



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:48 PM JST

PDB ID : 7E0O / pdb_00007e0o
Title : Crystal Structure of Human Indoleamine 2,3-dioxygenase 1 (hIDO1) Complexed with 6-Bromo-1H-indazol-4-amine (1)
Authors : Li, G.-B.; Ning, X.-L.
Deposited on : 2021-01-28
Resolution : 3.34 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

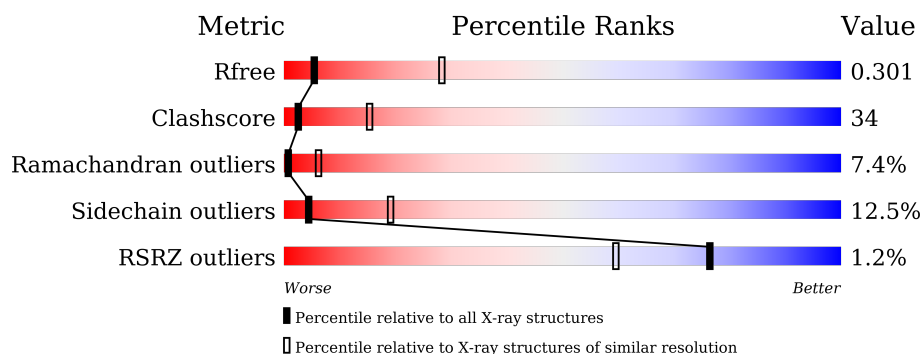
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	392	2% 37% 44% 12% 6%
1	B	392	% 39% 45% 10% 6%

2 Entry composition [i](#)

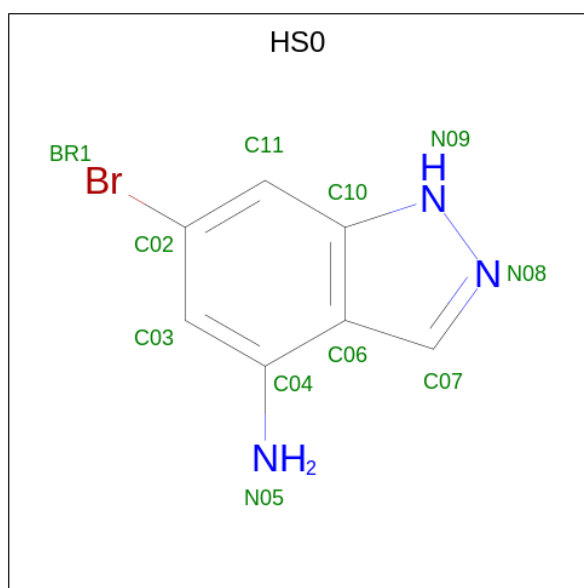
There are 3 unique types of molecules in this entry. The entry contains 5966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Indoleamine 2,3-dioxygenase 1.

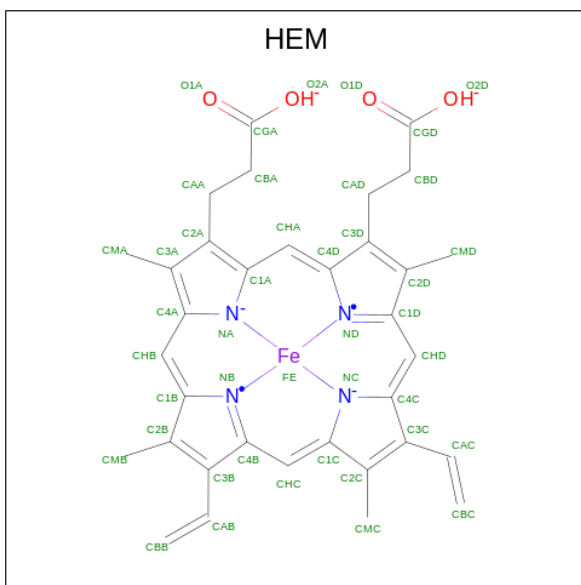
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2929	1883	499	530	17			
1	B	370	Total	C	N	O	S	0	0	0
			2929	1883	499	530	17			

- Molecule 2 is 6-bromanyl-1 {H}-indazol-4-amine (CCD ID: HS0) (formula: $C_7H_6BrN_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			11	1	7	3		
2	B	1	Total	Br	C	N	0	0
			11	1	7	3		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

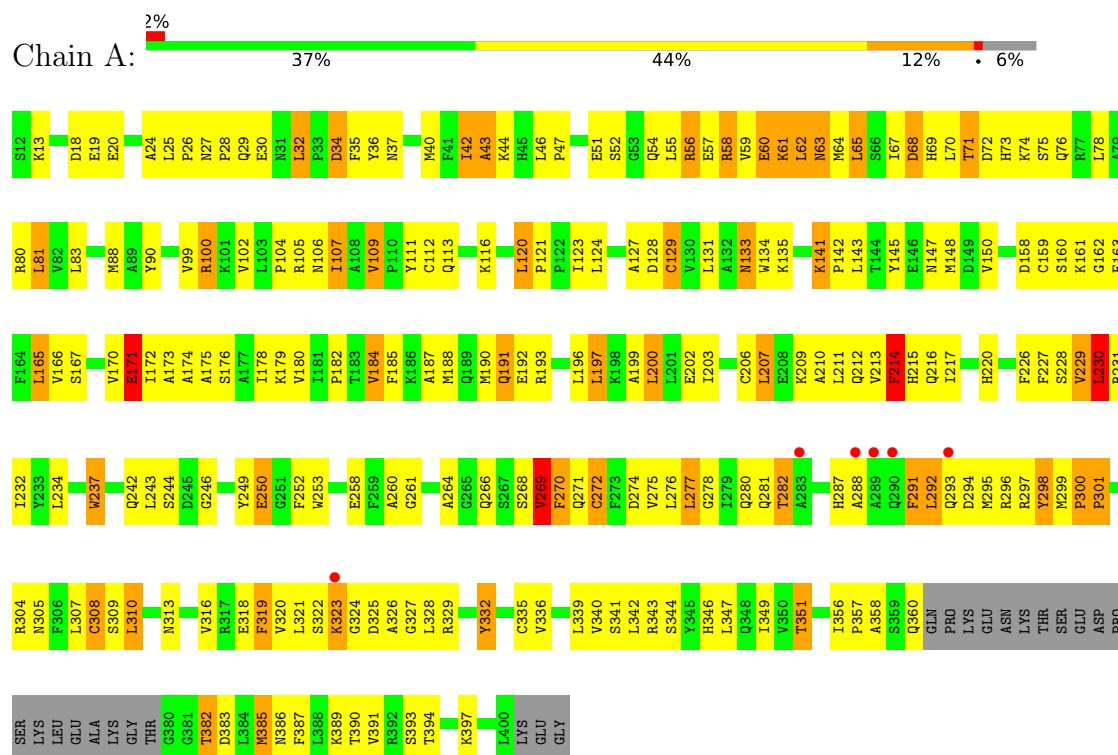


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

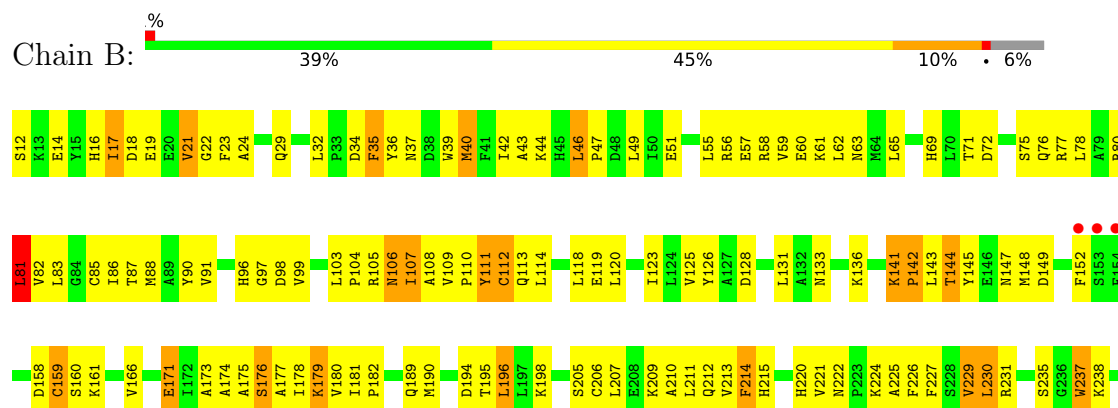
3 Residue-property plots [i](#)

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

• Molecule 1: Indoleamine 2,3-dioxygenase 1



• Molecule 1: Indoleamine 2,3-dioxygenase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.59Å 96.79Å 130.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.49 – 3.34 65.49 – 3.34	Depositor EDS
% Data completeness (in resolution range)	96.3 (65.49-3.34) 96.3 (65.49-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.211 , 0.302 0.223 , 0.301	Depositor DCC
R_{free} test set	1587 reflections (9.68%)	wwPDB-VP
Wilson B-factor (Å ²)	101.2	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5966	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: HS0, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	0/2997	0.93	1/4055 (0.0%)
1	B	0.76	2/2997 (0.1%)	0.95	2/4055 (0.0%)
All	All	0.76	2/5994 (0.0%)	0.94	3/8110 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	PRO	C-N	5.25	1.41	1.33
1	B	358	ALA	CA-C	5.11	1.59	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ILE	N-CA-C	-6.25	106.70	112.96
1	B	81	LEU	CA-C-N	5.98	128.18	120.70
1	B	81	LEU	C-N-CA	5.98	128.18	120.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2929	0	2934	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2929	0	2934	203	0
2	A	11	0	0	0	0
2	B	11	0	0	1	0
3	A	43	0	30	6	0
3	B	43	0	30	5	0
All	All	5966	0	5928	409	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 34.

All (409) 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:317:ARG:NH2	1:B:398:SER:O	2.07	0.87
1:A:109:VAL:O	1:A:113:GLN:HG3	1.76	0.84
1:A:80:ARG:NH2	1:A:128:ASP:OD2	2.09	0.84
1:B:274:ASP:OD2	1:B:343:ARG:NH2	2.14	0.79
1:A:64:MET:N	1:A:106:ASN:OD1	2.17	0.78
1:B:268:SER:O	1:B:270:PHE:N	2.18	0.77
1:B:342:LEU:O	1:B:345:TYR:N	2.13	0.77
1:B:87:THR:O	1:B:91:VAL:HG23	1.85	0.76
1:A:159:CYS:O	1:A:162:GLY:N	2.20	0.74
1:B:171:GLU:OE2	1:B:267:SER:OG	2.05	0.73
1:A:269:VAL:O	1:A:272:CYS:N	2.21	0.72
1:B:72:ASP:OD1	1:B:75:SER:OG	2.07	0.72
1:B:112:CYS:HB3	1:B:252:PHE:CE2	2.24	0.71
1:A:291:PHE:O	1:A:294:ASP:N	2.23	0.70
1:A:230:LEU:HD12	1:A:234:LEU:HD11	1.73	0.70
1:B:109:VAL:O	1:B:113:GLN:HG3	1.92	0.70
1:A:299:MET:O	1:A:300:PRO:O	2.10	0.70
1:A:176:SER:HB2	1:A:206:CYS:SG	2.32	0.69
1:A:269:VAL:HG23	1:A:270:PHE:CD2	2.29	0.68
1:A:55:LEU:C	1:A:55:LEU:HD23	2.20	0.66
1:B:29:GLN:OE1	1:B:75:SER:OG	2.09	0.65
1:A:322:SER:OG	1:A:323:LYS:N	2.29	0.65
1:B:158:ASP:OD1	1:B:159:CYS:N	2.30	0.65
1:B:21:VAL:HG12	1:B:24:ALA:HB3	1.79	0.64
1:A:193:ARG:HD3	1:A:193:ARG:C	2.23	0.64
1:A:34:ASP:OD1	1:A:34:ASP:N	2.28	0.64
1:A:105:ARG:HA	1:A:250:GLU:HB3	1.80	0.63
1:B:176:SER:HA	1:B:179:LYS:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:O	1:A:313:ASN:N	2.30	0.63
1:A:332:TYR:CD1	1:A:332:TYR:C	2.76	0.62
1:B:247:LEU:HD23	1:B:249:TYR:CZ	2.34	0.62
1:A:61:LYS:O	1:A:62:LEU:HD13	1.99	0.62
1:B:211:LEU:HD13	1:B:342:LEU:HD13	1.81	0.62
1:B:112:CYS:HB3	1:B:252:PHE:CZ	2.34	0.62
1:A:260:ALA:HB3	1:A:298:TYR:CE2	2.34	0.62
1:B:221:VAL:HG12	1:B:222:ASN:H	1.65	0.61
1:A:60:GLU:CD	1:A:60:GLU:H	2.09	0.61
1:A:188:MET:SD	1:A:316:VAL:HG22	2.40	0.61
1:A:274:ASP:OD2	1:A:281:GLN:HG3	2.01	0.60
1:B:281:GLN:O	1:B:289:ALA:HA	2.01	0.60
1:A:196:LEU:O	1:A:200:LEU:HD12	2.01	0.60
1:A:170:VAL:O	1:A:172:ILE:N	2.34	0.60
1:B:391:VAL:HG11	3:B:502:HEM:O1A	2.02	0.60
1:B:332:TYR:C	1:B:332:TYR:CD1	2.80	0.60
1:A:277:LEU:HD11	1:A:335:CYS:HB3	1.83	0.60
1:A:63:ASN:O	1:A:65:LEU:HD23	2.02	0.60
1:A:81:LEU:HD21	1:A:133:ASN:HB2	1.84	0.59
1:A:301:PRO:O	1:A:305:ASN:ND2	2.35	0.59
1:B:63:ASN:HA	1:B:106:ASN:OD1	2.03	0.59
1:B:214:PHE:O	1:B:214:PHE:HD1	1.86	0.59
1:B:226:PHE:CD1	1:B:226:PHE:C	2.80	0.59
1:B:12:SER:HB3	1:B:17:ILE:HD11	1.85	0.59
1:B:396:GLU:HG2	1:B:399:LEU:HD12	1.84	0.59
1:A:63:ASN:C	1:A:106:ASN:HD21	2.10	0.59
1:A:30:GLU:CD	1:A:135:LYS:HD2	2.28	0.58
1:B:271:GLN:NE2	1:B:292:LEU:O	2.27	0.58
1:A:291:PHE:O	1:A:293:GLN:N	2.35	0.58
1:B:336:VAL:O	1:B:340:VAL:HG23	2.03	0.58
1:A:170:VAL:O	1:A:173:ALA:N	2.36	0.58
1:B:175:ALA:HA	1:B:178:ILE:HD12	1.84	0.58
1:B:325:ASP:OD1	1:B:326:ALA:N	2.37	0.58
1:B:19:GLU:OE2	1:B:19:GLU:N	2.36	0.58
1:B:340:VAL:O	1:B:344:SER:HB2	2.03	0.58
1:B:103:LEU:HD23	1:B:108:ALA:HB2	1.86	0.57
1:A:29:GLN:O	1:A:78:LEU:HD22	2.04	0.57
1:B:221:VAL:HG12	1:B:222:ASN:N	2.19	0.57
1:B:260:ALA:O	1:B:261:GLY:O	2.22	0.57
1:B:252:PHE:HE2	1:B:253:TRP:CZ3	2.23	0.57
1:B:211:LEU:CD1	1:B:345:TYR:HD2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLY:O	1:B:99:VAL:HG23	2.04	0.57
1:B:32:LEU:HD12	1:B:40:MET:HG3	1.87	0.57
1:B:141:LYS:HB3	1:B:142:PRO:CD	2.34	0.56
1:B:214:PHE:CE1	1:B:349:ILE:HD12	2.40	0.56
1:B:281:GLN:OE1	1:B:343:ARG:NH2	2.37	0.56
1:A:161:LYS:O	1:A:165:LEU:HB2	2.05	0.56
1:B:272:CYS:HB2	1:B:307:LEU:CD2	2.35	0.56
1:B:90:TYR:CE2	1:B:104:PRO:HD3	2.41	0.56
1:A:326:ALA:HA	1:A:329:ARG:HG3	1.86	0.56
1:B:107:ILE:C	1:B:110:PRO:HD2	2.30	0.56
1:A:67:ILE:O	1:A:69:HIS:N	2.39	0.56
1:A:109:VAL:O	1:A:113:GLN:CG	2.50	0.56
1:A:178:ILE:HD11	1:A:269:VAL:HG12	1.87	0.56
1:A:269:VAL:O	1:A:270:PHE:C	2.48	0.56
1:B:12:SER:CB	1:B:17:ILE:HD11	2.35	0.55
1:B:17:ILE:HG22	1:B:22:GLY:O	2.06	0.55
1:B:55:LEU:C	1:B:55:LEU:HD23	2.30	0.55
1:B:332:TYR:CD1	1:B:332:TYR:O	2.59	0.55
1:B:56:ARG:O	1:B:60:GLU:HG3	2.06	0.55
1:A:143:LEU:HD23	1:A:148:MET:SD	2.47	0.55
1:A:99:VAL:HG11	1:A:243:LEU:HD11	1.88	0.55
1:B:29:GLN:O	1:B:78:LEU:HD22	2.06	0.55
1:A:347:LEU:O	1:A:351:THR:HG22	2.07	0.55
1:B:80:ARG:HH12	1:B:83:LEU:HD12	1.72	0.55
1:B:247:LEU:HD23	1:B:249:TYR:CE1	2.42	0.55
1:A:83:LEU:HD13	1:A:111:TYR:HA	1.88	0.55
1:B:43:ALA:HA	1:B:46:LEU:HD13	1.88	0.55
1:B:82:VAL:O	1:B:86:ILE:HG13	2.07	0.55
1:B:62:LEU:O	1:B:106:ASN:OD1	2.25	0.54
1:B:81:LEU:HD12	1:B:85:CYS:SG	2.47	0.54
1:B:189:GLN:HG2	1:B:190:MET:HE2	1.89	0.54
1:B:63:ASN:CA	1:B:106:ASN:OD1	2.56	0.54
1:A:27:ASN:O	1:A:74:LYS:HD3	2.08	0.54
1:A:269:VAL:HG23	1:A:270:PHE:H	1.73	0.54
1:A:332:TYR:C	1:A:332:TYR:HD1	2.16	0.53
1:B:271:GLN:NE2	1:B:292:LEU:HB3	2.23	0.53
1:A:175:ALA:HA	1:A:178:ILE:HD12	1.90	0.53
1:A:167:SER:HA	3:A:502:HEM:HBC2	1.91	0.53
1:B:277:LEU:HB2	1:B:279:ILE:HD12	1.90	0.53
1:A:158:ASP:O	1:A:230:LEU:CD2	2.57	0.53
1:A:133:ASN:OD1	1:A:133:ASN:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PHE:CE1	1:A:226:PHE:CE1	2.97	0.53
1:A:174:ALA:HB3	1:A:269:VAL:HG11	1.90	0.53
1:A:351:THR:O	1:A:356:ILE:HG13	2.08	0.53
1:B:35:PHE:CD1	1:B:35:PHE:C	2.87	0.53
1:B:264:ALA:O	1:B:267:SER:N	2.28	0.53
1:A:88:MET:HE1	1:A:123:ILE:HG13	1.92	0.52
1:B:290:GLN:O	1:B:293:GLN:N	2.34	0.52
1:A:56:ARG:NH2	1:A:100:ARG:HB2	2.24	0.52
1:B:118:LEU:O	1:B:120:LEU:HD12	2.09	0.52
1:A:296:ARG:HA	1:A:299:MET:HE3	1.91	0.52
1:B:319:PHE:O	1:B:323:LYS:HG2	2.09	0.52
1:A:332:TYR:CD1	1:A:332:TYR:O	2.63	0.52
1:B:342:LEU:O	1:B:344:SER:N	2.42	0.52
1:B:353:TYR:CB	3:B:502:HEM:HBC1	2.40	0.52
1:A:170:VAL:O	1:A:171:GLU:C	2.52	0.52
1:B:107:ILE:O	1:B:110:PRO:HG2	2.09	0.52
1:B:173:ALA:CB	1:B:210:ALA:HB2	2.40	0.52
1:B:384:LEU:HD12	1:B:385:MET:N	2.26	0.51
1:A:104:PRO:HB2	1:A:107:ILE:HG22	1.92	0.51
1:A:199:ALA:O	1:A:203:ILE:HG13	2.10	0.51
1:B:109:VAL:HG22	1:B:252:PHE:HB2	1.92	0.51
1:B:166:VAL:HG12	3:B:502:HEM:HBB1	1.93	0.51
1:A:56:ARG:NH2	1:A:100:ARG:HD3	2.26	0.51
1:B:179:LYS:O	1:B:182:PRO:HD2	2.08	0.51
1:B:282:THR:HG21	1:B:296:ARG:NH2	2.26	0.51
1:B:284:GLY:C	1:B:286:GLY:H	2.17	0.51
1:A:54:GLN:O	1:A:58:ARG:HG2	2.10	0.51
1:B:145:TYR:CE2	1:B:220:HIS:CD2	2.99	0.51
1:A:264:ALA:C	1:A:266:GLN:H	2.18	0.51
1:A:65:LEU:HD23	1:A:65:LEU:N	2.26	0.51
1:A:141:LYS:HB3	1:A:142:PRO:HD2	1.92	0.51
1:A:343:ARG:NH2	1:A:391:VAL:CG1	2.74	0.51
1:B:158:ASP:OD1	1:B:158:ASP:C	2.53	0.51
1:A:34:ASP:O	1:A:37:ASN:OD1	2.29	0.50
1:B:120:LEU:HD12	1:B:120:LEU:N	2.25	0.50
1:B:249:TYR:CD1	1:B:249:TYR:N	2.77	0.50
1:A:105:ARG:HA	1:A:250:GLU:CB	2.41	0.50
1:A:310:LEU:O	1:A:313:ASN:HB2	2.11	0.50
1:B:300:PRO:HG2	1:B:303:HIS:ND1	2.26	0.50
1:A:214:PHE:CE1	1:A:349:ILE:HD12	2.46	0.50
1:B:338:ALA:O	1:B:342:LEU:HD23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ILE:O	1:B:350:VAL:C	2.53	0.50
1:A:80:ARG:CZ	1:A:120:LEU:HD23	2.40	0.50
1:A:264:ALA:HB3	3:A:502:HEM:C1D	2.46	0.50
1:B:307:LEU:O	1:B:308:CYS:C	2.52	0.50
1:A:382:THR:O	1:A:385:MET:N	2.44	0.50
1:B:88:MET:HE1	1:B:123:ILE:HG13	1.92	0.50
1:A:393:SER:OG	1:A:394:THR:N	2.42	0.50
1:B:295:MET:N	1:B:295:MET:HE2	2.27	0.50
1:B:320:VAL:HG13	1:B:328:LEU:HB3	1.94	0.50
1:B:344:SER:OG	1:B:392:ARG:HD2	2.11	0.50
1:A:319:PHE:O	1:A:319:PHE:CD1	2.65	0.50
1:A:145:TYR:CD2	1:A:220:HIS:CE1	3.00	0.50
1:A:24:ALA:HA	1:A:131:LEU:HD22	1.93	0.49
1:A:305:ASN:HA	1:A:308:CYS:HB2	1.93	0.49
1:A:226:PHE:CD2	1:A:226:PHE:C	2.90	0.49
1:A:339:LEU:O	1:A:343:ARG:HG3	2.12	0.49
1:B:80:ARG:NH2	1:B:114:LEU:HB3	2.27	0.49
1:B:176:SER:HB2	1:B:206:CYS:SG	2.51	0.49
1:A:162:GLY:O	1:A:166:VAL:HG23	2.11	0.49
1:B:331:ALA:O	1:B:334:ALA:N	2.43	0.49
1:A:319:PHE:CD1	1:A:319:PHE:C	2.90	0.49
1:A:18:ASP:OD2	1:A:20:GLU:HB3	2.11	0.49
1:B:17:ILE:HA	1:B:22:GLY:O	2.12	0.49
1:A:55:LEU:C	1:A:55:LEU:CD2	2.85	0.49
1:A:134:TRP:CZ3	1:A:143:LEU:HD21	2.47	0.49
1:A:323:LYS:O	1:A:324:GLY:C	2.52	0.49
1:B:36:TYR:CD1	1:B:39:TRP:CZ3	3.01	0.49
1:B:123:ILE:HG13	1:B:237:TRP:CZ2	2.48	0.49
1:B:181:ILE:HG21	1:B:310:LEU:HD21	1.94	0.49
1:A:36:TYR:OH	1:A:69:HIS:HB2	2.13	0.49
1:B:252:PHE:HE2	1:B:253:TRP:CH2	2.30	0.49
1:B:221:VAL:CG1	1:B:222:ASN:H	2.26	0.48
1:A:120:LEU:HG	1:A:121:PRO:CD	2.43	0.48
1:B:34:ASP:OD1	1:B:34:ASP:N	2.43	0.48
1:B:119:GLU:C	1:B:120:LEU:HD12	2.39	0.48
1:B:158:ASP:OD1	1:B:160:SER:N	2.46	0.48
1:A:25:LEU:HD12	1:A:26:PRO:HD2	1.96	0.48
1:A:28:PRO:C	1:A:74:LYS:HD3	2.39	0.48
1:B:55:LEU:O	1:B:56:ARG:C	2.57	0.48
1:A:386:ASN:O	1:A:387:PHE:C	2.56	0.48
1:B:346:HIS:O	1:B:350:VAL:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:GLN:O	1:A:58:ARG:CG	2.62	0.48
1:A:116:LYS:CG	1:A:116:LYS:O	2.62	0.48
1:B:49:LEU:HD22	1:B:55:LEU:HA	1.95	0.48
1:B:284:GLY:C	1:B:286:GLY:N	2.72	0.48
1:B:353:TYR:HB3	3:B:502:HEM:HBC1	1.94	0.47
1:A:212:GLN:HA	1:A:215:HIS:ND1	2.29	0.47
1:A:127:ALA:HA	1:A:131:LEU:HB2	1.95	0.47
1:B:111:TYR:O	1:B:114:LEU:N	2.36	0.47
1:B:65:LEU:N	1:B:65:LEU:HD23	2.29	0.47
1:B:342:LEU:O	1:B:343:ARG:C	2.58	0.47
1:A:35:PHE:O	1:A:35:PHE:CD2	2.68	0.47
1:A:196:LEU:HG	1:A:200:LEU:HD11	1.96	0.47
1:B:63:ASN:O	1:B:65:LEU:CD2	2.63	0.47
1:B:112:CYS:CB	1:B:252:PHE:CE2	2.96	0.47
1:A:72:ASP:OD1	1:A:72:ASP:N	2.48	0.47
1:A:347:LEU:O	1:A:351:THR:CG2	2.63	0.47
1:B:293:GLN:HA	1:B:296:ARG:HG3	1.97	0.47
1:B:349:ILE:O	1:B:352:LYS:N	2.47	0.47
1:A:71:THR:HG23	1:A:72:ASP:H	1.79	0.46
1:A:288:ALA:HA	1:A:387:PHE:CD1	2.50	0.46
1:A:237:TRP:O	1:A:258:GLU:HA	2.16	0.46
1:A:287:HIS:O	1:A:288:ALA:C	2.57	0.46
1:A:184:VAL:HG23	1:A:199:ALA:HB1	1.97	0.46
1:B:238:LYS:HD2	1:B:260:ALA:HB2	1.98	0.46
1:A:124:LEU:HD12	1:A:128:ASP:CB	2.46	0.46
1:A:159:CYS:O	1:A:161:LYS:N	2.49	0.46
1:B:23:PHE:CE2	1:B:268:SER:CB	2.98	0.46
1:B:180:VAL:C	1:B:182:PRO:HD2	2.41	0.46
1:A:116:LYS:O	1:A:116:LYS:HG3	2.15	0.46
1:A:207:LEU:N	1:A:207:LEU:HD23	2.30	0.46
1:B:145:TYR:CE2	1:B:220:HIS:NE2	2.83	0.46
1:B:173:ALA:HB3	1:B:210:ALA:HB2	1.98	0.46
1:B:274:ASP:CG	1:B:343:ARG:HH22	2.18	0.46
1:B:225:ALA:O	1:B:226:PHE:C	2.59	0.46
1:B:392:ARG:O	1:B:393:SER:C	2.59	0.46
1:A:325:ASP:O	1:A:327:GLY:N	2.49	0.46
1:B:80:ARG:CZ	1:B:114:LEU:HB3	2.45	0.46
1:B:103:LEU:HD23	1:B:108:ALA:CB	2.45	0.46
1:B:343:ARG:HE	1:B:391:VAL:HG12	1.81	0.46
1:A:112:CYS:HB2	1:A:252:PHE:CE2	2.51	0.45
1:A:184:VAL:HG12	1:A:185:PHE:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PRO:O	1:A:304:ARG:NH2	2.49	0.45
1:B:46:LEU:N	1:B:47:PRO:HD3	2.31	0.45
1:B:56:ARG:NH2	1:B:98:ASP:O	2.35	0.45
1:B:108:ALA:O	1:B:111:TYR:HB3	2.16	0.45
1:A:158:ASP:HB2	1:A:230:LEU:HD22	1.98	0.45
1:A:316:VAL:O	1:A:320:VAL:HG23	2.16	0.45
1:B:227:PHE:HA	1:B:231:ARG:HD3	1.97	0.45
1:A:60:GLU:OE2	1:A:90:TYR:HE1	1.99	0.45
1:B:62:LEU:C	1:B:106:ASN:OD1	2.60	0.45
1:B:317:ARG:HG2	1:B:318:GLU:N	2.29	0.45
1:A:43:ALA:HA	1:A:46:LEU:CD2	2.46	0.45
1:A:56:ARG:HH21	1:A:100:ARG:HB2	1.81	0.45
1:B:75:SER:O	1:B:76:GLN:C	2.58	0.45
1:B:212:GLN:HA	1:B:215:HIS:CD2	2.51	0.45
1:A:51:GLU:OE2	1:A:52:SER:N	2.49	0.45
1:A:274:ASP:O	1:A:275:VAL:C	2.58	0.45
1:A:294:ASP:O	1:A:295:MET:HE2	2.17	0.45
1:B:180:VAL:C	1:B:182:PRO:CD	2.90	0.45
1:A:209:LYS:C	1:A:211:LEU:N	2.71	0.45
1:A:340:VAL:O	1:A:341:SER:C	2.58	0.45
1:B:77:ARG:HA	1:B:80:ARG:HG2	1.98	0.45
1:B:81:LEU:CD1	1:B:85:CYS:SG	3.04	0.45
1:B:276:LEU:HD11	1:B:316:VAL:HG21	1.97	0.45
1:A:43:ALA:HA	1:A:46:LEU:HD21	1.97	0.45
1:A:123:ILE:HD12	1:A:237:TRP:CZ2	2.52	0.45
1:A:158:ASP:O	1:A:159:CYS:HB2	2.17	0.45
1:B:23:PHE:CE2	1:B:268:SER:HB2	2.52	0.45
1:B:36:TYR:OH	1:B:69:HIS:HB2	2.17	0.45
1:B:141:LYS:HB2	1:B:147:ASN:ND2	2.32	0.44
1:B:266:GLN:HG2	1:B:298:TYR:HB2	1.98	0.44
1:A:105:ARG:CA	1:A:250:GLU:HB3	2.46	0.44
1:A:112:CYS:HB3	1:A:252:PHE:CZ	2.52	0.44
1:A:192:GLU:O	1:A:193:ARG:C	2.60	0.44
1:A:275:VAL:CG1	1:A:310:LEU:HB3	2.46	0.44
1:A:282:THR:HG21	1:A:296:ARG:NH2	2.32	0.44
1:B:229:VAL:O	1:B:230:LEU:C	2.59	0.44
1:A:90:TYR:CE2	1:A:100:ARG:HG2	2.52	0.44
1:A:59:VAL:O	1:A:62:LEU:CD2	2.65	0.44
1:B:46:LEU:N	1:B:47:PRO:CD	2.80	0.44
1:B:195:THR:O	1:B:196:LEU:C	2.60	0.44
1:A:83:LEU:CD1	1:A:111:TYR:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ASN:OD1	1:B:312:SER:HA	2.17	0.44
1:B:338:ALA:O	1:B:342:LEU:CD2	2.65	0.44
1:A:57:GLU:C	1:A:60:GLU:OE1	2.60	0.44
1:A:275:VAL:HG11	1:A:310:LEU:HB3	2.00	0.44
1:B:40:MET:HE1	1:B:44:LYS:HD3	1.99	0.44
1:B:80:ARG:NH1	1:B:114:LEU:HD23	2.32	0.44
1:B:175:ALA:C	1:B:177:ALA:H	2.25	0.44
1:A:190:MET:O	1:A:191:GLN:O	2.35	0.44
1:A:216:GLN:O	1:A:217:ILE:C	2.60	0.44
1:A:226:PHE:CE2	3:A:502:HEM:HMB2	2.52	0.44
1:A:63:ASN:C	1:A:106:ASN:OD1	2.60	0.44
1:A:180:VAL:HG21	1:A:202:GLU:HG3	2.00	0.44
1:B:214:PHE:O	1:B:214:PHE:CD1	2.70	0.44
1:B:227:PHE:CD2	1:B:357:PRO:HB2	2.52	0.44
1:A:124:LEU:HD11	1:A:129:CYS:HB3	1.99	0.44
1:A:185:PHE:CE1	1:A:313:ASN:HB3	2.53	0.44
1:A:197:LEU:HA	1:A:200:LEU:CD1	2.47	0.44
1:B:76:GLN:O	1:B:80:ARG:HD3	2.18	0.44
1:A:269:VAL:HG23	1:A:270:PHE:N	2.31	0.43
1:B:24:ALA:HB2	1:B:131:LEU:HD22	2.00	0.43
1:B:298:TYR:CD1	1:B:298:TYR:N	2.86	0.43
1:A:25:LEU:HD12	1:A:26:PRO:CD	2.48	0.43
1:A:209:LYS:C	1:A:211:LEU:H	2.26	0.43
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.82	0.43
1:B:142:PRO:O	1:B:144:THR:N	2.50	0.43
1:B:252:PHE:CE2	1:B:253:TRP:CZ3	3.05	0.43
1:A:60:GLU:OE1	1:A:60:GLU:N	2.52	0.43
1:B:14:GLU:C	1:B:16:HIS:N	2.75	0.43
1:B:268:SER:O	1:B:269:VAL:C	2.62	0.43
1:B:322:SER:OG	1:B:323:LYS:N	2.51	0.43
1:A:158:ASP:O	1:A:230:LEU:HD23	2.18	0.43
1:A:243:LEU:HB3	1:A:246:GLY:O	2.18	0.43
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.48	0.43
1:A:73:HIS:O	1:A:76:GLN:N	2.51	0.43
1:B:23:PHE:CD2	1:B:268:SER:HB2	2.54	0.43
1:B:149:ASP:OD1	1:B:161:LYS:HD2	2.18	0.43
1:B:76:GLN:O	1:B:80:ARG:CD	2.67	0.43
1:B:252:PHE:CE2	1:B:253:TRP:CH2	3.07	0.43
1:B:354:ILE:O	1:B:358:ALA:HB2	2.17	0.43
1:A:211:LEU:HD13	1:A:342:LEU:HD23	2.00	0.43
1:A:272:CYS:HB3	1:A:307:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:NH2	3:A:502:HEM:O1D	2.45	0.43
1:A:294:ASP:C	1:A:295:MET:HE2	2.43	0.43
1:A:389:LYS:C	1:A:391:VAL:N	2.76	0.43
1:B:29:GLN:HB3	1:B:78:LEU:HD22	2.00	0.43
1:B:63:ASN:O	1:B:65:LEU:HD23	2.19	0.43
1:B:328:LEU:C	1:B:330:GLU:N	2.76	0.43
1:B:356:ILE:HG22	1:B:357:PRO:HD3	2.01	0.43
1:A:170:VAL:HB	3:A:502:HEM:HBC1	2.01	0.43
1:A:179:LYS:C	1:A:182:PRO:HD2	2.43	0.43
1:A:264:ALA:C	1:A:266:GLN:N	2.76	0.43
1:B:347:LEU:HD21	1:B:388:LEU:HB3	2.01	0.43
1:B:103:LEU:O	1:B:104:PRO:C	2.62	0.42
1:A:59:VAL:O	1:A:62:LEU:HD22	2.19	0.42
1:A:159:CYS:C	1:A:161:LYS:N	2.77	0.42
1:A:170:VAL:C	1:A:172:ILE:N	2.77	0.42
1:A:188:MET:HG2	1:A:196:LEU:HD22	2.00	0.42
1:B:23:PHE:CE2	1:B:268:SER:HB3	2.54	0.42
1:B:126:TYR:OH	1:B:171:GLU:HG3	2.18	0.42
1:B:213:VAL:O	1:B:215:HIS:N	2.52	0.42
1:B:237:TRP:O	1:B:258:GLU:HG2	2.19	0.42
1:A:30:GLU:OE2	1:A:135:LYS:HD2	2.19	0.42
1:A:187:ALA:CB	1:A:196:LEU:HB2	2.49	0.42
1:A:229:VAL:O	1:A:232:ILE:HG12	2.20	0.42
1:A:295:MET:HE2	1:A:295:MET:HA	2.00	0.42
1:B:211:LEU:CD1	1:B:345:TYR:CD2	3.00	0.42
1:A:34:ASP:HA	1:A:37:ASN:OD1	2.19	0.42
1:A:90:TYR:CE2	1:A:104:PRO:HD3	2.54	0.42
1:A:175:ALA:HA	1:A:178:ILE:CD1	2.49	0.42
1:A:213:VAL:O	1:A:215:HIS:N	2.53	0.42
1:B:264:ALA:C	1:B:266:GLN:N	2.76	0.42
1:B:298:TYR:N	1:B:298:TYR:HD1	2.17	0.42
1:A:141:LYS:HB3	1:A:142:PRO:CD	2.50	0.42
1:B:23:PHE:O	1:B:303:HIS:HE1	2.02	0.42
1:A:32:LEU:HD22	1:A:40:MET:HG2	2.01	0.42
1:A:163:PHE:CE1	1:A:226:PHE:HE1	2.36	0.42
1:B:42:ILE:HD11	1:B:62:LEU:HD21	2.00	0.42
1:A:28:PRO:HG2	1:A:134:TRP:O	2.18	0.42
1:B:90:TYR:CZ	1:B:104:PRO:HD3	2.54	0.42
1:B:224:LYS:O	1:B:225:ALA:C	2.63	0.42
1:A:63:ASN:C	1:A:106:ASN:ND2	2.77	0.42
1:A:249:TYR:HB2	1:A:253:TRP:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:HIS:HE1	3:A:502:HEM:NA	2.18	0.42
1:A:269:VAL:O	1:A:271:GLN:N	2.52	0.42
1:A:67:ILE:O	1:A:68:ASP:C	2.63	0.41
1:B:118:LEU:O	1:B:120:LEU:CD1	2.68	0.41
2:B:501:HS0:C07	3:B:502:HEM:ND	2.81	0.41
1:A:298:TYR:N	1:A:298:TYR:CD1	2.88	0.41
1:B:133:ASN:CG	1:B:133:ASN:O	2.63	0.41
1:B:206:CYS:O	1:B:207:LEU:C	2.63	0.41
1:B:271:GLN:O	1:B:275:VAL:HG23	2.20	0.41
1:A:102:VAL:HG23	1:A:102:VAL:O	2.21	0.41
1:A:343:ARG:NH2	1:A:391:VAL:HG11	2.36	0.41
1:B:144:THR:O	1:B:148:MET:HG3	2.20	0.41
1:A:214:PHE:HE1	1:A:349:ILE:HD12	1.84	0.41
1:A:32:LEU:HA	1:A:32:LEU:HD12	1.91	0.41
1:B:18:ASP:HB3	1:B:21:VAL:HG23	2.02	0.41
1:A:42:ILE:O	1:A:43:ALA:C	2.63	0.41
1:B:88:MET:HE1	1:B:123:ILE:CG1	2.51	0.41
1:B:195:THR:O	1:B:198:LYS:N	2.51	0.41
1:A:55:LEU:O	1:A:59:VAL:HG23	2.20	0.41
1:A:227:PHE:CE2	1:A:358:ALA:HA	2.56	0.41
1:A:268:SER:O	1:A:269:VAL:O	2.39	0.41
1:A:276:LEU:C	1:A:278:GLY:H	2.29	0.41
1:A:277:LEU:HD13	1:A:336:VAL:HG22	2.02	0.41
1:B:34:ASP:O	1:B:37:ASN:OD1	2.39	0.41
1:B:82:VAL:HG22	1:B:152:PHE:CZ	2.56	0.41
1:A:228:SER:O	1:A:232:ILE:CG1	2.69	0.41
1:A:328:LEU:O	1:A:329:ARG:C	2.62	0.41
1:B:35:PHE:O	1:B:35:PHE:HD1	2.04	0.41
1:B:125:VAL:O	1:B:128:ASP:HB2	2.21	0.41
1:B:221:VAL:CG1	1:B:222:ASN:N	2.83	0.41
1:A:60:GLU:CD	1:A:60:GLU:N	2.77	0.40
1:A:320:VAL:HG13	1:A:328:LEU:HB2	2.04	0.40
1:B:56:ARG:O	1:B:57:GLU:C	2.64	0.40
1:A:34:ASP:C	1:A:36:TYR:H	2.29	0.40
1:A:46:LEU:N	1:A:47:PRO:CD	2.84	0.40
1:A:214:PHE:CE1	1:A:349:ILE:CD1	3.05	0.40
1:A:291:PHE:O	1:A:292:LEU:C	2.64	0.40
1:A:305:ASN:HB3	1:B:312:SER:HB3	2.04	0.40
1:A:133:ASN:OD1	1:A:150:VAL:HB	2.22	0.40
1:A:357:PRO:HA	1:A:360:GLN:OE1	2.21	0.40
1:B:88:MET:HE1	1:B:237:TRP:CH2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:HB2	1:B:301:PRO:HG3	2.03	0.40
1:B:173:ALA:HB1	1:B:210:ALA:HB2	2.03	0.40
1:B:284:GLY:O	1:B:286:GLY:N	2.54	0.40
1:B:288:ALA:O	1:B:289:ALA:C	2.63	0.40
1:A:42:ILE:O	1:A:44:LYS:N	2.54	0.40
1:A:124:LEU:CD1	1:A:128:ASP:HB3	2.52	0.40
1:B:269:VAL:HG23	1:B:270:PHE:HD1	1.86	0.40
1:B:343:ARG:HE	1:B:391:VAL:CG1	2.35	0.40
1:A:70:LEU:HD23	1:A:75:SER:HB3	2.03	0.40
1:A:105:ARG:O	1:A:109:VAL:HG23	2.21	0.40
1:B:59:VAL:C	1:B:61:LYS:N	2.79	0.40
1:B:72:ASP:O	1:B:76:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/392 (93%)	266 (73%)	72 (20%)	28 (8%)	1	5
1	B	366/392 (93%)	261 (71%)	79 (22%)	26 (7%)	1	7
All	All	732/784 (93%)	527 (72%)	151 (21%)	54 (7%)	1	6

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	160	SER
1	A	171	GLU
1	A	214	PHE
1	A	269	VAL
1	A	270	PHE

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Mol	Chain	Res	Type
1	A	291	PHE
1	A	300	PRO
1	B	269	VAL
1	B	343	ARG
1	A	60	GLU
1	A	68	ASP
1	A	133	ASN
1	A	191	GLN
1	A	231	ARG
1	A	261	GLY
1	A	292	LEU
1	A	390	THR
1	A	397	LYS
1	B	111	TYR
1	B	143	LEU
1	B	174	ALA
1	B	176	SER
1	B	196	LEU
1	B	214	PHE
1	B	261	GLY
1	B	268	SER
1	B	287	HIS
1	B	291	PHE
1	B	308	CYS
1	B	350	VAL
1	B	397	LYS
1	A	210	ALA
1	A	277	LEU
1	A	301	PRO
1	B	285	GLY
1	B	342	LEU
1	A	43	ALA
1	A	229	VAL
1	A	383	ASP
1	B	141	LYS
1	B	142	PRO
1	B	235	SER
1	B	307	LEU
1	B	354	ILE
1	A	42	ILE
1	A	230	LEU
1	A	382	THR

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Mol	Chain	Res	Type
1	B	252	PHE
1	A	109	VAL
1	B	112	CYS
1	A	141	LYS
1	B	229	VAL
1	B	286	GLY

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	319/339 (94%)	276 (86%)	43 (14%)	4	16
1	B	319/339 (94%)	282 (88%)	37 (12%)	5	21
All	All	638/678 (94%)	558 (88%)	80 (12%)	4	19

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	32	LEU
1	A	34	ASP
1	A	56	ARG
1	A	58	ARG
1	A	61	LYS
1	A	62	LEU
1	A	63	ASN
1	A	65	LEU
1	A	71	THR
1	A	81	LEU
1	A	100	ARG
1	A	120	LEU
1	A	129	CYS
1	A	147	ASN
1	A	165	LEU
1	A	171	GLU

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Mol	Chain	Res	Type
1	A	184	VAL
1	A	197	LEU
1	A	200	LEU
1	A	207	LEU
1	A	214	PHE
1	A	230	LEU
1	A	237	TRP
1	A	242	GLN
1	A	244	SER
1	A	250	GLU
1	A	269	VAL
1	A	272	CYS
1	A	280	GLN
1	A	282	THR
1	A	297	ARG
1	A	298	TYR
1	A	308	CYS
1	A	309	SER
1	A	310	LEU
1	A	318	GLU
1	A	319	PHE
1	A	323	LYS
1	A	332	TYR
1	A	344	SER
1	A	351	THR
1	A	385	MET
1	B	17	ILE
1	B	21	VAL
1	B	35	PHE
1	B	40	MET
1	B	46	LEU
1	B	51	GLU
1	B	58	ARG
1	B	71	THR
1	B	81	LEU
1	B	96	HIS
1	B	105	ARG
1	B	106	ASN
1	B	107	ILE
1	B	136	LYS
1	B	144	THR
1	B	159	CYS

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Mol	Chain	Res	Type
1	B	171	GLU
1	B	179	LYS
1	B	194	ASP
1	B	205	SER
1	B	209	LYS
1	B	230	LEU
1	B	237	TRP
1	B	242	GLN
1	B	269	VAL
1	B	272	CYS
1	B	292	LEU
1	B	297	ARG
1	B	308	CYS
1	B	318	GLU
1	B	322	SER
1	B	323	LYS
1	B	343	ARG
1	B	346	HIS
1	B	347	LEU
1	B	348	GLN
1	B	382	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	29	GLN
1	A	73	HIS
1	A	113	GLN
1	A	242	GLN
1	B	31	ASN
1	B	113	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HS0	A	501	3	12,12,12	1.38	2 (16%)	13,17,17	4.15	5 (38%)
2	HS0	B	501	3	12,12,12	1.81	3 (25%)	13,17,17	5.19	8 (61%)
3	HEM	B	502	1,2	50,50,50	1.66	9 (18%)	66,82,82	1.58	16 (24%)
3	HEM	A	502	1,2	50,50,50	1.55	8 (16%)	66,82,82	1.69	15 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HS0	A	501	3	-	-	0/2/2/2
2	HS0	B	501	3	-	-	0/2/2/2
3	HEM	B	502	1,2	-	6/14/54/54	-
3	HEM	A	502	1,2	-	5/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	HEM	FE-NB	5.28	2.11	1.94
3	A	502	HEM	FE-NC	4.94	2.11	1.95
3	B	502	HEM	FE-NA	4.62	2.10	1.95
3	A	502	HEM	FE-NB	3.86	2.06	1.94
2	B	501	HS0	C06-C10	-3.69	1.37	1.41
2	A	501	HS0	C06-C10	-3.34	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HEM	CAB-C3B	3.28	1.56	1.47
3	B	502	HEM	CAB-C3B	3.15	1.56	1.47
3	A	502	HEM	CAC-C3C	2.95	1.55	1.47
3	B	502	HEM	CAA-C2A	2.80	1.58	1.51
3	B	502	HEM	CAC-C3C	2.73	1.54	1.47
3	B	502	HEM	FE-ND	-2.53	1.86	1.94
3	A	502	HEM	CMA-C3A	2.52	1.56	1.50
3	B	502	HEM	CMC-C2C	2.51	1.56	1.50
3	A	502	HEM	C2A-C3A	-2.50	1.32	1.38
3	B	502	HEM	CMA-C3A	2.31	1.55	1.50
2	B	501	HS0	C04-N05	2.25	1.45	1.37
3	A	502	HEM	CMB-C2B	2.13	1.55	1.50
2	A	501	HS0	C04-N05	2.11	1.44	1.37
3	B	502	HEM	CMD-C2D	2.11	1.55	1.50
2	B	501	HS0	C03-C02	2.02	1.42	1.38
3	A	502	HEM	CMC-C2C	2.00	1.55	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HS0	C06-C07-N08	-14.25	106.89	111.41
2	A	501	HS0	C06-C07-N08	-10.51	108.07	111.41
2	B	501	HS0	C07-N08-N09	7.97	110.24	106.02
2	A	501	HS0	C07-N08-N09	7.42	109.95	106.02
2	A	501	HS0	C06-C10-N09	5.27	110.74	106.47
2	B	501	HS0	C06-C10-N09	5.12	110.61	106.47
2	B	501	HS0	BR1-C02-C03	4.80	125.93	119.27
3	A	502	HEM	CAA-CBA-CGA	-4.34	104.27	113.60
3	B	502	HEM	CAD-CBD-CGD	-4.13	104.72	113.60
3	A	502	HEM	CMB-C2B-C1B	-3.71	119.38	125.04
3	B	502	HEM	C4C-C3C-C2C	3.67	109.77	106.75
2	A	501	HS0	BR1-C02-C11	-3.36	114.59	119.27
2	A	501	HS0	C11-C10-C06	-3.28	118.84	122.22
3	A	502	HEM	C3B-C2B-C1B	3.27	108.91	106.49
3	A	502	HEM	CHD-C1D-ND	3.17	127.86	124.42
3	A	502	HEM	C2A-C1A-NA	-3.14	106.64	110.15
3	B	502	HEM	CMA-C3A-C4A	-3.09	120.66	125.37
3	A	502	HEM	CHC-C4B-NB	2.97	127.64	124.42
2	B	501	HS0	C11-C10-C06	-2.96	119.17	122.22
3	B	502	HEM	CHC-C4B-NB	2.86	127.53	124.42
3	A	502	HEM	CMA-C3A-C4A	2.85	129.71	125.37
3	A	502	HEM	C1A-C2A-C3A	2.81	111.31	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HS0	C10-C11-C02	2.79	122.80	117.46
3	A	502	HEM	C4A-NA-C1A	2.76	108.05	105.35
3	B	502	HEM	CAC-C3C-C4C	-2.74	118.27	124.90
3	A	502	HEM	CHB-C1B-NB	2.71	127.72	124.37
3	B	502	HEM	O1D-CGD-CBD	-2.66	114.53	123.08
3	A	502	HEM	CBA-CAA-C2A	-2.63	105.33	112.63
2	B	501	HS0	C11-C02-C03	-2.58	117.70	121.51
3	A	502	HEM	CHD-C4C-NC	2.55	127.20	124.44
3	B	502	HEM	C3D-C4D-ND	-2.54	107.34	110.17
3	A	502	HEM	O1D-CGD-CBD	-2.54	114.94	123.08
3	B	502	HEM	CMA-C3A-C2A	2.46	130.94	125.61
3	B	502	HEM	CHA-C4D-ND	2.46	127.40	124.37
3	B	502	HEM	CHD-C4C-NC	2.39	127.02	124.44
3	A	502	HEM	C3D-C4D-ND	-2.35	107.55	110.17
3	B	502	HEM	C3B-C2B-C1B	2.33	108.21	106.49
3	B	502	HEM	C4D-ND-C1D	2.29	107.44	105.07
3	B	502	HEM	CHB-C1B-NB	2.19	127.08	124.37
3	B	502	HEM	C4A-NA-C1A	2.13	107.44	105.35
2	B	501	HS0	BR1-C02-C11	-2.10	116.35	119.27
3	A	502	HEM	C4D-ND-C1D	2.07	107.22	105.07
3	B	502	HEM	CHD-C1D-ND	2.07	126.66	124.42
3	B	502	HEM	O2D-CGD-CBD	2.03	120.56	114.03

There are no chirality outliers.

All (11) torsion outliers are listed below:

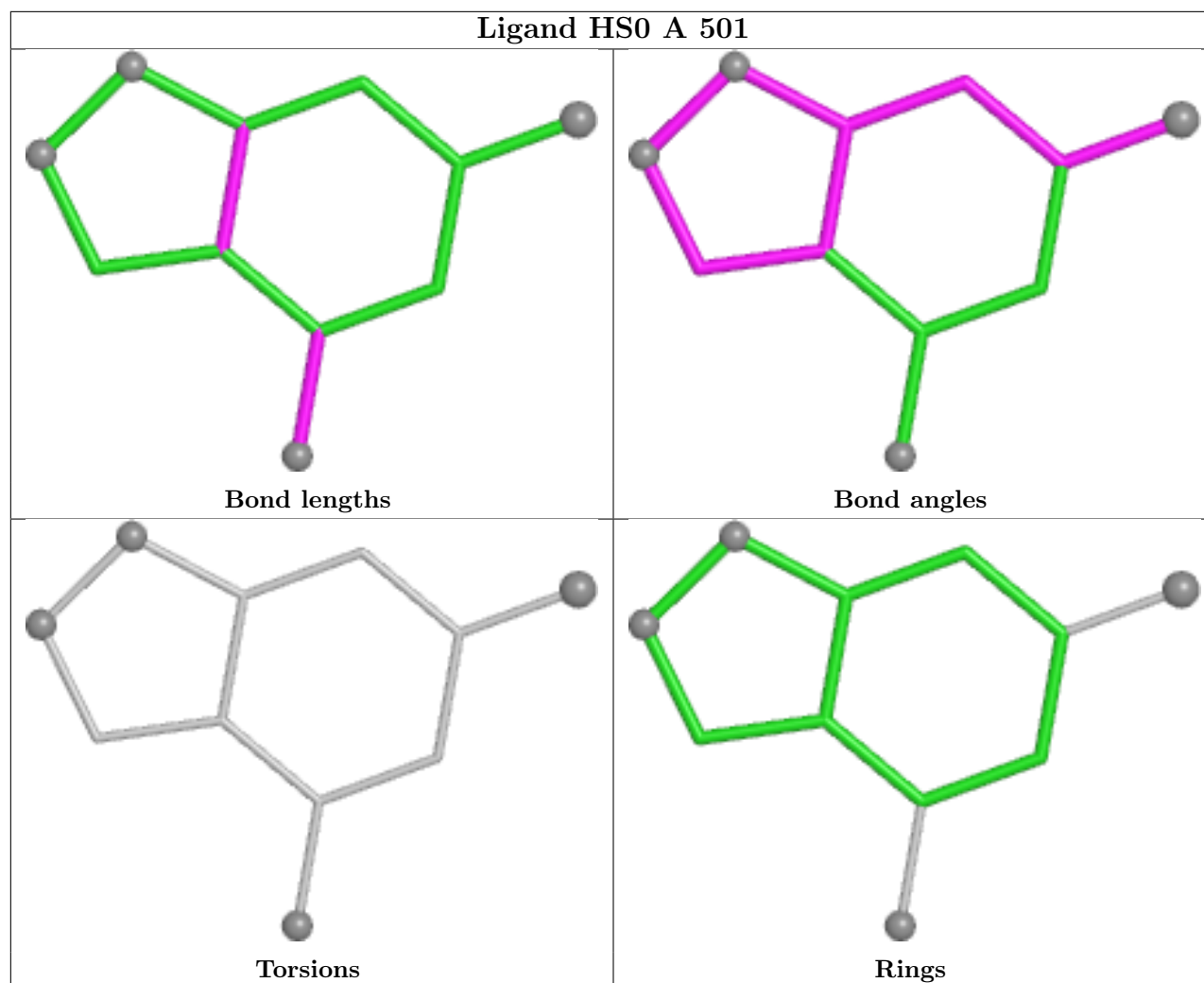
Mol	Chain	Res	Type	Atoms
3	B	502	HEM	C1A-C2A-CAA-CBA
3	B	502	HEM	C3A-C2A-CAA-CBA
3	A	502	HEM	C4D-C3D-CAD-CBD
3	A	502	HEM	C3D-CAD-CBD-CGD
3	A	502	HEM	C2D-C3D-CAD-CBD
3	B	502	HEM	CAA-CBA-CGA-O1A
3	B	502	HEM	CAA-CBA-CGA-O2A
3	B	502	HEM	CAD-CBD-CGD-O2D
3	B	502	HEM	CAD-CBD-CGD-O1D
3	A	502	HEM	CAD-CBD-CGD-O1D
3	A	502	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

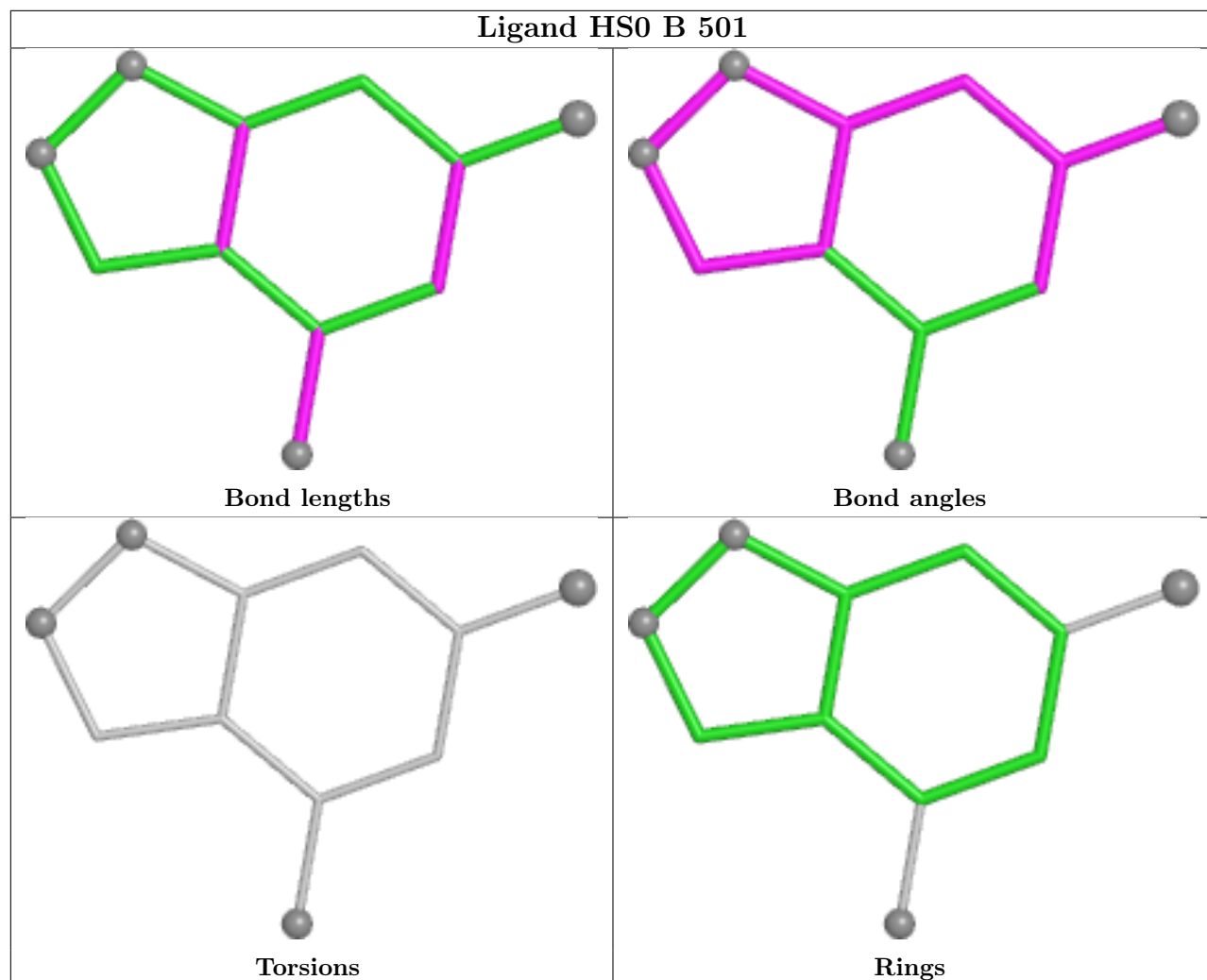
3 monomers are involved in 11 short contacts:

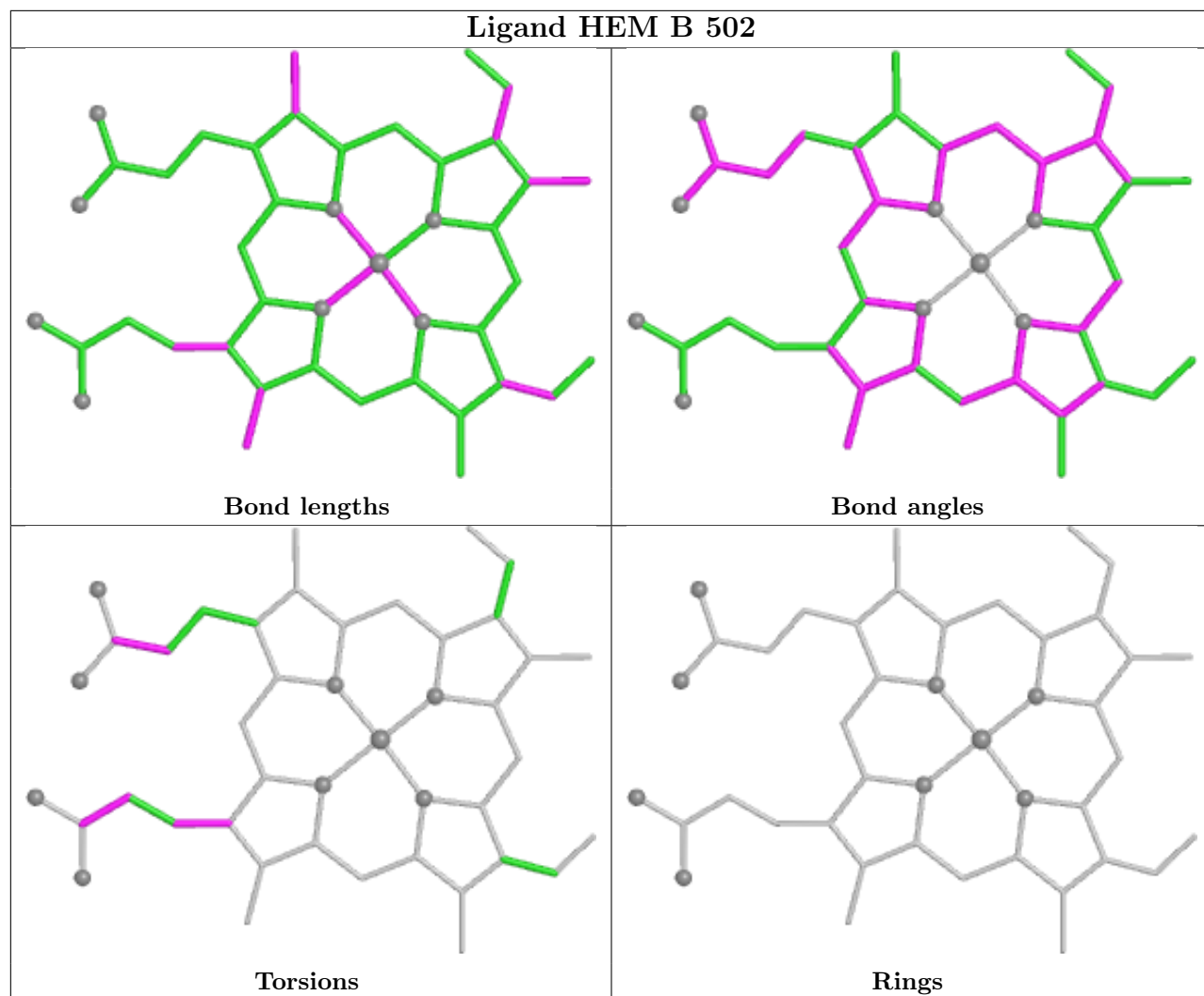
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HS0	1	0
3	B	502	HEM	5	0
3	A	502	HEM	6	0

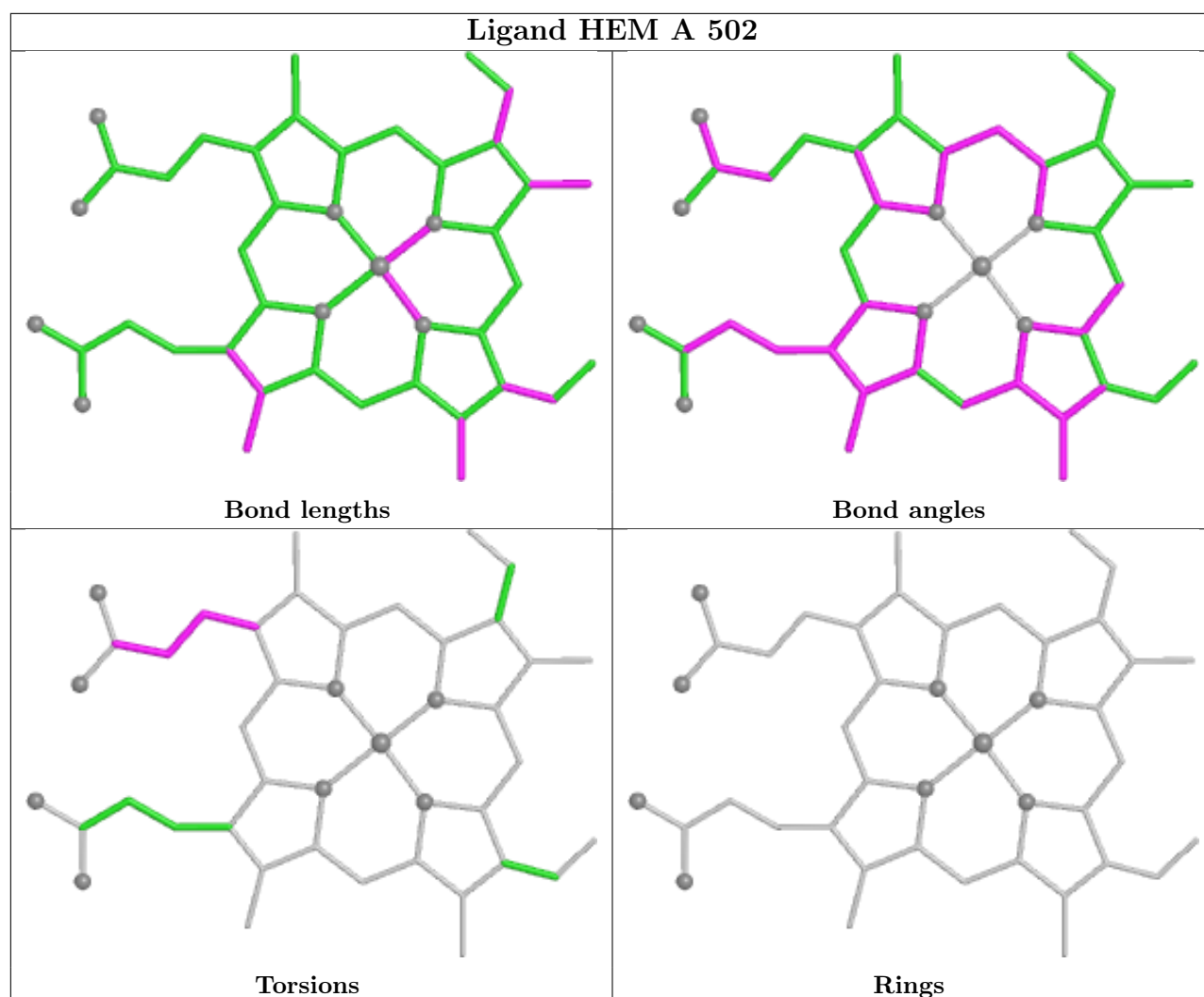
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand HS0 B 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	370/392 (94%)	-0.17	6 (1%)	70 52	67, 104, 131, 162	0
1	B	370/392 (94%)	-0.27	3 (0%)	82 69	72, 103, 131, 152	0
All	All	740/784 (94%)	-0.22	9 (1%)	76 59	67, 104, 131, 162	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	PHE	2.8
1	A	289	ALA	2.6
1	A	283	ALA	2.6
1	A	293	GLN	2.4
1	A	290	GLN	2.3
1	B	154	PHE	2.3
1	A	288	ALA	2.2
1	A	323	LYS	2.0
1	B	153	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

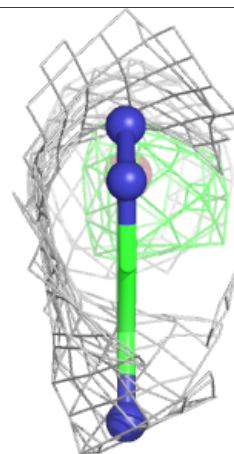
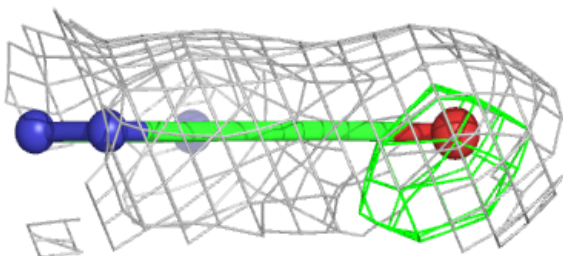
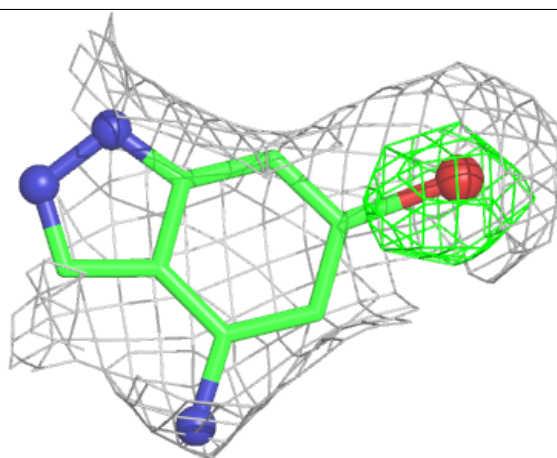
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HS0	B	501	11/11	0.87	0.12	93,108,129,192	0
2	HS0	A	501	11/11	0.93	0.08	88,100,116,128	0
3	HEM	B	502	43/43	0.95	0.10	67,91,117,131	0
3	HEM	A	502	43/43	0.97	0.09	74,91,110,118	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.

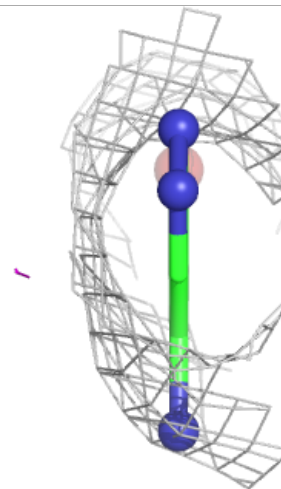
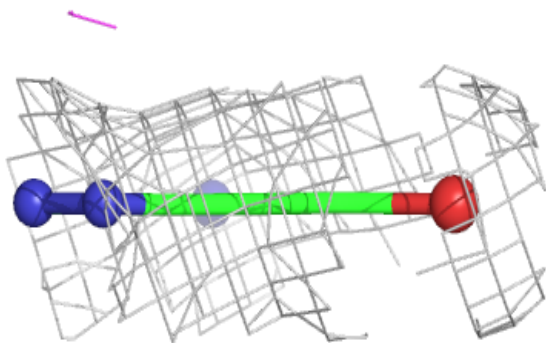
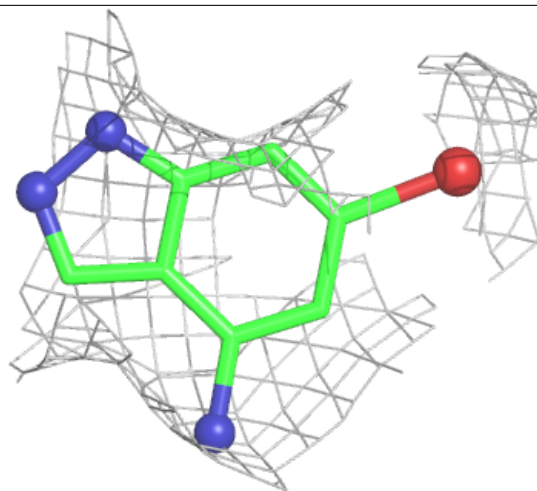
Electron density around HS0 B 501:

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



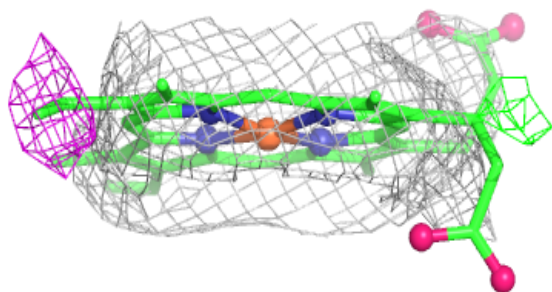
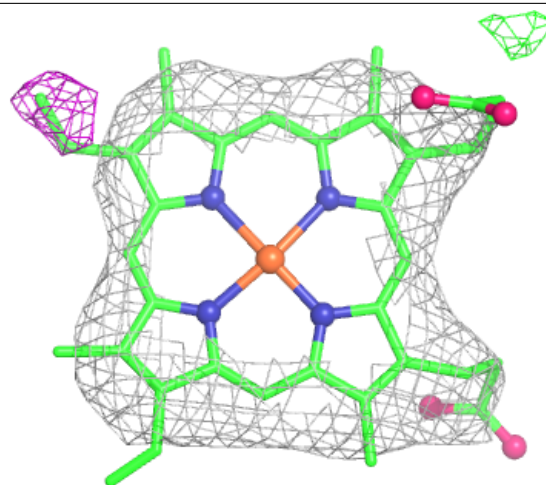
Electron density around HS0 A 501:

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



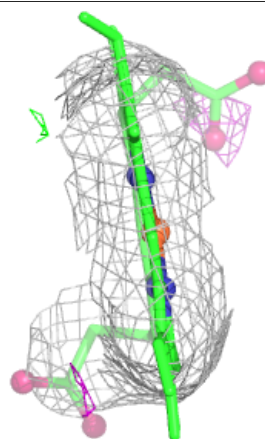
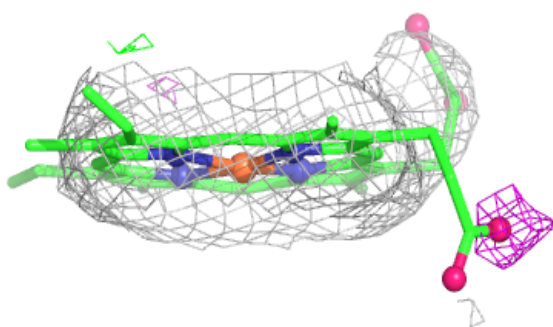
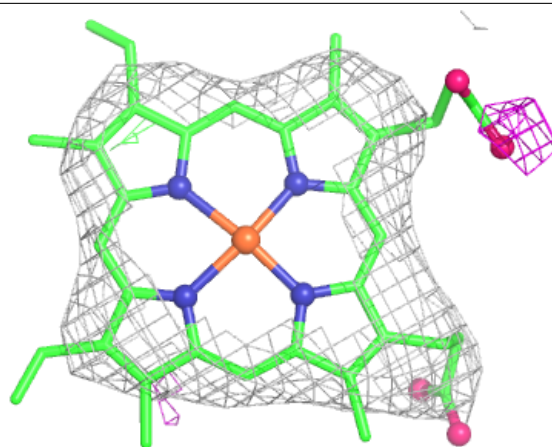
Electron density around HEM B 502:

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



Electron density around HEM A 502:

$2mF_o - DF_c$ (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.