



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:59 pm BST

PDB ID : 3O5A  
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](mailto: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.

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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 : 2.11  
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) : 2.11

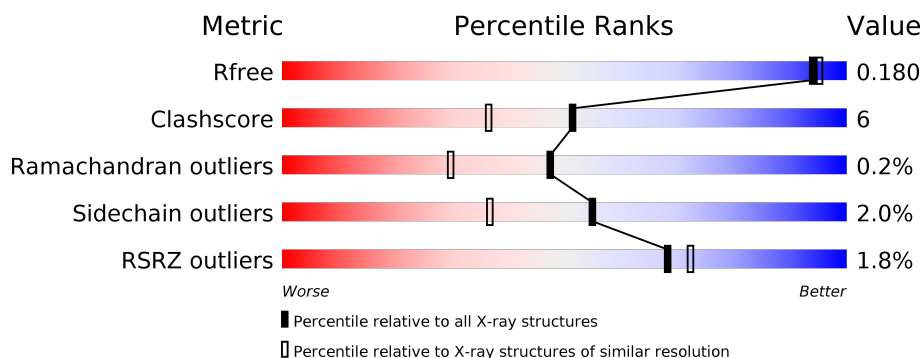
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

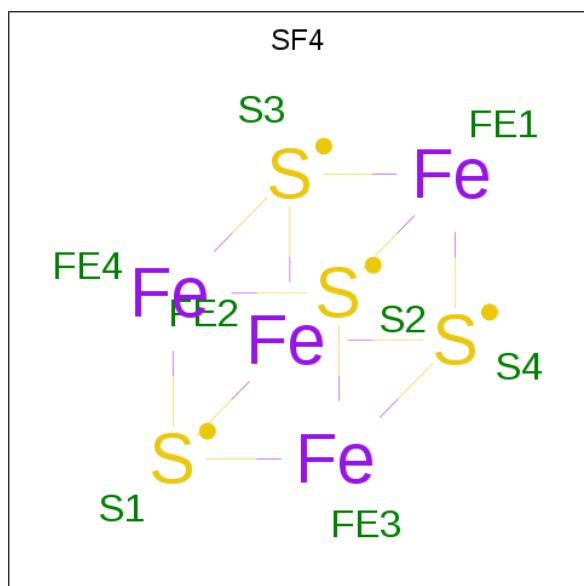
- Molecule 1 is a protein called Periplasmic nitrate reductase.

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.

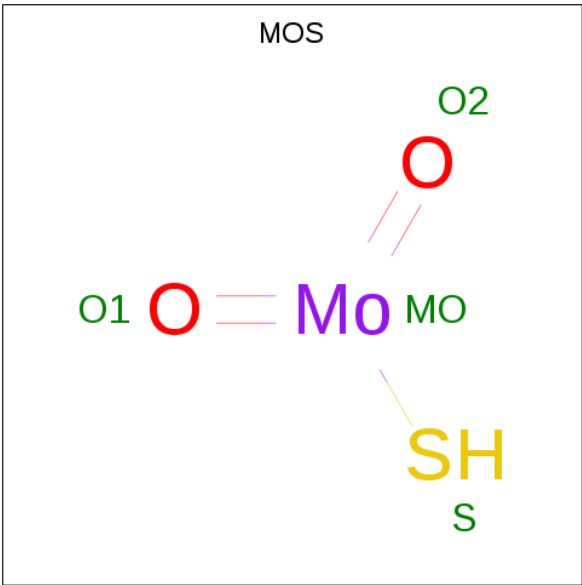
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	108	834	524	150	152	8	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



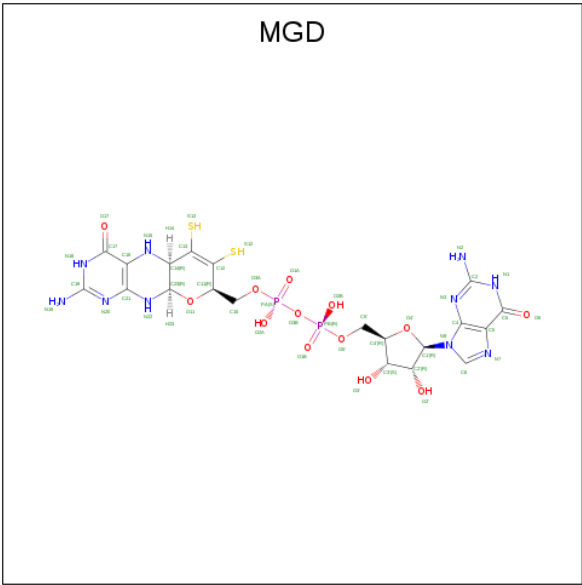
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0

- Molecule 4 is DIOXOTHIO MOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO<sub>2</sub>S).



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 (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



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

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



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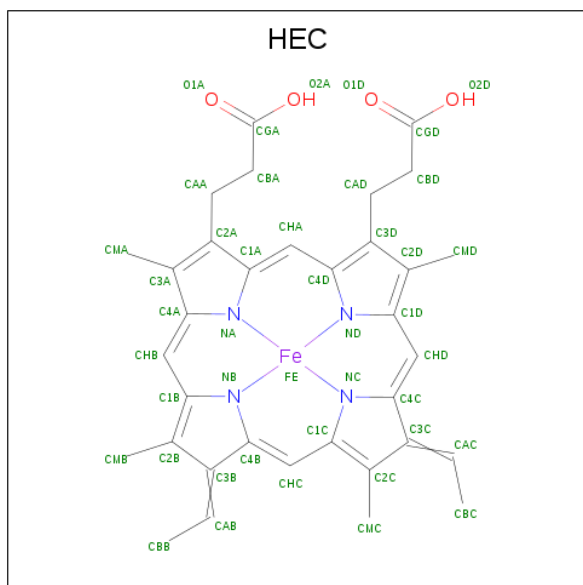
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 9 is water.

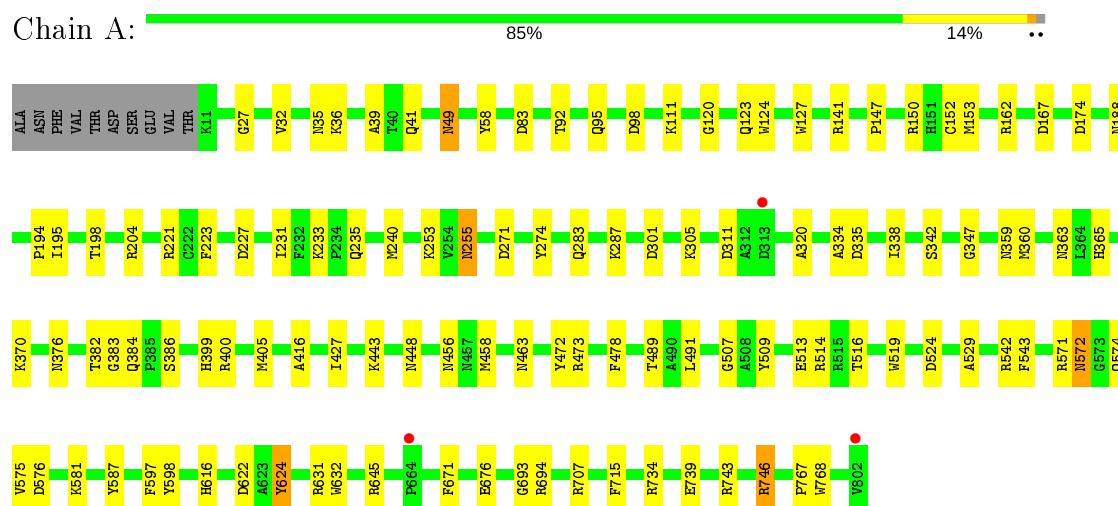
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	701	Total 701	O 701	0	0
9	B	86	Total 86	O 86	0	0



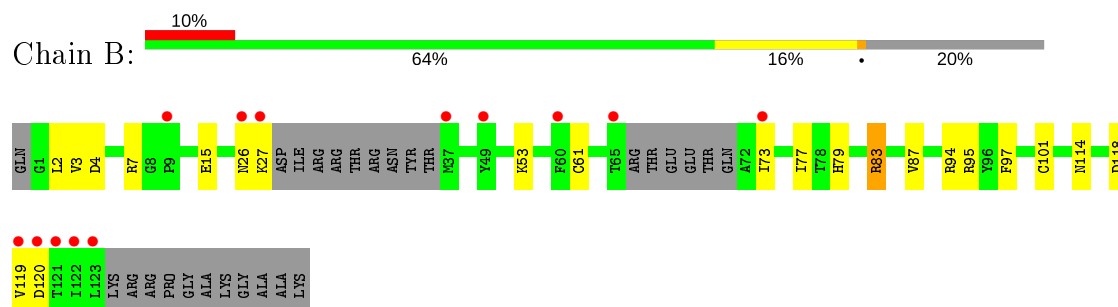
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MGD, MOS, SF4, CL, HEC, OCS, FMT

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	1.29	9/6474 (0.1%)	1.13	26/8780 (0.3%)
2	B	1.19	4/854 (0.5%)	1.11	4/1165 (0.3%)
All	All	1.28	13/7328 (0.2%)	1.12	30/9945 (0.3%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	ARG	CZ-NH1	8.05	1.43	1.33
1	A	472	TYR	CD2-CE2	5.98	1.48	1.39
2	B	15	GLU	CB-CG	-5.83	1.41	1.52
2	B	83	ARG	CZ-NH2	5.78	1.40	1.33
2	B	97	PHE	CE1-CZ	5.62	1.48	1.37
1	A	478	PHE	CE1-CZ	5.54	1.47	1.37
1	A	223	PHE	CE1-CZ	5.38	1.47	1.37
1	A	32	VAL	CB-CG2	5.37	1.64	1.52
1	A	543	PHE	CE1-CZ	5.35	1.47	1.37
1	A	624	TYR	CE2-CZ	5.12	1.45	1.38
1	A	320	ALA	CA-CB	5.12	1.63	1.52
1	A	676	GLU	CB-CG	5.08	1.61	1.52
1	A	768	TRP	CZ3-CH2	5.03	1.48	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	MET	CG-SD-CE	-11.04	82.54	100.20
1	A	301	ASP	CB-CG-OD1	-9.30	109.93	118.30
1	A	141	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	311	ASP	CB-CG-OD2	8.74	126.17	118.30
1	A	571	ARG	NE-CZ-NH1	-8.69	115.95	120.30
1	A	204	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	221	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	542	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	405	MET	CG-SD-CE	-6.65	89.56	100.20
1	A	746	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	746	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	443	LYS	CD-CE-NZ	6.42	126.46	111.70
1	A	400	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	83	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	587	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	A	473	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	622	ASP	CB-CG-OD1	6.01	123.71	118.30
2	B	7	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	645	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	94	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	743	ARG	CG-CD-NE	5.52	123.39	111.80
1	A	98	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	58	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	195	ILE	CG1-CB-CG2	-5.44	99.44	111.40
2	B	94	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	141	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	B	118	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	707	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	311	ASP	CB-CG-OD1	-5.12	113.70	118.30
1	A	514	ARG	NE-CZ-NH1	-5.10	117.75	120.30

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

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	60	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	79	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 (79) 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: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:41:GLN:CD	9:A:1513:HOH:O	2.37	0.62
1:A:342:SER:OG	1:A:365:HIS:HE1	1.83	0.61
1:A:49:ASN:H	1:A:49:ASN:HD22	1.48	0.61
1:A:360:MET:HB3	6:A:804:FMT:H	1.82	0.60
1:A:111:LYS:HZ2	1:A:448:ASN:HD21	1.50	0.59
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: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
2:B:95:ARG:HA	8:B:1129:HEC:HMC2	1.94	0.50
1:A:153:MET:HG3	1:A:382:THR:HG23	1.93	0.50
1:A:255:ASN:C	1:A:255:ASN:HD22	2.15	0.49
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:516:THR:HB	1:A:624:TYR:CE2	2.49	0.48
1:A:491:LEU:HD11	6:B:139:FMT:C	2.44	0.48
1:A:416:ALA:HB3	1:A:427:ILE:CD1	2.44	0.47
1:A:347:GLY:HA3	5:A:1804:MGD:N3	2.29	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:ND2	1:A:49:ASN:H	2.12	0.46
1:A:335:ASP:HB3	1:A:338:ILE:HD12	1.98	0.45
1:A:49:ASN:ND2	1:A:49:ASN:N	2.64	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:MET:H	1:A:489:THR:HG1	1.67	0.43
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: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:513:GLU:CD	1:A:631:ARG:HD3	2.39	0.42
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
2:B:79:HIS:HA	2:B:95:ARG:HG3	2.03	0.41
1:A:572:ASN:H	1:A:572:ASN:HD22	1.69	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 [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	792/802 (99%)	766 (97%)	25 (3%)	1 (0%)	51	33
2	B	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	15	4
All	All	894/937 (95%)	864 (97%)	28 (3%)	2 (0%)	47	30

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%)	639 (98%)	15 (2%)	50	31
2	B	90/118 (76%)	90 (100%)	0	100	100
All	All	744/782 (95%)	729 (98%)	15 (2%)	55	37

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

Mol	Chain	Res	Type
1	A	36	LYS
1	A	49	ASN
1	A	127	TRP
1	A	174	ASP
1	A	188	ASN
1	A	194	PRO
1	A	235	GLN
1	A	255	ASN
1	A	305	LYS
1	A	456	ASN
1	A	463	ASN
1	A	572	ASN
1	A	581	LYS
1	A	598	TYR
1	A	715	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	188	ASN
1	A	235	GLN
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	517	GLN
1	A	535	GLN
1	A	572	ASN
1	A	717	ASN
1	A	773	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	7,8,9	1.70	2 (28%)	6,11,13	1.15	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	784	OCS	OD3-SG	-2.77	1.36	1.45
1	A	784	OCS	OD1-SG	-2.00	1.39	1.45

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 carbohydrates 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	$\# Z  > 2$
6	FMT	B	135	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	140	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	139	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MOS	A	1802	1,5	0,1,3	0.00	-	-		
6	FMT	A	815	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	805	-	0,2,2	0.00	-	0,1,1	0.00	-
8	HEC	B	1129	2	26,50,50	2.26	7 (26%)	18,82,82	2.21	6 (33%)
6	FMT	A	813	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	804	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	810	-	0,2,2	0.00	-	0,1,1	0.00	-
5	MGD	A	1804	4	41,52,52	1.29	4 (9%)	43,81,81	2.44	17 (39%)
8	HEC	B	1128	2	26,50,50	2.18	9 (34%)	18,82,82	2.63	6 (33%)
6	FMT	A	806	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	808	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SF4	A	1801	1	0,12,12	0.00	-	-		
6	FMT	A	812	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	138	-	0,2,2	0.00	-	0,1,1	0.00	-
5	MGD	A	1803	4	41,52,52	1.48	8 (19%)	43,81,81	2.44	16 (37%)
6	FMT	A	814	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	136	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	811	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	809	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	137	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	803	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	807	-	0,2,2	0.00	-	0,1,1	0.00	-

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	SF4	A	1801	1	-	-	0/6/5/5
8	HEC	B	1129	2	-	0/6/54/54	-
5	MGD	A	1804	4	-	2/18/66/66	0/6/6/6
8	HEC	B	1128	2	-	0/6/54/54	-
5	MGD	A	1803	4	-	5/18/66/66	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1129	HEC	C3C-C2C	-6.69	1.33	1.40
8	B	1128	HEC	C3C-C2C	-5.90	1.34	1.40
8	B	1129	HEC	C3B-C2B	-5.45	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1803	MGD	C16-C21	4.80	1.50	1.41
8	B	1128	HEC	C3D-C2D	4.38	1.50	1.37
5	A	1803	MGD	C17-N18	3.89	1.39	1.33
5	A	1804	MGD	C6-C5	3.65	1.47	1.41
8	B	1129	HEC	C3D-C2D	3.59	1.48	1.37
8	B	1128	HEC	C3B-C2B	-3.47	1.37	1.40
8	B	1128	HEC	CAD-C3D	3.21	1.56	1.52
5	A	1804	MGD	C17-N18	2.91	1.38	1.33
5	A	1803	MGD	C17-C16	2.78	1.45	1.41
8	B	1128	HEC	CMD-C2D	2.70	1.57	1.51
8	B	1128	HEC	C1D-ND	2.51	1.41	1.36
5	A	1803	MGD	O6-C6	2.46	1.30	1.24
8	B	1129	HEC	C1D-ND	2.44	1.41	1.36
8	B	1129	HEC	CMC-C2C	2.33	1.57	1.51
8	B	1128	HEC	C1A-C2A	2.30	1.47	1.42
8	B	1129	HEC	C3C-C4C	2.28	1.47	1.43
5	A	1803	MGD	C6-N1	2.26	1.37	1.33
5	A	1803	MGD	C14-N15	2.23	1.48	1.45
8	B	1128	HEC	C3C-C4C	2.19	1.47	1.43
5	A	1803	MGD	C6-C5	2.18	1.45	1.41
8	B	1129	HEC	C2A-C3A	-2.15	1.31	1.37
5	A	1804	MGD	C16-C21	2.10	1.45	1.41
8	B	1128	HEC	CAA-C2A	2.08	1.55	1.52
5	A	1803	MGD	PA-O2A	-2.04	1.45	1.55
5	A	1804	MGD	O4'-C1'	2.04	1.43	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1804	MGD	C6-C5-C4	-7.73	113.42	120.80
5	A	1803	MGD	C5-C6-N1	-6.42	114.65	123.43
8	B	1128	HEC	CAD-CBD-CGD	-6.35	102.01	112.67
8	B	1128	HEC	CMC-C2C-C1C	-5.83	119.51	128.46
8	B	1129	HEC	CMC-C2C-C1C	-4.95	120.86	128.46
8	B	1129	HEC	CMC-C2C-C3C	4.88	131.56	125.82
5	A	1803	MGD	C17-C16-N15	4.83	123.18	119.12
5	A	1804	MGD	C6-N1-C2	4.73	123.45	115.93
5	A	1803	MGD	C6-N1-C2	4.47	123.04	115.93
5	A	1803	MGD	C4-C5-N7	-4.46	104.75	109.40
5	A	1804	MGD	C5-C6-N1	-4.31	117.54	123.43
5	A	1803	MGD	C1'-N9-C4	-4.23	119.20	126.64
5	A	1804	MGD	C16-C21-N22	4.22	121.99	118.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1804	MGD	C17-C16-N15	4.21	122.66	119.12
5	A	1803	MGD	C16-C21-N22	4.15	121.92	118.13
5	A	1803	MGD	O11-C23-N22	-3.86	104.60	108.57
5	A	1803	MGD	C17-N18-C19	3.78	121.93	115.93
5	A	1804	MGD	C21-N22-C23	-3.73	116.36	123.67
8	B	1128	HEC	CAA-CBA-CGA	-3.67	106.51	112.67
5	A	1803	MGD	C17-C16-C21	3.57	117.74	114.57
8	B	1128	HEC	CMC-C2C-C3C	3.53	129.97	125.82
5	A	1804	MGD	C23-C14-C13	-3.50	102.68	110.53
8	B	1128	HEC	CMB-C2B-C1B	-3.33	123.35	128.46
5	A	1804	MGD	O11-C23-N22	-3.23	105.25	108.57
5	A	1803	MGD	C19-N20-C21	3.22	121.76	114.54
8	B	1129	HEC	CBA-CAA-C2A	-3.02	106.92	112.48
5	A	1803	MGD	O11-C23-C14	-2.99	106.97	108.96
5	A	1804	MGD	C19-N20-C21	2.94	121.14	114.54
5	A	1804	MGD	N3-C2-N1	-2.73	123.58	127.22
5	A	1804	MGD	C17-C16-C21	2.70	116.97	114.57
5	A	1804	MGD	C17-N18-C19	2.68	120.19	115.93
5	A	1804	MGD	C5'-C4'-C3'	-2.68	105.14	115.18
8	B	1129	HEC	CBD-CAD-C3D	-2.49	107.89	112.49
5	A	1803	MGD	O4'-C4'-C3'	2.44	109.94	105.11
5	A	1803	MGD	C16-C17-N18	-2.26	117.57	124.01
5	A	1803	MGD	O2A-PA-O1A	2.23	123.28	112.24
5	A	1804	MGD	O2B-PB-O1B	2.23	123.24	112.24
8	B	1128	HEC	CMA-C3A-C2A	2.17	129.04	124.94
5	A	1804	MGD	N18-C19-N20	-2.14	122.06	125.42
8	B	1129	HEC	C3C-C4C-NC	-2.12	106.94	110.94
5	A	1804	MGD	N19-C19-N20	2.09	120.50	117.25
8	B	1129	HEC	CMA-C3A-C2A	2.07	128.85	124.94
5	A	1803	MGD	C16-N15-C14	-2.03	112.63	120.00
5	A	1804	MGD	O4'-C1'-C2'	-2.02	103.97	106.93
5	A	1803	MGD	N18-C19-N20	-2.01	122.26	125.42

There are no chirality outliers.

All (7) 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
5	A	1804	MGD	PB-O3B-PA-O1A
5	A	1803	MGD	C10-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	A	1804	MGD	PB-O3B-PA-O2A
5	A	1803	MGD	O4'-C4'-C5'-O5'

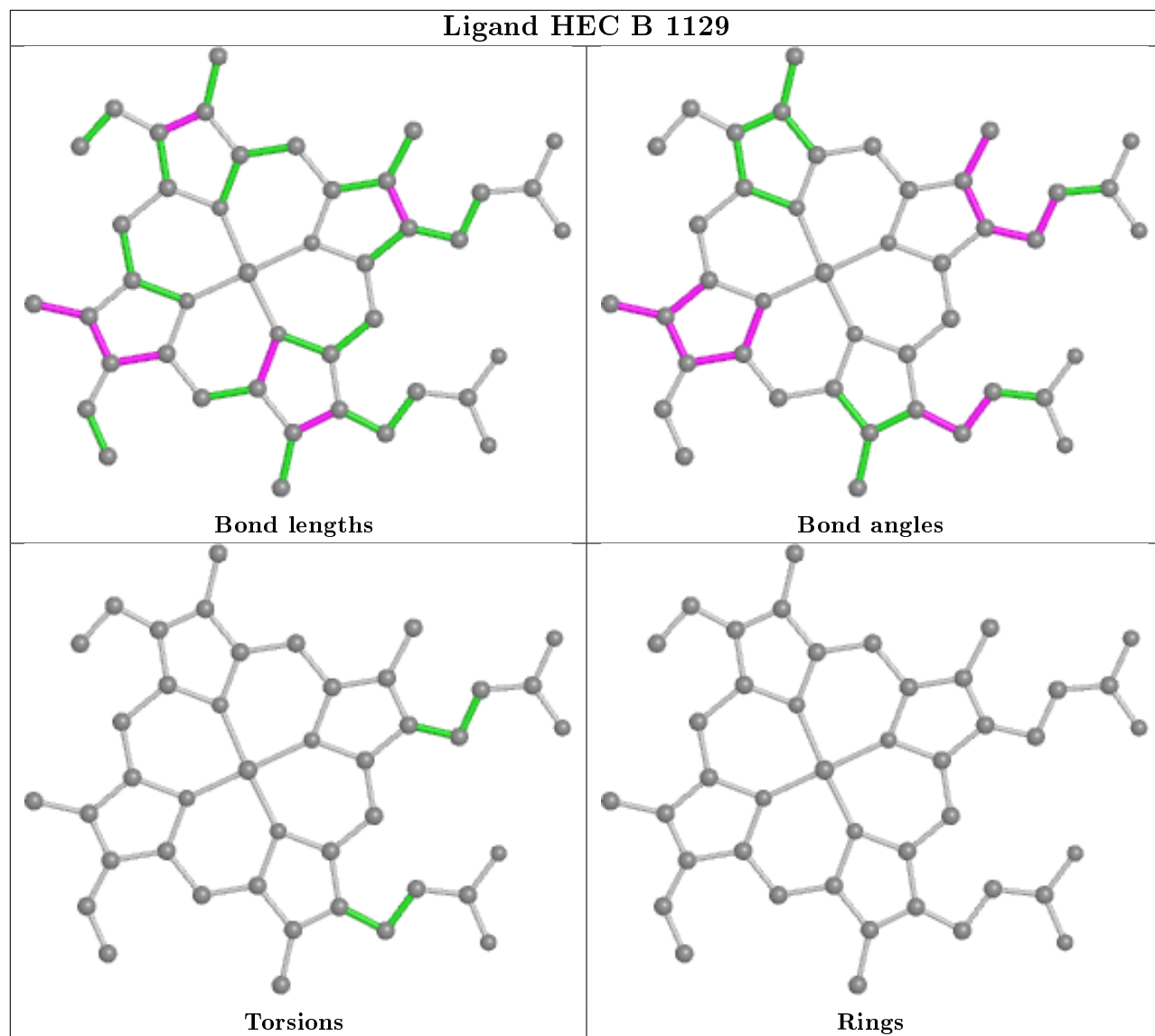
There are no ring outliers.

13 monomers are involved in 27 short contacts:

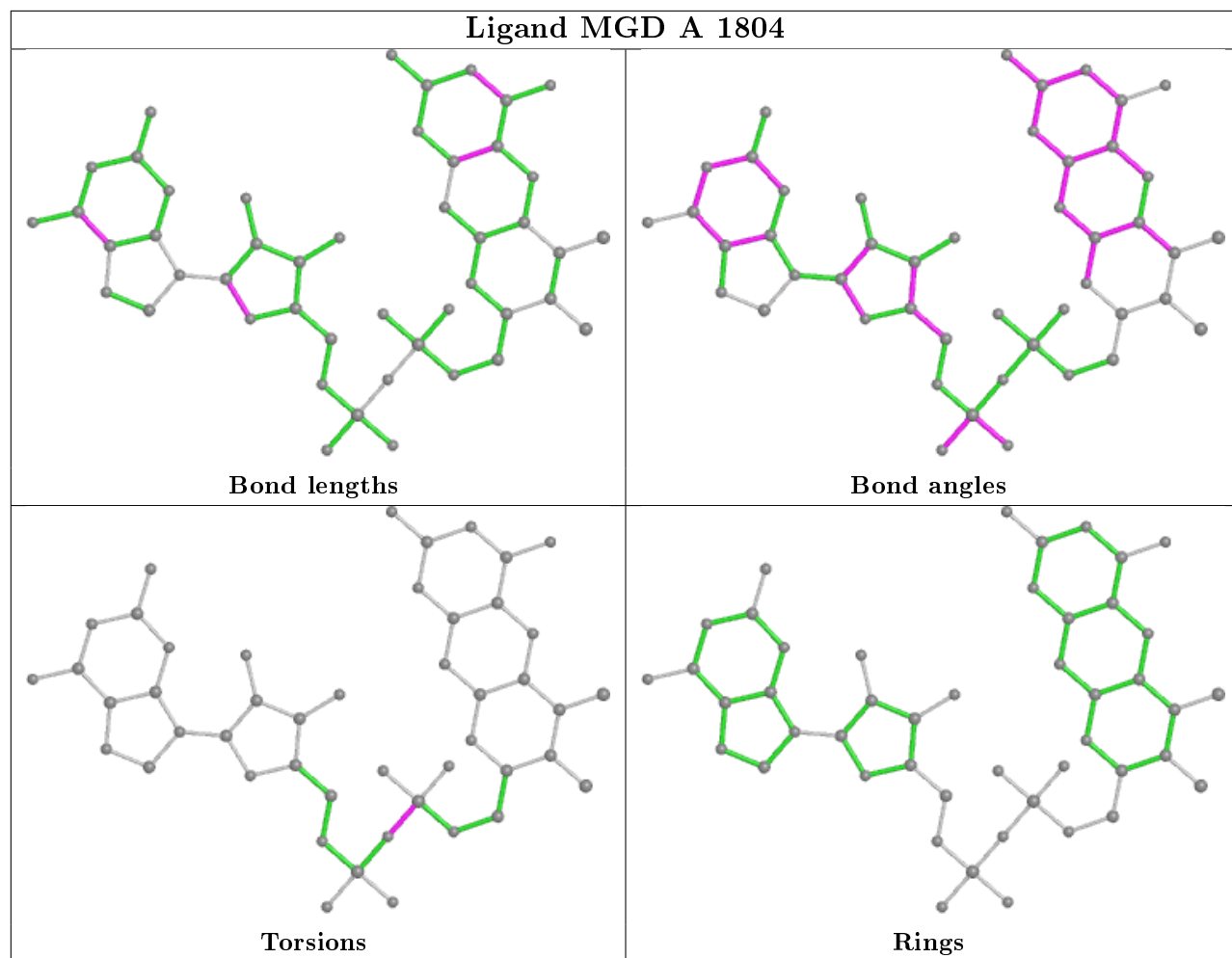
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	139	FMT	5	0
8	B	1129	HEC	4	0
6	A	804	FMT	1	0
5	A	1804	MGD	2	0
8	B	1128	HEC	4	0
6	A	806	FMT	2	0
6	B	138	FMT	1	0
5	A	1803	MGD	2	0
6	A	814	FMT	1	0
6	A	811	FMT	1	0
6	A	809	FMT	1	0
6	B	137	FMT	1	0
6	A	807	FMT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

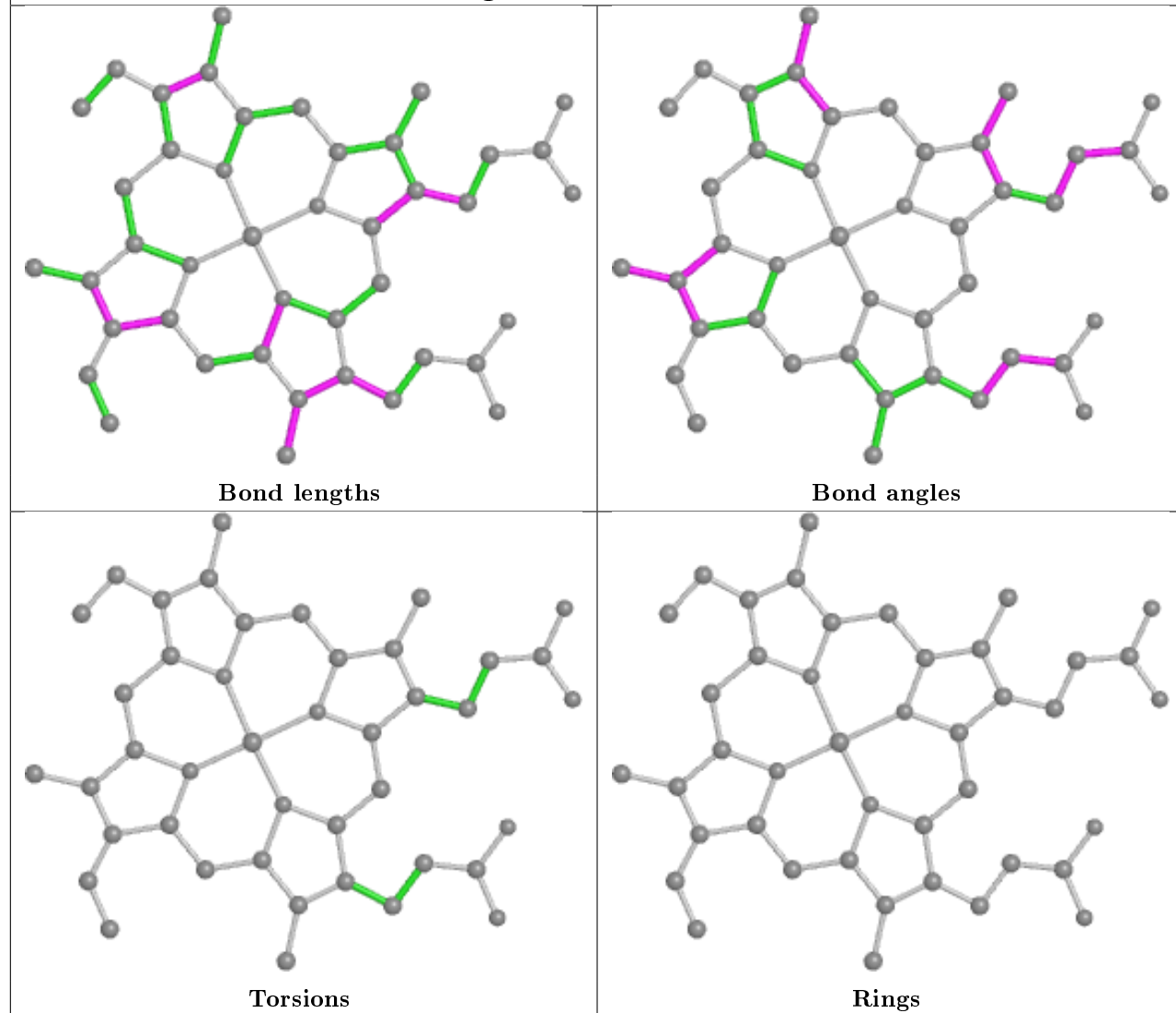


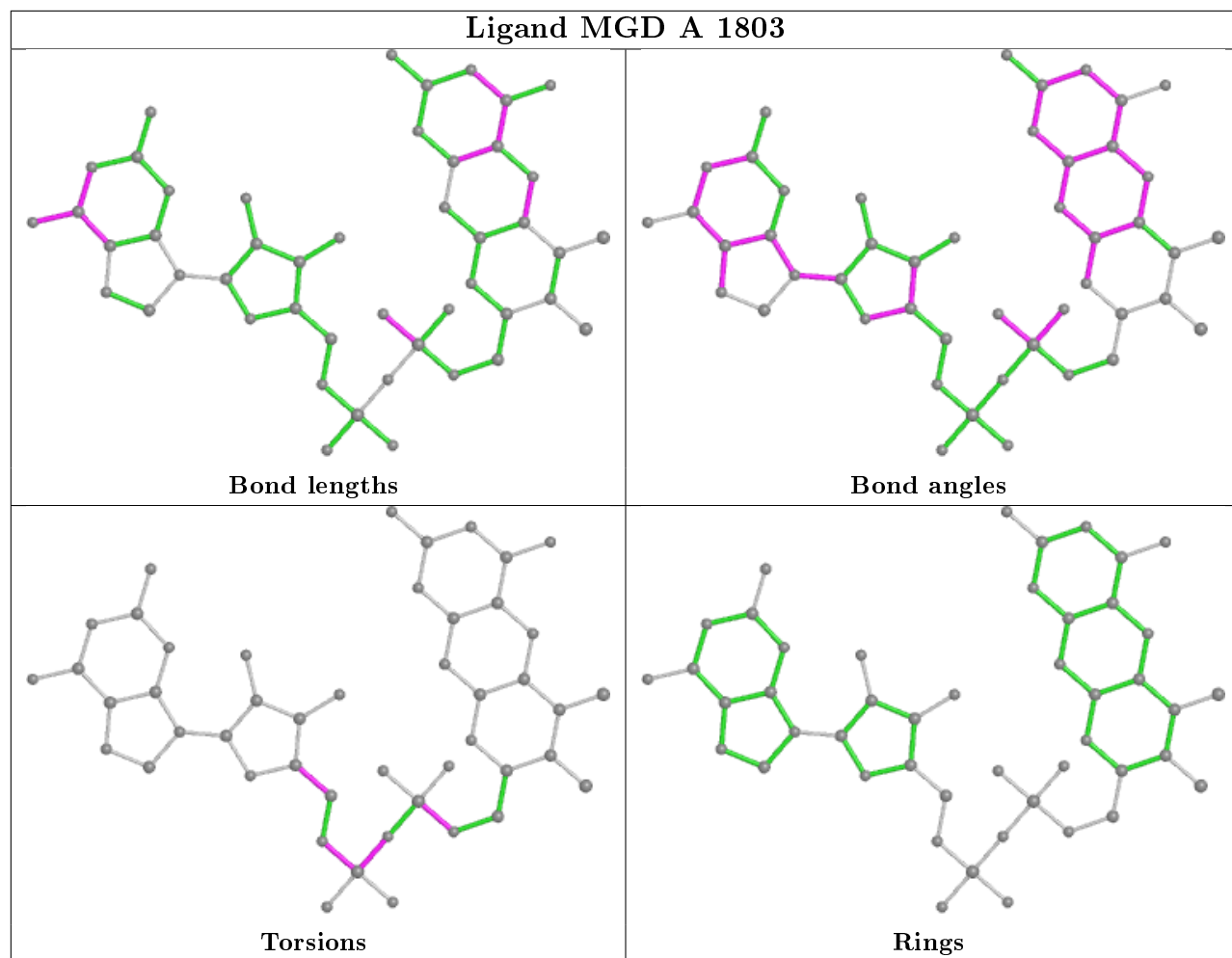
## Ligand MGD A 1804





## Ligand HEC B 1128





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	791/802 (98%)	-0.50	3 (0%) 92 93	4, 9, 19, 31	0
2	B	108/135 (80%)	0.23	13 (12%) 4 5	7, 17, 36, 48	0
All	All	899/937 (95%)	-0.42	16 (1%) 68 72	4, 10, 22, 48	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	121	THR	5.4
2	B	120	ASP	4.1
2	B	122	ILE	4.0
2	B	123	LEU	3.9
2	B	119	VAL	3.7
2	B	60	PHE	3.5
2	B	27	LYS	3.5
2	B	65	THR	3.4
1	A	802	VAL	2.6
2	B	9	PRO	2.6
2	B	37	MET	2.5
1	A	664	PRO	2.2
2	B	26	ASN	2.2
1	A	313	ASP	2.2
2	B	49	TYR	2.1
2	B	73	ILE	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	OCS	A	784	9/10	0.98	0.06	4,6,14,21	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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.

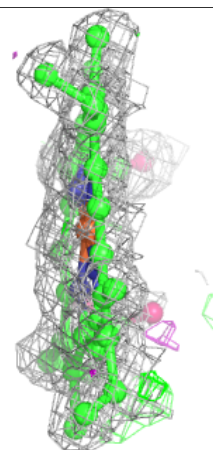
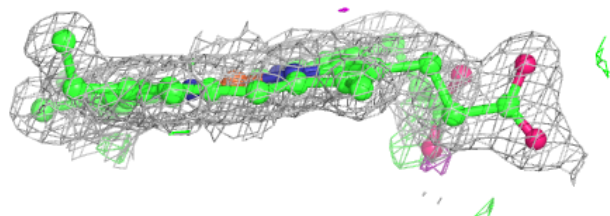
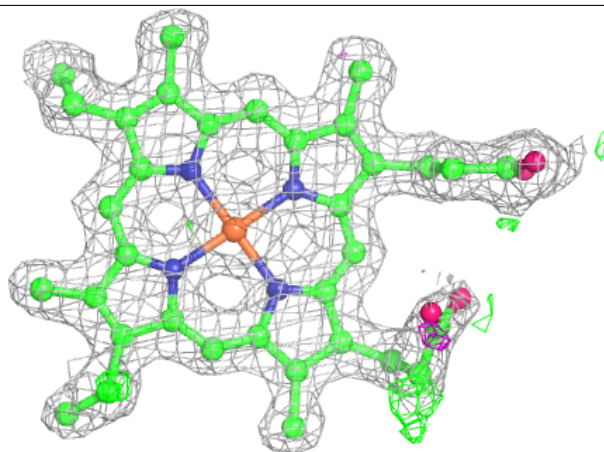
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	FMT	A	809	3/3	0.54	0.24	42,42,43,44	0
6	FMT	A	810	3/3	0.67	0.29	42,42,43,44	0
6	FMT	A	811	3/3	0.72	0.21	38,38,38,38	0
6	FMT	A	808	3/3	0.81	0.14	36,36,37,37	0
6	FMT	A	812	3/3	0.81	0.20	41,41,42,42	0
6	FMT	A	813	3/3	0.82	0.18	39,39,42,43	0
6	FMT	B	140	3/3	0.82	0.18	44,44,44,44	0
6	FMT	A	815	3/3	0.84	0.17	42,42,42,43	0
6	FMT	A	807	3/3	0.87	0.23	35,35,38,40	0
6	FMT	B	135	3/3	0.89	0.18	33,33,35,37	0
6	FMT	B	137	3/3	0.91	0.26	32,32,32,34	0
6	FMT	A	805	3/3	0.92	0.12	20,20,20,21	0
6	FMT	B	138	3/3	0.92	0.20	28,28,29,32	0
6	FMT	A	814	3/3	0.92	0.20	23,23,24,26	0
6	FMT	B	136	3/3	0.92	0.17	32,32,33,36	0
6	FMT	A	803	3/3	0.94	0.08	17,17,20,22	0
6	FMT	A	806	3/3	0.94	0.21	27,27,29,30	0
6	FMT	B	139	3/3	0.96	0.24	29,29,30,31	0
8	HEC	B	1128	43/43	0.97	0.10	9,16,30,41	0
6	FMT	A	804	3/3	0.97	0.10	23,23,24,29	0
5	MGD	A	1803	47/47	0.99	0.05	2,4,6,6	0
5	MGD	A	1804	47/47	0.99	0.05	2,5,7,8	0
7	CL	A	816	1/1	0.99	0.07	13,13,13,13	0
8	HEC	B	1129	43/43	0.99	0.07	3,9,20,26	0
4	MOS	A	1802	2/4	1.00	0.03	5,5,5,8	0
3	SF4	A	1801	8/8	1.00	0.06	5,6,7,7	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.

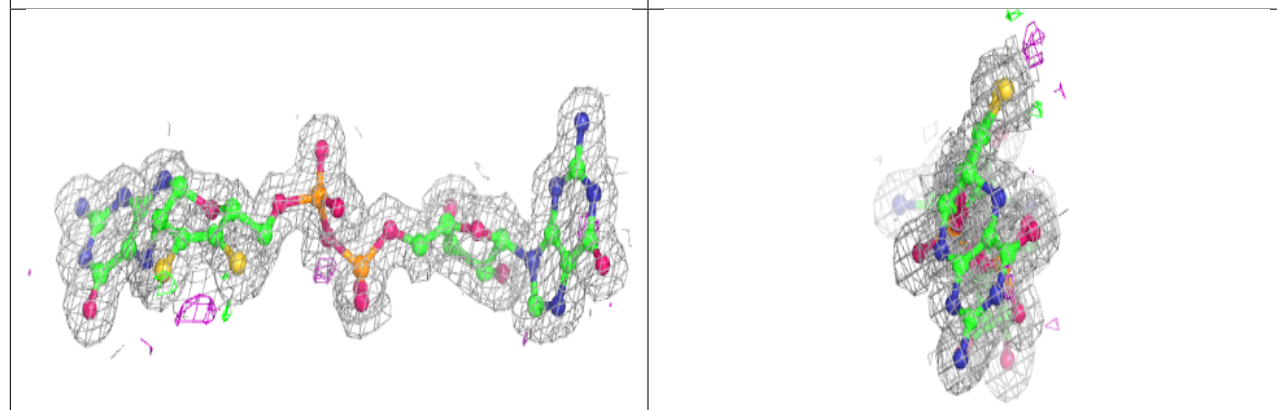
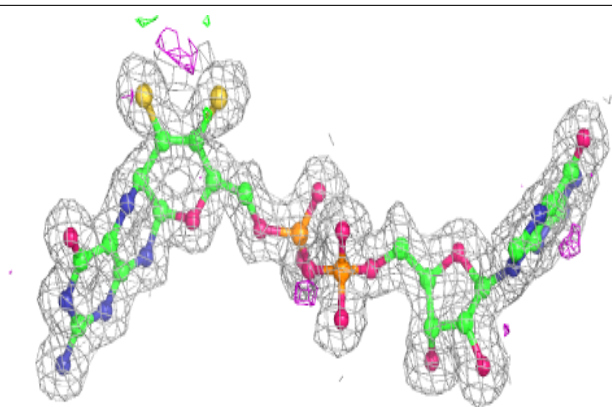
**Electron density around HEC B 1128:**

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

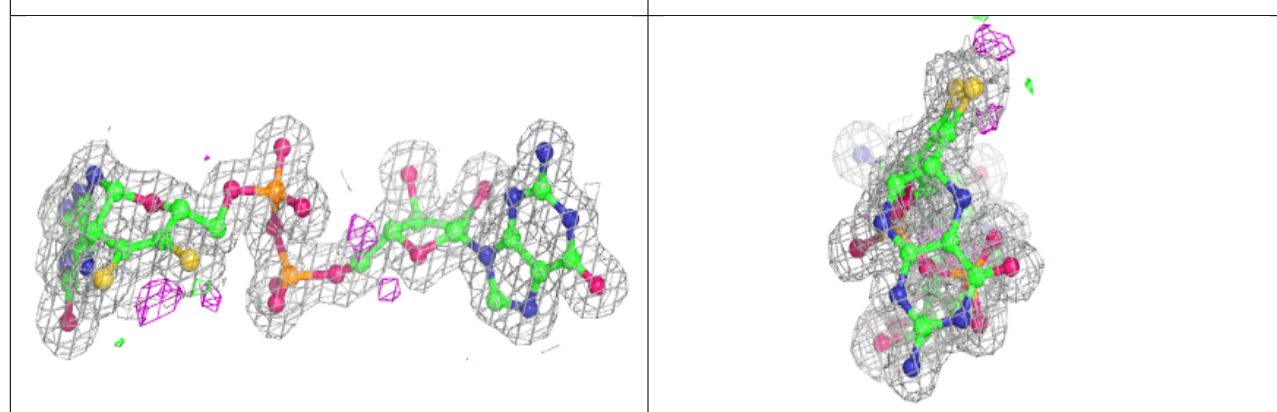
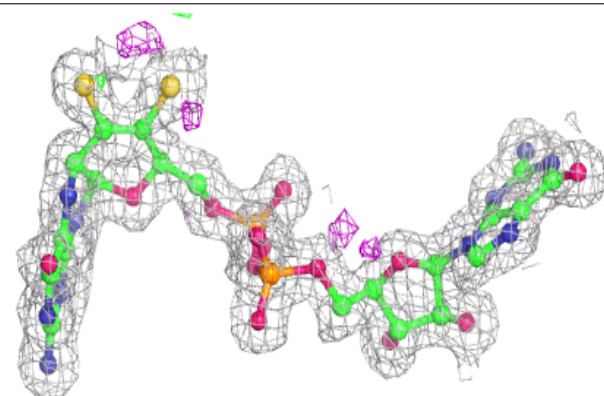


**Electron density around MGD A 1803:**

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

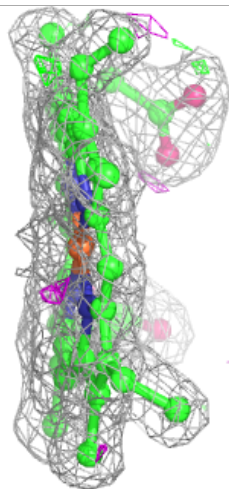
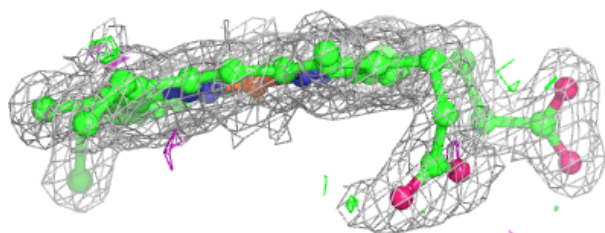
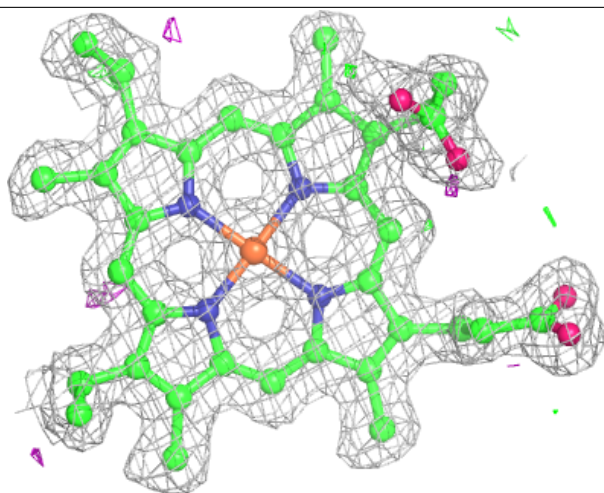
**Electron density around MGD A 1804:**

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



**Electron density around HEC B 1129:**

$2mF_o-DF_c$  (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.