Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2026 – 07:19 pm BST

PDB ID	:	5DOQ / pdb_00005doq
Title	:	The structure of bd oxidase from Geobacillus thermodenitrificans
Authors	:	Safarian, S.; Mueller, H.; Rajendran, C.; Preu, J.; Ovchinnikov, S.; Kusumoto, T.; Hirose, T.; Langer, J.; Sakamoto, J.; Michel, H.
Deposited on	:	2015-09-11
Resolution	:	3.05 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 (i) 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 (i)) were used in the production of this report:

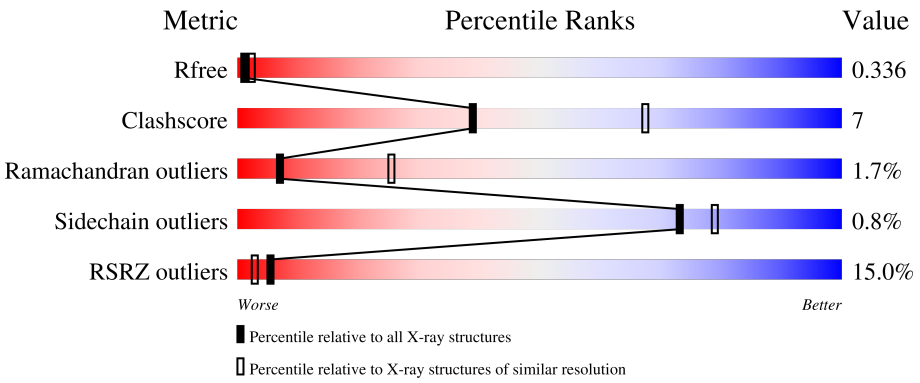
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	13% 76% 20% • •
2	B	342	16% 89% 7% •
3	C	33	18% 79% 12% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HEB	A	501	X	-	-	-
4	HEB	A	502	X	-	-	-
5	HDD	A	503	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6471 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 Bd-type quinol oxidase subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	432	3418	2270	555	574	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLU	LYS	conflict	UNP A4IKP6

- Molecule 2 is a protein called Bd-type quinol oxidase subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	330	2689	1832	409	442	6	0	0	0

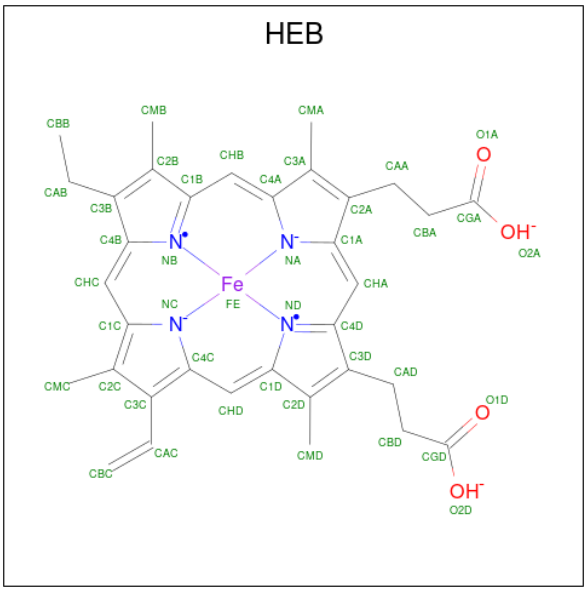
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	146	ASN	SER	conflict	UNP A4IKP7

- Molecule 3 is a protein called Putative membrane protein.

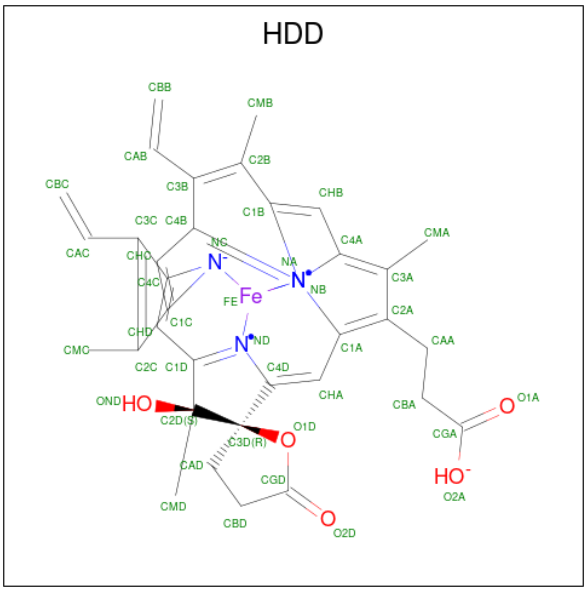
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	30	234	159	35	38	2	0	0	0

- Molecule 4 is HEME B/C (CCD ID: HEB) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 5 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



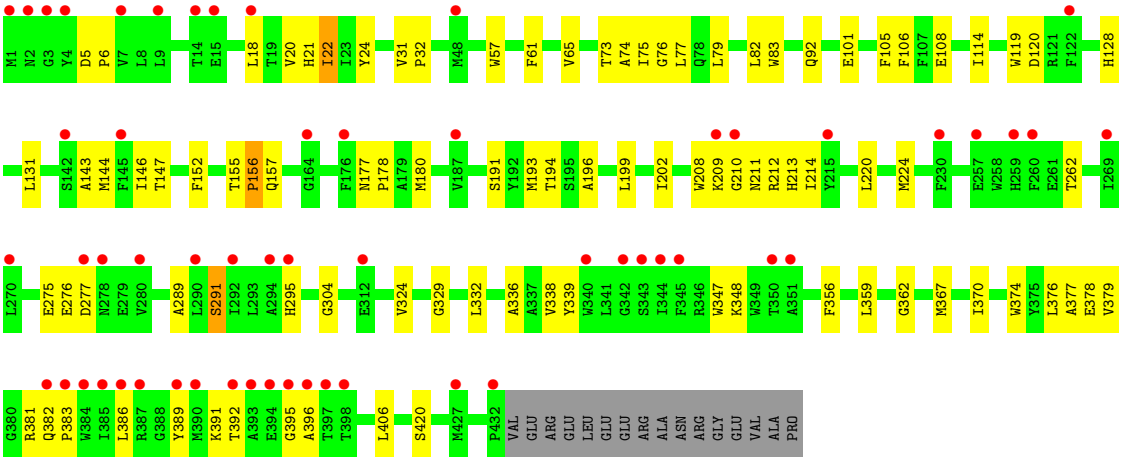
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	44	34	1	4	5	0	0

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.

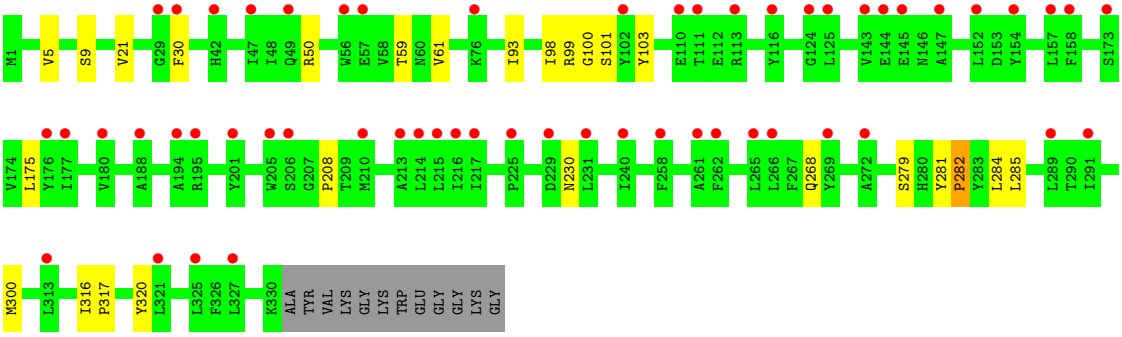
- Molecule 1: Bd-type quinol oxidase subunit I

Chain A:



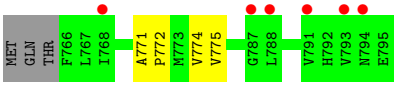
- Molecule 2: Bd-type quinol oxidase subunit II

Chain B:



- Molecule 3: Putative membrane protein

Chain C:


MET
GLN
THR
F766
L767
I768
A771
P772
M773
V774
V775
G787
L788
V791
H792
V793
N794
E795

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.06Å 120.86Å 122.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 20.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	57.0 (20.00-3.05) 57.3 (20.00-3.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.319 , 0.335 0.322 , 0.336	Depositor DCC
R_{free} test set	897 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å^2)	103.7	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -h,l,k	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6471	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HDD, HEB

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	0.56	0/3518	0.81	1/4802 (0.0%)
2	B	0.49	0/2781	0.77	0/3803
3	C	0.55	0/240	0.81	0/327
All	All	0.53	0/6539	0.79	1/8932 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	ILE	N-CA-C	-6.09	105.79	111.45

There are no chirality outliers.

There are no planarity outliers.

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	3418	0	3485	66	0
2	B	2689	0	2696	14	0
3	C	234	0	241	3	0
4	A	86	0	64	13	0
5	A	44	0	31	14	0
All	All	6471	0	6517	88	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 7.

All (88) 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)
4:A:501:HEB:HHD	4:A:501:HEB:HBC1	1.41	0.99
1:A:147:THR:HA	5:A:503:HDD:O2A	1.79	0.82
4:A:501:HEB:HBB2	4:A:501:HEB:HHC	1.63	0.81
4:A:502:HEB:HBB1	5:A:503:HDD:HMA2	1.72	0.72
4:A:501:HEB:HBC1	4:A:501:HEB:CHD	2.19	0.68
1:A:338:VAL:O	1:A:339:TYR:C	2.49	0.56
2:B:99:ARG:NH2	2:B:103:TYR:OH	2.38	0.56
1:A:374:TRP:CZ2	5:A:503:HDD:O2D	2.59	0.55
1:A:152:PHE:O	1:A:389:TYR:OH	2.22	0.55
2:B:316:ILE:HB	2:B:317:PRO:HD3	1.88	0.54
2:B:21:VAL:HG23	2:B:59:THR:HG22	1.90	0.54
1:A:289:ALA:O	1:A:291:SER:N	2.41	0.53
1:A:374:TRP:HA	4:A:501:HEB:HAD2	1.91	0.53
1:A:378:GLU:OE2	1:A:381:ARG:NH1	2.42	0.53
1:A:92:GLN:O	2:B:300:MET:SD	2.68	0.52
1:A:367:MET:O	1:A:370:ILE:HB	2.09	0.52
1:A:20:VAL:O	1:A:21:HIS:C	2.54	0.51
1:A:120:ASP:OD2	2:B:50:ARG:NH2	2.44	0.51
1:A:376:LEU:C	1:A:376:LEU:HD23	2.36	0.50
1:A:379:VAL:C	1:A:381:ARG:H	2.18	0.50
4:A:501:HEB:HHD	4:A:501:HEB:CBC	2.27	0.50
1:A:224:MET:CE	1:A:336:ALA:HA	2.42	0.50
1:A:378:GLU:O	1:A:381:ARG:HB3	2.12	0.50
2:B:317:PRO:HA	2:B:320:TYR:HB3	1.94	0.50
1:A:275:GLU:O	1:A:277:ASP:N	2.45	0.49
5:A:503:HDD:CBD	5:A:503:HDD:CHA	2.90	0.49
1:A:177:ASN:HB2	1:A:178:PRO:CD	2.43	0.49
1:A:5:ASP:N	1:A:6:PRO:HD2	2.28	0.49
1:A:210:GLY:O	1:A:212:ARG:N	2.46	0.48
2:B:5:VAL:O	2:B:9:SER:OG	2.31	0.48
1:A:378:GLU:HG2	5:A:503:HDD:NC	2.29	0.48
4:A:501:HEB:HBB2	4:A:501:HEB:CHC	2.40	0.48
1:A:18:LEU:HB3	5:A:503:HDD:HAD2	1.95	0.47
1:A:105:PHE:HA	1:A:108:GLU:HG2	1.96	0.47
1:A:105:PHE:CD1	4:A:502:HEB:HAD2	2.49	0.47
1:A:262:THR:OG1	1:A:304:GLY:N	2.47	0.47
1:A:32:PRO:HD3	1:A:61:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLN:N	1:A:383:PRO:CD	2.77	0.47
1:A:347:TRP:O	1:A:348:LYS:C	2.57	0.47
1:A:76:GLY:HA2	4:A:502:HEB:HMB1	1.97	0.46
1:A:386:LEU:HA	1:A:391:LYS:HA	1.97	0.46
1:A:18:LEU:HD21	1:A:75:ILE:HG12	1.97	0.46
1:A:147:THR:HA	5:A:503:HDD:CGA	2.46	0.46
1:A:6:PRO:HB2	1:A:396:ALA:HB1	1.98	0.45
1:A:24:TYR:OH	1:A:420:SER:OG	2.21	0.45
1:A:194:THR:OG1	1:A:370:ILE:HD11	2.17	0.45
1:A:83:TRP:HA	1:A:395:GLY:O	2.16	0.45
1:A:146:ILE:HG13	5:A:503:HDD:O1A	2.16	0.45
4:A:501:HEB:CHD	4:A:501:HEB:CBC	2.93	0.45
1:A:143:ALA:O	1:A:144:MET:C	2.60	0.44
1:A:156:PRO:HB3	1:A:157:GLN:HA	1.99	0.44
1:A:18:LEU:HB3	5:A:503:HDD:CAD	2.48	0.44
1:A:77:LEU:CB	2:B:93:ILE:HD11	2.48	0.44
1:A:374:TRP:CE2	5:A:503:HDD:O2D	2.70	0.44
1:A:332:LEU:HD11	1:A:362:GLY:HA2	2.00	0.44
2:B:281:TYR:HB3	2:B:282:PRO:HA	2.00	0.44
2:B:100:GLY:O	2:B:101:SER:C	2.61	0.44
2:B:230:ASN:HB3	2:B:279:SER:HA	2.00	0.43
1:A:22:ILE:HD12	1:A:22:ILE:HA	1.85	0.43
1:A:406:LEU:C	1:A:406:LEU:HD23	2.42	0.43
1:A:208:TRP:HB2	1:A:356:PHE:HB3	1.99	0.43
1:A:212:ARG:O	1:A:213:HIS:C	2.61	0.43
1:A:119:TRP:HA	1:A:128:HIS:NE2	2.33	0.43
3:C:774:VAL:O	3:C:775:VAL:C	2.61	0.43
1:A:291:SER:HA	1:A:295:HIS:HB2	2.01	0.42
1:A:180:MET:C	1:A:180:MET:SD	3.03	0.42
2:B:98:ILE:O	2:B:99:ARG:C	2.63	0.42
1:A:193:MET:O	1:A:196:ALA:HB3	2.20	0.42
1:A:73:THR:O	1:A:74:ALA:C	2.61	0.42
1:A:114:ILE:HG22	1:A:131:LEU:HD13	2.02	0.42
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.90	0.42
2:B:284:LEU:O	2:B:285:LEU:HB3	2.20	0.42
1:A:57:TRP:CH2	1:A:199:LEU:HD13	2.55	0.41
5:A:503:HDD:CHA	5:A:503:HDD:HBD1	2.51	0.41
1:A:101:GLU:HB2	1:A:146:ILE:HB	2.02	0.41
1:A:106:PHE:CD1	2:B:61:VAL:HG21	2.56	0.41
3:C:771:ALA:O	3:C:774:VAL:HB	2.20	0.41
1:A:18:LEU:HD13	5:A:503:HDD:HAD1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:N	1:A:32:PRO:HD2	2.35	0.41
1:A:177:ASN:HB2	1:A:178:PRO:HD2	2.03	0.41
1:A:374:TRP:CZ3	4:A:501:HEB:HBD1	2.55	0.41
1:A:377:ALA:HB2	4:A:501:HEB:HHA	2.03	0.41
1:A:82:LEU:O	1:A:396:ALA:HA	2.21	0.41
3:C:771:ALA:O	3:C:772:PRO:C	2.64	0.41
1:A:378:GLU:OE2	5:A:503:HDD:NA	2.54	0.40
1:A:146:ILE:HG23	5:A:503:HDD:O1A	2.20	0.40
1:A:329:GLY:CA	4:A:501:HEB:HMC2	2.52	0.40
1:A:339:TYR:CD1	1:A:359:LEU:HD11	2.55	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	430/448 (96%)	357 (83%)	64 (15%)	9 (2%)	5 21
2	B	328/342 (96%)	284 (87%)	40 (12%)	4 (1%)	10 32
3	C	28/33 (85%)	19 (68%)	9 (32%)	0	100 100
All	All	786/823 (96%)	660 (84%)	113 (14%)	13 (2%)	7 25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ILE
1	A	191	SER
1	A	211	ASN
1	A	276	GLU
2	B	30	PHE
1	A	79	LEU
1	A	209	LYS

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Mol	Chain	Res	Type
1	A	291	SER
2	B	268	GLN
1	A	156	PRO
2	B	208	PRO
1	A	324	VAL
2	B	282	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/370 (96%)	353 (99%)	4 (1%)	65	76
2	B	276/283 (98%)	275 (100%)	1 (0%)	84	84
3	C	25/28 (89%)	25 (100%)	0	100	100
All	All	658/681 (97%)	653 (99%)	5 (1%)	73	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	65	VAL
1	A	155	THR
1	A	392	THR
2	B	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	206	HIS
1	A	211	ASN
2	B	224	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	HDD	A	503	1	50,52,52	2.58	25 (50%)	56,89,89	2.66	23 (41%)
4	HEB	A	501	1	50,50,50	4.47	27 (54%)	65,82,82	5.44	40 (61%)
4	HEB	A	502	1	50,50,50	4.55	29 (58%)	65,82,82	5.41	42 (64%)

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
5	HDD	A	503	1	1/1/8/14	8/9/89/89	0/1/9/9
4	HEB	A	501	1	1/1/3/8	4/14/54/54	-
4	HEB	A	502	1	1/1/3/8	6/14/54/54	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	HEB	FE-ND	12.66	2.34	1.94
4	A	501	HEB	FE-ND	12.04	2.32	1.94
4	A	502	HEB	C1C-C2C	-8.64	1.22	1.43
4	A	501	HEB	C1C-C2C	-8.48	1.23	1.43
4	A	501	HEB	C1A-C2A	-8.03	1.30	1.45
4	A	502	HEB	C4A-NA	7.93	1.55	1.39
4	A	501	HEB	C1B-C2B	-7.63	1.29	1.44
4	A	502	HEB	C1A-C2A	-7.55	1.31	1.45
4	A	501	HEB	C4A-NA	7.49	1.54	1.39
4	A	502	HEB	C1B-C2B	-7.35	1.30	1.44
4	A	502	HEB	CHA-C4D	6.71	1.54	1.39
4	A	502	HEB	C4D-ND	6.59	1.52	1.38
4	A	501	HEB	C1D-C2D	-6.42	1.32	1.44
4	A	502	HEB	FE-NB	6.42	2.14	1.94
4	A	501	HEB	FE-NB	6.35	2.14	1.94
4	A	501	HEB	CHA-C4D	6.32	1.53	1.39
4	A	502	HEB	C1C-NC	6.17	1.51	1.39
4	A	501	HEB	C4D-ND	6.16	1.51	1.38
4	A	501	HEB	FE-NC	6.14	2.16	1.95
4	A	502	HEB	C1D-C2D	-5.96	1.33	1.44
4	A	502	HEB	FE-NC	5.91	2.15	1.95
4	A	501	HEB	C2A-C3A	-5.90	1.24	1.36
4	A	501	HEB	C1C-NC	5.87	1.51	1.39
4	A	502	HEB	C3B-C2B	-5.73	1.24	1.36
4	A	501	HEB	C3B-C2B	-5.64	1.24	1.36
4	A	502	HEB	C2A-C3A	-5.59	1.24	1.36
4	A	501	HEB	CHC-C1C	5.37	1.51	1.39
4	A	502	HEB	CHB-C4A	5.31	1.48	1.38
4	A	501	HEB	C3C-C2C	-5.31	1.23	1.41
4	A	502	HEB	CHD-C1D	5.27	1.49	1.38
4	A	502	HEB	C3C-C2C	-5.27	1.23	1.41
4	A	502	HEB	CHC-C1C	5.26	1.51	1.39
4	A	501	HEB	CHD-C1D	5.05	1.48	1.38
4	A	502	HEB	C4B-C3B	-5.02	1.36	1.45
4	A	502	HEB	C4B-NB	4.93	1.48	1.40
4	A	501	HEB	C4B-NB	4.91	1.48	1.40
4	A	501	HEB	CHB-C4A	4.90	1.47	1.38
5	A	503	HDD	O1D-CGD	4.90	1.43	1.35
4	A	501	HEB	C4A-C3A	-4.89	1.35	1.45
4	A	502	HEB	C4A-C3A	-4.78	1.35	1.45
4	A	501	HEB	FE-NA	4.74	2.11	1.95
4	A	502	HEB	FE-NA	4.74	2.11	1.95
5	A	503	HDD	C1A-NA	-4.68	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	HDD	C3B-C2B	4.55	1.46	1.37
4	A	502	HEB	CBC-CAC	4.43	1.52	1.30
4	A	501	HEB	CBC-CAC	4.30	1.51	1.30
5	A	503	HDD	CHB-C1B	4.21	1.47	1.38
4	A	501	HEB	C4B-C3B	-4.12	1.37	1.45
4	A	502	HEB	CHB-C1B	4.12	1.48	1.39
4	A	502	HEB	C1B-NB	4.11	1.47	1.38
5	A	503	HDD	O1D-C3D	-4.10	1.40	1.46
5	A	503	HDD	C4A-NA	-4.08	1.31	1.39
4	A	501	HEB	CHC-C4B	4.07	1.46	1.38
5	A	503	HDD	C4C-NC	-4.05	1.31	1.39
5	A	503	HDD	FE-NB	4.04	2.07	1.94
4	A	502	HEB	CHA-C1A	4.01	1.46	1.38
4	A	501	HEB	C1B-NB	3.84	1.46	1.38
4	A	501	HEB	CHB-C1B	3.80	1.47	1.39
5	A	503	HDD	CHC-C1C	3.76	1.45	1.38
5	A	503	HDD	CHD-C1D	-3.61	1.30	1.41
5	A	503	HDD	C1C-NC	-3.58	1.32	1.39
5	A	503	HDD	FE-NC	3.57	2.07	1.95
4	A	502	HEB	CHC-C4B	3.53	1.45	1.38
5	A	503	HDD	C3C-C2C	3.51	1.44	1.37
5	A	503	HDD	C1B-NB	-3.50	1.34	1.40
5	A	503	HDD	CHD-C4C	3.49	1.45	1.38
4	A	501	HEB	C4C-NC	3.32	1.46	1.39
4	A	501	HEB	CHA-C1A	3.28	1.44	1.38
5	A	503	HDD	CHC-C4B	3.27	1.46	1.39
5	A	503	HDD	C1D-ND	-3.20	1.33	1.35
5	A	503	HDD	CHB-C4A	3.17	1.46	1.39
5	A	503	HDD	FE-NA	3.14	2.05	1.95
4	A	502	HEB	C4C-NC	3.06	1.45	1.39
5	A	503	HDD	FE-ND	-2.89	1.85	1.94
5	A	503	HDD	CHA-C1A	2.68	1.45	1.39
4	A	502	HEB	C1A-NA	2.49	1.44	1.39
5	A	503	HDD	C2A-C3A	2.47	1.45	1.38
5	A	503	HDD	C4A-C3A	2.32	1.48	1.43
4	A	502	HEB	C1D-ND	2.04	1.43	1.40
5	A	503	HDD	C1C-C2C	2.02	1.49	1.45
5	A	503	HDD	C4B-NB	-2.01	1.34	1.38

All (105) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	HEB	C3C-C4C-NC	-17.81	99.29	110.25
4	A	501	HEB	C3C-C4C-NC	-17.36	99.57	110.25
4	A	501	HEB	C1D-C2D-C3D	15.62	123.38	106.96
4	A	502	HEB	C1D-C2D-C3D	14.75	122.46	106.96
4	A	501	HEB	C1B-C2B-C3B	13.12	120.75	106.96
4	A	502	HEB	C1B-C2B-C3B	12.81	120.42	106.96
4	A	501	HEB	C2D-C1D-ND	-11.01	96.80	109.84
4	A	501	HEB	C3D-C4D-ND	-10.93	99.77	110.36
4	A	501	HEB	C3C-C2C-C1C	10.89	120.31	107.16
4	A	502	HEB	C2A-C1A-NA	-10.88	99.74	110.32
4	A	502	HEB	C3C-C2C-C1C	10.75	120.14	107.16
4	A	502	HEB	C1A-C2A-C3A	10.36	120.62	107.13
4	A	502	HEB	C3D-C4D-ND	-10.28	100.39	110.36
4	A	501	HEB	C1D-ND-C4D	10.03	115.44	105.07
4	A	502	HEB	C2D-C1D-ND	-9.64	98.42	109.84
4	A	501	HEB	C1A-C2A-C3A	9.62	119.66	107.13
4	A	502	HEB	C2B-C1B-NB	-9.18	98.89	109.88
4	A	501	HEB	C2A-C1A-NA	-9.17	101.41	110.32
4	A	501	HEB	C2B-C1B-NB	-8.84	99.29	109.88
4	A	501	HEB	C3B-C4B-NB	-8.74	100.43	110.17
4	A	502	HEB	C3B-C4B-NB	-8.68	100.50	110.17
4	A	502	HEB	C1D-ND-C4D	8.62	113.98	105.07
5	A	503	HDD	C3C-C2C-C1C	-6.73	100.65	107.08
5	A	503	HDD	C2A-C1A-NA	6.15	117.02	110.15
4	A	502	HEB	CHB-C1B-C2B	5.96	134.29	124.98
5	A	503	HDD	C3B-C2B-C1B	-5.59	102.34	106.49
4	A	501	HEB	CMB-C2B-C1B	-5.50	116.66	125.04
4	A	502	HEB	C3A-C4A-NA	-5.50	99.54	109.69
4	A	501	HEB	CHB-C1B-C2B	5.41	133.43	124.98
4	A	502	HEB	C2C-C1C-NC	-5.26	102.07	110.08
4	A	501	HEB	CHA-C4D-ND	5.21	130.08	124.42
4	A	501	HEB	C3A-C4A-NA	-5.03	100.40	109.69
4	A	501	HEB	C2C-C1C-NC	-4.96	102.53	110.08
4	A	502	HEB	CHA-C1A-NA	4.93	129.77	124.44
4	A	502	HEB	CMD-C2D-C1D	-4.88	117.61	125.04
4	A	501	HEB	CMD-C2D-C1D	-4.80	117.73	125.04
5	A	503	HDD	C2D-C1D-CHD	-4.75	115.81	123.33
5	A	503	HDD	OND-C2D-CMD	-4.54	101.24	109.59
4	A	502	HEB	CMB-C2B-C1B	-4.35	118.41	125.04
5	A	503	HDD	C2B-C1B-NB	4.29	114.92	109.84
5	A	503	HDD	CMC-C2C-C1C	4.29	132.28	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	503	HDD	C4A-C3A-C2A	-4.29	101.81	106.83
4	A	501	HEB	CHC-C4B-C3B	4.24	133.29	125.33
4	A	502	HEB	CHA-C4D-C3D	4.23	131.05	124.84
5	A	503	HDD	CAA-CBA-CGA	-4.20	104.57	113.60
4	A	501	HEB	CHA-C1A-NA	4.19	128.97	124.44
4	A	501	HEB	CMC-C2C-C1C	-4.18	119.01	125.37
4	A	501	HEB	CAA-C2A-C1A	-4.01	117.33	124.89
4	A	502	HEB	CAA-C2A-C3A	-3.82	120.77	127.88
4	A	502	HEB	CHA-C4D-ND	3.80	128.55	124.42
5	A	503	HDD	C4B-C3B-C2B	-3.67	104.20	107.11
4	A	501	HEB	C4B-NB-C1B	3.63	108.83	105.07
4	A	501	HEB	CHA-C4D-C3D	3.61	130.15	124.84
4	A	502	HEB	C4B-NB-C1B	3.56	108.75	105.07
4	A	501	HEB	CHD-C1D-ND	3.51	128.70	124.37
4	A	502	HEB	CHC-C4B-C3B	3.48	131.86	125.33
4	A	502	HEB	CHA-C1A-C2A	3.43	130.49	124.94
5	A	503	HDD	CAA-C2A-C3A	3.41	134.89	127.07
4	A	502	HEB	CHB-C4A-NA	3.40	128.12	124.44
4	A	502	HEB	C4A-C3A-C2A	3.40	111.91	106.94
5	A	503	HDD	C2C-C1C-NC	3.38	115.92	109.69
5	A	503	HDD	C3A-C4A-NA	3.37	115.22	110.08
4	A	502	HEB	CHD-C4C-NC	3.37	130.04	123.85
4	A	502	HEB	CMC-C2C-C1C	-3.36	120.25	125.37
4	A	502	HEB	CAA-C2A-C1A	-3.35	118.58	124.89
5	A	503	HDD	CAD-CBD-CGD	-3.34	99.39	104.56
5	A	503	HDD	C4C-C3C-C2C	-3.28	104.06	106.75
4	A	502	HEB	CHB-C4A-C3A	3.27	132.34	125.48
4	A	501	HEB	C4A-C3A-C2A	3.25	111.69	106.94
5	A	503	HDD	CHD-C4C-C3C	-3.14	119.89	125.26
4	A	502	HEB	C4B-C3B-C2B	3.12	111.44	106.90
4	A	501	HEB	CHB-C4A-C3A	3.10	131.98	125.48
5	A	503	HDD	C1A-C2A-C3A	-3.04	102.12	106.89
4	A	501	HEB	CHB-C4A-NA	2.94	127.62	124.44
5	A	503	HDD	O1D-CGD-O2D	2.90	123.39	120.80
4	A	502	HEB	C4A-NA-C1A	2.90	108.19	105.35
4	A	501	HEB	CHA-C1A-C2A	2.90	129.62	124.94
4	A	502	HEB	CMC-C2C-C3C	-2.88	119.61	126.59
4	A	501	HEB	CHD-C1D-C2D	2.80	134.49	126.73
5	A	503	HDD	CHC-C1C-NC	-2.78	121.43	124.44
4	A	502	HEB	CHD-C1D-C2D	2.75	134.36	126.73
4	A	501	HEB	CMD-C2D-C3D	-2.66	118.89	126.12
4	A	502	HEB	CHC-C1C-NC	2.65	128.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	HEB	O2A-CGA-CBA	2.64	122.53	114.03
4	A	502	HEB	CHC-C4B-NB	2.64	127.63	124.37
5	A	503	HDD	CHB-C1B-C2B	-2.64	119.40	126.73
4	A	501	HEB	CHB-C1B-NB	2.63	127.28	124.42
4	A	501	HEB	CAA-C2A-C3A	-2.62	123.01	127.88
4	A	501	HEB	C4B-C3B-C2B	2.61	110.69	106.90
4	A	501	HEB	CBC-CAC-C3C	-2.60	114.68	127.62
4	A	501	HEB	CHD-C4C-NC	2.52	128.48	123.85
5	A	503	HDD	OND-C2D-C3D	2.51	116.70	110.45
4	A	501	HEB	CMC-C2C-C3C	-2.44	120.67	126.59
4	A	501	HEB	CHC-C1C-NC	2.33	128.13	123.85
4	A	502	HEB	CBC-CAC-C3C	-2.32	116.09	127.62
4	A	502	HEB	CHD-C1D-ND	2.31	127.22	124.37
4	A	502	HEB	CMD-C2D-C3D	-2.28	119.93	126.12
5	A	503	HDD	C4C-NC-C1C	-2.25	103.15	105.35
4	A	502	HEB	CHB-C1B-NB	2.21	126.82	124.42
4	A	501	HEB	CMA-C3A-C4A	-2.15	120.93	124.71
4	A	502	HEB	O2D-CGD-CBD	2.08	120.72	114.03
4	A	502	HEB	CBB-CAB-C3B	-2.05	106.79	112.43
5	A	503	HDD	CMA-C3A-C2A	2.02	129.99	125.61
4	A	501	HEB	C4C-CHD-C1D	-2.01	121.57	126.34
4	A	502	HEB	CAA-CBA-CGA	-2.01	109.29	113.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	501	HEB	NA
4	A	502	HEB	NA
5	A	503	HDD	NC

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	HEB	C2C-C3C-CAC-CBC
4	A	502	HEB	C4C-C3C-CAC-CBC
4	A	501	HEB	C2B-C3B-CAB-CBB
4	A	501	HEB	C4B-C3B-CAB-CBB
5	A	503	HDD	C3A-C2A-CAA-CBA
5	A	503	HDD	C1A-C2A-CAA-CBA
5	A	503	HDD	C2B-C3B-CAB-CBB
5	A	503	HDD	C4B-C3B-CAB-CBB
5	A	503	HDD	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	A	503	HDD	C4C-C3C-CAC-CBC
5	A	503	HDD	CAA-CBA-CGA-O1A
4	A	501	HEB	CAD-CBD-CGD-O2D
5	A	503	HDD	CAA-CBA-CGA-O2A
4	A	502	HEB	CAD-CBD-CGD-O1D
4	A	502	HEB	CAD-CBD-CGD-O2D
4	A	501	HEB	CAD-CBD-CGD-O1D
4	A	502	HEB	CAA-CBA-CGA-O1A
4	A	502	HEB	CAA-CBA-CGA-O2A

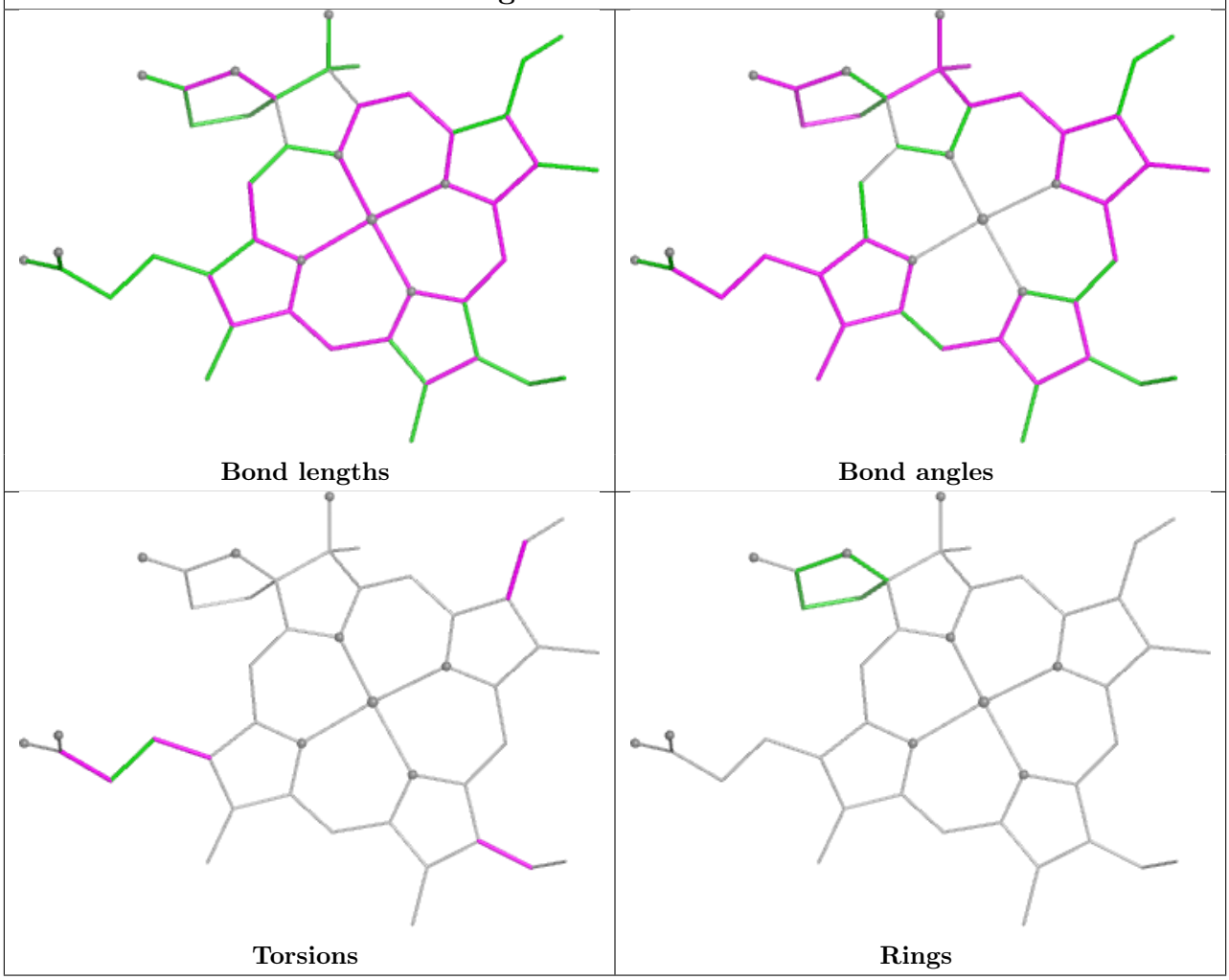
There are no ring outliers.

3 monomers are involved in 26 short contacts:

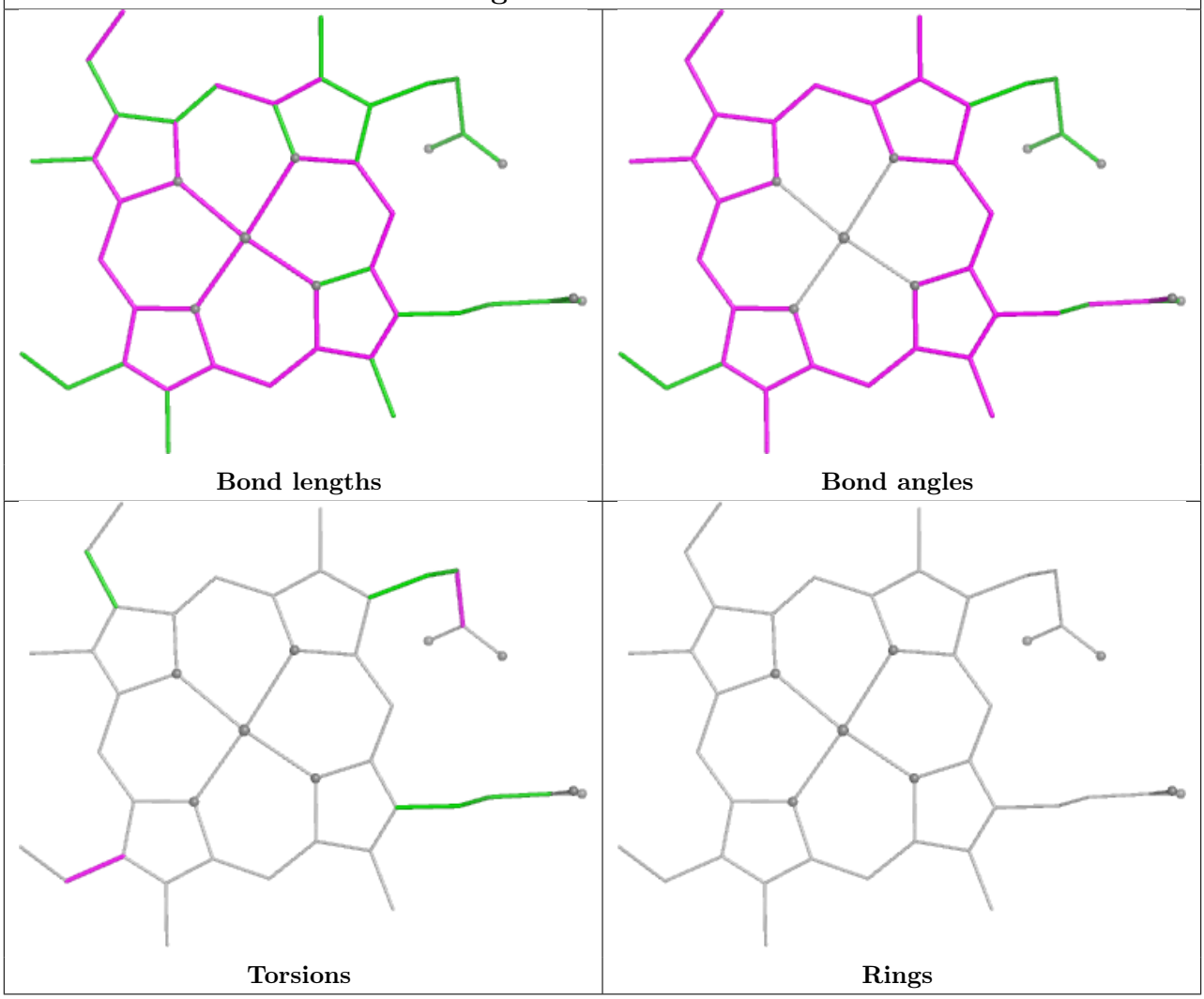
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	HDD	14	0
4	A	501	HEB	10	0
4	A	502	HEB	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

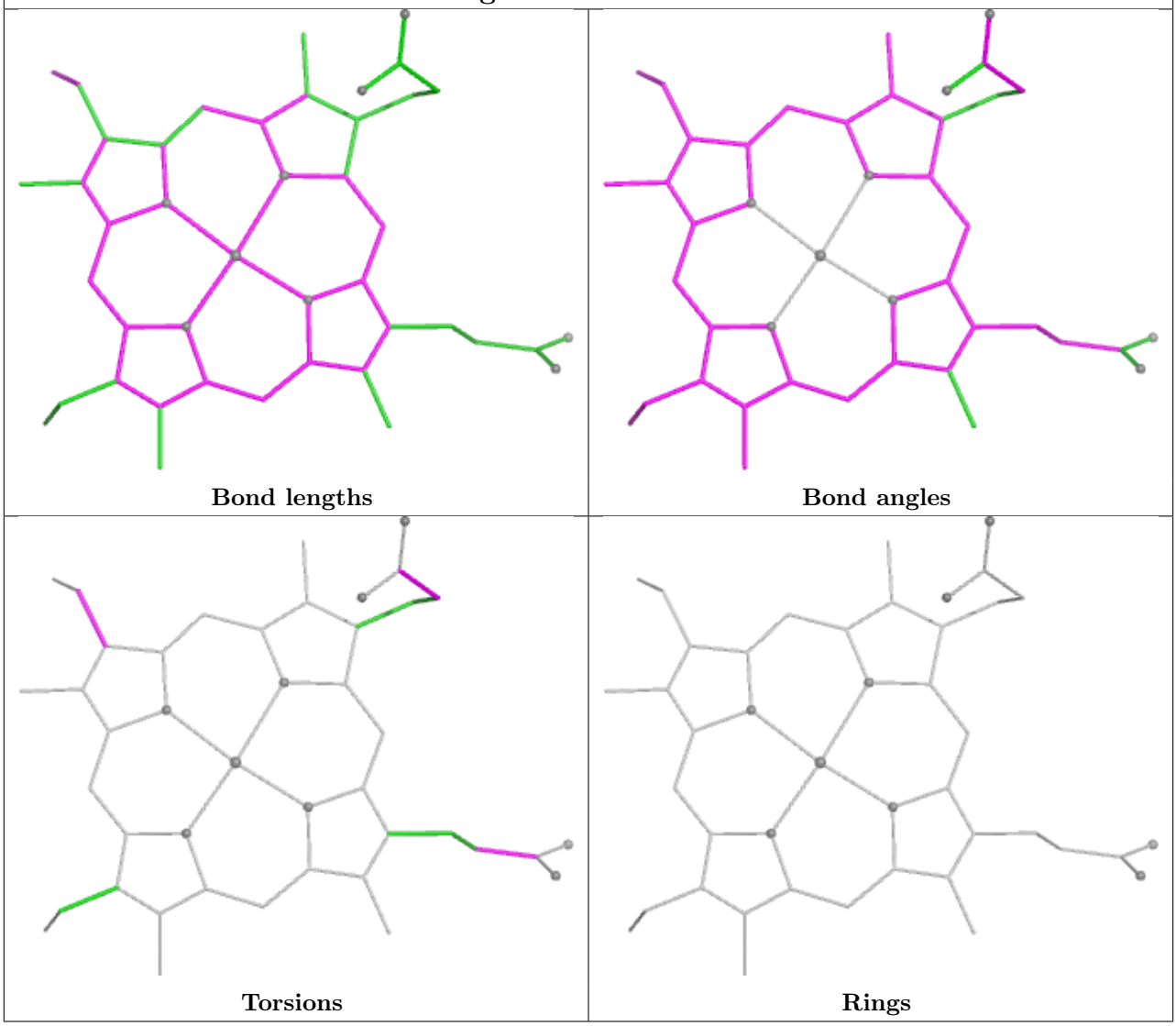
Ligand HDD A 503



Ligand HEB A 501



Ligand HEB A 502



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	432/448 (96%)	0.78	57 (13%)	7	4	50, 90, 158, 205	0
2	B	330/342 (96%)	1.08	56 (16%)	4	2	78, 151, 202, 224	0
3	C	30/33 (90%)	0.97	6 (20%)	3	1	71, 118, 179, 194	0
All	All	792/823 (96%)	0.91	119 (15%)	5	3	50, 120, 192, 224	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	GLY	5.9
2	B	205	TRP	5.5
1	A	270	LEU	4.8
1	A	397	THR	4.4
1	A	292	ILE	4.3
2	B	206	SER	4.2
1	A	215	TYR	4.2
1	A	209	LYS	4.2
2	B	111	THR	4.1
1	A	259	HIS	4.0
1	A	277	ASP	4.0
1	A	392	THR	4.0
3	C	788	LEU	3.8
1	A	394	GLU	3.8
2	B	214	LEU	3.8
1	A	142	SER	3.7
2	B	154	TYR	3.6
1	A	351	ALA	3.5
3	C	793	VAL	3.5
1	A	389	TYR	3.5
1	A	432	PRO	3.4
2	B	217	ILE	3.4
1	A	393	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	110	GLU	3.4
1	A	3	GLY	3.4
1	A	18	LEU	3.3
1	A	427	MET	3.3
1	A	15	GLU	3.3
2	B	145	GLU	3.3
1	A	387	ARG	3.3
1	A	164	GLY	3.3
1	A	385	ILE	3.3
2	B	216	ILE	3.2
2	B	29	GLY	3.2
1	A	48	MET	3.2
2	B	116	TYR	3.1
2	B	272	ALA	3.1
2	B	325	LEU	3.1
1	A	386	LEU	3.0
1	A	395	GLY	3.0
1	A	343	SER	3.0
1	A	280	VAL	3.0
2	B	313	LEU	2.9
1	A	384	TRP	2.9
2	B	258	PHE	2.9
1	A	278	ASN	2.9
1	A	396	ALA	2.9
1	A	4	TYR	2.9
1	A	312	GLU	2.8
1	A	290	LEU	2.8
2	B	49	GLN	2.8
2	B	152	LEU	2.8
2	B	269	TYR	2.8
2	B	195	ARG	2.8
3	C	794	ASN	2.8
1	A	340	TRP	2.8
1	A	257	GLU	2.8
2	B	291	ILE	2.8
1	A	390	MET	2.7
2	B	30	PHE	2.7
1	A	342	GLY	2.7
2	B	261	ALA	2.7
1	A	14	THR	2.7
2	B	147	ALA	2.7
2	B	180	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	240	ILE	2.6
1	A	230	PHE	2.6
3	C	787	GLY	2.6
2	B	144	GLU	2.6
2	B	265	LEU	2.6
1	A	294	ALA	2.6
2	B	194	ALA	2.6
1	A	350	THR	2.5
2	B	213	ALA	2.5
2	B	210	MET	2.5
2	B	231	LEU	2.5
2	B	57	GLU	2.5
2	B	321	LEU	2.5
2	B	124	GLY	2.5
2	B	42	HIS	2.4
1	A	176	PHE	2.4
1	A	260	PHE	2.4
1	A	9	LEU	2.4
1	A	398	THR	2.4
2	B	177	ILE	2.4
2	B	173	SER	2.4
2	B	225	PRO	2.4
1	A	344	ILE	2.4
2	B	266	LEU	2.3
2	B	327	LEU	2.3
1	A	345	PHE	2.3
1	A	382	GLN	2.3
2	B	113	ARG	2.3
1	A	269	ILE	2.3
3	C	768	ILE	2.3
1	A	145	PHE	2.3
1	A	295	HIS	2.3
2	B	158	PHE	2.3
2	B	76	LYS	2.3
2	B	229	ASP	2.3
1	A	2	ASN	2.2
2	B	176	TYR	2.2
2	B	47	ILE	2.2
1	A	1	MET	2.2
2	B	102	TYR	2.1
2	B	262	PHE	2.1
2	B	157	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	188	ALA	2.1
1	A	122	PHE	2.1
2	B	56	TRP	2.1
2	B	201	TYR	2.1
2	B	215	LEU	2.1
1	A	7	VAL	2.1
3	C	791	VAL	2.1
1	A	187	VAL	2.0
1	A	383	PRO	2.0
2	B	143	VAL	2.0
2	B	125	LEU	2.0
2	B	289	LEU	2.0

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)

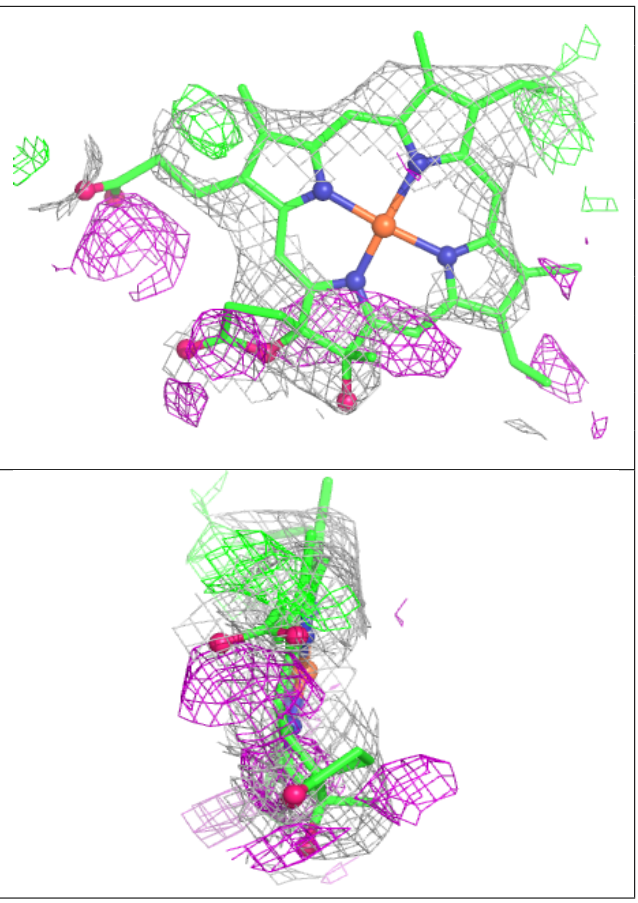
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

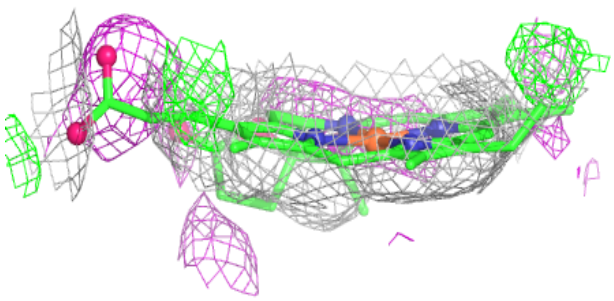
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	HDD	A	503	44/44	0.87	0.22	113,113,113,113	0
4	HEB	A	502	43/43	0.96	0.16	92,92,92,92	0
4	HEB	A	501	43/43	0.96	0.16	75,75,75,75	0

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 HDD A 503:

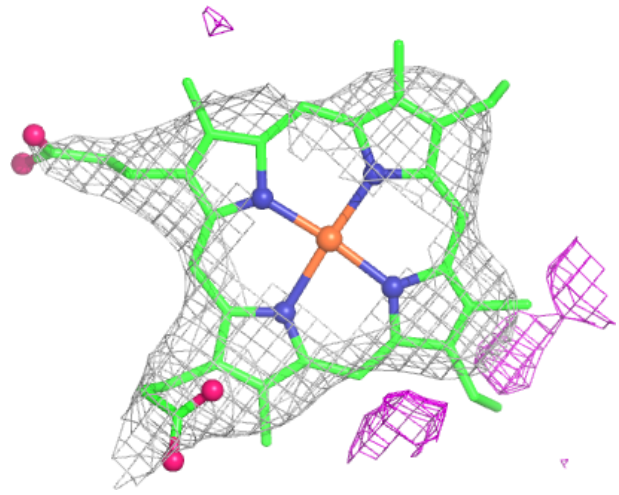
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

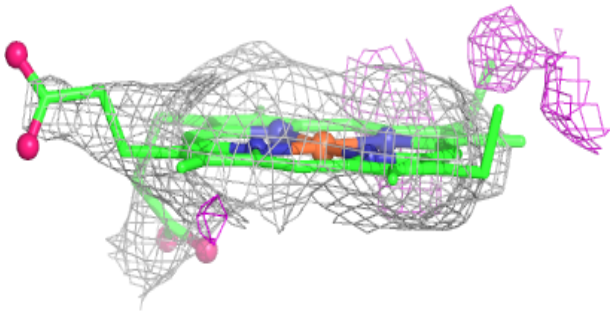


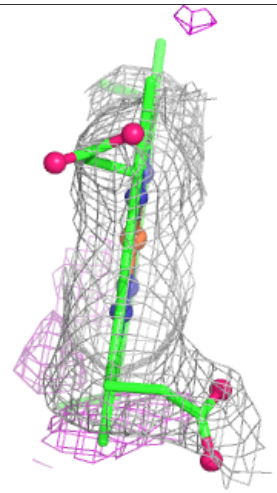


Electron density around HEB A 502:

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

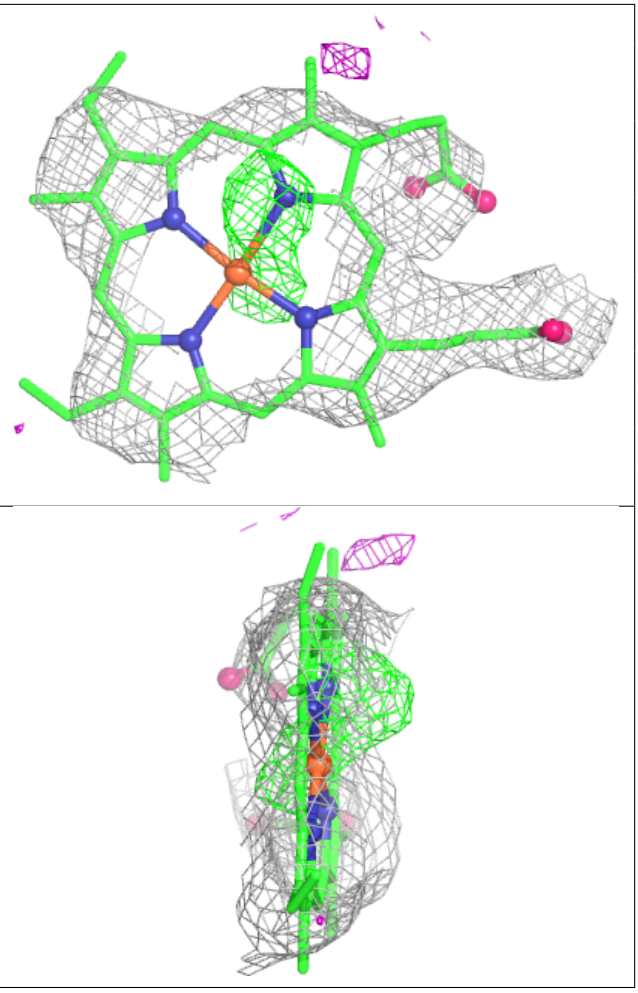






Electron density around HEB A 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.