Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 11:15 PM EDT

PDB ID	:	4HGI
Title	:	Crystal structure of P450 BM3 5F5 heme domain variant complexed with styrene (dataset II)
Authors	:	Shehzad, A.; Panneerselvam, S.; Bocola, M.; Mueller-Dieckmann, J.; Wilmanns, M.; Schwaneberg, U.
Deposited on	:	2012-10-08
Resolution	:	1.50 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	Percentile Ranks	Value
Rfree		0.197
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		5.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
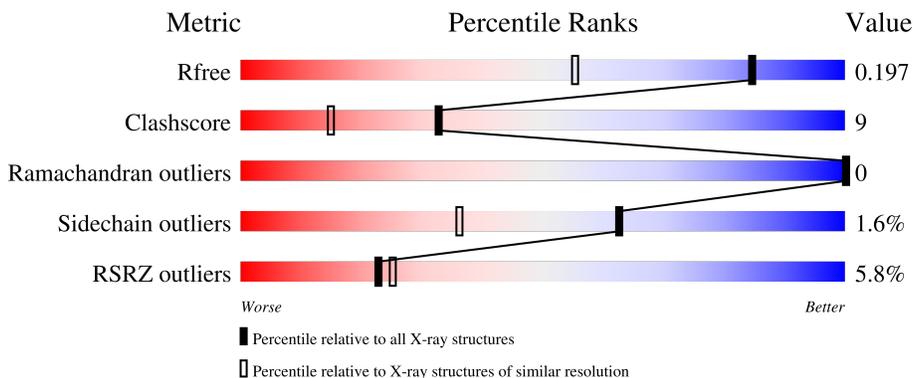
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	455	5% / 88% / 12% / •
1	B	455	6% / 84% / 14% / •

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	SYN	A	502[A]	-	-	X	-
3	SYN	B	503[A]	-	-	X	-
5	PEG	A	505	-	X	X	-

2 Entity composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8715 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 Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total 3824	C 2461	N 635	O 707	S 21	0	31	0
1	B	453	Total 3808	C 2454	N 631	O 704	S 19	0	31	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	PHE	engineered mutation	UNP P14779
A	235	ALA	THR	engineered mutation	UNP P14779
B	87	ALA	PHE	engineered mutation	UNP P14779
B	235	ALA	THR	engineered mutation	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
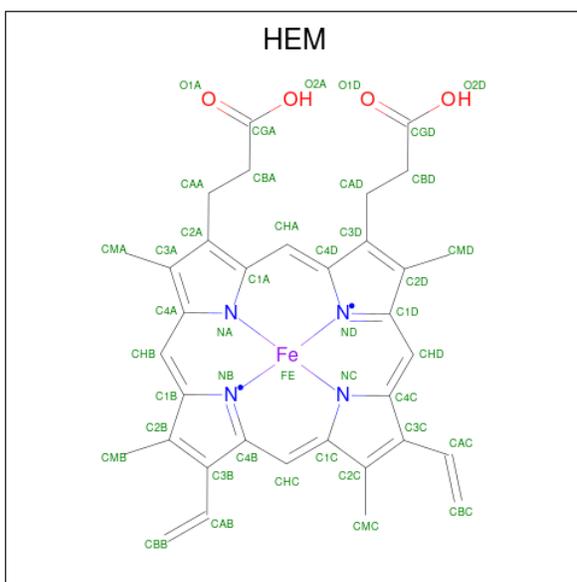
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ethenylbenzene (three-letter code: SYN) (formula: C_8H_8).
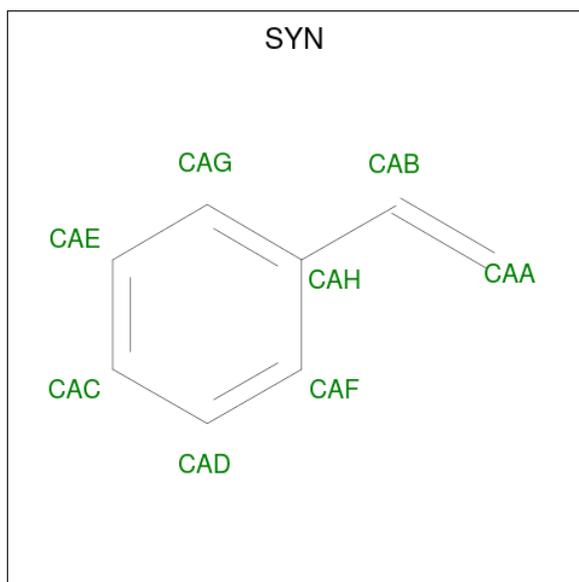
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	1
			16	16		
3	B	1	Total	C	0	1
			16	16		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

WORLDWIDE
PDB
PROTEIN DATA BANK
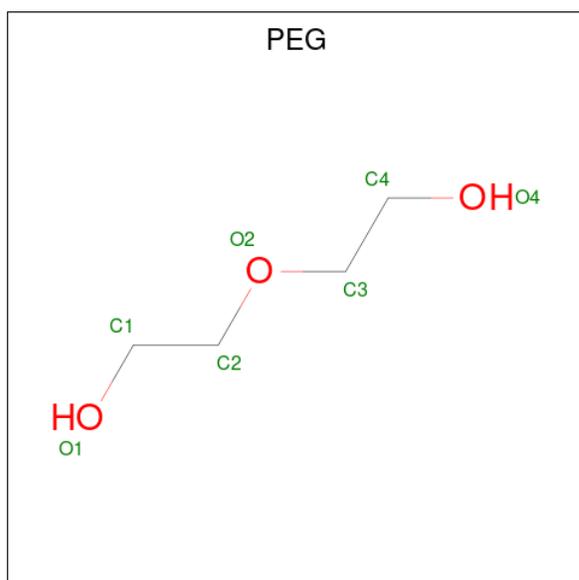
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).
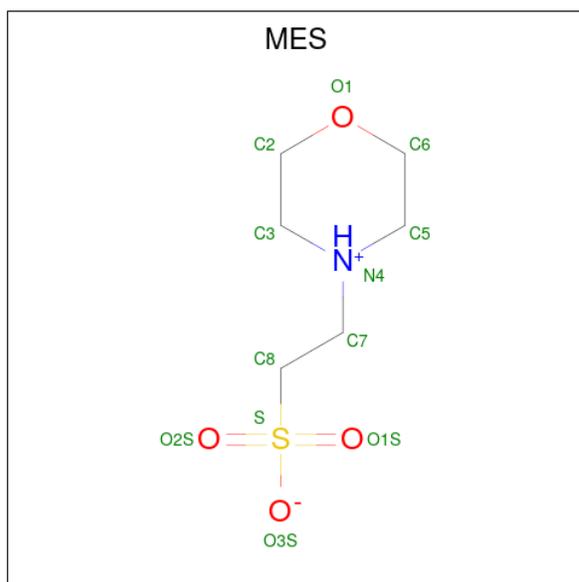
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	489	Total	O	0	2
			489	489		
7	B	427	Total	O	0	0
			427	427		

3 Residue-property plots ⓘ

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

- Molecule 1: Bifunctional P-450/NADPH-P450 reductase
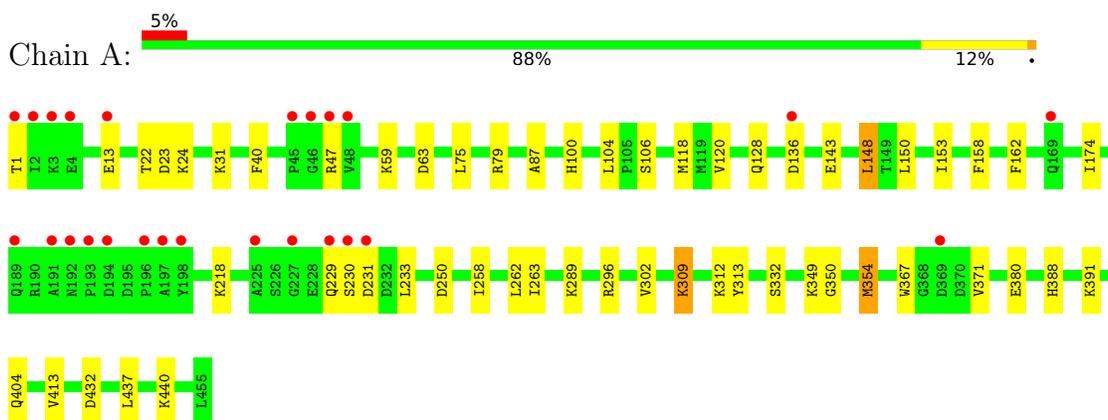
- Molecule 1: Bifunctional P-450/NADPH-P450 reductase
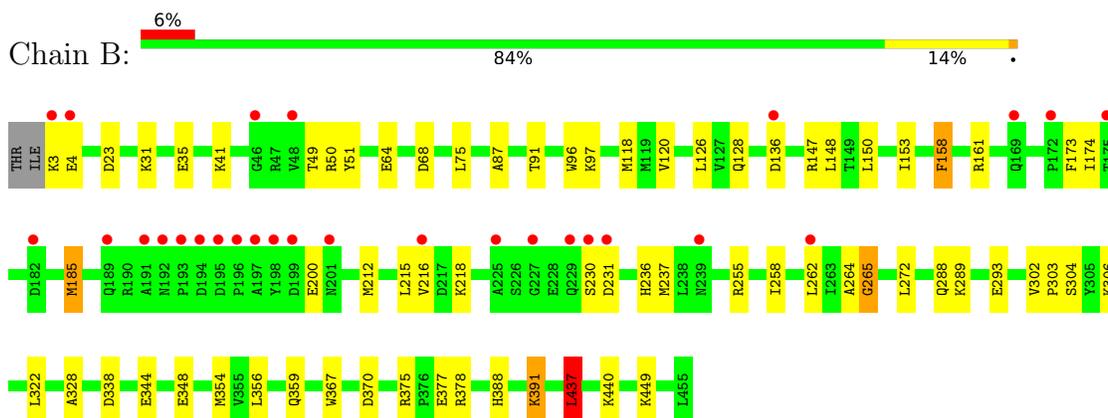
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.99Å 148.89Å 64.82Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	19.99 – 1.50 19.98 – 1.50	Depositor EDS
% Data completeness (in resolution range)	88.5 (19.99-1.50) 88.5 (19.98-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.178 , 0.199 0.176 , 0.197	Depositor DCC
R_{free} test set	839 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å^2)	14.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8715	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MES, GOL, SYN, PEG, 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	1.22	3/3998 (0.1%)	1.04	9/5398 (0.2%)
1	B	1.18	7/3983 (0.2%)	1.07	13/5378 (0.2%)
All	All	1.20	10/7981 (0.1%)	1.05	22/10776 (0.2%)

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLU	CD-OE1	-7.57	1.17	1.25
1	B	64	GLU	CD-OE2	-5.88	1.19	1.25
1	B	367	TRP	CD2-CE2	5.84	1.48	1.41
1	B	348	GLU	CD-OE2	-5.81	1.19	1.25
1	A	40	PHE	CG-CD2	5.35	1.46	1.38
1	B	96	TRP	CD2-CE2	5.32	1.47	1.41
1	B	293	GLU	CD-OE2	5.31	1.31	1.25
1	B	377	GLU	CD-OE1	5.24	1.31	1.25
1	B	304	SER	CB-OG	5.06	1.48	1.42
1	A	380	GLU	C-O	5.03	1.32	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ASP	CB-CG-OD1	7.32	124.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	50	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	161	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	250	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	437	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	147	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	354[A]	MET	CG-SD-CE	5.69	109.31	100.20
1	A	354[B]	MET	CG-SD-CE	5.69	109.31	100.20
1	B	147	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	432	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	378	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	79	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	59[A]	LYS	CD-CE-NZ	5.45	124.24	111.70
1	A	59[B]	LYS	CD-CE-NZ	5.45	124.24	111.70
1	B	237	MET	CG-SD-CE	5.45	108.92	100.20
1	B	158[A]	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	B	158[B]	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	A	63	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	391[A]	LYS	CD-CE-NZ	5.22	123.71	111.70
1	B	391[B]	LYS	CD-CE-NZ	5.22	123.71	111.70
1	A	309	LYS	CD-CE-NZ	5.15	123.56	111.70
1	B	96	TRP	CA-CB-CG	-5.05	104.10	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	265[A]	GLY	Peptide

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	3824	0	3900	60	0
1	B	3808	0	3878	77	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	16	0	16	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	16	11	0
4	A	18	0	24	1	0
4	B	12	0	15	2	0
5	A	7	0	10	6	0
6	B	12	0	12	1	0
7	A	489	0	0	9	0
7	B	427	0	0	14	0
All	All	8715	0	7931	137	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 9.

All (137) 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:150[A]:LEU:HD21	1:B:174:ILE:CD1	1.23	1.66
1:B:150[A]:LEU:CD2	1:B:174:ILE:CD1	1.96	1.43
1:B:158[A]:PHE:CE1	1:B:258:ILE:HG12	1.62	1.34
1:A:289[B]:LYS:CB	1:A:289[B]:LYS:NZ	1.79	1.31
1:B:150[A]:LEU:CD2	1:B:174:ILE:HD13	1.60	1.28
1:A:289[B]:LYS:CB	1:A:289[B]:LYS:HZ3	1.21	1.23
1:B:370:ASP:OD2	1:B:375:ARG:NH1	1.74	1.21
1:B:264:ALA:O	3:B:503[A]:SYN:CAA	1.91	1.18
1:A:289[B]:LYS:NZ	1:A:289[B]:LYS:HB3	0.91	1.15
1:A:22[B]:THR:HG22	1:A:24:LYS:H	1.17	1.10
1:B:212:MET:O	1:B:216[B]:VAL:HG23	1.55	1.07
1:B:150[A]:LEU:CD2	1:B:174:ILE:HD11	1.72	0.97
1:B:158[A]:PHE:HE1	1:B:258:ILE:HG12	1.23	0.95
1:B:150[A]:LEU:HD21	1:B:174:ILE:CG1	1.98	0.92
1:B:440:LYS:HD3	7:B:995:HOH:O	1.70	0.91
1:B:150[A]:LEU:HD21	1:B:174:ILE:HD11	0.91	0.89
1:B:264:ALA:O	3:B:503[A]:SYN:H9	1.72	0.89
1:A:87:ALA:HB1	3:A:502[A]:SYN:H4	1.57	0.87
1:A:22[B]:THR:HG22	1:A:24:LYS:N	1.92	0.83
1:B:118[B]:MET:SD	7:B:799:HOH:O	2.36	0.83
1:A:349:LYS:HG2	5:A:505:PEG:H32	1.59	0.82
1:A:289[B]:LYS:HB3	1:A:289[B]:LYS:HZ2	0.94	0.77
1:B:158[A]:PHE:CE1	1:B:258:ILE:CG1	2.58	0.76
1:B:264:ALA:HB1	3:B:503[A]:SYN:H8	1.66	0.76
1:B:356[A]:LEU:HD23	1:B:359[A]:GLN:HG3	1.67	0.76
1:B:264:ALA:O	3:B:503[A]:SYN:H8	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[B]:THR:CG2	1:A:24:LYS:H	1.96	0.75
1:B:150[A]:LEU:HD23	1:B:174:ILE:HD13	1.66	0.74
1:B:150[A]:LEU:HD22	1:B:174:ILE:HD13	1.66	0.73
1:A:148[B]:LEU:HD11	1:A:413:VAL:HG21	1.69	0.73
1:B:49[A]:THR:CG2	1:B:354[A]:MET:HG2	2.19	0.73
1:B:49[A]:THR:HG21	1:B:354[A]:MET:HG2	1.72	0.72
1:A:289[B]:LYS:HE3	1:A:313:TYR:CZ	2.25	0.71
1:B:288[B]:GLN:OE1	7:B:753:HOH:O	2.08	0.71
1:A:332:SER:HB2	1:A:354[B]:MET:CE	2.21	0.71
1:A:75:LEU:HD21	3:A:502[A]:SYN:H3	1.71	0.70
1:B:23:ASP:OD2	7:B:976:HOH:O	2.10	0.69
1:A:158:PHE:CD1	1:A:258[A]:ILE:HD12	2.28	0.69
1:B:150[A]:LEU:HD23	1:B:174:ILE:CD1	2.18	0.69
1:B:264:ALA:HB1	3:B:503[A]:SYN:H5	1.74	0.69
1:B:185:MET:HE1	1:B:437:LEU:HD23	1.74	0.68
1:B:158[B]:PHE:CZ	1:B:262[B]:LEU:HD21	2.30	0.66
1:A:349:LYS:HE2	5:A:505:PEG:H21	1.77	0.66
1:A:230[A]:SER:OG	1:A:231:ASP:N	2.29	0.64
1:A:263:ILE:HG22	3:A:502[B]:SYN:H6	1.79	0.64
1:A:153[B]:ILE:HG23	1:A:262:LEU:HD23	1.80	0.63
1:A:136:ASP:OD1	1:B:218:LYS:CE	2.47	0.63
1:A:440:LYS:HE2	7:A:970:HOH:O	1.99	0.63
1:A:296[B]:ARG:NH2	7:A:975:HOH:O	2.34	0.61
1:B:236:HIS:CE1	7:B:921:HOH:O	2.53	0.61
1:B:153[B]:ILE:HG13	7:B:809:HOH:O	1.99	0.61
1:A:332:SER:HB2	1:A:354[B]:MET:HE2	1.83	0.59
1:A:153[A]:ILE:HG13	7:A:964:HOH:O	2.01	0.59
1:B:185:MET:CE	1:B:437:LEU:HD23	2.33	0.59
1:A:289[B]:LYS:HZ3	1:A:289[B]:LYS:CA	2.10	0.58
1:A:120:VAL:HG11	1:A:302[A]:VAL:HG13	1.84	0.58
1:B:3:LYS:HG3	1:B:344:GLU:OE2	2.05	0.56
1:B:264:ALA:C	3:B:503[A]:SYN:H8	2.25	0.56
1:B:264:ALA:CB	3:B:503[A]:SYN:H8	2.34	0.56
1:B:388:HIS:ND1	1:B:391[B]:LYS:HE3	2.21	0.56
1:A:75:LEU:HD21	3:A:502[A]:SYN:CAC	2.35	0.55
1:B:4:GLU:OE2	1:B:4:GLU:N	2.36	0.55
1:B:49[A]:THR:HG21	1:B:354[A]:MET:CG	2.35	0.55
1:B:288[B]:GLN:CD	7:B:753:HOH:O	2.45	0.54
1:A:437:LEU:HD23	7:A:1044:HOH:O	2.08	0.54
1:A:100:HIS:HE1	4:A:506:GOL:O2	1.91	0.54
1:A:136:ASP:OD1	1:B:218:LYS:HE3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:CG	5:A:505:PEG:H32	2.37	0.54
1:B:158[B]:PHE:HZ	1:B:262[B]:LEU:HD21	1.72	0.52
1:B:158[A]:PHE:HE1	1:B:258:ILE:CG1	2.10	0.52
1:B:153[A]:ILE:CG2	1:B:262[A]:LEU:HD23	2.40	0.52
1:A:128[A]:GLN:NE2	7:A:961:HOH:O	2.42	0.52
1:B:264:ALA:CA	3:B:503[A]:SYN:H8	2.40	0.52
1:B:158[B]:PHE:CE1	1:B:262[B]:LEU:HD21	2.44	0.51
1:A:309:LYS:O	1:A:312:LYS:HE3	2.11	0.51
1:B:265[A]:GLY:HA3	2:B:502:HEM:C2C	2.47	0.50
1:B:173:PHE:CE2	1:B:262[B]:LEU:HD13	2.46	0.50
1:A:150[B]:LEU:CD1	1:A:162:PHE:CD2	2.95	0.50
1:B:158[A]:PHE:CZ	1:B:258:ILE:HG12	2.36	0.50
1:B:68:ASP:CG	4:B:504:GOL:H32	2.33	0.50
1:B:153[A]:ILE:HG23	1:B:262[A]:LEU:HD23	1.95	0.48
1:B:87:ALA:HB1	3:B:503[A]:SYN:H4	1.96	0.48
1:A:120:VAL:HG11	1:A:302[A]:VAL:CG1	2.43	0.48
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.94	0.48
1:A:23[B]:ASP:HB3	1:A:24:LYS:HG3	1.95	0.47
1:A:349:LYS:HG2	5:A:505:PEG:H21	1.95	0.47
1:B:328:ALA:HB2	3:B:503[B]:SYN:H3	1.97	0.47
1:B:35[A]:GLU:HG3	7:B:1007:HOH:O	2.15	0.46
1:A:118[B]:MET:HE1	7:A:806:HOH:O	2.14	0.46
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.97	0.46
1:B:288[B]:GLN:NE2	1:B:288[B]:GLN:HA	2.31	0.46
1:A:153[B]:ILE:CG2	1:A:262:LEU:HD23	2.46	0.46
1:B:216[B]:VAL:HG11	1:B:255:ARG:HG2	1.97	0.46
1:B:288[B]:GLN:NE2	7:B:753:HOH:O	2.49	0.46
1:A:218:LYS:HE3	1:B:136:ASP:OD2	2.16	0.46
1:A:350:GLY:CA	5:A:505:PEG:H12	2.46	0.45
1:B:153[A]:ILE:HG23	1:B:262[A]:LEU:CD2	2.47	0.45
1:A:100:HIS:NE2	1:A:104[B]:LEU:HD11	2.32	0.44
1:A:350:GLY:HA2	5:A:505:PEG:H12	1.99	0.44
6:B:505:MES:H51	7:B:684:HOH:O	2.18	0.44
1:B:75:LEU:HD21	3:B:503[A]:SYN:H3	1.98	0.44
1:B:272:LEU:HD13	1:B:322:LEU:HG	1.99	0.44
1:A:150[B]:LEU:CD1	1:A:174:ILE:HD11	2.48	0.43
1:B:200:GLU:HA	1:B:200:GLU:OE1	2.16	0.43
1:B:216[B]:VAL:HG11	1:B:255:ARG:CG	2.48	0.43
1:B:303:PRO:HG3	7:B:928:HOH:O	2.18	0.43
1:B:150[A]:LEU:HD21	1:B:174:ILE:HG12	1.91	0.43
1:B:128[A]:GLN:NE2	7:B:938:HOH:O	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LYS:HE3	7:B:763:HOH:O	2.18	0.43
1:A:148[A]:LEU:HD21	1:A:413:VAL:HG21	1.99	0.43
1:B:289[A]:LYS:HG3	7:B:821:HOH:O	2.19	0.42
1:B:150[A]:LEU:CD2	1:B:174:ILE:CG1	2.76	0.42
1:B:173:PHE:HB2	1:B:215:LEU:HD22	2.01	0.42
1:B:354[B]:MET:HE3	1:B:354[B]:MET:HB2	1.75	0.42
1:A:31[A]:LYS:HG3	7:A:747:HOH:O	2.20	0.42
1:A:404[B]:GLN:NE2	7:A:967:HOH:O	2.50	0.42
1:A:106[A]:SER:HB3	1:A:233:LEU:HD23	2.02	0.42
3:A:502[A]:SYN:H1	7:A:1043:HOH:O	2.19	0.42
1:A:87:ALA:HB1	3:A:502[A]:SYN:CAE	2.39	0.42
1:A:388:HIS:HA	1:A:391:LYS:HD3	2.02	0.41
1:A:150[B]:LEU:HG	1:A:174:ILE:CD1	2.51	0.41
1:A:104[B]:LEU:HD23	1:A:104[B]:LEU:HA	1.95	0.41
3:A:502[B]:SYN:H8	3:A:502[B]:SYN:H5	1.79	0.41
1:A:100:HIS:CE1	1:A:104[B]:LEU:HD11	2.56	0.41
1:A:263:ILE:HG21	1:A:263:ILE:HD13	1.83	0.41
1:B:306:LYS:HB2	1:B:306:LYS:HE2	1.37	0.41
1:A:120:VAL:CG1	1:A:302[B]:VAL:CG2	2.98	0.41
1:B:91:THR:CG2	4:B:504:GOL:H2	2.51	0.40
1:B:185:MET:HE2	1:B:437:LEU:HA	2.02	0.40
1:B:97[B]:LYS:HD2	1:B:97[B]:LYS:HA	1.85	0.40
1:B:51:TYR:CE2	1:B:354[B]:MET:HG2	2.56	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	484/455 (106%)	467 (96%)	17 (4%)	0	100	100
1	B	482/455 (106%)	469 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	966/910 (106%)	936 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	427/397 (108%)	421 (99%)	6 (1%)	67	42
1	B	425/397 (107%)	416 (98%)	9 (2%)	53	23
All	All	852/794 (107%)	837 (98%)	15 (2%)	62	30

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	13	GLU
1	A	47	ARG
1	A	148[A]	LEU
1	A	148[B]	LEU
1	A	229	GLN
1	B	31	LYS
1	B	41	LYS
1	B	148	LEU
1	B	185	MET
1	B	230[A]	SER
1	B	230[B]	SER
1	B	231	ASP
1	B	437	LEU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	189	GLN
1	A	206	GLN
1	B	201	ASN
1	B	204	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	SYN	A	502[A]	-	8,8,8	1.61	2 (25%)	9,9,9	1.14	1 (11%)
4	GOL	B	501	-	5,5,5	0.46	0	5,5,5	0.46	0
4	GOL	A	506	-	5,5,5	0.91	0	5,5,5	0.97	0
5	PEG	A	505	-	6,6,6	1.02	0	5,5,5	1.71	2 (40%)
4	GOL	A	503	-	5,5,5	0.56	0	5,5,5	1.79	2 (40%)
6	MES	B	505	-	12,12,12	2.43	1 (8%)	14,16,16	7.11	9 (64%)
2	HEM	B	502	1,7	41,50,50	1.92	7 (17%)	45,82,82	2.54	17 (37%)
4	GOL	B	504	-	5,5,5	1.02	1 (20%)	5,5,5	1.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SYN	B	503[A]	-	8,8,8	1.80	2 (25%)	9,9,9	1.33	1 (11%)
2	HEM	A	501	1,7	41,50,50	1.89	8 (19%)	45,82,82	2.76	20 (44%)
3	SYN	B	503[B]	-	8,8,8	1.53	2 (25%)	9,9,9	0.75	0
4	GOL	A	504	-	5,5,5	0.52	0	5,5,5	1.20	0
3	SYN	A	502[B]	-	8,8,8	1.76	2 (25%)	9,9,9	1.34	3 (33%)

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	SYN	A	502[A]	-	-	0/2/2/2	0/1/1/1
4	GOL	B	501	-	-	3/4/4/4	-
4	GOL	A	506	-	-	0/4/4/4	-
5	PEG	A	505	-	-	4/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
6	MES	B	505	-	-	2/6/14/14	0/1/1/1
2	HEM	B	502	1,7	-	2/12/54/54	-
4	GOL	B	504	-	-	2/4/4/4	-
3	SYN	B	503[A]	-	-	0/2/2/2	0/1/1/1
2	HEM	A	501	1,7	-	1/12/54/54	-
3	SYN	B	503[B]	-	-	2/2/2/2	0/1/1/1
4	GOL	A	504	-	-	2/4/4/4	-
3	SYN	A	502[B]	-	-	0/2/2/2	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	505	MES	C8-S	-8.13	1.65	1.77
2	B	502	HEM	C3D-C2D	5.65	1.48	1.36
2	A	501	HEM	C3D-C2D	5.59	1.48	1.36
2	A	501	HEM	C3C-C2C	-5.25	1.33	1.40
2	B	502	HEM	C3C-C2C	-4.90	1.33	1.40
2	B	502	HEM	FE-NB	4.09	2.17	1.96
2	A	501	HEM	FE-ND	3.63	2.14	1.96
3	A	502[A]	SYN	CAA-CAB	3.57	1.53	1.29
3	B	503[A]	SYN	CAA-CAB	3.52	1.52	1.29
2	B	502	HEM	O2D-CGD	-3.43	1.19	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[B]	SYN	CAA-CAB	3.40	1.51	1.29
3	B	503[A]	SYN	CAH-CAB	-3.38	1.36	1.49
2	B	502	HEM	O2A-CGA	-3.35	1.19	1.30
3	B	503[B]	SYN	CAA-CAB	3.22	1.50	1.29
2	A	501	HEM	CAA-C2A	3.08	1.56	1.52
3	A	502[B]	SYN	CAH-CAB	-3.03	1.37	1.49
2	B	502	HEM	C3C-CAC	2.91	1.53	1.47
2	A	501	HEM	O2D-CGD	-2.86	1.21	1.30
3	A	502[A]	SYN	CAH-CAB	-2.49	1.39	1.49
2	A	501	HEM	O2A-CGA	-2.34	1.22	1.30
3	B	503[B]	SYN	CAH-CAB	-2.34	1.40	1.49
2	B	502	HEM	CAA-C2A	2.26	1.55	1.52
2	A	501	HEM	C4B-NB	-2.16	1.34	1.38
2	A	501	HEM	C4D-ND	-2.09	1.36	1.40
4	B	504	GOL	O3-C3	-2.02	1.33	1.42

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	505	MES	O1S-S-C8	-19.50	83.43	106.92
6	B	505	MES	O3S-S-C8	-10.83	88.25	105.77
6	B	505	MES	O2S-S-C8	-10.30	94.51	106.92
2	A	501	HEM	C4D-ND-C1D	7.75	113.08	105.07
2	B	502	HEM	C4D-ND-C1D	7.68	113.00	105.07
2	A	501	HEM	C1B-NB-C4B	7.23	112.54	105.07
2	B	502	HEM	C1B-NB-C4B	7.15	112.45	105.07
2	A	501	HEM	C4A-C3A-C2A	6.56	111.56	107.00
6	B	505	MES	C5-N4-C3	5.52	121.26	108.83
6	B	505	MES	O3S-S-O1S	4.95	123.36	111.27
2	B	502	HEM	CHD-C1D-ND	4.65	129.48	124.43
2	A	501	HEM	C2B-C1B-NB	-4.27	104.78	109.84
2	A	501	HEM	CMA-C3A-C4A	-4.25	121.94	128.46
2	B	502	HEM	C2B-C1B-NB	-4.18	104.89	109.84
6	B	505	MES	C7-N4-C3	4.12	121.78	111.23
2	A	501	HEM	CHD-C1D-ND	4.03	128.81	124.43
2	A	501	HEM	CHB-C1B-NB	3.83	129.12	124.38
6	B	505	MES	C2-C3-N4	-3.80	104.35	110.10
2	A	501	HEM	CHA-C4D-ND	3.76	129.03	124.38
2	A	501	HEM	C4B-CHC-C1C	3.47	127.14	122.56
2	B	502	HEM	C4B-C3B-C2B	3.36	109.78	107.11
2	A	501	HEM	CAD-C3D-C4D	3.25	130.34	124.66
2	B	502	HEM	O1A-CGA-CBA	-3.03	113.34	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	HEM	CHB-C1B-NB	3.03	128.12	124.38
2	B	502	HEM	C4B-CHC-C1C	3.01	126.53	122.56
2	B	502	HEM	C3D-C4D-ND	-2.96	106.87	110.17
2	B	502	HEM	CMA-C3A-C4A	-2.91	124.00	128.46
2	B	502	HEM	CHC-C4B-C3B	2.82	128.89	124.57
2	A	501	HEM	C3B-C2B-C1B	2.82	108.58	106.49
2	B	502	HEM	C2C-C3C-C4C	2.79	108.84	106.90
2	B	502	HEM	CMC-C2C-C3C	2.74	129.81	124.68
4	A	503	GOL	O3-C3-C2	-2.72	97.17	110.20
2	B	502	HEM	CHA-C4D-ND	2.67	127.68	124.38
2	A	501	HEM	C3D-C4D-ND	-2.64	107.22	110.17
2	A	501	HEM	C2C-C3C-C4C	2.60	108.72	106.90
2	A	501	HEM	C3C-C4C-NC	-2.56	106.11	110.94
3	B	503[A]	SYN	CAG-CAH-CAF	2.54	121.40	117.64
6	B	505	MES	O3S-S-O2S	2.53	117.47	111.27
4	A	503	GOL	O1-C1-C2	-2.53	98.08	110.20
2	B	502	HEM	C3C-C4C-NC	-2.52	106.19	110.94
2	A	501	HEM	C4B-C3B-C2B	2.48	109.09	107.11
2	A	501	HEM	O1D-CGD-CBD	-2.44	115.25	123.08
2	A	501	HEM	C2D-C1D-ND	-2.43	106.97	109.88
2	B	502	HEM	CMD-C2D-C1D	2.42	128.73	125.04
5	A	505	PEG	O2-C3-C4	2.39	120.58	110.07
2	A	501	HEM	CHC-C4B-NB	2.35	126.98	124.43
3	A	502[B]	SYN	CAH-CAB-CAA	-2.25	113.05	125.66
2	A	501	HEM	CHC-C4B-C3B	2.24	128.00	124.57
6	B	505	MES	C7-N4-C5	2.24	116.95	111.23
3	A	502[B]	SYN	CAG-CAH-CAF	2.22	120.92	117.64
2	A	501	HEM	CAD-C3D-C2D	-2.16	123.86	127.88
3	A	502[A]	SYN	CAH-CAB-CAA	-2.14	113.66	125.66
2	B	502	HEM	C2D-C1D-ND	-2.10	107.36	109.88
5	A	505	PEG	O2-C2-C1	2.10	119.29	110.07
3	A	502[B]	SYN	CAE-CAG-CAH	-2.03	118.19	120.65

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	GOL	C1-C2-C3-O3
4	B	501	GOL	O2-C2-C3-O3
4	B	504	GOL	C1-C2-C3-O3
6	B	505	MES	C8-C7-N4-C5
3	B	503[B]	SYN	CAA-CAB-CAH-CAG

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Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O2-C2-C3-O3
5	A	505	PEG	O1-C1-C2-O2
3	B	503[B]	SYN	CAA-CAB-CAH-CAF
4	A	503	GOL	C1-C2-C3-O3
4	A	504	GOL	O1-C1-C2-C3
4	B	501	GOL	O1-C1-C2-C3
5	A	505	PEG	O2-C3-C4-O4
4	B	504	GOL	O2-C2-C3-O3
5	A	505	PEG	C4-C3-O2-C2
5	A	505	PEG	C1-C2-O2-C3
4	A	504	GOL	O1-C1-C2-O2
2	B	502	HEM	CAD-CBD-CGD-O1D
2	B	502	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
6	B	505	MES	C7-C8-S-O1S

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[A]	SYN	5	0
4	A	506	GOL	1	0
5	A	505	PEG	6	0
6	B	505	MES	1	0
2	B	502	HEM	1	0
4	B	504	GOL	2	0
3	B	503[A]	SYN	10	0
3	B	503[B]	SYN	1	0
3	A	502[B]	SYN	2	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 then 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 HEM B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings
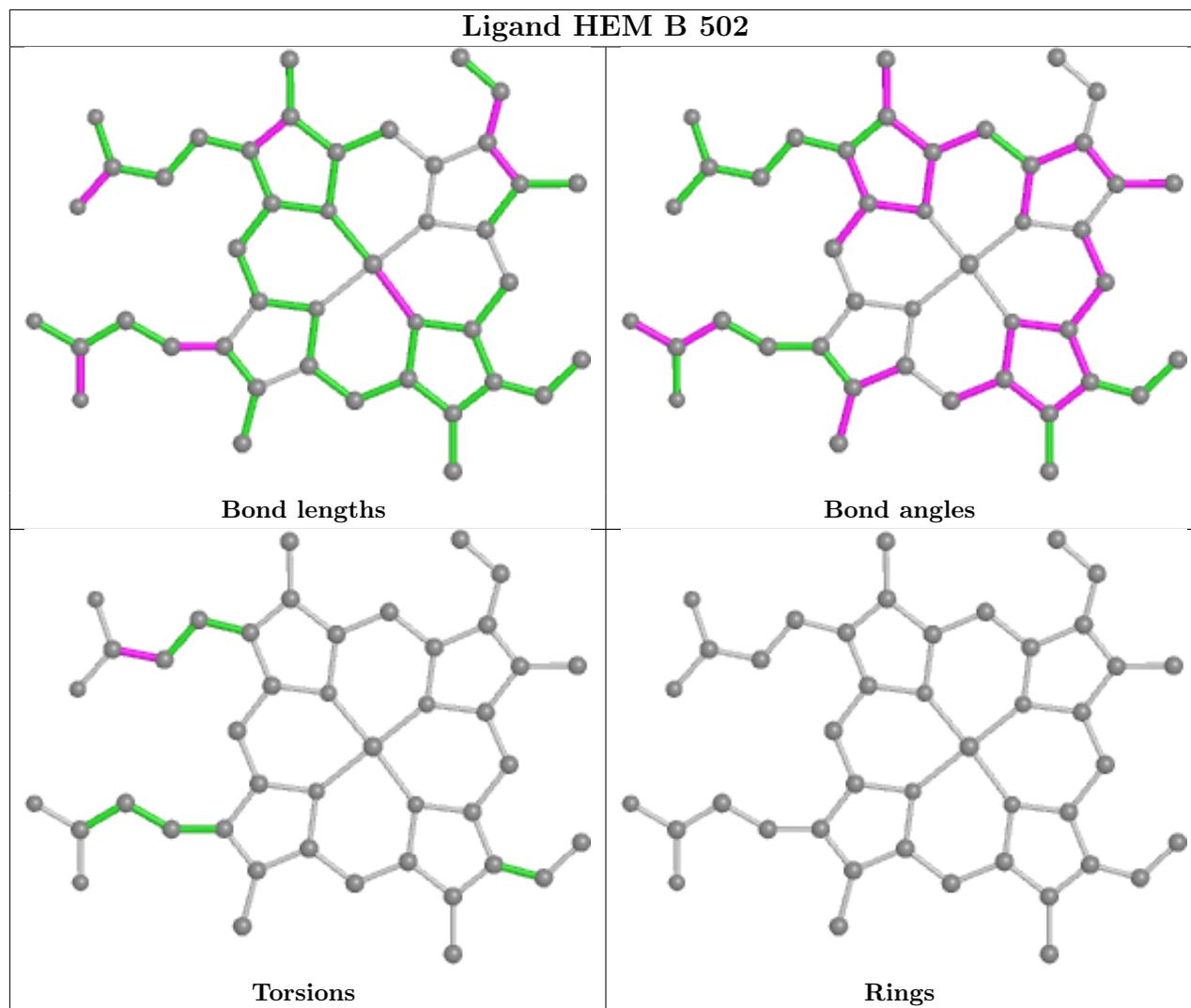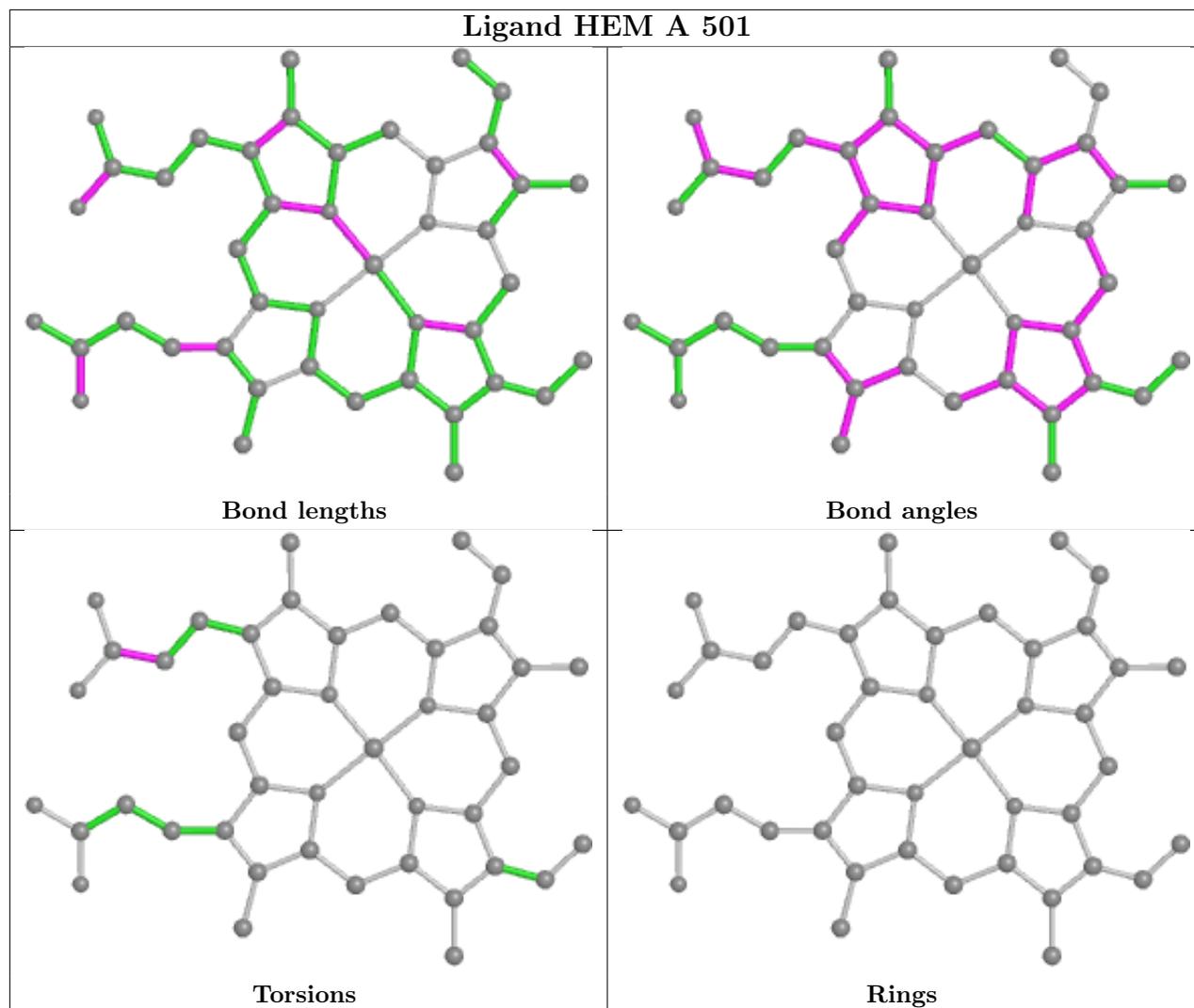
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	455/455 (100%)	0.13	25 (5%)	25	27	8, 15, 33, 95	0
1	B	453/455 (99%)	0.35	28 (6%)	20	22	8, 16, 51, 128	0
All	All	908/910 (99%)	0.24	53 (5%)	23	25	8, 15, 41, 128	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	PRO	9.1
1	B	191	ALA	9.0
1	B	197	ALA	8.0
1	A	1	THR	7.4
1	B	192	ASN	7.0
1	B	225	ALA	5.9
1	B	198	TYR	5.8
1	B	4	GLU	5.7
1	B	194	ASP	5.1
1	B	231	ASP	5.0
1	A	191	ALA	4.7
1	B	199	ASP	4.4
1	A	2	ILE	4.4
1	B	193	PRO	4.4
1	B	195	ASP	3.7
1	A	229	GLN	3.6
1	A	46	GLY	3.5
1	B	46	GLY	3.5
1	B	169	GLN	3.5
1	B	189	GLN	3.4
1	B	227	GLY	3.3
1	A	169	GLN	3.2
1	B	3	LYS	3.2
1	B	229	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	230[A]	SER	3.1
1	A	192	ASN	3.1
1	A	4	GLU	3.1
1	B	182	ASP	3.0
1	B	239	ASN	2.9
1	B	175	THR	2.9
1	A	231	ASP	2.9
1	A	194	ASP	2.9
1	A	48	VAL	2.8
1	A	3	LYS	2.8
1	A	13	GLU	2.7
1	A	45	PRO	2.7
1	A	227	GLY	2.7
1	A	136	ASP	2.7
1	B	136	ASP	2.6
1	A	197	ALA	2.5
1	A	369	ASP	2.5
1	A	196	PRO	2.4
1	B	262[A]	LEU	2.4
1	A	225	ALA	2.4
1	B	216[A]	VAL	2.3
1	B	230[A]	SER	2.3
1	A	193	PRO	2.3
1	A	47	ARG	2.2
1	A	189	GLN	2.2
1	B	201	ASN	2.2
1	B	48	VAL	2.1
1	A	198	TYR	2.1
1	B	172	PRO	2.1

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 monosaccharides 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($\mathring{A}^2$)	Q<0.9
6	MES	B	505	12/12	0.66	0.21	40,57,94,99	0
5	PEG	A	505	7/7	0.78	0.22	35,35,41,42	0
4	GOL	B	504	6/6	0.84	0.20	29,42,56,58	0
3	SYN	A	502[B]	8/8	0.86	0.18	17,22,24,28	8
3	SYN	A	502[A]	8/8	0.86	0.18	17,22,24,28	8
3	SYN	B	503[B]	8/8	0.88	0.19	21,23,25,30	8
3	SYN	B	503[A]	8/8	0.88	0.19	21,23,25,30	8
4	GOL	A	506	6/6	0.90	0.10	22,26,29,33	0
4	GOL	A	503	6/6	0.91	0.16	23,39,41,42	0
4	GOL	A	504	6/6	0.93	0.12	19,37,45,51	0
4	GOL	B	501	6/6	0.96	0.12	19,41,44,61	0
2	HEM	B	502	43/43	0.98	0.08	7,9,12,19	0
2	HEM	A	501	43/43	0.98	0.07	5,8,12,22	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 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 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.