



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:23 PM UTC

PDB ID : 2QD2 / pdb_00002qd2
Title : F110A variant of human ferrochelatase with protoheme bound
Authors : Medlock, A.E.; Dailey, T.A.; Ross, T.A.; Dailey, H.A.; Lanzilota, W.N.
Deposited on : 2007-06-20
Resolution : 2.20 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

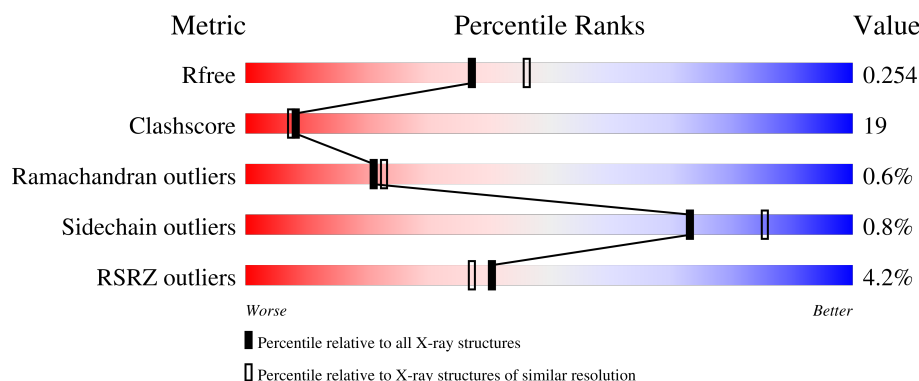
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	359	
1	B	359	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6480 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.

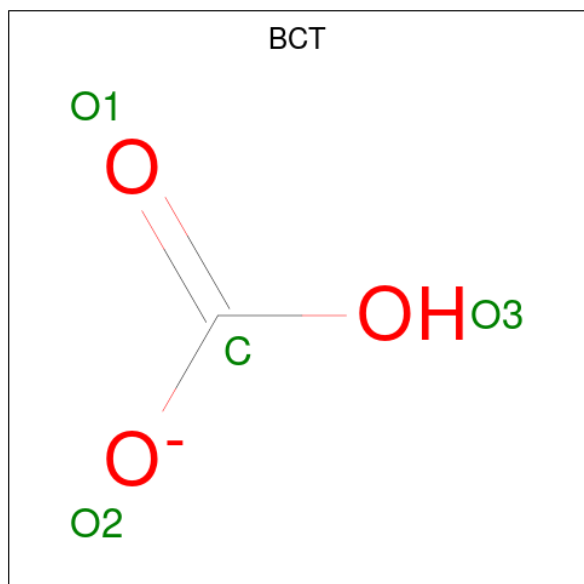
- Molecule 1 is a protein called Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	5	0
			2929	1860	513	537	19			
1	B	359	Total	C	N	O	S	0	6	0
			2933	1861	510	543	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	PHE	engineered mutation	UNP Q7KZA3
B	110	ALA	PHE	engineered mutation	UNP Q7KZA3

- Molecule 2 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



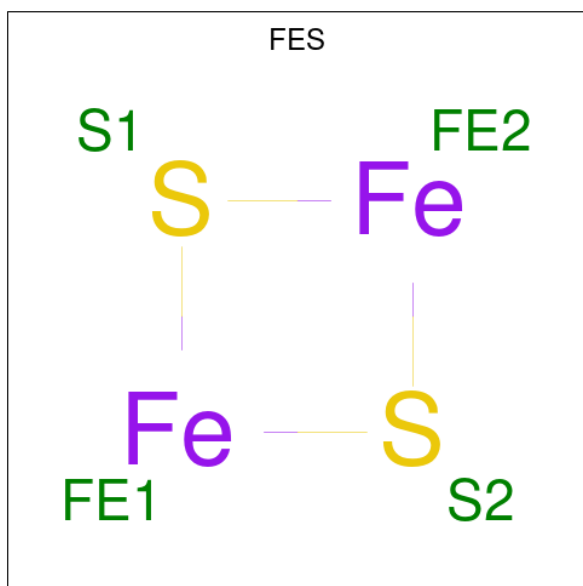
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		

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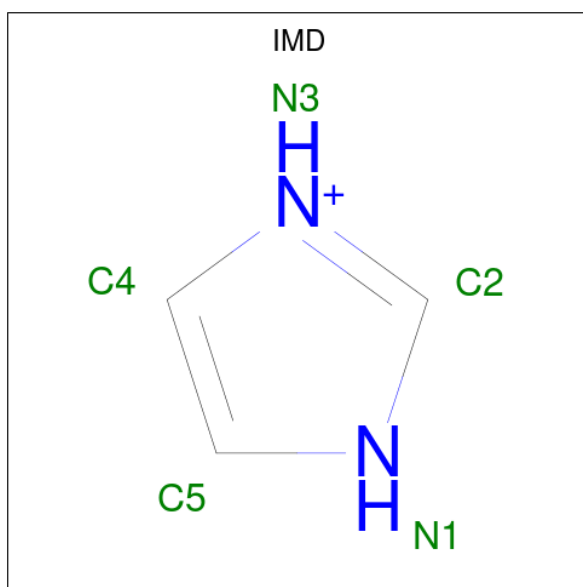
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



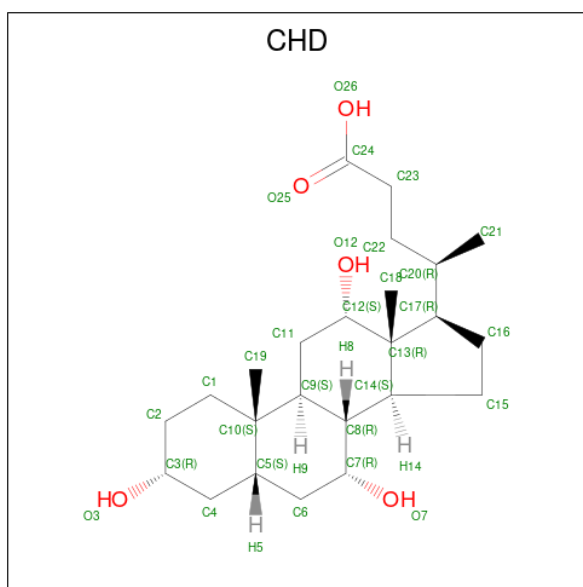
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $\text{C}_3\text{H}_5\text{N}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



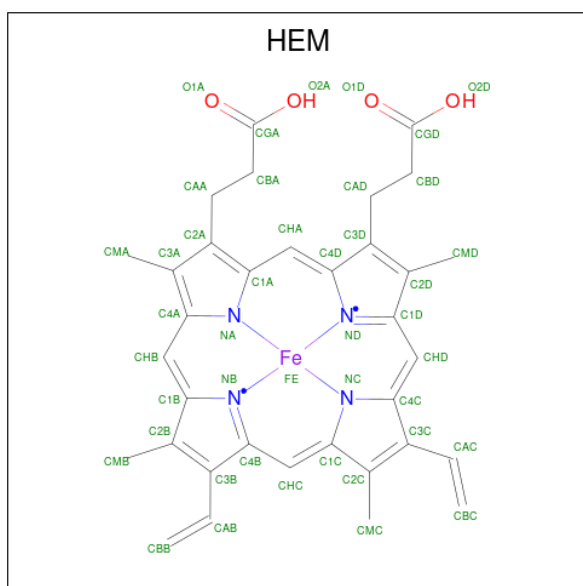
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			29	24	5		
5	B	1	Total	C	O	0	0
			29	24	5		
5	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 6 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	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

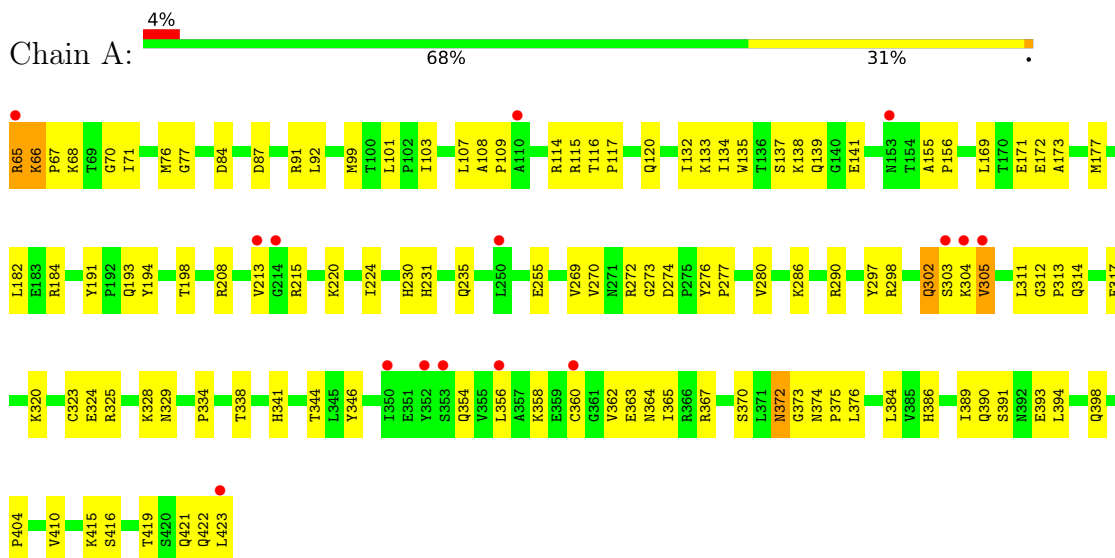
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O	0	0
			199	199		
7	B	186	Total	O	0	0
			186	186		

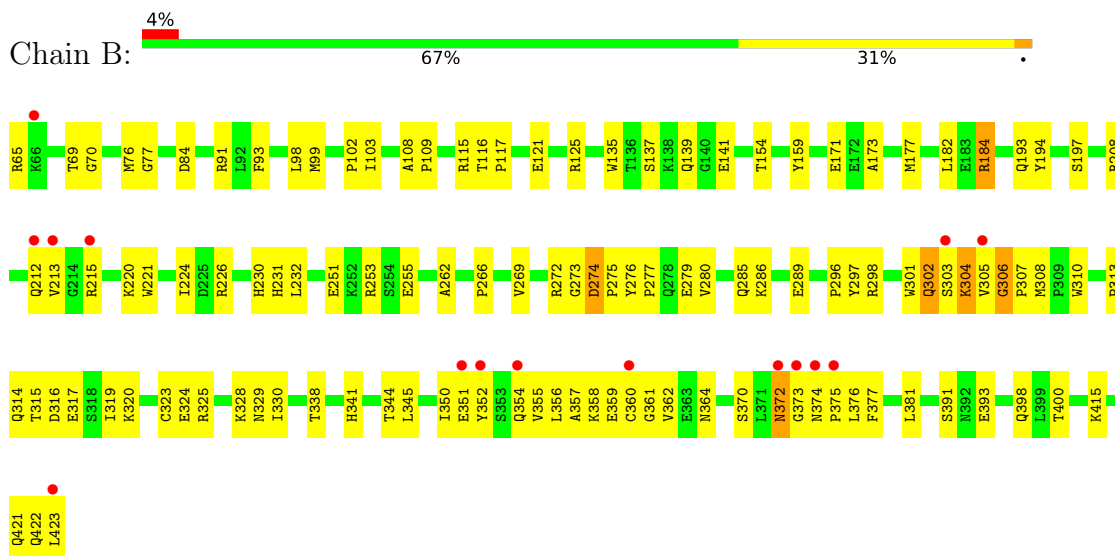
3 Residue-property plots

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: Ferrochelatase



• Molecule 1: Ferrochelatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.20Å 92.64Å 109.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 2.20 46.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.99-2.20) 100.0 (46.99-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.90 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.261 0.215 , 0.254	Depositor DCC
R_{free} test set	2274 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6480	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0170e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CHD, BCT, HEM, IMD, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2998	0.91	8/4059 (0.2%)
1	B	0.38	0/3002	0.91	10/4066 (0.2%)
All	All	0.38	0/6000	0.91	18/8125 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ASP	CA-C-N	7.53	127.17	119.19
1	B	274	ASP	C-N-CA	7.53	127.17	119.19
1	B	302	GLN	N-CA-C	6.64	119.51	109.95
1	A	302	GLN	N-CA-C	6.62	119.49	109.95
1	A	338	THR	N-CA-C	6.47	120.89	113.19
1	A	274	ASP	CA-C-N	6.18	125.81	119.56
1	A	274	ASP	C-N-CA	6.18	125.81	119.56
1	B	338	THR	N-CA-C	6.06	120.40	113.19
1	A	224	ILE	N-CA-C	-5.88	97.11	109.34
1	B	224	ILE	N-CA-C	-5.86	97.15	109.34
1	A	194	TYR	N-CA-C	5.42	118.46	109.46
1	B	194	TYR	N-CA-C	5.37	118.30	109.76
1	A	305	VAL	N-CA-C	5.26	115.43	107.75
1	B	330	ILE	N-CA-C	5.22	115.42	108.11
1	A	231	HIS	N-CA-C	5.13	117.53	111.33
1	B	231	HIS	N-CA-C	5.11	117.51	111.33
1	B	306	GLY	CA-C-N	5.10	126.21	119.84
1	B	306	GLY	C-N-CA	5.10	126.21	119.84

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	2929	0	2935	119	0
1	B	2933	0	2926	127	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	10	0	9	1	0
4	B	5	0	5	3	0
5	A	58	0	78	6	0
5	B	58	0	78	9	0
6	A	43	0	30	1	0
6	B	43	0	30	6	0
7	A	199	0	0	6	0
7	B	186	0	0	8	0
All	All	6480	0	6091	235	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 (235) 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:304:LYS:HD3	1:B:314:GLN:HG3	1.36	1.01
1:B:266:PRO:HD3	6:B:601:HEM:HAB	1.53	0.90
1:B:323[A]:CYS:SG	1:B:362:VAL:HG22	2.15	0.86
1:A:297:TYR:H	1:B:398:GLN:HE22	1.22	0.84
1:A:323[B]:CYS:SG	1:A:360:CYS:HB2	2.19	0.82
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.46	0.81
1:B:358:LYS:HA	1:B:358:LYS:HE2	1.62	0.81
1:A:65:ARG:HE	1:A:65:ARG:N	1.77	0.80
1:B:115:ARG:HH11	1:B:115:ARG:HG2	1.47	0.80
1:A:235:GLN:HE21	1:A:376:LEU:HD21	1.48	0.79
1:A:398:GLN:HE22	1:B:297:TYR:H	1.32	0.78
1:A:139:GLN:HE21	1:A:373:GLY:HA2	1.50	0.77
1:B:208:ARG:HB3	1:B:212[A]:GLN:HE21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLN:O	1:A:423:LEU:HB2	1.87	0.74
1:A:304[B]:LYS:NZ	1:A:312:GLY:HA2	2.03	0.73
1:B:301:TRP:O	1:B:304:LYS:HE3	1.88	0.73
1:B:422:GLN:HG2	1:B:423:LEU:HD13	1.70	0.73
1:A:101:LEU:HD21	5:A:2:CHD:H151	1.69	0.73
1:A:208:ARG:HH21	1:A:410:VAL:HG21	1.54	0.72
1:A:184:ARG:HD3	7:A:776:HOH:O	1.89	0.72
1:B:115:ARG:CZ	5:B:1:CHD:H231	2.19	0.72
1:B:272:ARG:HD2	7:B:612:HOH:O	1.87	0.72
1:A:65:ARG:N	1:A:65:ARG:NE	2.37	0.71
1:B:215:ARG:HD2	7:B:748:HOH:O	1.90	0.71
1:B:304:LYS:H	1:B:304:LYS:HD2	1.53	0.71
1:B:323[A]:CYS:SG	1:B:360:CYS:HB3	2.30	0.71
1:A:220:LYS:HE3	1:A:423:LEU:HD22	1.73	0.71
1:A:415:LYS:HE2	1:A:419:THR:HG21	1.72	0.71
1:A:87:ASP:HB3	1:A:91[A]:ARG:HH12	1.56	0.70
1:B:305:VAL:HB	5:B:1:CHD:C21	2.21	0.70
1:B:305:VAL:HB	5:B:1:CHD:H211	1.73	0.70
1:A:415:LYS:HD3	1:A:416:SER:N	2.07	0.70
1:A:328:LYS:HB3	1:A:363:GLU:HG3	1.74	0.69
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.75	0.69
1:A:67:PRO:HA	1:A:156:PRO:HG2	1.76	0.68
1:A:354:GLN:HE21	1:A:358:LYS:HZ3	1.42	0.68
1:A:208:ARG:HG3	1:A:208:ARG:NH1	2.08	0.68
1:A:304[B]:LYS:HZ1	1:A:312:GLY:HA2	1.59	0.68
1:B:400:THR:HA	1:B:415:LYS:HD2	1.76	0.68
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.76	0.67
1:B:370:SER:HB2	1:B:372:ASN:ND2	2.10	0.67
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.76	0.67
1:B:308:MET:HB2	7:B:737:HOH:O	1.95	0.66
1:A:290:ARG:HG2	1:A:290:ARG:HH11	1.58	0.66
1:A:304[A]:LYS:HZ2	1:A:314:GLN:HB2	1.61	0.66
1:A:354:GLN:HE21	1:A:358:LYS:NZ	1.93	0.66
1:A:313:PRO:HG2	1:B:273:GLY:HA2	1.78	0.66
1:B:422:GLN:O	1:B:423:LEU:HB2	1.96	0.66
1:A:297:TYR:N	1:B:398:GLN:HE22	1.94	0.65
1:A:323[B]:CYS:SG	1:A:360:CYS:CB	2.84	0.65
1:B:213:VAL:O	1:B:215:ARG:HG3	1.96	0.65
1:A:314:GLN:HB3	1:A:317:GLU:HG2	1.78	0.65
1:B:314:GLN:HB3	1:B:317[A]:GLU:HG2	1.79	0.65
1:B:374:ASN:HD22	1:B:375:PRO:N	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:HG3	7:A:699:HOH:O	1.98	0.64
1:A:220:LYS:HD2	1:A:423:LEU:HD13	1.79	0.64
1:A:374:ASN:C	1:A:374:ASN:HD22	2.05	0.64
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.62	0.64
1:B:269:VAL:O	1:B:272:ARG:HG2	1.98	0.63
1:B:374:ASN:ND2	1:B:376:LEU:H	1.96	0.63
1:B:304:LYS:CD	1:B:314:GLN:HG3	2.22	0.62
1:A:334:PRO:HG3	1:A:367:ARG:HH11	1.64	0.62
1:A:137:SER:O	1:A:141:GLU:HG3	1.98	0.62
1:B:69:THR:HG23	1:B:184:ARG:HD2	1.82	0.62
1:B:344:THR:HG22	7:B:769:HOH:O	1.98	0.61
1:A:374:ASN:ND2	1:A:376:LEU:H	1.99	0.61
1:A:304[B]:LYS:HE3	1:A:314:GLN:HA	1.83	0.61
1:A:235:GLN:HE21	1:A:376:LEU:CD2	2.14	0.61
1:B:137:SER:O	1:B:141:GLU:HG3	2.01	0.60
1:A:220:LYS:CE	1:A:423:LEU:HD22	2.30	0.60
1:B:266:PRO:CD	6:B:601:HEM:HAB	2.29	0.60
1:A:374:ASN:HD22	1:A:375:PRO:N	1.98	0.60
1:B:370:SER:C	1:B:372:ASN:H	2.08	0.60
1:A:235:GLN:NE2	1:A:376:LEU:HD21	2.16	0.60
1:A:415:LYS:HD3	1:A:415:LYS:C	2.27	0.60
1:A:184:ARG:NH1	1:A:389:ILE:HG23	2.17	0.60
1:B:356:LEU:O	1:B:360:CYS:HB2	2.00	0.60
1:A:398:GLN:HE22	1:B:297:TYR:N	1.99	0.60
1:A:184:ARG:HH12	1:A:389:ILE:HG23	1.66	0.60
1:A:362:VAL:HG21	1:A:365:ILE:HD11	1.83	0.60
1:A:286:LYS:HE3	1:B:286:LYS:NZ	2.17	0.59
1:B:84:ASP:HB3	7:B:752:HOH:O	2.03	0.59
1:B:116:THR:HB	1:B:117:PRO:HD3	1.83	0.58
1:B:220:LYS:HG3	1:B:220:LYS:O	2.03	0.58
1:B:374:ASN:HD22	1:B:374:ASN:C	2.11	0.58
1:B:221:TRP:H	1:B:421:GLN:NE2	2.02	0.58
1:B:303:SER:O	1:B:305:VAL:HG13	2.03	0.58
1:B:341:HIS:HB2	6:B:601:HEM:O2D	2.03	0.58
1:B:374:ASN:HD22	1:B:375:PRO:CD	2.16	0.58
1:B:305:VAL:C	5:B:1:CHD:H213	2.29	0.58
1:A:116:THR:HB	1:A:117:PRO:HD3	1.84	0.57
1:A:139:GLN:NE2	1:A:373:GLY:HA2	2.17	0.57
1:B:314:GLN:O	1:B:317[A]:GLU:HG2	2.03	0.57
1:B:139:GLN:NE2	1:B:373:GLY:HA2	2.18	0.57
1:A:213:VAL:HG23	1:A:215:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLN:OE1	1:B:317[B]:GLU:HG3	2.04	0.57
1:A:391:SER:OG	1:A:393[A]:GLU:HG3	2.05	0.56
1:B:422:GLN:HG2	1:B:423:LEU:CD1	2.35	0.56
1:B:173:ALA:O	1:B:177:MET:HG3	2.06	0.56
1:B:304:LYS:HD3	1:B:314:GLN:CG	2.24	0.56
1:B:303:SER:CB	4:B:425:IMD:HN1	2.19	0.56
1:A:115:ARG:HD2	5:A:2:CHD:H231	1.87	0.56
1:A:273:GLY:HA3	1:A:404:PRO:HD2	1.87	0.56
1:A:215:ARG:HB3	1:A:215:ARG:NH1	2.22	0.55
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.89	0.55
1:B:102:PRO:O	1:B:103:ILE:C	2.48	0.55
1:A:370:SER:C	1:A:372:ASN:H	2.13	0.55
1:B:320:LYS:O	1:B:324:GLU:HG3	2.06	0.55
1:A:87:ASP:HB3	1:A:91[A]:ARG:NH1	2.22	0.54
1:A:344:THR:HG22	7:A:739:HOH:O	2.06	0.54
1:B:208:ARG:HB3	1:B:212[A]:GLN:NE2	2.19	0.54
1:B:139:GLN:HE21	1:B:373:GLY:HA2	1.72	0.54
1:B:115:ARG:HG2	1:B:115:ARG:NH1	2.19	0.54
1:A:134:ILE:O	1:A:138:LYS:HG2	2.08	0.54
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.72	0.54
1:A:173:ALA:O	1:A:177:MET:HG3	2.08	0.53
1:A:320:LYS:O	1:A:324:GLU:HG3	2.08	0.53
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.21	0.53
1:B:302:GLN:HB3	1:B:315:THR:OG1	2.08	0.53
1:B:99:MET:HG3	5:B:1:CHD:C19	2.39	0.53
1:A:114:ARG:HH12	5:A:426:CHD:H5	1.74	0.53
1:A:286:LYS:HE3	1:B:286:LYS:HZ2	1.73	0.53
1:A:114:ARG:HH12	5:A:426:CHD:C5	2.22	0.53
1:A:235:GLN:HA	1:A:290:ARG:NH1	2.24	0.53
1:A:269:VAL:O	1:A:272:ARG:HG2	2.08	0.53
1:B:303:SER:HB2	4:B:425:IMD:HN1	1.74	0.52
1:A:171:GLU:CD	1:A:171:GLU:H	2.18	0.52
1:A:103:ILE:HG13	1:A:107:LEU:HD13	1.90	0.52
1:A:68:LYS:HE3	1:A:155:ALA:O	2.10	0.52
1:A:313:PRO:CG	1:B:273:GLY:HA2	2.39	0.52
1:B:76:MET:HE1	6:B:601:HEM:CHD	2.40	0.52
1:A:370:SER:HB2	1:A:372:ASN:ND2	2.25	0.52
1:B:230:HIS:CE1	1:B:232:LEU:HB2	2.46	0.51
1:A:135:TRP:CE2	1:A:372:ASN:HB3	2.46	0.51
1:B:305:VAL:HG11	6:B:601:HEM:O2A	2.11	0.50
1:A:422:GLN:HG2	1:A:423:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLU:OE2	1:B:351:GLU:HA	2.10	0.50
1:B:350:ILE:O	1:B:354:GLN:HG3	2.11	0.50
1:B:306:GLY:N	5:B:1:CHD:H213	2.26	0.50
1:B:70:GLY:HA3	1:B:182:LEU:HD13	1.93	0.49
1:B:135:TRP:CE2	1:B:372:ASN:HB3	2.47	0.49
1:A:84:ASP:HB3	7:A:681:HOH:O	2.12	0.49
1:A:99:MET:HB2	5:A:2:CHD:H62	1.94	0.49
1:A:116:THR:O	1:A:120:GLN:HG3	2.12	0.49
1:B:356:LEU:HG	1:B:362:VAL:CG2	2.42	0.49
1:B:220:LYS:HD3	1:B:423:LEU:HD22	1.93	0.49
1:B:355:VAL:O	1:B:359:GLU:HG2	2.11	0.49
1:B:303:SER:HB2	4:B:425:IMD:N1	2.26	0.49
1:A:191:TYR:CZ	1:A:198:THR:HB	2.48	0.49
1:A:304[A]:LYS:HZ1	1:A:312:GLY:HA2	1.77	0.49
1:B:139:GLN:HG3	7:B:726:HOH:O	2.13	0.49
1:A:169:LEU:HB2	1:A:172:GLU:HG3	1.95	0.48
1:A:273:GLY:O	1:B:298:ARG:NH1	2.46	0.48
1:A:386:HIS:O	1:A:390:GLN:HG3	2.13	0.48
1:A:208:ARG:NH2	1:A:410:VAL:HG21	2.26	0.48
1:A:341:HIS:HB2	6:A:602:HEM:O2D	2.12	0.48
1:B:370:SER:C	1:B:372:ASN:N	2.72	0.48
1:A:71:ILE:N	1:A:71:ILE:HD12	2.28	0.48
1:B:208:ARG:O	1:B:212[A]:GLN:HG3	2.14	0.47
1:B:121:GLU:O	1:B:125:ARG:HG2	2.15	0.47
1:B:171:GLU:H	1:B:171:GLU:CD	2.21	0.47
1:B:374:ASN:ND2	1:B:374:ASN:C	2.72	0.47
1:B:351:GLU:O	1:B:355:VAL:HG23	2.14	0.47
1:A:374:ASN:C	1:A:374:ASN:ND2	2.70	0.47
1:B:374:ASN:HD22	1:B:375:PRO:HD2	1.78	0.47
1:A:91[B]:ARG:NH2	1:A:169:LEU:HD11	2.30	0.47
1:A:193:GLN:HG2	1:A:280:VAL:HA	1.96	0.46
1:A:155:ALA:HB1	1:A:156:PRO:HA	1.97	0.46
1:B:357:ALA:HA	1:B:362:VAL:HG23	1.96	0.46
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.81	0.46
1:B:314:GLN:HB3	1:B:317[A]:GLU:CG	2.45	0.46
1:A:101:LEU:HD21	5:A:2:CHD:H7	1.96	0.46
1:A:215:ARG:HB3	1:A:215:ARG:HH11	1.80	0.46
1:B:391:SER:OG	1:B:393[B]:GLU:HG3	2.16	0.45
1:A:394:LEU:HD22	1:A:421:GLN:HB2	1.97	0.45
1:A:66:LYS:HG2	1:A:67:PRO:HD2	1.97	0.45
1:A:235:GLN:HG3	1:A:290:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:HH11	1:B:253:ARG:HG2	1.82	0.45
1:B:325:ARG:HG3	1:B:325:ARG:HH11	1.81	0.45
1:B:193:GLN:HG2	1:B:280:VAL:HA	1.97	0.45
1:A:370:SER:C	1:A:372:ASN:N	2.74	0.45
1:A:398:GLN:NE2	1:B:296:PRO:HA	2.31	0.45
1:B:76:MET:HG3	1:B:77:GLY:O	2.16	0.45
1:B:93:PHE:CZ	1:B:115:ARG:HD3	2.52	0.45
1:B:285:GLN:O	1:B:289:GLU:HB2	2.16	0.45
1:B:314:GLN:H	1:B:317[A]:GLU:CD	2.24	0.45
1:A:304[A]:LYS:HE2	1:A:311:LEU:O	2.17	0.44
1:A:334:PRO:HG3	1:A:367:ARG:NH1	2.30	0.44
1:B:356:LEU:HG	1:B:362:VAL:HG21	1.99	0.44
1:A:374:ASN:HD22	1:A:375:PRO:HD2	1.81	0.44
1:A:132:ILE:HG23	1:A:133:LYS:N	2.32	0.44
1:B:98:LEU:HD12	1:B:197:SER:HB2	1.99	0.44
1:B:226:ARG:HD3	1:B:279:GLU:OE2	2.17	0.44
1:B:316:ASP:OD1	1:B:344:THR:HB	2.17	0.44
1:A:302:GLN:NE2	7:A:789:HOH:O	2.45	0.44
1:A:70:GLY:HA3	1:A:182:LEU:HD13	2.00	0.44
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.74	0.43
1:A:91[A]:ARG:NH1	7:A:695:HOH:O	2.51	0.43
1:B:159:TYR:CD1	1:B:159:TYR:C	2.96	0.43
1:A:76:MET:HG3	1:A:77:GLY:O	2.19	0.43
1:A:213:VAL:CG2	1:A:215:ARG:HG2	2.49	0.43
1:B:91:ARG:NH1	7:B:698:HOH:O	2.52	0.43
1:B:99:MET:HG3	5:B:1:CHD:H192	2.01	0.43
1:B:304:LYS:H	1:B:304:LYS:CD	2.26	0.43
1:B:303:SER:O	1:B:304:LYS:C	2.60	0.43
1:A:346:TYR:CD2	1:A:356:LEU:HD22	2.54	0.42
1:B:115:ARG:NH1	5:B:1:CHD:H231	2.34	0.42
1:B:230:HIS:HE1	1:B:232:LEU:HB2	1.84	0.42
1:B:251:GLU:CD	1:B:251:GLU:H	2.26	0.42
1:A:415:LYS:O	1:A:419:THR:HG23	2.19	0.42
1:B:304:LYS:HD2	1:B:304:LYS:N	2.26	0.42
1:B:99:MET:HG3	5:B:1:CHD:H191	2.01	0.42
1:B:65:ARG:HH11	1:B:65:ARG:HG2	1.84	0.42
1:B:115:ARG:NH1	1:B:115:ARG:CG	2.80	0.42
1:B:315:THR:O	1:B:319:ILE:HG13	2.19	0.42
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.85	0.42
1:B:325:ARG:HG3	1:B:325:ARG:NH1	2.35	0.41
1:A:103:ILE:HG13	1:A:103:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:O	1:B:313:PRO:HD3	2.20	0.41
1:A:171:GLU:CD	1:A:171:GLU:N	2.79	0.41
1:A:230:HIS:CD2	1:A:384:LEU:HG	2.56	0.41
1:A:290:ARG:HG2	1:A:290:ARG:NH1	2.29	0.41
1:B:310:TRP:NE1	7:B:737:HOH:O	2.53	0.41
1:A:303:SER:O	1:A:305:VAL:HG13	2.21	0.41
1:B:262:ALA:O	1:B:301:TRP:HA	2.20	0.41
1:B:354:GLN:O	1:B:358:LYS:HG2	2.20	0.41
1:B:377:PHE:O	1:B:381:LEU:HG	2.21	0.41
1:A:303:SER:O	4:A:425:IMD:N1	2.43	0.41
1:A:422:GLN:HG2	1:A:423:LEU:HD13	2.03	0.41
1:A:92:LEU:C	1:A:92:LEU:HD23	2.46	0.41
1:B:69:THR:OG1	1:B:154:THR:HB	2.21	0.40
1:B:102:PRO:C	1:B:103:ILE:HG12	2.46	0.40
1:B:328:LYS:HD3	1:B:361:GLY:O	2.22	0.40
1:B:345:LEU:HD11	1:B:352:TYR:CD2	2.56	0.40
1:B:115:ARG:HH21	6:B:601:HEM:CGA	2.34	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	362/359 (101%)	347 (96%)	13 (4%)	2 (1%)	21	23
1	B	363/359 (101%)	351 (97%)	10 (3%)	2 (1%)	21	23
All	All	725/718 (101%)	698 (96%)	23 (3%)	4 (1%)	21	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	ASN

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Mol	Chain	Res	Type
1	B	372	ASN
1	A	66	LYS
1	B	307	PRO

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	328/323 (102%)	326 (99%)	2 (1%)	78	89
1	B	329/323 (102%)	325 (99%)	4 (1%)	63	78
All	All	657/646 (102%)	651 (99%)	6 (1%)	73	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	255	GLU
1	B	184	ARG
1	B	255[A]	GLU
1	B	255[B]	GLU
1	B	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	211	ASN
1	A	231	HIS
1	A	235	GLN
1	A	278	GLN
1	A	302	GLN
1	A	329	ASN
1	A	354	GLN
1	A	374	ASN

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Mol	Chain	Res	Type
1	A	390	GLN
1	A	398	GLN
1	A	421	GLN
1	B	120	GLN
1	B	153	ASN
1	B	235	GLN
1	B	329	ASN
1	B	354	GLN
1	B	364	ASN
1	B	374	ASN
1	B	392	ASN
1	B	398	GLN
1	B	421	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	CHD	B	1	-	32,32,32	1.48	7 (21%)	51,51,51	1.46	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHD	B	4	-	32,32,32	1.55	7 (21%)	51,51,51	1.55	9 (17%)
6	HEM	A	602	4,2	50,50,50	1.83	14 (28%)	67,82,82	1.63	15 (22%)
3	FES	A	424	1	0,4,4	-	-	-	-	-
2	BCT	B	2	-	3,3,3	0.79	0	2,3,3	0.26	0
2	BCT	A	1	6	3,3,3	0.59	0	2,3,3	0.17	0
4	IMD	B	425	6	5,5,5	0.35	0	5,5,5	0.50	0
6	HEM	B	601	4	50,50,50	1.79	14 (28%)	67,82,82	1.57	12 (17%)
5	CHD	A	426	-	32,32,32	1.55	7 (21%)	51,51,51	1.55	9 (17%)
4	IMD	A	425	6	5,5,5	0.37	0	5,5,5	0.50	0
5	CHD	A	2	-	32,32,32	1.51	6 (18%)	51,51,51	1.51	9 (17%)
4	IMD	A	3	-	5,5,5	0.38	0	5,5,5	0.46	0
3	FES	B	424	1	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHD	B	1	-	-	0/9/74/74	0/4/4/4
5	CHD	B	4	-	-	0/9/74/74	0/4/4/4
4	IMD	A	3	-	-	-	0/1/1/1
3	FES	A	424	1	-	-	0/1/1/1
4	IMD	B	425	6	-	-	0/1/1/1
6	HEM	B	601	4	-	8/14/54/54	-
5	CHD	A	426	-	-	0/9/74/74	0/4/4/4
4	IMD	A	425	6	-	-	0/1/1/1
5	CHD	A	2	-	-	0/9/74/74	0/4/4/4
6	HEM	A	602	4,2	-	8/14/54/54	-
3	FES	B	424	1	-	-	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	HEM	CAC-C3C	-4.20	1.36	1.47
6	A	602	HEM	C1B-NB	-4.07	1.33	1.40
6	A	602	HEM	CAC-C3C	-3.99	1.36	1.47
6	B	601	HEM	C1B-NB	-3.67	1.33	1.40
6	A	602	HEM	C3B-C2B	3.43	1.44	1.37
6	B	601	HEM	C3C-C4C	3.37	1.51	1.46
6	B	601	HEM	O2A-CGA	-3.35	1.19	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	HEM	O2A-CGA	-3.34	1.19	1.30
6	B	601	HEM	C3B-C2B	3.31	1.43	1.37
6	A	602	HEM	C4C-NC	-3.29	1.33	1.39
6	A	602	HEM	C3C-C4C	3.13	1.51	1.46
6	A	602	HEM	CBD-CGD	-3.06	1.43	1.50
6	B	601	HEM	C4C-NC	-3.06	1.33	1.39
5	A	2	CHD	C10-C9	2.97	1.61	1.56
6	B	601	HEM	CBD-CGD	-2.96	1.43	1.50
5	A	426	CHD	C18-C13	2.90	1.58	1.54
5	B	4	CHD	C18-C13	2.89	1.58	1.54
5	B	1	CHD	C18-C13	2.75	1.58	1.54
5	A	2	CHD	C11-C9	2.70	1.58	1.53
6	A	602	HEM	C4D-C3D	2.68	1.49	1.45
5	A	426	CHD	C20-C17	2.65	1.58	1.54
5	B	1	CHD	C8-C9	2.65	1.59	1.53
5	B	4	CHD	C20-C17	2.64	1.58	1.54
5	A	2	CHD	C18-C13	2.61	1.58	1.54
5	A	2	CHD	C11-C12	2.54	1.57	1.53
6	B	601	HEM	CHB-C4A	-2.51	1.33	1.39
5	B	1	CHD	C20-C17	2.49	1.58	1.54
6	B	601	HEM	C1D-C2D	2.45	1.49	1.44
6	A	602	HEM	CHD-C4C	-2.44	1.33	1.38
6	A	602	HEM	CHB-C4A	-2.42	1.34	1.39
5	A	426	CHD	C8-C9	2.42	1.58	1.53
5	B	4	CHD	C8-C9	2.42	1.58	1.53
5	B	1	CHD	C6-C7	2.35	1.57	1.52
5	B	4	CHD	C6-C5	2.34	1.57	1.53
5	A	426	CHD	C6-C5	2.34	1.57	1.53
6	B	601	HEM	C4D-C3D	2.30	1.48	1.45
6	B	601	HEM	FE-NB	2.28	2.01	1.94
5	B	1	CHD	C6-C5	2.27	1.57	1.53
6	A	602	HEM	CMA-C3A	2.24	1.55	1.50
6	B	601	HEM	CMA-C3A	2.22	1.55	1.50
6	A	602	HEM	FE-NB	2.21	2.01	1.94
5	B	4	CHD	C6-C7	2.20	1.56	1.52
5	A	426	CHD	C6-C7	2.18	1.56	1.52
6	A	602	HEM	C1D-ND	-2.17	1.34	1.38
5	A	426	CHD	C10-C9	2.17	1.59	1.56
6	B	601	HEM	C1D-ND	-2.16	1.34	1.38
5	B	4	CHD	C10-C9	2.15	1.59	1.56
5	A	2	CHD	C8-C9	2.14	1.58	1.53
6	A	602	HEM	C1D-C2D	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2	CHD	C20-C17	2.09	1.58	1.54
6	B	601	HEM	CHD-C4C	-2.07	1.34	1.38
5	B	1	CHD	C16-C17	2.04	1.58	1.54
5	B	4	CHD	C4-C3	2.04	1.55	1.52
5	B	1	CHD	C10-C9	2.03	1.59	1.56
5	A	426	CHD	C4-C3	2.03	1.55	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	HEM	C4C-C3C-C2C	-4.23	103.14	106.81
6	B	601	HEM	C4C-C3C-C2C	-4.15	103.21	106.81
5	B	1	CHD	C9-C11-C12	-4.09	108.95	114.29
6	B	601	HEM	C3B-C4B-NB	4.04	112.37	109.47
6	A	602	HEM	C3B-C4B-NB	3.92	112.28	109.47
6	A	602	HEM	C2B-C1B-NB	3.89	114.31	109.84
6	B	601	HEM	C2B-C1B-NB	3.83	114.24	109.84
5	A	2	CHD	C17-C13-C12	3.65	120.95	117.67
5	A	2	CHD	C9-C11-C12	-3.64	109.53	114.29
6	A	602	HEM	C3B-C2B-C1B	-3.43	103.84	106.41
6	B	601	HEM	C3B-C2B-C1B	-3.42	103.84	106.41
5	A	426	CHD	C13-C17-C20	-3.31	115.47	119.48
5	B	4	CHD	C13-C17-C20	-3.29	115.50	119.48
5	B	4	CHD	C9-C11-C12	-3.27	110.01	114.29
5	A	426	CHD	C9-C11-C12	-3.27	110.01	114.29
5	A	426	CHD	C17-C13-C12	3.20	120.55	117.67
5	B	4	CHD	C17-C13-C12	3.20	120.55	117.67
5	A	426	CHD	C13-C14-C8	-3.12	110.77	114.72
5	B	1	CHD	C19-C10-C9	-3.11	107.00	111.18
5	B	4	CHD	C13-C14-C8	-3.10	110.79	114.72
5	A	2	CHD	C19-C10-C9	-3.01	107.13	111.18
5	A	426	CHD	C19-C10-C9	-2.99	107.16	111.18
5	B	4	CHD	C19-C10-C9	-2.95	107.22	111.18
5	B	1	CHD	C16-C15-C14	-2.82	99.63	105.14
6	A	602	HEM	CAA-C2A-C1A	2.78	130.37	124.94
5	A	426	CHD	C11-C9-C10	-2.75	110.91	113.70
5	B	4	CHD	C11-C9-C10	-2.74	110.92	113.70
6	A	602	HEM	CBD-CAD-C3D	-2.72	105.03	112.53
5	B	1	CHD	C11-C9-C10	-2.69	110.97	113.70
5	B	1	CHD	C13-C14-C8	-2.64	111.37	114.72
5	A	2	CHD	C16-C15-C14	-2.60	100.05	105.14
5	A	2	CHD	C10-C9-C8	-2.59	108.95	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	HEM	CBC-CAC-C3C	2.52	140.14	127.53
6	B	601	HEM	CBD-CAD-C3D	-2.50	105.62	112.53
5	B	1	CHD	C6-C5-C10	-2.48	110.02	112.66
5	A	426	CHD	C16-C15-C14	-2.48	100.29	105.14
6	B	601	HEM	CBC-CAC-C3C	2.46	139.84	127.53
5	B	4	CHD	C16-C15-C14	-2.46	100.33	105.14
6	A	602	HEM	CAD-C3D-C4D	2.45	128.97	124.70
6	A	602	HEM	CHB-C1B-NB	-2.44	121.35	124.37
5	A	2	CHD	C6-C5-C10	-2.41	110.10	112.66
6	B	601	HEM	CHB-C1B-NB	-2.40	121.40	124.37
6	B	601	HEM	CAA-C2A-C1A	2.38	129.58	124.94
6	B	601	HEM	CHC-C1C-NC	2.36	127.03	124.45
6	A	602	HEM	C4A-C3A-C2A	2.33	109.48	106.82
5	B	4	CHD	C6-C5-C10	-2.25	110.27	112.66
5	A	426	CHD	C6-C5-C10	-2.24	110.27	112.66
6	A	602	HEM	CHC-C1C-NC	2.23	126.88	124.45
5	A	2	CHD	C16-C17-C20	-2.22	108.82	112.18
5	A	426	CHD	C18-C13-C14	-2.19	107.78	111.20
5	A	2	CHD	C13-C14-C8	-2.18	111.96	114.72
6	A	602	HEM	C1D-C2D-C3D	-2.17	104.69	106.98
6	B	601	HEM	C4A-C3A-C2A	2.17	109.30	106.82
5	B	4	CHD	C18-C13-C14	-2.14	107.84	111.20
5	B	1	CHD	C4-C5-C10	-2.14	110.38	112.66
5	B	1	CHD	C13-C17-C20	-2.06	116.99	119.48
6	B	601	HEM	CAD-C3D-C4D	2.05	128.27	124.70
6	A	602	HEM	CMD-C2D-C3D	2.04	131.68	126.15
6	A	602	HEM	CAD-C3D-C2D	-2.04	124.04	127.87
6	B	601	HEM	C1D-C2D-C3D	-2.03	104.84	106.98
5	A	2	CHD	C5-C4-C3	-2.03	109.64	112.71
6	A	602	HEM	CHD-C1D-C2D	-2.02	121.84	125.03

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	HEM	C2C-C3C-CAC-CBC
6	B	601	HEM	C2B-C3B-CAB-CBB
6	B	601	HEM	C4B-C3B-CAB-CBB
6	B	601	HEM	C2C-C3C-CAC-CBC
6	A	602	HEM	C2A-CAA-CBA-CGA
6	A	602	HEM	C3D-CAD-CBD-CGD
6	A	602	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	B	601	HEM	C4C-C3C-CAC-CBC
6	A	602	HEM	CAD-CBD-CGD-O1D
6	B	601	HEM	CAD-CBD-CGD-O2D
6	B	601	HEM	CAD-CBD-CGD-O1D
6	A	602	HEM	CAD-CBD-CGD-O2D
6	A	602	HEM	C2B-C3B-CAB-CBB
6	A	602	HEM	C4B-C3B-CAB-CBB
6	B	601	HEM	CAA-CBA-CGA-O2A
6	B	601	HEM	CAA-CBA-CGA-O1A

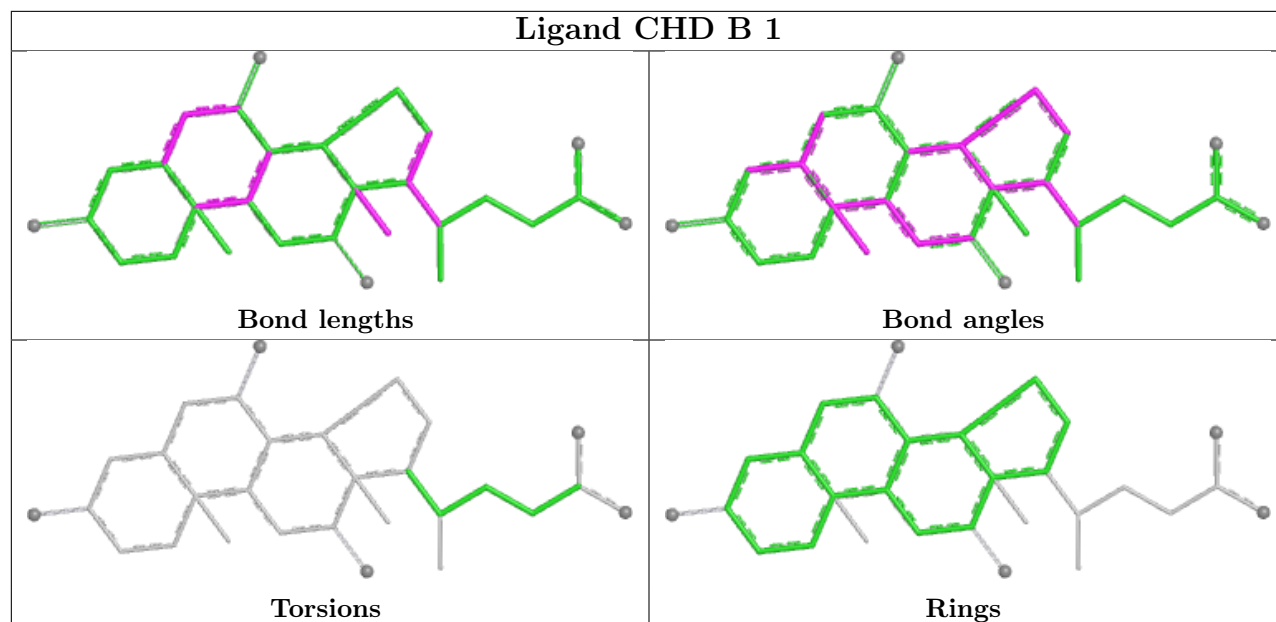
There are no ring outliers.

7 monomers are involved in 26 short contacts:

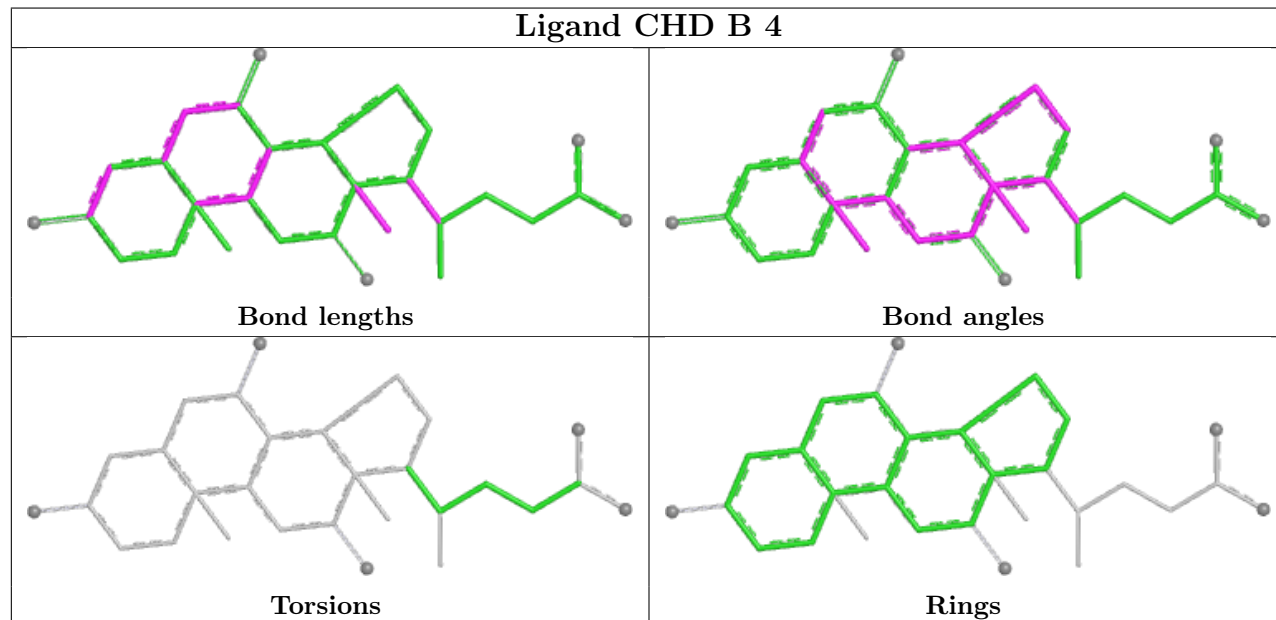
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	CHD	9	0
6	A	602	HEM	1	0
4	B	425	IMD	3	0
6	B	601	HEM	6	0
5	A	426	CHD	2	0
4	A	425	IMD	1	0
5	A	2	CHD	4	0

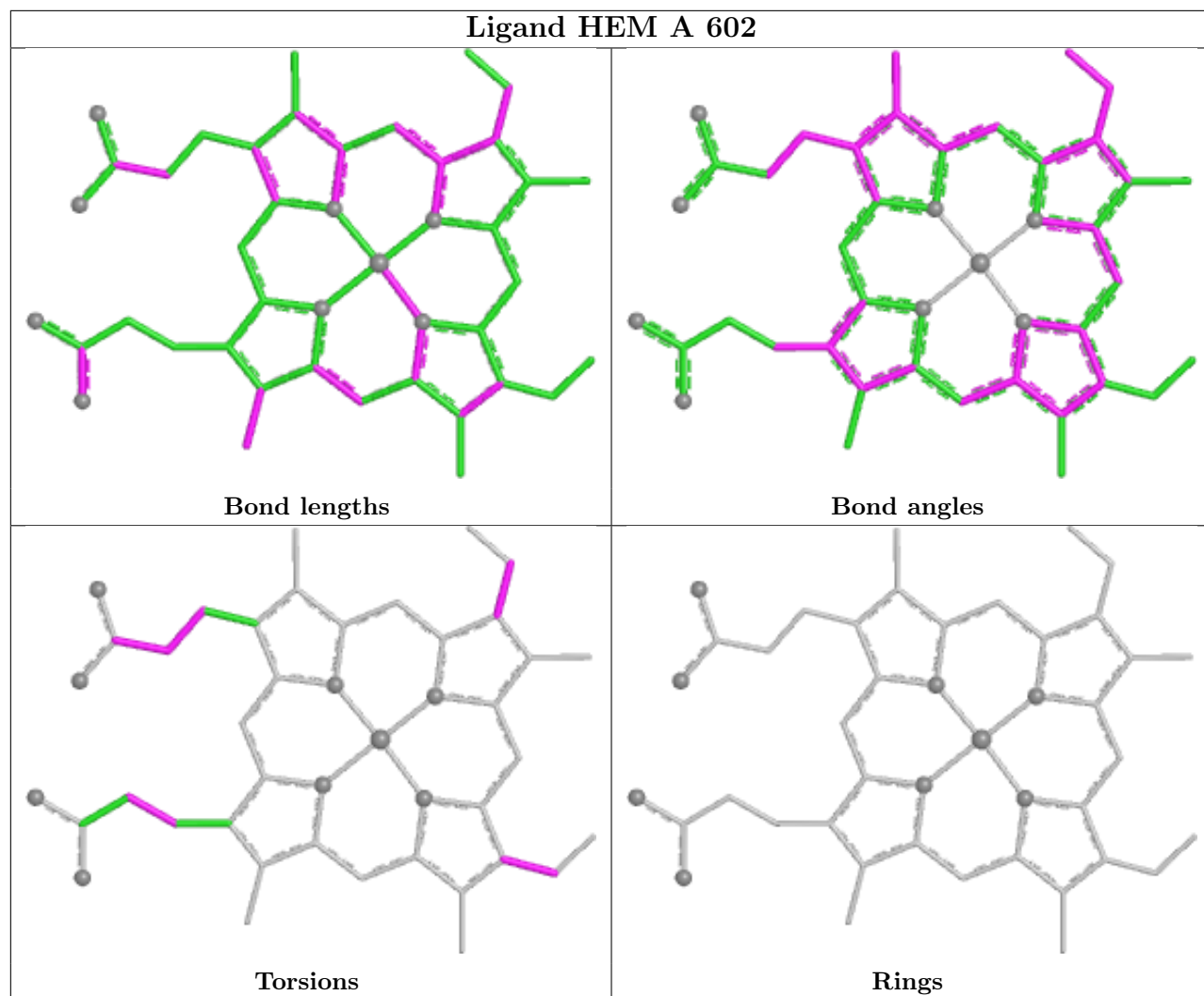
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

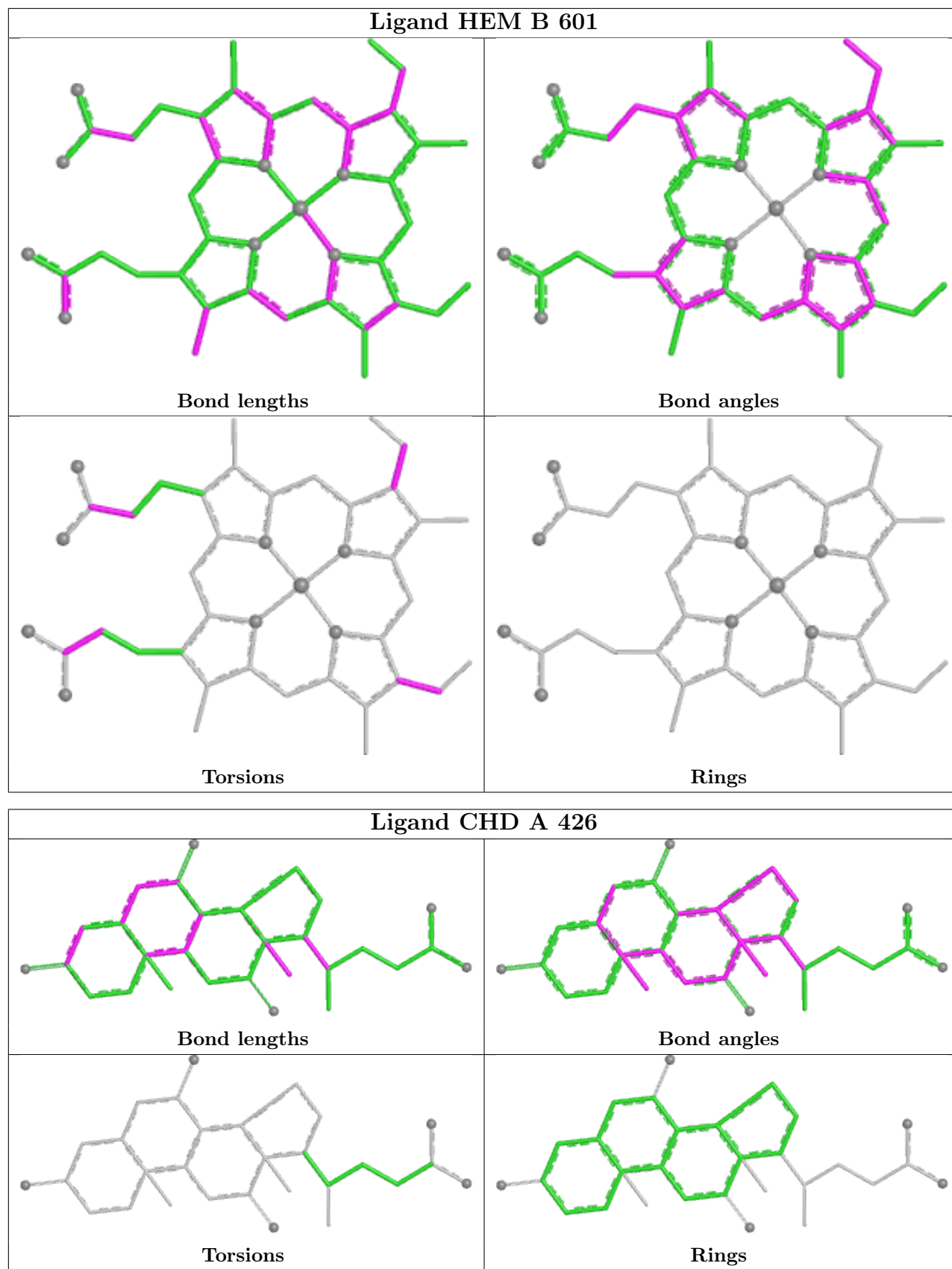
Ligand CHD B 1

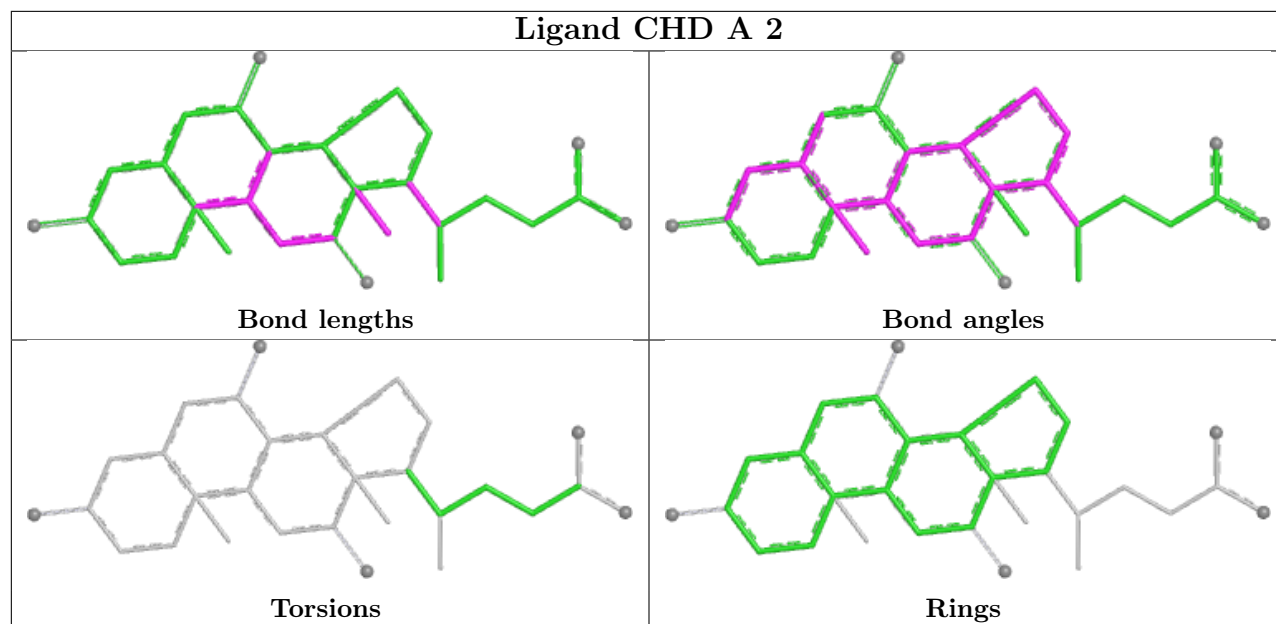


Ligand CHD B 4









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

6.1 Protein, DNA and RNA chains

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	359/359 (100%)	0.32	15 (4%)	40	37	14, 30, 50, 59	5 (1%)
1	B	359/359 (100%)	0.34	15 (4%)	40	37	13, 29, 50, 59	6 (1%)
All	All	718/718 (100%)	0.33	30 (4%)	40	37	13, 30, 50, 59	11 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	SER	4.2
1	A	303	SER	3.7
1	A	305	VAL	3.0
1	A	213	VAL	3.0
1	B	423	LEU	2.8
1	B	372	ASN	2.8
1	B	305	VAL	2.8
1	B	213	VAL	2.8
1	B	215	ARG	2.7
1	B	374	ASN	2.7
1	A	352	TYR	2.7
1	B	352	TYR	2.6
1	A	65	ARG	2.6
1	B	354	GLN	2.5
1	B	373	GLY	2.4
1	B	360	CYS	2.4
1	A	153	ASN	2.3
1	A	110	ALA	2.3
1	A	304[A]	LYS	2.3
1	A	350	ILE	2.1
1	A	353	SER	2.1
1	A	423	LEU	2.1
1	B	351	GLU	2.1
1	A	214	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	212[A]	GLN	2.1
1	B	375	PRO	2.1
1	A	360	CYS	2.1
1	A	250	LEU	2.1
1	B	66	LYS	2.0
1	A	356	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

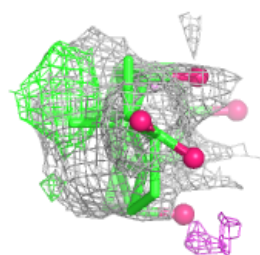
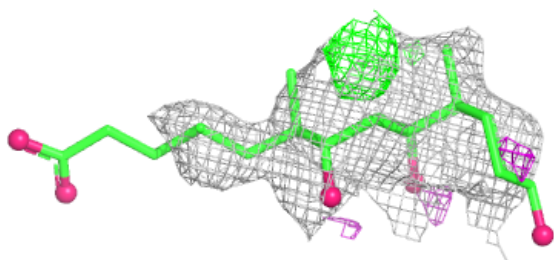
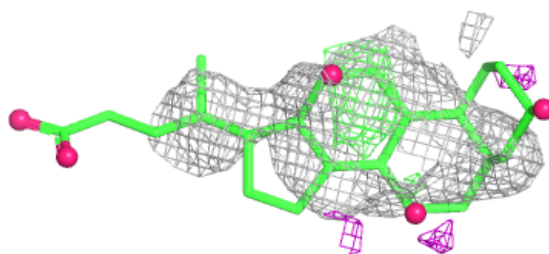
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CHD	B	4	29/29	0.56	0.26	95,95,96,96	0
5	CHD	A	2	29/29	0.71	0.28	81,81,83,84	0
5	CHD	B	1	29/29	0.73	0.31	90,91,93,93	0
5	CHD	A	426	29/29	0.77	0.21	89,89,91,91	0
2	BCT	B	2	4/4	0.84	0.20	30,31,32,32	0
2	BCT	A	1	4/4	0.87	0.17	50,51,51,51	0
4	IMD	A	3	5/5	0.90	0.11	32,32,32,32	0
6	HEM	A	602	43/43	0.94	0.11	24,28,33,35	0
4	IMD	A	425	5/5	0.95	0.08	34,34,34,34	0
6	HEM	B	601	43/43	0.95	0.11	26,27,33,35	0
4	IMD	B	425	5/5	0.96	0.07	27,27,28,28	0
3	FES	B	424	4/4	0.98	0.04	23,24,25,25	0
3	FES	A	424	4/4	0.98	0.05	24,24,25,26	0

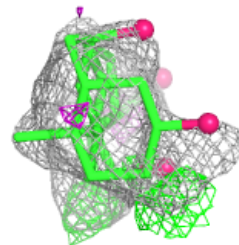
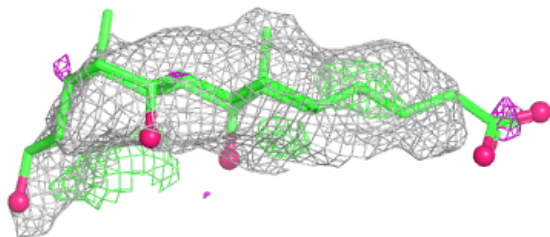
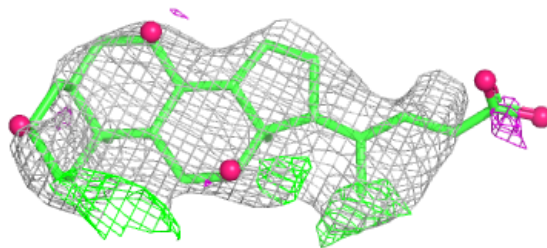
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD B 4:

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

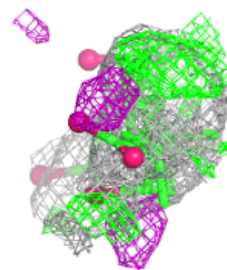
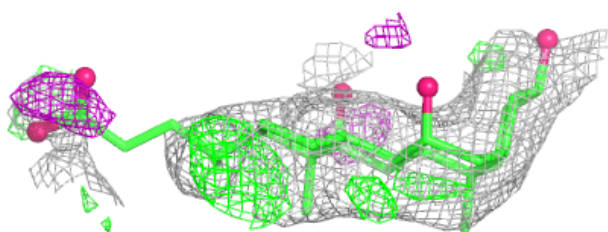
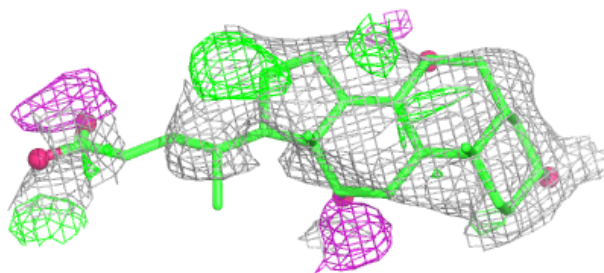
**Electron density around CHD A 2:**

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

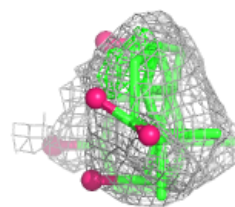
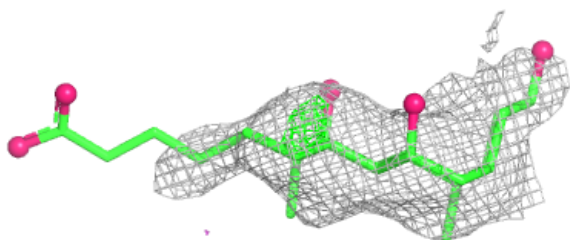
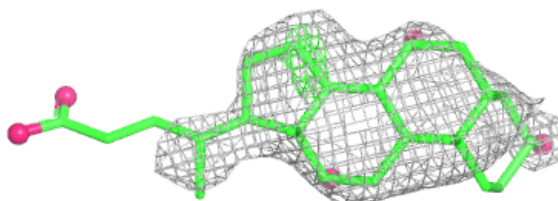


Electron density around CHD B 1:

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

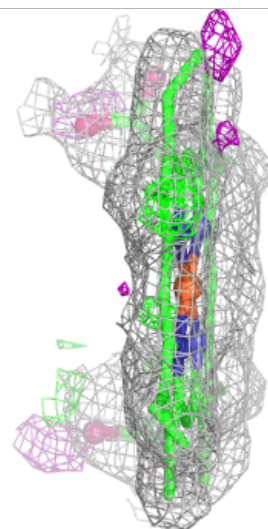
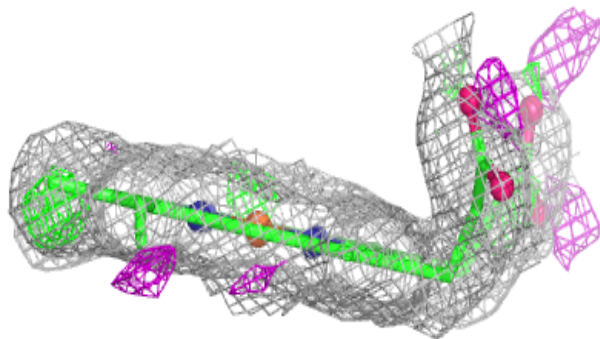
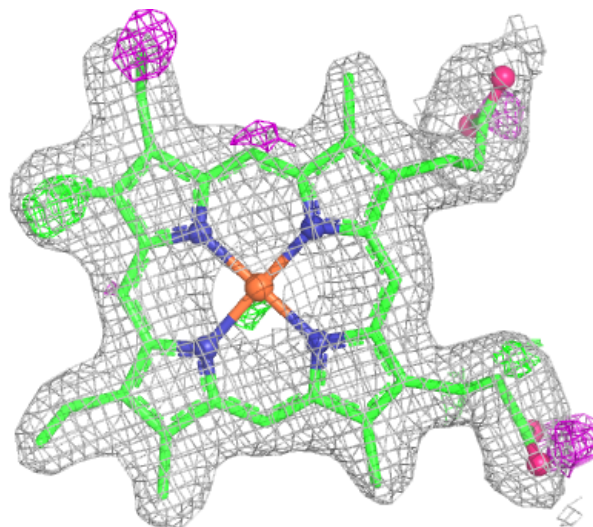
**Electron density around CHD A 426:**

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



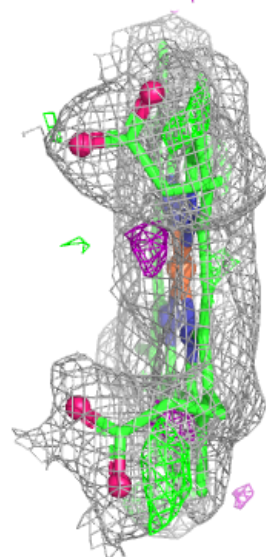
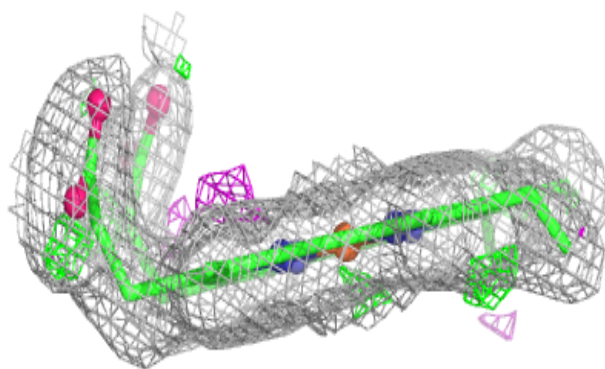
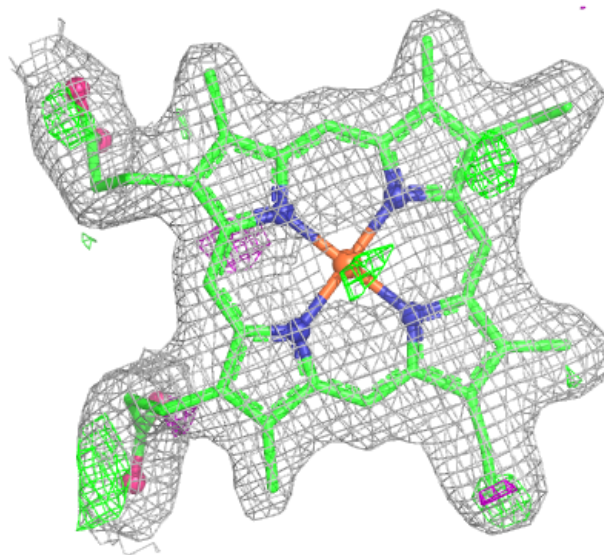
Electron density around HEM A 602:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.