



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 3O5A / pdb_00003o5a
Title : Crystal Structure of partially reduced Periplasmic Nitrate Reductase from
Cupriavidus necator using Ionic Liquids
Authors : Coelho, C.; Trincao, J.; Romao, M.J.
Deposited on : 2010-07-28
Resolution : 1.72 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

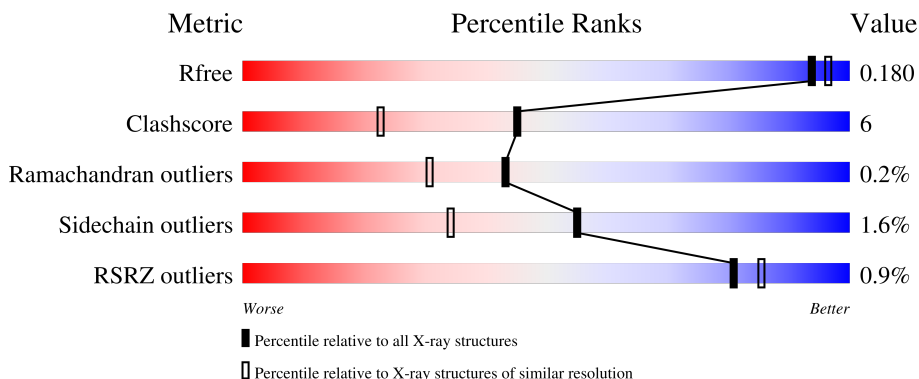
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	802	
2	B	135	

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
6	FMT	A	806	-	-	X	-
6	FMT	A	807	-	-	X	-
6	FMT	B	139	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8171 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.

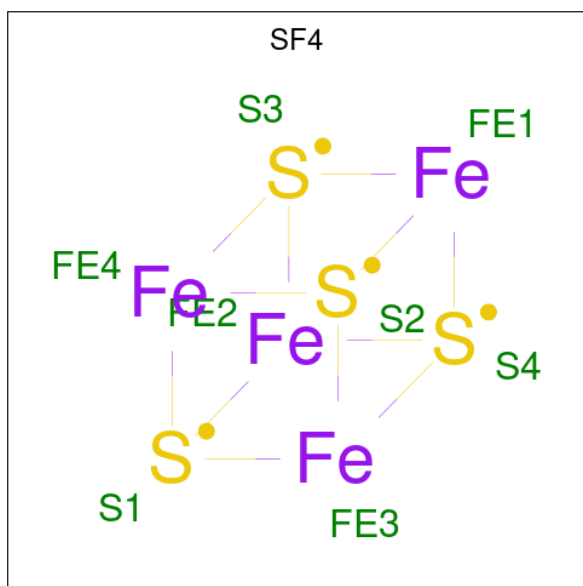
- Molecule 1 is a protein called Periplasmic nitrate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	792	6302	4027	1106	1135	34	0	3	0

- Molecule 2 is a protein called Diheme cytochrome c napB.

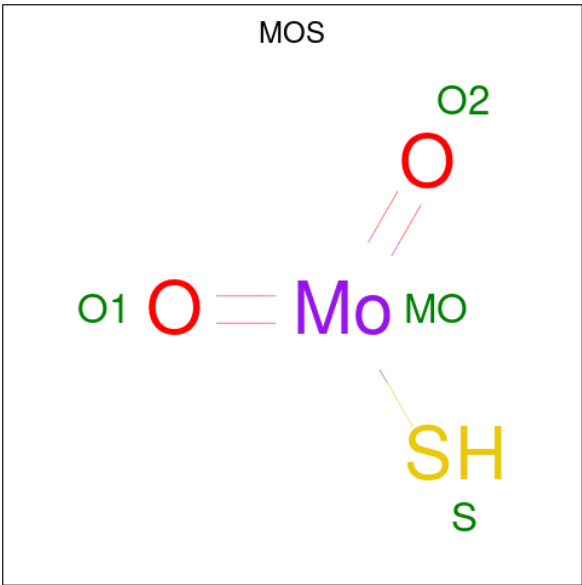
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	108	834	524	150	152	8	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



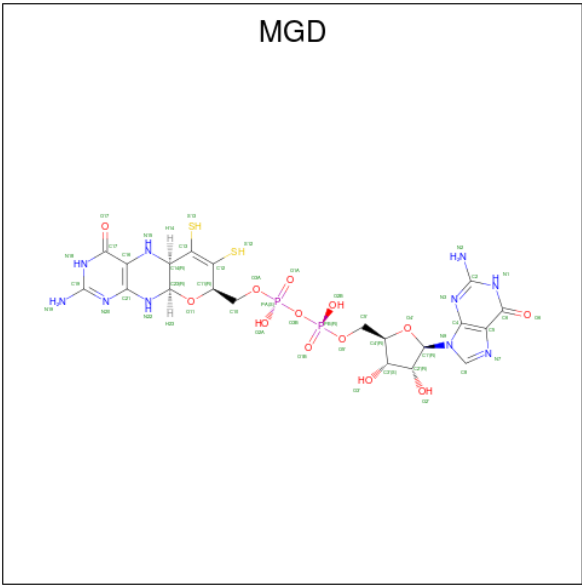
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0

- Molecule 4 is DIOXOTHIO MOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



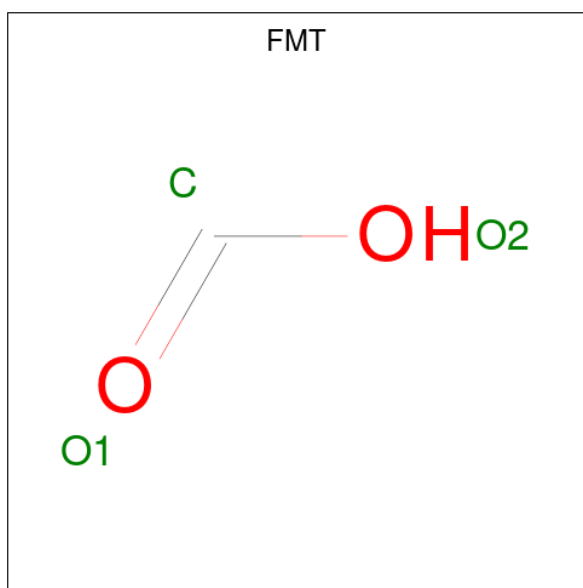
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Mo	S	0	0
			2	1	1		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

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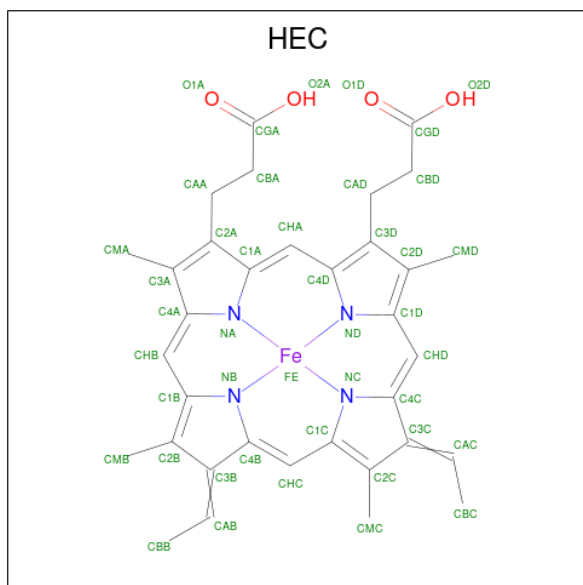
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

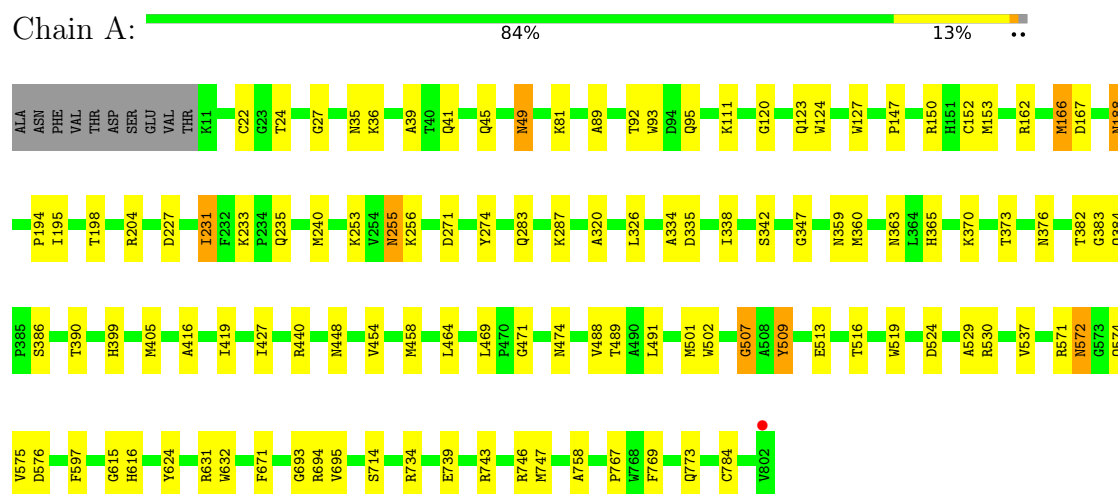
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	701	Total 701	O 701	0	0
9	B	86	Total 86	O 86	0	0

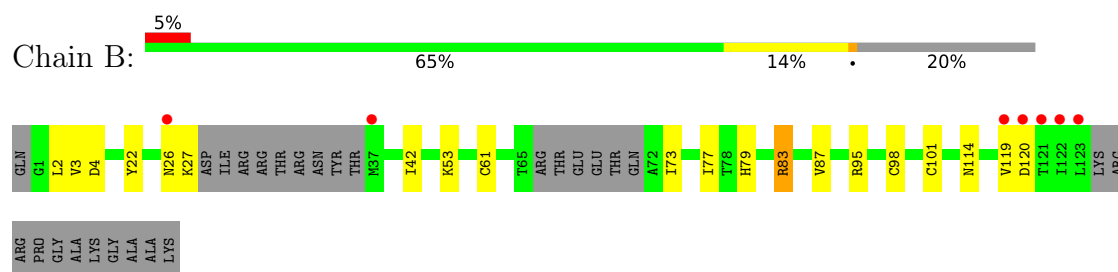
3 Residue-property plots [i](#)

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: Periplasmic nitrate reductase



• Molecule 2: Diheme cytochrome c napB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.40Å 71.41Å 128.41Å 90.00° 121.04° 90.00°	Depositor
Resolution (Å)	27.63 – 1.72 27.63 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.63-1.72) 99.6 (27.63-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.143 , 0.181 0.142 , 0.180	Depositor DCC
R_{free} test set	4889 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8171	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: HEC, MGD, FMT, OCS, SF4, MOS, CL

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	1.49	21/6474 (0.3%)	1.25	13/8780 (0.1%)
2	B	1.43	2/854 (0.2%)	1.29	4/1165 (0.3%)
All	All	1.48	23/7328 (0.3%)	1.25	17/9945 (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	A	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	MET	SD-CE	-8.71	1.57	1.79
1	A	89	ALA	CA-CB	-7.70	1.42	1.54
2	B	83	ARG	CZ-NH1	7.69	1.43	1.32
1	A	93	TRP	N-CA	6.41	1.54	1.46
1	A	320	ALA	CA-CB	6.21	1.63	1.53
1	A	22	CYS	N-CA	6.14	1.53	1.45
1	A	419	ILE	C-O	-5.78	1.17	1.24
1	A	373	THR	N-CA	5.61	1.50	1.45
1	A	390	THR	CA-CB	5.60	1.62	1.53
1	A	405	MET	SD-CE	-5.54	1.65	1.79
2	B	83	ARG	CZ-NH2	5.47	1.40	1.33
1	A	166	MET	CB-CG	-5.37	1.36	1.52
1	A	471	GLY	N-CA	5.29	1.52	1.45
1	A	714	SER	CA-C	-5.21	1.45	1.52
1	A	695	VAL	N-CA	5.18	1.51	1.46
1	A	507	GLY	N-CA	5.17	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ILE	C-O	5.15	1.29	1.24
1	A	758	ALA	CA-CB	5.11	1.60	1.53
1	A	24	THR	C-O	5.06	1.29	1.24
1	A	373	THR	CA-CB	5.06	1.60	1.54
1	A	474	ASN	CA-C	5.04	1.59	1.52
1	A	509	TYR	N-CA	5.03	1.52	1.46
1	A	488	VAL	C-O	-5.01	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	MET	CG-SD-CE	-8.35	82.54	100.90
1	A	469	LEU	CA-C-N	-6.04	113.46	119.56
1	A	469	LEU	C-N-CA	-6.04	113.46	119.56
1	A	571	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	A	440	ARG	N-CA-C	-5.33	105.55	111.36
2	B	22	TYR	CA-C-N	-5.32	114.76	120.03
2	B	22	TYR	C-N-CA	-5.32	114.76	120.03
1	A	537	VAL	N-CA-C	-5.29	105.24	111.00
1	A	743	ARG	CG-CD-NE	5.18	123.39	112.00
1	A	204	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	B	42	ILE	N-CA-C	-5.17	102.54	107.76
1	A	405	MET	CG-SD-CE	-5.16	89.56	100.90
2	B	98	CYS	CB-CA-C	-5.09	102.35	110.79
1	A	530	ARG	CA-CB-CG	-5.08	103.95	114.10
1	A	45	GLN	CA-C-N	-5.05	114.28	121.50
1	A	45	GLN	C-N-CA	-5.05	114.28	121.50
1	A	326	LEU	N-CA-C	-5.05	105.78	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	ASN	Peptide
1	A	632	TRP	Peptide

5.2 Too-close contacts [i](#)

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	6302	0	6168	64	0
2	B	834	0	795	21	0
3	A	8	0	0	0	0
4	A	2	0	0	0	0
5	A	94	0	44	4	0
6	A	39	0	13	8	0
6	B	18	0	6	7	0
7	A	1	0	0	0	0
8	B	86	0	62	8	0
9	A	701	0	0	2	0
9	B	86	0	0	5	0
All	All	8171	0	7088	83	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 6.

All (83) 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)
2:B:73:ILE:HG22	8:B:1128:HEC:O2D	1.49	1.11
2:B:61:CYS:SG	8:B:1128:HEC:HAC	1.95	1.05
1:A:35:ASN:HD21	1:A:524:ASP:H	1.07	1.02
2:B:101:CYS:SG	8:B:1129:HEC:HAC	2.04	0.94
1:A:162:ARG:HE	1:A:359:ASN:HD21	1.15	0.91
1:A:274:TYR:H	1:A:283:GLN:HE22	1.15	0.90
2:B:83:ARG:CD	9:B:700:HOH:O	2.21	0.86
2:B:4:ASP:H	6:B:139:FMT:H	1.39	0.86
1:A:198:THR:HG21	9:B:298:HOH:O	1.76	0.85
1:A:572:ASN:HD21	1:A:575:VAL:H	1.24	0.84
1:A:271:ASP:OD2	1:A:287:LYS:HG2	1.82	0.79
2:B:83:ARG:HD3	9:B:700:HOH:O	1.81	0.78
1:A:233[A]:LYS:HE2	9:A:1438:HOH:O	1.83	0.78
1:A:123:GLN:HG3	1:A:384:GLN:HE21	1.48	0.77
2:B:73:ILE:CG2	8:B:1128:HEC:O2D	2.33	0.76
2:B:4:ASP:H	6:B:139:FMT:C	2.01	0.72
2:B:61:CYS:SG	8:B:1128:HEC:C3C	2.80	0.70
2:B:101:CYS:SG	8:B:1129:HEC:C3C	2.81	0.69
1:A:363:ASN:HD21	1:A:671:PHE:H	1.40	0.69
1:A:41:GLN:CD	9:A:1513:HOH:O	2.37	0.67
1:A:616:HIS:NE2	6:A:807:FMT:O2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ILE:HD11	2:B:87:VAL:HG11	1.78	0.64
1:A:491:LEU:HD11	6:B:139:FMT:H	1.81	0.62
1:A:342:SER:OG	1:A:365:HIS:HE1	1.83	0.61
1:A:49:ASN:HD22	1:A:49:ASN:H	1.48	0.61
1:A:360:MET:HB3	6:A:804:FMT:H	1.82	0.60
1:A:365:HIS:HD2	1:A:370:LYS:O	1.84	0.59
1:A:529:ALA:O	6:A:814:FMT:H	2.02	0.59
1:A:49:ASN:HD22	1:A:49:ASN:N	2.00	0.58
1:A:35:ASN:HD21	1:A:524:ASP:N	1.89	0.58
1:A:572:ASN:ND2	1:A:575:VAL:H	1.97	0.57
1:A:27:GLY:H	1:A:49:ASN:HD21	1.53	0.56
2:B:2:LEU:HD12	6:B:138:FMT:H	1.88	0.56
1:A:399:HIS:ND1	6:A:806:FMT:H	2.21	0.55
1:A:572:ASN:ND2	1:A:574:GLN:H	2.06	0.54
1:A:255:ASN:C	1:A:255:ASN:HD22	2.15	0.54
1:A:35:ASN:ND2	1:A:524:ASP:H	1.90	0.53
1:A:111:LYS:NZ	1:A:448:ASN:HD21	2.05	0.53
2:B:83:ARG:NE	9:B:700:HOH:O	2.39	0.53
1:A:92:THR:H	1:A:95:GLN:HE21	1.57	0.52
1:A:231:ILE:H	6:A:811:FMT:C	2.25	0.50
1:A:153:MET:HG3	1:A:382:THR:HG23	1.93	0.50
2:B:26:ASN:O	2:B:27:LYS:CB	2.59	0.49
2:B:101:CYS:SG	8:B:1129:HEC:CBC	2.99	0.49
1:A:27:GLY:H	1:A:49:ASN:ND2	2.10	0.48
1:A:491:LEU:HD11	6:B:139:FMT:C	2.44	0.48
1:A:516:THR:HB	1:A:624:TYR:CE2	2.49	0.48
1:A:416:ALA:HB3	1:A:427:ILE:CD1	2.44	0.47
1:A:513:GLU:CD	1:A:631:ARG:HD3	2.39	0.47
1:A:347:GLY:HA3	5:A:1804:MGD:N3	2.29	0.46
2:B:61:CYS:HG	8:B:1128:HEC:HAC	1.78	0.46
1:A:227:ASP:OD1	2:B:53:LYS:NZ	2.48	0.46
1:A:734:ARG:HH11	6:A:809:FMT:C	2.29	0.46
1:A:49:ASN:H	1:A:49:ASN:ND2	2.12	0.46
1:A:166:MET:HE1	1:A:615:GLY:HA3	1.99	0.45
1:A:335:ASP:HB3	1:A:338:ILE:HD12	1.98	0.45
1:A:167:ASP:HB3	6:A:807:FMT:C	2.46	0.44
2:B:114:ASN:H	6:B:137:FMT:C	2.29	0.44
1:A:92:THR:H	1:A:95:GLN:NE2	2.15	0.44
1:A:39:ALA:HB2	2:B:119:VAL:HG23	1.98	0.44
1:A:233[A]:LYS:HA	1:A:233[A]:LYS:HD2	1.78	0.44
1:A:458:MET:H	1:A:489:THR:HG1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:HIS:CD2	1:A:370:LYS:O	2.70	0.43
1:A:198:THR:CG2	9:B:298:HOH:O	2.50	0.43
1:A:501:MET:O	1:A:502:TRP:C	2.62	0.43
1:A:386:SER:HB2	1:A:509:TYR:CD2	2.54	0.43
1:A:693:GLY:O	1:A:767:PRO:HA	2.19	0.42
2:B:3:VAL:HG13	6:B:139:FMT:O2	2.19	0.42
1:A:120:GLY:HA3	1:A:124:TRP:CH2	2.54	0.42
1:A:694:ARG:HH22	5:A:1803:MGD:H15	1.65	0.42
1:A:507:GLY:HA3	1:A:519:TRP:CZ2	2.54	0.42
1:A:188:ASN:C	1:A:188:ASN:HD22	2.27	0.41
1:A:383:GLY:HA3	5:A:1804:MGD:C12	2.50	0.41
1:A:150:ARG:HH12	6:A:806:FMT:C	2.33	0.41
1:A:739:GLU:OE2	1:A:746:ARG:HD3	2.19	0.41
1:A:464:LEU:HD23	1:A:464:LEU:C	2.45	0.41
1:A:747:MET:HE2	1:A:773:GLN:HB3	2.01	0.41
2:B:79:HIS:HA	2:B:95:ARG:HG3	2.03	0.41
1:A:572:ASN:HD22	1:A:572:ASN:H	1.69	0.41
1:A:769:PHE:CD2	1:A:769:PHE:C	2.99	0.41
1:A:152[A]:CYS:HB2	5:A:1803:MGD:S13	2.62	0.40
1:A:576:ASP:HA	1:A:597:PHE:CD2	2.55	0.40
1:A:253:LYS:HG3	1:A:334:ALA:HB1	2.03	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	792/802 (99%)	766 (97%)	25 (3%)	1 (0%)	48	34
2	B	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	12	4
All	All	894/937 (95%)	864 (97%)	28 (3%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	ASP
1	A	147	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	654/664 (98%)	642 (98%)	12 (2%)	51	29
2	B	90/118 (76%)	90 (100%)	0	100	100
All	All	744/782 (95%)	732 (98%)	12 (2%)	55	34

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	49	ASN
1	A	81	LYS
1	A	127	TRP
1	A	188	ASN
1	A	194	PRO
1	A	195	ILE
1	A	235	GLN
1	A	255	ASN
1	A	256	LYS
1	A	454	VAL
1	A	572	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	ASN
1	A	95	GLN

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	235	GLN
1	A	251	ASN
1	A	255	ASN
1	A	283	GLN
1	A	350	GLN
1	A	359	ASN
1	A	363	ASN
1	A	365	HIS
1	A	384	GLN
1	A	448	ASN
1	A	456	ASN
1	A	463	ASN
1	A	572	ASN
1	A	773	GLN
2	B	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	OCS	A	784	1	6,8,9	1.89	3 (50%)	7,11,13	1.17	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
1	OCS	A	784	1	-	1/4/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	784	OCS	OD3-SG	-2.93	1.36	1.45
1	A	784	OCS	OD1-SG	-2.13	1.39	1.45
1	A	784	OCS	CB-CA	-2.07	1.52	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	784	OCS	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\# Z > 2$
8	HEC	B	1129	2	46,50,50	2.03	9 (19%)	58,82,82	2.05	17 (29%)
6	FMT	B	140	-	2,2,2	0.71	0	1,1,1	0.12	0
6	FMT	A	811	-	2,2,2	0.60	0	1,1,1	0.18	0
6	FMT	A	804	-	2,2,2	0.99	0	1,1,1	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	A	810	-	2,2,2	0.67	0	1,1,1	0.18	0
3	SF4	A	1801	1	0,12,12	-	-	-	-	-
6	FMT	A	806	-	2,2,2	0.63	0	1,1,1	0.01	0
6	FMT	B	139	-	2,2,2	0.93	0	1,1,1	0.26	0
6	FMT	A	807	-	2,2,2	0.55	0	1,1,1	0.02	0
4	MOS	A	1802	1,5	0,1,3	-	-	-	-	-
6	FMT	A	812	-	2,2,2	0.78	0	1,1,1	0.72	0
5	MGD	A	1803	4	47,52,52	1.51	5 (10%)	58,81,81	2.02	17 (29%)
5	MGD	A	1804	4	47,52,52	1.31	4 (8%)	58,81,81	2.19	17 (29%)
6	FMT	A	815	-	2,2,2	0.67	0	1,1,1	0.39	0
6	FMT	B	137	-	2,2,2	0.86	0	1,1,1	0.01	0
6	FMT	A	814	-	2,2,2	0.75	0	1,1,1	0.36	0
6	FMT	B	136	-	2,2,2	0.66	0	1,1,1	0.19	0
6	FMT	B	138	-	2,2,2	0.85	0	1,1,1	0.18	0
6	FMT	A	803	-	2,2,2	0.87	0	1,1,1	0.93	0
6	FMT	A	808	-	2,2,2	0.66	0	1,1,1	0.17	0
6	FMT	A	809	-	2,2,2	0.76	0	1,1,1	0.18	0
6	FMT	B	135	-	2,2,2	0.89	0	1,1,1	0.80	0
8	HEC	B	1128	2	46,50,50	1.93	6 (13%)	58,82,82	1.94	12 (20%)
6	FMT	A	813	-	2,2,2	0.74	0	1,1,1	0.26	0
6	FMT	A	805	-	2,2,2	0.66	0	1,1,1	0.50	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
8	HEC	B	1129	2	-	6/14/54/54	-
3	SF4	A	1801	1	-	-	0/6/5/5
5	MGD	A	1803	4	-	4/22/66/66	0/6/6/6
5	MGD	A	1804	4	-	2/22/66/66	0/6/6/6
8	HEC	B	1128	2	-	7/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1128	HEC	CAC-C3C	7.49	1.59	1.35
8	B	1129	HEC	CAC-C3C	7.12	1.58	1.35
5	A	1803	MGD	C16-C21	6.94	1.50	1.38
8	B	1129	HEC	CAB-C3B	6.28	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1128	HEC	CAB-C3B	5.50	1.52	1.35
8	B	1128	HEC	C3D-C2D	4.51	1.50	1.38
5	A	1804	MGD	C16-C21	3.95	1.45	1.38
5	A	1803	MGD	O6-C6	3.78	1.30	1.23
8	B	1129	HEC	C3D-C2D	3.61	1.48	1.38
8	B	1129	HEC	C1A-NA	-3.35	1.33	1.39
5	A	1804	MGD	C8-N9	3.18	1.44	1.37
8	B	1128	HEC	CMD-C2D	3.17	1.57	1.50
8	B	1129	HEC	CMC-C2C	3.09	1.57	1.50
5	A	1804	MGD	C6-N1	-3.01	1.33	1.38
5	A	1804	MGD	PA-O3B	2.58	1.62	1.59
8	B	1129	HEC	C2A-C3A	-2.54	1.31	1.36
5	A	1803	MGD	O17-C17	2.47	1.28	1.23
8	B	1128	HEC	CMB-C2B	2.24	1.55	1.50
8	B	1129	HEC	C3B-C4B	-2.23	1.42	1.46
8	B	1129	HEC	C3C-C2C	-2.19	1.33	1.41
8	B	1128	HEC	CAD-C3D	2.11	1.56	1.51
5	A	1803	MGD	PA-O2A	-2.07	1.45	1.55
8	B	1129	HEC	CMB-C2B	2.04	1.55	1.50
5	A	1803	MGD	C5-C4	2.04	1.44	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1128	HEC	CBB-CAB-C3B	-8.61	110.22	127.43
8	B	1129	HEC	CBB-CAB-C3B	-7.76	111.92	127.43
5	A	1804	MGD	C23-C14-N15	7.06	114.80	107.87
5	A	1803	MGD	C23-C14-N15	5.88	113.64	107.87
5	A	1804	MGD	N9-C8-N7	-5.00	104.12	113.40
5	A	1803	MGD	C19-N20-C21	4.76	121.76	113.36
5	A	1804	MGD	O17-C17-C16	-4.43	116.58	127.26
5	A	1803	MGD	O11-C23-N22	-4.41	104.60	108.61
5	A	1804	MGD	C19-N20-C21	4.41	121.14	113.36
8	B	1128	HEC	CAD-CBD-CGD	-4.39	102.01	113.67
8	B	1129	HEC	CHD-C4C-NC	4.16	128.98	124.45
8	B	1129	HEC	CHB-C4A-NA	3.88	128.68	124.45
8	B	1128	HEC	CMC-C2C-C1C	-3.88	119.51	125.42
8	B	1129	HEC	C2A-C1A-NA	-3.79	106.67	110.32
5	A	1803	MGD	C4-C5-N7	-3.74	104.75	110.67
5	A	1804	MGD	O11-C23-N22	-3.70	105.25	108.61
5	A	1804	MGD	C6-C5-C4	-3.59	113.42	118.83
5	A	1804	MGD	C6-C5-N7	3.55	136.76	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1129	HEC	CBC-CAC-C3C	-3.38	120.68	127.43
5	A	1803	MGD	O6-C6-N1	3.37	126.45	120.11
8	B	1128	HEC	CBC-CAC-C3C	-3.34	120.76	127.43
8	B	1129	HEC	CAD-C3D-C4D	3.31	131.40	124.94
5	A	1803	MGD	C6-C5-N7	3.22	136.14	130.29
5	A	1803	MGD	C8-N7-C5	3.21	109.99	104.26
5	A	1804	MGD	C8-N7-C5	3.17	109.90	104.26
5	A	1804	MGD	C8-N9-C4	3.13	111.88	106.03
5	A	1803	MGD	O17-C17-C16	-3.09	119.81	127.26
8	B	1129	HEC	CMC-C2C-C1C	-2.99	120.86	125.42
8	B	1129	HEC	CHA-C1A-NA	2.99	127.70	124.45
5	A	1803	MGD	O11-C23-C14	-2.99	106.97	108.96
5	A	1804	MGD	O6-C6-C5	-2.98	118.66	126.53
8	B	1129	HEC	CHC-C4B-C3B	-2.98	120.19	125.21
8	B	1128	HEC	C4D-ND-C1D	2.97	110.67	105.82
5	A	1803	MGD	O6-C6-C5	-2.91	118.85	126.53
8	B	1128	HEC	C2B-C1B-NB	-2.89	105.50	110.14
8	B	1129	HEC	O2A-CGA-O1A	-2.87	115.96	123.33
5	A	1803	MGD	C4'-O4'-C1'	-2.81	103.26	109.47
5	A	1804	MGD	C5'-C4'-C3'	-2.80	105.14	115.21
5	A	1804	MGD	C19-N18-C17	-2.71	120.19	125.11
5	A	1803	MGD	C5-C4-N3	-2.70	124.08	128.39
8	B	1128	HEC	CAA-CBA-CGA	-2.70	106.51	113.67
5	A	1804	MGD	O3A-C10-C11	-2.65	102.05	108.58
8	B	1129	HEC	C4A-NA-C1A	2.63	110.11	105.82
5	A	1804	MGD	C16-C17-N18	2.59	119.25	112.13
8	B	1129	HEC	O2A-CGA-CBA	2.59	122.19	114.00
8	B	1128	HEC	O2A-CGA-O1A	-2.59	116.68	123.33
8	B	1128	HEC	O2A-CGA-CBA	2.57	122.11	114.00
5	A	1803	MGD	C17-C16-N15	2.53	123.18	116.27
8	B	1129	HEC	CHC-C4B-NB	2.52	127.19	124.45
8	B	1128	HEC	C4B-NB-C1B	2.51	109.92	105.82
5	A	1803	MGD	C1'-N9-C4	-2.47	119.20	126.49
5	A	1803	MGD	O4'-C4'-C3'	2.41	109.94	105.15
5	A	1803	MGD	C5-C4-N9	2.35	109.86	105.66
5	A	1804	MGD	C17-C16-N15	2.34	122.66	116.27
5	A	1803	MGD	O2A-PA-O1A	2.33	123.28	112.44
8	B	1129	HEC	CHA-C4D-ND	2.33	128.08	123.86
5	A	1804	MGD	O2B-PB-O1B	2.32	123.24	112.44
5	A	1804	MGD	C4'-O4'-C1'	-2.31	104.36	109.47
8	B	1128	HEC	CHD-C1D-ND	2.20	127.85	123.86
8	B	1129	HEC	CHA-C4D-C3D	-2.16	120.56	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1129	HEC	CMC-C2C-C3C	2.13	131.56	126.55
8	B	1129	HEC	CBA-CAA-C2A	-2.03	106.92	112.53
8	B	1128	HEC	CHB-C1B-NB	2.03	127.54	123.86

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1803	MGD	PA-O3B-PB-O5'
5	A	1803	MGD	C5'-O5'-PB-O2B
5	A	1803	MGD	C5'-O5'-PB-O3B
8	B	1128	HEC	C2B-C3B-CAB-CBB
8	B	1128	HEC	C4B-C3B-CAB-CBB
8	B	1128	HEC	C2C-C3C-CAC-CBC
8	B	1128	HEC	C4C-C3C-CAC-CBC
8	B	1129	HEC	C2B-C3B-CAB-CBB
8	B	1129	HEC	C4B-C3B-CAB-CBB
8	B	1129	HEC	C2C-C3C-CAC-CBC
8	B	1129	HEC	C4C-C3C-CAC-CBC
5	A	1804	MGD	PB-O3B-PA-O1A
5	A	1803	MGD	C10-O3A-PA-O2A
5	A	1804	MGD	PB-O3B-PA-O2A
8	B	1129	HEC	CAD-CBD-CGD-O1D
8	B	1129	HEC	CAD-CBD-CGD-O2D
8	B	1128	HEC	CAD-CBD-CGD-O2D
8	B	1128	HEC	CAD-CBD-CGD-O1D
8	B	1128	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1129	HEC	3	0
6	A	811	FMT	1	0
6	A	804	FMT	1	0
6	A	806	FMT	2	0
6	B	139	FMT	5	0
6	A	807	FMT	2	0
5	A	1803	MGD	2	0
5	A	1804	MGD	2	0
6	B	137	FMT	1	0

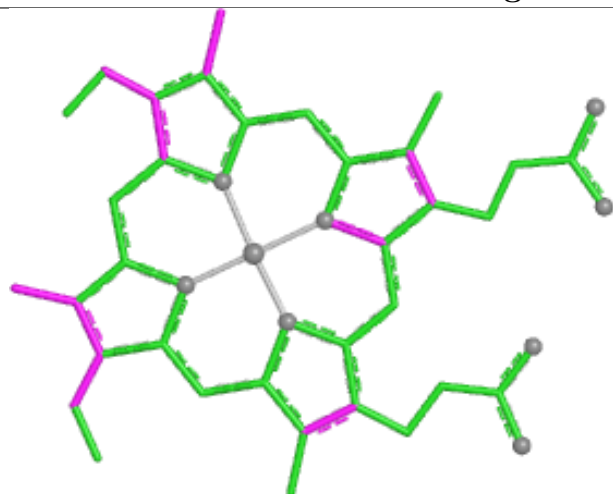
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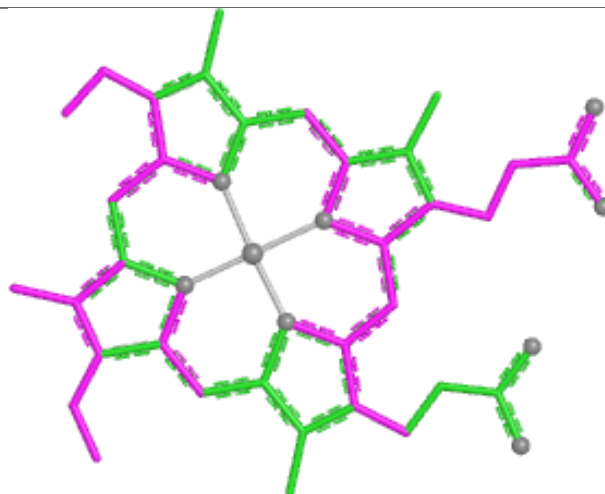
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	814	FMT	1	0
6	B	138	FMT	1	0
6	A	809	FMT	1	0
8	B	1128	HEC	5	0

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

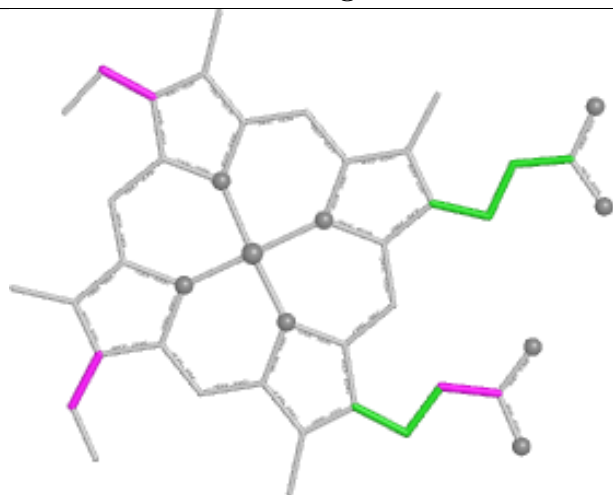
Ligand HEC B 1129



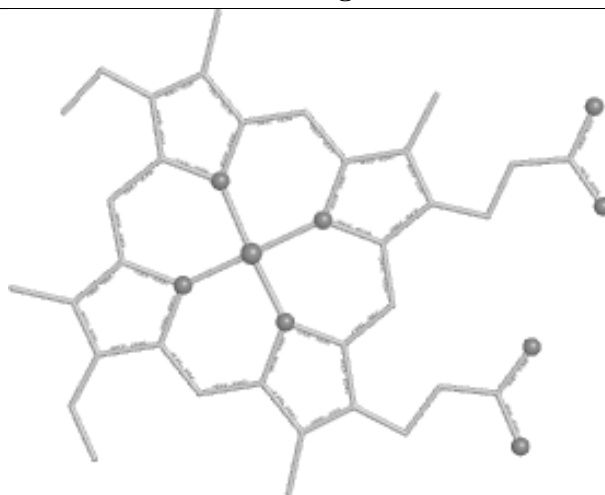
Bond lengths



Bond angles

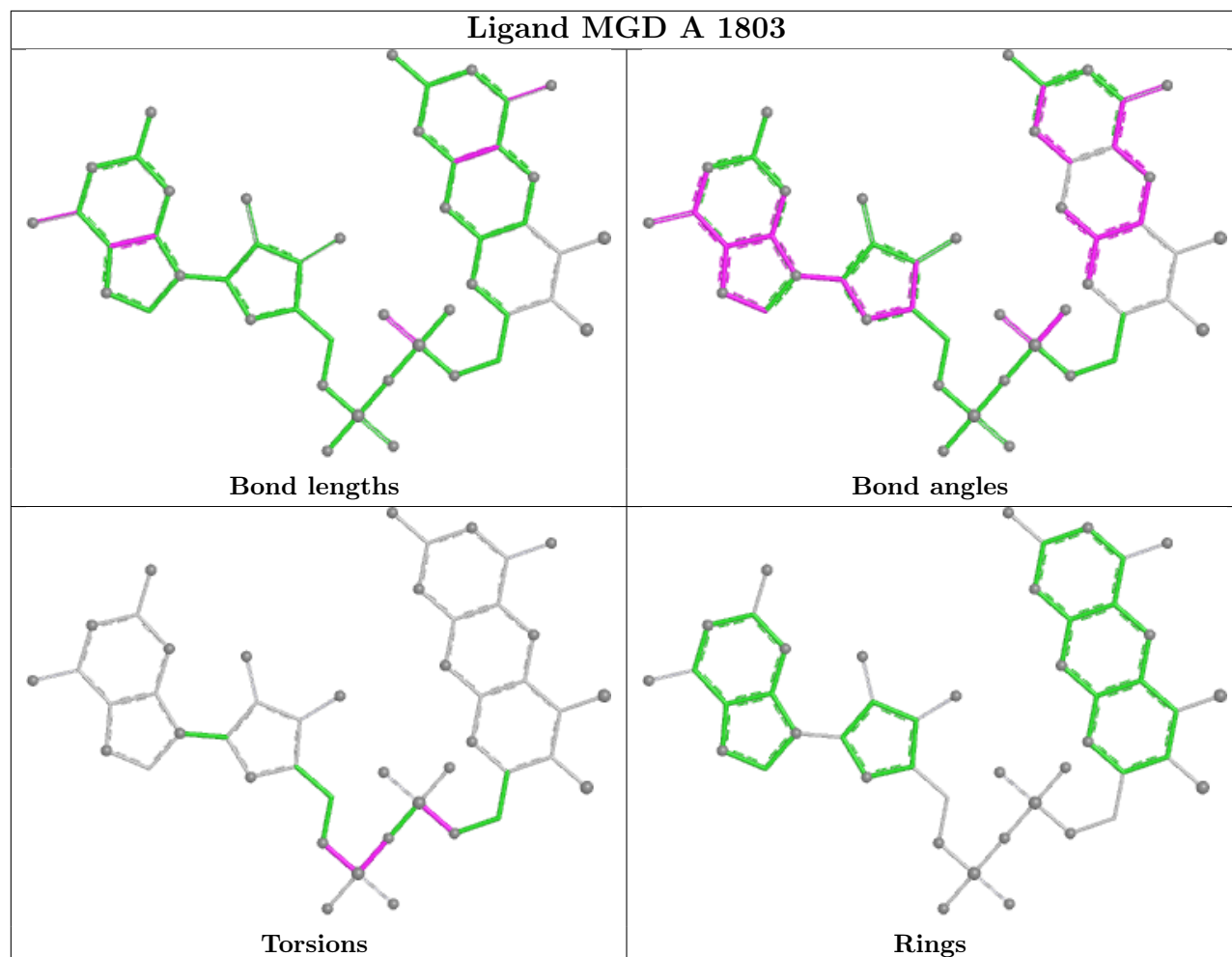


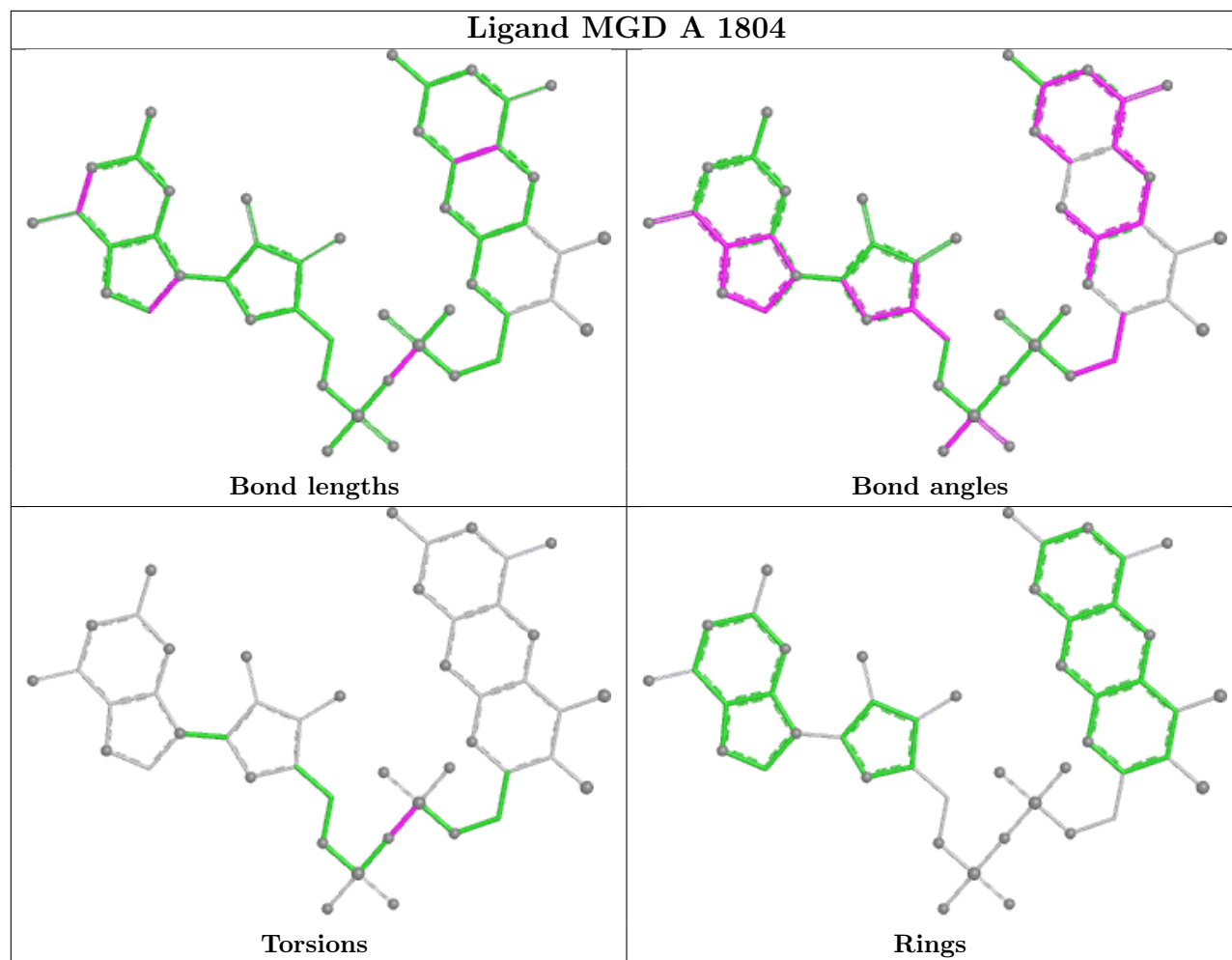
Torsions

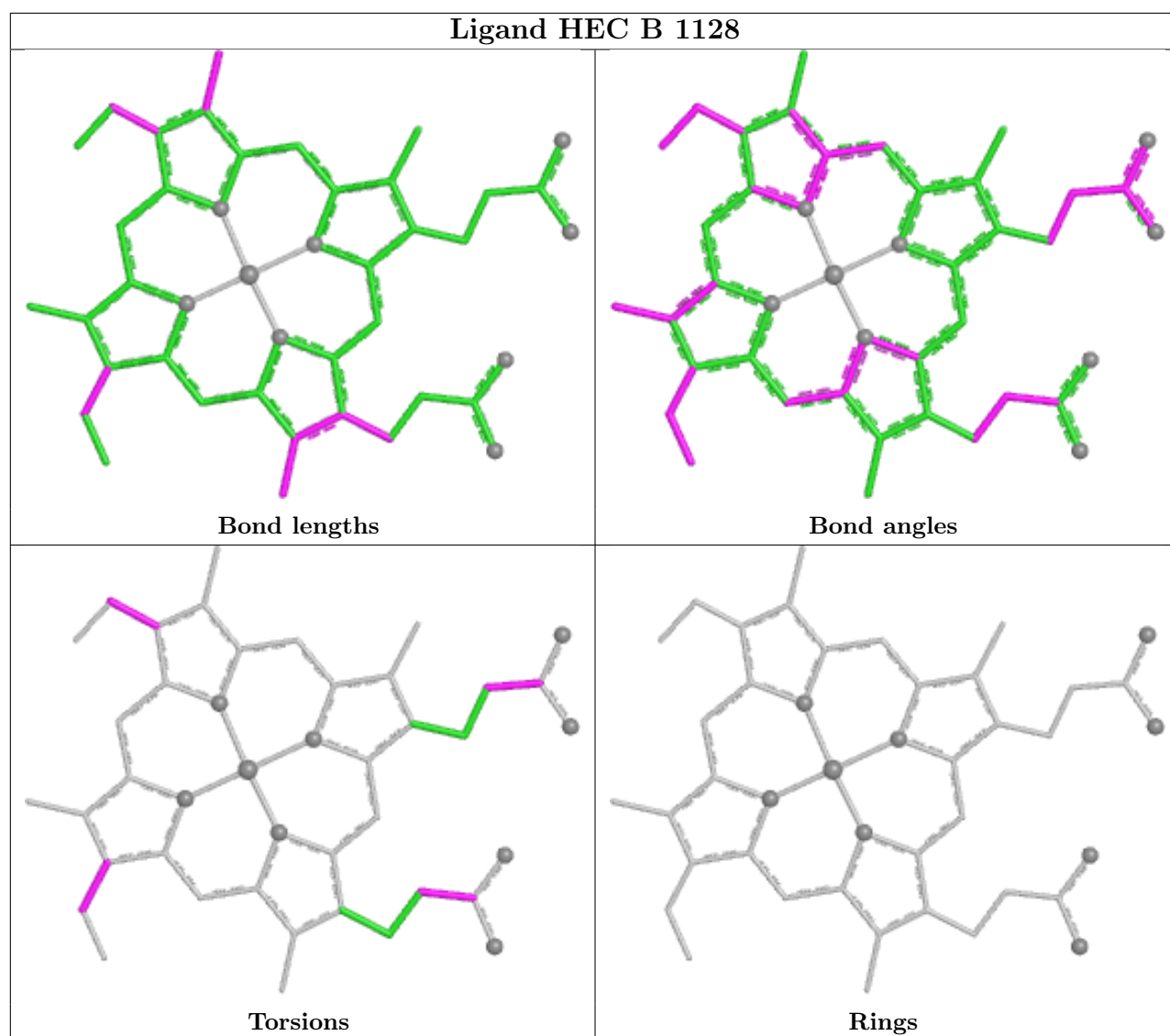


Rings

Ligand MGD A 1803







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	791/802 (98%)	-0.83	1 (0%) 92 93	2, 9, 19, 31	3 (0%)
2	B	108/135 (80%)	-0.09	7 (6%) 25 30	7, 17, 36, 48	0
All	All	899/937 (95%)	-0.74	8 (0%) 81 85	2, 10, 22, 48	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	123	LEU	3.3
2	B	122	ILE	2.9
2	B	37	MET	2.7
2	B	120	ASP	2.7
1	A	802	VAL	2.7
2	B	121	THR	2.5
2	B	119	VAL	2.5
2	B	26	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	A	784	9/10	0.98	0.05	4,6,14,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

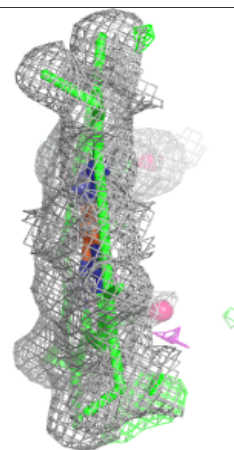
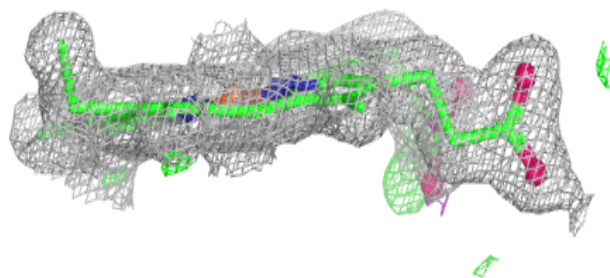
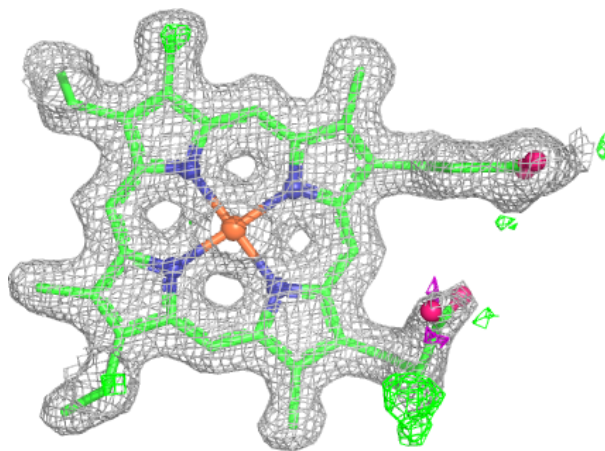
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	FMT	A	812	3/3	0.69	0.14	41,41,42,42	0
6	FMT	A	811	3/3	0.79	0.17	38,38,38,38	0
6	FMT	A	810	3/3	0.81	0.16	42,42,43,44	0
6	FMT	A	809	3/3	0.84	0.12	42,42,43,44	0
6	FMT	A	815	3/3	0.84	0.11	42,42,42,43	0
6	FMT	B	135	3/3	0.85	0.11	33,33,35,37	0
6	FMT	A	813	3/3	0.86	0.10	39,39,42,43	0
6	FMT	B	136	3/3	0.86	0.16	32,32,33,36	0
6	FMT	A	807	3/3	0.87	0.27	35,35,38,40	0
6	FMT	A	806	3/3	0.88	0.18	27,27,29,30	0
6	FMT	B	137	3/3	0.88	0.14	32,32,32,34	0
6	FMT	B	140	3/3	0.89	0.10	44,44,44,44	0
6	FMT	B	139	3/3	0.91	0.19	29,29,30,31	0
6	FMT	A	808	3/3	0.92	0.09	36,36,37,37	0
6	FMT	A	803	3/3	0.93	0.08	17,17,20,22	0
6	FMT	A	814	3/3	0.93	0.16	23,23,24,26	0
6	FMT	A	804	3/3	0.94	0.14	23,23,24,29	0
6	FMT	B	138	3/3	0.95	0.10	28,28,29,32	0
6	FMT	A	805	3/3	0.96	0.09	20,20,20,21	0
8	HEC	B	1128	43/43	0.98	0.07	9,16,30,41	0
5	MGD	A	1803	47/47	0.99	0.03	2,4,6,6	0
7	CL	A	816	1/1	0.99	0.02	13,13,13,13	0
5	MGD	A	1804	47/47	0.99	0.03	2,5,7,8	0
8	HEC	B	1129	43/43	0.99	0.05	3,9,20,26	0
3	SF4	A	1801	8/8	1.00	0.02	5,6,7,7	0
4	MOS	A	1802	2/4	1.00	0.01	5,5,5,8	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.

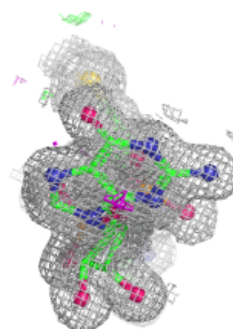
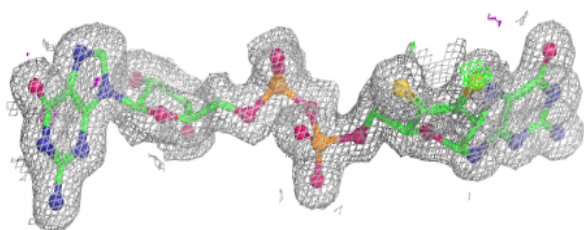
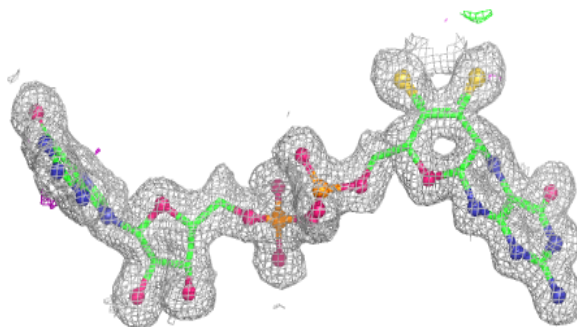
Electron density around HEC B 1128:

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

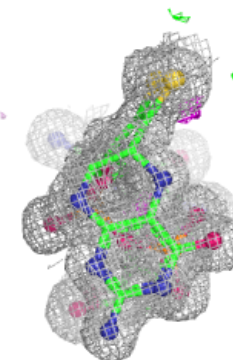
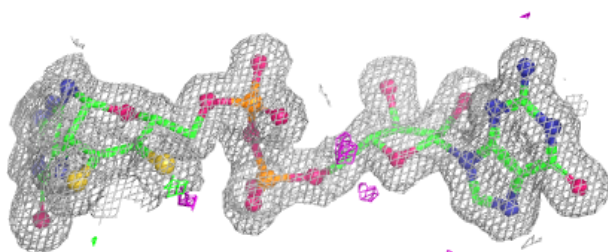
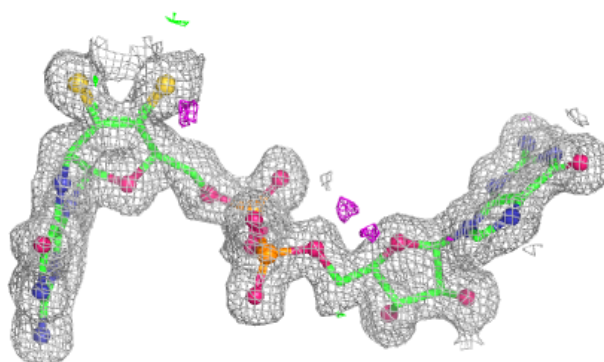


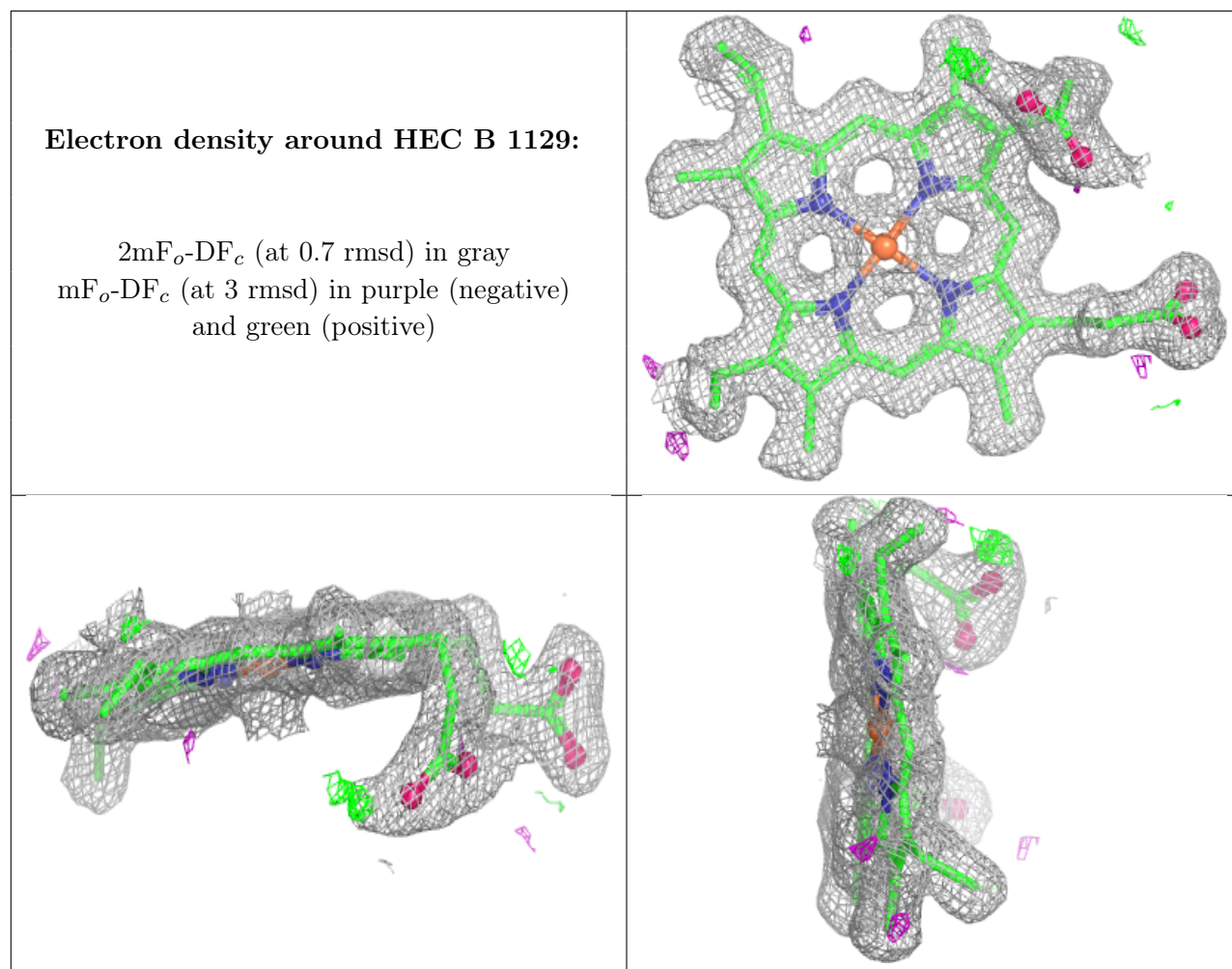
Electron density around MGD A 1803:

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

**Electron density around MGD A 1804:**

$2mF_o-DF_c$ (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.