



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:07 AM EST

PDB ID : 6DPR
Title : Mapping the binding trajectory of a suicide inhibitor in human indoleamine 2,3-dioxygenase 1
Authors : Pham, K.N.; Yeh, S.R.
Deposited on : 2018-06-09
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

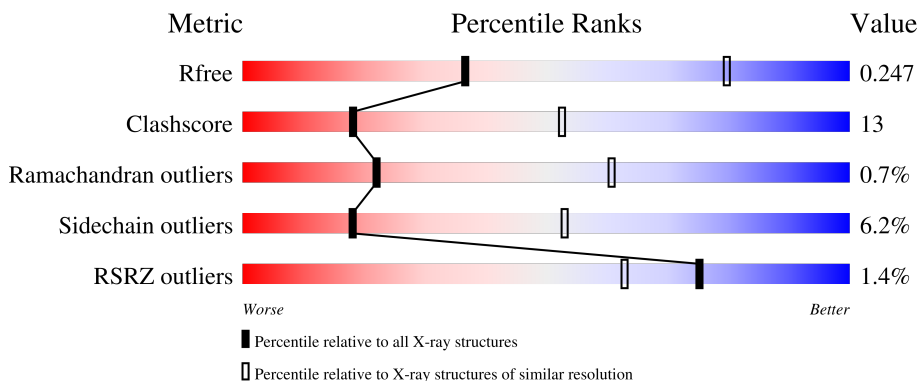
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	424	 59% 22% 16%
1	B	424	 65% 21% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	504	-	-	-	X
4	EDO	A	505	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5969 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
			Total	C	N	O	S			
1	A	358	2836	1820	488	510	18	0	0	0
1	B	371	2950	1898	503	532	17	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P14902
A	404	LYS	-	expression tag	UNP P14902
A	405	GLY	-	expression tag	UNP P14902
A	406	GLU	-	expression tag	UNP P14902
A	407	LEU	-	expression tag	UNP P14902
A	408	ASN	-	expression tag	UNP P14902
A	409	SER	-	expression tag	UNP P14902
A	410	LYS	-	expression tag	UNP P14902
A	411	LEU	-	expression tag	UNP P14902
A	412	GLU	-	expression tag	UNP P14902
A	413	GLY	-	expression tag	UNP P14902
A	414	LYS	-	expression tag	UNP P14902
A	415	PRO	-	expression tag	UNP P14902
A	416	ILE	-	expression tag	UNP P14902
A	417	PRO	-	expression tag	UNP P14902
A	418	ASN	-	expression tag	UNP P14902
A	419	PRO	-	expression tag	UNP P14902
A	420	LEU	-	expression tag	UNP P14902
A	421	LEU	-	expression tag	UNP P14902
A	422	GLY	-	expression tag	UNP P14902
A	423	LEU	-	expression tag	UNP P14902
A	424	ASP	-	expression tag	UNP P14902
A	425	SER	-	expression tag	UNP P14902
A	426	THR	-	expression tag	UNP P14902
A	427	ARG	-	expression tag	UNP P14902

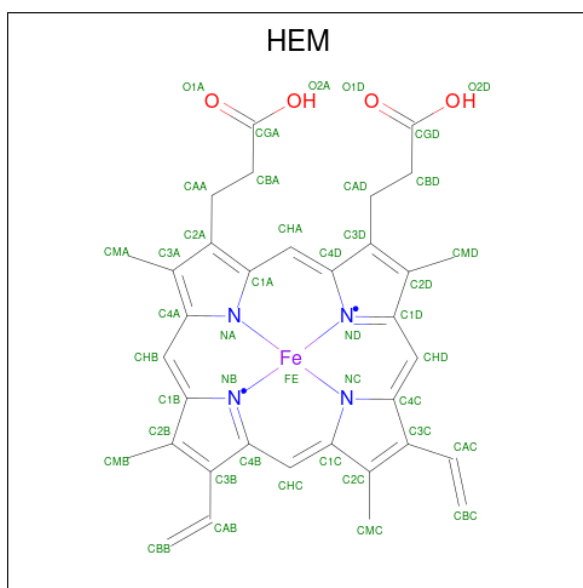
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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	THR	-	expression tag	UNP P14902
A	429	GLY	-	expression tag	UNP P14902
A	430	HIS	-	expression tag	UNP P14902
A	431	HIS	-	expression tag	UNP P14902
A	432	HIS	-	expression tag	UNP P14902
A	433	HIS	-	expression tag	UNP P14902
A	434	HIS	-	expression tag	UNP P14902
A	435	HIS	-	expression tag	UNP P14902
B	12	MET	-	initiating methionine	UNP P14902
B	404	LYS	-	expression tag	UNP P14902
B	405	GLY	-	expression tag	UNP P14902
B	406	GLU	-	expression tag	UNP P14902
B	407	LEU	-	expression tag	UNP P14902
B	408	ASN	-	expression tag	UNP P14902
B	409	SER	-	expression tag	UNP P14902
B	410	LYS	-	expression tag	UNP P14902
B	411	LEU	-	expression tag	UNP P14902
B	412	GLU	-	expression tag	UNP P14902
B	413	GLY	-	expression tag	UNP P14902
B	414	LYS	-	expression tag	UNP P14902
B	415	PRO	-	expression tag	UNP P14902
B	416	ILE	-	expression tag	UNP P14902
B	417	PRO	-	expression tag	UNP P14902
B	418	ASN	-	expression tag	UNP P14902
B	419	PRO	-	expression tag	UNP P14902
B	420	LEU	-	expression tag	UNP P14902
B	421	LEU	-	expression tag	UNP P14902
B	422	GLY	-	expression tag	UNP P14902
B	423	LEU	-	expression tag	UNP P14902
B	424	ASP	-	expression tag	UNP P14902
B	425	SER	-	expression tag	UNP P14902
B	426	THR	-	expression tag	UNP P14902
B	427	ARG	-	expression tag	UNP P14902
B	428	THR	-	expression tag	UNP P14902
B	429	GLY	-	expression tag	UNP P14902
B	430	HIS	-	expression tag	UNP P14902
B	431	HIS	-	expression tag	UNP P14902
B	432	HIS	-	expression tag	UNP P14902
B	433	HIS	-	expression tag	UNP P14902
B	434	HIS	-	expression tag	UNP P14902
B	435	HIS	-	expression tag	UNP P14902

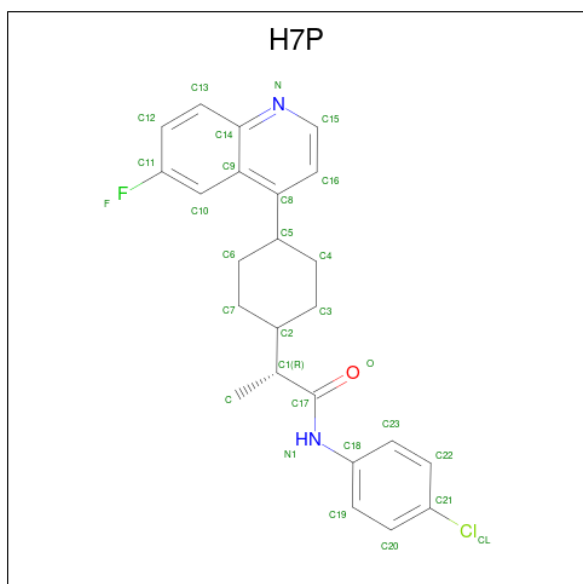
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 3 is (2R)-N-(4-chlorophenyl)-2-[cis-4-(6-fluoroquinolin-4-yl)cyclohexyl]propanamide (three-letter code: H7P) (formula: C₂₄H₂₄ClFN₂O).



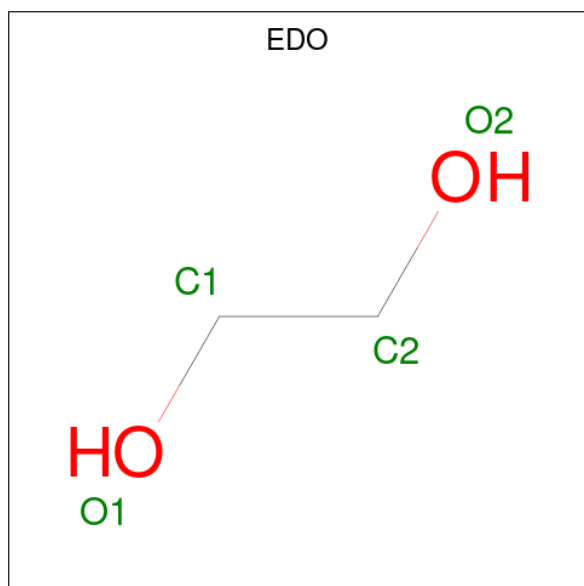
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
3	A	1	29	24	1	1	2	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
3	B	1	29	24	1	1	2	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	4	2	0	0
4	A	1	4	2	0	0
4	A	1	4	2	0	0
4	A	1	4	2	0	0
4	A	1	4	2	0	0
4	B	1	4	2	0	0

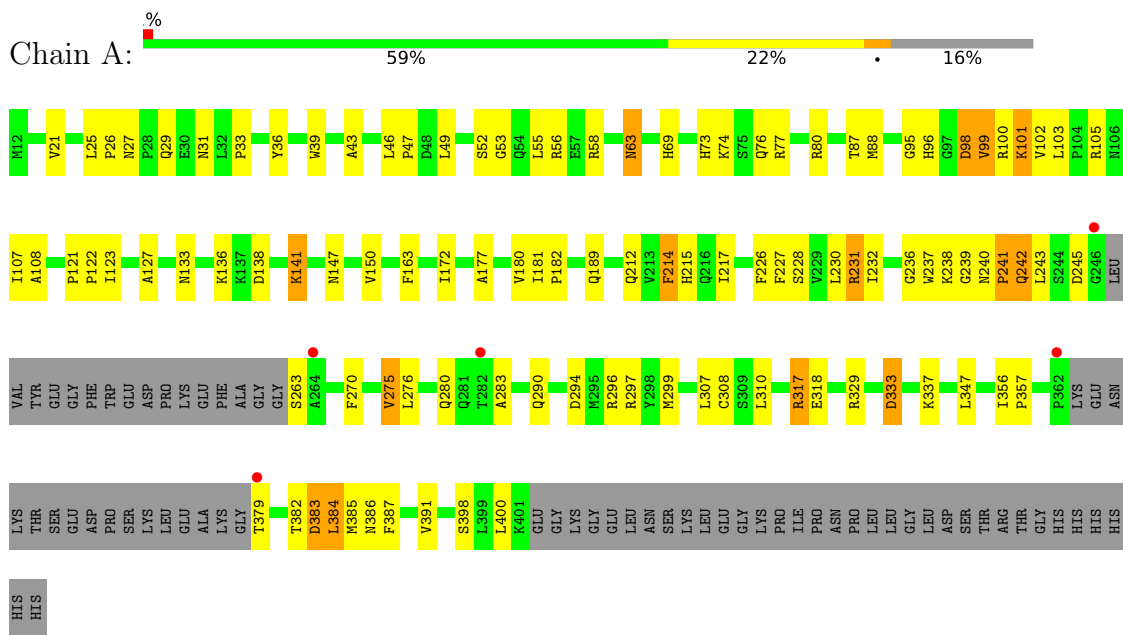
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	38	38	38	0	0
5	B	20	20	20	0	0

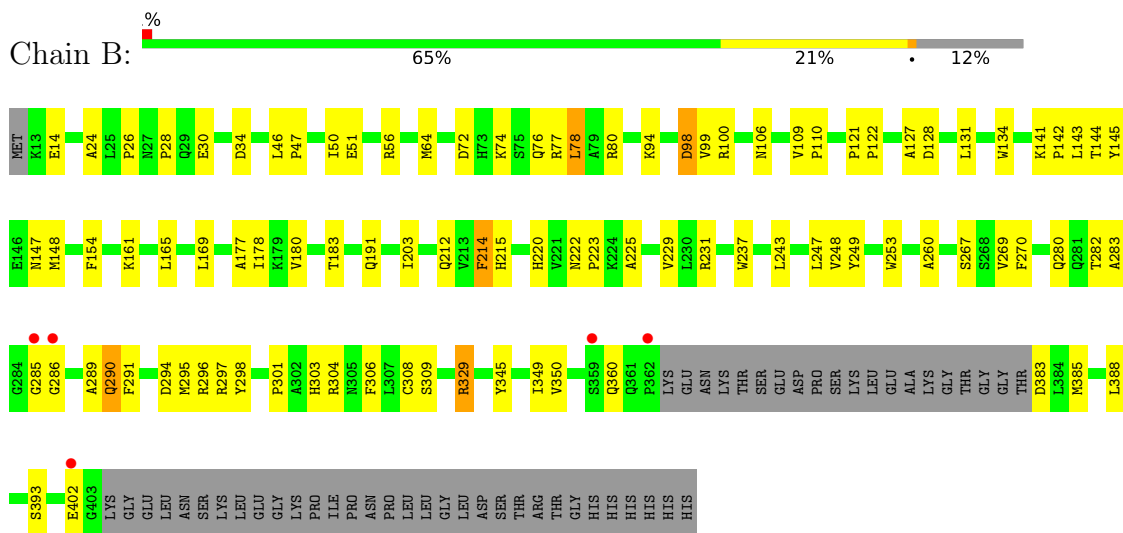
3 Residue-property plots i

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	85.53Å 97.23Å 128.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 3.20 29.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.50-3.20) 100.0 (29.50-3.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.196 , 0.242 0.204 , 0.247	Depositor DCC
R_{free} test set	906 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5969	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: H7P, EDO, 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	0.26	0/2898	0.45	0/3917
1	B	0.26	0/3019	0.44	0/4083
All	All	0.26	0/5917	0.45	0/8000

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PRO	Peptide
1	A	231	ARG	Sidechain
1	A	297	ARG	Sidechain
1	A	58	ARG	Sidechain
1	B	100	ARG	Sidechain
1	B	231	ARG	Sidechain
1	B	285	GLY	Peptide
1	B	297	ARG	Sidechain
1	B	329	ARG	Sidechain

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	2836	0	2870	86	0
1	B	2950	0	2964	63	0
2	A	43	0	30	7	0
3	A	29	0	0	6	0
3	B	29	0	0	3	0
4	A	20	0	30	1	0
4	B	4	0	6	0	0
5	A	38	0	0	9	0
5	B	20	0	0	3	0
All	All	5969	0	5900	158	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 13.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLY:O	1:A:240:ASN:ND2	1.65	1.26
1:A:239:GLY:C	1:A:240:ASN:HD22	1.47	1.15
1:A:102:VAL:HG23	1:A:241:PRO:O	1.56	1.03
1:A:108:ALA:CB	1:A:243:LEU:HD21	1.90	1.01
1:A:80:ARG:NH1	1:A:121:PRO:O	1.99	0.94
1:A:133:ASN:ND2	1:A:150:VAL:HB	1.88	0.88
1:A:263:SER:HA	3:A:502:H7P:F	1.65	0.87
1:A:108:ALA:HB2	1:A:243:LEU:HD21	1.59	0.82
2:A:501:HEM:O1A	5:A:601:HOH:O	1.99	0.80
3:A:502:H7P:C19	3:A:502:H7P:O	2.33	0.76
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.65	0.76
1:A:99:VAL:HG21	5:A:634:HOH:O	1.86	0.76
1:A:56:ARG:NH2	1:A:98:ASP:O	2.22	0.73
2:A:501:HEM:HMB1	2:A:501:HEM:HBB2	1.70	0.73
1:A:101:LYS:N	1:A:101:LYS:HE2	2.03	0.72
1:A:383:ASP:O	1:A:386:ASN:HB2	1.91	0.69
1:A:133:ASN:HD21	1:A:150:VAL:HB	1.54	0.69
1:A:63:ASN:OD1	1:A:63:ASN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:HG21	1:A:242:GLN:O	1.92	0.69
1:A:102:VAL:HG21	1:A:242:GLN:C	2.13	0.68
1:A:108:ALA:HB1	1:A:243:LEU:HD21	1.75	0.68
1:A:99:VAL:CG2	1:A:99:VAL:O	2.43	0.67
1:B:109:VAL:HB	1:B:110:PRO:HD3	1.77	0.67
1:A:215:HIS:ND1	5:A:602:HOH:O	2.28	0.65
1:A:102:VAL:CG2	1:A:241:PRO:O	2.39	0.64
1:B:161:LYS:O	1:B:165:LEU:HB2	1.98	0.63
1:A:356:ILE:HB	1:A:357:PRO:CD	2.29	0.63
1:A:133:ASN:ND2	1:A:133:ASN:O	2.32	0.63
3:A:502:H7P:C4	5:A:628:HOH:O	2.47	0.63
1:B:212:GLN:OE1	5:B:601:HOH:O	2.16	0.62
1:A:382:THR:CG2	1:A:385:MET:HG2	2.30	0.62
1:B:148:MET:SD	1:B:169:LEU:HD21	2.40	0.61
1:A:239:GLY:C	1:A:240:ASN:ND2	2.29	0.61
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.31	0.61
3:A:502:H7P:C10	5:A:607:HOH:O	2.48	0.61
1:A:105:ARG:HA	1:A:108:ALA:HB3	1.82	0.60
1:B:329:ARG:HD2	1:B:402:GLU:HA	1.83	0.60
1:A:384:LEU:HD11	2:A:501:HEM:HMA3	1.83	0.60
1:A:307:LEU:O	1:A:310:LEU:HB2	2.01	0.60
1:A:46:LEU:N	1:A:47:PRO:CD	2.65	0.59
1:B:178:ILE:HG13	5:B:612:HOH:O	2.02	0.59
1:B:77:ARG:NH2	1:B:127:ALA:O	2.36	0.59
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.33	0.59
1:B:345:TYR:O	1:B:349:ILE:HG12	2.03	0.59
1:A:77:ARG:NH2	1:A:127:ALA:O	2.35	0.58
1:B:26:PRO:O	1:B:74:LYS:NZ	2.33	0.58
1:A:317:ARG:NH1	1:A:398:SER:O	2.37	0.57
1:A:177:ALA:O	1:A:180:VAL:HG22	2.05	0.57
1:B:109:VAL:HB	1:B:110:PRO:CD	2.36	0.55
1:A:384:LEU:C	1:A:384:LEU:CD2	2.75	0.55
1:B:295:MET:HA	1:B:295:MET:CE	2.37	0.54
1:A:237:TRP:HB2	3:A:502:H7P:C20	2.38	0.54
1:A:400:LEU:O	1:A:400:LEU:HG	2.08	0.54
1:B:122:PRO:HB2	1:B:249:TYR:CE2	2.43	0.54
1:A:238:LYS:HE2	5:A:622:HOH:O	2.07	0.53
1:A:227:PHE:CE1	1:A:231:ARG:NH1	2.75	0.53
1:A:329:ARG:O	1:A:333:ASP:HB2	2.09	0.53
1:B:46:LEU:N	1:B:47:PRO:HD2	2.24	0.53
1:A:87:THR:HG23	1:A:103:LEU:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ALA:O	1:B:229:VAL:HB	2.10	0.52
1:B:385:MET:O	1:B:388:LEU:N	2.42	0.52
1:B:80:ARG:NH2	1:B:128:ASP:OD2	2.42	0.52
1:B:329:ARG:HH11	1:B:402:GLU:HA	1.74	0.52
1:A:95:GLY:O	1:A:96:HIS:ND1	2.43	0.52
1:B:145:TYR:CE2	1:B:220:HIS:CE1	2.97	0.52
1:A:98:ASP:OD1	1:A:98:ASP:N	2.29	0.51
1:B:72:ASP:O	1:B:76:GLN:HG3	2.11	0.51
1:A:227:PHE:O	1:A:231:ARG:HG2	2.10	0.51
1:A:290:GLN:O	1:A:294:ASP:OD1	2.29	0.51
1:A:181:ILE:N	1:A:182:PRO:CD	2.74	0.50
1:A:88:MET:HE2	5:A:604:HOH:O	2.11	0.50
1:A:87:THR:HG23	1:A:103:LEU:HD11	1.94	0.50
1:A:108:ALA:HB1	1:A:243:LEU:CD2	2.42	0.50
1:B:222:ASN:ND2	1:B:223:PRO:HD2	2.27	0.50
1:B:56:ARG:NH2	1:B:98:ASP:O	2.44	0.49
1:A:101:LYS:HE2	1:A:101:LYS:CA	2.42	0.49
1:A:275:VAL:O	4:A:506:EDO:H21	2.13	0.49
1:A:356:ILE:CB	1:A:357:PRO:CD	2.89	0.49
1:B:141:LYS:HB3	1:B:142:PRO:HD2	1.93	0.49
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.93	0.49
1:B:180:VAL:HG21	1:B:203:ILE:HG13	1.95	0.49
1:B:28:PRO:HG2	1:B:134:TRP:O	2.13	0.48
1:B:290:GLN:OE1	1:B:290:GLN:HA	2.12	0.48
1:A:99:VAL:O	1:A:99:VAL:HG23	2.13	0.48
1:B:147:ASN:CG	1:B:147:ASN:O	2.52	0.48
1:A:214:PHE:O	1:A:217:ILE:HG22	2.13	0.48
1:B:99:VAL:HG23	1:B:99:VAL:O	2.13	0.48
1:B:269:VAL:HG12	3:B:501:H7P:F	2.04	0.48
1:A:26:PRO:O	1:A:74:LYS:NZ	2.44	0.47
1:A:46:LEU:H	1:A:47:PRO:CD	2.27	0.47
1:A:99:VAL:O	1:A:99:VAL:HG22	2.14	0.47
1:A:387:PHE:O	1:A:391:VAL:HG23	2.15	0.47
1:B:80:ARG:NH1	1:B:121:PRO:O	2.37	0.47
1:B:215:HIS:HA	1:B:345:TYR:OH	2.15	0.47
1:B:269:VAL:CG1	3:B:501:H7P:F	2.52	0.47
1:A:382:THR:HG21	1:A:385:MET:HG2	1.97	0.47
1:B:47:PRO:O	1:B:51:GLU:HG2	2.14	0.46
1:B:50:ILE:O	1:B:94:LYS:HE3	2.15	0.46
1:A:29:GLN:NE2	5:A:603:HOH:O	2.48	0.46
1:A:46:LEU:N	1:A:47:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:HB	1:A:242:GLN:HB2	1.97	0.46
1:B:47:PRO:HA	1:B:154:PHE:O	2.16	0.45
1:B:280:GLN:HB3	1:B:283:ALA:HB3	1.99	0.45
1:B:350:VAL:HG12	1:B:385:MET:HE2	1.99	0.45
1:B:30:GLU:O	1:B:78:LEU:HD11	2.17	0.45
1:A:133:ASN:HD22	1:A:150:VAL:HB	1.73	0.45
1:B:212:GLN:O	1:B:215:HIS:HB2	2.16	0.45
1:B:267:SER:HB3	1:B:270:PHE:HB2	1.99	0.45
1:B:24:ALA:HA	1:B:131:LEU:HD22	1.98	0.45
1:A:270:PHE:CD2	2:A:501:HEM:HMD3	2.52	0.44
1:B:180:VAL:O	1:B:183:THR:N	2.49	0.44
1:A:73:HIS:O	1:A:76:GLN:N	2.51	0.44
1:A:98:ASP:C	1:A:100:ARG:H	2.20	0.44
1:A:384:LEU:C	1:A:384:LEU:HD22	2.38	0.44
1:B:64:MET:HG3	1:B:106:ASN:HA	1.98	0.44
1:B:301:PRO:HA	1:B:304:ARG:NH2	2.32	0.44
1:A:43:ALA:O	1:A:46:LEU:HB2	2.17	0.44
1:B:280:GLN:HB3	1:B:283:ALA:CB	2.48	0.44
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.84	0.43
1:B:214:PHE:O	1:B:214:PHE:CD1	2.70	0.43
1:B:260:ALA:HB3	1:B:298:TYR:CE2	2.53	0.43
1:A:21:VAL:HG23	1:A:172:ILE:HG12	1.99	0.43
1:A:49:LEU:HB3	1:A:55:LEU:HB2	1.99	0.43
1:A:138:ASP:OD2	1:A:141:LYS:HG3	2.18	0.43
1:B:286:GLY:HA2	1:B:289:ALA:HB3	2.00	0.43
1:B:122:PRO:HG3	1:B:253:TRP:HZ3	1.83	0.43
1:B:14:GLU:HA	1:B:14:GLU:OE1	2.18	0.43
1:A:136:LYS:HA	1:A:147:ASN:O	2.18	0.43
1:A:356:ILE:HB	1:A:357:PRO:HD2	2.00	0.42
1:A:384:LEU:O	1:A:387:PHE:HB3	2.18	0.42
1:A:296:ARG:HA	1:A:299:MET:SD	2.59	0.42
1:A:36:TYR:CD1	1:A:39:TRP:CZ3	3.08	0.42
1:A:25:LEU:HA	1:A:26:PRO:HD3	1.89	0.42
1:B:109:VAL:CB	1:B:110:PRO:HD3	2.46	0.42
3:B:501:H7P:O	3:B:501:H7P:C23	2.68	0.42
1:B:141:LYS:HB3	1:B:142:PRO:CD	2.49	0.42
1:B:282:THR:HG21	1:B:296:ARG:HH21	1.85	0.42
1:A:102:VAL:HB	1:A:242:GLN:CB	2.50	0.42
1:A:237:TRP:HB2	3:A:502:H7P:C19	2.50	0.42
1:B:291:PHE:O	1:B:295:MET:HG2	2.20	0.42
1:B:296:ARG:O	1:B:304:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ASP:OD1	1:B:98:ASP:N	2.51	0.41
1:A:212:GLN:O	1:A:215:HIS:HB2	2.20	0.41
1:A:52:SER:OG	1:A:53:GLY:N	2.54	0.41
1:A:69:HIS:CD2	5:A:620:HOH:O	2.73	0.41
1:A:230:LEU:HD12	1:A:230:LEU:O	2.21	0.41
1:B:109:VAL:CB	1:B:110:PRO:CD	2.96	0.41
1:A:108:ALA:CA	1:A:243:LEU:HD21	2.48	0.41
1:A:163:PHE:CE2	1:A:226:PHE:CE1	3.09	0.41
1:B:177:ALA:O	1:B:178:ILE:C	2.59	0.40
1:B:303:HIS:O	1:B:306:PHE:N	2.54	0.40
1:A:280:GLN:HB3	1:A:283:ALA:HB3	2.04	0.40
1:A:400:LEU:O	1:A:400:LEU:CG	2.69	0.40
1:B:214:PHE:O	1:B:214:PHE:HD1	2.04	0.40
1:B:243:LEU:HD23	1:B:247:LEU:HB2	2.02	0.40
1:B:134:TRP:CZ3	1:B:143:LEU:HD21	2.56	0.40
1:B:178:ILE:CG1	5:B:612:HOH:O	2.67	0.40
1:A:102:VAL:HG21	1:A:242:GLN:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	352/424 (83%)	317 (90%)	31 (9%)	4 (1%)	14 51
1	B	367/424 (87%)	332 (90%)	34 (9%)	1 (0%)	41 74
All	All	719/848 (85%)	649 (90%)	65 (9%)	5 (1%)	22 61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLY

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Mol	Chain	Res	Type
1	B	98	ASP
1	A	123	ILE
1	A	33	PRO
1	A	241	PRO

5.3.2 Protein sidechains [i](#)

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	312/367 (85%)	287 (92%)	25 (8%)	12	42
1	B	322/367 (88%)	308 (96%)	14 (4%)	29	64
All	All	634/734 (86%)	595 (94%)	39 (6%)	18	53

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	31	ASN
1	A	63	ASN
1	A	98	ASP
1	A	99	VAL
1	A	101	LYS
1	A	107	ILE
1	A	141	LYS
1	A	189	GLN
1	A	214	PHE
1	A	228	SER
1	A	232	ILE
1	A	242	GLN
1	A	245	ASP
1	A	275	VAL
1	A	276	LEU
1	A	308	CYS
1	A	317	ARG
1	A	318	GLU

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Mol	Chain	Res	Type
1	A	333	ASP
1	A	337	LYS
1	A	347	LEU
1	A	379	THR
1	A	383	ASP
1	A	384	LEU
1	B	34	ASP
1	B	78	LEU
1	B	144	THR
1	B	191	GLN
1	B	214	PHE
1	B	237	TRP
1	B	248	VAL
1	B	290	GLN
1	B	294	ASP
1	B	308	CYS
1	B	309	SER
1	B	360	GLN
1	B	383	ASP
1	B	393	SER

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	240	ASN
1	A	266	GLN
1	B	140	ASN
1	B	222	ASN
1	B	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	H7P	B	501	-	32,32,32	1.48	5 (15%)	45,45,45	1.54	6 (13%)
3	H7P	A	502	-	32,32,32	1.43	5 (15%)	45,45,45	1.80	9 (20%)
4	EDO	A	503	-	3,3,3	0.53	0	2,2,2	0.16	0
4	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.28	0
2	HEM	A	501	1	41,50,50	1.31	5 (12%)	45,82,82	1.79	7 (15%)
4	EDO	A	505	-	3,3,3	0.51	0	2,2,2	0.21	0
4	EDO	A	507	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.28	0
4	EDO	B	502	-	3,3,3	0.51	0	2,2,2	0.22	0

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	H7P	B	501	-	-	4/16/26/26	0/4/4/4
3	H7P	A	502	-	-	10/16/26/26	0/4/4/4
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
2	HEM	A	501	1	-	3/12/54/54	-
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	B	502	-	-	1/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	H7P	C8-C9	4.05	1.50	1.43
3	B	501	H7P	C8-C9	3.98	1.49	1.43
3	B	501	H7P	C9-C14	3.90	1.48	1.42
3	A	502	H7P	C9-C14	3.70	1.48	1.42
2	A	501	HEM	C1B-NB	-3.44	1.34	1.40
2	A	501	HEM	C4D-ND	-2.95	1.35	1.40
2	A	501	HEM	FE-NB	2.80	2.10	1.96
3	B	501	H7P	C18-N1	-2.76	1.36	1.41
3	B	501	H7P	C10-C11	2.60	1.40	1.36
3	B	501	H7P	C21-CL	2.60	1.80	1.74
3	A	502	H7P	C21-CL	2.58	1.80	1.74
3	A	502	H7P	C18-N1	-2.46	1.36	1.41
3	A	502	H7P	C10-C11	2.44	1.40	1.36
2	A	501	HEM	CHB-C1B	2.13	1.40	1.35
2	A	501	HEM	C4B-NB	-2.00	1.34	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H7P	C1-C17-N1	5.62	122.97	114.38
2	A	501	HEM	CHC-C4B-NB	5.29	130.18	124.43
3	B	501	H7P	C5-C8-C9	5.09	125.99	120.67
2	A	501	HEM	CHD-C1D-ND	4.42	129.24	124.43
2	A	501	HEM	C1B-NB-C4B	4.17	109.38	105.07
3	A	502	H7P	C2-C1-C17	3.99	117.50	110.42
3	B	501	H7P	C3-C2-C7	3.64	115.86	109.44
3	B	501	H7P	C16-C8-C5	-3.58	116.85	120.55
3	A	502	H7P	C18-N1-C17	-3.52	118.98	127.40
3	A	502	H7P	C15-N-C14	3.41	122.22	116.93
3	A	502	H7P	C7-C6-C5	3.40	116.91	110.52
3	B	501	H7P	C15-N-C14	3.33	122.08	116.93
2	A	501	HEM	CHB-C1B-NB	3.15	128.27	124.38
2	A	501	HEM	CHD-C1D-C2D	-3.08	120.17	124.98
3	A	502	H7P	C9-C14-N	-2.97	119.67	122.83
3	A	502	H7P	C5-C8-C9	2.82	123.61	120.67
3	A	502	H7P	O-C17-C1	-2.80	115.97	121.02
2	A	501	HEM	CHA-C4D-ND	2.79	127.83	124.38
3	B	501	H7P	C9-C14-N	-2.42	120.25	122.83
2	A	501	HEM	CAD-C3D-C4D	2.26	128.60	124.66
3	A	502	H7P	C4-C5-C8	-2.06	108.20	112.28
3	B	501	H7P	C6-C7-C2	2.05	116.85	112.24

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	H7P	C6-C5-C8-C9
3	A	502	H7P	C17-C1-C2-C3
3	A	502	H7P	C-C1-C2-C3
3	A	502	H7P	C2-C1-C17-N1
3	A	502	H7P	C2-C1-C17-O
3	B	501	H7P	C4-C5-C8-C9
3	A	502	H7P	C6-C5-C8-C16
3	B	501	H7P	C6-C5-C8-C16
3	B	501	H7P	C4-C5-C8-C16
3	A	502	H7P	C4-C5-C8-C16
4	A	506	EDO	O1-C1-C2-O2
2	A	501	HEM	C2A-CAA-CBA-CGA
4	A	505	EDO	O1-C1-C2-O2
3	A	502	H7P	C4-C5-C8-C9
3	A	502	H7P	C17-C1-C2-C7
4	A	507	EDO	O1-C1-C2-O2
3	A	502	H7P	C-C1-C2-C7
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O2A
3	B	501	H7P	C-C1-C17-O
4	B	502	EDO	O1-C1-C2-O2

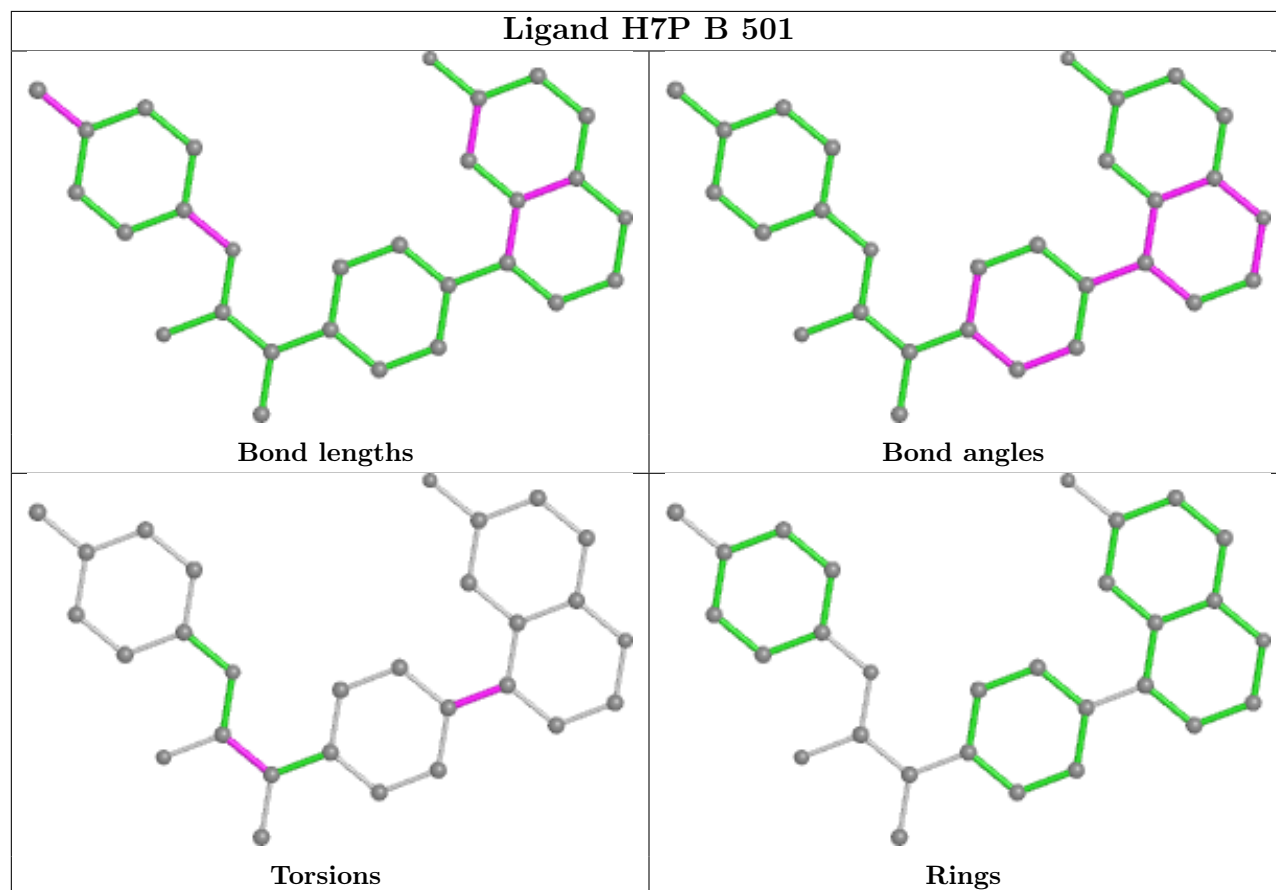
There are no ring outliers.

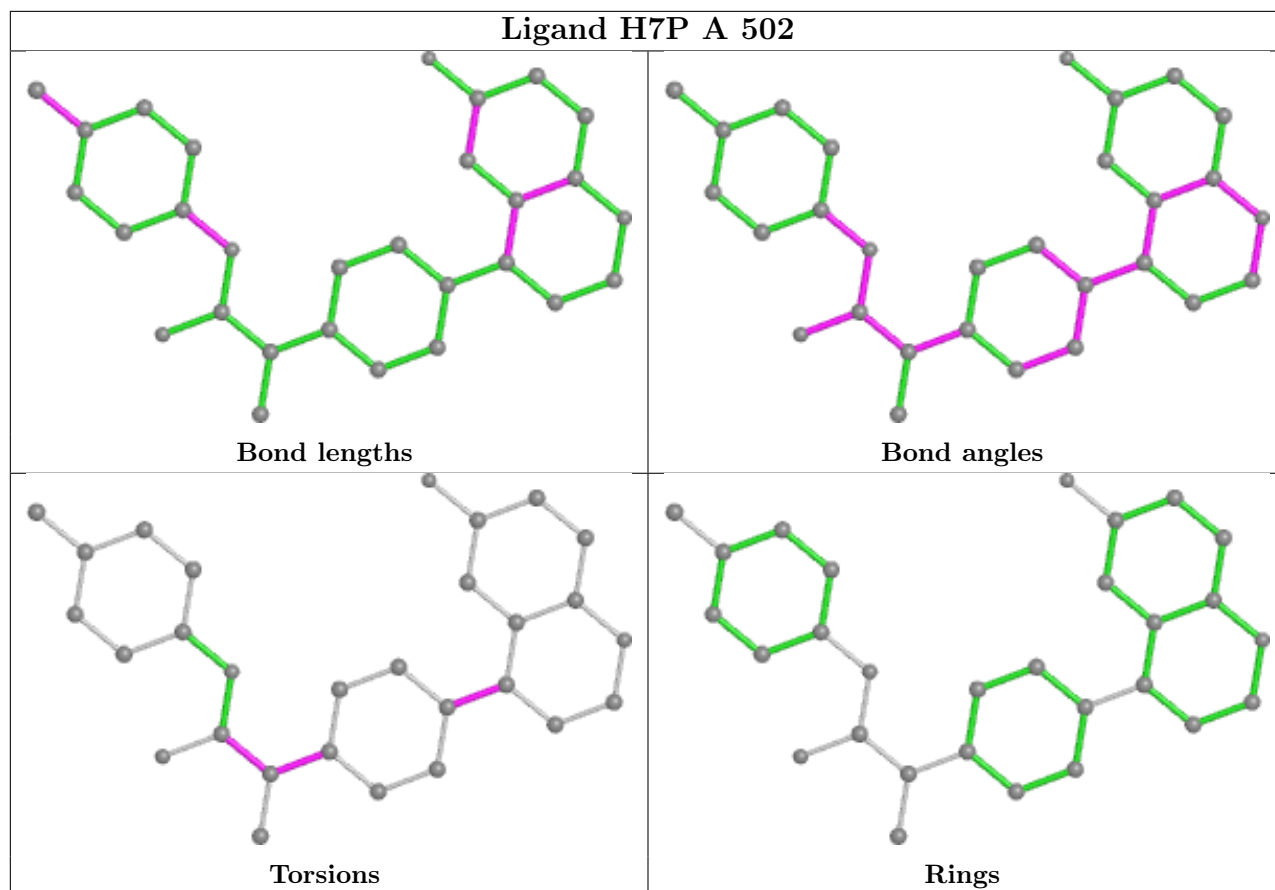
4 monomers are involved in 17 short contacts:

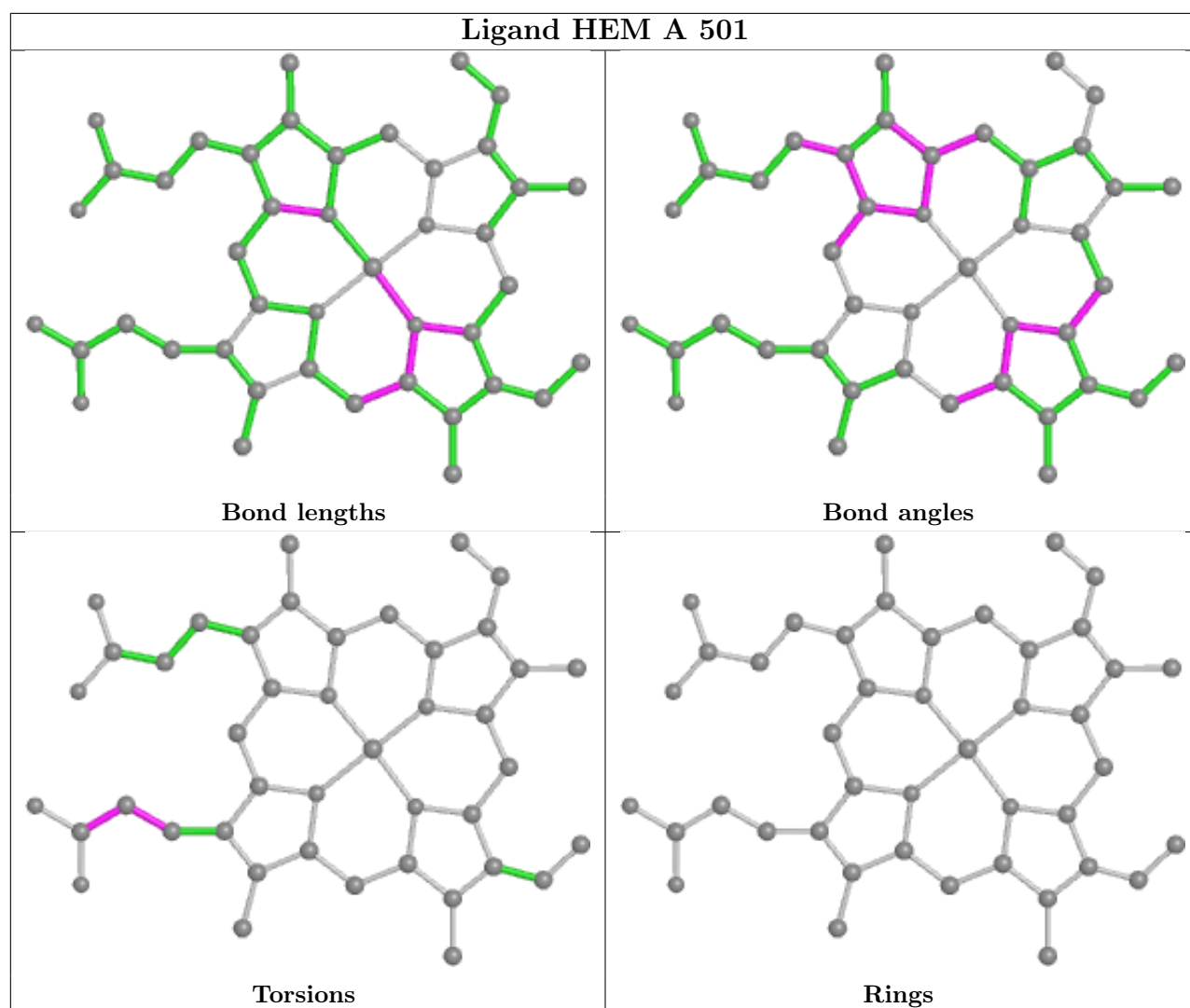
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	H7P	3	0
3	A	502	H7P	6	0
4	A	506	EDO	1	0
2	A	501	HEM	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	358/424 (84%)	-0.37	5 (1%) 75 63	55, 88, 130, 158	0
1	B	371/424 (87%)	-0.37	5 (1%) 77 65	49, 84, 119, 154	0
All	All	729/848 (85%)	-0.37	10 (1%) 75 63	49, 86, 125, 158	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	PRO	3.7
1	B	286	GLY	3.0
1	B	285	GLY	2.9
1	A	264	ALA	2.8
1	A	362	PRO	2.6
1	B	402	GLU	2.6
1	A	246	GLY	2.4
1	B	359	SER	2.2
1	A	379	THR	2.2
1	A	282	THR	2.1

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](#)

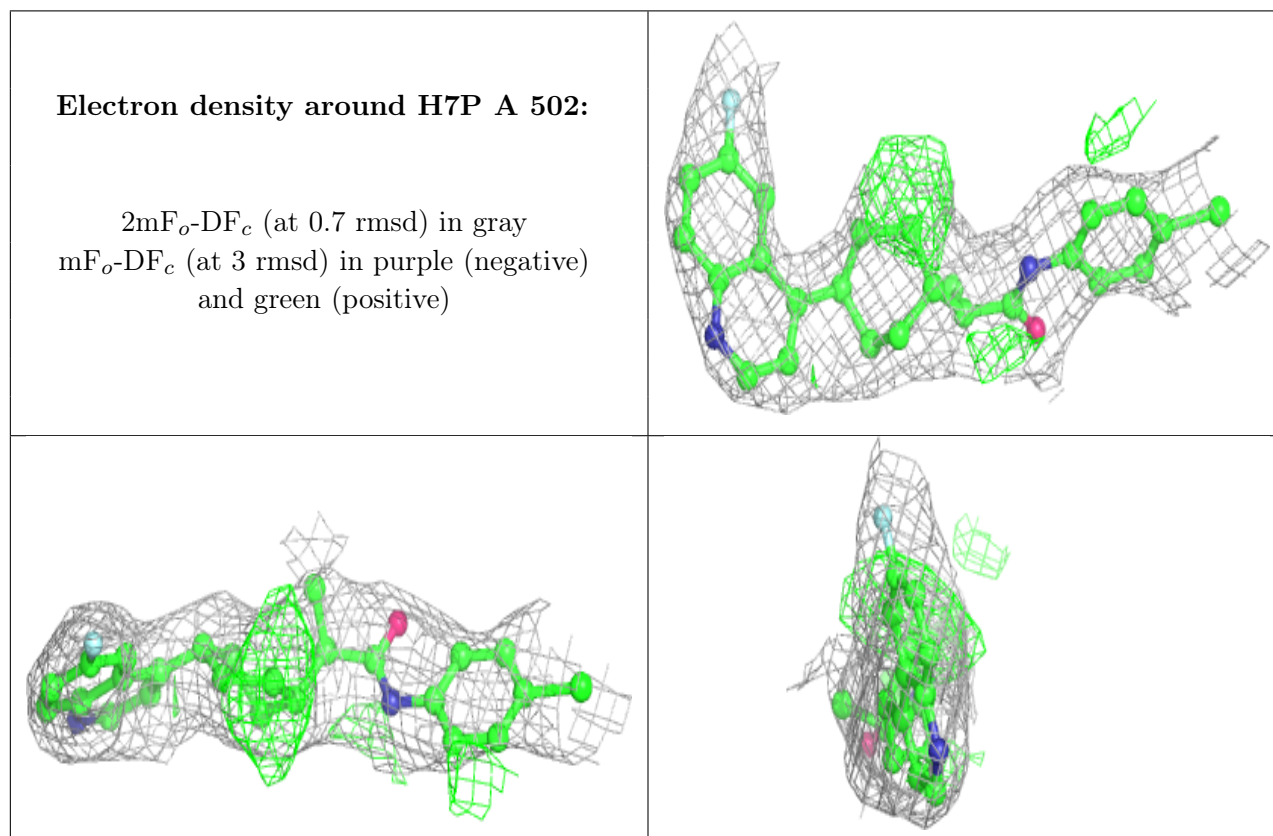
There are no monosaccharides in this entry.

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.

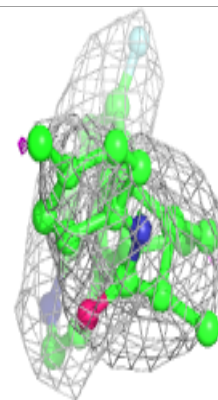
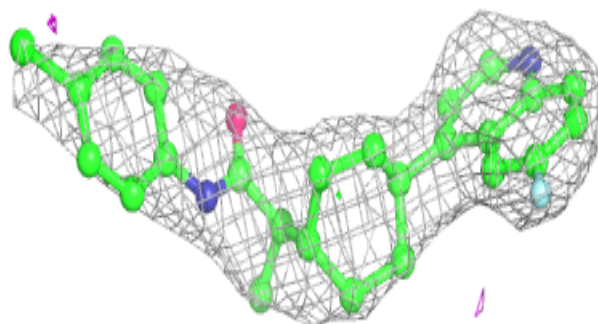
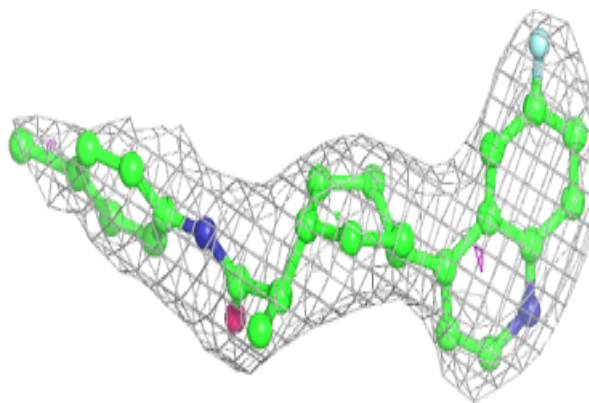
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	505	4/4	0.57	0.52	91,105,106,109	0
4	EDO	A	504	4/4	0.74	0.58	97,100,102,107	0
4	EDO	A	506	4/4	0.77	0.38	88,100,106,107	0
4	EDO	A	503	4/4	0.81	0.40	71,85,86,91	0
3	H7P	A	502	29/29	0.82	0.24	87,104,122,131	0
4	EDO	B	502	4/4	0.82	0.18	86,86,92,94	0
4	EDO	A	507	4/4	0.91	0.21	87,88,88,89	0
3	H7P	B	501	29/29	0.96	0.20	59,66,99,111	0
2	HEM	A	501	43/43	0.97	0.20	70,81,90,100	0

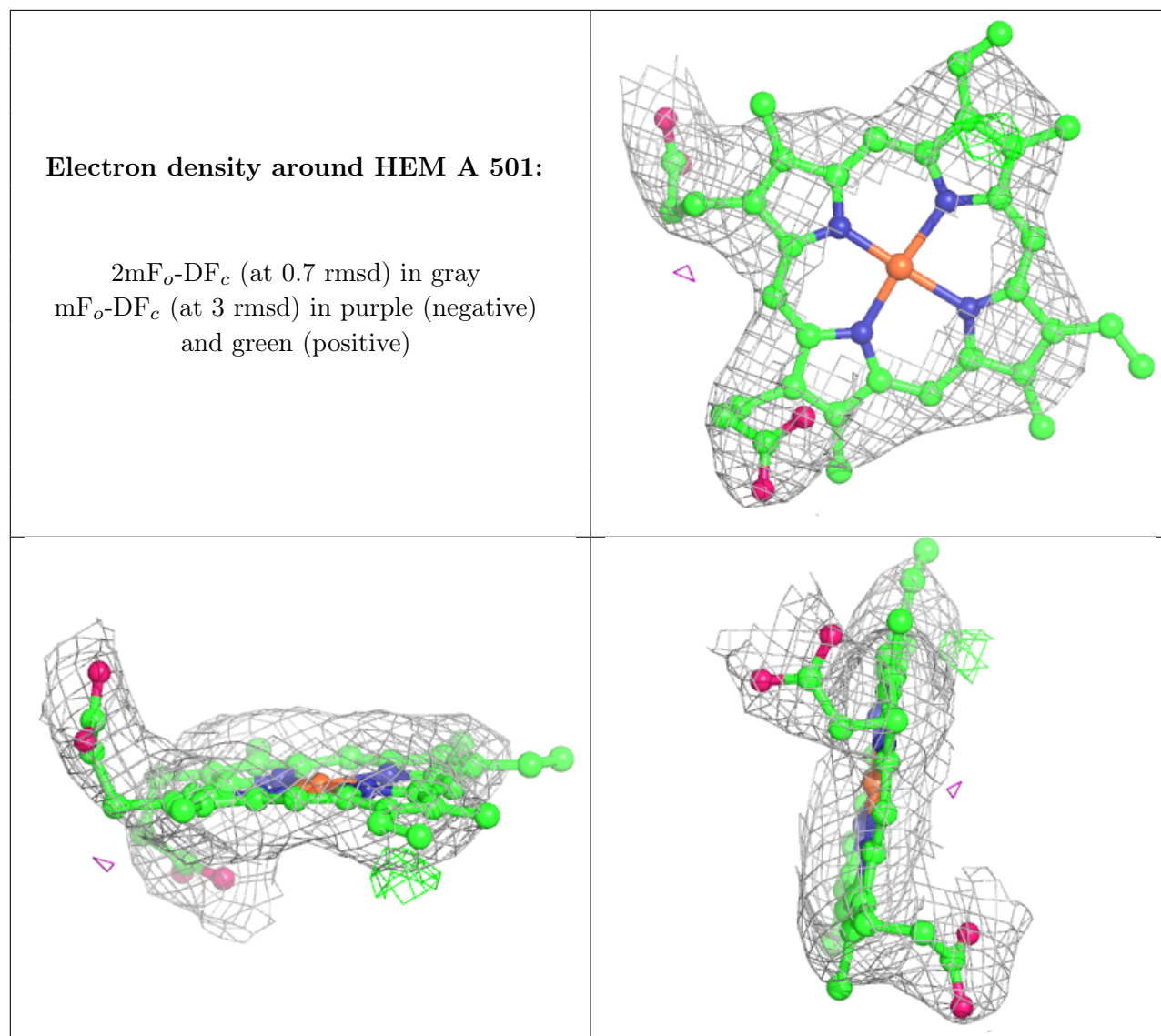
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around H7P 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)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.