



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:41 PM UTC

PDB ID : 1P6N / pdb_00001p6n
Title : Bovine endothelial NOS heme domain with L-N(omega)-nitroarginine-(4R)-amino-L-proline amide bound
Authors : Flinspach, M.L.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Hah, J.-M.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.
Deposited on : 2003-04-29
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

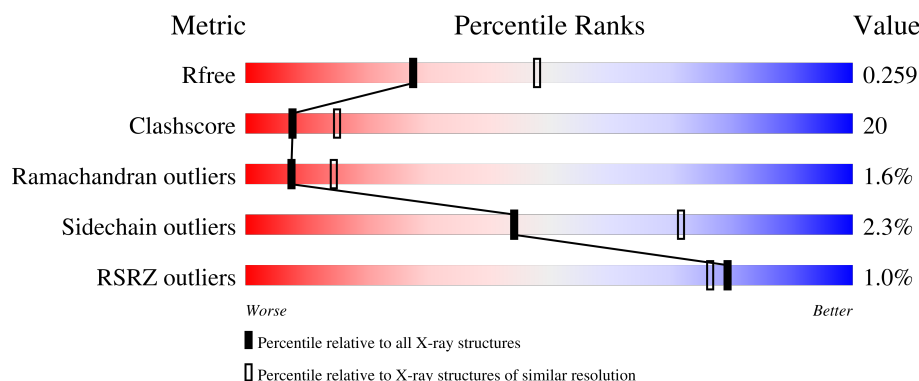
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	417	% 61% 33% • •
1	B	417	% 61% 32% • •

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
2	CAC	B	852	-	-	X	-
3	ACT	A	860	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6921 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.

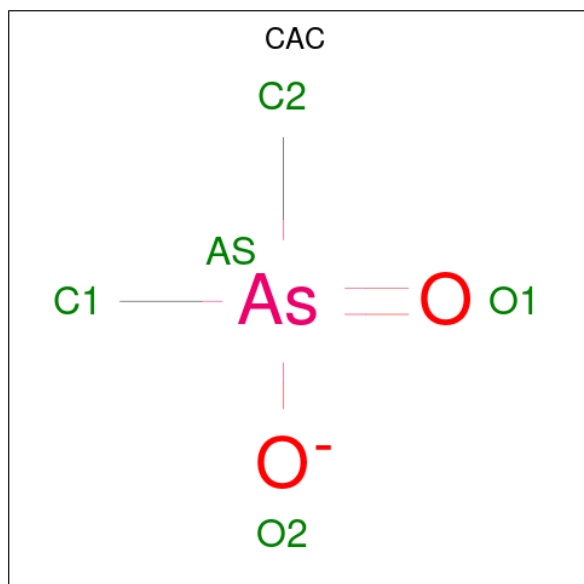
- Molecule 1 is a protein called Nitric-oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3226	2052	569	589	16			
1	B	404	Total	C	N	O	S	0	0	0
			3215	2045	567	587	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 2 is CACODYLATE ION (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



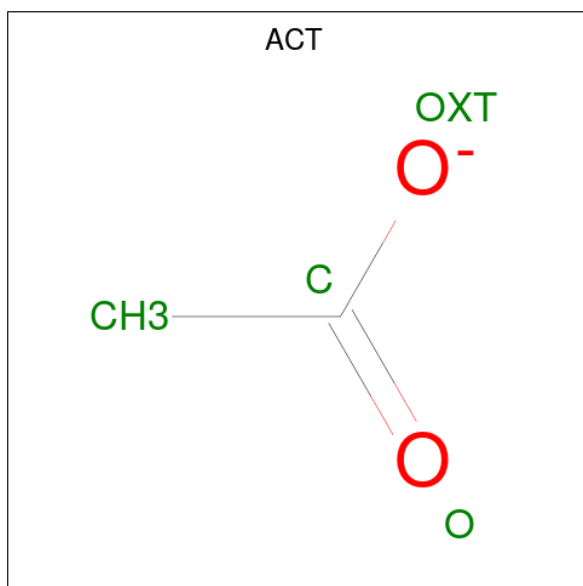
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	As C	0	0
			3	1 2		

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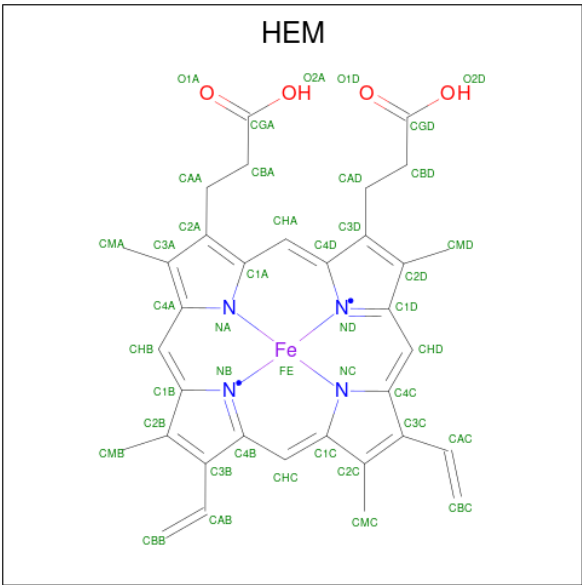
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



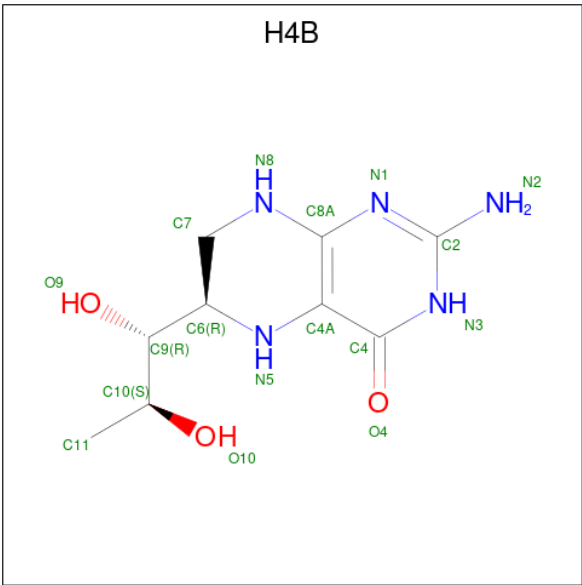
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



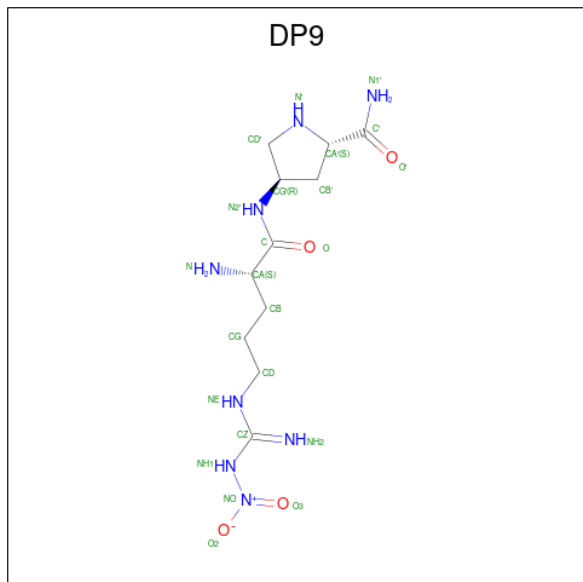
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



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

- Molecule 6 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINE AMIDE (CCD ID: DP9) (formula: $C_{11}H_{22}N_8O_4$).

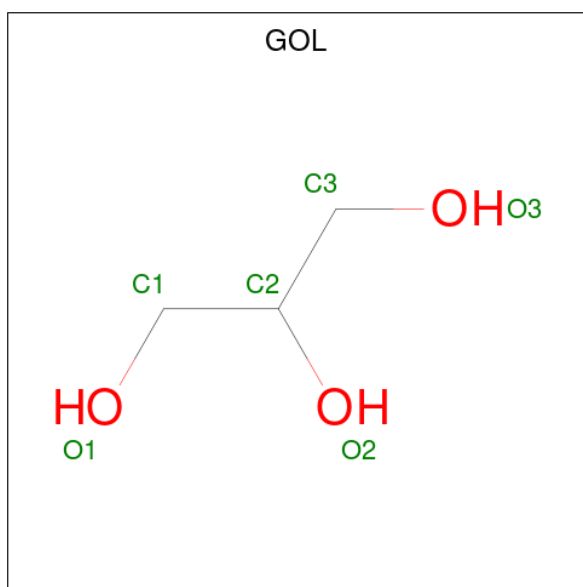


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			23	11	8	4		
6	B	1	Total	C	N	O	0	0
			23	11	8	4		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

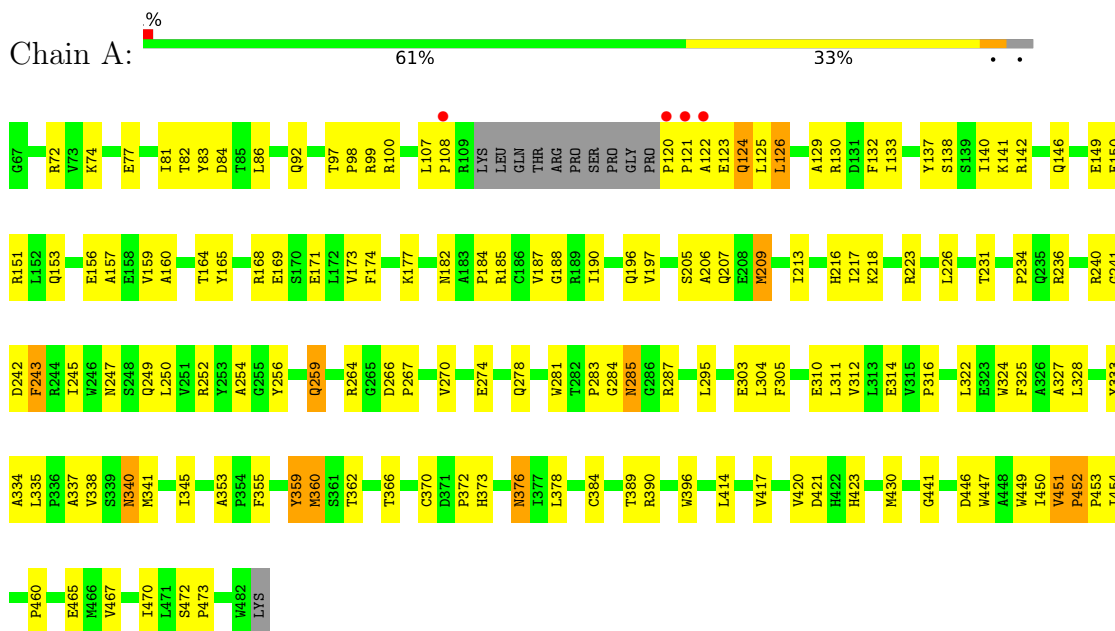
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	151	Total	O	0	0
			151	151		
9	B	136	Total	O	0	0
			136	136		

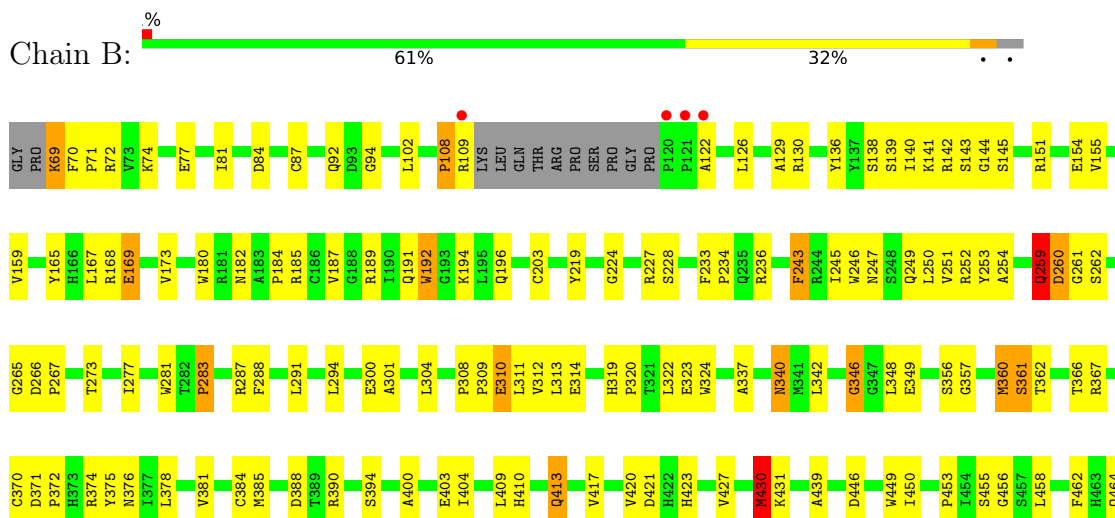
3 Residue-property plots

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: Nitric-oxide synthase, endothelial



- Molecule 1: Nitric-oxide synthase, endothelial



Y469	I470	L471	S472	P473	A474	W482	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.67Å 106.29Å 156.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.55 – 2.50 42.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.55-2.50) 99.8 (42.55-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.278 0.209 , 0.259	Depositor DCC
R_{free} test set	1836 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6921	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: DP9, CAC, ZN, H4B, HEM, GOL, ACT

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	0.49	0/3317	1.05	19/4520 (0.4%)
1	B	0.47	0/3305	1.02	15/4503 (0.3%)
All	All	0.48	0/6622	1.03	34/9023 (0.4%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	VAL	CA-C-N	9.35	126.48	119.66
1	A	451	VAL	C-N-CA	9.35	126.48	119.66
1	A	284	GLY	N-CA-C	-8.33	102.79	112.79
1	B	245	ILE	N-CA-C	-8.15	95.99	107.80
1	A	107	LEU	CA-C-N	7.78	129.57	119.84
1	A	107	LEU	C-N-CA	7.78	129.57	119.84
1	A	360	MET	N-CA-C	-7.69	95.98	108.52
1	A	312	VAL	N-CA-C	7.07	113.78	106.21
1	A	243	PHE	N-CA-C	-6.74	98.27	109.46
1	A	335	LEU	N-CA-C	6.74	120.81	108.69
1	A	245	ILE	N-CA-C	-6.70	97.97	107.75
1	A	452	PRO	N-CA-C	6.63	116.83	110.47
1	B	243	PHE	N-CA-C	-6.60	100.06	109.96
1	A	359	TYR	N-CA-C	6.29	119.37	110.50
1	B	138	SER	N-CA-C	-6.23	104.59	111.82
1	A	226	LEU	N-CA-C	6.16	118.25	110.24
1	A	452	PRO	CA-C-N	6.06	125.75	119.56
1	A	452	PRO	C-N-CA	6.06	125.75	119.56
1	B	394	SER	N-CA-C	-5.98	105.99	113.28
1	B	266	ASP	CA-C-N	5.86	126.27	119.47
1	B	266	ASP	C-N-CA	5.86	126.27	119.47
1	B	470	ILE	N-CA-C	5.73	116.05	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	MET	N-CA-C	-5.70	105.14	111.36
1	B	94	GLY	CA-C-N	5.55	125.07	119.19
1	B	94	GLY	C-N-CA	5.55	125.07	119.19
1	B	312	VAL	N-CA-C	5.46	114.47	106.55
1	B	439	ALA	N-CA-C	5.46	119.11	112.23
1	A	460	PRO	N-CA-C	5.44	120.66	113.86
1	B	301	ALA	CA-C-N	5.30	125.22	119.76
1	B	301	ALA	C-N-CA	5.30	125.22	119.76
1	A	197	VAL	N-CA-C	5.23	115.88	107.73
1	A	337	ALA	N-CA-C	5.18	118.50	107.67
1	B	360	MET	N-CA-C	-5.10	99.09	108.02
1	B	430	MET	N-CA-C	-5.02	105.08	111.11

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	3226	0	3135	133	0
1	B	3215	0	3125	124	0
2	A	3	0	0	3	0
2	B	3	0	0	4	0
3	A	4	0	3	3	0
3	B	4	0	3	0	0
4	A	43	0	30	3	0
4	B	43	0	30	1	0
5	A	17	0	15	2	0
5	B	17	0	15	0	0
6	A	23	0	21	1	0
6	B	23	0	21	3	0
7	B	1	0	0	0	0
8	B	12	0	16	3	0
9	A	151	0	0	16	0
9	B	136	0	0	9	0
All	All	6921	0	6414	261	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 20.

All (261) 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:92:GLN:HE21	1:A:470:ILE:HD13	1.32	0.93
1:A:384:CYS:SG	2:A:850:CAC:AS	2.89	0.91
1:A:360:MET:HE3	1:A:362:THR:OG1	1.79	0.83
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.65	0.79
1:B:191:GLN:HE22	1:B:194:LYS:HE2	1.50	0.76
1:B:384:CYS:SG	2:B:852:CAC:AS	3.04	0.75
1:B:249:GLN:HB3	9:B:982:HOH:O	1.86	0.75
1:B:126:LEU:O	1:B:130:ARG:HG3	1.87	0.75
1:B:313:LEU:HD12	1:B:314:GLU:H	1.52	0.74
1:A:126:LEU:HD12	1:A:130:ARG:CZ	2.18	0.73
1:B:310:GLU:CD	1:B:310:GLU:H	1.96	0.73
1:B:300:GLU:HG3	9:B:1015:HOH:O	1.88	0.72
1:A:126:LEU:HD11	1:A:156:GLU:HG3	1.71	0.72
1:A:99:ARG:NH1	1:A:99:ARG:HB2	2.06	0.70
1:A:168:ARG:HD3	9:A:943:HOH:O	1.92	0.70
1:A:285:ASN:HD22	1:A:285:ASN:N	1.89	0.70
1:A:149:GLU:O	1:A:153:GLN:HG3	1.91	0.70
1:B:169:GLU:O	1:B:173:VAL:HG23	1.91	0.70
1:B:136:TYR:O	1:B:139:SER:HB3	1.92	0.69
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.27	0.69
4:A:500:HEM:HMC2	4:A:500:HEM:HBC2	1.75	0.68
1:A:254:ALA:HB2	9:A:973:HOH:O	1.92	0.68
1:B:310:GLU:N	1:B:310:GLU:OE2	2.28	0.67
4:A:500:HEM:HBA2	6:A:799:DP9:HG1	1.77	0.66
1:B:313:LEU:HD12	1:B:314:GLU:N	2.11	0.66
1:B:277:ILE:HG12	1:B:283:PRO:HG3	1.78	0.65
1:B:324:TRP:HB2	2:B:852:CAC:C1	2.27	0.64
1:B:423:HIS:O	1:B:427:VAL:HG23	1.97	0.64
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.37	0.64
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.63	0.64
1:A:472:SER:HA	1:A:473:PRO:C	2.23	0.64
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.78	0.64
1:B:250:LEU:N	9:B:982:HOH:O	2.30	0.63
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.79	0.63
1:A:274:GLU:O	1:A:278:GLN:HG3	1.99	0.63
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.64	0.62
1:A:146:GLN:O	1:A:150:GLU:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:TYR:HA	9:A:1010:HOH:O	2.01	0.61
1:A:378:LEU:HB2	9:A:861:HOH:O	2.00	0.60
1:A:125:LEU:O	1:A:125:LEU:HD23	2.02	0.60
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.84	0.60
1:B:360:MET:HE3	1:B:362:THR:OG1	2.02	0.59
1:A:125:LEU:HD23	1:A:125:LEU:C	2.27	0.59
1:B:191:GLN:NE2	1:B:194:LYS:HE2	2.16	0.59
1:A:372:PRO:HA	1:A:376:ASN:ND2	2.18	0.59
1:B:378:LEU:HB2	9:B:906:HOH:O	2.02	0.59
1:B:182:ASN:O	1:B:184:PRO:HD3	2.03	0.58
1:B:265:GLY:O	1:B:267:PRO:HD3	2.03	0.58
1:A:338:VAL:HG11	1:A:341:MET:HG3	1.85	0.58
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.33	0.58
1:A:206:ALA:HB3	1:A:303:GLU:OE2	2.04	0.58
1:A:285:ASN:HD22	1:A:285:ASN:H	1.50	0.58
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.85	0.57
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.86	0.57
1:B:155:VAL:O	1:B:159:VAL:HG23	2.05	0.57
1:A:120:PRO:HA	1:A:124:GLN:NE2	2.20	0.56
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.87	0.56
1:A:472:SER:HA	1:A:473:PRO:O	2.06	0.56
1:A:310:GLU:OE1	1:A:310:GLU:N	2.24	0.56
1:B:385:MET:CE	1:B:403:GLU:HG3	2.36	0.56
1:A:99:ARG:HH11	1:A:99:ARG:CB	2.19	0.56
1:A:360:MET:HA	1:A:420:VAL:O	2.05	0.56
6:B:800:DP9:HN'	8:B:882:GOL:H32	1.70	0.56
1:A:121:PRO:O	1:A:123:GLU:N	2.39	0.55
1:B:227:ARG:HA	9:B:961:HOH:O	2.05	0.55
4:A:500:HEM:HHC	4:A:500:HEM:HBB2	1.87	0.55
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.42	0.55
1:B:234:PRO:HB2	1:B:243:PHE:CE1	2.42	0.55
1:B:385:MET:HE1	1:B:403:GLU:HG3	1.87	0.55
1:B:381:VAL:O	1:B:385:MET:HG3	2.06	0.55
1:B:371:ASP:HB2	1:B:374:ARG:HG2	1.89	0.54
1:B:236:ARG:HG3	1:B:349:GLU:O	2.06	0.54
1:A:389:THR:HA	1:A:396:TRP:CD1	2.43	0.54
1:B:472:SER:HA	1:B:473:PRO:C	2.32	0.54
1:B:196:GLN:HG2	1:B:219:TYR:CZ	2.43	0.54
1:B:430:MET:HE1	1:B:464:GLN:HG2	1.89	0.54
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.43	0.54
1:A:338:VAL:CG1	1:A:341:MET:HG3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HD22	1:A:340:ASN:H	1.54	0.53
1:A:259:GLN:HE21	1:A:259:GLN:HA	1.72	0.53
1:A:384:CYS:HB3	2:A:850:CAC:AS	2.68	0.53
1:B:409:LEU:O	1:B:413:GLN:HB2	2.09	0.53
1:B:69:LYS:HB2	1:B:69:LYS:NZ	2.23	0.53
1:B:388:ASP:OD1	1:B:390:ARG:HB2	2.09	0.53
1:B:249:GLN:CB	1:B:252:ARG:HD3	2.36	0.53
1:A:236:ARG:HG2	1:A:242:ASP:OD2	2.09	0.53
1:B:366:THR:HG21	1:B:453:PRO:HB2	1.90	0.52
1:A:92:GLN:HG2	1:A:470:ILE:HD12	1.90	0.52
1:A:249:GLN:HB3	9:A:868:HOH:O	2.09	0.52
1:A:168:ARG:HD2	9:A:984:HOH:O	2.10	0.52
1:A:188:GLY:HA2	3:A:860:ACT:H1	1.90	0.52
1:A:360:MET:HE3	1:A:362:THR:HG1	1.71	0.52
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.40	0.51
1:A:207:GLN:NE2	1:A:305:PHE:HE2	2.08	0.51
1:A:384:CYS:CB	2:A:850:CAC:AS	3.18	0.51
1:A:74:LYS:O	1:A:465:GLU:HG3	2.10	0.51
1:B:400:ALA:O	1:B:404:ILE:HG13	2.10	0.51
1:B:129:ALA:HB1	1:B:155:VAL:HG11	1.93	0.51
1:A:138:SER:O	1:A:141:LYS:HD3	2.11	0.51
1:A:325:PHE:HA	1:A:328:LEU:HD23	1.92	0.51
1:A:316:PRO:HD2	9:A:898:HOH:O	2.11	0.50
1:B:151:ARG:O	1:B:155:VAL:HG23	2.11	0.50
1:B:340:ASN:H	1:B:340:ASN:HD22	1.59	0.50
1:A:285:ASN:N	1:A:285:ASN:ND2	2.60	0.50
1:B:224:GLY:O	1:B:417:VAL:HA	2.11	0.50
1:A:120:PRO:HA	1:A:124:GLN:CD	2.37	0.49
1:B:259:GLN:HG3	1:B:260:ASP:OD1	2.11	0.49
1:A:159:VAL:HA	1:A:164:THR:O	2.12	0.49
1:A:390:ARG:HD3	9:A:950:HOH:O	2.11	0.49
1:A:97:THR:HB	1:A:98:PRO:HD2	1.94	0.49
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.48	0.49
1:B:72:ARG:HD2	1:B:81:ILE:HD13	1.94	0.49
1:B:371:ASP:CB	1:B:374:ARG:HG2	2.43	0.49
1:B:143:SER:O	1:B:145:SER:N	2.46	0.49
1:B:287:ARG:HB2	1:B:288:PHE:CD1	2.48	0.49
1:B:430:MET:HE1	1:B:464:GLN:CG	2.43	0.48
1:B:366:THR:O	1:B:370:CYS:HB2	2.13	0.48
1:B:342:LEU:C	1:B:342:LEU:HD23	2.38	0.48
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:NH1	1:A:242:ASP:OD1	2.42	0.48
1:A:187:VAL:HG22	1:A:187:VAL:O	2.12	0.48
1:B:87:CYS:HA	1:B:469:TYR:CE1	2.49	0.48
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.79	0.48
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.96	0.48
1:A:188:GLY:HA2	3:A:860:ACT:CH3	2.44	0.48
1:B:281:TRP:O	1:B:283:PRO:HD3	2.14	0.47
1:B:234:PRO:HB2	1:B:243:PHE:CD1	2.50	0.47
1:A:453:PRO:HG3	9:A:885:HOH:O	2.14	0.47
1:B:246:TRP:HB2	1:B:294:LEU:HB2	1.95	0.47
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.96	0.47
1:B:471:LEU:O	1:B:474:ALA:HB2	2.15	0.47
1:A:190:ILE:HG22	3:A:860:ACT:H2	1.96	0.47
1:A:209:MET:HE2	1:A:295:LEU:HB3	1.97	0.47
1:A:213:ILE:HG23	1:A:250:LEU:HD13	1.97	0.46
1:A:196:GLN:HG3	9:A:977:HOH:O	2.15	0.46
1:B:287:ARG:HB2	1:B:288:PHE:CE1	2.50	0.46
1:A:125:LEU:C	1:A:125:LEU:CD2	2.88	0.46
1:A:141:LYS:O	1:A:142:ARG:NH1	2.48	0.46
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.51	0.46
1:A:259:GLN:HE21	1:A:259:GLN:CA	2.28	0.46
1:A:72:ARG:NH1	1:A:81:ILE:HD12	2.30	0.46
1:A:414:LEU:C	1:A:414:LEU:HD23	2.41	0.46
1:B:308:PRO:O	1:B:310:GLU:N	2.49	0.46
1:B:367:ARG:HG3	1:B:367:ARG:HH11	1.81	0.46
1:A:92:GLN:NE2	1:A:470:ILE:HD13	2.14	0.46
1:A:205:SER:HB3	9:A:889:HOH:O	2.16	0.46
1:B:260:ASP:C	1:B:262:SER:H	2.23	0.46
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.98	0.46
6:B:800:DP9:N'	8:B:882:GOL:H32	2.31	0.46
1:A:421:ASP:OD2	1:A:423:HIS:HB2	2.15	0.46
1:B:252:ARG:HB2	1:B:291:LEU:HD12	1.97	0.46
1:B:384:CYS:HB3	2:B:852:CAC:AS	2.76	0.46
1:A:340:ASN:HD22	1:A:340:ASN:N	2.12	0.45
1:A:467:VAL:HG22	1:B:102:LEU:CD2	2.46	0.45
1:B:180:TRP:CZ3	1:B:192:TRP:HA	2.51	0.45
1:B:251:VAL:C	1:B:252:ARG:HG2	2.42	0.45
1:B:361:SER:HB3	1:B:409:LEU:CD2	2.46	0.45
1:B:431:LYS:HE3	1:B:431:LYS:HB2	1.82	0.45
1:A:264:ARG:HG3	1:A:264:ARG:NH1	2.30	0.45
1:B:92:GLN:HG3	1:B:470:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:OG1	1:A:165:TYR:N	2.49	0.45
1:A:295:LEU:HD12	1:A:305:PHE:CD1	2.51	0.45
1:A:334:ALA:CB	1:A:417:VAL:HG11	2.47	0.45
1:B:320:PRO:HG3	1:B:410:HIS:CG	2.52	0.45
4:B:500:HEM:O2A	6:B:800:DP9:HA	2.17	0.45
1:A:316:PRO:HB2	9:A:898:HOH:O	2.16	0.45
1:A:340:ASN:H	1:A:340:ASN:ND2	2.14	0.45
1:A:446:ASP:O	1:A:450:ILE:HG12	2.17	0.44
1:A:281:TRP:HH2	9:A:973:HOH:O	1.98	0.44
1:A:287:ARG:HD3	9:A:879:HOH:O	2.17	0.44
1:A:373:HIS:ND1	1:B:77:GLU:HA	2.32	0.44
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.52	0.44
1:A:338:VAL:HG23	9:A:1011:HOH:O	2.17	0.44
1:A:72:ARG:HH12	1:A:81:ILE:HD12	1.82	0.44
1:B:361:SER:OG	1:B:421:ASP:HA	2.17	0.44
1:A:86:LEU:HD12	1:A:86:LEU:O	2.17	0.44
1:A:234:PRO:HB2	1:A:243:PHE:CD1	2.52	0.44
1:A:324:TRP:O	1:A:327:ALA:HB3	2.18	0.44
1:B:187:VAL:O	1:B:187:VAL:HG22	2.18	0.44
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.99	0.44
1:A:216:HIS:C	1:A:216:HIS:CD2	2.95	0.44
1:B:191:GLN:HB3	9:B:974:HOH:O	2.16	0.44
1:A:97:THR:C	1:A:99:ARG:H	2.26	0.44
1:B:340:ASN:HD22	1:B:340:ASN:N	2.14	0.44
1:B:249:GLN:CG	1:B:252:ARG:HD3	2.48	0.44
1:B:390:ARG:HH11	1:B:390:ARG:CB	2.30	0.44
1:A:310:GLU:H	1:A:310:GLU:CD	2.15	0.43
1:B:253:TYR:CE2	1:B:288:PHE:HD2	2.35	0.43
1:B:360:MET:HA	1:B:420:VAL:O	2.18	0.43
1:A:338:VAL:HG12	9:A:864:HOH:O	2.18	0.43
1:B:324:TRP:CZ3	1:B:384:CYS:HB3	2.53	0.43
1:A:141:LYS:C	1:A:142:ARG:HG2	2.43	0.43
1:A:247:ASN:OD1	1:A:247:ASN:N	2.52	0.43
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.99	0.43
1:B:182:ASN:O	1:B:184:PRO:CD	2.66	0.43
1:A:81:ILE:HG22	1:A:82:THR:N	2.32	0.43
1:A:281:TRP:O	1:A:283:PRO:HD3	2.19	0.43
1:A:84:ASP:HA	1:A:441:GLY:O	2.19	0.43
1:B:141:LYS:C	1:B:143:SER:H	2.26	0.43
1:B:308:PRO:O	1:B:311:LEU:N	2.49	0.43
1:B:384:CYS:CB	2:B:852:CAC:AS	3.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ALA:HA	9:B:983:HOH:O	2.19	0.43
1:A:240:ARG:HG2	1:A:241:GLY:N	2.34	0.43
1:B:140:ILE:O	1:B:141:LYS:HB2	2.18	0.43
1:A:420:VAL:O	1:A:420:VAL:HG13	2.19	0.43
1:B:324:TRP:CZ3	1:B:384:CYS:CB	3.02	0.43
1:A:452:PRO:HA	1:A:453:PRO:HD3	1.79	0.43
1:B:74:LYS:HD2	9:B:953:HOH:O	2.18	0.43
1:B:376:ASN:HA	9:B:906:HOH:O	2.18	0.43
1:B:390:ARG:HH11	1:B:390:ARG:HB3	1.84	0.43
1:A:314:GLU:HA	1:A:333:TYR:HA	2.00	0.42
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.54	0.42
1:A:449:TRP:HA	5:A:760:H4B:N1	2.35	0.42
1:B:247:ASN:OD1	1:B:247:ASN:N	2.52	0.42
1:B:168:ARG:O	1:B:169:GLU:C	2.61	0.42
1:A:124:GLN:C	1:A:124:GLN:HE21	2.28	0.42
1:A:137:TYR:HA	1:A:140:ILE:HG12	2.02	0.42
1:B:254:ALA:HB1	1:B:273:THR:HG21	2.02	0.42
1:A:182:ASN:O	1:A:184:PRO:HD3	2.20	0.42
1:B:360:MET:O	1:B:361:SER:C	2.62	0.42
1:B:337:ALA:CB	1:B:356:SER:HB3	2.49	0.42
1:A:146:GLN:HG2	1:A:150:GLU:OE2	2.20	0.42
1:A:231:THR:O	1:A:353:ALA:HA	2.20	0.42
1:A:270:VAL:O	1:A:274:GLU:HG3	2.19	0.42
1:B:340:ASN:H	1:B:340:ASN:ND2	2.17	0.42
1:A:249:GLN:HB2	1:A:252:ARG:HG2	2.02	0.42
1:B:167:LEU:HG	1:B:348:LEU:CD1	2.46	0.42
1:B:370:CYS:HB3	1:B:378:LEU:HD13	2.01	0.42
1:B:165:TYR:OH	1:B:346:GLY:O	2.27	0.41
1:B:151:ARG:O	1:B:151:ARG:HD2	2.20	0.41
1:B:403:GLU:OE2	1:B:403:GLU:HA	2.20	0.41
5:A:760:H4B:O4	8:B:880:GOL:C3	2.69	0.41
1:B:228:SER:HA	1:B:357:GLY:HA2	2.01	0.41
1:A:129:ALA:O	1:A:133:ILE:HG12	2.20	0.41
1:A:173:VAL:O	1:A:177:LYS:HG3	2.21	0.41
1:A:213:ILE:O	1:A:217:ILE:HG13	2.21	0.41
1:B:446:ASP:O	1:B:450:ILE:HG12	2.20	0.41
1:A:236:ARG:HH11	1:A:242:ASP:CG	2.28	0.41
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.56	0.41
1:B:69:LYS:HB2	1:B:70:PHE:H	1.70	0.41
1:B:154:GLU:OE2	1:B:168:ARG:NH2	2.53	0.41
1:B:361:SER:HB3	1:B:409:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:HIS:HA	1:B:320:PRO:HD3	1.93	0.41
1:A:72:ARG:HD2	1:A:83:TYR:OH	2.20	0.41
1:B:108:PRO:C	1:B:109:ARG:HD2	2.46	0.41
1:B:189:ARG:O	1:B:192:TRP:HD1	2.04	0.41
1:A:97:THR:C	1:A:99:ARG:N	2.79	0.41
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.86	0.41
1:A:259:GLN:CA	1:A:259:GLN:NE2	2.82	0.41
1:B:340:ASN:ND2	1:B:340:ASN:C	2.79	0.41
1:A:157:ALA:O	1:A:160:ALA:HB3	2.21	0.41
1:A:266:ASP:HA	1:A:267:PRO:HD3	1.95	0.41
1:B:375:TYR:O	1:B:376:ASN:C	2.63	0.41
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.82	0.40
1:A:168:ARG:O	1:A:169:GLU:C	2.63	0.40
1:A:132:PHE:CE1	1:A:174:PHE:CD2	3.10	0.40
1:B:259:GLN:NE2	1:B:260:ASP:OD1	2.54	0.40
1:B:281:TRP:HB2	1:B:304:LEU:HD21	2.04	0.40
1:B:456:GLY:O	1:B:462:PHE:HB2	2.21	0.40
1:A:256:TYR:CE1	1:A:285:ASN:HA	2.56	0.40
1:A:345:ILE:HG12	1:A:473:PRO:HB3	2.02	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	402/417 (96%)	364 (90%)	36 (9%)	2 (0%)	24	43
1	B	400/417 (96%)	356 (89%)	33 (8%)	11 (3%)	4	6
All	All	802/834 (96%)	720 (90%)	69 (9%)	13 (2%)	7	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	PRO
1	A	122	ALA
1	B	108	PRO
1	B	144	GLY
1	B	259	GLN
1	B	361	SER
1	B	192	TRP
1	B	283	PRO
1	B	122	ALA
1	B	309	PRO
1	B	260	ASP
1	B	346	GLY
1	B	261	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	345/355 (97%)	338 (98%)	7 (2%)	48	75
1	B	344/355 (97%)	335 (97%)	9 (3%)	40	68
All	All	689/710 (97%)	673 (98%)	16 (2%)	44	72

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	126	LEU
1	A	209	MET
1	A	259	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	B	69	LYS
1	B	169	GLU
1	B	203	CYS
1	B	259	GLN

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Mol	Chain	Res	Type
1	B	310	GLU
1	B	323	GLU
1	B	340	ASN
1	B	413	GLN
1	B	430	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	124	GLN
1	A	153	GLN
1	A	166	HIS
1	A	191	GLN
1	A	207	GLN
1	A	249	GLN
1	A	258	GLN
1	A	259	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	410	HIS
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	128	GLN
1	B	146	GLN
1	B	153	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	249	GLN
1	B	278	GLN
1	B	340	ASN
1	B	405	ASN
1	B	410	HIS
1	B	413	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	HEM	B	500	1	50,50,50	0.97	2 (4%)	67,82,82	1.23	5 (7%)
2	CAC	B	852	-	0,2,4	-	-	0,1,6	-	-
8	GOL	B	882	-	5,5,5	0.26	0	5,5,5	0.34	0
5	H4B	A	760	-	17,18,18	1.60	2 (11%)	14,26,26	1.92	3 (21%)
3	ACT	A	860	-	3,3,3	1.00	0	3,3,3	0.52	0
6	DP9	A	799	-	17,23,23	0.98	2 (11%)	20,30,30	1.94	6 (30%)
3	ACT	B	861	-	3,3,3	1.03	0	3,3,3	0.56	0
8	GOL	B	880	-	5,5,5	0.17	0	5,5,5	0.31	0
5	H4B	B	761	-	17,18,18	1.47	2 (11%)	14,26,26	1.93	3 (21%)
6	DP9	B	800	-	17,23,23	0.80	0	20,30,30	1.97	5 (25%)
2	CAC	A	850	-	0,2,4	-	-	0,1,6	-	-
4	HEM	A	500	1	50,50,50	1.20	5 (10%)	67,82,82	1.47	11 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	500	1	-	2/14/54/54	-
8	GOL	B	882	-	-	2/4/4/4	-
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	DP9	A	799	-	-	4/20/32/32	0/1/1/1
8	GOL	B	880	-	-	2/4/4/4	-
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2
6	DP9	B	800	-	-	7/20/32/32	0/1/1/1
4	HEM	A	500	1	-	5/14/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	760	H4B	C6-N5	3.96	1.54	1.47
5	B	761	H4B	C4A-N5	3.93	1.47	1.37
5	A	760	H4B	C4A-N5	3.83	1.46	1.37
4	A	500	HEM	CAB-C3B	-3.59	1.37	1.47
5	B	761	H4B	C6-N5	3.19	1.53	1.47
4	A	500	HEM	C1B-NB	-2.67	1.35	1.40
6	A	799	DP9	CG'-N2'	2.62	1.52	1.46
4	B	500	HEM	CAB-C3B	-2.49	1.40	1.47
4	A	500	HEM	CMD-C2D	2.28	1.55	1.50
4	B	500	HEM	CAC-C3C	-2.26	1.41	1.47
6	A	799	DP9	O3-NO	2.26	1.30	1.24
4	A	500	HEM	CHD-C1D	-2.16	1.34	1.39
4	A	500	HEM	FE-ND	2.13	2.01	1.94

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	H4B	C2-N1-C8A	5.02	122.22	113.36
5	B	761	H4B	C2-N1-C8A	4.92	122.05	113.36
6	B	800	DP9	C'-CA'-N'	-4.52	101.84	111.16
6	A	799	DP9	CD-NE-CZ	4.46	131.64	123.46
4	A	500	HEM	CMD-C2D-C1D	3.72	130.85	125.03
6	B	800	DP9	O'-C'-N1'	-3.66	116.57	123.04
6	B	800	DP9	CD-NE-CZ	3.66	130.18	123.46
4	A	500	HEM	C4C-C3C-C2C	-3.66	103.64	106.81
6	A	799	DP9	O'-C'-N1'	-3.48	116.90	123.04
4	A	500	HEM	C4A-C3A-C2A	-3.10	103.27	106.82
6	B	800	DP9	CA'-C'-N1'	3.04	121.93	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	799	DP9	C'-CA'-N'	-3.03	104.91	111.16
5	B	761	H4B	N3-C2-N1	-3.03	117.78	123.32
5	B	761	H4B	O10-C10-C9	-3.01	104.79	109.77
4	B	500	HEM	C4B-C3B-C2B	-3.00	104.52	107.28
5	A	760	H4B	N3-C2-N1	-2.92	117.98	123.32
4	A	500	HEM	C2D-C1D-ND	2.91	113.27	109.90
4	B	500	HEM	CBA-CAA-C2A	-2.88	104.56	112.53
5	A	760	H4B	O10-C10-C9	-2.87	105.02	109.77
4	B	500	HEM	C3B-C4B-NB	2.87	111.53	109.47
6	A	799	DP9	CG'-N2'-C	2.73	127.69	123.29
4	B	500	HEM	CMA-C3A-C4A	2.73	129.57	125.42
4	B	500	HEM	C3B-C2B-C1B	2.68	108.42	106.41
4	A	500	HEM	C1D-C2D-C3D	-2.66	104.18	106.98
4	A	500	HEM	CMA-C3A-C4A	2.62	129.40	125.42
6	B	800	DP9	CG'-N2'-C	2.49	127.30	123.29
6	A	799	DP9	CA'-C'-N1'	2.47	120.96	116.76
4	A	500	HEM	C2B-C1B-NB	2.30	112.49	109.84
4	A	500	HEM	C1A-C2A-C3A	2.28	110.40	106.87
4	A	500	HEM	C3C-C2C-C1C	2.18	109.11	107.05
6	A	799	DP9	NE-CZ-NH2	-2.11	116.38	120.26
4	A	500	HEM	C4B-C3B-C2B	-2.10	105.35	107.28
4	A	500	HEM	CHD-C1D-C2D	-2.05	121.79	125.03

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	882	GOL	O1-C1-C2-O2
8	B	882	GOL	O1-C1-C2-C3
6	A	799	DP9	NE-CD-CG-CB
8	B	880	GOL	O1-C1-C2-C3
8	B	880	GOL	O1-C1-C2-O2
6	B	800	DP9	CA-CB-CG-CD
6	B	800	DP9	O-C-CA-N
6	B	800	DP9	N2'-C-CA-CB
4	A	500	HEM	C4B-C3B-CAB-CBB
6	B	800	DP9	O-C-CA-CB
6	B	800	DP9	N2'-C-CA-N
6	B	800	DP9	CG-CD-NE-CZ
6	A	799	DP9	O-C-CA-N
4	A	500	HEM	CAA-CBA-CGA-O2A
6	A	799	DP9	N2'-C-CA-N

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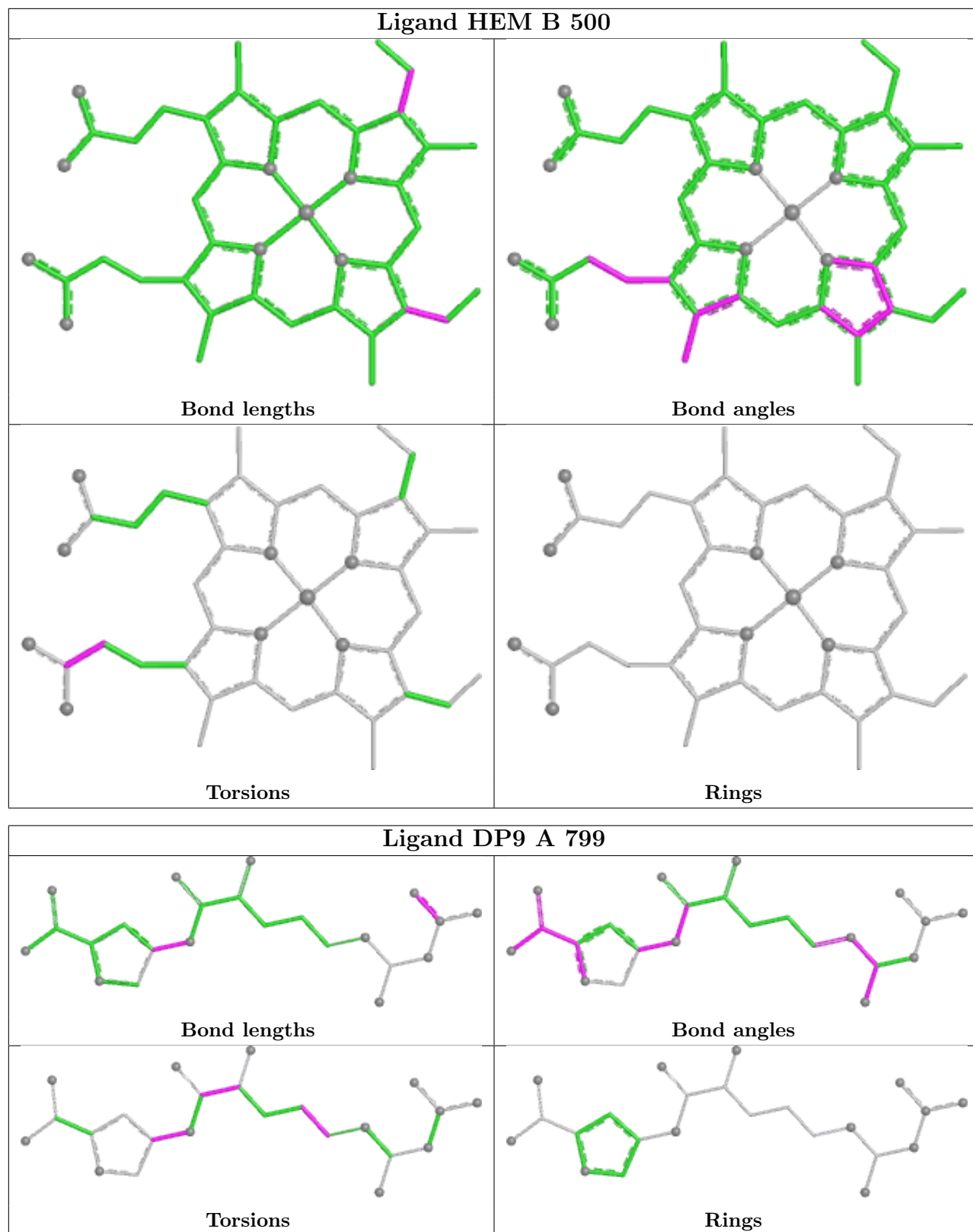
Mol	Chain	Res	Type	Atoms
4	B	500	HEM	CAA-CBA-CGA-O2A
4	B	500	HEM	CAA-CBA-CGA-O1A
6	A	799	DP9	CD'-CG'-N2'-C
4	A	500	HEM	CAA-CBA-CGA-O1A
4	A	500	HEM	CAD-CBD-CGD-O2D
6	B	800	DP9	N-CA-CB-CG
4	A	500	HEM	CAD-CBD-CGD-O1D

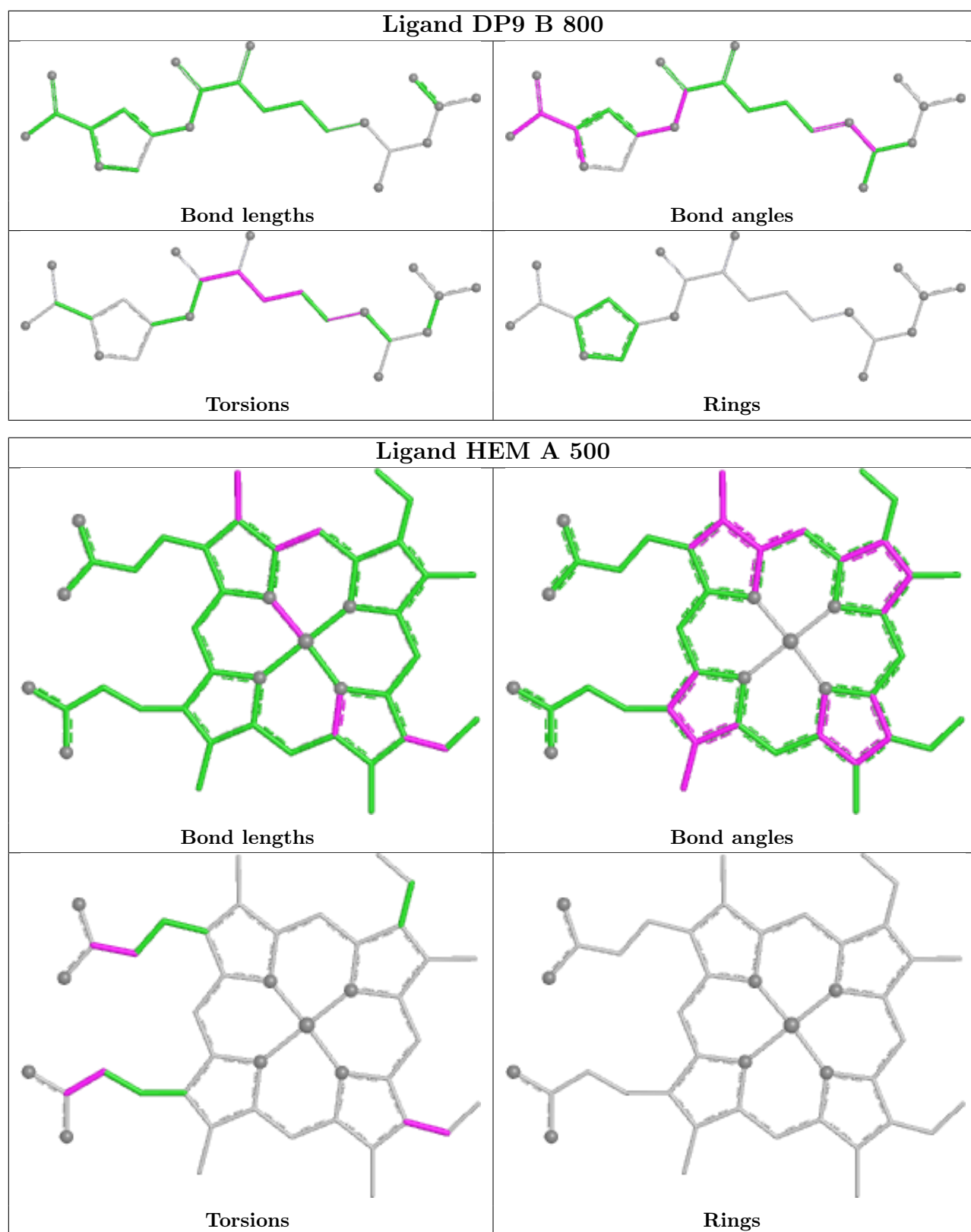
There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500	HEM	1	0
2	B	852	CAC	4	0
8	B	882	GOL	2	0
5	A	760	H4B	2	0
3	A	860	ACT	3	0
6	A	799	DP9	1	0
8	B	880	GOL	1	0
6	B	800	DP9	3	0
2	A	850	CAC	3	0
4	A	500	HEM	3	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 ⓘ

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	406/417 (97%)	-0.11	4 (0%) 79 76	31, 49, 73, 119	0
1	B	404/417 (96%)	0.02	4 (0%) 79 76	32, 53, 78, 115	0
All	All	810/834 (97%)	-0.05	8 (0%) 79 76	31, 50, 76, 119	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	PRO	5.5
1	A	120	PRO	4.4
1	B	121	PRO	4.0
1	A	108	PRO	3.5
1	A	121	PRO	3.1
1	B	122	ALA	2.8
1	A	122	ALA	2.4
1	B	109	ARG	2.4

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,

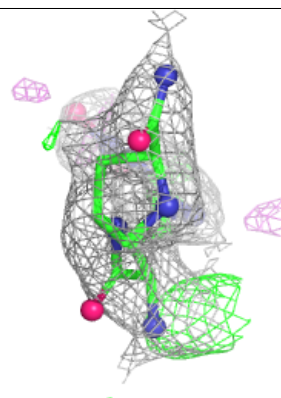
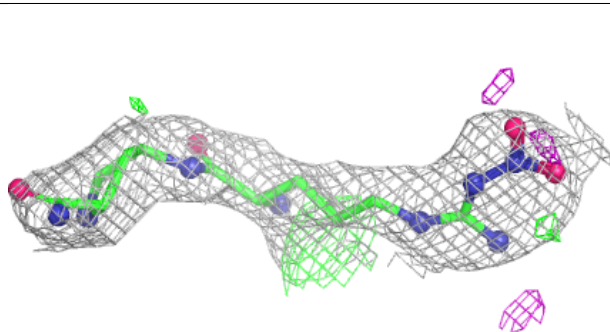
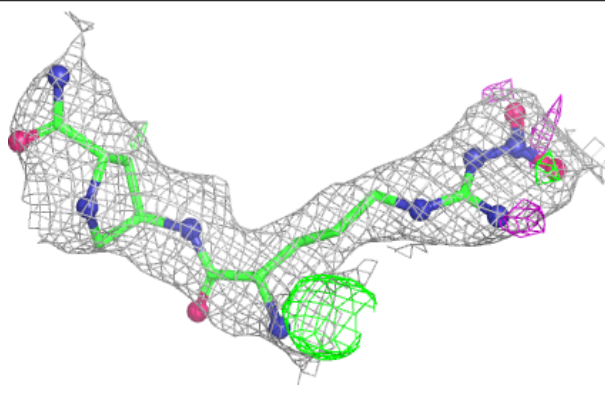
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACT	A	860	4/4	0.82	0.17	40,43,49,52	0
6	DP9	A	799	23/23	0.85	0.13	52,69,72,75	0
6	DP9	B	800	23/23	0.86	0.15	48,66,68,70	0
8	GOL	B	882	6/6	0.89	0.14	67,70,71,72	0
8	GOL	B	880	6/6	0.90	0.11	61,65,68,70	0
2	CAC	B	852	3/5	0.94	0.14	92,92,96,97	0
3	ACT	B	861	4/4	0.95	0.11	46,46,47,47	0
5	H4B	A	760	17/17	0.96	0.06	45,47,49,50	0
5	H4B	B	761	17/17	0.96	0.07	39,41,44,45	0
2	CAC	A	850	3/5	0.97	0.12	83,83,83,84	0
4	HEM	A	500	43/43	0.98	0.07	24,34,50,54	0
4	HEM	B	500	43/43	0.98	0.06	27,33,48,51	0
7	ZN	B	900	1/1	0.99	0.04	50,50,50,50	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.

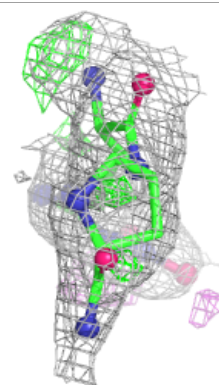
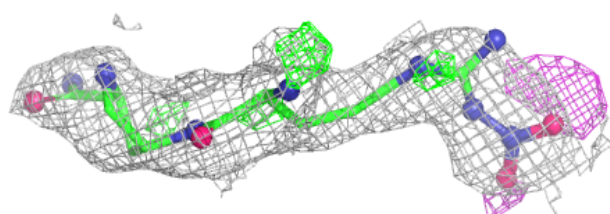
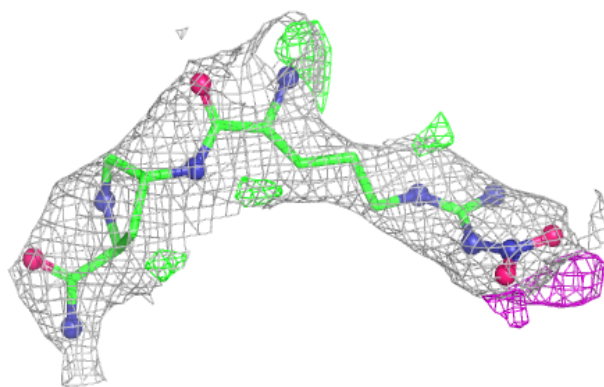
Electron density around DP9 A 799:

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



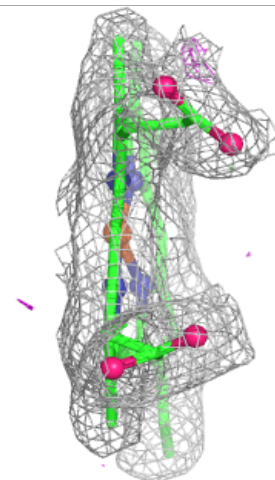
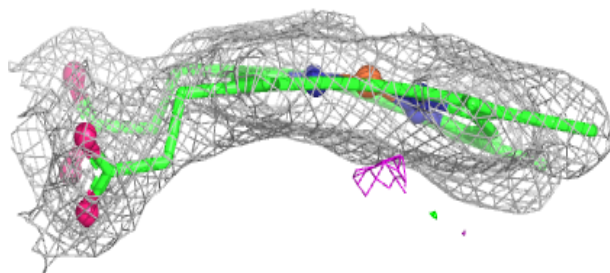
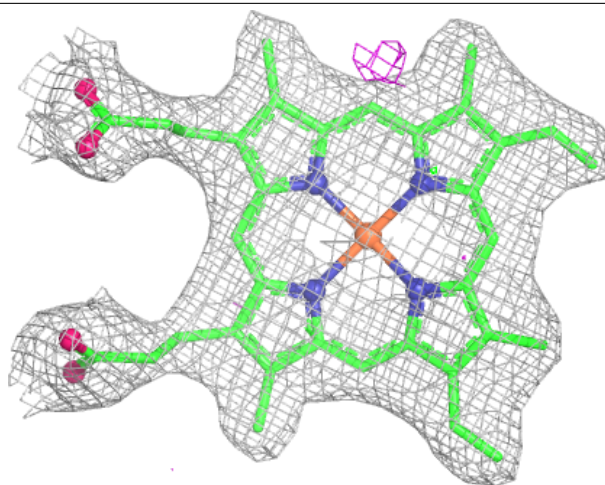
Electron density around DP9 B 800:

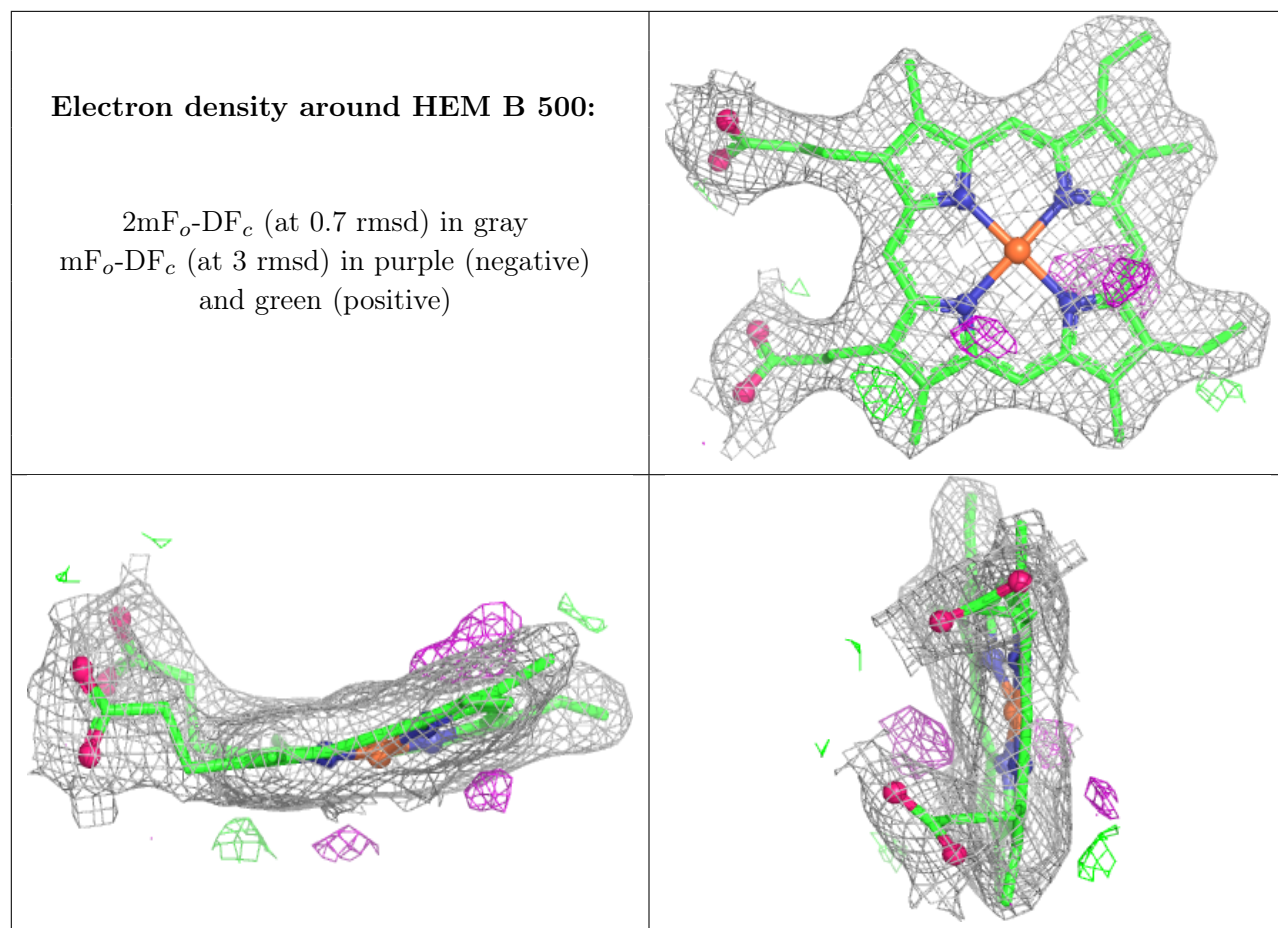
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 500:

$2mF_o-DF_c$ (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.