



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:41 PM EDT

PDB ID : 4CAT
Title : THREE-DIMENSIONAL STRUCTURE OF CATALASE FROM PENICILLIUM VITALE AT 2.0 ANGSTROMS RESOLUTION
Authors : Vainshtein, B.K.; Melik-Adamyanyan, W.R.; Barynin, V.V.; Vagin, A.A.; Grebenko, A.I.
Deposited on : 1983-02-24
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

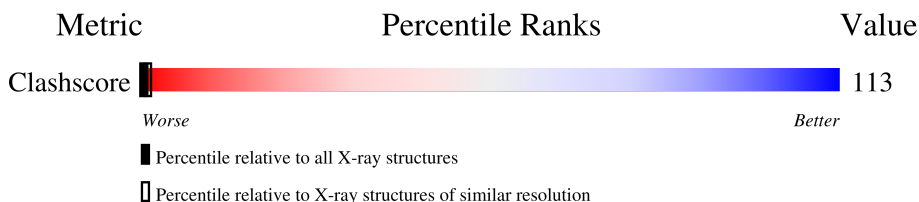
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.



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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	659	 51% 49% .
1	B	659	 51% 48% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5360 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 CATALASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	659	2637	1318	659	660	0	0	0
1	B	659	2637	1318	659	660	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



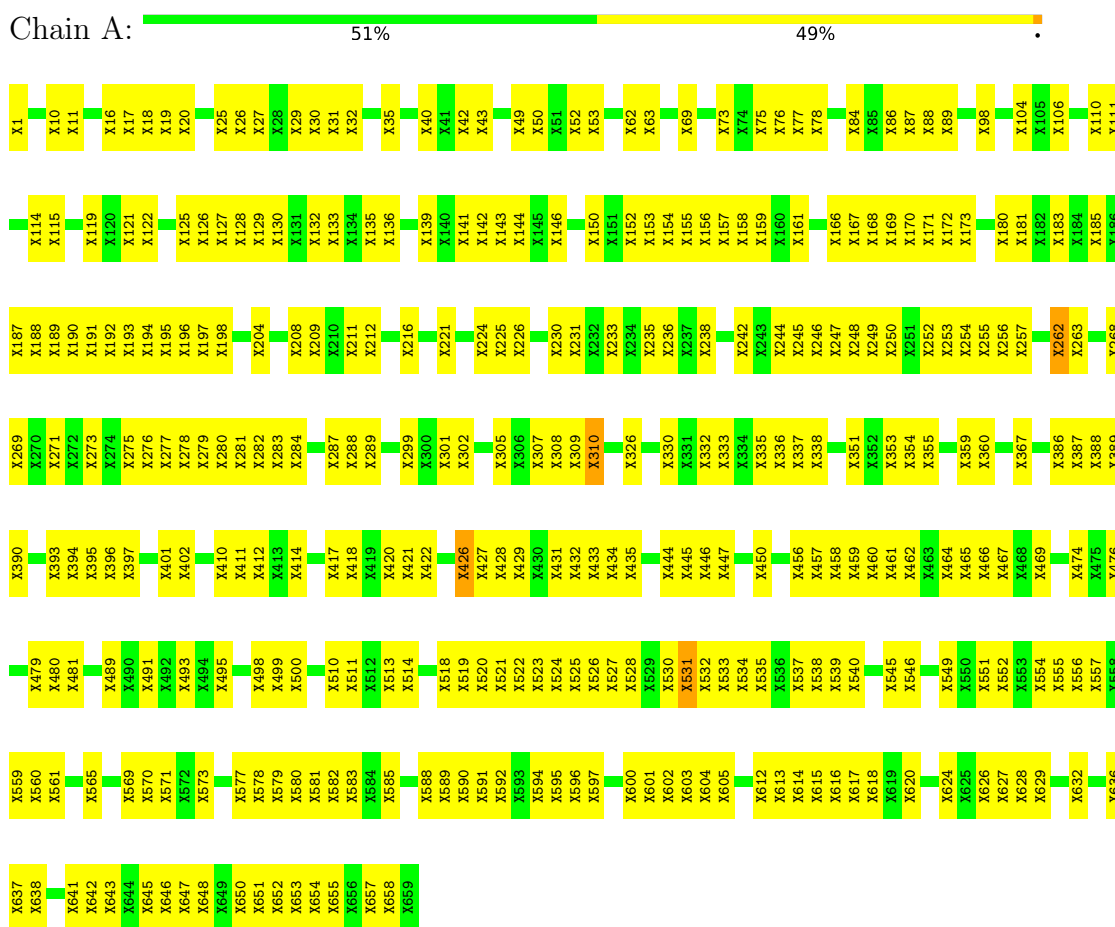
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

3 Residue-property plots

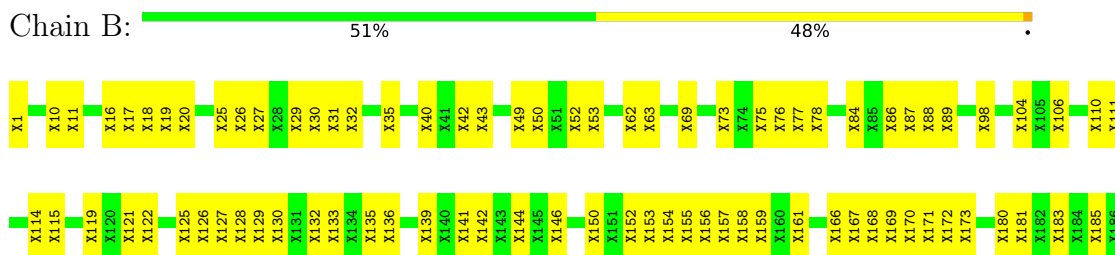
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: CATALASE



- Molecule 1: CATALASE



X187	X269	X390	X559	X637
X188	X270	X399	X479	X638
X189	X271	X394	X480	X641
X190	X272	X395	X481	X642
X191	X273	X396	X489	X643
X192	X274	X397	X490	X644
X193	X275	X401	X491	X645
X194	X276	X402	X492	X646
X195	X277	X410	X493	X647
X196	X278	X411	X494	X648
X197	X279	X412	X495	X649
X198	X280	X413	X498	X650
X204	X281	X414	X499	X651
X208	X282	X418	X500	X652
X209	X283	X419	X510	X653
X210	X284	X420	X511	X654
X211	X287	X421	X512	X655
X212	X288	X422	X513	X656
X216	X289	X426	X514	X657
X221	X299	X427	X518	X658
X224	X301	X428	X519	X659
X225	X302	X429	X520	
X226	X305	X430	X521	
X230	X306	X431	X522	
X231	X307	X432	X523	
X232	X308	X433	X524	
X233	X309	X434	X525	
X234	X310	X435	X526	
X235	X326	X444	X527	
X236	X330	X445	X528	
X237	X331	X446	X530	
X238	X332	X447	X531	
X242	X333	X450	X532	
X243	X334	X456	X533	
X244	X335	X457	X534	
X245	X336	X458	X535	
X246	X337	X459	X536	
X247	X338	X460	X537	
X248	X351	X461	X538	
X249	X352	X462	X539	
X250	X353	X463	X540	
X251	X354	X464	X545	
X252	X355	X465	X546	
X253	X359	X466	X549	
X254	X360	X467	X550	
X255	X367	X468	X551	
X256	X386	X469	X552	
X257	X387	X474	X553	
X262	X388	X475	X554	
X263	X389	X476	X555	
X268			X556	
			X557	
			X558	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.40Å 144.40Å 133.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5360	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
1	B	0	14
All	All	0	28

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	UNK	Peptide
1	A	226	UNK	Mainchain
1	A	262	UNK	Peptide
1	A	263	UNK	Peptide
1	A	310	UNK	Peptide
1	A	326	UNK	Peptide
1	A	351	UNK	Peptide
1	A	387	UNK	Peptide
1	A	412	UNK	Peptide
1	A	426	UNK	Peptide
1	A	435	UNK	Mainchain
1	A	511	UNK	Peptide
1	A	531	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	A	585	UNK	Peptide
1	B	17	UNK	Peptide
1	B	226	UNK	Mainchain
1	B	262	UNK	Peptide
1	B	263	UNK	Peptide
1	B	310	UNK	Peptide
1	B	326	UNK	Peptide
1	B	351	UNK	Peptide
1	B	387	UNK	Peptide
1	B	412	UNK	Peptide
1	B	426	UNK	Peptide
1	B	435	UNK	Mainchain
1	B	511	UNK	Peptide
1	B	531	UNK	Mainchain
1	B	585	UNK	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2637	0	97	319	6
1	B	2637	0	99	312	6
2	A	43	0	30	5	0
2	B	43	0	30	6	0
All	All	5360	0	256	634	6

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 113.

All (634) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:UNK:C	1:A:533:UNK:CA	1.76	1.59
1:B:533:UNK:C	1:B:533:UNK:CA	1.76	1.58
1:A:534:UNK:N	1:A:534:UNK:CA	1.70	1.53
1:A:535:UNK:N	1:A:535:UNK:CA	1.69	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:UNK:CA	1:A:533:UNK:N	1.72	1.53
1:B:535:UNK:N	1:B:535:UNK:CA	1.69	1.53
1:B:533:UNK:CA	1:B:533:UNK:N	1.72	1.51
1:A:1:UNK:N	1:A:1:UNK:CA	1.73	1.50
1:B:534:UNK:N	1:B:534:UNK:CA	1.70	1.49
1:B:1:UNK:N	1:B:1:UNK:CA	1.73	1.48
2:A:660:HEM:HHC	2:A:660:HEM:HBB2	1.34	1.08
2:B:660:HEM:HHC	2:B:660:HEM:HBB2	1.34	1.07
1:A:305:UNK:O	1:B:154:UNK:CA	2.04	1.06
2:A:660:HEM:HBC2	2:A:660:HEM:HMC1	1.38	1.06
1:A:287:UNK:O	1:A:289:UNK:N	1.90	1.05
1:A:154:UNK:CA	1:B:305:UNK:O	2.04	1.05
1:B:287:UNK:O	1:B:289:UNK:N	1.90	1.04
2:B:660:HEM:HMC1	2:B:660:HEM:HBC2	1.38	1.03
1:A:555:UNK:C	1:A:557:UNK:N	2.24	0.99
1:B:555:UNK:C	1:B:557:UNK:N	2.24	0.98
1:B:444:UNK:O	1:B:447:UNK:N	1.96	0.98
1:A:444:UNK:O	1:A:447:UNK:N	1.96	0.97
1:B:152:UNK:O	1:B:155:UNK:O	1.82	0.97
1:B:524:UNK:O	1:B:526:UNK:N	1.98	0.96
1:A:524:UNK:O	1:A:526:UNK:N	1.98	0.96
1:B:577:UNK:O	1:B:579:UNK:N	1.99	0.96
1:A:577:UNK:O	1:A:579:UNK:N	1.99	0.96
1:A:152:UNK:O	1:A:155:UNK:O	1.82	0.95
1:A:221:UNK:N	1:A:262:UNK:O	2.00	0.94
1:B:581:UNK:O	1:B:583:UNK:N	2.00	0.94
1:A:581:UNK:O	1:A:583:UNK:N	2.00	0.93
1:B:221:UNK:N	1:B:262:UNK:O	2.00	0.93
1:A:281:UNK:O	1:A:283:UNK:N	2.05	0.90
1:A:353:UNK:O	1:A:355:UNK:N	2.05	0.90
1:B:353:UNK:O	1:B:355:UNK:N	2.05	0.90
1:B:281:UNK:O	1:B:283:UNK:N	2.05	0.89
1:A:474:UNK:C	1:A:476:UNK:N	2.35	0.89
1:A:307:UNK:O	1:A:310:UNK:N	2.06	0.88
1:B:426:UNK:O	1:B:427:UNK:C	2.22	0.88
1:B:474:UNK:C	1:B:476:UNK:N	2.35	0.88
1:B:307:UNK:O	1:B:310:UNK:N	2.06	0.87
1:A:278:UNK:O	1:A:281:UNK:N	2.07	0.87
1:B:278:UNK:O	1:B:281:UNK:N	2.07	0.87
1:B:533:UNK:C	1:B:533:UNK:N	2.37	0.87
1:B:224:UNK:O	1:B:225:UNK:O	1.92	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:UNK:C	1:A:533:UNK:N	2.37	0.86
1:A:624:UNK:O	1:A:626:UNK:N	2.09	0.86
1:A:426:UNK:O	1:A:427:UNK:C	2.22	0.86
1:B:555:UNK:O	1:B:557:UNK:N	2.09	0.86
1:A:335:UNK:O	1:A:337:UNK:N	2.09	0.85
1:B:577:UNK:C	1:B:579:UNK:N	2.37	0.85
1:A:224:UNK:O	1:A:225:UNK:O	1.92	0.85
1:A:126:UNK:O	1:A:128:UNK:N	2.09	0.85
1:A:242:UNK:O	1:A:244:UNK:N	2.10	0.85
1:B:624:UNK:O	1:B:626:UNK:N	2.09	0.85
1:A:555:UNK:O	1:A:557:UNK:N	2.09	0.85
1:B:335:UNK:O	1:B:337:UNK:N	2.09	0.85
1:B:242:UNK:O	1:B:244:UNK:N	2.10	0.85
1:B:153:UNK:O	1:B:155:UNK:N	2.11	0.84
1:A:603:UNK:C	1:A:605:UNK:N	2.37	0.84
1:A:115:UNK:O	1:A:129:UNK:O	1.94	0.84
1:A:464:UNK:C	1:A:466:UNK:N	2.36	0.84
1:B:126:UNK:O	1:B:128:UNK:N	2.09	0.84
1:A:577:UNK:C	1:A:579:UNK:N	2.37	0.84
2:B:660:HEM:HBC2	2:B:660:HEM:CMC	2.08	0.84
1:B:115:UNK:O	1:B:129:UNK:O	1.94	0.84
1:A:153:UNK:O	1:A:155:UNK:N	2.11	0.83
2:A:660:HEM:HBC2	2:A:660:HEM:CMC	2.08	0.83
1:A:191:UNK:O	1:A:192:UNK:O	1.96	0.83
1:A:650:UNK:O	1:A:651:UNK:C	2.26	0.83
1:B:191:UNK:O	1:B:192:UNK:O	1.96	0.83
1:A:396:UNK:O	1:A:397:UNK:O	1.97	0.83
1:A:141:UNK:O	1:A:144:UNK:N	2.12	0.83
1:B:603:UNK:C	1:B:605:UNK:N	2.37	0.83
1:B:396:UNK:O	1:B:397:UNK:O	1.97	0.82
1:A:489:UNK:O	1:A:491:UNK:N	2.11	0.82
1:B:489:UNK:O	1:B:491:UNK:N	2.11	0.82
1:B:141:UNK:O	1:B:144:UNK:N	2.12	0.82
1:A:76:UNK:O	1:A:78:UNK:N	2.13	0.82
1:B:650:UNK:O	1:B:651:UNK:C	2.26	0.82
1:B:281:UNK:O	1:B:282:UNK:C	2.29	0.81
1:A:281:UNK:O	1:A:282:UNK:C	2.29	0.81
1:B:221:UNK:O	1:B:262:UNK:N	2.14	0.81
1:B:76:UNK:O	1:B:78:UNK:N	2.13	0.80
1:A:278:UNK:O	1:A:280:UNK:N	2.14	0.80
1:A:333:UNK:C	1:A:335:UNK:N	2.37	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:UNK:O	1:A:466:UNK:N	2.14	0.80
1:A:139:UNK:O	1:A:141:UNK:N	2.15	0.80
1:B:110:UNK:O	1:B:111:UNK:O	2.00	0.80
1:B:139:UNK:O	1:B:141:UNK:N	2.15	0.80
1:A:221:UNK:O	1:A:262:UNK:N	2.14	0.80
1:A:110:UNK:O	1:A:111:UNK:O	2.00	0.80
1:B:464:UNK:C	1:B:466:UNK:N	2.36	0.80
1:A:524:UNK:O	1:A:527:UNK:N	2.15	0.80
1:B:278:UNK:O	1:B:280:UNK:N	2.14	0.79
1:B:333:UNK:C	1:B:335:UNK:N	2.37	0.79
1:B:464:UNK:O	1:B:466:UNK:N	2.14	0.79
1:A:393:UNK:O	1:A:396:UNK:N	2.14	0.79
1:B:393:UNK:O	1:B:396:UNK:N	2.14	0.79
1:B:146:UNK:O	1:B:150:UNK:N	2.16	0.79
1:A:146:UNK:O	1:A:150:UNK:N	2.16	0.79
1:A:426:UNK:C	1:A:428:UNK:N	2.37	0.79
1:B:421:UNK:O	1:B:422:UNK:C	2.27	0.79
1:B:524:UNK:O	1:B:527:UNK:N	2.15	0.78
1:B:519:UNK:O	1:B:520:UNK:O	2.01	0.78
1:A:519:UNK:O	1:A:520:UNK:O	2.01	0.78
1:B:426:UNK:C	1:B:428:UNK:N	2.37	0.78
1:B:624:UNK:C	1:B:626:UNK:N	2.44	0.78
1:B:648:UNK:O	1:B:650:UNK:N	2.16	0.78
1:A:153:UNK:O	1:A:155:UNK:O	2.00	0.78
1:A:159:UNK:O	1:A:161:UNK:N	2.17	0.78
1:B:159:UNK:O	1:B:161:UNK:N	2.17	0.78
1:B:153:UNK:O	1:B:155:UNK:O	2.00	0.78
1:A:426:UNK:O	1:A:428:UNK:N	2.17	0.77
1:A:428:UNK:O	1:A:431:UNK:N	2.18	0.76
1:A:624:UNK:C	1:A:626:UNK:N	2.44	0.76
1:A:248:UNK:O	1:A:252:UNK:N	2.19	0.76
1:B:428:UNK:O	1:B:431:UNK:N	2.18	0.76
1:A:648:UNK:O	1:A:650:UNK:N	2.16	0.76
1:B:333:UNK:O	1:B:335:UNK:N	2.19	0.76
1:B:426:UNK:O	1:B:428:UNK:N	2.17	0.76
1:A:466:UNK:O	1:A:469:UNK:N	2.20	0.75
1:A:519:UNK:C	1:A:520:UNK:O	2.34	0.75
1:A:230:UNK:O	1:A:233:UNK:N	2.19	0.75
1:A:130:UNK:O	1:A:198:UNK:O	2.04	0.75
1:A:333:UNK:O	1:A:335:UNK:N	2.19	0.75
1:B:230:UNK:O	1:B:233:UNK:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:UNK:O	1:B:252:UNK:N	2.19	0.75
1:B:466:UNK:O	1:B:469:UNK:N	2.20	0.74
1:B:519:UNK:C	1:B:520:UNK:O	2.35	0.74
1:A:307:UNK:O	1:A:309:UNK:N	2.21	0.74
1:B:581:UNK:O	1:B:582:UNK:C	2.35	0.74
1:B:130:UNK:O	1:B:198:UNK:O	2.04	0.74
1:A:581:UNK:O	1:A:582:UNK:C	2.35	0.73
1:B:474:UNK:O	1:B:476:UNK:N	2.20	0.73
1:A:84:UNK:C	1:A:86:UNK:H	2.00	0.73
1:B:307:UNK:O	1:B:309:UNK:N	2.21	0.73
1:A:474:UNK:O	1:A:476:UNK:N	2.20	0.73
1:B:40:UNK:C	1:B:42:UNK:N	2.47	0.73
1:B:84:UNK:C	1:B:86:UNK:H	2.00	0.73
1:A:554:UNK:O	1:A:557:UNK:N	2.22	0.73
1:B:603:UNK:O	1:B:605:UNK:N	2.22	0.73
1:B:554:UNK:O	1:B:557:UNK:N	2.22	0.72
1:B:335:UNK:C	1:B:337:UNK:N	2.51	0.72
1:B:388:UNK:O	1:B:389:UNK:C	2.37	0.72
1:A:388:UNK:O	1:A:389:UNK:C	2.37	0.72
1:A:524:UNK:C	1:A:526:UNK:N	2.47	0.72
1:B:330:UNK:C	1:B:332:UNK:N	2.49	0.72
1:A:10:UNK:O	1:A:11:UNK:C	2.38	0.72
1:A:493:UNK:O	1:A:495:UNK:N	2.23	0.72
1:A:591:UNK:O	1:A:592:UNK:C	2.38	0.72
1:B:493:UNK:O	1:B:495:UNK:N	2.23	0.72
1:B:119:UNK:O	1:B:125:UNK:N	2.23	0.71
1:B:29:UNK:CA	1:B:35:UNK:O	2.39	0.71
1:B:591:UNK:O	1:B:592:UNK:C	2.38	0.71
1:A:18:UNK:O	1:A:20:UNK:N	2.23	0.71
1:A:29:UNK:CA	1:A:35:UNK:O	2.39	0.71
1:A:421:UNK:O	1:A:422:UNK:C	2.27	0.71
1:B:524:UNK:C	1:B:526:UNK:N	2.47	0.71
1:A:603:UNK:O	1:A:605:UNK:N	2.22	0.71
1:B:18:UNK:O	1:B:20:UNK:N	2.23	0.70
1:B:193:UNK:C	1:B:195:UNK:N	2.52	0.70
1:B:393:UNK:O	1:B:394:UNK:C	2.39	0.70
1:A:393:UNK:O	1:A:394:UNK:C	2.39	0.70
1:A:40:UNK:C	1:A:42:UNK:N	2.47	0.70
1:A:188:UNK:C	1:A:190:UNK:H2	2.04	0.70
1:A:268:UNK:O	1:A:271:UNK:N	2.25	0.70
1:A:335:UNK:C	1:A:337:UNK:N	2.51	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:UNK:O	1:A:125:UNK:N	2.23	0.70
1:A:193:UNK:O	1:A:195:UNK:N	2.25	0.69
1:B:10:UNK:O	1:B:11:UNK:C	2.38	0.69
1:B:268:UNK:O	1:B:271:UNK:N	2.25	0.69
1:B:278:UNK:O	1:B:279:UNK:C	2.40	0.69
1:A:191:UNK:O	1:A:192:UNK:C	2.41	0.69
1:A:299:UNK:O	1:A:301:UNK:N	2.25	0.69
1:A:330:UNK:C	1:A:332:UNK:N	2.49	0.69
1:A:461:UNK:O	1:A:462:UNK:C	2.40	0.69
1:A:461:UNK:O	1:A:464:UNK:N	2.26	0.69
1:A:278:UNK:O	1:A:279:UNK:C	2.40	0.69
1:B:104:UNK:O	1:B:106:UNK:N	2.25	0.69
1:B:193:UNK:O	1:B:195:UNK:N	2.25	0.68
1:B:461:UNK:O	1:B:462:UNK:C	2.40	0.68
1:A:104:UNK:O	1:A:106:UNK:N	2.25	0.68
1:A:193:UNK:C	1:A:195:UNK:N	2.52	0.68
1:B:191:UNK:O	1:B:192:UNK:C	2.41	0.68
1:B:299:UNK:O	1:B:301:UNK:N	2.25	0.68
1:A:510:UNK:O	1:A:538:UNK:C	2.41	0.68
1:A:636:UNK:C	1:A:638:UNK:N	2.54	0.68
1:B:510:UNK:O	1:B:538:UNK:C	2.41	0.68
1:B:461:UNK:O	1:B:464:UNK:N	2.26	0.67
1:A:246:UNK:O	1:A:248:UNK:N	2.27	0.67
1:B:188:UNK:C	1:B:190:UNK:H2	2.04	0.67
1:B:76:UNK:C	1:B:78:UNK:N	2.57	0.67
1:A:75:UNK:O	1:A:88:UNK:CA	2.43	0.67
1:B:636:UNK:C	1:B:638:UNK:N	2.54	0.67
1:A:513:UNK:N	1:A:540:UNK:O	2.28	0.67
1:B:246:UNK:O	1:B:248:UNK:N	2.27	0.67
1:A:569:UNK:O	1:A:570:UNK:C	2.42	0.67
1:B:75:UNK:O	1:B:88:UNK:CA	2.43	0.67
1:B:513:UNK:N	1:B:540:UNK:O	2.28	0.66
1:A:532:UNK:C	1:A:533:UNK:CA	2.69	0.66
1:A:27:UNK:O	1:B:414:UNK:CA	2.44	0.66
1:A:498:UNK:O	1:A:500:UNK:N	2.29	0.66
1:A:414:UNK:CA	1:B:27:UNK:O	2.44	0.66
1:A:168:UNK:O	1:A:170:UNK:N	2.29	0.66
1:A:386:UNK:O	1:A:388:UNK:N	2.28	0.66
1:B:275:UNK:O	1:B:276:UNK:C	2.44	0.66
1:B:386:UNK:O	1:B:388:UNK:N	2.28	0.66
1:B:549:UNK:O	1:B:551:UNK:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:UNK:O	1:B:570:UNK:C	2.43	0.66
1:A:335:UNK:O	1:A:338:UNK:N	2.28	0.65
1:A:426:UNK:O	1:A:429:UNK:N	2.29	0.65
1:B:153:UNK:C	1:B:155:UNK:N	2.58	0.65
1:B:76:UNK:CA	1:B:87:UNK:O	2.45	0.65
1:B:168:UNK:O	1:B:170:UNK:N	2.29	0.65
1:B:335:UNK:O	1:B:338:UNK:N	2.28	0.65
1:B:426:UNK:O	1:B:429:UNK:N	2.29	0.65
1:B:615:UNK:C	1:B:617:UNK:N	2.57	0.65
1:A:76:UNK:C	1:A:78:UNK:N	2.57	0.65
1:A:549:UNK:O	1:A:551:UNK:N	2.29	0.65
1:A:275:UNK:O	1:A:276:UNK:C	2.44	0.65
2:A:660:HEM:HMC1	2:A:660:HEM:CBC	2.22	0.65
1:B:498:UNK:O	1:B:500:UNK:N	2.29	0.65
1:A:76:UNK:CA	1:A:87:UNK:O	2.45	0.65
1:A:645:UNK:O	1:A:648:UNK:N	2.30	0.65
1:B:645:UNK:O	1:B:648:UNK:N	2.30	0.64
1:B:524:UNK:O	1:B:525:UNK:C	2.45	0.64
1:A:533:UNK:N	1:A:534:UNK:N	2.45	0.64
1:A:62:UNK:O	1:A:63:UNK:C	2.45	0.64
1:A:278:UNK:C	1:A:280:UNK:N	2.60	0.64
1:A:524:UNK:O	1:A:525:UNK:C	2.45	0.64
1:A:154:UNK:N	1:B:305:UNK:O	2.30	0.64
1:A:305:UNK:O	1:B:154:UNK:N	2.30	0.64
1:B:62:UNK:O	1:B:63:UNK:C	2.45	0.64
1:A:615:UNK:C	1:A:617:UNK:N	2.57	0.63
1:B:18:UNK:O	1:B:19:UNK:C	2.46	0.63
1:B:533:UNK:N	1:B:534:UNK:N	2.45	0.63
1:A:98:UNK:CA	1:A:114:UNK:O	2.47	0.63
1:B:98:UNK:CA	1:B:114:UNK:O	2.47	0.63
1:B:594:UNK:O	1:B:595:UNK:C	2.47	0.63
1:B:278:UNK:C	1:B:280:UNK:N	2.60	0.63
1:A:153:UNK:C	1:A:155:UNK:N	2.58	0.63
1:A:255:UNK:O	1:A:256:UNK:C	2.47	0.63
1:B:613:UNK:O	1:B:615:UNK:N	2.32	0.62
1:A:594:UNK:O	1:A:595:UNK:C	2.47	0.62
1:B:657:UNK:O	1:B:658:UNK:C	2.47	0.62
1:A:613:UNK:O	1:A:615:UNK:N	2.32	0.62
1:B:255:UNK:O	1:B:256:UNK:C	2.47	0.62
1:A:18:UNK:O	1:A:19:UNK:C	2.46	0.62
1:A:601:UNK:O	1:A:602:UNK:C	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:UNK:O	1:A:658:UNK:C	2.48	0.61
1:A:410:UNK:O	1:A:411:UNK:C	2.48	0.61
1:A:520:UNK:O	1:A:522:UNK:N	2.33	0.61
1:B:156:UNK:O	1:B:157:UNK:O	2.18	0.61
1:B:532:UNK:C	1:B:533:UNK:CA	2.69	0.61
1:B:571:UNK:C	1:B:573:UNK:N	2.61	0.61
1:A:40:UNK:O	1:A:42:UNK:N	2.33	0.61
1:A:456:UNK:O	1:A:458:UNK:N	2.34	0.61
1:B:188:UNK:C	1:B:190:UNK:N	2.63	0.61
1:B:236:UNK:C	1:B:238:UNK:N	2.63	0.61
1:B:410:UNK:O	1:B:411:UNK:C	2.48	0.61
1:A:156:UNK:O	1:A:157:UNK:O	2.18	0.61
1:A:654:UNK:O	1:A:655:UNK:C	2.49	0.61
1:B:189:UNK:O	1:B:190:UNK:C	2.49	0.61
1:B:601:UNK:O	1:B:602:UNK:C	2.48	0.61
1:B:40:UNK:O	1:B:42:UNK:N	2.33	0.61
1:B:456:UNK:O	1:B:458:UNK:N	2.34	0.61
1:B:520:UNK:O	1:B:522:UNK:N	2.33	0.61
1:B:410:UNK:O	1:B:411:UNK:O	2.19	0.60
1:B:654:UNK:O	1:B:655:UNK:C	2.49	0.60
1:A:613:UNK:O	1:A:616:UNK:N	2.35	0.60
1:A:236:UNK:C	1:A:238:UNK:N	2.63	0.60
1:B:50:UNK:C	1:B:52:UNK:H	2.14	0.60
1:B:588:UNK:O	1:B:589:UNK:C	2.49	0.60
1:A:410:UNK:O	1:A:411:UNK:O	2.19	0.60
1:B:534:UNK:O	1:B:537:UNK:N	2.35	0.60
1:A:188:UNK:C	1:A:190:UNK:N	2.63	0.59
1:A:534:UNK:O	1:A:537:UNK:N	2.35	0.59
1:B:520:UNK:O	1:B:521:UNK:C	2.49	0.59
1:A:520:UNK:O	1:A:521:UNK:C	2.49	0.59
1:A:588:UNK:O	1:A:589:UNK:C	2.49	0.59
1:B:612:UNK:O	1:B:632:UNK:C	2.50	0.59
1:A:50:UNK:C	1:A:52:UNK:H	2.14	0.59
1:A:189:UNK:O	1:A:190:UNK:C	2.49	0.59
1:B:335:UNK:O	1:B:336:UNK:C	2.51	0.59
1:B:166:UNK:O	1:B:167:UNK:C	2.51	0.59
1:B:170:UNK:C	1:B:172:UNK:N	2.65	0.59
1:B:617:UNK:O	1:B:620:UNK:N	2.36	0.59
1:B:613:UNK:O	1:B:616:UNK:N	2.35	0.59
1:A:534:UNK:O	1:A:537:UNK:O	2.21	0.58
1:B:242:UNK:C	1:B:244:UNK:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:UNK:O	1:B:277:UNK:C	2.50	0.58
1:A:522:UNK:O	1:A:523:UNK:C	2.51	0.58
1:B:522:UNK:O	1:B:524:UNK:N	2.36	0.58
1:A:242:UNK:C	1:A:244:UNK:N	2.66	0.58
1:A:571:UNK:C	1:A:573:UNK:N	2.61	0.58
1:B:591:UNK:O	1:B:592:UNK:O	2.21	0.58
2:B:660:HEM:HMC1	2:B:660:HEM:CBC	2.23	0.58
1:A:135:UNK:O	1:A:136:UNK:C	2.51	0.58
1:A:166:UNK:O	1:A:167:UNK:C	2.51	0.58
1:A:335:UNK:O	1:A:336:UNK:C	2.51	0.58
1:A:612:UNK:O	1:A:632:UNK:C	2.50	0.58
1:B:168:UNK:C	1:B:170:UNK:N	2.63	0.58
1:A:276:UNK:O	1:A:277:UNK:C	2.50	0.58
1:A:168:UNK:C	1:A:170:UNK:N	2.63	0.58
1:B:135:UNK:O	1:B:136:UNK:C	2.51	0.58
1:B:388:UNK:O	1:B:390:UNK:N	2.36	0.58
1:B:522:UNK:O	1:B:523:UNK:C	2.51	0.58
1:A:281:UNK:C	1:A:283:UNK:N	2.67	0.58
1:A:388:UNK:O	1:A:390:UNK:N	2.36	0.58
1:A:591:UNK:O	1:A:592:UNK:O	2.21	0.58
1:A:522:UNK:O	1:A:524:UNK:N	2.36	0.58
1:A:466:UNK:O	1:A:467:UNK:C	2.52	0.57
2:B:660:HEM:HBB2	2:B:660:HEM:CHC	2.17	0.57
1:A:617:UNK:O	1:A:620:UNK:N	2.36	0.57
1:B:637:UNK:O	1:B:641:UNK:N	2.38	0.57
1:A:456:UNK:O	1:A:459:UNK:N	2.38	0.57
1:B:627:UNK:O	1:B:629:UNK:N	2.37	0.57
1:A:627:UNK:O	1:A:629:UNK:N	2.37	0.57
1:B:456:UNK:O	1:B:459:UNK:N	2.38	0.57
1:A:187:UNK:O	1:A:188:UNK:C	2.52	0.57
1:A:170:UNK:C	1:A:172:UNK:N	2.65	0.57
1:B:534:UNK:O	1:B:537:UNK:O	2.21	0.57
1:A:444:UNK:O	1:A:445:UNK:C	2.52	0.57
1:A:479:UNK:O	1:A:481:UNK:O	2.23	0.57
1:B:16:UNK:O	1:B:18:UNK:C	2.53	0.57
1:B:256:UNK:O	1:B:257:UNK:C	2.52	0.57
1:B:444:UNK:O	1:B:445:UNK:C	2.52	0.57
1:B:466:UNK:O	1:B:467:UNK:C	2.52	0.57
1:A:256:UNK:O	1:A:257:UNK:C	2.52	0.56
1:A:643:UNK:C	1:A:645:UNK:N	2.66	0.56
1:B:417:UNK:O	1:B:418:UNK:C	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:UNK:O	1:B:188:UNK:C	2.52	0.56
1:A:246:UNK:C	1:A:248:UNK:N	2.67	0.56
1:B:281:UNK:C	1:B:283:UNK:N	2.67	0.56
1:A:16:UNK:O	1:A:18:UNK:C	2.53	0.56
1:A:637:UNK:O	1:A:641:UNK:N	2.38	0.56
1:B:627:UNK:O	1:B:628:UNK:C	2.54	0.56
1:B:153:UNK:O	1:B:154:UNK:C	2.54	0.56
1:B:158:UNK:O	1:B:159:UNK:O	2.24	0.56
1:B:643:UNK:C	1:B:645:UNK:N	2.66	0.56
1:A:183:UNK:C	1:A:185:UNK:N	2.67	0.56
1:B:193:UNK:O	1:B:196:UNK:N	2.38	0.56
1:A:158:UNK:O	1:A:159:UNK:O	2.24	0.55
1:A:627:UNK:O	1:A:628:UNK:C	2.54	0.55
1:A:193:UNK:O	1:A:196:UNK:N	2.38	0.55
1:A:417:UNK:O	1:A:418:UNK:C	2.53	0.55
1:B:188:UNK:O	1:B:190:UNK:N	2.40	0.55
1:A:121:UNK:O	1:A:122:UNK:C	2.55	0.55
1:A:188:UNK:O	1:A:190:UNK:N	2.40	0.55
1:B:269:UNK:C	1:B:271:UNK:N	2.66	0.55
1:B:479:UNK:O	1:B:481:UNK:O	2.23	0.55
1:A:224:UNK:O	1:A:225:UNK:C	2.55	0.55
1:B:152:UNK:O	1:B:153:UNK:O	2.25	0.55
1:B:645:UNK:C	1:B:647:UNK:N	2.67	0.55
1:A:554:UNK:O	1:A:556:UNK:C	2.55	0.55
1:B:1:UNK:N	1:B:1:UNK:C	2.65	0.55
1:B:31:UNK:O	1:B:32:UNK:C	2.55	0.55
1:A:152:UNK:O	1:A:153:UNK:O	2.25	0.55
1:B:183:UNK:C	1:B:185:UNK:N	2.67	0.55
1:A:31:UNK:O	1:A:32:UNK:C	2.55	0.54
1:B:307:UNK:O	1:B:308:UNK:C	2.55	0.54
1:B:121:UNK:O	1:B:122:UNK:C	2.55	0.54
1:B:276:UNK:O	1:B:277:UNK:O	2.25	0.54
1:B:446:UNK:O	1:B:450:UNK:N	2.41	0.54
1:B:554:UNK:O	1:B:556:UNK:C	2.55	0.54
1:A:1:UNK:N	1:A:1:UNK:C	2.65	0.54
1:A:40:UNK:O	1:A:43:UNK:N	2.40	0.54
1:A:287:UNK:C	1:A:289:UNK:N	2.69	0.54
1:A:446:UNK:O	1:A:450:UNK:N	2.41	0.54
1:A:249:UNK:O	1:A:252:UNK:N	2.40	0.54
1:A:269:UNK:C	1:A:271:UNK:N	2.66	0.54
1:B:249:UNK:O	1:B:252:UNK:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:UNK:C	1:B:616:UNK:N	2.68	0.54
1:A:276:UNK:O	1:A:277:UNK:O	2.25	0.54
1:A:614:UNK:C	1:A:616:UNK:N	2.67	0.54
1:A:153:UNK:O	1:A:154:UNK:C	2.54	0.54
1:A:180:UNK:O	1:A:183:UNK:N	2.41	0.54
1:A:538:UNK:C	1:A:539:UNK:O	2.56	0.54
1:B:287:UNK:C	1:B:289:UNK:N	2.69	0.54
1:B:40:UNK:O	1:B:43:UNK:N	2.40	0.54
1:B:180:UNK:O	1:B:183:UNK:N	2.41	0.54
1:B:396:UNK:C	1:B:397:UNK:O	2.56	0.54
1:B:246:UNK:O	1:B:249:UNK:N	2.41	0.54
1:B:246:UNK:C	1:B:248:UNK:N	2.67	0.54
1:A:139:UNK:C	1:A:141:UNK:N	2.71	0.53
1:A:170:UNK:O	1:A:173:UNK:N	2.42	0.53
1:A:396:UNK:C	1:A:397:UNK:O	2.56	0.53
1:B:577:UNK:O	1:B:580:UNK:N	2.41	0.53
1:A:307:UNK:O	1:A:308:UNK:C	2.55	0.53
1:B:224:UNK:O	1:B:225:UNK:C	2.55	0.53
1:A:246:UNK:O	1:A:249:UNK:N	2.40	0.53
1:B:551:UNK:O	1:B:552:UNK:O	2.26	0.53
1:A:551:UNK:O	1:A:552:UNK:O	2.26	0.53
1:A:645:UNK:C	1:A:647:UNK:N	2.67	0.53
1:A:577:UNK:O	1:A:580:UNK:N	2.42	0.53
1:B:386:UNK:C	1:B:388:UNK:N	2.72	0.53
1:B:538:UNK:C	1:B:539:UNK:O	2.56	0.53
1:B:139:UNK:C	1:B:141:UNK:N	2.71	0.53
1:B:555:UNK:O	1:B:557:UNK:O	2.27	0.53
1:B:224:UNK:C	1:B:225:UNK:O	2.57	0.53
1:B:464:UNK:O	1:B:465:UNK:C	2.56	0.53
1:A:77:UNK:O	1:A:78:UNK:C	2.57	0.52
1:A:353:UNK:O	1:A:354:UNK:C	2.57	0.52
1:A:555:UNK:O	1:A:557:UNK:O	2.27	0.52
1:B:170:UNK:O	1:B:173:UNK:N	2.42	0.52
1:A:464:UNK:O	1:A:465:UNK:C	2.56	0.52
1:B:255:UNK:O	1:B:257:UNK:N	2.42	0.52
1:A:386:UNK:C	1:A:388:UNK:N	2.72	0.52
1:A:538:UNK:O	1:A:539:UNK:C	2.57	0.52
1:B:132:UNK:O	1:B:133:UNK:C	2.57	0.52
1:A:16:UNK:C	1:A:18:UNK:N	2.71	0.52
1:B:191:UNK:C	1:B:192:UNK:O	2.58	0.52
1:A:432:UNK:O	1:A:433:UNK:C	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:UNK:O	1:B:646:UNK:C	2.58	0.52
1:B:432:UNK:O	1:B:433:UNK:C	2.57	0.52
1:B:538:UNK:O	1:B:539:UNK:C	2.57	0.52
1:B:16:UNK:C	1:B:18:UNK:N	2.71	0.52
1:B:527:UNK:O	1:B:531:UNK:N	2.43	0.52
1:A:168:UNK:O	1:A:169:UNK:C	2.58	0.52
1:A:645:UNK:O	1:A:646:UNK:C	2.58	0.52
1:A:191:UNK:C	1:A:192:UNK:O	2.58	0.51
1:A:224:UNK:C	1:A:225:UNK:O	2.57	0.51
1:B:77:UNK:O	1:B:78:UNK:C	2.57	0.51
1:A:255:UNK:O	1:A:257:UNK:N	2.42	0.51
1:A:115:UNK:C	1:A:129:UNK:O	2.58	0.51
1:A:132:UNK:O	1:A:133:UNK:C	2.57	0.51
1:A:627:UNK:C	1:A:629:UNK:N	2.71	0.51
1:B:126:UNK:O	1:B:127:UNK:C	2.56	0.51
1:A:268:UNK:O	1:A:269:UNK:C	2.59	0.51
1:A:527:UNK:O	1:A:531:UNK:N	2.43	0.51
1:B:535:UNK:N	1:B:535:UNK:C	2.67	0.51
1:B:594:UNK:O	1:B:597:UNK:N	2.44	0.51
1:B:168:UNK:O	1:B:169:UNK:C	2.58	0.51
1:A:594:UNK:O	1:A:597:UNK:N	2.44	0.51
1:B:170:UNK:O	1:B:172:UNK:N	2.44	0.51
1:B:268:UNK:O	1:B:269:UNK:C	2.59	0.51
1:A:244:UNK:C	1:A:246:UNK:N	2.73	0.50
1:A:456:UNK:O	1:A:457:UNK:C	2.60	0.50
1:A:577:UNK:O	1:A:578:UNK:C	2.57	0.50
1:B:353:UNK:O	1:B:354:UNK:C	2.58	0.50
1:B:456:UNK:O	1:B:457:UNK:C	2.60	0.50
1:B:627:UNK:C	1:B:629:UNK:N	2.71	0.50
1:B:141:UNK:O	1:B:142:UNK:C	2.59	0.50
1:B:197:UNK:O	1:B:198:UNK:C	2.60	0.50
1:A:170:UNK:O	1:A:172:UNK:N	2.44	0.50
1:B:444:UNK:O	1:B:447:UNK:CA	2.60	0.50
1:A:141:UNK:O	1:A:142:UNK:C	2.59	0.49
1:A:231:UNK:O	1:A:235:UNK:N	2.44	0.49
1:A:393:UNK:O	1:A:395:UNK:N	2.45	0.49
1:B:187:UNK:O	1:B:190:UNK:N	2.42	0.49
1:B:588:UNK:O	1:B:590:UNK:N	2.45	0.49
1:B:231:UNK:O	1:B:235:UNK:N	2.44	0.49
1:A:126:UNK:O	1:A:127:UNK:C	2.56	0.49
1:B:115:UNK:C	1:B:129:UNK:O	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:UNK:O	1:B:254:UNK:C	2.60	0.49
1:B:600:UNK:O	1:B:604:UNK:N	2.45	0.49
1:A:287:UNK:O	1:A:288:UNK:C	2.59	0.49
1:A:613:UNK:O	1:A:614:UNK:C	2.60	0.49
1:B:156:UNK:O	1:B:157:UNK:C	2.60	0.49
1:A:197:UNK:O	1:A:198:UNK:C	2.60	0.49
1:A:253:UNK:O	1:A:254:UNK:C	2.60	0.49
1:A:535:UNK:N	1:A:535:UNK:C	2.67	0.49
1:B:613:UNK:O	1:B:614:UNK:C	2.60	0.49
1:A:156:UNK:O	1:A:157:UNK:C	2.60	0.49
1:A:166:UNK:O	1:A:168:UNK:N	2.46	0.49
1:A:588:UNK:O	1:A:590:UNK:N	2.45	0.49
1:B:244:UNK:C	1:B:246:UNK:N	2.73	0.49
1:B:393:UNK:O	1:B:395:UNK:N	2.45	0.49
1:B:29:UNK:O	1:B:30:UNK:C	2.61	0.49
1:B:211:UNK:O	1:B:212:UNK:C	2.61	0.49
1:B:166:UNK:O	1:B:169:UNK:N	2.46	0.48
1:A:600:UNK:O	1:A:604:UNK:N	2.45	0.48
1:A:307:UNK:C	1:A:309:UNK:N	2.74	0.48
1:B:551:UNK:O	1:B:552:UNK:C	2.61	0.48
1:A:244:UNK:O	1:A:245:UNK:C	2.57	0.48
1:B:577:UNK:O	1:B:578:UNK:C	2.57	0.48
1:A:110:UNK:O	1:A:111:UNK:C	2.61	0.48
1:A:211:UNK:O	1:A:212:UNK:C	2.61	0.48
1:A:444:UNK:O	1:A:447:UNK:CA	2.60	0.48
1:B:307:UNK:C	1:B:309:UNK:N	2.74	0.48
1:A:29:UNK:O	1:A:30:UNK:C	2.61	0.48
1:A:551:UNK:O	1:A:552:UNK:C	2.61	0.48
1:B:166:UNK:O	1:B:168:UNK:N	2.46	0.48
1:A:69:UNK:CA	1:A:299:UNK:O	2.62	0.48
1:A:166:UNK:O	1:A:169:UNK:N	2.46	0.48
1:B:612:UNK:O	1:B:632:UNK:O	2.32	0.47
1:A:527:UNK:O	1:A:528:UNK:C	2.61	0.47
1:B:69:UNK:CA	1:B:299:UNK:O	2.62	0.47
1:B:110:UNK:O	1:B:111:UNK:C	2.61	0.47
1:B:645:UNK:O	1:B:647:UNK:N	2.47	0.47
1:A:638:UNK:O	1:A:642:UNK:N	2.48	0.47
1:A:645:UNK:O	1:A:647:UNK:N	2.47	0.47
1:B:527:UNK:O	1:B:530:UNK:N	2.47	0.47
1:B:638:UNK:O	1:B:642:UNK:N	2.48	0.47
1:B:527:UNK:O	1:B:528:UNK:C	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:UNK:O	1:B:596:UNK:C	2.62	0.47
1:A:30:UNK:O	1:B:410:UNK:O	2.33	0.47
1:A:521:UNK:O	1:A:522:UNK:C	2.63	0.47
1:B:479:UNK:O	1:B:480:UNK:C	2.62	0.47
1:A:230:UNK:O	1:A:231:UNK:C	2.63	0.47
1:A:527:UNK:O	1:A:530:UNK:N	2.47	0.47
1:B:166:UNK:C	1:B:168:UNK:N	2.78	0.47
1:B:208:UNK:O	1:B:209:UNK:C	2.63	0.47
1:A:479:UNK:O	1:A:480:UNK:C	2.62	0.47
1:B:230:UNK:O	1:B:231:UNK:C	2.63	0.47
1:A:166:UNK:C	1:A:168:UNK:N	2.78	0.47
1:A:410:UNK:O	1:B:30:UNK:O	2.32	0.47
1:B:489:UNK:C	1:B:491:UNK:N	2.78	0.47
1:A:170:UNK:O	1:A:172:UNK:C	2.63	0.46
1:A:560:UNK:O	1:A:561:UNK:O	2.33	0.46
1:B:170:UNK:O	1:B:172:UNK:C	2.63	0.46
1:B:244:UNK:O	1:B:245:UNK:C	2.57	0.46
1:B:521:UNK:O	1:B:522:UNK:C	2.63	0.46
1:A:249:UNK:O	1:A:252:UNK:CA	2.64	0.46
1:A:595:UNK:O	1:A:596:UNK:C	2.62	0.46
1:A:612:UNK:O	1:A:632:UNK:O	2.32	0.46
1:B:560:UNK:O	1:B:561:UNK:O	2.33	0.46
1:B:50:UNK:C	1:B:52:UNK:N	2.79	0.46
1:B:514:UNK:O	1:B:565:UNK:CA	2.63	0.46
1:A:187:UNK:O	1:A:190:UNK:N	2.42	0.46
1:A:432:UNK:C	1:A:434:UNK:N	2.79	0.46
1:A:559:UNK:O	1:A:560:UNK:C	2.64	0.46
1:A:514:UNK:O	1:A:565:UNK:CA	2.63	0.46
1:A:650:UNK:O	1:A:651:UNK:O	2.33	0.46
1:A:646:UNK:C	1:A:648:UNK:H	2.29	0.46
1:B:249:UNK:O	1:B:252:UNK:CA	2.64	0.46
1:B:417:UNK:O	1:B:420:UNK:N	2.49	0.45
1:A:648:UNK:C	1:A:650:UNK:N	2.79	0.45
1:B:533:UNK:C	1:B:534:UNK:CA	2.83	0.45
1:A:417:UNK:O	1:A:420:UNK:N	2.49	0.45
1:B:559:UNK:O	1:B:560:UNK:C	2.64	0.45
1:B:648:UNK:C	1:B:650:UNK:N	2.79	0.45
1:A:194:UNK:O	1:A:224:UNK:O	2.34	0.45
1:A:208:UNK:O	1:A:209:UNK:C	2.63	0.45
1:B:646:UNK:C	1:B:648:UNK:H	2.29	0.45
1:B:545:UNK:O	1:B:546:UNK:C	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:UNK:C	1:A:537:UNK:O	2.65	0.45
1:B:650:UNK:O	1:B:651:UNK:O	2.33	0.45
1:A:49:UNK:O	1:A:52:UNK:N	2.50	0.45
1:B:535:UNK:C	1:B:537:UNK:O	2.65	0.45
1:A:589:UNK:O	1:A:590:UNK:C	2.65	0.45
1:B:49:UNK:O	1:B:52:UNK:N	2.50	0.45
1:A:489:UNK:C	1:A:491:UNK:N	2.78	0.44
1:A:534:UNK:N	1:A:534:UNK:C	2.76	0.44
1:A:545:UNK:O	1:A:546:UNK:C	2.65	0.44
1:B:25:UNK:O	1:B:26:UNK:C	2.66	0.44
1:B:194:UNK:O	1:B:224:UNK:O	2.34	0.44
1:B:432:UNK:C	1:B:434:UNK:N	2.79	0.44
1:A:432:UNK:O	1:A:434:UNK:N	2.50	0.44
1:A:141:UNK:C	1:A:143:UNK:N	2.79	0.44
1:B:458:UNK:C	1:B:460:UNK:N	2.81	0.44
1:B:636:UNK:O	1:B:638:UNK:N	2.50	0.44
1:A:170:UNK:O	1:A:171:UNK:C	2.66	0.44
1:A:204:UNK:O	1:A:216:UNK:N	2.51	0.44
1:B:432:UNK:O	1:B:434:UNK:N	2.50	0.44
1:A:73:UNK:O	1:A:89:UNK:CA	2.66	0.43
1:B:589:UNK:O	1:B:590:UNK:C	2.65	0.43
1:A:104:UNK:C	1:A:106:UNK:N	2.81	0.43
1:A:458:UNK:C	1:A:460:UNK:N	2.81	0.43
1:B:159:UNK:C	1:B:161:UNK:N	2.81	0.43
1:B:170:UNK:O	1:B:171:UNK:C	2.66	0.43
1:A:159:UNK:C	1:A:161:UNK:N	2.81	0.43
1:A:189:UNK:O	1:A:190:UNK:O	2.37	0.43
1:A:353:UNK:C	1:A:355:UNK:N	2.71	0.43
1:A:498:UNK:O	1:A:499:UNK:C	2.67	0.43
1:B:73:UNK:O	1:B:89:UNK:CA	2.66	0.43
1:A:636:UNK:O	1:A:638:UNK:N	2.50	0.43
1:B:104:UNK:C	1:B:106:UNK:N	2.81	0.43
1:A:180:UNK:O	1:A:181:UNK:C	2.67	0.43
1:A:519:UNK:O	1:A:520:UNK:C	2.66	0.43
1:B:273:UNK:O	1:B:276:UNK:O	2.37	0.43
1:A:142:UNK:C	1:A:144:UNK:N	2.81	0.43
1:B:275:UNK:O	1:B:276:UNK:O	2.36	0.43
1:A:50:UNK:C	1:A:52:UNK:N	2.79	0.43
1:A:275:UNK:O	1:A:276:UNK:O	2.36	0.43
1:B:498:UNK:O	1:B:499:UNK:C	2.66	0.43
1:A:560:UNK:O	1:A:561:UNK:C	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:UNK:O	1:B:181:UNK:C	2.67	0.42
1:B:534:UNK:N	1:B:534:UNK:C	2.76	0.42
1:B:456:UNK:C	1:B:458:UNK:N	2.82	0.42
1:A:25:UNK:O	1:A:26:UNK:C	2.66	0.42
1:A:456:UNK:C	1:A:458:UNK:N	2.83	0.42
1:A:642:UNK:O	1:A:645:UNK:N	2.52	0.42
1:B:204:UNK:O	1:B:216:UNK:N	2.51	0.42
1:B:281:UNK:O	1:B:284:UNK:N	2.52	0.42
1:B:554:UNK:O	1:B:555:UNK:C	2.66	0.42
1:A:401:UNK:C	1:A:402:UNK:O	2.68	0.42
1:A:554:UNK:O	1:A:555:UNK:C	2.66	0.42
1:B:560:UNK:O	1:B:561:UNK:C	2.67	0.42
1:B:642:UNK:O	1:B:645:UNK:N	2.52	0.42
1:A:16:UNK:O	1:A:18:UNK:N	2.52	0.42
1:A:273:UNK:O	1:A:276:UNK:O	2.37	0.42
1:B:301:UNK:O	1:B:302:UNK:O	2.37	0.42
1:A:281:UNK:O	1:A:284:UNK:N	2.52	0.42
1:A:615:UNK:O	1:A:618:UNK:N	2.53	0.42
1:B:144:UNK:C	1:B:146:UNK:N	2.81	0.42
1:A:246:UNK:O	1:A:247:UNK:C	2.68	0.42
1:A:301:UNK:O	1:A:302:UNK:O	2.37	0.42
1:A:359:UNK:O	1:A:360:UNK:O	2.38	0.42
1:A:250:UNK:C	1:A:252:UNK:N	2.83	0.42
1:A:278:UNK:O	1:A:280:UNK:C	2.68	0.41
1:B:615:UNK:O	1:B:618:UNK:N	2.53	0.41
1:A:393:UNK:C	1:A:395:UNK:N	2.83	0.41
1:B:189:UNK:O	1:B:190:UNK:O	2.37	0.41
1:B:393:UNK:C	1:B:395:UNK:N	2.83	0.41
1:A:518:UNK:O	1:A:520:UNK:C	2.68	0.41
1:A:615:UNK:O	1:A:617:UNK:N	2.53	0.41
1:B:16:UNK:O	1:B:18:UNK:N	2.53	0.41
1:B:518:UNK:O	1:B:520:UNK:C	2.68	0.41
1:B:401:UNK:C	1:B:402:UNK:O	2.68	0.41
1:B:617:UNK:O	1:B:618:UNK:C	2.69	0.41
1:B:652:UNK:O	1:B:653:UNK:C	2.68	0.41
1:B:330:UNK:O	1:B:331:UNK:C	2.68	0.41
1:A:652:UNK:O	1:A:653:UNK:C	2.68	0.41
2:A:660:HEM:HHC	2:A:660:HEM:CBB	2.22	0.41
1:B:353:UNK:O	1:B:355:UNK:C	2.69	0.41
1:A:613:UNK:C	1:A:615:UNK:N	2.84	0.41
1:A:617:UNK:O	1:A:618:UNK:C	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:UNK:O	1:A:185:UNK:N	2.54	0.41
1:B:250:UNK:C	1:B:252:UNK:N	2.83	0.41
1:B:428:UNK:O	1:B:431:UNK:CA	2.69	0.41
1:B:522:UNK:C	1:B:524:UNK:N	2.84	0.41
1:A:353:UNK:O	1:A:355:UNK:C	2.69	0.41
1:A:193:UNK:O	1:A:194:UNK:C	2.69	0.40
1:B:142:UNK:C	1:B:144:UNK:N	2.81	0.40
1:A:75:UNK:O	1:A:88:UNK:C	2.69	0.40
1:B:480:UNK:C	1:B:481:UNK:O	2.69	0.40
1:B:359:UNK:O	1:B:360:UNK:O	2.38	0.40
1:A:428:UNK:O	1:A:431:UNK:CA	2.69	0.40
1:A:491:UNK:O	1:A:493:UNK:N	2.54	0.40
2:B:660:HEM:HHC	2:B:660:HEM:CBB	2.22	0.40
1:A:533:UNK:C	1:A:534:UNK:CA	2.83	0.40
1:B:615:UNK:O	1:B:617:UNK:N	2.53	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:UNK:O	1:B:367:UNK:O[4_555]	1.64	0.56
1:A:367:UNK:O	1:B:53:UNK:O[4_555]	1.64	0.56
1:A:53:UNK:C	1:B:367:UNK:O[4_555]	2.09	0.11
1:A:367:UNK:O	1:B:53:UNK:C[4_555]	2.09	0.11
1:A:53:UNK:CA	1:B:367:UNK:O[4_555]	2.12	0.08
1:A:367:UNK:O	1:B:53:UNK:CA[4_555]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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](#)

2 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
2	HEM	A	660	-	41,50,50	1.46	5 (12%)	45,82,82	1.36	7 (15%)
2	HEM	B	660	-	41,50,50	1.45	5 (12%)	45,82,82	1.36	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	660	-	-	6/12/54/54	-
2	HEM	B	660	-	-	6/12/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	660	HEM	C3C-C2C	-4.25	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	HEM	C3C-C2C	-4.20	1.34	1.40
2	A	660	HEM	O2A-CGA	-3.10	1.20	1.30
2	B	660	HEM	O2A-CGA	-3.08	1.20	1.30
2	B	660	HEM	O2D-CGD	-3.04	1.20	1.30
2	A	660	HEM	O2D-CGD	-3.02	1.20	1.30
2	A	660	HEM	C1B-NB	-2.88	1.35	1.40
2	B	660	HEM	C1B-NB	-2.88	1.35	1.40
2	A	660	HEM	FE-NB	2.18	2.07	1.96
2	B	660	HEM	FE-NB	2.17	2.07	1.96

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	660	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
2	B	660	HEM	CBA-CAA-C2A	-2.70	108.02	112.62
2	A	660	HEM	C4B-CHC-C1C	2.59	125.98	122.56
2	A	660	HEM	CAD-CBD-CGD	-2.59	108.04	113.60
2	B	660	HEM	C4B-CHC-C1C	2.58	125.96	122.56
2	B	660	HEM	CAD-CBD-CGD	-2.57	108.07	113.60
2	A	660	HEM	C4C-CHD-C1D	2.49	125.85	122.56
2	B	660	HEM	C4C-CHD-C1D	2.48	125.83	122.56
2	A	660	HEM	CHC-C4B-NB	2.40	127.04	124.43
2	B	660	HEM	CHC-C4B-NB	2.39	127.03	124.43
2	B	660	HEM	CHA-C4D-ND	2.19	127.09	124.38
2	A	660	HEM	CHA-C4D-ND	2.16	127.05	124.38
2	A	660	HEM	CAA-CBA-CGA	-2.06	107.99	113.76
2	B	660	HEM	CAA-CBA-CGA	-2.04	108.04	113.76

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	660	HEM	C4B-C3B-CAB-CBB
2	B	660	HEM	C4B-C3B-CAB-CBB
2	A	660	HEM	CAD-CBD-CGD-O2D
2	B	660	HEM	CAD-CBD-CGD-O2D
2	A	660	HEM	CAD-CBD-CGD-O1D
2	B	660	HEM	CAD-CBD-CGD-O1D
2	B	660	HEM	CAA-CBA-CGA-O2A
2	A	660	HEM	CAA-CBA-CGA-O2A
2	B	660	HEM	C3D-CAD-CBD-CGD
2	A	660	HEM	CAA-CBA-CGA-O1A

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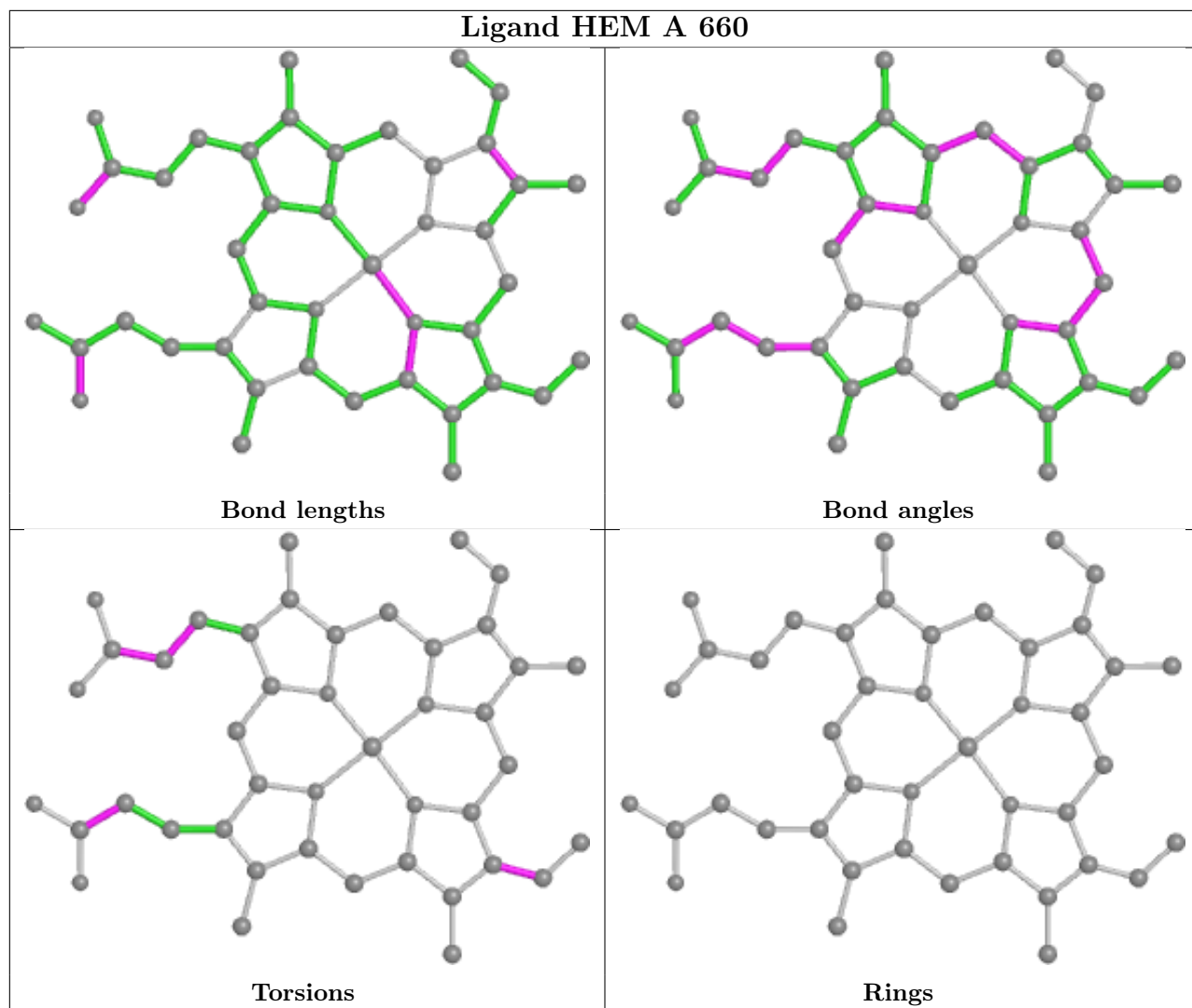
Mol	Chain	Res	Type	Atoms
2	B	660	HEM	CAA-CBA-CGA-O1A
2	A	660	HEM	C3D-CAD-CBD-CGD

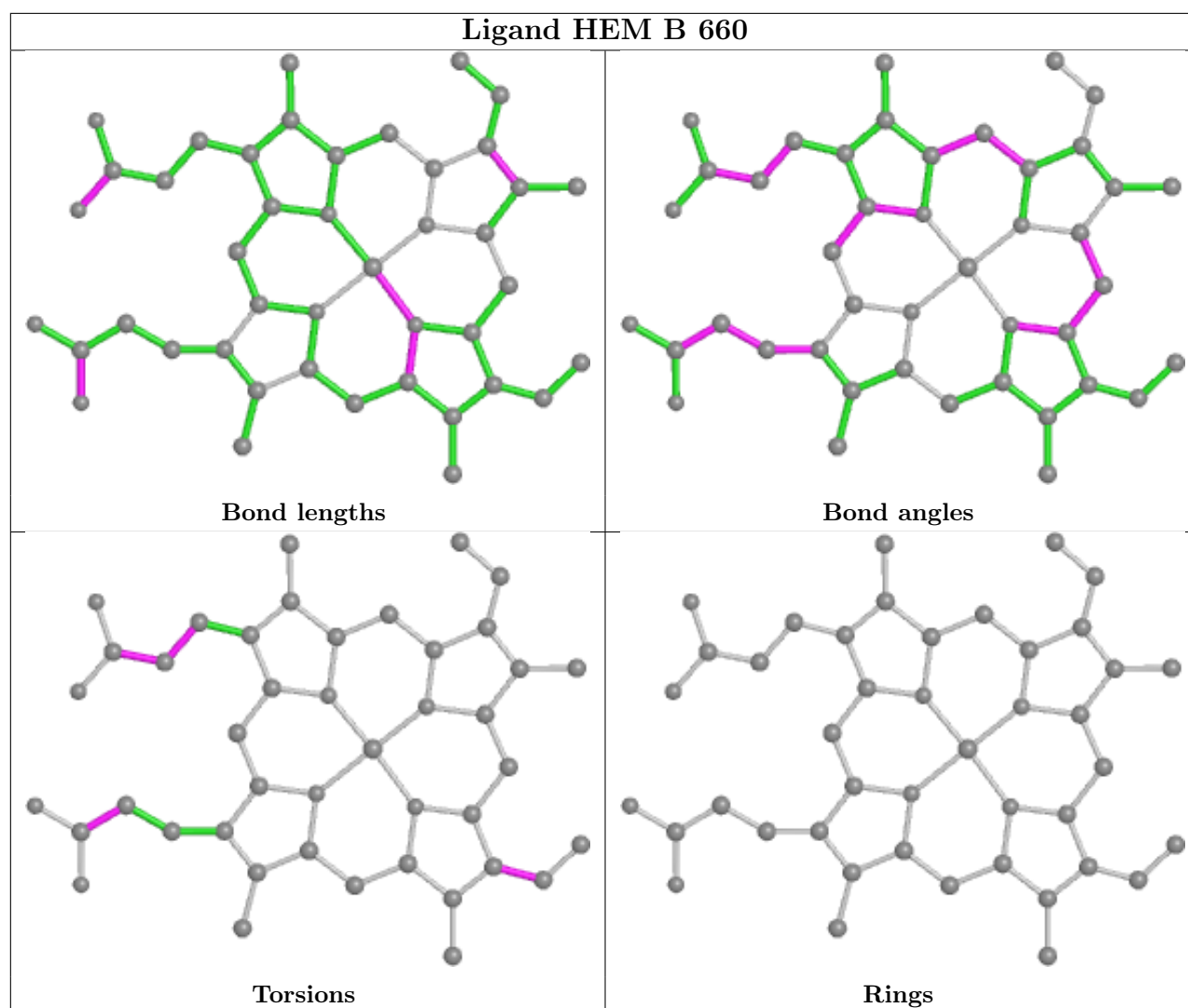
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	660	HEM	5	0
2	B	660	HEM	6	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	390:UNK	C	391:UNK	N	1.20
1	B	390:UNK	C	391:UNK	N	1.20
1	A	421:UNK	C	422:UNK	N	1.14
1	B	421:UNK	C	422:UNK	N	1.14
1	A	244:UNK	C	245:UNK	N	1.12
1	B	244:UNK	C	245:UNK	N	1.12
1	B	531:UNK	C	532:UNK	N	1.10
1	A	531:UNK	C	532:UNK	N	1.09

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.