



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:45 AM UTC

PDB ID : 3E6O / pdb_00003e6o
Title : Structure of murine INOS oxygenase domain with inhibitor AR-C124355
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-15
Resolution : 2.60 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](#) ①) 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

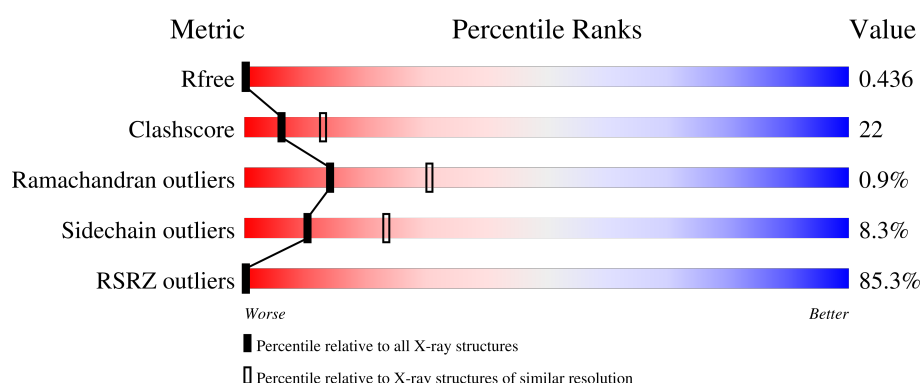
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	433	81% 53% 37% 5% • •
1	B	433	82% 58% 32% 5% 5%

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:

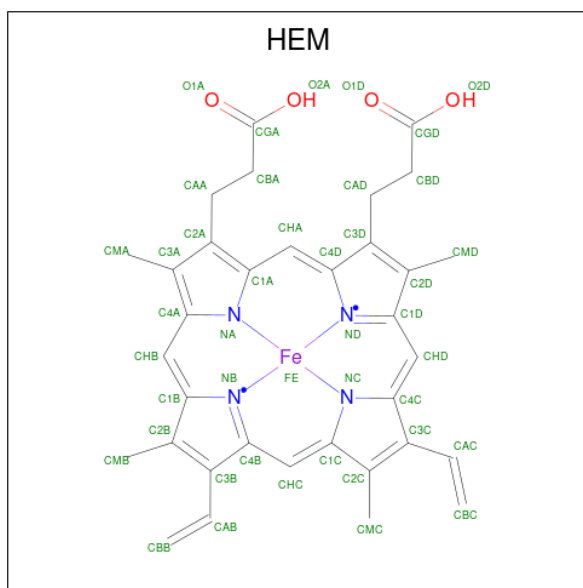
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	H4B	A	902	X	-	-	-

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 Nitric oxide synthase, inducible.

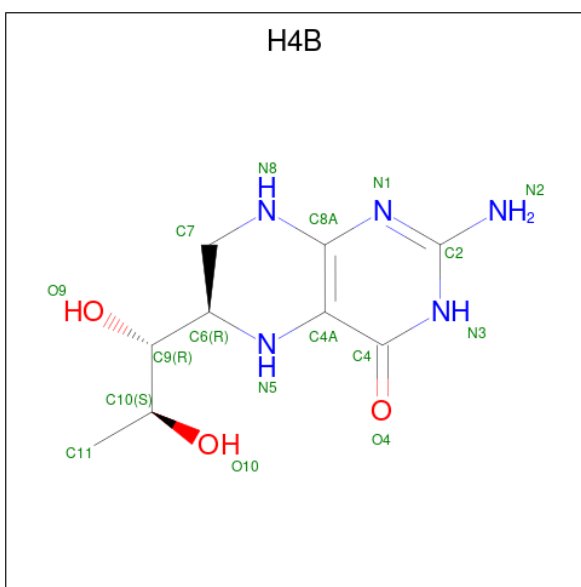
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total 3385	C 2171	N 582	O 612	S 20	0	0	0
1	B	410	Total 3347	C 2148	N 577	O 602	S 20	0	0	0

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



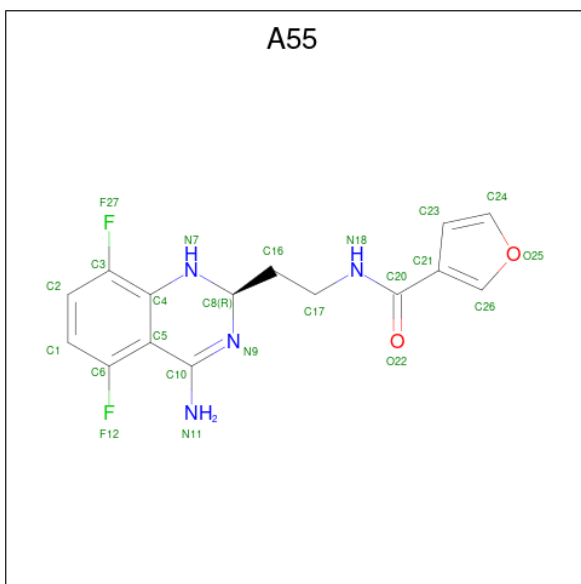
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-[2-(4-AMINO-5,8-DIFLUORO-1,2-DIHYDROQUINAZOLIN-2-YL)ETHYL]-3-FURAMIDE (CCD ID: A55) (formula: C₁₅H₁₄F₂N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			23	15	2	4	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			23	15	2	4	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	153	Total	O	0	0
			153	153		

I487	I488	I489	I490	I491	I492	I493	I494	I495	
GLN	ASN	GLU							
I427	I428	I429	I430	I431	I432	I433	I434	I435	I436
I437	I438	I439	I440	I441	I442	I443	I444	I445	I446
I447	I448	I449	I450	I451	I452	I453	I454	I455	I456
I457	I458	I459	I460	I461	I462	I463	I464	I465	I466
I467	I468	I469	I470	I471	I472	I473	I474	I475	I476
I477	I478	I479	I480	I481	I482	I483	I484	I485	I486
I487	I488	I489	I490	I491	I492	I493	I494	I495	I496
I497	I498	I499	I500	I501	I502	I503	I504	I505	I506
I507	I508	I509	I510	I511	I512	I513	I514	I515	I516
I517	I518	I519	I520	I521	I522	I523	I524	I525	I526
I527	I528	I529	I530	I531	I532	I533	I534	I535	I536
I537	I538	I539	I540	I541	I542	I543	I544	I545	I546
I547	I548	I549	I550	I551	I552	I553	I554	I555	I556
I557	I558	I559	I560	I561	I562	I563	I564	I565	I566
I567	I568	I569	I570	I571	I572	I573	I574	I575	I576
I577	I578	I579	I580	I581	I582	I583	I584	I585	I586
I587	I588	I589	I590	I591	I592	I593	I594	I595	I596
I597	I598	I599	I600	I601	I602	I603	I604	I605	I606
I607	I608	I609	I610	I611	I612	I613	I614	I615	I616
I617	I618	I619	I620	I621	I622	I623	I624	I625	I626
I627	I628	I629	I630	I631	I632	I633	I634	I635	I636
I637	I638	I639	I640	I641	I642	I643	I644	I645	I646
I647	I648	I649	I650	I651	I652	I653	I654	I655	I656
I657	I658	I659	I660	I661	I662	I663	I664	I665	I666
I667	I668	I669	I670	I671	I672	I673	I674	I675	I676
I677	I678	I679	I680	I681	I682	I683	I684	I685	I686
I687	I688	I689	I690	I691	I692	I693	I694	I695	I696
I697	I698	I699	I700	I701	I702	I703	I704	I705	I706
I707	I708	I709	I710	I711	I712	I713	I714	I715	I716
I717	I718	I719	I720	I721	I722	I723	I724	I725	I726
I727	I728	I729	I730	I731	I732	I733	I734	I735	I736
I737	I738	I739	I740	I741	I742	I743	I744	I745	I746
I747	I748	I749	I750	I751	I752	I753	I754	I755	I756
I757	I758	I759	I760	I761	I762	I763	I764	I765	I766
I767	I768	I769	I770	I771	I772	I773	I774	I775	I776
I777	I778	I779	I780	I781	I782	I783	I784	I785	I786
I787	I788	I789	I790	I791	I792	I793	I794	I795	I796
I797	I798	I799	I800	I801	I802	I803	I804	I805	I806
I807	I808	I809	I810	I811	I812	I813	I814	I815	I816
I817	I818	I819	I820	I821	I822	I823	I824	I825	I826
I827	I828	I829	I830	I831	I832	I833	I834	I835	I836
I837	I838	I839	I840	I841	I842	I843	I844	I845	I846
I847	I848	I849	I850	I851	I852	I853	I854	I855	I856
I857	I858	I859	I860	I861	I862	I863	I864	I865	I866
I867	I868	I869	I870	I871	I872	I873	I874	I875	I876
I877	I878	I879	I880	I881	I882	I883	I884	I885	I886
I887	I888	I889	I890	I891	I892	I893	I894	I895	I896
I897	I898	I899	I900	I901	I902	I903	I904	I905	I906
I907	I908	I909	I910	I911	I912	I913	I914	I915	I916
I917	I918	I919	I920	I921	I922	I923	I924	I925	I926
I927	I928	I929	I930	I931	I932	I933	I934	I935	I936
I937	I938	I939	I940	I941	I942	I943	I944	I945	I946
I947	I948	I949	I950	I951	I952	I953	I954	I955	I956
I957	I958	I959	I960	I961	I962	I963	I964	I965	I966
I967	I968	I969	I970	I971	I972	I973	I974	I975	I976
I977	I978	I979	I980	I981	I982	I983	I984	I985	I986
I987	I988	I989	I990	I991	I992	I993	I994	I995	I996
I997	I998	I999							
D306	G307	D308	D309	D310	D311	D312	D313	D314	D315
D316	D317	D318	D319	D320	D321	D322	D323	D324	D325
D326	D327	D328	D329	D330	D331	D332	D333	D334	D335
D336	D337	D338	D339	D340	D341	D342	D343	D344	D345
D346	D347	D348	D349	D350	D351	D352	D353	D354	D355
D356	D357	D358	D359	D360	D361	D362	D363	D364	D365
D366	D367	D368	D369	D370	D371	D372	D373	D374	D375
D376	D377	D378	D379	D380	D381	D382	D383	D384	D385
D386	D387	D388	D389	D390	D391	D392	D393	D394	D395
D396	D397	D398	D399	D400	D401	D402	D403	D404	D405
D406	D407	D408	D409	D410	D411	D412	D413	D414	D415
D416	D417	D418	D419	D420	D421	D422	D423	D424	D425
D426	D427	D428	D429	D430	D431	D432	D433	D434	D435
D436	D437	D438	D439	D440	D441	D442	D443	D444	D445
D446	D447	D448	D449	D450	D451	D452	D453	D454	D455
D456	D457	D458	D459	D460	D461	D462	D463	D464	D465
D466	D467	D468	D469	D470	D471	D472	D473	D474	D475
D476	D477	D478	D479	D480	D481	D482	D483	D484	D485
D486	D487	D488	D489	D490	D491	D492	D493	D494	D495
D496	D497	D498	D499	D500	D501	D502	D503	D504	D505
D506	D507	D508	D509	D510	D511	D512	D513	D514	D515
D516	D517	D518	D519	D520	D521	D522	D523	D524	D525
D526	D527	D528	D529	D530	D531	D532	D533	D534	D535
D536	D537	D538	D539	D540	D541	D542	D543	D544	D545
D546	D547	D548	D549	D550	D551	D552	D553	D554	D555
D556	D557	D558	D559	D560	D561	D562	D563	D564	D565
D566	D567	D568	D569	D570	D571	D572	D573	D574	D575
D576	D577	D578	D579	D580	D581	D582	D583	D584	D585
D586	D587	D588	D589	D590	D591	D592	D593	D594	D595
D596	D597	D598	D599	D600	D601	D602	D603	D604	D605
D606	D607	D608	D609	D610	D611	D612	D613	D614	D615
D616	D617	D618	D619	D620	D621	D622	D623	D624	D625
D626	D627	D628	D629	D630	D631	D632	D633	D634	D635
D636	D637	D638	D639	D640	D641	D642	D643	D644	D645
D646	D647	D648	D649	D650	D651	D652	D653	D654	D655
D656	D657	D658	D659	D660	D661	D662	D663	D664	D665
D666	D667	D668	D669	D670	D671	D672	D673	D674	D675
D676	D677	D678	D679	D680	D681	D682	D683	D684	D685
D686	D687	D688	D689	D690	D691	D692	D693	D694	D695
D696	D697	D698	D699	D700	D701	D702	D703	D704	D705
D706	D707	D708	D709	D710	D711	D712	D713	D714	D715
D716	D717	D718	D719	D720	D721	D722	D723	D724	D725
D726	D727	D728	D729	D730	D731	D732	D733	D734	D735
D736	D737	D738	D739	D740	D741	D742	D743	D744	D745
D746	D747	D748	D749	D750	D751	D752	D753	D754	D755
D756	D757	D758	D759	D760	D761	D762	D763	D764	D765
D766	D767	D768	D769	D770	D771	D772	D773	D774	D775
D776	D777	D778	D779	D780	D781	D782	D783	D784	D785
D786	D787	D788	D789	D790	D791	D792	D793	D794	D795
D796	D797	D798	D799	D800	D801	D802	D803	D804	D805
D806	D807	D808	D809	D810	D811	D812	D813	D814	D815
D816	D817	D818	D819	D820	D821	D822	D823	D824	D825
D826	D827	D828	D829	D830	D831	D832	D833	D834	D835
D836	D837	D838	D839	D840	D841	D842	D843	D844	D845
D846	D847	D848	D849	D850	D851	D852	D853	D854	D855
D856	D857	D858	D859	D860	D861	D862	D863	D864	D865
D866	D867	D868	D869	D870	D871	D872	D873	D874	D875
D876	D877	D878	D879	D880	D881	D882	D883	D884	D885
D886	D887	D888	D889	D890	D891	D892	D893	D894	D895
D896	D897	D898	D899	D900	D901	D902	D903	D904	D905
D906	D907	D908	D909	D910	D911	D912	D913	D914	D915
D916	D917	D918	D919	D920	D921	D922	D923	D924	D925
D926	D927	D928	D929	D930	D931	D932	D933	D934	D935
D936	D937	D938	D939	D940	D941	D942	D943	D944	D945
D946	D947	D948	D949	D950	D951	D952	D953	D954	D955
D956	D957	D958	D959	D960	D961	D962	D963	D964	D965
D966	D967	D968	D969	D970	D971	D972	D973	D974	D975
D976	D977	D978	D979	D980	D981	D982	D983	D984	D985
D986	D987	D988	D989	D990	D991	D992	D993	D994	D995
D996	D997	D998	D999						

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	213.90Å 213.90Å 116.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.60 19.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-2.60) 93.4 (19.96-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.262 0.416 , 0.436	Depositor DCC
R_{free} test set	2686 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	7171	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, H4B, A55

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	0.44	0/3484	0.94	11/4737 (0.2%)
1	B	0.43	0/3445	0.92	9/4684 (0.2%)
All	All	0.44	0/6929	0.93	20/9421 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	N-CA-C	-9.61	97.93	110.33
1	A	365	GLY	N-CA-C	-7.88	98.25	110.77
1	A	367	TYR	N-CA-C	6.85	119.80	110.55
1	B	386	LEU	N-CA-C	6.67	119.16	111.02
1	A	485	TYR	N-CA-C	-6.64	100.69	110.52
1	B	485	TYR	N-CA-C	-6.50	100.90	110.52
1	B	367	TYR	N-CA-C	6.08	119.48	110.48
1	A	348	ASN	N-CA-C	6.06	119.62	112.72
1	B	348	ASN	N-CA-C	5.63	119.74	112.41
1	A	176	THR	N-CA-C	-5.60	102.99	110.55
1	B	368	MET	N-CA-C	-5.50	99.45	108.41
1	A	251	PHE	N-CA-C	-5.34	100.98	109.96
1	A	378	CYS	N-CA-C	5.26	119.85	113.38
1	B	303	LEU	N-CA-C	5.23	118.00	109.59
1	B	365	GLY	N-CA-C	-5.18	100.91	113.18
1	B	478	VAL	N-CA-C	5.16	115.20	107.51
1	A	386	LEU	N-CA-C	5.13	116.56	111.07
1	B	308	GLN	N-CA-C	5.08	116.89	110.33
1	A	389	VAL	N-CA-C	-5.08	104.75	111.09
1	A	253	LEU	N-CA-C	-5.05	100.93	108.96

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	3385	0	3278	167	4
1	B	3347	0	3248	135	4
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	17	0	14	0	1
3	B	17	0	14	0	0
4	A	23	0	14	0	0
4	B	23	0	14	0	0
5	A	120	0	0	12	1
5	B	153	0	0	10	1
All	All	7171	0	6642	304	8

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 22.

All (304) 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:195:ILE:HB	5:B:1937:HOH:O	1.33	1.26
1:A:195:ILE:HB	5:A:1043:HOH:O	1.43	1.18
1:B:438:MET:HE3	1:B:469:VAL:HG12	1.45	0.96
1:A:438:MET:HE3	1:A:469:VAL:HG12	1.47	0.94
1:A:153:ILE:HD12	1:A:153:ILE:H	1.31	0.94
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.55	0.89
1:A:428:MET:HB3	5:A:1050:HOH:O	1.74	0.87
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.15	0.81
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.65	0.79
1:B:292:ARG:HH11	1:B:292:ARG:HB2	1.48	0.79
1:A:195:ILE:HG12	1:A:458:LEU:HD22	1.64	0.79
1:A:102:PHE:C	1:A:103:THR:HG23	2.06	0.77
1:B:182:PHE:CZ	1:B:186:MET:HE2	2.19	0.77
1:B:129:PRO:HB2	1:B:131:GLU:OE2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.67	0.74
1:A:217:MET:CE	1:A:303:LEU:HB3	2.18	0.72
1:A:290:LYS:CE	1:A:290:LYS:H	2.03	0.72
1:B:215:GLN:HG2	5:B:1949:HOH:O	1.89	0.71
1:A:189:ARG:HD2	1:A:200:TRP:CE3	2.26	0.71
1:A:281:THR:O	1:A:285:ILE:HG12	1.90	0.71
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.56	0.70
1:B:197:ARG:NE	5:B:2015:HOH:O	2.23	0.70
1:A:304:GLN:O	1:A:304:GLN:HG3	1.91	0.70
1:B:215:GLN:O	1:B:219:GLN:HG3	1.92	0.70
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.22	0.68
1:A:102:PHE:CG	1:A:102:PHE:O	2.45	0.68
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.75	0.68
1:A:290:LYS:H	1:A:290:LYS:CD	2.08	0.67
1:A:102:PHE:O	1:A:103:THR:HG23	1.95	0.67
1:B:195:ILE:CG2	1:B:437:PHE:HB2	2.25	0.67
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.30	0.67
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.30	0.66
1:A:195:ILE:HD11	1:A:458:LEU:O	1.95	0.66
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.24	0.66
1:A:333:PHE:HB3	5:A:1099:HOH:O	1.95	0.66
1:B:210:ASN:N	1:B:210:ASN:HD22	1.94	0.66
1:B:84:TRP:CD2	1:B:114:MET:HE3	2.31	0.66
1:B:249:HIS:C	1:B:306:ASP:O	2.39	0.65
1:B:197:ARG:CZ	5:B:2015:HOH:O	2.43	0.65
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.77	0.65
1:B:190:ASN:O	1:B:192:PRO:HD3	1.97	0.65
1:A:465:SER:O	1:A:471:HIS:HE1	1.80	0.64
1:B:464:GLY:O	1:B:467:THR:HB	1.96	0.64
1:B:149:LYS:HG2	1:B:150:GLU:HG3	1.78	0.64
1:B:141:ILE:HD11	1:B:163:VAL:HG21	1.79	0.64
1:B:210:ASN:HD22	1:B:210:ASN:H	1.43	0.64
1:A:144:TYR:O	1:A:147:SER:HB3	1.97	0.64
1:B:244:ARG:HA	5:B:1958:HOH:O	1.96	0.64
1:B:266:MET:HE2	1:B:272:ARG:HE	1.63	0.64
1:A:195:ILE:HG22	1:A:195:ILE:O	1.98	0.63
1:A:249:HIS:C	1:A:306:ASP:O	2.42	0.62
1:B:438:MET:HE2	1:B:438:MET:HA	1.82	0.62
1:B:195:ILE:HD11	1:B:458:LEU:O	2.00	0.62
1:A:410:THR:O	1:A:414:VAL:HG23	2.00	0.62
1:A:124:ARG:HD3	5:A:1020:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:THR:HG21	1:B:469:VAL:HG22	1.81	0.61
1:A:290:LYS:H	1:A:290:LYS:HE3	1.65	0.61
1:B:292:ARG:NH1	1:B:297:ASP:HB3	2.16	0.61
1:A:334:GLN:HA	5:A:1098:HOH:O	2.00	0.61
1:B:209:ARG:O	1:B:242:PRO:HG3	2.00	0.61
1:A:206:PHE:HB2	1:A:239:THR:HG22	1.83	0.61
1:A:224:HIS:ND1	1:A:239:THR:HG23	2.16	0.61
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.15	0.60
1:B:387:GLU:HG3	1:B:397:THR:HG21	1.84	0.60
1:B:195:ILE:O	1:B:195:ILE:HG22	2.02	0.60
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.84	0.60
1:A:332:TRP:CE3	1:A:392:ARG:HD2	2.37	0.59
1:A:217:MET:HE2	1:A:305:ALA:HB2	1.83	0.59
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.84	0.59
1:A:246:ASP:OD2	1:A:248:LYS:HB3	2.02	0.59
1:B:177:LEU:O	1:B:181:ILE:HD13	2.03	0.59
1:B:301:LEU:HG	1:B:303:LEU:HD11	1.83	0.59
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.37	0.59
1:A:134:LEU:O	1:A:138:ILE:HG12	2.02	0.59
1:B:210:ASN:H	1:B:210:ASN:ND2	1.99	0.59
1:B:141:ILE:CD1	1:B:163:VAL:HG21	2.32	0.59
1:A:252:ARG:HB2	1:A:304:GLN:HG2	1.83	0.59
1:A:149:LYS:HG2	1:A:150:GLU:HG2	1.85	0.59
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.03	0.58
1:B:438:MET:HG3	1:B:468:PRO:HB2	1.86	0.58
1:A:290:LYS:H	1:A:290:LYS:HD2	1.68	0.58
1:B:149:LYS:HG2	1:B:150:GLU:N	2.19	0.58
1:B:281:THR:O	1:B:285:ILE:HG12	2.04	0.58
1:A:149:LYS:HG2	1:A:150:GLU:N	2.19	0.57
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.34	0.57
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.20	0.56
1:A:223:ARG:HD3	5:A:1061:HOH:O	2.04	0.56
1:A:480:SER:HA	1:A:481:PRO:C	2.29	0.56
1:B:78:TYR:CD1	1:B:78:TYR:C	2.84	0.56
1:B:195:ILE:HG23	1:B:437:PHE:HB2	1.87	0.56
1:A:132:GLU:O	1:A:135:PRO:HD2	2.06	0.56
1:B:156:HIS:ND1	5:B:1922:HOH:O	2.33	0.56
1:B:195:ILE:HG22	1:B:437:PHE:HB2	1.87	0.56
1:B:410:THR:O	1:B:414:VAL:HG13	2.06	0.56
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.87	0.55
1:B:131:GLU:CD	1:B:131:GLU:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TRP:CE2	1:B:114:MET:HE3	2.42	0.55
1:B:441:MET:HE1	1:B:472:GLN:CD	2.32	0.55
1:B:221:ILE:HD12	1:B:303:LEU:HD21	1.88	0.55
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.88	0.55
1:A:102:PHE:C	1:A:103:THR:CG2	2.78	0.55
1:B:292:ARG:HH11	1:B:292:ARG:CB	2.18	0.55
1:A:439:LYS:O	1:A:442:GLN:HG2	2.07	0.54
1:B:152:LYS:HD2	1:B:155:GLU:OE2	2.07	0.54
1:B:239:THR:O	1:B:361:CYS:HA	2.07	0.54
1:B:445:TYR:HA	1:B:450:GLY:H	1.73	0.54
1:B:84:TRP:CG	1:B:114:MET:HE3	2.43	0.54
1:A:209:ARG:O	1:A:242:PRO:HG3	2.07	0.54
1:A:283:LEU:O	1:A:287:LEU:HG	2.07	0.54
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.08	0.54
1:A:405:LYS:O	1:A:409:VAL:HG23	2.08	0.54
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.90	0.53
1:B:175:LEU:HD13	1:B:356:LEU:CD1	2.37	0.53
1:A:189:ARG:HD2	1:A:200:TRP:CZ3	2.42	0.53
1:A:290:LYS:HD3	1:A:292:ARG:HH22	1.74	0.53
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.90	0.53
1:A:332:TRP:O	1:A:335:GLU:HB2	2.08	0.53
1:B:195:ILE:HG12	1:B:458:LEU:HD22	1.91	0.53
1:B:191:ALA:O	1:B:197:ARG:NH1	2.42	0.53
1:A:195:ILE:CG2	1:A:437:PHE:HB2	2.38	0.52
1:B:131:GLU:CD	1:B:131:GLU:N	2.67	0.52
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.44	0.52
1:A:78:TYR:C	1:A:78:TYR:CD1	2.87	0.52
1:A:303:LEU:O	1:A:310:PRO:HA	2.09	0.52
1:B:331:GLU:OE1	1:B:331:GLU:HA	2.08	0.52
1:A:132:GLU:C	1:A:135:PRO:HD2	2.35	0.52
1:A:206:PHE:HD2	1:A:239:THR:HG22	1.74	0.52
1:A:257:GLN:OE1	1:A:260:ARG:NH1	2.36	0.52
1:B:387:GLU:O	1:B:391:ARG:HG3	2.09	0.52
1:A:264:TYR:HB2	1:A:266:MET:CE	2.40	0.52
1:B:194:CYS:O	1:B:197:ARG:HG3	2.10	0.52
1:B:332:TRP:O	1:B:335:GLU:HB2	2.09	0.52
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.40	0.52
1:A:102:PHE:C	1:A:103:THR:O	2.53	0.51
1:A:172:THR:OG1	1:A:173:TYR:N	2.42	0.51
1:A:185:LYS:O	1:A:189:ARG:HG3	2.09	0.51
1:B:177:LEU:HD13	1:B:181:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.45	0.51
1:B:333:PHE:HA	1:B:336:LEU:CD2	2.40	0.51
1:A:159:ARG:O	1:A:163:VAL:HG23	2.10	0.51
1:A:434:SER:HB3	1:A:468:PRO:HD2	1.91	0.51
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.91	0.51
1:A:189:ARG:HH21	1:A:444:GLU:CD	2.19	0.51
1:A:301:LEU:HB3	1:A:303:LEU:HD13	1.91	0.51
1:A:290:LYS:HE3	1:A:290:LYS:N	2.25	0.51
1:A:164:THR:O	1:A:168:GLU:HG2	2.12	0.50
1:A:464:GLY:O	1:A:467:THR:HB	2.12	0.50
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.40	0.50
1:A:190:ASN:O	1:A:192:PRO:HD3	2.12	0.50
1:B:124:ARG:HH21	1:B:128:THR:HB	1.76	0.50
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.26	0.50
1:A:153:ILE:HD12	1:A:153:ILE:N	2.14	0.50
1:A:266:MET:HE1	1:A:293:TYR:HD1	1.77	0.50
1:B:165:LYS:O	1:B:169:THR:HG23	2.12	0.50
1:B:266:MET:HE2	1:B:272:ARG:HH21	1.76	0.50
1:B:434:SER:HB3	1:B:468:PRO:HD2	1.94	0.50
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.76	0.50
1:B:251:PHE:O	1:B:360:ALA:HB2	2.11	0.50
1:A:195:ILE:HG23	1:A:437:PHE:HB2	1.94	0.50
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.27	0.50
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.47	0.50
1:A:233:ASN:ND2	5:A:1066:HOH:O	2.44	0.49
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.94	0.49
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.93	0.49
1:B:379:ASP:HB3	1:B:381:GLN:OE1	2.12	0.49
1:B:411:GLU:O	1:B:414:VAL:HG22	2.13	0.49
1:B:480:SER:HA	1:B:481:PRO:C	2.38	0.49
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.28	0.49
1:A:467:THR:HG21	1:A:469:VAL:HG22	1.95	0.49
1:B:195:ILE:HG23	1:B:437:PHE:CB	2.43	0.49
1:A:129:PRO:HG3	5:A:1021:HOH:O	2.13	0.48
1:A:88:GLU:HG2	1:A:89:ILE:N	2.28	0.48
1:B:445:TYR:CZ	1:B:450:GLY:HA2	2.48	0.48
1:A:290:LYS:HG2	1:A:292:ARG:HH12	1.77	0.48
1:B:88:GLU:C	1:B:89:ILE:HD12	2.38	0.48
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.29	0.48
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.44	0.48
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD13	1:B:177:LEU:C	2.39	0.48
1:A:214:ALA:HA	1:A:217:MET:HE2	1.95	0.48
1:B:295:ARG:HD2	5:B:2027:HOH:O	2.14	0.48
1:B:252:ARG:HD3	1:B:359:PRO:HB2	1.96	0.47
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.44	0.47
1:A:330:TYR:HD2	1:A:332:TRP:HE1	1.62	0.47
1:B:303:LEU:O	1:B:310:PRO:HA	2.15	0.47
1:A:180:LEU:O	1:A:184:THR:HG23	2.14	0.47
1:A:252:ARG:CD	1:A:359:PRO:HB2	2.44	0.47
1:A:350:LEU:C	1:A:350:LEU:HD23	2.39	0.47
1:A:301:LEU:HB3	1:A:303:LEU:CD1	2.45	0.47
1:A:348:ASN:H	1:A:348:ASN:ND2	2.13	0.47
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.44	0.47
1:A:487:ILE:HD12	1:A:487:ILE:N	2.30	0.47
1:A:360:ALA:HA	5:A:1075:HOH:O	2.14	0.47
2:A:901:HEM:HBC2	2:A:901:HEM:HMC1	1.97	0.47
1:A:78:TYR:CE1	1:A:91:HIS:ND1	2.82	0.46
1:A:80:ARG:NH1	5:A:1136:HOH:O	2.48	0.46
1:A:103:THR:O	1:A:103:THR:OG1	2.31	0.46
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.50	0.46
1:A:393:MET:HB2	1:A:395:LEU:HD22	1.96	0.46
1:B:292:ARG:N	1:B:292:ARG:HD3	2.30	0.46
1:A:305:ALA:O	1:A:307:GLY:N	2.49	0.46
1:B:194:CYS:O	1:B:197:ARG:NH1	2.49	0.46
1:A:290:LYS:CD	1:A:290:LYS:N	2.77	0.46
1:B:182:PHE:CE2	1:B:186:MET:HE2	2.49	0.46
1:A:253:LEU:HD12	1:A:253:LEU:N	2.30	0.46
1:A:290:LYS:HD2	1:A:290:LYS:N	2.30	0.46
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.97	0.46
1:A:100:SER:C	1:A:101:ASP:O	2.53	0.45
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.99	0.45
1:A:375:ARG:O	1:A:379:ASP:HB2	2.16	0.45
1:B:213:THR:N	1:B:216:GLU:OE1	2.50	0.45
1:A:328:PRO:HB3	1:A:418:HIS:CD2	2.51	0.45
1:A:489:PRO:C	1:A:491:LYS:H	2.25	0.45
1:A:102:PHE:O	1:A:102:PHE:CD1	2.70	0.45
1:B:375:ARG:O	1:B:379:ASP:HB2	2.16	0.45
1:B:441:MET:HE1	1:B:472:GLN:CG	2.47	0.45
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.98	0.45
1:B:350:LEU:C	1:B:350:LEU:HD23	2.42	0.45
1:A:194:CYS:HB2	2:A:901:HEM:ND	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:GLU:HB3	1:A:490:TRP:CE2	2.52	0.44
1:B:190:ASN:O	1:B:192:PRO:CD	2.65	0.44
1:A:77:GLN:O	1:A:78:TYR:HB3	2.18	0.44
1:A:290:LYS:HG2	1:A:292:ARG:NH1	2.32	0.44
1:B:258:LEU:HD13	1:B:347:ALA:HB2	1.99	0.44
1:A:371:GLU:O	1:A:375:ARG:HB2	2.17	0.44
1:A:195:ILE:HG12	1:A:458:LEU:CD2	2.42	0.44
1:A:102:PHE:O	1:A:103:THR:CG2	2.65	0.44
1:A:290:LYS:CD	1:A:292:ARG:HH22	2.29	0.44
1:B:141:ILE:HD11	1:B:163:VAL:HG11	2.00	0.44
1:A:83:ASN:O	1:A:87:GLY:N	2.50	0.44
1:B:453:ALA:O	1:B:476:ASN:HB2	2.17	0.44
1:A:206:PHE:CD2	1:A:239:THR:HG22	2.53	0.43
1:A:349:MET:HE3	1:A:485:TYR:CD1	2.53	0.43
1:A:167:ILE:HA	1:A:172:THR:O	2.18	0.43
1:A:289:TRP:CD1	1:A:290:LYS:HZ2	2.36	0.43
1:A:377:PHE:O	1:A:385:ILE:HG12	2.17	0.43
1:B:188:TRP:HB2	2:B:1901:HEM:CBC	2.48	0.43
1:B:351:LEU:HB3	1:B:358:PHE:HB2	1.99	0.43
1:B:466:ILE:O	1:B:466:ILE:HG22	2.18	0.43
1:A:290:LYS:CG	1:A:292:ARG:HH12	2.30	0.43
1:B:342:ALA:HB1	1:B:425:VAL:HG11	2.00	0.43
1:A:344:PRO:HG3	1:A:366:TRP:C	2.43	0.43
1:B:292:ARG:HH12	1:B:297:ASP:HB3	1.82	0.43
1:A:194:CYS:SG	1:A:197:ARG:HG3	2.58	0.43
1:B:195:ILE:CG1	1:B:458:LEU:HD22	2.49	0.43
1:B:348:ASN:HD22	1:B:348:ASN:H	1.67	0.43
1:A:188:TRP:CD2	1:A:200:TRP:HA	2.53	0.43
1:A:221:ILE:HD12	1:A:303:LEU:HD21	2.01	0.43
1:A:80:ARG:NH2	1:A:89:ILE:HD13	2.34	0.43
1:A:266:MET:SD	1:A:272:ARG:HD3	2.58	0.43
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.79	0.43
1:A:470:PHE:CD1	1:A:470:PHE:C	2.97	0.43
1:B:262:ALA:HB2	1:B:299:LEU:CD2	2.49	0.43
1:A:224:HIS:C	1:A:224:HIS:CD2	2.97	0.42
1:A:234:ILE:HG21	1:A:366:TRP:HB3	2.01	0.42
1:A:368:MET:HE3	1:A:370:THR:OG1	2.19	0.42
1:B:134:LEU:HB3	1:B:135:PRO:HD3	2.00	0.42
1:B:136:HIS:O	1:B:139:GLU:HB3	2.19	0.42
1:A:242:PRO:HG2	1:A:251:PHE:CZ	2.54	0.42
1:A:134:LEU:HB3	1:A:135:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:C	1:B:303:LEU:HD12	2.44	0.42
2:A:901:HEM:HBC2	2:A:901:HEM:CMC	2.49	0.42
1:A:80:ARG:HH22	1:A:89:ILE:HD13	1.84	0.42
1:A:466:ILE:HG22	1:A:466:ILE:O	2.20	0.42
1:A:482:PHE:HB3	1:A:484:TYR:CE1	2.54	0.42
1:A:124:ARG:CD	5:A:1020:HOH:O	2.63	0.42
1:B:223:ARG:HD3	5:B:1950:HOH:O	2.19	0.42
1:B:289:TRP:NE1	1:B:314:GLU:OE1	2.51	0.42
1:A:374:VAL:O	1:A:378:CYS:HB2	2.20	0.42
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.55	0.42
1:A:438:MET:HE3	1:A:469:VAL:CG1	2.34	0.42
1:A:489:PRO:C	1:A:491:LYS:N	2.76	0.42
1:A:195:ILE:HG21	1:A:195:ILE:HD13	1.81	0.42
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.55	0.42
1:A:153:ILE:H	1:A:153:ILE:CD1	2.06	0.41
1:A:453:ALA:O	1:A:476:ASN:HB2	2.20	0.41
1:B:78:TYR:C	1:B:78:TYR:HD1	2.26	0.41
1:B:188:TRP:CD2	1:B:200:TRP:HA	2.55	0.41
1:B:257:GLN:CB	1:B:345:ALA:O	2.68	0.41
1:B:79:VAL:HG23	1:B:95:HIS:NE2	2.34	0.41
1:B:175:LEU:HD13	1:B:356:LEU:HD11	2.02	0.41
1:A:121:ARG:HA	1:A:121:ARG:HD3	1.87	0.41
1:B:472:GLN:O	1:B:474:MET:HG2	2.20	0.41
1:B:175:LEU:HD13	1:B:356:LEU:HD12	2.03	0.41
1:B:345:ALA:HB2	1:B:364:ASN:HB3	2.03	0.41
1:B:486:GLN:HB2	5:B:1917:HOH:O	2.20	0.41
1:A:303:LEU:CD1	1:A:303:LEU:N	2.83	0.41
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.20	0.41
1:B:283:LEU:O	1:B:287:LEU:HG	2.20	0.41
1:B:305:ALA:O	1:B:307:GLY:N	2.53	0.41
1:A:183:ALA:HB2	1:A:353:VAL:HG21	2.03	0.41
1:A:262:ALA:HB2	1:A:299:LEU:HG	2.03	0.41
1:A:407:ARG:HD2	5:A:1117:HOH:O	2.21	0.41
1:A:266:MET:HE3	1:A:272:ARG:HB2	2.03	0.41
1:B:163:VAL:O	1:B:167:ILE:HG13	2.21	0.41
1:B:333:PHE:O	1:B:336:LEU:HD23	2.21	0.41
1:B:454:ASP:O	1:B:455:TRP:C	2.64	0.41
1:B:386:LEU:HB2	5:B:1990:HOH:O	2.21	0.41
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.56	0.40
1:B:257:GLN:HE21	1:B:257:GLN:HB3	1.68	0.40
1:A:254:TRP:HB2	1:A:302:VAL:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:GLU:O	1:A:491:LYS:HB2	2.22	0.40
1:B:161:GLU:CG	1:B:165:LYS:HE2	2.51	0.40
1:B:172:THR:OG1	1:B:173:TYR:N	2.54	0.40

All (8) 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:B:406:ASP:OD2	1:B:463:SER:OG[9_766]	1.72	0.48
1:A:103:THR:CG2	1:A:118:SER:OG[11_655]	1.87	0.33
1:B:231:ASN:N	1:B:318:ASP:OD2[11_656]	1.99	0.21
1:B:318:ASP:N	5:B:1954:HOH:O[11_656]	1.99	0.21
1:A:470:PHE:O	3:A:902:H4B:O9[11_655]	2.00	0.20
1:A:461:PRO:O	1:A:464:GLY:N[11_655]	2.12	0.08
1:B:99:THR:OG1	1:B:478:VAL:O[9_766]	2.12	0.08
1:A:318:ASP:OD2	5:A:1065:HOH:O[9_765]	2.19	0.01

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	411/433 (95%)	370 (90%)	35 (8%)	6 (2%)	8	18
1	B	406/433 (94%)	367 (90%)	38 (9%)	1 (0%)	43	66
All	All	817/866 (94%)	737 (90%)	73 (9%)	7 (1%)	14	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	200	TRP
1	A	306	ASP

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Mol	Chain	Res	Type
1	B	306	ASP
1	A	307	GLY
1	A	369	GLY
1	A	344	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	363/381 (95%)	334 (92%)	29 (8%)	11	25
1	B	358/381 (94%)	327 (91%)	31 (9%)	9	21
All	All	721/762 (95%)	661 (92%)	60 (8%)	10	23

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	94	LEU
1	A	101	ASP
1	A	102	PHE
1	A	114	MET
1	A	119	LEU
1	A	125	ASP
1	A	148	PHE
1	A	153	ILE
1	A	154	GLU
1	A	157	LEU
1	A	161	GLU
1	A	180	LEU
1	A	257	GLN
1	A	258	LEU
1	A	265	GLN
1	A	290	LYS
1	A	301	LEU
1	A	303	LEU

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Mol	Chain	Res	Type
1	A	324	THR
1	A	325	MET
1	A	338	LEU
1	A	348	ASN
1	A	386	LEU
1	A	395	LEU
1	A	417	LEU
1	A	467	THR
1	A	469	VAL
1	A	475	LEU
1	B	114	MET
1	B	119	LEU
1	B	125	ASP
1	B	128	THR
1	B	130	LEU
1	B	131	GLU
1	B	134	LEU
1	B	148	PHE
1	B	175	LEU
1	B	178	ASP
1	B	186	MET
1	B	210	ASN
1	B	215	GLN
1	B	226	LEU
1	B	257	GLN
1	B	258	LEU
1	B	265	GLN
1	B	292	ARG
1	B	301	LEU
1	B	317	PRO
1	B	325	MET
1	B	331	GLU
1	B	336	LEU
1	B	348	ASN
1	B	407	ARG
1	B	414	VAL
1	B	417	LEU
1	B	421	GLN
1	B	423	GLN
1	B	462	VAL
1	B	467	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	96	HIS
1	A	115	ASN
1	A	142	ASN
1	A	202	ASN
1	A	204	GLN
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	249	HIS
1	A	348	ASN
1	A	431	HIS
1	A	442	GLN
1	A	471	HIS
1	B	96	HIS
1	B	115	ASN
1	B	143	GLN
1	B	199	GLN
1	B	210	ASN
1	B	215	GLN
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN
1	B	423	GLN
1	B	431	HIS
1	B	476	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

6 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
3	H4B	B	1902	-	17,18,18	2.77	3 (17%)	14,26,26	1.95	5 (35%)
4	A55	B	904	-	23,25,25	1.59	5 (21%)	25,35,35	2.04	10 (40%)
4	A55	A	903	-	23,25,25	1.62	5 (21%)	25,35,35	2.04	10 (40%)
2	HEM	B	1901	-	50,50,50	1.60	6 (12%)	67,82,82	1.14	5 (7%)
2	HEM	A	901	-	50,50,50	1.49	7 (14%)	67,82,82	1.32	8 (11%)
3	H4B	A	902	-	17,18,18	2.53	4 (23%)	14,26,26	1.97	4 (28%)

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
3	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
4	A55	B	904	-	-	3/9/22/22	0/2/3/3
4	A55	A	903	-	-	2/9/22/22	0/2/3/3
2	HEM	B	1901	-	-	2/14/54/54	-
2	HEM	A	901	-	-	1/14/54/54	-
3	H4B	A	902	-	1/1/3/5	4/8/17/17	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1902	H4B	C7-N8	-7.89	1.38	1.46
3	A	902	H4B	C7-N8	-7.37	1.39	1.46
3	B	1902	H4B	C7-C6	-6.81	1.45	1.52
3	A	902	H4B	C7-C6	-5.75	1.46	1.52
2	B	1901	HEM	FE-NB	4.71	2.09	1.94
4	A	903	A55	C5-C10	4.46	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	904	A55	C5-C10	4.35	1.53	1.45
2	B	1901	HEM	FE-ND	4.17	2.07	1.94
2	A	901	HEM	FE-NB	3.89	2.06	1.94
2	A	901	HEM	FE-NC	3.64	2.07	1.95
2	A	901	HEM	FE-NA	3.63	2.07	1.95
2	B	1901	HEM	FE-NC	3.60	2.07	1.95
2	A	901	HEM	FE-ND	3.00	2.04	1.94
2	B	1901	HEM	CAB-C3B	-2.93	1.39	1.47
3	A	902	H4B	C4-N3	-2.90	1.33	1.38
2	A	901	HEM	C3B-C4B	2.84	1.50	1.44
2	B	1901	HEM	CAC-C3C	-2.77	1.40	1.47
4	A	903	A55	C1-C2	2.77	1.43	1.38
3	B	1902	H4B	C4-N3	-2.76	1.33	1.38
2	B	1901	HEM	FE-NA	2.73	2.04	1.95
4	B	904	A55	C20-N18	2.66	1.38	1.33
2	A	901	HEM	CAC-C3C	-2.54	1.40	1.47
4	A	903	A55	C1-C6	2.41	1.42	1.37
4	A	903	A55	O22-C20	2.32	1.28	1.23
4	B	904	A55	C23-C21	2.31	1.49	1.43
4	B	904	A55	C1-C2	2.21	1.42	1.38
2	A	901	HEM	CBB-CAB	2.11	1.40	1.30
4	A	903	A55	C2-C3	2.11	1.42	1.37
3	A	902	H4B	C4A-N5	-2.05	1.33	1.37
4	B	904	A55	O22-C20	2.04	1.27	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	904	A55	O25-C26-C21	5.36	115.48	110.81
4	A	903	A55	O25-C26-C21	5.15	115.31	110.81
2	A	901	HEM	CMD-C2D-C1D	4.24	131.65	125.03
3	A	902	H4B	O4-C4-C4A	-4.14	117.27	127.26
2	A	901	HEM	C4B-C3B-C2B	-4.09	103.52	107.28
3	B	1902	H4B	C2-N1-C8A	3.83	120.12	113.36
3	B	1902	H4B	O4-C4-C4A	-3.78	118.15	127.26
2	A	901	HEM	C3B-C2B-C1B	3.64	109.14	106.41
3	A	902	H4B	C2-N1-C8A	3.46	119.47	113.36
2	B	1901	HEM	CAD-C3D-C2D	-3.27	121.73	127.87
4	A	903	A55	C5-C4-C3	3.05	121.82	117.93
4	B	904	A55	C23-C21-C26	-2.95	103.40	105.59
4	A	903	A55	O25-C24-C23	2.92	115.91	110.10
4	B	904	A55	C5-C4-C3	2.85	121.57	117.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1901	HEM	C3B-C2B-C1B	2.85	108.55	106.41
4	A	903	A55	C24-C23-C21	-2.84	103.52	107.01
3	A	902	H4B	C4A-C4-N3	2.82	119.88	112.13
3	A	902	H4B	C2-N3-C4	-2.77	120.09	125.11
2	B	1901	HEM	CMD-C2D-C1D	2.75	129.32	125.03
3	B	1902	H4B	C4A-C4-N3	2.74	119.64	112.13
4	B	904	A55	O25-C24-C23	2.72	115.51	110.10
3	B	1902	H4B	C2-N3-C4	-2.68	120.25	125.11
4	A	903	A55	C26-O25-C24	-2.61	101.29	106.24
4	B	904	A55	C26-O25-C24	-2.54	101.41	106.24
4	B	904	A55	C16-C8-N7	-2.49	105.80	111.32
2	A	901	HEM	CAD-C3D-C2D	-2.42	123.33	127.87
4	A	903	A55	O22-C20-C21	-2.35	118.07	120.83
4	B	904	A55	C24-C23-C21	-2.29	104.20	107.01
4	B	904	A55	O22-C20-C21	-2.29	118.14	120.83
4	B	904	A55	N11-C10-N9	2.27	121.87	118.72
2	A	901	HEM	CAA-C2A-C1A	2.26	129.35	124.94
4	B	904	A55	C21-C20-N18	2.24	119.05	116.75
2	B	1901	HEM	CAD-C3D-C4D	2.20	128.53	124.70
4	A	903	A55	C2-C3-C4	-2.18	119.70	122.83
4	A	903	A55	C23-C21-C26	-2.18	103.98	105.59
2	B	1901	HEM	CAA-C2A-C1A	2.14	129.12	124.94
2	A	901	HEM	CBA-CAA-C2A	-2.08	106.77	112.53
4	A	903	A55	C1-C6-C5	-2.08	119.66	123.48
2	A	901	HEM	C3B-C4B-NB	2.05	110.94	109.47
2	A	901	HEM	C4D-C3D-C2D	2.04	109.86	106.89
3	B	1902	H4B	C4-C4A-N5	2.02	121.78	116.27
4	A	903	A55	N11-C10-N9	2.01	121.51	118.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	H4B	N5-C6-C9-O9
3	A	902	H4B	C7-C6-C9-O9
3	A	902	H4B	C7-C6-C9-C10
4	B	904	A55	C17-C16-C8-N7
2	B	1901	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	A	902	H4B	N5-C6-C9-C10
4	A	903	A55	O22-C20-C21-C26
4	A	903	A55	N18-C20-C21-C26
4	B	904	A55	N18-C20-C21-C26
2	A	901	HEM	C4B-C3B-CAB-CBB
2	B	1901	HEM	C4B-C3B-CAB-CBB
4	B	904	A55	O22-C20-C21-C26

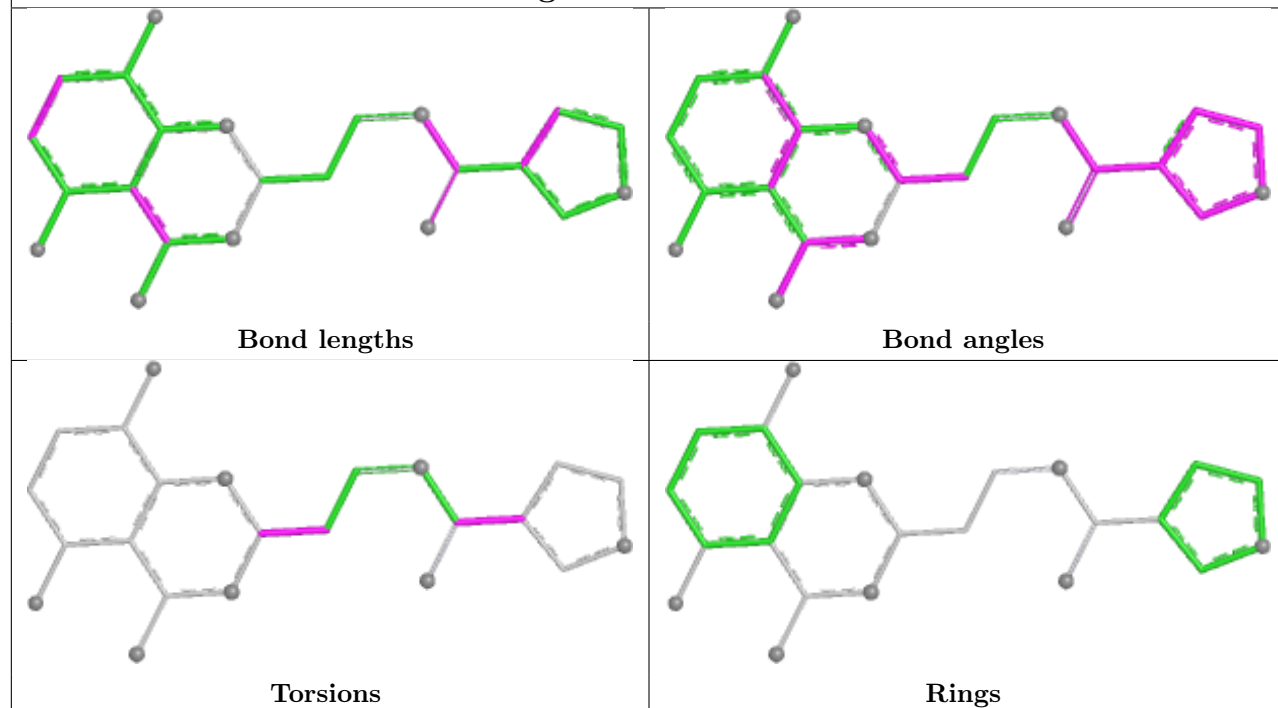
There are no ring outliers.

3 monomers are involved in 5 short contacts:

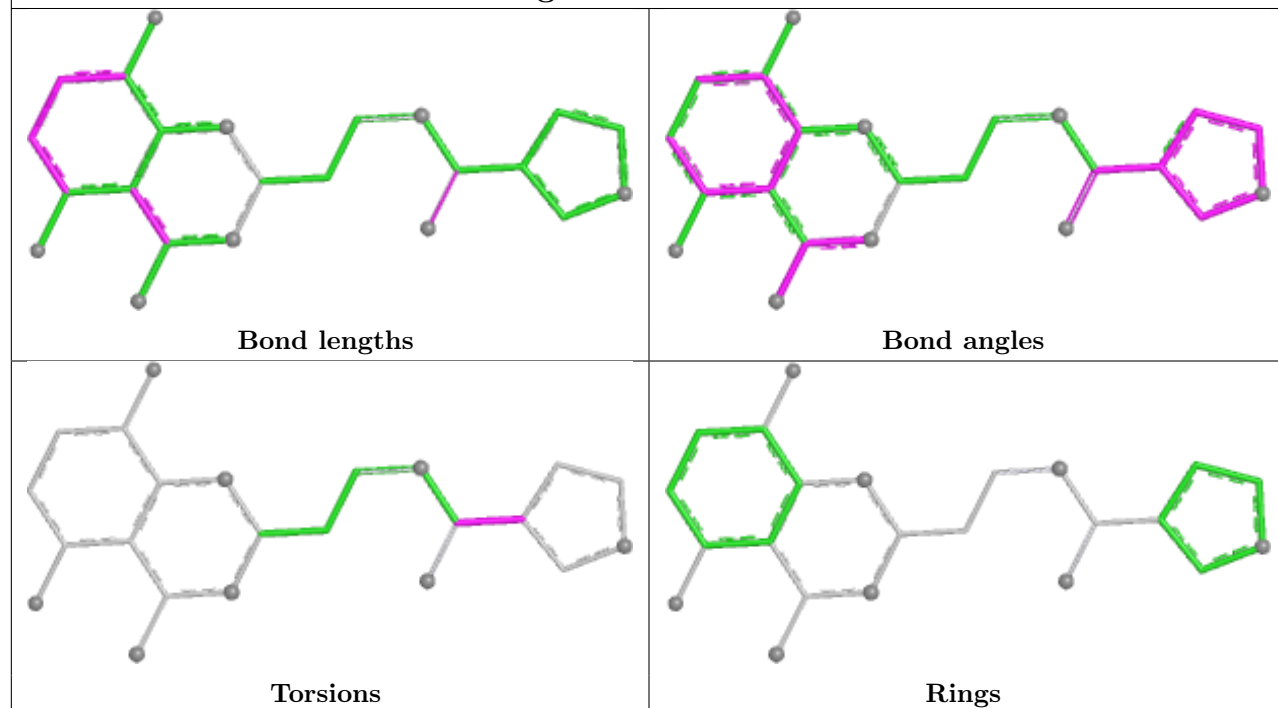
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1901	HEM	1	0
2	A	901	HEM	3	0
3	A	902	H4B	0	1

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.

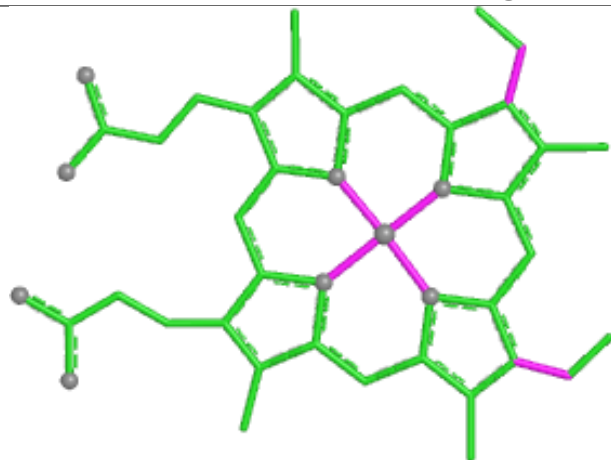
Ligand A55 B 904



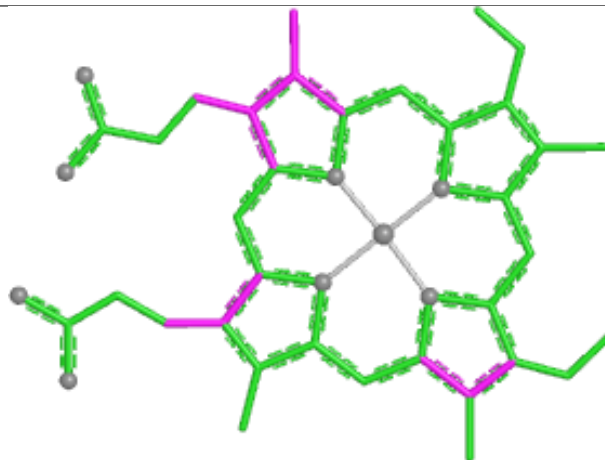
Ligand A55 A 903



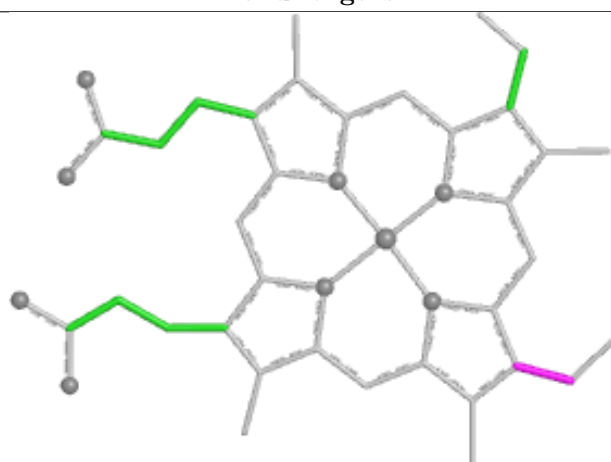
Ligand HEM B 1901



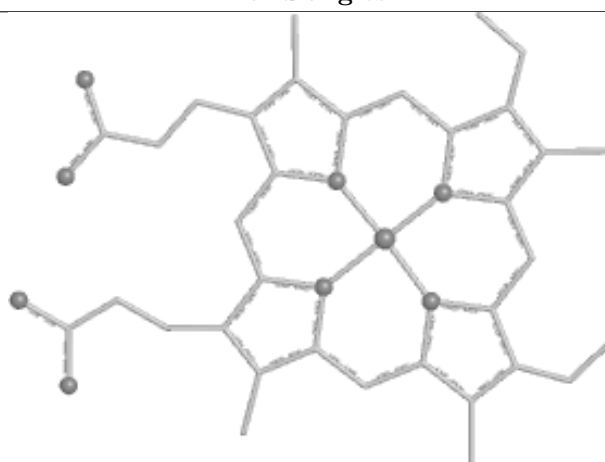
Bond lengths



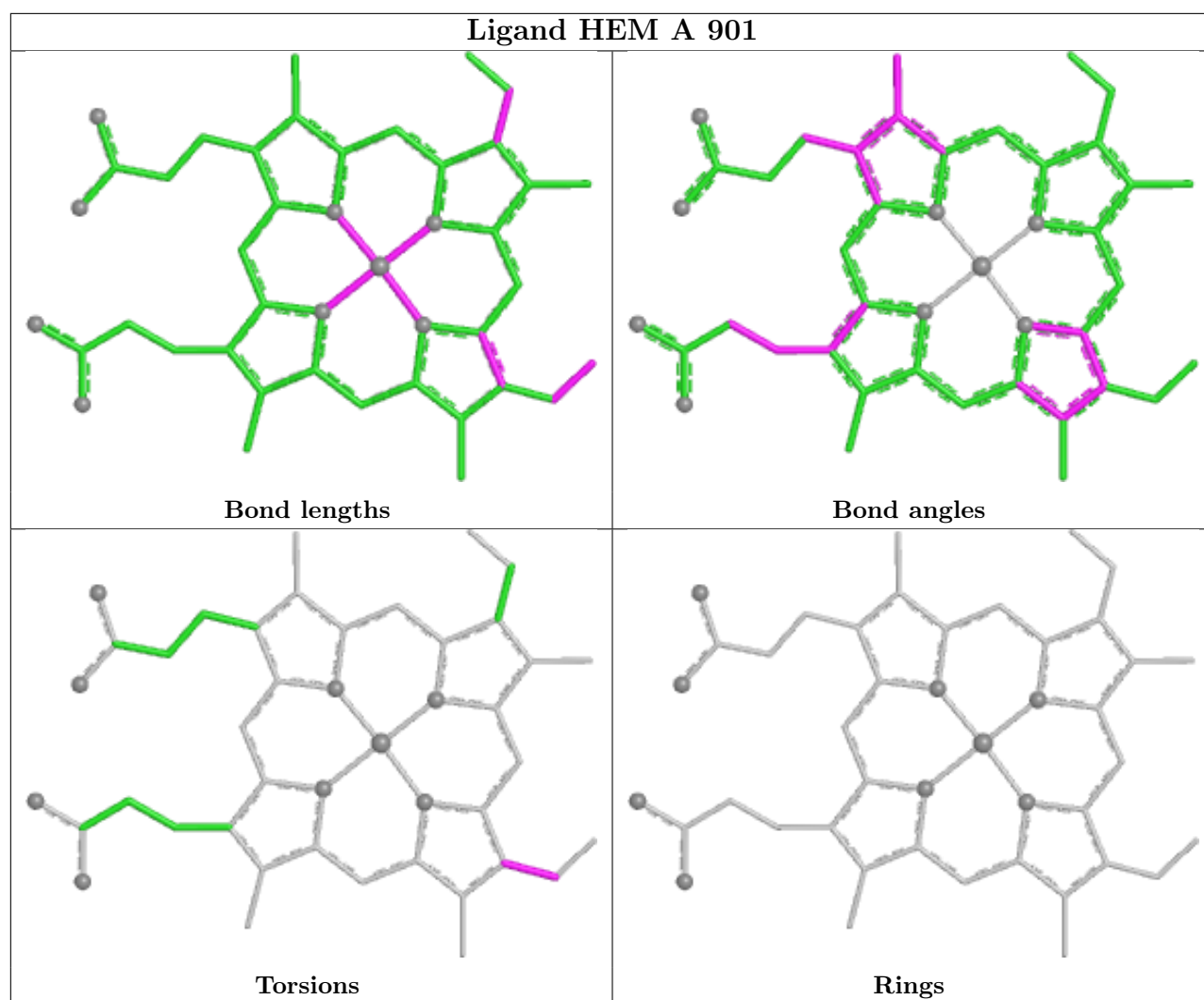
Bond angles



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

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	415/433 (95%)	3.07	349 (84%) 0 0	26, 45, 74, 99	0
1	B	410/433 (94%)	3.16	355 (86%) 0 0	25, 43, 68, 94	0
All	All	825/866 (95%)	3.12	704 (85%) 0 0	25, 44, 70, 99	0

All (704) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	CYS	7.8
1	A	102	PHE	7.3
1	B	494	ILE	6.8
1	B	112	SER	6.4
1	A	171	GLY	6.3
1	A	294	GLY	6.2
1	A	409	VAL	6.2
1	A	323	VAL	6.2
1	A	203	LEU	6.2
1	A	423	GLN	5.9
1	B	330	TYR	5.9
1	A	263	GLY	5.9
1	A	232	GLY	5.8
1	B	416	VAL	5.8
1	B	305	ALA	5.8
1	B	372	ILE	5.8
1	B	148	PHE	5.7
1	B	192	PRO	5.7
1	A	390	GLY	5.6
1	B	87	GLY	5.6
1	B	379	ASP	5.5
1	A	256	SER	5.5
1	B	170	THR	5.5
1	A	164	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	397	THR	5.5
1	A	237	ALA	5.4
1	B	420	PHE	5.4
1	B	425	VAL	5.4
1	B	196	GLY	5.3
1	A	337	GLY	5.3
1	B	489	PRO	5.2
1	B	338	LEU	5.2
1	B	340	TRP	5.2
1	B	191	ALA	5.1
1	A	278	LEU	5.1
1	B	273	GLY	5.1
1	B	288	GLY	5.1
1	A	312	VAL	5.1
1	A	401	ALA	5.1
1	B	157	LEU	5.1
1	B	490	TRP	5.0
1	B	350	LEU	5.0
1	A	89	ILE	5.0
1	A	306	ASP	5.0
1	A	152	LYS	5.0
1	A	168	GLU	5.0
1	B	261	TYR	4.9
1	B	445	TYR	4.9
1	A	84	TRP	4.9
1	B	117	LYS	4.9
1	A	283	LEU	4.9
1	A	103	THR	4.9
1	A	229	THR	4.9
1	B	99	THR	4.9
1	B	432	THR	4.9
1	B	163	VAL	4.9
1	A	108	SER	4.8
1	A	396	GLU	4.8
1	B	495	TRP	4.8
1	B	400	LEU	4.8
1	A	296	PHE	4.8
1	B	84	TRP	4.8
1	A	494	ILE	4.7
1	A	118	SER	4.7
1	B	142	ASN	4.7
1	A	202	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	476	ASN	4.7
1	B	298	VAL	4.7
1	B	229	THR	4.7
1	B	293	TYR	4.7
1	B	395	LEU	4.7
1	A	225	ILE	4.6
1	B	153	ILE	4.6
1	A	187	ALA	4.6
1	A	330	TYR	4.6
1	B	98	ALA	4.6
1	B	337	GLY	4.6
1	B	200	TRP	4.5
1	B	79	VAL	4.5
1	B	433	ALA	4.5
1	B	267	PRO	4.5
1	B	353	VAL	4.5
1	B	190	ASN	4.5
1	B	194	CYS	4.5
1	B	156	HIS	4.5
1	A	218	PHE	4.5
1	B	272	ARG	4.5
1	A	303	LEU	4.5
1	A	162	ALA	4.4
1	B	90	LEU	4.4
1	B	458	LEU	4.4
1	A	101	ASP	4.4
1	B	454	ASP	4.4
1	B	430	HIS	4.4
1	B	123	PRO	4.4
1	B	481	PRO	4.4
1	B	332	TRP	4.4
1	A	214	ALA	4.4
1	A	495	TRP	4.4
1	A	313	PHE	4.4
1	A	100	SER	4.4
1	B	333	PHE	4.4
1	B	417	LEU	4.3
1	B	152	LYS	4.3
1	B	354	GLY	4.3
1	B	147	SER	4.3
1	B	402	SER	4.3
1	A	389	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	PRO	4.3
1	B	426	THR	4.3
1	B	126	LYS	4.3
1	A	183	ALA	4.3
1	A	344	PRO	4.3
1	A	412	ILE	4.3
1	B	409	VAL	4.3
1	B	448	ARG	4.2
1	A	247	GLY	4.2
1	B	375	ARG	4.2
1	B	392	ARG	4.2
1	B	131	GLU	4.2
1	B	81	ILE	4.2
1	B	280	PHE	4.2
1	A	302	VAL	4.2
1	B	328	PRO	4.2
1	B	453	ALA	4.2
1	B	197	ARG	4.2
1	A	88	GLU	4.2
1	B	355	GLY	4.2
1	B	277	THR	4.2
1	B	483	TYR	4.1
1	A	366	TRP	4.1
1	A	87	GLY	4.1
1	B	307	GLY	4.1
1	A	420	PHE	4.1
1	A	159	ARG	4.1
1	A	110	LEU	4.1
1	B	247	GLY	4.1
1	B	80	ARG	4.1
1	B	382	ARG	4.1
1	A	90	LEU	4.1
1	A	148	PHE	4.1
1	B	451	CYS	4.1
1	A	304	GLN	4.1
1	A	471	HIS	4.1
1	B	95	HIS	4.1
1	A	192	PRO	4.0
1	A	441	MET	4.0
1	A	150	GLU	4.0
1	A	367	TYR	4.0
1	A	167	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	450	GLY	4.0
1	A	317	PRO	4.0
1	B	369	GLY	4.0
1	A	437	PHE	4.0
1	B	230	ASN	4.0
1	A	257	GLN	4.0
1	B	311	GLU	4.0
1	A	220	HIS	4.0
1	A	308	GLN	4.0
1	A	259	ILE	4.0
1	B	113	ILE	4.0
1	B	303	LEU	4.0
1	B	440	HIS	4.0
1	A	414	VAL	4.0
1	A	128	THR	3.9
1	A	236	SER	3.9
1	B	208	ALA	3.9
1	A	455	TRP	3.9
1	B	140	PHE	3.9
1	B	251	PHE	3.9
1	B	484	TYR	3.9
1	A	292	ARG	3.9
1	A	195	ILE	3.9
1	A	415	ALA	3.9
1	B	466	ILE	3.9
1	B	144	TYR	3.9
1	B	264	TYR	3.9
1	A	120	THR	3.9
1	A	382	ARG	3.9
1	B	283	LEU	3.9
1	B	437	PHE	3.9
1	A	416	VAL	3.9
1	B	188	TRP	3.9
1	A	310	PRO	3.8
1	B	270	THR	3.8
1	A	321	LEU	3.8
1	B	486	GLN	3.8
1	B	335	GLU	3.8
1	A	198	ILE	3.8
1	A	400	LEU	3.8
1	B	125	ASP	3.8
1	A	179	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	351	LEU	3.8
1	A	434	SER	3.8
1	B	111	GLY	3.8
1	B	171	GLY	3.8
1	A	222	CYS	3.8
1	B	285	ILE	3.8
1	B	456	ILE	3.8
1	A	447	ALA	3.8
1	A	449	GLY	3.8
1	B	377	PHE	3.8
1	A	381	GLN	3.7
1	A	210	ASN	3.7
1	B	467	THR	3.7
1	A	458	LEU	3.7
1	B	110	LEU	3.7
1	B	342	ALA	3.7
1	B	257	GLN	3.7
1	A	467	THR	3.7
1	A	293	TYR	3.7
1	B	138	ILE	3.7
1	A	342	ALA	3.7
1	B	265	GLN	3.7
1	A	81	ILE	3.7
1	A	196	GLY	3.7
1	A	251	PHE	3.7
1	B	441	MET	3.7
1	A	417	LEU	3.7
1	B	412	ILE	3.7
1	B	367	TYR	3.7
1	B	162	ALA	3.7
1	B	442	GLN	3.7
1	A	189	ARG	3.6
1	A	289	TRP	3.6
1	A	276	ALA	3.6
1	B	263	GLY	3.6
1	B	212	SER	3.6
1	A	265	GLN	3.6
1	B	336	LEU	3.6
1	B	475	LEU	3.6
1	B	89	ILE	3.6
1	B	487	ILE	3.6
1	A	121	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	347	ALA	3.6
1	A	460	PRO	3.6
1	B	143	GLN	3.6
1	A	329	LYS	3.6
1	A	285	ILE	3.6
1	B	239	THR	3.6
1	B	274	ASP	3.6
1	B	476	ASN	3.6
1	A	114	MET	3.6
1	A	264	TYR	3.6
1	B	78	TYR	3.6
1	A	361	CYS	3.6
1	A	212	SER	3.6
1	A	442	GLN	3.6
1	B	292	ARG	3.6
1	B	228	ALA	3.6
1	B	262	ALA	3.6
1	B	266	MET	3.6
1	A	123	PRO	3.6
1	B	206	PHE	3.6
1	A	320	VAL	3.6
1	A	95	HIS	3.5
1	A	428	MET	3.5
1	B	474	MET	3.5
1	A	161	GLU	3.5
1	A	241	PHE	3.5
1	B	211	CYS	3.5
1	A	141	ILE	3.5
1	B	181	ILE	3.5
1	A	213	THR	3.5
1	A	126	LYS	3.5
1	B	371	GLU	3.5
1	B	241	PHE	3.5
1	A	386	LEU	3.5
1	B	306	ASP	3.5
1	A	452	PRO	3.5
1	B	366	TRP	3.5
1	A	485	TYR	3.5
1	B	141	ILE	3.5
1	A	207	ASP	3.5
1	A	328	PRO	3.5
1	A	371	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	133	LEU	3.5
1	B	470	PHE	3.5
1	B	374	VAL	3.5
1	B	462	VAL	3.5
1	A	391	ARG	3.5
1	A	385	ILE	3.4
1	A	275	ALA	3.4
1	A	305	ALA	3.4
1	A	335	GLU	3.4
1	A	489	PRO	3.4
1	B	205	VAL	3.4
1	A	372	ILE	3.4
1	B	172	THR	3.4
1	A	137	ALA	3.4
1	A	360	ALA	3.4
1	A	404	TRP	3.4
1	A	383	TYR	3.4
1	A	483	TYR	3.4
1	B	439	LYS	3.4
1	B	463	SER	3.4
1	A	492	THR	3.4
1	A	253	LEU	3.4
1	A	295	ARG	3.4
1	A	364	ASN	3.4
1	A	472	GLN	3.4
1	B	83	ASN	3.4
1	B	413	ASN	3.4
1	A	112	SER	3.4
1	A	419	SER	3.4
1	B	383	TYR	3.4
1	B	132	GLU	3.4
1	B	317	PRO	3.4
1	A	299	LEU	3.4
1	A	345	ALA	3.4
1	B	360	ALA	3.4
1	B	231	ASN	3.4
1	B	318	ASP	3.4
1	A	240	VAL	3.4
1	A	346	VAL	3.4
1	B	459	VAL	3.4
1	B	271	ILE	3.3
1	A	261	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	242	PRO	3.3
1	B	295	ARG	3.3
1	B	460	PRO	3.3
1	B	468	PRO	3.3
1	A	334	GLN	3.3
1	B	214	ALA	3.3
1	B	114	MET	3.3
1	A	280	PHE	3.3
1	B	406	ASP	3.3
1	A	149	LYS	3.3
1	A	405	LYS	3.3
1	A	370	THR	3.3
1	B	399	THR	3.3
1	B	243	GLN	3.3
1	B	472	GLN	3.3
1	A	254	TRP	3.3
1	A	93	THR	3.3
1	A	176	THR	3.3
1	A	336	LEU	3.3
1	B	94	LEU	3.3
1	A	327	HIS	3.3
1	A	82	LYS	3.3
1	A	231	ASN	3.3
1	B	92	ASP	3.3
1	A	200	TRP	3.3
1	A	463	SER	3.3
1	B	343	LEU	3.3
1	B	452	PRO	3.3
1	B	82	LYS	3.3
1	B	269	GLY	3.3
1	A	163	VAL	3.3
1	A	255	ASN	3.3
1	B	469	VAL	3.3
1	B	155	GLU	3.2
1	A	91	HIS	3.2
1	A	339	LYS	3.2
1	B	436	SER	3.2
1	B	137	ALA	3.2
1	A	125	ASP	3.2
1	A	160	LEU	3.2
1	B	279	GLU	3.2
1	B	349	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	362	PRO	3.2
1	B	334	GLN	3.2
1	B	401	ALA	3.2
1	A	298	VAL	3.2
1	A	392	ARG	3.2
1	A	331	GLU	3.2
1	B	139	GLU	3.2
1	B	331	GLU	3.2
1	A	172	THR	3.2
1	B	282	GLN	3.2
1	B	323	VAL	3.2
1	A	233	ASN	3.2
1	A	158	ALA	3.2
1	A	113	ILE	3.2
1	B	227	TYR	3.2
1	B	312	VAL	3.2
1	B	320	VAL	3.2
1	A	309	ASP	3.1
1	A	94	LEU	3.1
1	B	479	LEU	3.1
1	A	332	TRP	3.1
1	B	464	GLY	3.1
1	B	275	ALA	3.1
1	B	195	ILE	3.1
1	B	221	ILE	3.1
1	A	227	TYR	3.1
1	B	91	HIS	3.1
1	B	136	HIS	3.1
1	A	369	GLY	3.1
1	A	490	TRP	3.1
1	B	159	ARG	3.1
1	A	204	GLN	3.1
1	B	294	GLY	3.1
1	A	80	ARG	3.1
1	A	459	VAL	3.1
1	A	133	LEU	3.1
1	B	386	LEU	3.1
1	B	359	PRO	3.1
1	A	146	GLY	3.1
1	B	93	THR	3.1
1	B	324	THR	3.1
1	A	109	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	222	CYS	3.1
1	B	304	GLN	3.0
1	A	184	THR	3.0
1	A	464	GLY	3.0
1	B	169	THR	3.0
1	A	325	MET	3.0
1	B	438	MET	3.0
1	A	287	LEU	3.0
1	B	134	LEU	3.0
1	A	144	TYR	3.0
1	A	154	GLU	3.0
1	A	348	ASN	3.0
1	B	424	ASN	3.0
1	B	297	ASP	3.0
1	B	370	THR	3.0
1	B	158	ALA	3.0
1	B	447	ALA	3.0
1	A	130	LEU	3.0
1	A	338	LEU	3.0
1	A	351	LEU	3.0
1	B	431	HIS	3.0
1	A	461	PRO	3.0
1	A	478	VAL	3.0
1	B	278	LEU	3.0
1	B	418	HIS	3.0
1	A	215	GLN	3.0
1	A	477	TYR	3.0
1	A	486	GLN	3.0
1	B	308	GLN	3.0
1	A	124	ARG	3.0
1	B	428	MET	3.0
1	B	234	ILE	3.0
1	A	155	GLU	2.9
1	B	291	PRO	2.9
1	A	282	GLN	2.9
1	A	230	ASN	2.9
1	B	145	TYR	2.9
1	A	268	ASP	2.9
1	B	177	LEU	2.9
1	B	286	ASP	2.9
1	A	208	ALA	2.9
1	B	151	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	345	ALA	2.9
1	A	79	VAL	2.9
1	A	206	PHE	2.9
1	A	469	VAL	2.9
1	B	121	ARG	2.9
1	A	190	ASN	2.9
1	A	445	TYR	2.9
1	A	484	TYR	2.9
1	B	427	ILE	2.9
1	A	85	GLY	2.9
1	A	270	THR	2.9
1	A	136	HIS	2.9
1	A	431	HIS	2.9
1	B	493	HIS	2.9
1	A	127	PRO	2.9
1	A	272	ARG	2.9
1	A	142	ASN	2.9
1	A	194	CYS	2.9
1	A	122	GLY	2.9
1	B	130	LEU	2.9
1	B	403	LEU	2.9
1	B	182	PHE	2.9
1	A	440	HIS	2.9
1	A	421	GLN	2.8
1	A	340	TRP	2.8
1	A	153	ILE	2.8
1	B	329	LYS	2.8
1	B	341	TYR	2.8
1	B	485	TYR	2.8
1	A	356	LEU	2.8
1	B	128	THR	2.8
1	B	203	LEU	2.8
1	B	218	PHE	2.8
1	B	313	PHE	2.8
1	A	488	GLU	2.8
1	B	357	GLU	2.8
1	A	209	ARG	2.8
1	B	124	ARG	2.8
1	A	77	GLN	2.8
1	B	423	GLN	2.8
1	B	254	TRP	2.8
1	A	307	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLY	2.8
1	B	258	LEU	2.8
1	B	326	GLU	2.8
1	A	446	ARG	2.8
1	B	391	ARG	2.8
1	B	461	PRO	2.8
1	B	160	LEU	2.8
1	B	376	ASP	2.8
1	A	341	TYR	2.8
1	B	179	GLU	2.8
1	A	267	PRO	2.8
1	B	193	ARG	2.8
1	A	188	TRP	2.8
1	B	419	SER	2.8
1	B	301	LEU	2.8
1	A	376	ASP	2.8
1	A	98	ALA	2.8
1	A	99	THR	2.8
1	A	482	PHE	2.8
1	B	363	PHE	2.8
1	A	252	ARG	2.8
1	A	271	ILE	2.7
1	A	258	LEU	2.7
1	B	226	LEU	2.7
1	A	169	THR	2.7
1	A	191	ALA	2.7
1	A	377	PHE	2.7
1	A	407	ARG	2.7
1	A	174	GLN	2.7
1	A	456	ILE	2.7
1	A	180	LEU	2.7
1	B	319	LEU	2.7
1	B	449	GLY	2.7
1	A	448	ARG	2.7
1	B	116	PRO	2.7
1	B	109	CYS	2.7
1	A	238	ILE	2.7
1	A	119	LEU	2.7
1	A	266	MET	2.7
1	B	364	ASN	2.7
1	A	151	ALA	2.7
1	B	175	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	96	HIS	2.7
1	B	161	GLU	2.7
1	B	210	ASN	2.7
1	A	97	LYS	2.7
1	A	262	ALA	2.7
1	A	277	THR	2.7
1	B	184	THR	2.7
1	B	281	THR	2.7
1	B	378	CYS	2.6
1	A	249	HIS	2.6
1	A	357	GLU	2.6
1	A	147	SER	2.6
1	A	408	ALA	2.6
1	B	240	VAL	2.6
1	B	455	TRP	2.6
1	A	116	PRO	2.6
1	A	316	PRO	2.6
1	A	78	TYR	2.6
1	A	173	TYR	2.6
1	A	315	ILE	2.6
1	A	475	LEU	2.6
1	A	493	HIS	2.6
1	A	443	ASN	2.6
1	B	242	PRO	2.6
1	B	207	ASP	2.6
1	B	250	ASP	2.6
1	A	175	LEU	2.6
1	A	403	LEU	2.6
1	A	473	GLU	2.6
1	A	273	GLY	2.6
1	B	284	CYS	2.6
1	A	359	PRO	2.6
1	A	453	ALA	2.6
1	B	389	VAL	2.6
1	B	164	THR	2.6
1	B	393	MET	2.6
1	B	356	LEU	2.6
1	A	165	LYS	2.6
1	B	202	ASN	2.6
1	A	380	THR	2.5
1	B	325	MET	2.5
1	B	198	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	253	LEU	2.5
1	B	168	GLU	2.5
1	B	276	ALA	2.5
1	B	118	SER	2.5
1	A	178	ASP	2.5
1	B	166	GLU	2.5
1	B	388	GLU	2.5
1	B	309	ASP	2.5
1	B	339	LYS	2.5
1	B	249	HIS	2.5
1	A	311	GLU	2.5
1	B	477	TYR	2.5
1	B	176	THR	2.5
1	B	446	ARG	2.5
1	B	246	ASP	2.5
1	A	362	PRO	2.5
1	B	316	PRO	2.5
1	B	302	VAL	2.5
1	B	381	GLN	2.5
1	B	290	LYS	2.4
1	B	223	ARG	2.4
1	A	319	LEU	2.4
1	B	245	SER	2.4
1	B	289	TRP	2.4
1	B	390	GLY	2.4
1	A	143	GLN	2.4
1	A	260	ARG	2.4
1	B	315	ILE	2.4
1	B	434	SER	2.4
1	A	297	ASP	2.4
1	B	235	ARG	2.4
1	A	324	THR	2.4
1	A	451	CYS	2.4
1	B	186	MET	2.4
1	A	491	LYS	2.4
1	A	394	GLY	2.4
1	B	310	PRO	2.4
1	B	373	GLY	2.4
1	B	244	ARG	2.4
1	A	139	GLU	2.4
1	A	399	THR	2.3
1	A	413	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLU	2.3
1	A	438	MET	2.3
1	A	250	ASP	2.3
1	A	457	TRP	2.3
1	B	457	TRP	2.3
1	A	363	PHE	2.3
1	A	226	LEU	2.3
1	A	228	ALA	2.3
1	B	225	ILE	2.3
1	A	166	GLU	2.3
1	A	387	GLU	2.3
1	B	86	SER	2.3
1	B	404	TRP	2.3
1	A	244	ARG	2.3
1	A	374	VAL	2.3
1	B	119	LEU	2.3
1	B	287	LEU	2.3
1	B	167	ILE	2.3
1	A	465	SER	2.3
1	A	111	GLY	2.3
1	B	77	GLN	2.3
1	B	327	HIS	2.3
1	A	368	MET	2.3
1	B	491	LYS	2.3
1	A	301	LEU	2.3
1	B	97	LYS	2.2
1	B	405	LYS	2.2
1	A	397	THR	2.2
1	B	213	THR	2.2
1	A	314	GLU	2.2
1	A	145	TYR	2.2
1	A	201	SER	2.2
1	A	354	GLY	2.2
1	A	248	LYS	2.2
1	A	358	PHE	2.2
1	B	149	LYS	2.2
1	B	236	SER	2.2
1	B	365	GLY	2.2
1	A	96	HIS	2.2
1	A	224	HIS	2.2
1	A	300	PRO	2.2
1	A	117	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	373	GLY	2.2
1	B	122	GLY	2.2
1	A	402	SER	2.2
1	A	140	PHE	2.2
1	B	224	HIS	2.2
1	B	358	PHE	2.2
1	B	415	ALA	2.2
1	A	239	THR	2.2
1	B	361	CYS	2.2
1	A	129	PRO	2.2
1	A	384	ASN	2.2
1	B	368	MET	2.2
1	B	256	SER	2.2
1	B	471	HIS	2.2
1	B	396	GLU	2.1
1	B	173	TYR	2.1
1	A	393	MET	2.1
1	B	217	MET	2.1
1	A	365	GLY	2.1
1	B	346	VAL	2.1
1	B	385	ILE	2.1
1	A	223	ARG	2.1
1	A	411	GLU	2.1
1	B	314	GLU	2.1
1	B	387	GLU	2.1
1	A	197	ARG	2.1
1	B	422	LYS	2.1
1	A	395	LEU	2.1
1	A	156	HIS	2.1
1	B	444	GLU	2.1
1	B	115	ASN	2.1
1	B	233	ASN	2.1
1	A	353	VAL	2.1
1	B	414	VAL	2.1
1	A	379	ASP	2.0
1	A	290	LYS	2.0
1	A	410	THR	2.0
1	A	157	LEU	2.0
1	A	243	GLN	2.0
1	B	299	LEU	2.0
1	B	348	ASN	2.0
1	B	259	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	ARG	2.0
1	A	185	LYS	2.0
1	A	422	LYS	2.0
1	B	183	ALA	2.0
1	B	237	ALA	2.0
1	A	217	MET	2.0
1	B	189	ARG	2.0
1	B	260	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

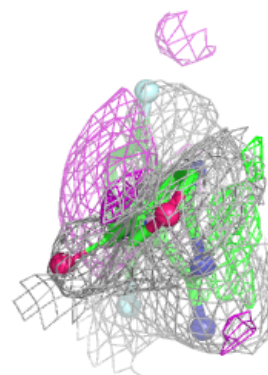
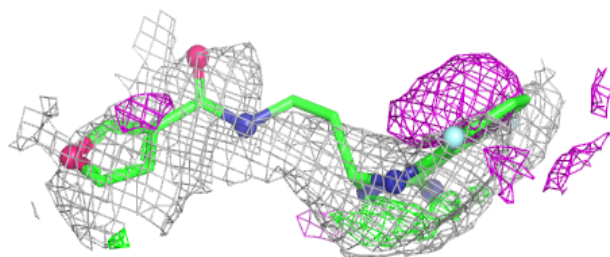
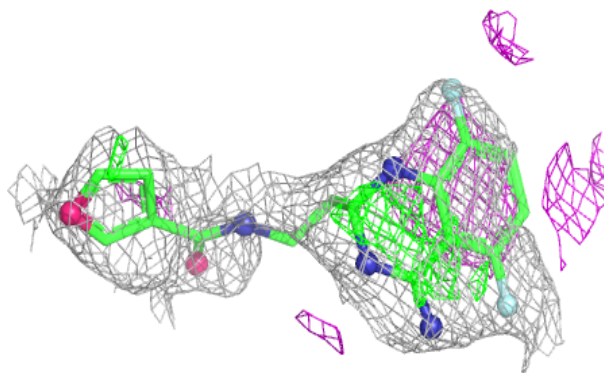
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A55	B	904	23/23	0.51	0.27	23,31,54,56	0
3	H4B	B	1902	17/17	0.67	0.24	26,29,34,34	0
4	A55	A	903	23/23	0.71	0.21	28,32,46,48	0
2	HEM	B	1901	43/43	0.76	0.25	23,25,29,37	0
2	HEM	A	901	43/43	0.79	0.22	24,26,30,30	0
3	H4B	A	902	17/17	0.80	0.16	28,30,31,32	0

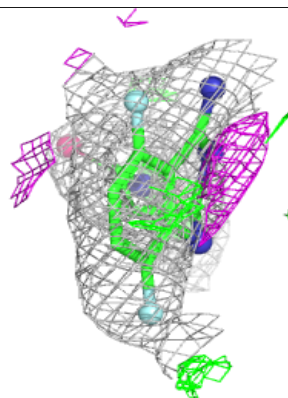
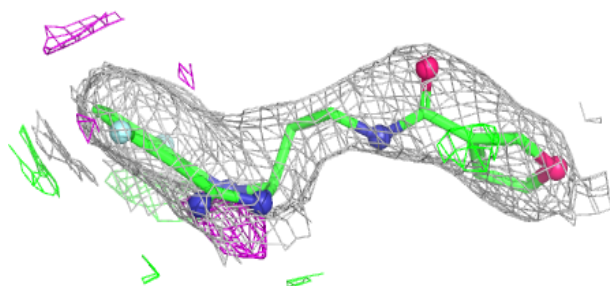
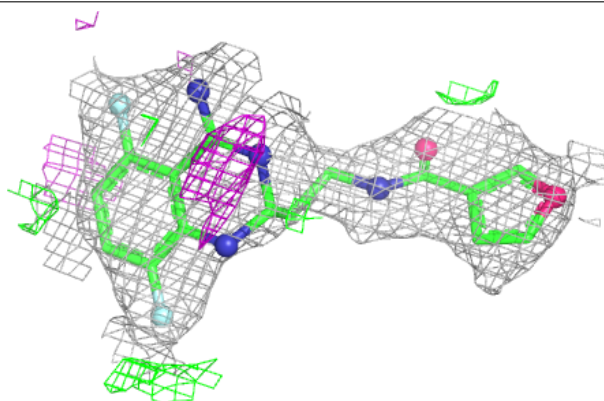
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A55 B 904:

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

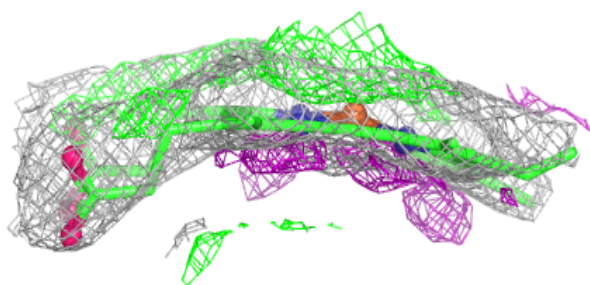
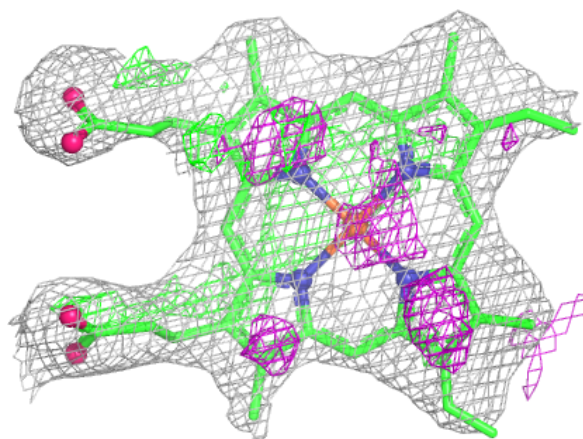
**Electron density around A55 A 903:**

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



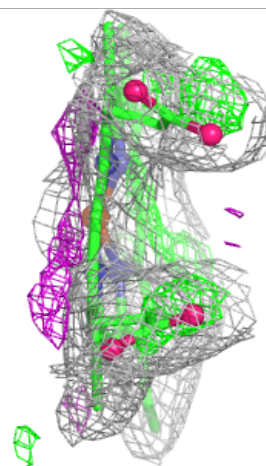
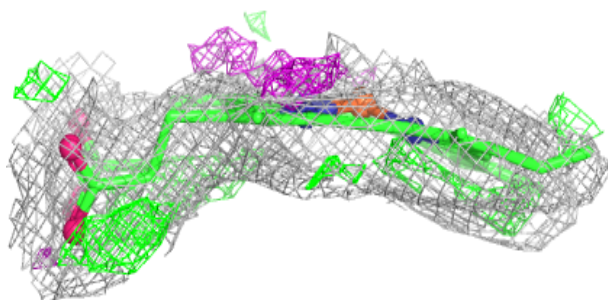
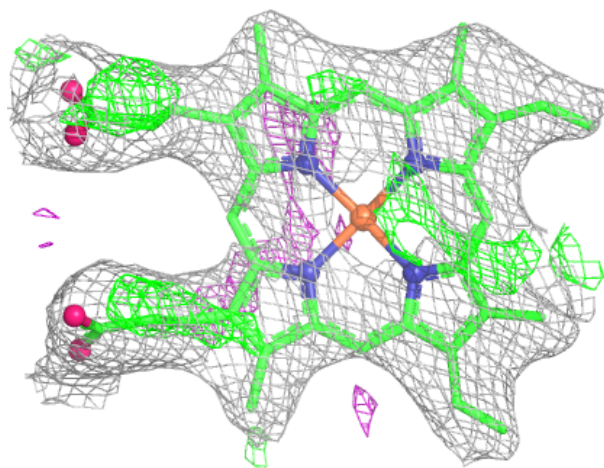
Electron density around HEM B 1901:

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



Electron density around HEM A 901:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.