



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:34 PM EDT

PDB ID : 1IQC / pdb_00001iqc
Title : Crystal structure of Di-Heme Peroxidase from Nitrosomonas europaea
Authors : Shimizu, H.
Deposited on : 2001-07-20
Resolution : 1.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

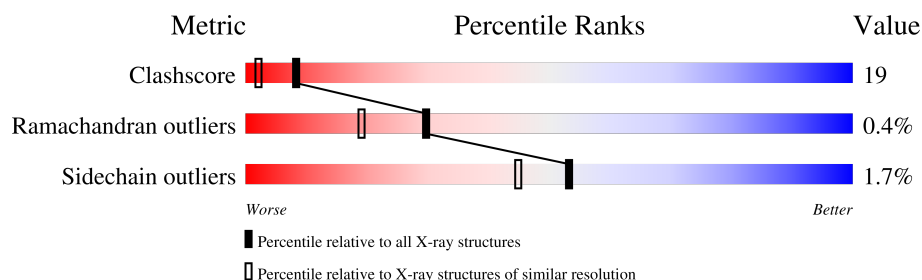
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	308	80% 19% .
1	B	308	72% 26% .
1	C	308	85% 14% .
1	D	308	50% 46% .

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
4	HEC	A	401	X	-	-	-
4	HEC	A	402	X	-	-	-
4	HEC	B	401	X	-	-	-
4	HEC	B	402	X	-	-	-
4	HEC	C	401	X	-	-	-
4	HEC	C	402	X	-	-	-
4	HEC	D	401	X	-	-	-
4	HEC	D	402	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10767 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 di-heme peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	B	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	C	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	D	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			

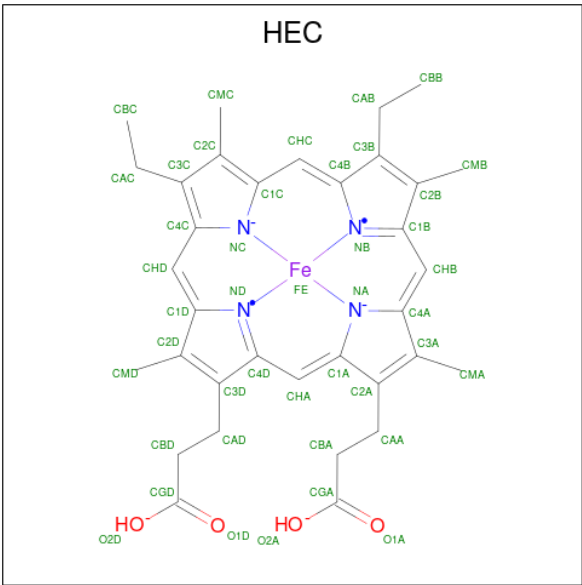
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

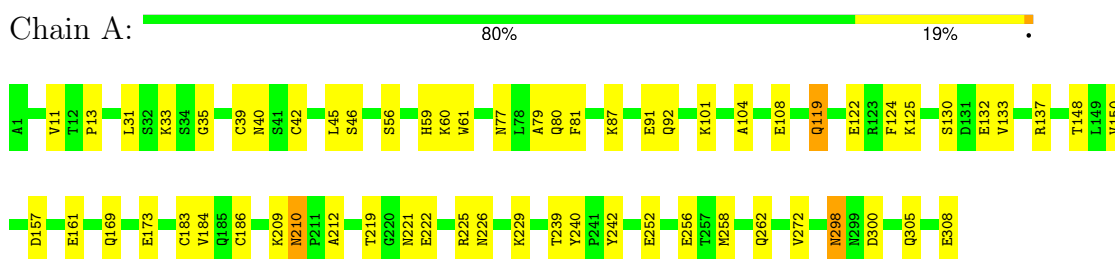
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	260	Total	O	0	0
			260	260		
6	B	199	Total	O	0	0
			199	199		
6	C	279	Total	O	0	0
			279	279		
6	D	120	Total	O	0	0
			120	120		

3 Residue-property plots

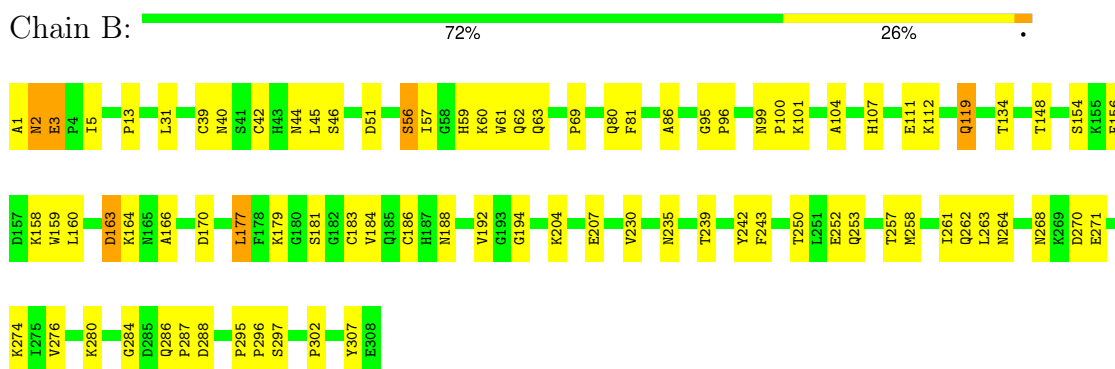
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

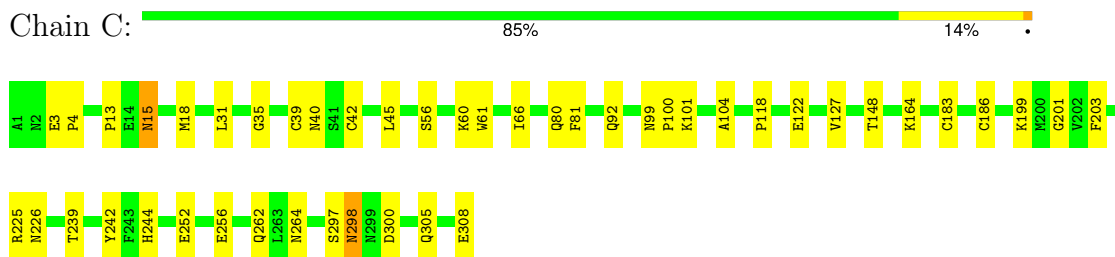
- Molecule 1: di-heme peroxidase



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A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19	A20	A21	A22	A23	A24	A25	A26	A27	A28	A29	A30	A31	A32	A33	A34	A35	A36	A37	A38	A39	A40	A41	A42	A43	A44	A45	A46	A47	A48	A49	A50	A51	A52	A53	A54	A55	A56	A57	A58	A59	A60	A61	A62	A63	A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	A97	A98	A99	A100	A101	A102	A103	A104	A105	A106	A107	A108	A109	A110	A111	A112	A113	A114	A115	A116	A117	A118	A119	A120	A121	A122	A123	A124	A125	A126	A127	A128	A129	A130	A131	A132	A133	A134	A135	A136	A137	A138	A139	A140	A141	A142	A143	A144	A145	A146	A147	A148	A149	A150	A151	A152	A153	A154	A155	A156	A157	A158	A159	A160	A161	A162	A163	A164	A165	A166	A167	A168	A169	A170	A171	A172	A173	A174	A175	A176	A177	A178	A179	A180	A181	A182	A183	A184	A185	A186	A187	A188	A189	A190	A191	A192	A193	A194	A195	A196	A197	A198	A199	A200	A201	A202	A203	A204	A205	A206	A207	A208	A209	A210	A211	A212	A213	A214	A215	A216	A217	A218	A219	A220	A221	A222	A223	A224	A225	A226	A227	A228	A229	A230	A231	A232	A233	A234	A235	A236	A237	A238	A239	A240	A241	A242	A243	A244	A245	A246	A247	A248	A249	A250	A251	A252	A253	A254	A255	A256	A257	A258	A259	A260	A261	A262	A263	A264	A265	A266	A267	A268	A269	A270	A271	A272	A273	A274	A275	A276	A277	A278	A279	A280	A281	A282	A283	A284	A285	A286	A287	A288	A289	A290	A291	A292	A293	A294	A295	A296	A297	A298	A299	A300	A301	A302	A303	A304	A305	A306	A307	A308	A309	A310	A311	A312	A313	A314	A315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.13Å 55.11Å 144.00Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.9 (30.00-1.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: CA, HEC, MG, GOL

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	0.36	0/2441	0.91	8/3304 (0.2%)
1	B	0.33	0/2441	0.93	10/3304 (0.3%)
1	C	0.38	0/2441	0.92	8/3304 (0.2%)
1	D	0.32	0/2441	0.85	2/3304 (0.1%)
All	All	0.35	0/9764	0.90	28/13216 (0.2%)

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

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

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	SER	N-CA-C	7.22	120.97	110.28
1	C	56	SER	N-CA-C	6.88	120.45	110.28
1	C	127	VAL	N-CA-C	6.52	117.14	110.82
1	B	239	THR	N-CA-C	6.20	120.45	112.26
1	B	56	SER	N-CA-C	6.13	119.15	110.50
1	A	242	TYR	N-CA-C	6.13	119.64	110.14
1	B	95	GLY	CA-C-N	6.09	125.57	119.24
1	B	95	GLY	C-N-CA	6.09	125.57	119.24
1	C	242	TYR	N-CA-C	5.97	119.40	110.14
1	A	31	LEU	N-CA-C	-5.81	105.69	112.89
1	C	297	SER	N-CA-C	-5.56	103.19	110.53
1	B	3	GLU	CA-C-N	5.52	126.58	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	GLU	C-N-CA	5.52	126.58	120.45
1	B	31	LEU	N-CA-C	-5.52	106.50	113.18
1	B	104	ALA	N-CA-C	5.38	119.43	112.86
1	B	297	SER	N-CA-C	-5.36	103.45	110.53
1	C	104	ALA	N-CA-C	5.33	119.07	112.24
1	C	35	GLY	N-CA-C	-5.21	108.06	115.30
1	A	46	SER	N-CA-C	-5.21	106.93	113.28
1	B	3	GLU	N-CA-C	5.20	121.30	109.81
1	D	78	LEU	N-CA-C	-5.18	106.47	112.89
1	A	229	LYS	N-CA-C	-5.17	102.63	110.28
1	D	260	ARG	N-CA-C	5.14	116.57	110.97
1	A	104	ALA	N-CA-C	5.10	118.76	112.24
1	A	35	GLY	N-CA-C	-5.09	108.22	115.30
1	C	31	LEU	N-CA-C	-5.08	106.59	112.89
1	C	239	THR	N-CA-C	5.06	118.93	112.26
1	A	239	THR	N-CA-C	5.00	118.92	111.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2331	58	0
1	B	2388	0	2331	86	0
1	C	2388	0	2331	46	0
1	D	2388	0	2331	195	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	86	0	64	16	0
4	B	86	0	64	18	0
4	C	86	0	64	18	0
4	D	86	0	64	20	0
5	B	6	0	8	0	0
6	A	260	0	0	4	0
6	B	199	0	0	4	0
6	C	279	0	0	0	0
6	D	120	0	0	6	0
All	All	10767	0	9588	375	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 (375) 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:186:CYS:SG	4:B:402:HEC:HAC	1.50	1.50
1:C:39:CYS:SG	4:C:401:HEC:CAB	2.08	1.41
1:A:39:CYS:SG	4:A:401:HEC:CAB	2.12	1.38
1:B:39:CYS:SG	4:B:401:HEC:CAB	2.13	1.37
1:A:42:CYS:SG	4:A:401:HEC:CAC	2.14	1.36
1:C:183:CYS:SG	4:C:402:HEC:CAB	2.13	1.36
1:A:183:CYS:SG	4:A:402:HEC:CAB	2.13	1.36
1:C:42:CYS:SG	4:C:401:HEC:CAC	2.12	1.36
1:C:186:CYS:SG	4:C:402:HEC:CAC	2.15	1.35
1:A:186:CYS:SG	4:A:402:HEC:CAC	2.14	1.34
1:B:42:CYS:SG	4:B:401:HEC:CAC	2.17	1.33
1:B:186:CYS:SG	4:B:402:HEC:CAC	2.16	1.32
1:B:183:CYS:SG	4:B:402:HEC:CAB	2.18	1.31
1:D:42:CYS:SG	4:D:401:HEC:HAC	1.70	1.31
1:D:183:CYS:SG	4:D:402:HEC:CAB	2.19	1.31
1:D:39:CYS:SG	4:D:401:HEC:CAB	2.19	1.30
1:D:186:CYS:SG	4:D:402:HEC:CAC	2.19	1.30
1:D:42:CYS:SG	4:D:401:HEC:CAC	2.20	1.29
1:C:39:CYS:SG	4:C:401:HEC:HAB	1.72	1.25
1:A:183:CYS:SG	4:A:402:HEC:HAB	1.75	1.21
1:A:39:CYS:SG	4:A:401:HEC:HAB	1.77	1.15
1:B:183:CYS:SG	4:B:402:HEC:HAB	1.79	1.15
1:D:183:CYS:SG	4:D:402:HEC:HAB	1.86	1.13
1:B:39:CYS:SG	4:B:401:HEC:HAB	1.86	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:CYS:SG	4:C:402:HEC:HAC	1.90	1.06
1:A:42:CYS:SG	4:A:401:HEC:HAC	1.87	1.05
1:D:39:CYS:SG	4:D:401:HEC:HAB	1.91	1.04
1:C:42:CYS:SG	4:C:401:HEC:HAC	1.97	1.03
1:C:183:CYS:SG	4:C:402:HEC:HAB	1.95	1.03
1:A:186:CYS:SG	4:A:402:HEC:HAC	1.98	1.01
1:D:151:THR:HG21	1:D:235:ASN:HD21	1.23	1.00
1:D:125:LYS:HE2	1:D:131:ASP:HB3	1.42	1.00
1:D:73:ASN:HD21	1:D:151:THR:HG22	1.25	0.98
1:D:186:CYS:SG	4:D:402:HEC:HAC	2.02	0.97
1:B:119:GLN:H	1:B:119:GLN:HE21	0.97	0.95
1:A:298:ASN:HD22	1:A:300:ASP:H	1.19	0.90
1:B:42:CYS:SG	4:B:401:HEC:HAC	2.10	0.90
1:D:225:ARG:HB2	1:D:225:ARG:HH11	1.38	0.88
1:B:119:GLN:H	1:B:119:GLN:NE2	1.70	0.88
1:D:224:ASP:O	1:D:227:VAL:HG12	1.74	0.88
1:D:201:GLY:H	1:D:262:GLN:HE22	1.20	0.87
1:D:268:ASN:ND2	1:D:271:GLU:H	1.72	0.87
1:D:201:GLY:H	1:D:262:GLN:NE2	1.72	0.87
1:D:40:ASN:HD21	1:D:45:LEU:H	1.22	0.86
1:A:33:LYS:HD3	6:A:1640:HOH:O	1.74	0.85
1:C:201:GLY:H	1:C:262:GLN:HE22	1.27	0.83
1:B:119:GLN:HE21	1:B:119:GLN:N	1.77	0.82
1:D:122:GLU:O	1:D:126:LYS:HD3	1.79	0.82
1:C:298:ASN:HD22	1:C:300:ASP:H	1.24	0.81
1:D:164:LYS:HE3	1:D:164:LYS:HA	1.61	0.81
1:D:103:MET:HE1	6:D:2502:HOH:O	1.80	0.80
1:D:151:THR:HG21	1:D:235:ASN:ND2	1.98	0.79
1:C:42:CYS:SG	4:C:401:HEC:CBC	2.70	0.79
1:C:183:CYS:SG	4:C:402:HEC:CBB	2.71	0.78
1:D:268:ASN:HD21	1:D:271:GLU:H	1.32	0.78
1:D:113:VAL:HG22	1:D:302:PRO:HG2	1.66	0.78
1:B:5:ILE:HD12	1:B:192:VAL:HG22	1.67	0.77
1:C:39:CYS:SG	4:C:401:HEC:CBB	2.71	0.77
1:B:39:CYS:SG	4:B:401:HEC:CBB	2.73	0.77
1:D:31:LEU:HB2	6:D:2502:HOH:O	1.84	0.76
1:A:210:ASN:HD22	1:A:212:ALA:H	1.33	0.76
1:D:40:ASN:ND2	1:D:45:LEU:H	1.83	0.75
1:B:44:ASN:HD22	1:B:46:SER:H	1.33	0.75
1:B:204:LYS:HB2	1:B:261:ILE:HG22	1.69	0.75
1:D:73:ASN:ND2	1:D:151:THR:HG22	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ASN:HD22	1:D:300:ASP:H	1.35	0.74
1:B:42:CYS:SG	4:B:401:HEC:C3C	2.75	0.74
1:B:42:CYS:SG	4:B:401:HEC:CBC	2.75	0.74
1:A:119:GLN:H	1:A:119:GLN:NE2	1.84	0.74
1:D:66:ILE:HD11	1:D:244:HIS:HB2	1.69	0.73
1:A:186:CYS:SG	4:A:402:HEC:CBC	2.75	0.73
1:D:130:SER:HB2	1:D:137:ARG:HH12	1.54	0.73
1:B:46:SER:OG	1:D:291:LEU:HD21	1.89	0.73
1:A:42:CYS:SG	4:A:401:HEC:C3C	2.76	0.72
1:D:125:LYS:CE	1:D:131:ASP:HB3	2.19	0.72
1:A:252:GLU:O	1:A:256:GLU:HG3	1.90	0.72
1:B:13:PRO:HG3	1:B:148:THR:CG2	2.19	0.71
1:D:3:GLU:O	1:D:188:ASN:HB2	1.89	0.71
1:D:73:ASN:HD21	1:D:151:THR:CG2	2.00	0.71
1:B:44:ASN:ND2	1:B:46:SER:H	1.88	0.71
1:D:130:SER:HB2	1:D:137:ARG:HH22	1.54	0.70
1:D:186:CYS:SG	4:D:402:HEC:C3C	2.79	0.70
1:D:221:ASN:HB2	1:D:224:ASP:OD2	1.91	0.70
1:D:216:MET:SD	1:D:225:ARG:NH1	2.65	0.70
1:D:42:CYS:SG	4:D:401:HEC:C3C	2.80	0.70
1:A:308:GLU:HG3	1:A:308:GLU:OXT	1.92	0.70
1:B:186:CYS:SG	4:B:402:HEC:C3C	2.80	0.69
1:A:39:CYS:SG	4:A:401:HEC:CBB	2.79	0.69
1:D:215:ARG:HB3	1:D:227:VAL:HG13	1.73	0.69
1:A:308:GLU:OXT	1:A:308:GLU:CG	2.40	0.69
1:C:186:CYS:SG	4:C:402:HEC:C3C	2.81	0.69
1:D:169:GLN:HG3	1:D:170:ASP:N	2.08	0.69
1:B:170:ASP:OD1	1:B:274:LYS:HE3	1.93	0.69
1:D:268:ASN:HD22	1:D:268:ASN:C	2.01	0.69
1:D:183:CYS:SG	4:D:402:HEC:CBB	2.81	0.68
1:C:80:GLN:O	1:C:81:PHE:HB2	1.93	0.68
1:D:108:GLU:OE1	1:D:109:ILE:HG13	1.94	0.68
1:D:298:ASN:HD21	1:D:300:ASP:HB2	1.59	0.67
1:D:3:GLU:HG3	1:D:189:GLY:HA2	1.77	0.67
1:D:114:VAL:HG21	1:D:133:VAL:HG11	1.77	0.67
1:A:184:VAL:HG22	6:A:1464:HOH:O	1.95	0.67
1:A:186:CYS:SG	4:A:402:HEC:C3C	2.81	0.67
1:A:169:GLN:O	1:A:173:GLU:HG3	1.95	0.67
1:B:13:PRO:HG3	1:B:148:THR:HG21	1.77	0.67
1:D:188:ASN:C	1:D:188:ASN:HD22	2.03	0.66
1:C:201:GLY:H	1:C:262:GLN:NE2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ARG:HB3	1:D:227:VAL:CG1	2.26	0.66
1:A:80:GLN:O	1:A:81:PHE:HB2	1.96	0.66
1:C:42:CYS:SG	4:C:401:HEC:C3C	2.81	0.66
1:B:96:PRO:HG3	6:B:1609:HOH:O	1.96	0.66
1:D:18:MET:HB3	1:D:144:GLN:HG2	1.77	0.66
1:D:110:ALA:O	1:D:114:VAL:HG22	1.96	0.65
1:D:1:ALA:O	1:D:2:ASN:HB2	1.96	0.65
1:D:108:GLU:CD	1:D:109:ILE:HG13	2.22	0.65
1:C:15:ASN:C	1:C:15:ASN:HD22	2.05	0.65
1:D:20:GLU:O	1:D:23:LYS:HG2	1.97	0.64
1:D:186:CYS:SG	4:D:402:HEC:CBC	2.86	0.64
1:C:186:CYS:SG	4:C:402:HEC:CBC	2.84	0.64
1:D:298:ASN:ND2	1:D:300:ASP:HB2	2.13	0.64
1:C:298:ASN:ND2	1:C:300:ASP:H	1.96	0.64
1:C:183:CYS:SG	4:C:402:HEC:C3B	2.85	0.64
1:D:225:ARG:HB2	1:D:225:ARG:NH1	2.12	0.63
1:A:125:LYS:HA	1:A:130:SER:O	1.98	0.63
1:A:298:ASN:ND2	1:A:300:ASP:H	1.94	0.63
1:B:286:GLN:HB3	1:B:287:PRO:HD2	1.80	0.63
1:B:270:ASP:O	1:B:274:LYS:HD3	1.99	0.62
1:D:78:LEU:C	1:D:78:LEU:HD12	2.23	0.62
1:C:252:GLU:O	1:C:256:GLU:HG3	1.99	0.62
1:D:39:CYS:SG	4:D:401:HEC:CBB	2.87	0.62
1:B:80:GLN:O	1:B:81:PHE:HB2	1.99	0.62
1:B:1:ALA:O	1:B:2:ASN:HB2	1.99	0.62
1:D:66:ILE:HG13	1:D:244:HIS:O	2.00	0.62
1:B:268:ASN:HB2	1:B:271:GLU:HG3	1.82	0.62
1:A:210:ASN:ND2	1:A:212:ALA:H	1.96	0.61
1:D:125:LYS:HA	1:D:130:SER:O	2.00	0.61
1:A:42:CYS:SG	4:A:401:HEC:CBC	2.87	0.61
1:D:198:GLN:C	1:D:227:VAL:HG23	2.25	0.61
1:D:80:GLN:O	1:D:81:PHE:HB2	1.99	0.61
1:A:130:SER:HB3	1:A:137:ARG:HH12	1.65	0.60
1:B:44:ASN:HD22	1:B:44:ASN:C	2.09	0.60
1:A:183:CYS:SG	4:A:402:HEC:CBB	2.86	0.60
1:B:183:CYS:SG	4:B:402:HEC:CBB	2.88	0.60
1:D:96:PRO:HG3	6:D:2540:HOH:O	2.02	0.60
1:D:135:ILE:HD13	1:D:135:ILE:O	2.01	0.60
1:B:264:ASN:C	1:B:264:ASN:HD22	2.10	0.59
1:C:13:PRO:HG3	1:C:148:THR:HG22	1.83	0.59
1:D:3:GLU:HG3	1:D:189:GLY:CA	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:CYS:SG	4:B:401:HEC:C3B	2.89	0.59
1:B:107:HIS:O	1:B:111:GLU:HG3	2.03	0.58
1:D:29:PRO:O	1:D:35:GLY:HA2	2.04	0.58
1:D:155:LYS:O	1:D:166:ALA:HB1	2.04	0.58
1:A:298:ASN:HD21	1:A:300:ASP:HB2	1.68	0.58
1:A:119:GLN:H	1:A:119:GLN:HE21	1.47	0.58
1:D:130:SER:HB2	1:D:137:ARG:NH2	2.18	0.58
1:D:225:ARG:HH11	1:D:225:ARG:CB	2.14	0.58
1:C:298:ASN:HD21	1:C:300:ASP:HB2	1.68	0.58
1:D:39:CYS:SG	4:D:401:HEC:C3B	2.89	0.58
1:D:130:SER:HB2	1:D:137:ARG:NH1	2.17	0.58
1:D:2:ASN:ND2	1:D:3:GLU:H	2.03	0.57
1:B:163:ASP:OD2	1:B:166:ALA:HB2	2.05	0.57
1:B:61:TRP:HB2	1:D:61:TRP:HB2	1.87	0.57
1:A:157:ASP:O	1:A:161:GLU:HG3	2.05	0.56
1:C:118:PRO:O	1:C:122:GLU:HG3	2.05	0.56
1:B:288:ASP:HA	6:B:1514:HOH:O	2.06	0.56
1:C:13:PRO:HG3	1:C:148:THR:CG2	2.36	0.56
1:B:13:PRO:HG3	1:B:148:THR:HG22	1.86	0.56
1:D:291:LEU:C	1:D:291:LEU:HD23	2.31	0.56
1:D:15:ASN:OD1	1:D:18:MET:HB2	2.06	0.55
1:C:99:ASN:C	1:C:99:ASN:HD22	2.13	0.55
1:D:124:PHE:CE2	1:D:133:VAL:HG13	2.41	0.55
1:D:268:ASN:ND2	1:D:268:ASN:C	2.62	0.55
1:A:13:PRO:HG3	1:A:148:THR:CG2	2.36	0.55
1:B:1:ALA:O	1:B:2:ASN:CB	2.54	0.55
1:D:21:LEU:O	1:D:25:LEU:HD23	2.06	0.55
1:D:5:ILE:HD12	1:D:5:ILE:H	1.72	0.55
1:D:151:THR:HG23	1:D:151:THR:O	2.06	0.55
1:A:305:GLN:HB3	1:A:308:GLU:HG2	1.89	0.54
1:A:183:CYS:SG	4:A:402:HEC:C3B	2.89	0.54
1:B:258:MET:O	1:B:262:GLN:HB2	2.07	0.54
1:B:242:TYR:O	1:B:243:PHE:HB2	2.08	0.54
1:D:130:SER:CB	1:D:137:ARG:HH12	2.19	0.54
1:D:28:ASP:OD1	1:D:30:ARG:HB2	2.08	0.54
1:C:39:CYS:SG	4:C:401:HEC:C3B	2.91	0.54
1:D:215:ARG:CB	1:D:227:VAL:HG13	2.37	0.54
1:D:298:ASN:ND2	1:D:300:ASP:H	2.02	0.54
1:D:263:LEU:HD21	4:D:402:HEC:HMC2	1.89	0.54
1:D:135:ILE:HD13	1:D:135:ILE:C	2.33	0.54
1:D:2:ASN:CG	1:D:3:GLU:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:HD12	1:D:5:ILE:N	2.22	0.53
1:B:134:THR:HG22	6:B:1575:HOH:O	2.09	0.53
1:B:235:ASN:HD21	1:B:284:GLY:H	1.54	0.53
1:D:5:ILE:HA	1:D:189:GLY:O	2.09	0.53
1:D:209:LYS:O	1:D:211:PRO:HD3	2.09	0.53
1:D:268:ASN:HD21	1:D:271:GLU:HG3	1.73	0.53
1:D:114:VAL:CG2	1:D:133:VAL:HG11	2.38	0.53
1:D:42:CYS:HA	1:D:51:ASP:HB3	1.90	0.53
1:A:13:PRO:HG3	1:A:148:THR:HG21	1.91	0.53
1:D:135:ILE:HA	1:D:138:ILE:HD12	1.90	0.53
1:B:194:GLY:HA2	1:B:230:VAL:O	2.08	0.53
1:C:99:ASN:ND2	1:C:101:LYS:H	2.07	0.53
1:D:134:THR:O	1:D:138:ILE:HG13	2.10	0.52
1:D:37:ILE:HD12	1:D:37:ILE:N	2.23	0.52
1:D:82:TRP:HZ3	4:D:402:HEC:HBD2	1.75	0.52
1:A:39:CYS:SG	4:A:401:HEC:C3B	2.91	0.52
1:D:78:LEU:HD23	1:D:195:SER:C	2.34	0.52
1:D:194:GLY:N	1:D:230:VAL:O	2.43	0.52
1:B:183:CYS:SG	4:B:402:HEC:C3B	2.94	0.52
1:C:40:ASN:HD21	1:C:45:LEU:H	1.57	0.52
1:D:78:LEU:HD11	1:D:197:TYR:OH	2.10	0.51
1:D:132:GLU:OE1	1:D:132:GLU:HA	2.08	0.51
1:D:169:GLN:O	1:D:173:GLU:HG3	2.10	0.51
1:A:130:SER:OG	1:A:132:GLU:HG2	2.10	0.51
1:D:306:PRO:HG2	1:D:307:TYR:CD1	2.45	0.51
1:A:60:LYS:HA	1:C:61:TRP:CD2	2.45	0.51
1:B:5:ILE:HD11	1:B:188:ASN:HA	1.93	0.51
1:D:229:LYS:NZ	4:D:401:HEC:O1A	2.43	0.51
1:D:168:ASN:OD1	1:D:171:GLU:HG3	2.11	0.51
1:D:177:LEU:HD21	1:D:271:GLU:HB3	1.92	0.51
1:D:258:MET:O	1:D:262:GLN:HB2	2.10	0.51
1:D:268:ASN:HD21	1:D:271:GLU:N	2.03	0.50
1:D:270:ASP:OD2	1:D:274:LYS:HE2	2.10	0.50
1:D:242:TYR:O	1:D:243:PHE:HB2	2.12	0.50
1:A:40:ASN:HD21	1:A:45:LEU:H	1.60	0.50
1:D:8:ILE:O	1:D:152:PRO:HB3	2.11	0.50
1:B:40:ASN:ND2	1:B:45:LEU:H	2.10	0.50
1:D:256:GLU:CD	1:D:260:ARG:HH12	2.19	0.50
1:B:44:ASN:HD21	1:B:46:SER:HB2	1.76	0.50
1:D:80:GLN:HB2	1:D:86:ALA:HB3	1.94	0.50
1:B:56:SER:HB3	4:B:401:HEC:HAC	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TRP:HB2	1:C:61:TRP:HB2	1.93	0.49
1:B:60:LYS:HA	1:D:61:TRP:CD2	2.47	0.49
1:D:201:GLY:N	1:D:262:GLN:HE22	2.00	0.49
1:B:5:ILE:CD1	1:B:188:ASN:HA	2.41	0.49
1:B:59:HIS:O	1:B:62:GLN:HG3	2.12	0.49
1:D:32:SER:HB3	1:D:103:MET:HE2	1.95	0.49
1:D:77:ASN:HB3	1:D:79:ALA:O	2.12	0.49
1:D:268:ASN:ND2	1:D:271:GLU:HB2	2.27	0.49
1:A:256:GLU:HG2	1:A:272:VAL:HG21	1.95	0.49
1:A:108:GLU:CD	1:A:108:GLU:H	2.20	0.49
1:C:40:ASN:ND2	1:C:45:LEU:H	2.11	0.49
1:B:99:ASN:C	1:B:99:ASN:HD22	2.19	0.49
1:D:24:MET:HE2	1:D:120:TYR:CE1	2.48	0.49
1:A:61:TRP:CD2	1:C:60:LYS:HA	2.48	0.48
1:D:215:ARG:O	1:D:218:VAL:HG12	2.13	0.48
1:D:34:SER:HB3	1:D:59:HIS:CE1	2.47	0.48
1:D:183:CYS:CB	4:D:402:HEC:HAB	2.42	0.48
1:D:183:CYS:C	1:D:185:GLN:H	2.21	0.48
1:D:218:VAL:HG13	1:D:219:THR:HG23	1.95	0.48
1:D:222:GLU:OE2	1:D:225:ARG:NH1	2.46	0.48
1:B:112:LYS:HD3	1:B:302:PRO:HG3	1.94	0.48
1:D:78:LEU:HD11	1:D:197:TYR:CZ	2.48	0.48
1:B:40:ASN:HD21	1:B:45:LEU:H	1.62	0.48
1:D:96:PRO:HA	1:D:102:GLU:OE1	2.14	0.48
1:D:291:LEU:HD23	1:D:292:PRO:N	2.28	0.47
1:B:57:ILE:HD11	1:D:306:PRO:HB2	1.97	0.47
1:C:15:ASN:ND2	1:C:18:MET:H	2.13	0.47
1:A:101:LYS:HD3	6:A:1524:HOH:O	2.12	0.47
1:B:119:GLN:CD	1:B:295:PRO:HB3	2.40	0.47
1:B:177:LEU:HD23	1:B:181:SER:HG	1.79	0.47
1:B:57:ILE:HD13	1:D:307:TYR:CZ	2.49	0.47
1:C:66:ILE:HD11	1:C:244:HIS:HB2	1.97	0.47
1:C:308:GLU:OXT	1:C:308:GLU:HG2	2.15	0.47
1:D:155:LYS:HD3	1:D:166:ALA:O	2.14	0.47
1:D:188:ASN:C	1:D:188:ASN:ND2	2.69	0.47
1:D:1:ALA:HB2	1:D:184:VAL:HG23	1.97	0.47
1:D:80:GLN:HA	1:D:80:GLN:NE2	2.30	0.47
1:D:183:CYS:SG	4:D:402:HEC:C3B	2.97	0.47
1:B:296:PRO:HB3	1:D:238:LEU:HD22	1.97	0.46
1:D:113:VAL:HG22	1:D:302:PRO:CG	2.41	0.46
1:D:167:LEU:HD22	1:D:281:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:PHE:CD2	1:C:264:ASN:HB2	2.51	0.46
1:D:80:GLN:O	1:D:84:GLY:HA2	2.15	0.46
1:B:99:ASN:HD22	1:B:100:PRO:N	2.14	0.46
1:B:99:ASN:HD22	1:B:100:PRO:CD	2.27	0.46
1:B:181:SER:O	1:B:263:LEU:HD13	2.16	0.46
1:D:128:PHE:HE2	1:D:140:THR:HG21	1.81	0.46
1:D:134:THR:OG1	1:D:137:ARG:HG3	2.16	0.46
1:D:200:MET:HE3	1:D:206:TYR:CG	2.51	0.46
1:D:225:ARG:O	1:D:226:ASN:HB2	2.16	0.46
1:D:240:TYR:HB2	6:D:2535:HOH:O	2.15	0.46
1:B:288:ASP:OD1	1:D:290:LYS:HD3	2.16	0.46
1:C:183:CYS:HG	4:C:402:HEC:HAB	1.78	0.46
1:C:99:ASN:HD22	1:C:100:PRO:N	2.13	0.45
1:D:100:PRO:HA	1:D:104:ALA:HA	1.98	0.45
1:D:146:GLU:HA	1:D:149:LEU:HG	1.99	0.45
1:B:177:LEU:HD11	1:B:271:GLU:HB3	1.98	0.45
4:C:402:HEC:HMB3	4:C:402:HEC:HBB3	1.98	0.45
1:D:23:LYS:HB2	1:D:23:LYS:NZ	2.32	0.45
1:B:63:GLN:HG3	1:D:307:TYR:CZ	2.51	0.45
1:A:40:ASN:ND2	1:A:45:LEU:H	2.14	0.45
1:B:42:CYS:HA	1:B:51:ASP:HB3	1.99	0.45
1:D:78:LEU:HD12	1:D:79:ALA:HB2	1.99	0.45
1:D:150:VAL:HG23	1:D:152:PRO:HD3	1.99	0.45
1:A:59:HIS:CD2	1:A:60:LYS:HG3	2.52	0.45
1:D:142:ILE:O	1:D:146:GLU:HG3	2.16	0.45
4:B:401:HEC:HBC3	4:B:401:HEC:HMC3	2.00	0.44
1:D:15:ASN:HB3	1:D:18:MET:HE3	1.98	0.44
1:D:268:ASN:ND2	1:D:271:GLU:CB	2.80	0.44
1:D:72:LEU:O	1:D:73:ASN:HB2	2.18	0.44
1:B:99:ASN:HD22	1:B:100:PRO:HD2	1.83	0.44
1:D:92:GLN:C	1:D:92:GLN:CD	2.85	0.44
1:B:179:LYS:HG2	1:B:184:VAL:HG11	2.00	0.44
1:D:260:ARG:O	1:D:264:ASN:HA	2.18	0.44
1:D:270:ASP:O	1:D:274:LYS:HG3	2.18	0.44
1:C:305:GLN:HB3	1:C:308:GLU:HB3	1.99	0.44
1:B:257:THR:O	1:B:261:ILE:HG12	2.18	0.44
1:C:199:LYS:HE3	1:C:226:ASN:HB2	2.00	0.44
1:B:307:TYR:CZ	1:D:63:GLN:HG3	2.53	0.43
1:D:194:GLY:HA2	1:D:230:VAL:O	2.18	0.43
1:B:207:GLU:H	1:B:207:GLU:CD	2.26	0.43
1:B:235:ASN:ND2	1:B:284:GLY:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LYS:HE2	6:B:1474:HOH:O	2.18	0.43
1:B:177:LEU:HD23	1:B:181:SER:OG	2.18	0.43
1:D:26:PHE:O	1:D:39:CYS:HB2	2.18	0.43
1:B:99:ASN:ND2	1:B:101:LYS:H	2.16	0.43
1:A:298:ASN:ND2	1:A:300:ASP:HB2	2.32	0.43
1:D:11:VAL:HG12	1:D:12:THR:N	2.33	0.43
1:D:59:HIS:O	1:D:60:LYS:HB2	2.18	0.43
1:D:236:ILE:HA	6:D:2461:HOH:O	2.18	0.43
1:B:44:ASN:ND2	1:B:46:SER:HB2	2.33	0.43
1:B:250:THR:HG23	1:B:253:GLN:H	1.84	0.43
1:C:225:ARG:O	1:C:226:ASN:HB2	2.18	0.43
1:A:92:GLN:C	1:A:92:GLN:CD	2.86	0.42
1:D:157:ASP:O	1:D:161:GLU:HG3	2.18	0.42
1:D:229:LYS:HE2	1:D:229:LYS:HB3	1.89	0.42
1:A:87:LYS:HG2	1:A:91:GLU:OE1	2.19	0.42
1:D:164:LYS:HA	1:D:164:LYS:CE	2.42	0.42
1:D:294:LEU:HA	1:D:295:PRO:HD3	1.89	0.42
1:A:225:ARG:O	1:A:226:ASN:HB2	2.18	0.42
1:D:199:LYS:HA	1:D:227:VAL:HA	2.02	0.42
1:B:276:VAL:HG12	1:B:280:LYS:HE3	2.01	0.42
1:D:199:LYS:N	1:D:227:VAL:HG23	2.34	0.42
1:B:69:PRO:HG2	4:B:401:HEC:HBA1	2.02	0.42
1:D:258:MET:SD	1:D:262:GLN:HG3	2.60	0.42
1:A:219:THR:HB	1:A:221:ASN:ND2	2.35	0.42
1:B:252:GLU:CD	1:B:252:GLU:H	2.28	0.42
1:D:32:SER:HB3	1:D:37:ILE:O	2.20	0.42
1:D:99:ASN:CG	1:D:102:GLU:HG3	2.44	0.42
1:D:115:ALA:O	1:D:121:ARG:HD3	2.19	0.42
1:D:192:VAL:HG12	1:D:192:VAL:O	2.20	0.42
1:D:198:GLN:HA	1:D:198:GLN:NE2	2.34	0.42
1:D:268:ASN:HD21	1:D:271:GLU:CG	2.32	0.42
1:A:77:ASN:HB3	1:A:79:ALA:O	2.20	0.41
1:D:5:ILE:H	1:D:5:ILE:CD1	2.33	0.41
1:A:11:VAL:HG23	1:A:150:VAL:HG21	2.01	0.41
1:A:258:MET:O	1:A:262:GLN:HB2	2.20	0.41
1:B:112:LYS:HD3	1:B:302:PRO:CG	2.50	0.41
1:B:154:SER:O	1:B:158:LYS:HG3	2.20	0.41
1:D:130:SER:HB2	1:D:137:ARG:CZ	2.50	0.41
1:D:183:CYS:CB	4:D:402:HEC:CAB	2.98	0.41
1:C:92:GLN:CD	1:C:92:GLN:C	2.89	0.41
1:D:200:MET:HE3	1:D:206:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HE2	6:A:1550:HOH:O	2.21	0.41
1:B:80:GLN:HB2	1:B:86:ALA:HB3	2.02	0.41
1:C:164:LYS:HA	1:C:164:LYS:HD3	1.87	0.41
1:D:183:CYS:C	1:D:185:GLN:N	2.79	0.41
1:B:156:PHE:CE2	1:B:160:LEU:HD11	2.56	0.41
1:C:3:GLU:HA	1:C:4:PRO:HD3	1.82	0.41
1:D:15:ASN:C	1:D:15:ASN:HD22	2.28	0.41
1:D:119:GLN:NE2	1:D:296:PRO:HD2	2.36	0.41
1:D:141:ALA:O	1:D:144:GLN:HB3	2.21	0.41
1:D:78:LEU:HD12	1:D:79:ALA:CB	2.51	0.41
1:D:201:GLY:N	1:D:262:GLN:NE2	2.54	0.41
1:D:236:ILE:HG13	1:D:251:LEU:HD21	2.03	0.41
1:A:13:PRO:HG3	1:A:148:THR:HG22	2.03	0.41
1:B:159:TRP:CD1	1:B:164:LYS:HA	2.56	0.41
1:D:21:LEU:O	1:D:25:LEU:CD2	2.69	0.41
1:D:119:GLN:HE22	1:D:296:PRO:HD2	1.86	0.41
1:D:291:LEU:C	1:D:291:LEU:CD2	2.94	0.41
1:A:80:GLN:O	1:A:81:PHE:CB	2.68	0.40
1:A:124:PHE:CE2	1:A:133:VAL:HG13	2.55	0.40
1:D:128:PHE:C	1:D:130:SER:H	2.29	0.40
1:D:80:GLN:HA	1:D:80:GLN:HE21	1.85	0.40
1:D:151:THR:HG23	6:D:2519:HOH:O	2.20	0.40
1:D:15:ASN:CB	1:D:18:MET:HE3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/308 (99%)	296 (97%)	10 (3%)	0	100	100
1	B	306/308 (99%)	287 (94%)	16 (5%)	3 (1%)	12	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	306/308 (99%)	298 (97%)	8 (3%)	0	100	100
1	D	306/308 (99%)	285 (93%)	19 (6%)	2 (1%)	18	8
All	All	1224/1232 (99%)	1166 (95%)	53 (4%)	5 (0%)	30	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	D	2	ASN
1	B	163	ASP
1	D	215	ARG
1	B	3	GLU

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	260/260 (100%)	254 (98%)	6 (2%)	44	33
1	B	260/260 (100%)	258 (99%)	2 (1%)	73	70
1	C	260/260 (100%)	258 (99%)	2 (1%)	73	70
1	D	260/260 (100%)	252 (97%)	8 (3%)	35	23
All	All	1040/1040 (100%)	1022 (98%)	18 (2%)	53	45

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	122	GLU
1	A	209	LYS
1	A	210	ASN
1	A	222	GLU
1	A	298	ASN
1	B	119	GLN

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Mol	Chain	Res	Type
1	B	177	LEU
1	C	15	ASN
1	C	298	ASN
1	D	23	LYS
1	D	132	GLU
1	D	135	ILE
1	D	164	LYS
1	D	188	ASN
1	D	225	ARG
1	D	268	ASN
1	D	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	165	ASN
1	A	185	GLN
1	A	198	GLN
1	A	210	ASN
1	A	221	ASN
1	A	226	ASN
1	A	298	ASN
1	A	299	ASN
1	B	40	ASN
1	B	44	ASN
1	B	52	ASN
1	B	59	HIS
1	B	63	GLN
1	B	99	ASN
1	B	119	GLN
1	B	165	ASN
1	B	176	ASN
1	B	198	GLN
1	B	235	ASN
1	B	264	ASN
1	B	268	ASN
1	B	286	GLN
1	B	299	ASN
1	C	2	ASN
1	C	15	ASN
1	C	63	GLN

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Mol	Chain	Res	Type
1	C	99	ASN
1	C	144	GLN
1	C	176	ASN
1	C	185	GLN
1	C	221	ASN
1	C	226	ASN
1	C	253	GLN
1	C	262	GLN
1	C	264	ASN
1	C	298	ASN
1	D	2	ASN
1	D	40	ASN
1	D	62	GLN
1	D	63	GLN
1	D	73	ASN
1	D	77	ASN
1	D	80	GLN
1	D	119	GLN
1	D	198	GLN
1	D	226	ASN
1	D	262	GLN
1	D	264	ASN
1	D	268	ASN
1	D	298	ASN
1	D	299	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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
4	HEC	C	402	1	50,50,50	1.19	2 (4%)	68,82,82	1.10	2 (2%)
5	GOL	B	1410	-	5,5,5	0.30	0	5,5,5	0.29	0
4	HEC	A	401	1,6	50,50,50	1.25	2 (4%)	68,82,82	1.18	2 (2%)
4	HEC	D	401	1,6	50,50,50	1.21	2 (4%)	68,82,82	0.95	2 (2%)
4	HEC	D	402	1	50,50,50	1.26	2 (4%)	68,82,82	1.33	7 (10%)
4	HEC	A	402	1	50,50,50	1.15	2 (4%)	68,82,82	1.08	2 (2%)
4	HEC	C	401	1,6	50,50,50	1.28	2 (4%)	68,82,82	1.17	2 (2%)
4	HEC	B	401	1,6	50,50,50	1.15	2 (4%)	68,82,82	1.15	2 (2%)
4	HEC	B	402	1	50,50,50	1.28	3 (6%)	68,82,82	1.10	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	C	402	1	1/1/3/7	6/14/54/54	-
5	GOL	B	1410	-	-	0/4/4/4	-
4	HEC	A	401	1,6	1/1/3/7	5/14/54/54	-
4	HEC	D	401	1,6	1/1/3/7	10/14/54/54	-
4	HEC	D	402	1	1/1/3/7	8/14/54/54	-
4	HEC	A	402	1	1/1/3/7	6/14/54/54	-
4	HEC	C	401	1,6	1/1/3/7	6/14/54/54	-
4	HEC	B	401	1,6	1/1/3/7	6/14/54/54	-
4	HEC	B	402	1	1/1/3/7	5/14/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	HEC	CAC-C3C	-4.91	1.38	1.51
4	D	402	HEC	CAB-C3B	-4.67	1.39	1.51
4	C	401	HEC	CAB-C3B	-4.59	1.39	1.51
4	B	402	HEC	CAC-C3C	-4.57	1.39	1.51
4	A	402	HEC	CAC-C3C	-4.36	1.40	1.51
4	D	402	HEC	CAC-C3C	-4.33	1.40	1.51
4	B	401	HEC	CAB-C3B	-4.33	1.40	1.51
4	D	401	HEC	CAB-C3B	-4.31	1.40	1.51
4	D	401	HEC	CAC-C3C	-4.28	1.40	1.51
4	C	402	HEC	CAC-C3C	-4.28	1.40	1.51
4	C	402	HEC	CAB-C3B	-4.24	1.40	1.51
4	C	401	HEC	CAC-C3C	-4.24	1.40	1.51
4	B	402	HEC	CAB-C3B	-4.23	1.40	1.51
4	A	402	HEC	CAB-C3B	-4.11	1.40	1.51
4	A	401	HEC	CAB-C3B	-4.02	1.40	1.51
4	B	401	HEC	CAC-C3C	-3.74	1.41	1.51
4	B	402	HEC	FE-NC	2.07	2.02	1.95

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	HEC	CBC-CAC-C3C	5.39	127.04	112.42
4	B	402	HEC	CBC-CAC-C3C	5.30	126.80	112.42
4	A	401	HEC	CBC-CAC-C3C	5.10	126.24	112.42
4	B	401	HEC	CBB-CAB-C3B	4.80	125.43	112.42
4	C	401	HEC	CBB-CAB-C3B	4.78	125.38	112.42
4	A	401	HEC	CBB-CAB-C3B	4.74	125.28	112.42
4	C	402	HEC	CBC-CAC-C3C	4.71	125.18	112.42
4	C	401	HEC	CBC-CAC-C3C	4.66	125.05	112.42
4	D	402	HEC	CBC-CAC-C3C	4.51	124.65	112.42
4	C	402	HEC	CBB-CAB-C3B	4.42	124.39	112.42
4	A	402	HEC	CBB-CAB-C3B	4.39	124.31	112.42
4	A	402	HEC	CBC-CAC-C3C	4.38	124.29	112.42
4	D	402	HEC	CBB-CAB-C3B	4.37	124.26	112.42
4	D	402	HEC	CBD-CAD-C3D	4.33	124.51	112.53
4	B	402	HEC	CBB-CAB-C3B	4.15	123.67	112.42
4	D	401	HEC	CBC-CAC-C3C	4.11	123.56	112.42
4	D	401	HEC	CBB-CAB-C3B	4.05	123.40	112.42
4	D	402	HEC	C3D-C4D-ND	2.73	112.99	110.35
4	D	402	HEC	C1D-ND-C4D	-2.64	102.08	105.21
4	D	402	HEC	CHA-C4D-C3D	-2.14	121.66	124.77
4	D	402	HEC	C4D-C3D-C2D	-2.06	103.90	106.89

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	401	HEC	NA
4	A	402	HEC	NA
4	B	401	HEC	NA
4	B	402	HEC	NA
4	C	401	HEC	NA
4	C	402	HEC	NA
4	D	401	HEC	NA
4	D	402	HEC	NA

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	HEC	C2C-C3C-CAC-CBC
4	B	401	HEC	C2C-C3C-CAC-CBC
4	D	402	HEC	C2C-C3C-CAC-CBC
4	A	402	HEC	C4C-C3C-CAC-CBC
4	B	401	HEC	C4C-C3C-CAC-CBC
4	C	401	HEC	C4C-C3C-CAC-CBC
4	C	401	HEC	C2C-C3C-CAC-CBC
4	C	402	HEC	C2B-C3B-CAB-CBB
4	D	401	HEC	C2B-C3B-CAB-CBB
4	A	402	HEC	C2B-C3B-CAB-CBB
4	B	401	HEC	C2B-C3B-CAB-CBB
4	D	402	HEC	C4C-C3C-CAC-CBC
4	D	402	HEC	C2B-C3B-CAB-CBB
4	C	402	HEC	C2C-C3C-CAC-CBC
4	D	402	HEC	C4D-C3D-CAD-CBD
4	A	401	HEC	C2C-C3C-CAC-CBC
4	A	401	HEC	C2B-C3B-CAB-CBB
4	B	402	HEC	C2B-C3B-CAB-CBB
4	C	402	HEC	C4C-C3C-CAC-CBC
4	A	401	HEC	C4C-C3C-CAC-CBC
4	C	401	HEC	C2B-C3B-CAB-CBB
4	D	401	HEC	C4B-C3B-CAB-CBB
4	C	402	HEC	C4B-C3B-CAB-CBB
4	B	401	HEC	C4B-C3B-CAB-CBB
4	D	402	HEC	C4B-C3B-CAB-CBB
4	A	402	HEC	C4B-C3B-CAB-CBB
4	A	401	HEC	C4B-C3B-CAB-CBB
4	B	402	HEC	C4B-C3B-CAB-CBB
4	D	401	HEC	C4C-C3C-CAC-CBC
4	D	401	HEC	C3A-C2A-CAA-CBA

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	D	401	HEC	C2C-C3C-CAC-CBC
4	C	401	HEC	C4B-C3B-CAB-CBB
4	D	402	HEC	C2D-C3D-CAD-CBD
4	D	402	HEC	CAD-CBD-CGD-O2D
4	B	402	HEC	CAD-CBD-CGD-O2D
4	C	402	HEC	CAD-CBD-CGD-O2D
4	C	401	HEC	CAA-CBA-CGA-O2A
4	A	402	HEC	CAD-CBD-CGD-O2D
4	C	402	HEC	CAD-CBD-CGD-O1D
4	D	401	HEC	CAA-CBA-CGA-O2A
4	B	402	HEC	CAD-CBD-CGD-O1D
4	D	402	HEC	CAD-CBD-CGD-O1D
4	C	401	HEC	CAA-CBA-CGA-O1A
4	D	401	HEC	CAA-CBA-CGA-O1A
4	D	401	HEC	CAD-CBD-CGD-O2D
4	B	402	HEC	C4C-C3C-CAC-CBC
4	A	402	HEC	CAD-CBD-CGD-O1D
4	D	401	HEC	CAD-CBD-CGD-O1D
4	D	401	HEC	C2D-C3D-CAD-CBD
4	B	401	HEC	CAD-CBD-CGD-O2D
4	B	401	HEC	CAD-CBD-CGD-O1D
4	A	401	HEC	CAA-CBA-CGA-O2A

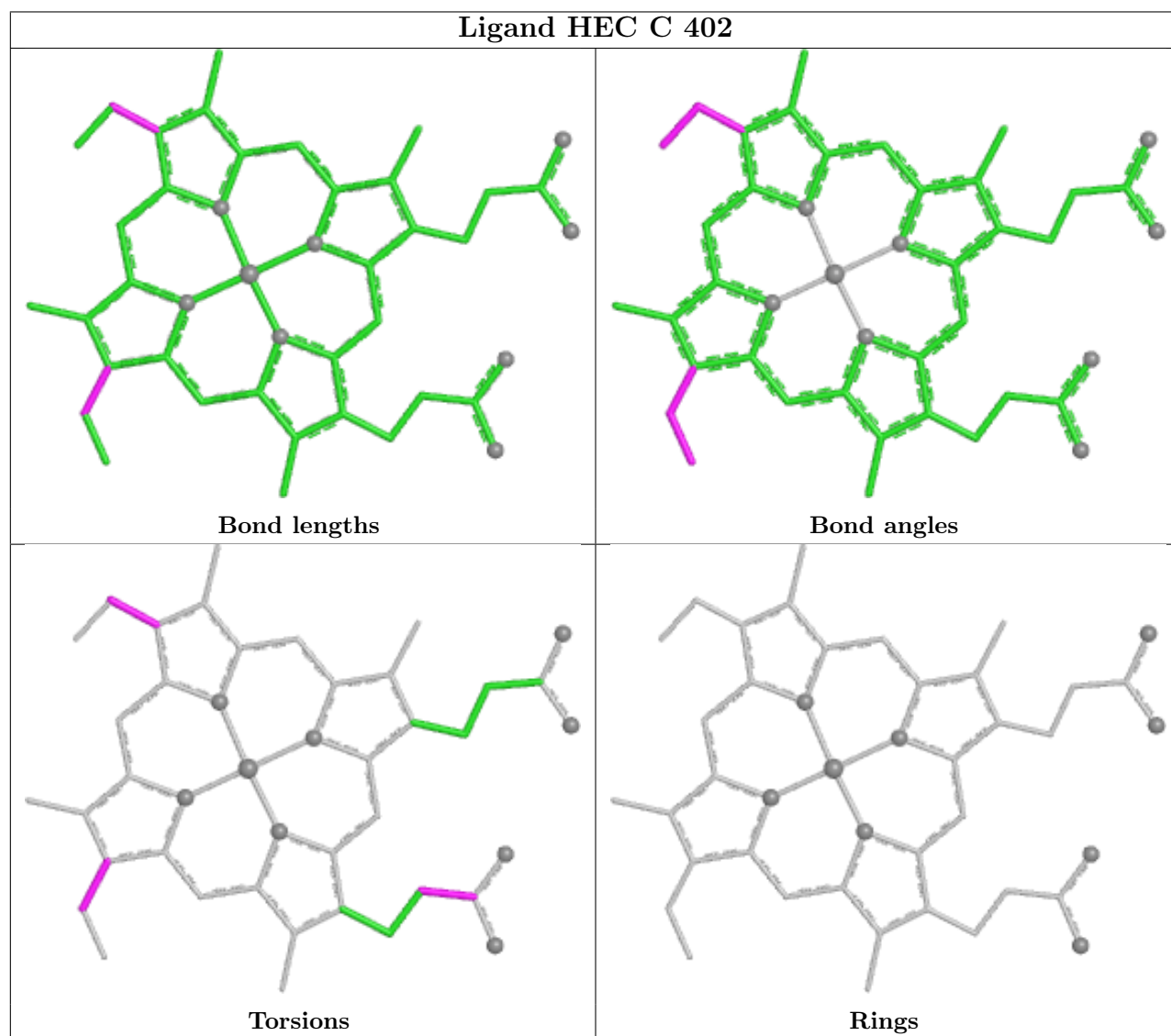
There are no ring outliers.

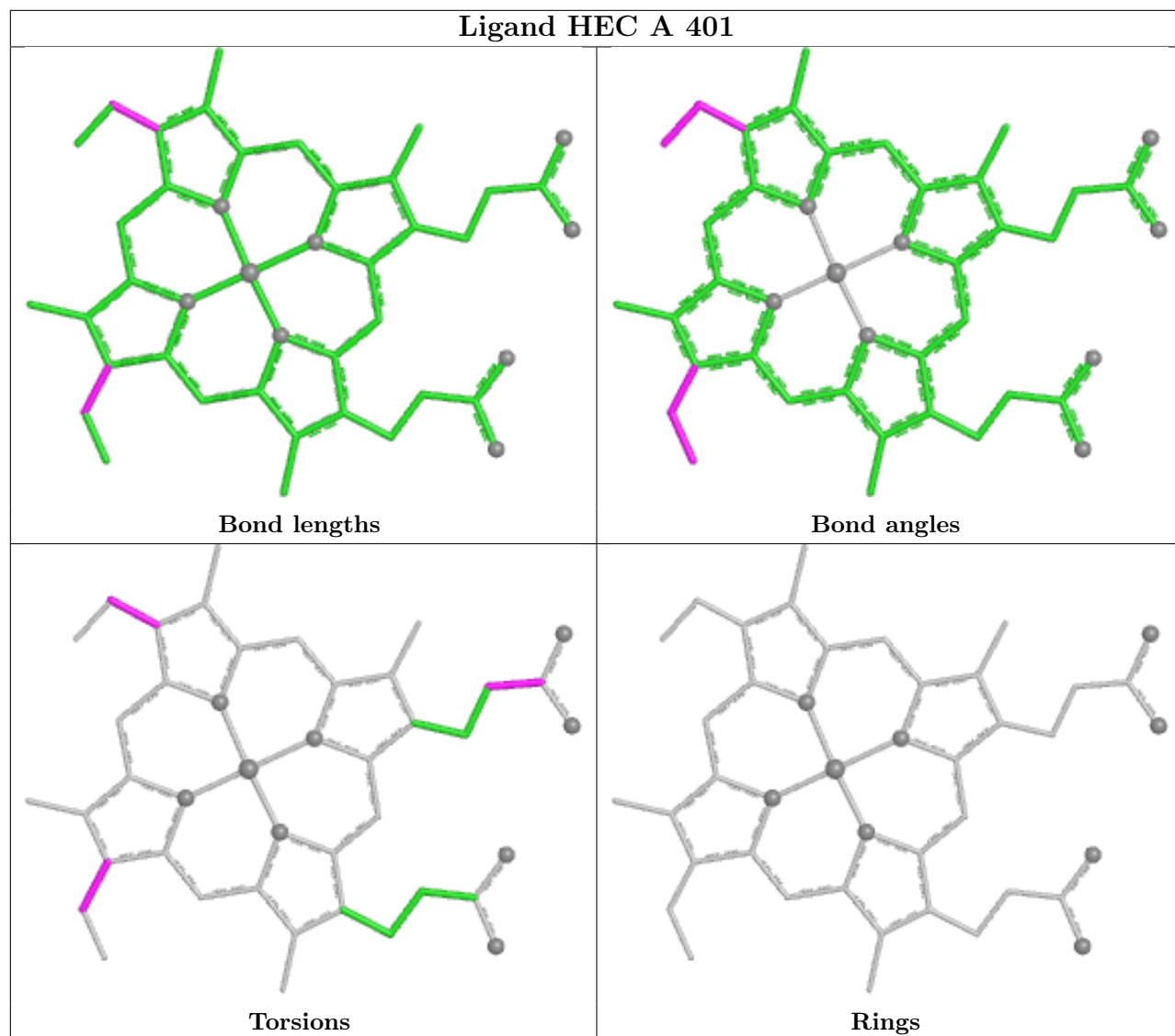
8 monomers are involved in 72 short contacts:

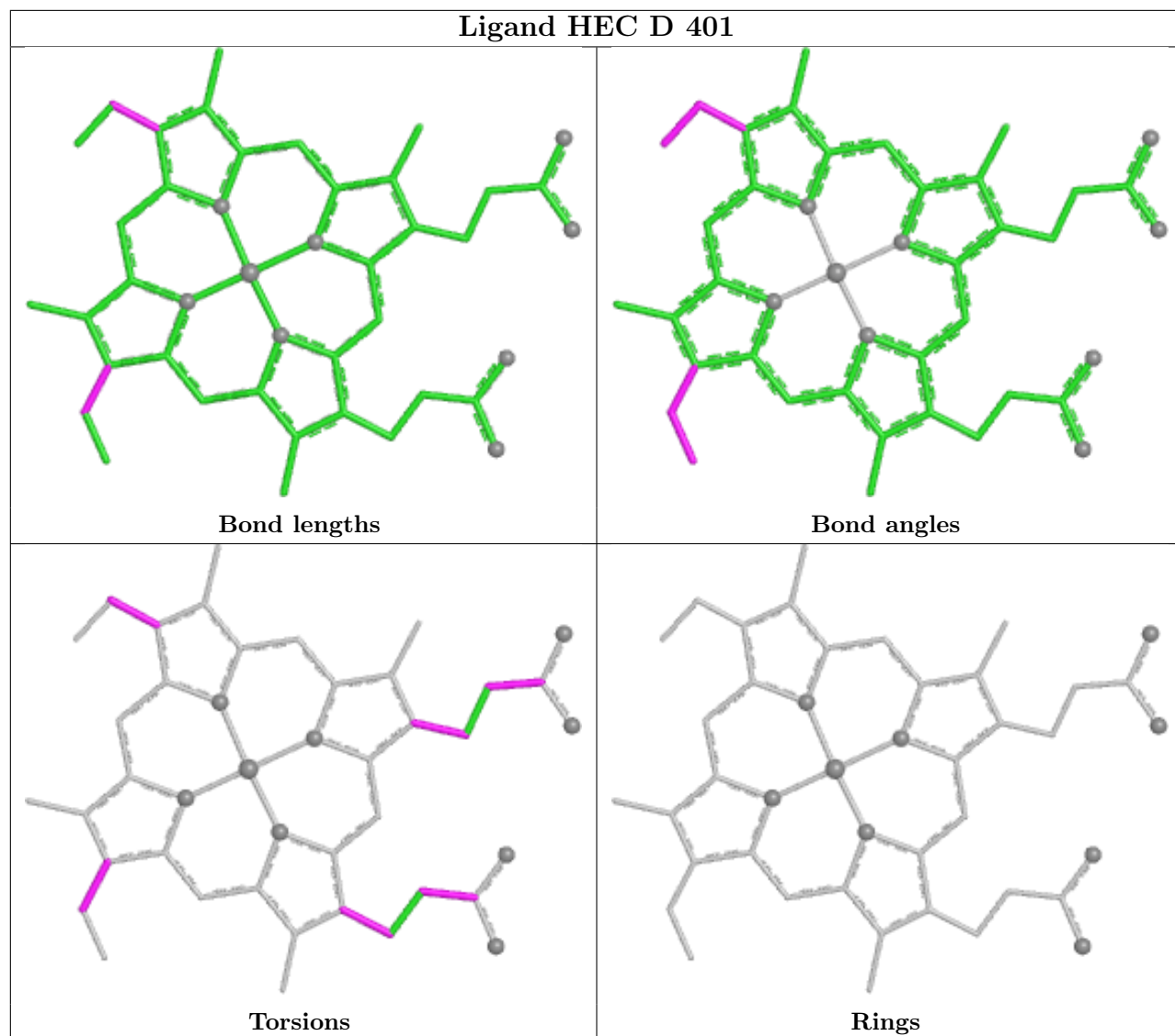
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	HEC	10	0
4	A	401	HEC	8	0
4	D	401	HEC	8	0
4	D	402	HEC	12	0
4	A	402	HEC	8	0
4	C	401	HEC	8	0
4	B	401	HEC	11	0
4	B	402	HEC	7	0

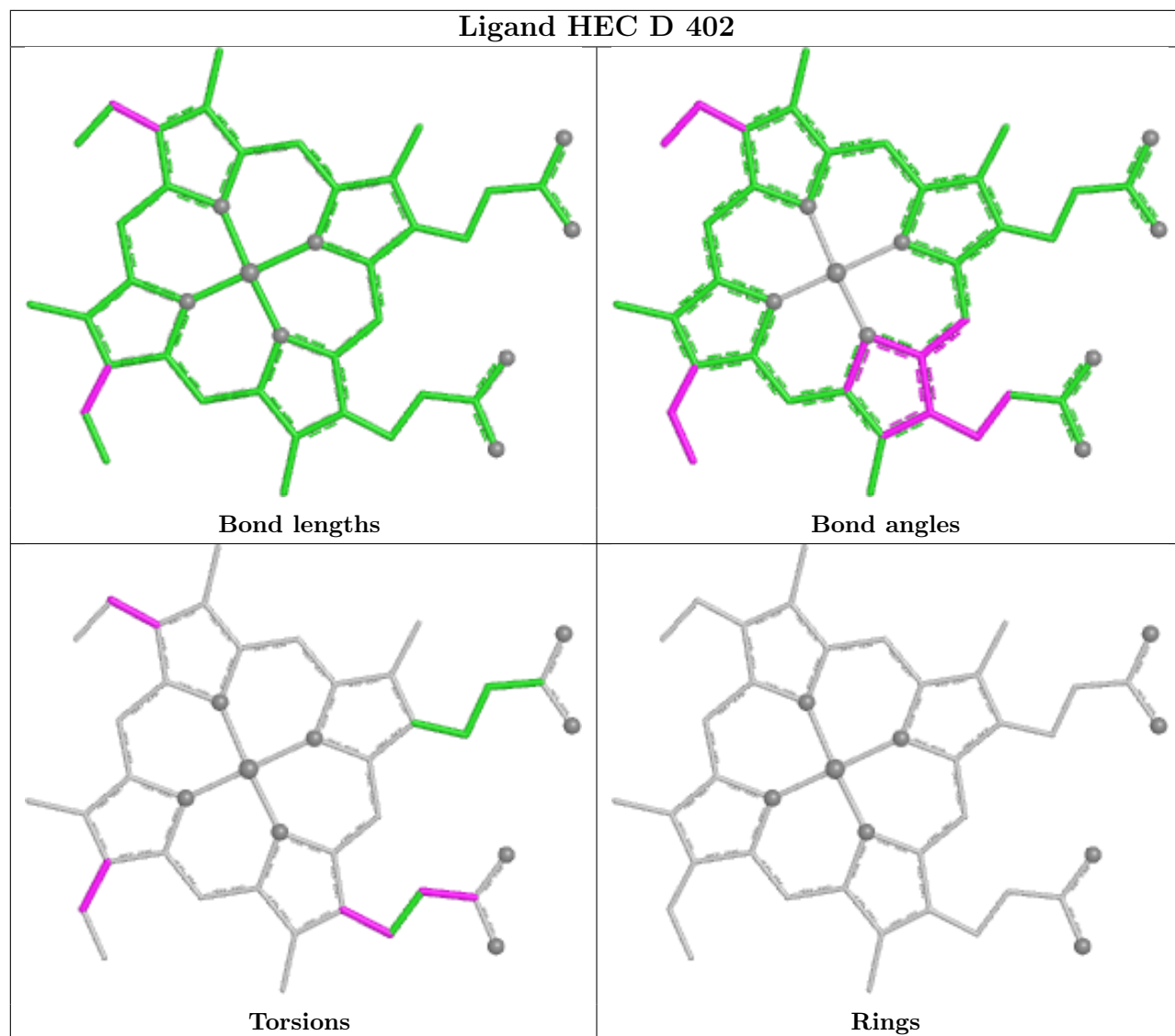
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

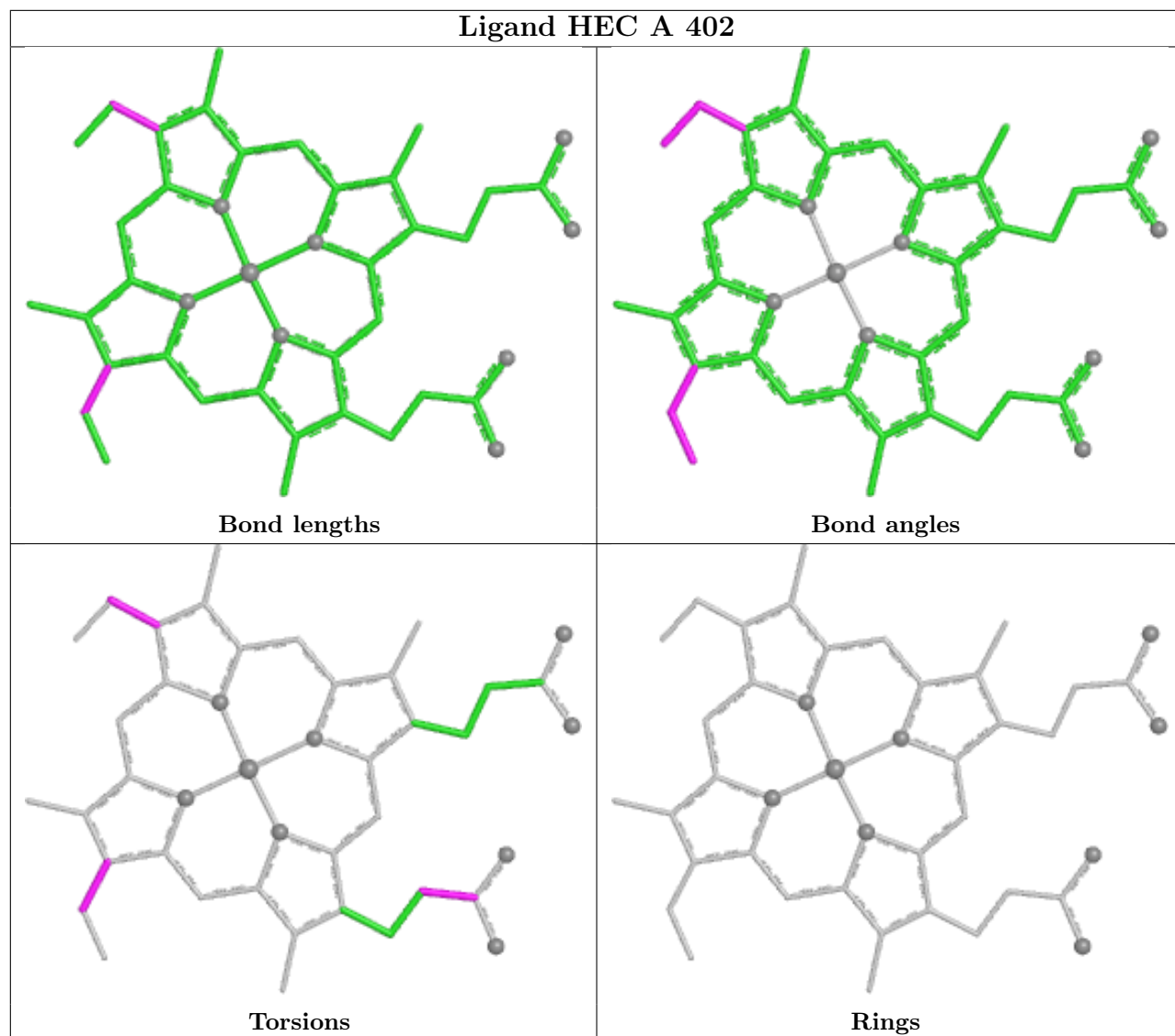
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



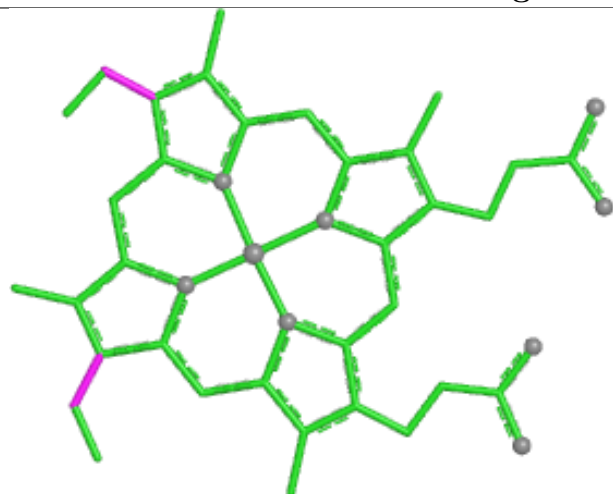




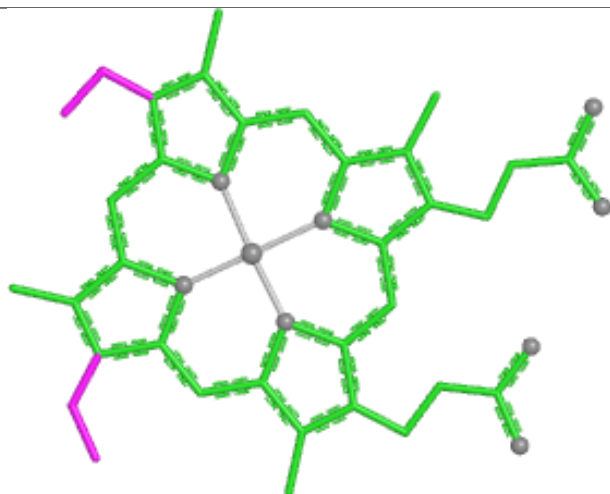




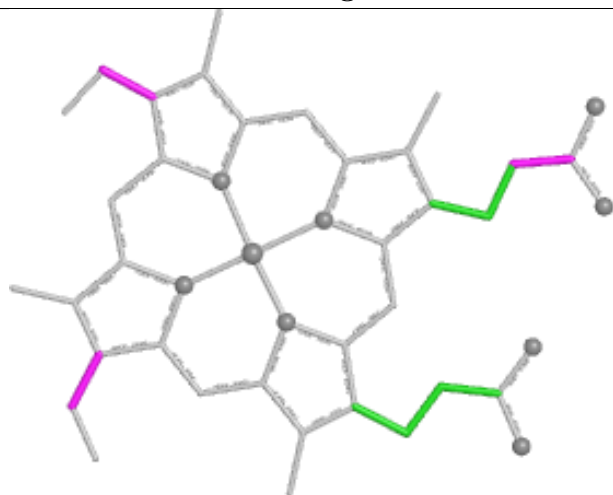
Ligand HEC C 401



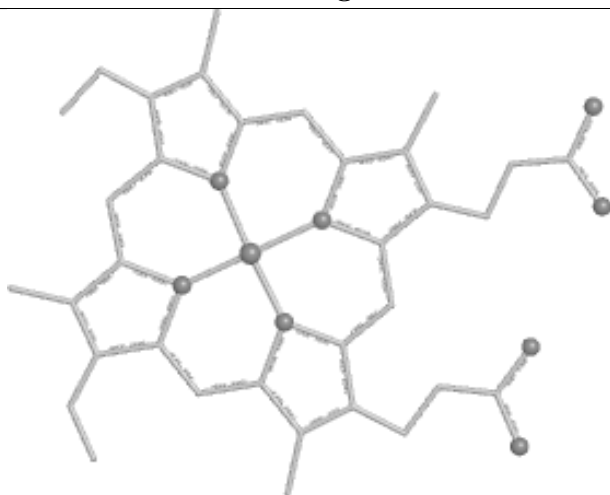
Bond lengths



Bond angles

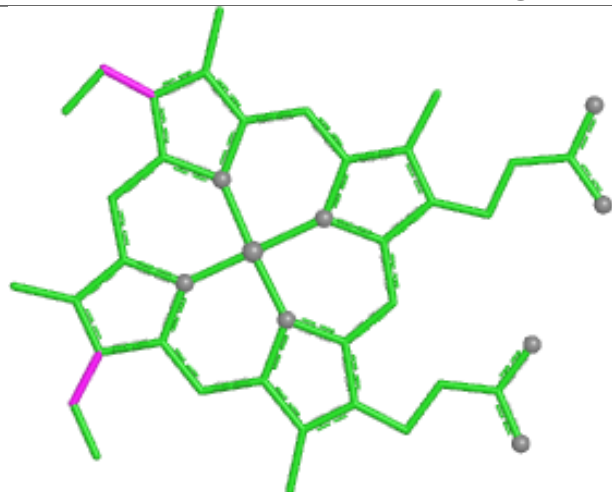


Torsions

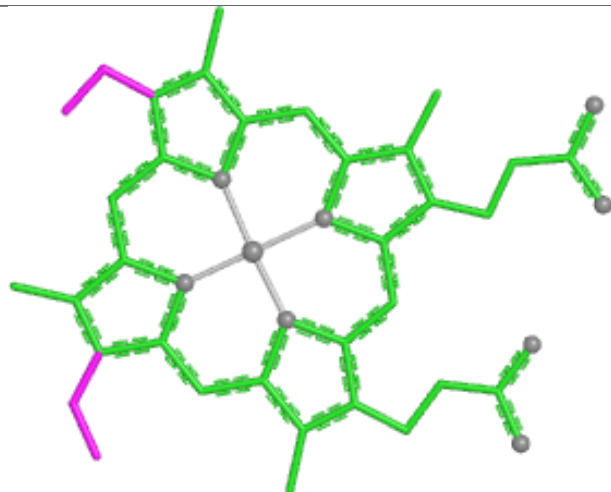


Rings

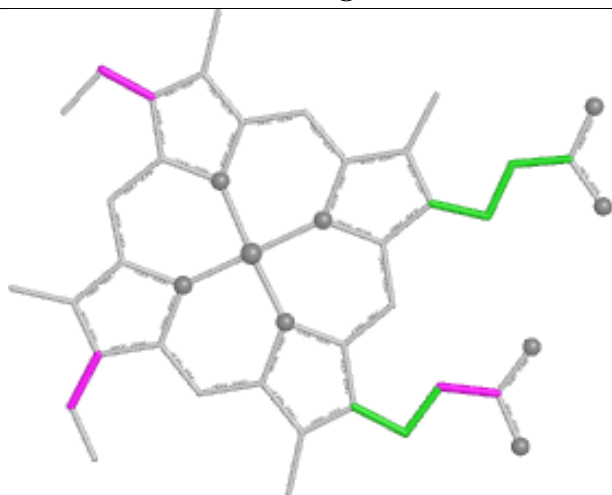
Ligand HEC B 401



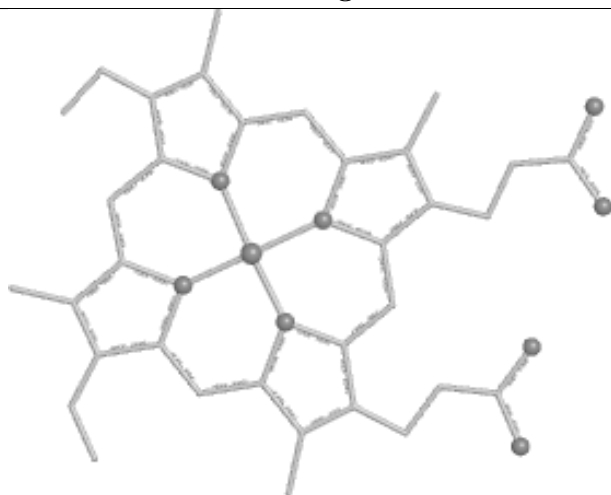
Bond lengths



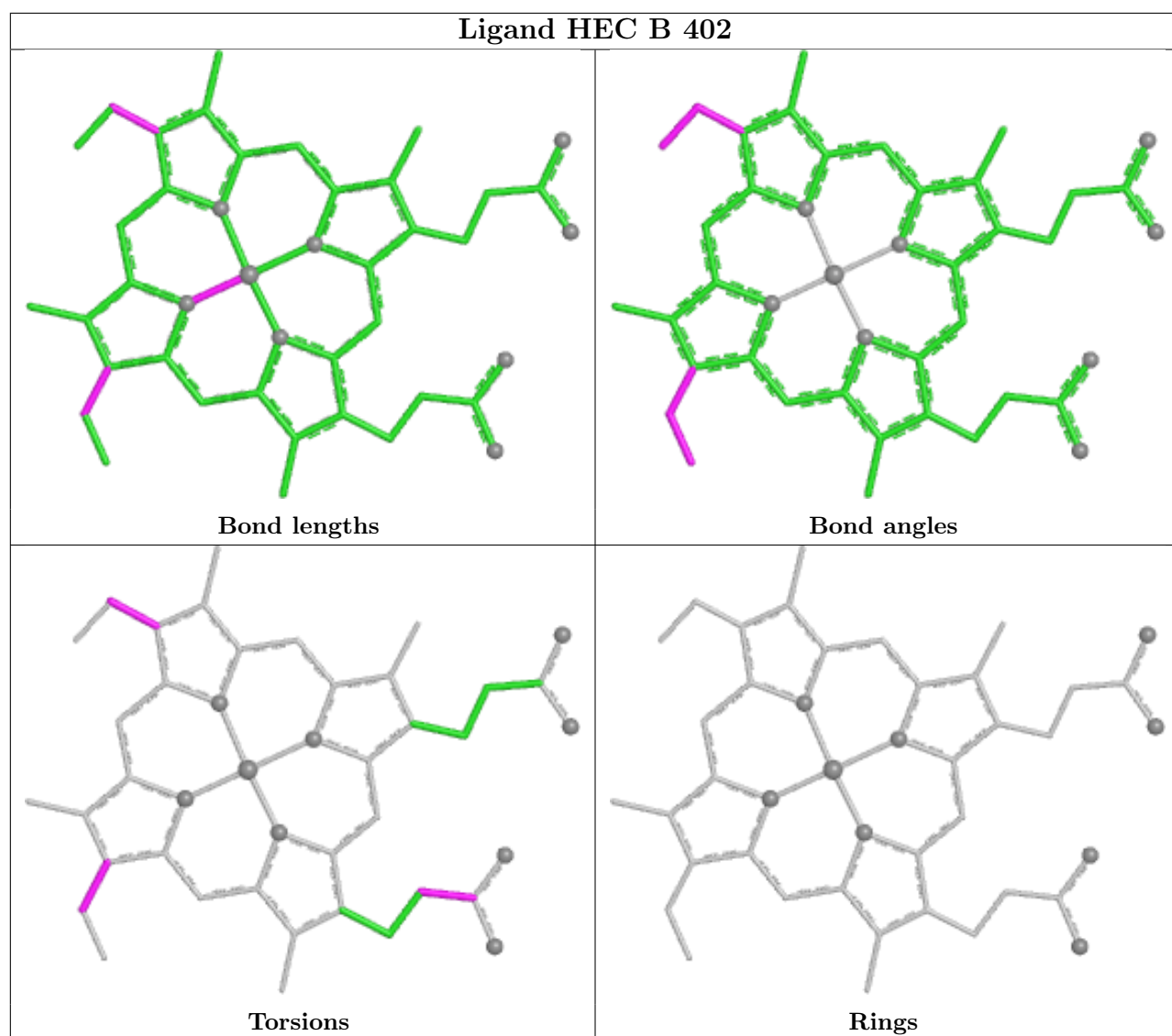
Bond angles



Torsions



Rings



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

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.