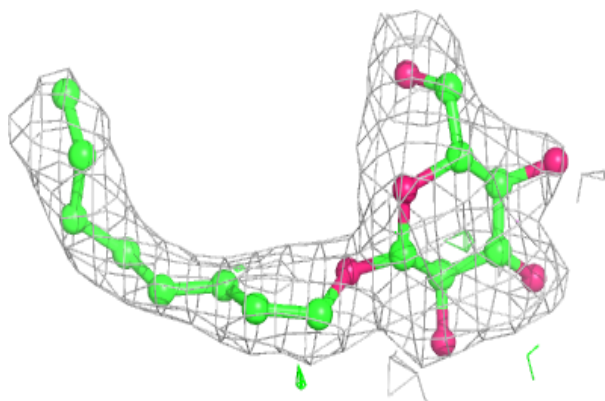
**Electron density around BOG B 620:**

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

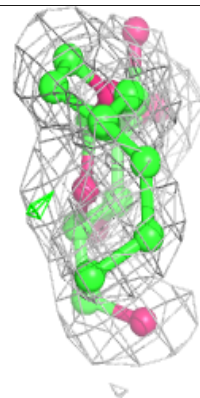
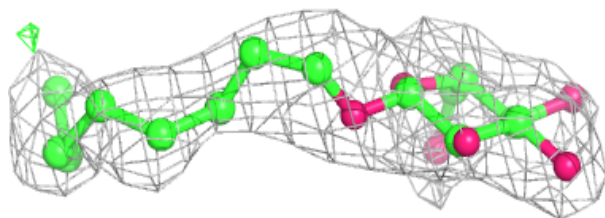
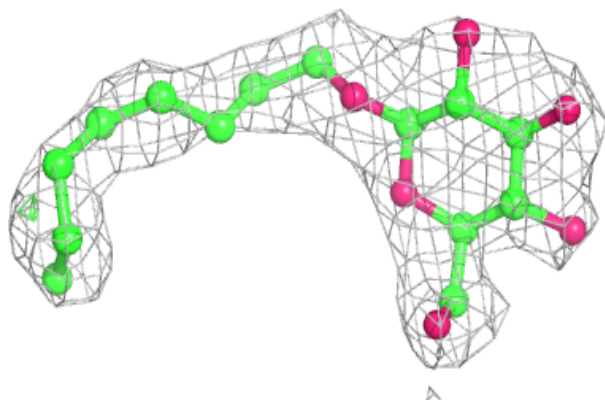


Electron density around BOG A 6:

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

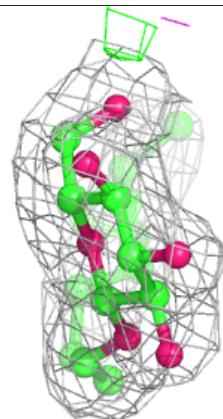
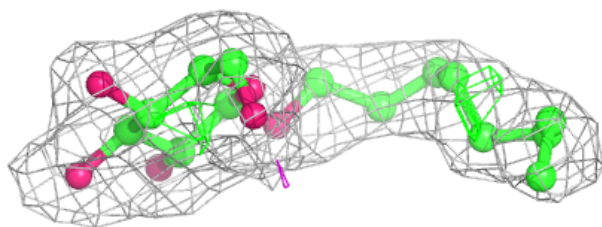
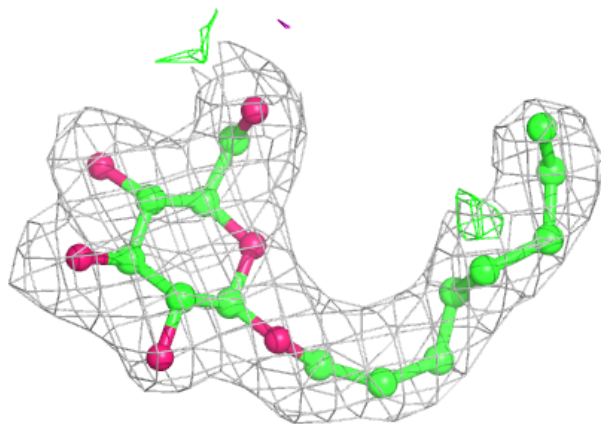
**Electron density around BOG B 3:**

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



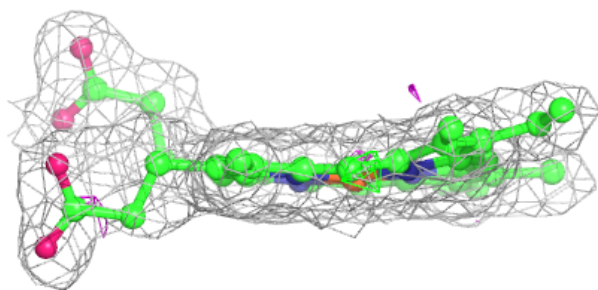
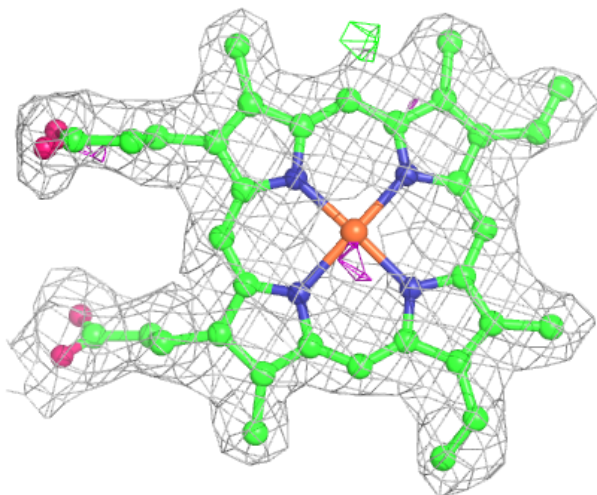
Electron density around BOG A 3:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



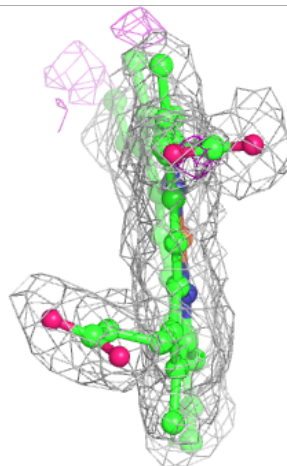
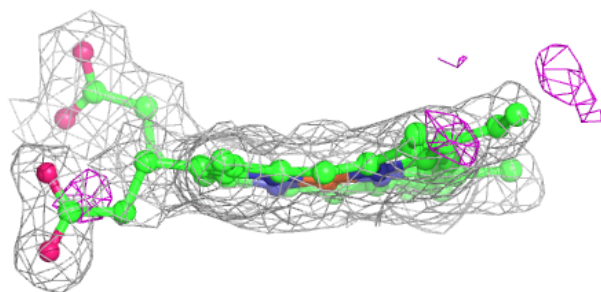
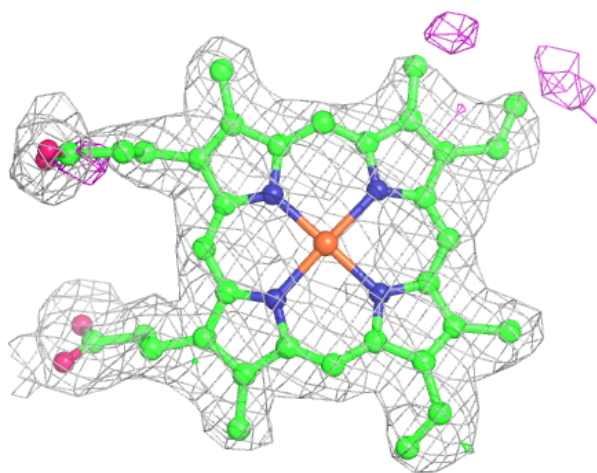
Electron density around HEM A 682:

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



Electron density around HEM B 682:

$2mF_o-DF_c$ (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.