



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:39 PM EDT

PDB ID : 3O0R / pdb_00003o0r
Title : Crystal structure of nitric oxide reductase from *Pseudomonas aeruginosa* in complex with antibody fragment
Authors : Hino, T.; Matsumoto, Y.; Nagano, S.; Sugimoto, H.; Fukumori, Y.; Murata, T.; Iwata, S.; Shiro, Y.
Deposited on : 2010-07-20
Resolution : 2.70 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	:	9.0.015 (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

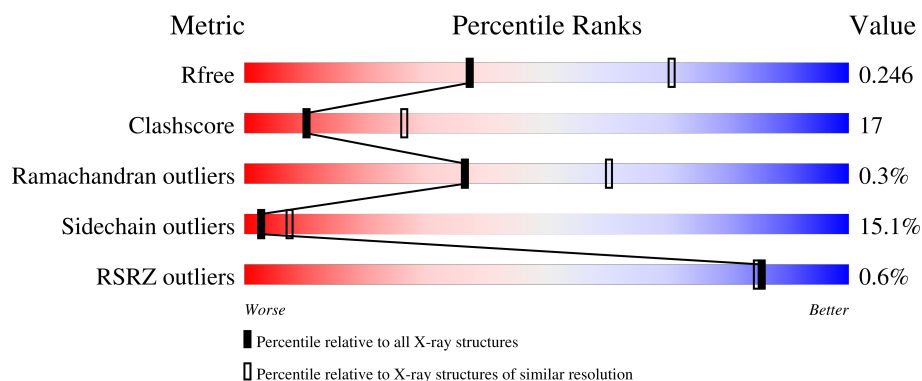
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 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	L	213	 70% 23% . .
2	H	225	 2% 68% 25% 6%
3	B	465	 56% 33% 7% . .
4	C	146	 62% 31% 5% .

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
9	HEC	C	201	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8364 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 antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1669	1047	277	338	7			

- Molecule 2 is a protein called antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1692	1065	280	338	9			

- Molecule 3 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	SEE REMARK 999	UNP Q59647

- Molecule 4 is a protein called Nitric oxide reductase subunit C.

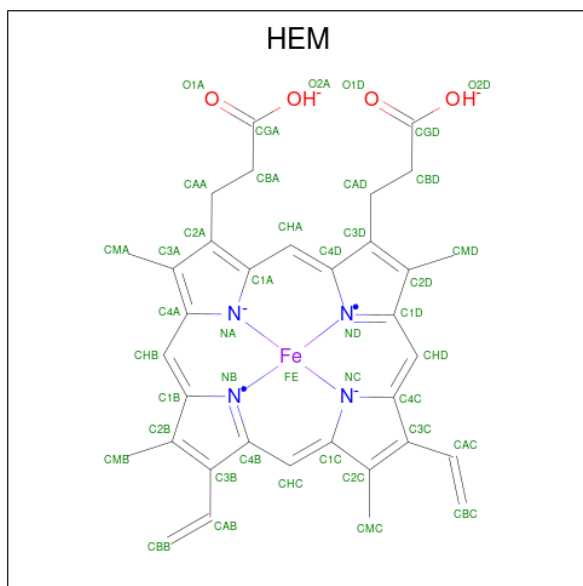
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	LYS	ASN	conflict	UNP Q59646

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe		
			1	1	0	0

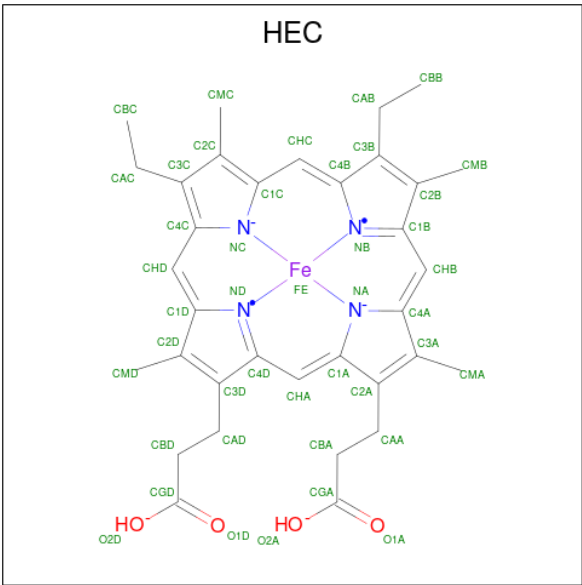
- Molecule 7 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca		
			1	1	0	0

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

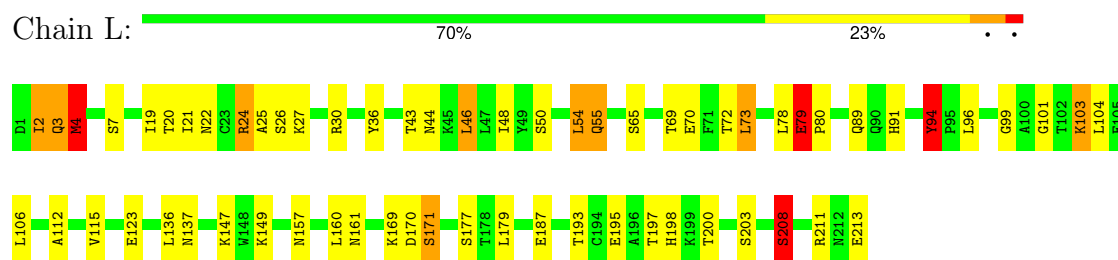
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	44	Total	O	0	0
			44	44		
10	H	46	Total	O	0	0
			46	46		
10	B	38	Total	O	0	0
			38	38		
10	C	44	Total	O	0	0
			44	44		

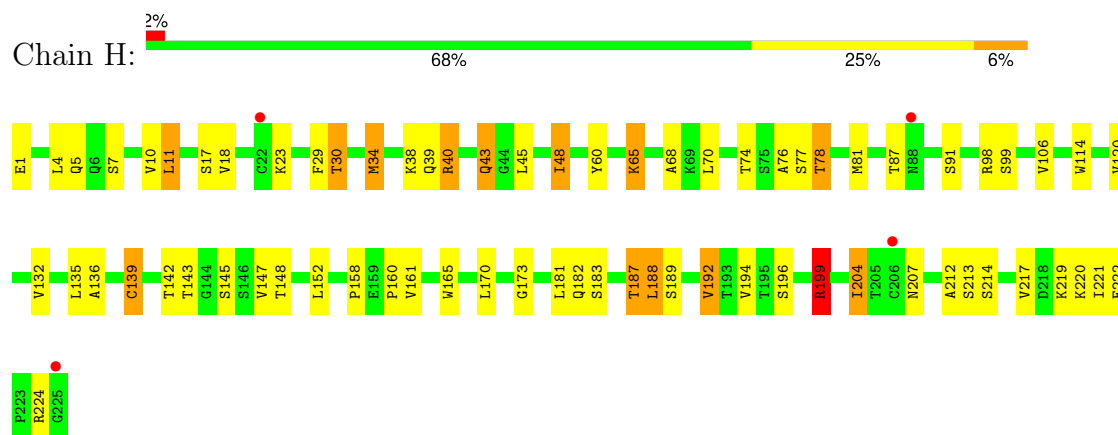
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

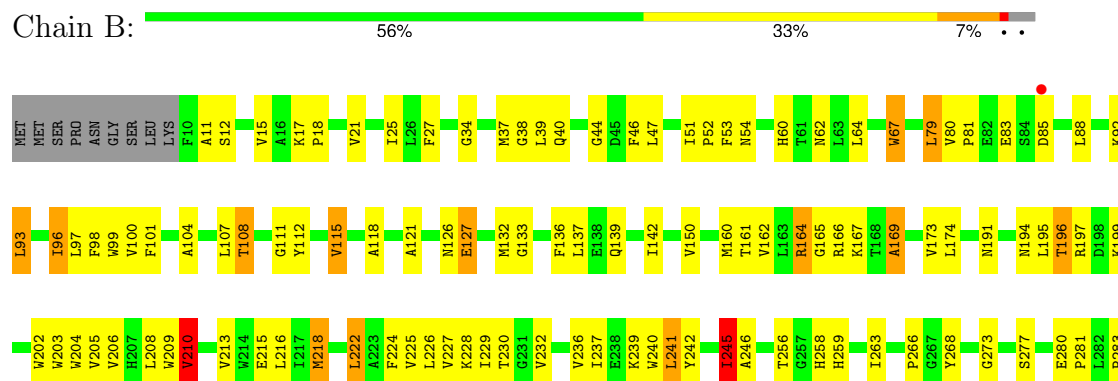
- Molecule 1: antibody fab fragment light chain



- Molecule 2: antibody fab fragment heavy chain

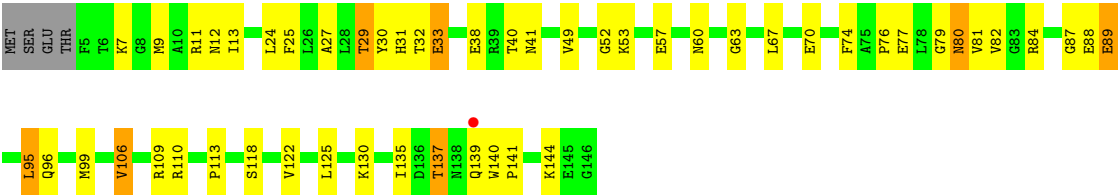


- Molecule 3: Nitric oxide reductase subunit B





● Molecule 4: Nitric oxide reductase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.47Å 104.52Å 195.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.70) 97.2 (20.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.247 0.185 , 0.246	Depositor DCC
R_{free} test set	2559 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.4	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	8364	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: CA, FE, HEC, O, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	1.12	2/1709 (0.1%)	1.26	12/2317 (0.5%)
2	H	1.09	1/1735 (0.1%)	1.24	8/2367 (0.3%)
3	B	0.95	0/3693	1.20	12/5039 (0.2%)
4	C	1.04	0/1153	1.17	4/1559 (0.3%)
All	All	1.03	3/8290 (0.0%)	1.22	36/11282 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	79	GLU	N-CA	-7.62	1.39	1.45
1	L	79	GLU	CA-CB	-5.38	1.47	1.54
2	H	183	SER	CA-C	5.01	1.58	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	417	MET	CA-C-N	-9.78	110.35	120.03
3	B	417	MET	C-N-CA	-9.78	110.35	120.03
3	B	245	ILE	CB-CA-C	-8.84	100.20	112.14
3	B	11	ALA	N-CA-C	7.27	118.99	111.14
1	L	101	GLY	N-CA-C	6.90	121.37	112.68
2	H	192	VAL	CB-CA-C	-6.55	101.21	110.12
3	B	191	ASN	CA-C-N	6.55	126.58	119.90
3	B	191	ASN	C-N-CA	6.55	126.58	119.90
3	B	165	GLY	N-CA-C	6.41	119.47	112.29
1	L	208	SER	N-CA-C	6.36	117.52	108.74
1	L	203	SER	N-CA-C	6.05	117.28	109.72
2	H	181	LEU	N-CA-C	6.03	118.48	109.25
4	C	95	LEU	N-CA-C	-6.01	104.84	111.82
1	L	137	ASN	N-CA-C	5.92	119.37	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	48	ILE	N-CA-C	5.84	116.02	110.53
2	H	145	SER	N-CA-C	-5.74	106.32	113.38
4	C	76	PRO	N-CA-C	5.66	120.21	111.21
3	B	413	TRP	N-CA-C	5.65	117.44	111.28
1	L	203	SER	CA-C-N	5.65	125.66	119.90
1	L	203	SER	C-N-CA	5.65	125.66	119.90
1	L	112	ALA	CA-C-N	-5.56	114.25	120.14
1	L	112	ALA	C-N-CA	-5.56	114.25	120.14
2	H	207	ASN	CB-CA-C	-5.55	101.81	110.74
3	B	427	MET	N-CA-C	-5.41	106.19	112.89
3	B	169	ALA	N-CA-C	-5.40	105.42	112.23
1	L	4	MET	CB-CA-C	-5.36	100.44	109.72
3	B	295	ILE	N-CA-C	-5.35	106.21	111.88
3	B	210	VAL	CB-CA-C	5.33	119.17	111.65
4	C	89	GLU	N-CA-C	5.26	117.44	111.02
2	H	199	ARG	CG-CD-NE	-5.18	100.60	112.00
1	L	171	SER	N-CA-C	5.16	119.15	112.86
2	H	43	GLN	N-CA-C	5.13	120.67	113.02
2	H	173	GLY	N-CA-C	-5.10	108.24	115.43
4	C	52	GLY	N-CA-C	-5.08	106.60	112.50
1	L	157	ASN	N-CA-C	5.06	117.64	110.50
1	L	94	TYR	N-CA-C	-5.01	103.46	109.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1669	0	1606	44	0
2	H	1692	0	1647	39	0
3	B	3576	0	3619	162	0
4	C	1123	0	1092	48	0
5	B	86	0	60	8	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
9	C	43	0	30	7	0
10	B	38	0	0	3	0
10	C	44	0	0	2	0
10	H	46	0	0	6	0
10	L	44	0	0	3	0
All	All	8364	0	8054	277	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 17.

All (277) 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:H:182:GLN:HE21	2:H:187:THR:HG21	1.03	1.12
3:B:372:ARG:HG2	3:B:372:ARG:HH11	1.14	1.09
3:B:226:LEU:O	3:B:230:THR:HG22	1.56	1.05
3:B:104:ALA:O	3:B:108:THR:HG22	1.61	1.01
3:B:121:ALA:HA	3:B:132:MET:HE1	1.02	1.00
3:B:127:GLU:OE2	3:B:127:GLU:HA	1.62	0.99
3:B:121:ALA:CA	3:B:132:MET:HE1	1.93	0.98
2:H:30:THR:HB	10:H:338:HOH:O	1.64	0.97
2:H:48:ILE:HG21	2:H:81:MET:HE1	1.50	0.94
2:H:70:LEU:HD21	2:H:81:MET:HE3	1.50	0.94
3:B:300:ARG:HG3	3:B:300:ARG:HH11	1.31	0.91
3:B:425:THR:O	3:B:429:THR:HG23	1.72	0.90
2:H:182:GLN:NE2	2:H:187:THR:HG21	1.87	0.88
3:B:384:VAL:HA	3:B:387:MET:HE2	1.53	0.87
3:B:121:ALA:HA	3:B:132:MET:CE	1.98	0.86
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.57	0.85
4:C:106:VAL:HG22	4:C:109:ARG:HB2	1.60	0.83
3:B:338:THR:O	3:B:341:THR:HB	1.79	0.82
2:H:165:TRP:HZ3	2:H:221:ILE:HD11	1.42	0.81
3:B:350:MET:HB2	3:B:401:THR:HG21	1.63	0.81
1:L:79:GLU:CG	1:L:80:PRO:HD2	2.11	0.80
3:B:314:THR:HG23	3:B:358:MET:HB2	1.63	0.79
3:B:126:ASN:HB2	3:B:132:MET:HE2	1.66	0.78
9:C:201:HEC:CGA	10:C:332:HOH:O	2.31	0.78
3:B:225:VAL:O	3:B:229:ILE:HB	1.84	0.77
1:L:79:GLU:HG2	1:L:80:PRO:HD2	1.66	0.77
2:H:182:GLN:HE21	2:H:187:THR:CG2	1.93	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:381:ARG:HH11	3:B:381:ARG:HB3	1.48	0.77
4:C:137:THR:HG21	4:C:140:TRP:O	1.87	0.75
3:B:427:MET:HE1	4:C:110:ARG:HD2	1.69	0.75
4:C:88:GLU:HG3	4:C:89:GLU:N	2.00	0.74
1:L:79:GLU:HG3	1:L:80:PRO:CD	2.18	0.74
1:L:79:GLU:CG	1:L:80:PRO:CD	2.66	0.73
3:B:104:ALA:O	3:B:108:THR:CG2	2.36	0.73
2:H:38:LYS:HE2	2:H:40:ARG:HD3	1.71	0.72
3:B:162:VAL:O	3:B:167:LYS:HE3	1.88	0.72
4:C:84:ARG:O	4:C:84:ARG:HG2	1.88	0.72
3:B:341:THR:HG22	3:B:343:LEU:H	1.55	0.71
3:B:372:ARG:HG2	3:B:372:ARG:NH1	1.93	0.71
1:L:79:GLU:HG3	1:L:80:PRO:HD3	1.72	0.71
3:B:137:LEU:HA	3:B:139:GLN:NE2	2.05	0.71
1:L:160:LEU:HD11	2:H:182:GLN:HG2	1.72	0.70
4:C:88:GLU:HG3	4:C:89:GLU:H	1.55	0.70
3:B:304:ASN:OD1	3:B:306:ALA:HB3	1.91	0.70
3:B:85:ASP:HB2	3:B:166:ARG:HG3	1.74	0.70
1:L:4:MET:N	1:L:4:MET:HE3	2.07	0.70
2:H:65:LYS:HE2	2:H:65:LYS:HA	1.73	0.70
4:C:113:PRO:HD3	9:C:201:HEC:CBC	2.22	0.69
3:B:93:LEU:O	3:B:97:LEU:HG	1.92	0.69
4:C:25:PHE:O	4:C:29:THR:HG23	1.93	0.68
3:B:302:TYR:OH	3:B:370:ARG:NH1	2.26	0.68
3:B:196:THR:HG22	4:C:135:ILE:HD13	1.77	0.67
3:B:51:ILE:O	3:B:51:ILE:HG22	1.95	0.66
3:B:300:ARG:HG3	3:B:300:ARG:NH1	2.05	0.65
2:H:165:TRP:HZ3	2:H:221:ILE:CD1	2.09	0.65
4:C:113:PRO:HD3	9:C:201:HEC:HBC2	1.76	0.65
2:H:76:ALA:O	2:H:78:THR:HG22	1.97	0.65
2:H:70:LEU:CD2	2:H:81:MET:HE3	2.26	0.64
2:H:60:TYR:CD2	2:H:65:LYS:HE3	2.33	0.64
3:B:17:LYS:HG3	3:B:368:MET:HE1	1.79	0.63
1:L:115:VAL:HG22	1:L:136:LEU:HD23	1.79	0.63
3:B:126:ASN:HB2	3:B:132:MET:CE	2.27	0.63
3:B:353:TYR:N	5:B:801:HEM:HBC1	2.14	0.63
3:B:199:LYS:HG2	4:C:70:GLU:OE1	1.98	0.63
3:B:381:ARG:HB3	3:B:381:ARG:NH1	2.14	0.62
3:B:83:GLU:OE2	3:B:83:GLU:HA	2.00	0.62
3:B:222:LEU:HD12	3:B:287:MET:CE	2.29	0.62
3:B:266:PRO:HD2	4:C:32:THR:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:220:LYS:HE3	2:H:222:GLU:OE2	2.00	0.61
3:B:67:TRP:HZ3	3:B:360:VAL:HG11	1.65	0.61
3:B:137:LEU:HA	3:B:139:GLN:HE22	1.66	0.60
3:B:196:THR:CG2	4:C:135:ILE:HD13	2.31	0.60
1:L:48:ILE:HD13	1:L:54:LEU:HD23	1.82	0.60
2:H:68:ALA:HB1	2:H:81:MET:HE2	1.84	0.60
3:B:230:THR:HG23	3:B:232:VAL:H	1.66	0.60
3:B:295:ILE:O	3:B:295:ILE:HG23	2.00	0.60
3:B:291:ALA:HB2	3:B:315:THR:HG21	1.84	0.60
3:B:425:THR:O	3:B:429:THR:CG2	2.49	0.60
3:B:126:ASN:CB	3:B:132:MET:HE2	2.32	0.60
3:B:230:THR:OG1	3:B:232:VAL:HG23	2.03	0.59
3:B:197:ARG:HD3	4:C:33:GLU:OE2	2.03	0.59
3:B:341:THR:CG2	3:B:343:LEU:H	2.16	0.59
4:C:82:VAL:HG21	4:C:130:LYS:HA	1.85	0.58
2:H:74:THR:HG23	10:H:336:HOH:O	2.03	0.58
3:B:372:ARG:HH11	3:B:372:ARG:CG	2.01	0.58
2:H:165:TRP:CZ3	2:H:221:ILE:HD11	2.33	0.58
4:C:137:THR:CG2	4:C:140:TRP:O	2.52	0.58
1:L:50:SER:H	1:L:91:HIS:HE1	1.50	0.57
3:B:397:MET:O	3:B:401:THR:HG23	2.04	0.57
3:B:27:PHE:HE1	3:B:361:MET:HE3	1.68	0.57
3:B:205:VAL:O	3:B:209:TRP:HB2	2.04	0.57
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.85	0.57
3:B:350:MET:HE3	3:B:401:THR:CG2	2.34	0.57
4:C:99:MET:HE1	9:C:201:HEC:HBB3	1.87	0.57
1:L:46:LEU:HD13	1:L:55:GLN:CG	2.36	0.56
1:L:3:GLN:HG2	1:L:26:SER:HB3	1.87	0.56
3:B:341:THR:HG22	3:B:343:LEU:N	2.20	0.56
4:C:84:ARG:NH1	9:C:201:HEC:O2A	2.35	0.56
3:B:139:GLN:NE2	3:B:139:GLN:H	2.03	0.56
3:B:430:GLN:NE2	4:C:110:ARG:HH12	2.04	0.56
1:L:160:LEU:CD1	2:H:182:GLN:HG2	2.34	0.56
3:B:17:LYS:HB3	3:B:18:PRO:CD	2.36	0.56
2:H:30:THR:CB	10:H:338:HOH:O	2.37	0.56
3:B:136:PHE:O	3:B:137:LEU:HD23	2.06	0.55
1:L:19:ILE:O	1:L:19:ILE:HD12	2.05	0.55
1:L:2:ILE:HG23	10:L:305:HOH:O	2.05	0.55
3:B:415:GLN:HB2	3:B:429:THR:HG21	1.88	0.55
1:L:115:VAL:HG22	1:L:136:LEU:CD2	2.36	0.55
3:B:21:VAL:O	3:B:25:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:PHE:CD1	2:H:77:SER:HA	2.42	0.54
3:B:310:TRP:CZ3	3:B:358:MET:HE3	2.43	0.54
1:L:198:HIS:CD2	1:L:200:THR:OG1	2.49	0.54
3:B:390:PHE:CD1	3:B:390:PHE:C	2.86	0.54
1:L:161:ASN:ND2	1:L:177:SER:OG	2.41	0.53
3:B:93:LEU:HA	3:B:96:ILE:HG22	1.91	0.53
3:B:126:ASN:CG	3:B:132:MET:HE2	2.34	0.52
3:B:314:THR:HG23	3:B:358:MET:CB	2.34	0.52
3:B:118:ALA:O	3:B:121:ALA:HB3	2.08	0.52
1:L:4:MET:HB3	1:L:99:GLY:HA2	1.91	0.52
3:B:27:PHE:CE1	3:B:361:MET:HE3	2.43	0.52
3:B:226:LEU:O	3:B:230:THR:CG2	2.45	0.52
3:B:38:GLY:HA3	3:B:441:GLU:OE1	2.08	0.52
2:H:40:ARG:NH1	10:H:319:HOH:O	2.43	0.52
4:C:96:GLN:HA	4:C:96:GLN:NE2	2.25	0.52
3:B:197:ARG:CD	4:C:33:GLU:OE2	2.57	0.52
4:C:77:GLU:OE1	4:C:79:GLY:HA3	2.10	0.52
10:H:338:HOH:O	3:B:424:MET:HE3	2.10	0.51
1:L:193:THR:HA	1:L:208:SER:HB3	1.92	0.51
3:B:202:TRP:CH2	3:B:206:VAL:HG21	2.44	0.51
1:L:46:LEU:HB3	1:L:55:GLN:HG3	1.92	0.51
1:L:19:ILE:HD12	1:L:19:ILE:C	2.36	0.51
3:B:34:GLY:HA2	3:B:37:MET:HE3	1.93	0.51
2:H:11:LEU:HD21	2:H:158:PRO:HG3	1.93	0.50
3:B:339:HIS:HA	5:B:802:HEM:O1D	2.10	0.50
3:B:283:PRO:O	3:B:287:MET:HG3	2.11	0.50
3:B:378:MET:HB3	3:B:382:SER:HB2	1.93	0.50
3:B:196:THR:HB	3:B:263:ILE:O	2.12	0.50
3:B:350:MET:O	3:B:354:GLY:N	2.41	0.50
1:L:4:MET:CE	1:L:4:MET:CA	2.89	0.50
1:L:21:ILE:HD11	1:L:73:LEU:HD23	1.93	0.50
3:B:142:ILE:HG12	10:B:926:HOH:O	2.11	0.50
3:B:203:TRP:CE2	3:B:259:HIS:HB3	2.47	0.50
3:B:111:GLY:O	3:B:115:VAL:HG13	2.11	0.50
3:B:424:MET:HG2	3:B:429:THR:HG22	1.94	0.50
1:L:50:SER:H	1:L:91:HIS:CE1	2.29	0.50
1:L:24:ARG:HG3	1:L:25:ALA:N	2.21	0.49
3:B:194:ASN:HB3	3:B:197:ARG:NH1	2.27	0.49
1:L:70:GLU:HG3	10:L:327:HOH:O	2.13	0.49
3:B:242:TYR:CZ	4:C:11:ARG:HG3	2.47	0.49
3:B:342:GLN:OE1	10:B:935:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:352:PHE:HB3	5:B:801:HEM:HBC1	1.94	0.49
3:B:204:TRP:HZ2	4:C:29:THR:HG21	1.78	0.49
1:L:94:TYR:CD1	1:L:94:TYR:C	2.90	0.49
3:B:273:GLY:O	3:B:277:SER:HB2	2.12	0.49
3:B:341:THR:HG22	3:B:343:LEU:HB2	1.94	0.49
4:C:80:ASN:HD22	4:C:80:ASN:H	1.60	0.49
3:B:173:VAL:HG11	3:B:241:LEU:HD11	1.94	0.48
3:B:230:THR:HG23	3:B:232:VAL:N	2.28	0.48
3:B:127:GLU:OE2	3:B:127:GLU:CA	2.46	0.48
1:L:46:LEU:HD13	1:L:55:GLN:HG3	1.94	0.48
3:B:216:LEU:HD11	3:B:245:ILE:CG2	2.44	0.48
4:C:113:PRO:HD3	9:C:201:HEC:HBC3	1.94	0.48
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.62	0.48
3:B:79:LEU:HD22	3:B:80:VAL:N	2.28	0.48
3:B:382:SER:HB3	3:B:457:SER:O	2.14	0.48
2:H:132:VAL:HG21	2:H:217:VAL:HG21	1.96	0.48
3:B:359:ILE:HG23	3:B:360:VAL:N	2.28	0.48
3:B:332:ALA:HB3	3:B:333:PRO:HD3	1.95	0.47
3:B:300:ARG:NH1	3:B:300:ARG:CG	2.74	0.47
3:B:368:MET:HA	3:B:368:MET:HE2	1.96	0.47
3:B:204:TRP:O	3:B:208:LEU:HB2	2.14	0.47
3:B:218:MET:HG3	3:B:359:ILE:HD13	1.95	0.47
3:B:258:HIS:CD2	3:B:259:HIS:CD2	3.02	0.47
3:B:310:TRP:CE3	3:B:358:MET:HE3	2.50	0.47
3:B:350:MET:HE2	3:B:398:VAL:HA	1.97	0.47
4:C:140:TRP:CD2	4:C:141:PRO:HA	2.49	0.47
1:L:4:MET:N	1:L:4:MET:CE	2.76	0.47
5:B:802:HEM:O1A	10:B:906:HOH:O	2.20	0.47
2:H:139:CYS:HB2	2:H:224:ARG:HB2	1.96	0.47
1:L:44:ASN:HB2	2:H:114:TRP:CG	2.49	0.47
3:B:210:VAL:HG22	5:B:802:HEM:HMB2	1.96	0.46
3:B:239:LYS:HE2	3:B:240:TRP:HZ3	1.80	0.46
3:B:309:LEU:HD12	3:B:387:MET:HG2	1.95	0.46
3:B:312:MET:O	3:B:313:GLY:C	2.57	0.46
3:B:424:MET:HB3	3:B:429:THR:HG22	1.97	0.46
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.98	0.46
4:C:106:VAL:HG13	4:C:109:ARG:HD3	1.97	0.46
2:H:98:ARG:HD3	2:H:99:SER:O	2.15	0.46
3:B:258:HIS:HD2	3:B:259:HIS:CD2	2.34	0.46
2:H:188:LEU:C	2:H:188:LEU:HD23	2.40	0.46
10:H:301:HOH:O	3:B:427:MET:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:239:LYS:HE2	3:B:240:TRP:CZ3	2.50	0.46
4:C:25:PHE:O	4:C:29:THR:CG2	2.62	0.46
3:B:341:THR:CG2	3:B:343:LEU:HB2	2.46	0.46
3:B:46:PHE:O	3:B:47:LEU:HB2	2.15	0.46
1:L:4:MET:HB3	1:L:99:GLY:CA	2.46	0.45
1:L:149:LYS:HD2	1:L:195:GLU:OE1	2.16	0.45
3:B:216:LEU:CD1	3:B:245:ILE:HG23	2.46	0.45
1:L:187:GLU:HG2	1:L:211:ARG:NH1	2.31	0.45
4:C:53:LYS:O	4:C:57:GLU:HG3	2.17	0.45
2:H:213:SER:O	2:H:214:SER:HB2	2.16	0.45
4:C:96:GLN:HA	4:C:96:GLN:HE21	1.82	0.45
3:B:37:MET:HE1	3:B:60:HIS:CD2	2.52	0.45
3:B:203:TRP:HH2	5:B:802:HEM:HBA1	1.82	0.45
3:B:160:MET:O	3:B:164:ARG:HD3	2.17	0.45
3:B:215:GLU:OE2	3:B:284:PHE:CZ	2.70	0.45
3:B:306:ALA:O	3:B:310:TRP:CD1	2.70	0.45
3:B:426:PHE:O	3:B:430:GLN:HG2	2.16	0.45
3:B:430:GLN:NE2	4:C:110:ARG:NH1	2.65	0.45
4:C:125:LEU:HD23	4:C:125:LEU:HA	1.86	0.44
3:B:372:ARG:NH1	3:B:372:ARG:CG	2.68	0.44
4:C:82:VAL:O	4:C:87:GLY:HA2	2.18	0.44
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.50	0.44
1:L:170:ASP:OD2	1:L:170:ASP:C	2.59	0.44
3:B:305:ARG:HE	3:B:305:ARG:HB3	1.61	0.44
4:C:77:GLU:HG3	4:C:80:ASN:ND2	2.31	0.44
3:B:126:ASN:ND2	3:B:132:MET:HE2	2.32	0.44
3:B:229:ILE:HD11	3:B:366:TYR:CD2	2.53	0.44
3:B:245:ILE:O	3:B:246:ALA:C	2.60	0.44
4:C:137:THR:HG23	4:C:140:TRP:H	1.82	0.44
3:B:353:TYR:N	5:B:801:HEM:CBC	2.80	0.44
3:B:27:PHE:HE1	3:B:361:MET:CE	2.31	0.43
4:C:81:VAL:HG21	9:C:201:HEC:HBA2	2.00	0.43
3:B:169:ALA:O	3:B:173:VAL:HG23	2.19	0.43
3:B:368:MET:HE2	3:B:371:LEU:HD23	2.00	0.43
2:H:4:LEU:HD21	2:H:34:MET:HE1	2.00	0.43
3:B:17:LYS:O	3:B:18:PRO:C	2.62	0.43
1:L:78:LEU:HD21	1:L:104:LEU:HD21	2.00	0.43
3:B:350:MET:HE3	3:B:401:THR:HG21	2.00	0.43
3:B:280:GLU:N	3:B:281:PRO:HD2	2.34	0.43
3:B:344:THR:HG23	5:B:802:HEM:HBD1	2.01	0.43
1:L:103:LYS:HA	1:L:103:LYS:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:424:MET:CG	3:B:429:THR:HG22	2.49	0.43
2:H:40:ARG:H	2:H:40:ARG:HG2	1.79	0.43
1:L:149:LYS:HB2	1:L:193:THR:HB	2.00	0.42
2:H:199:ARG:HG2	2:H:204:ILE:HG13	2.00	0.42
3:B:47:LEU:HD23	3:B:47:LEU:HA	1.74	0.42
2:H:4:LEU:CD2	2:H:34:MET:HE1	2.49	0.42
3:B:304:ASN:ND2	3:B:307:VAL:HG22	2.34	0.42
3:B:197:ARG:NE	4:C:33:GLU:OE2	2.53	0.42
3:B:12:SER:O	3:B:15:VAL:HG22	2.19	0.42
4:C:110:ARG:HG3	10:C:921:HOH:O	2.19	0.42
3:B:126:ASN:CB	3:B:132:MET:CE	2.95	0.42
3:B:451:LEU:HD22	3:B:455:LEU:HD12	2.01	0.42
4:C:12:ASN:O	4:C:13:ILE:C	2.63	0.42
3:B:216:LEU:CD1	3:B:245:ILE:CG2	2.97	0.42
3:B:224:PHE:O	3:B:228:LYS:HG2	2.20	0.42
3:B:101:PHE:HB2	3:B:150:VAL:HG11	2.01	0.42
3:B:227:VAL:HG23	3:B:237:ILE:HG21	2.01	0.42
4:C:40:THR:O	4:C:41:ASN:HB2	2.19	0.42
3:B:53:PHE:CE1	4:C:74:PHE:HB2	2.54	0.42
3:B:52:PRO:HB2	3:B:54:ASN:ND2	2.35	0.42
3:B:268:TYR:OH	4:C:31:HIS:CD2	2.73	0.42
3:B:346:ALA:HB2	3:B:404:LEU:HB3	2.00	0.42
3:B:40:GLN:O	3:B:44:GLY:HA2	2.20	0.41
3:B:194:ASN:OD1	3:B:194:ASN:C	2.62	0.41
3:B:451:LEU:HD22	3:B:455:LEU:CD1	2.50	0.41
3:B:292:PHE:O	3:B:296:ASN:HB2	2.20	0.41
1:L:46:LEU:HD13	1:L:55:GLN:HG2	2.01	0.41
4:C:27:ALA:O	4:C:30:TYR:HB3	2.21	0.41
1:L:22:ASN:HD22	1:L:72:THR:HG22	1.85	0.41
3:B:99:TRP:O	3:B:100:VAL:C	2.63	0.41
3:B:126:ASN:CG	3:B:132:MET:CE	2.94	0.41
3:B:307:VAL:O	3:B:308:ALA:C	2.63	0.41
4:C:60:ASN:ND2	4:C:63:GLY:HA3	2.36	0.41
1:L:147:LYS:HB2	10:L:321:HOH:O	2.19	0.41
2:H:136:ALA:O	2:H:224:ARG:NH1	2.54	0.41
3:B:88:LEU:HA	3:B:161:THR:HG21	2.02	0.41
4:C:118:SER:O	4:C:122:VAL:HG23	2.21	0.41
4:C:77:GLU:HG3	4:C:80:ASN:HD22	1.86	0.40
2:H:158:PRO:HD2	2:H:212:ALA:CB	2.51	0.40
1:L:21:ILE:O	1:L:72:THR:HA	2.21	0.40
2:H:68:ALA:HB1	2:H:81:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:97:LEU:O	3:B:98:PHE:C	2.65	0.40
2:H:91:SER:HA	2:H:120:VAL:O	2.22	0.40
3:B:80:VAL:HB	3:B:81:PRO:HD3	2.03	0.40
3:B:133:GLY:HA3	4:C:57:GLU:O	2.21	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	L	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
2	H	223/225 (99%)	210 (94%)	12 (5%)	1 (0%)	30	54
3	B	447/465 (96%)	411 (92%)	34 (8%)	2 (0%)	30	54
4	C	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
All	All	1021/1049 (97%)	955 (94%)	63 (6%)	3 (0%)	36	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	256	THR
3	B	380	ASN
2	H	196	SER

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	L	189/189 (100%)	162 (86%)	27 (14%)	3	8
2	H	192/192 (100%)	158 (82%)	34 (18%)	2	5
3	B	360/371 (97%)	306 (85%)	54 (15%)	3	7
4	C	116/120 (97%)	102 (88%)	14 (12%)	5	12
All	All	857/872 (98%)	728 (85%)	129 (15%)	3	7

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	3	GLN
1	L	4	MET
1	L	7	SER
1	L	20	THR
1	L	24	ARG
1	L	27	LYS
1	L	30	ARG
1	L	43	THR
1	L	46	LEU
1	L	54	LEU
1	L	55	GLN
1	L	65	SER
1	L	69	THR
1	L	73	LEU
1	L	79	GLU
1	L	94	TYR
1	L	96	LEU
1	L	103	LYS
1	L	106	LEU
1	L	123	GLU
1	L	169	LYS
1	L	171	SER
1	L	179	LEU
1	L	197	THR
1	L	208	SER
1	L	213	GLU
2	H	1	GLU
2	H	5	GLN
2	H	7	SER
2	H	10	VAL

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Mol	Chain	Res	Type
2	H	11	LEU
2	H	17	SER
2	H	18	VAL
2	H	23	LYS
2	H	30	THR
2	H	34	MET
2	H	40	ARG
2	H	43	GLN
2	H	65	LYS
2	H	78	THR
2	H	87	THR
2	H	106	VAL
2	H	135	LEU
2	H	139	CYS
2	H	142	THR
2	H	143	THR
2	H	147	VAL
2	H	148	THR
2	H	152	LEU
2	H	160	PRO
2	H	161	VAL
2	H	170	LEU
2	H	187	THR
2	H	188	LEU
2	H	189	SER
2	H	192	VAL
2	H	194	VAL
2	H	199	ARG
2	H	204	ILE
2	H	219	LYS
3	B	39	LEU
3	B	64	LEU
3	B	67	TRP
3	B	79	LEU
3	B	92	LYS
3	B	93	LEU
3	B	96	ILE
3	B	107	LEU
3	B	108	THR
3	B	115	VAL
3	B	127	GLU
3	B	164	ARG

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Mol	Chain	Res	Type
3	B	174	LEU
3	B	195	LEU
3	B	196	THR
3	B	210	VAL
3	B	213	VAL
3	B	218	MET
3	B	222	LEU
3	B	236	VAL
3	B	241	LEU
3	B	245	ILE
3	B	288	VAL
3	B	296	ASN
3	B	297	ARG
3	B	298	ARG
3	B	300	ARG
3	B	305	ARG
3	B	307	VAL
3	B	309	LEU
3	B	328	MET
3	B	341	THR
3	B	343	LEU
3	B	358	MET
3	B	359	ILE
3	B	363	ILE
3	B	368	MET
3	B	372	ARG
3	B	381	ARG
3	B	385	LEU
3	B	387	MET
3	B	398	VAL
3	B	401	THR
3	B	404	LEU
3	B	410	LEU
3	B	413	TRP
3	B	427	MET
3	B	429	THR
3	B	433	LEU
3	B	435	ILE
3	B	440	ARG
3	B	448	LEU
3	B	451	LEU
3	B	452	VAL

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Mol	Chain	Res	Type
4	C	7	LYS
4	C	9	MET
4	C	24	LEU
4	C	29	THR
4	C	33	GLU
4	C	38	GLU
4	C	49	VAL
4	C	67	LEU
4	C	80	ASN
4	C	95	LEU
4	C	106	VAL
4	C	137	THR
4	C	139	GLN
4	C	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	22	ASN
1	L	89	GLN
1	L	91	HIS
1	L	137	ASN
1	L	161	ASN
1	L	198	HIS
2	H	43	GLN
2	H	175	HIS
2	H	182	GLN
3	B	30	GLN
3	B	54	ASN
3	B	62	ASN
3	B	139	GLN
3	B	329	HIS
3	B	383	GLN
3	B	411	GLN
3	B	430	GLN
4	C	31	HIS
4	C	60	ASN
4	C	80	ASN
4	C	96	GLN
4	C	102	GLN
4	C	105	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
5	HEM	B	801	8,3	50,50,50	1.85	10 (20%)	67,82,82	2.19	24 (35%)
9	HEC	C	201	4	50,50,50	1.71	6 (12%)	68,82,82	1.61	14 (20%)
5	HEM	B	802	8,7,3	50,50,50	1.81	8 (16%)	67,82,82	1.42	9 (13%)

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
9	HEC	C	201	4	1/1/3/7	2/14/54/54	-
5	HEM	B	801	8,3	-	9/14/54/54	-
5	HEM	B	802	8,7,3	-	6/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	HEM	C3D-C2D	7.86	1.53	1.36
9	C	201	HEC	C3D-C2D	7.28	1.52	1.36
5	B	801	HEM	C3D-C2D	6.63	1.51	1.36
5	B	801	HEM	FE-NC	5.35	2.12	1.95
9	C	201	HEC	FE-ND	5.06	2.10	1.94
5	B	802	HEM	FE-ND	4.58	2.09	1.94
5	B	801	HEM	FE-ND	3.34	2.05	1.94
9	C	201	HEC	FE-NA	3.18	2.05	1.95
5	B	802	HEM	CAC-C3C	2.60	1.54	1.47
5	B	801	HEM	C3C-C4C	-2.52	1.41	1.46
5	B	802	HEM	CAB-C3B	2.47	1.54	1.47
5	B	801	HEM	FE-NA	2.42	2.03	1.95
5	B	802	HEM	C2A-C3A	-2.36	1.32	1.38
5	B	801	HEM	C3B-C2B	-2.34	1.32	1.37
5	B	802	HEM	CHC-C1C	-2.32	1.33	1.38
5	B	802	HEM	FE-NB	2.30	2.02	1.94
5	B	801	HEM	CMB-C2B	2.29	1.55	1.50
9	C	201	HEC	O2A-CGA	-2.25	1.23	1.30
5	B	801	HEM	CMC-C2C	2.25	1.55	1.50
5	B	801	HEM	CBA-CGA	2.23	1.55	1.50
9	C	201	HEC	C3C-C2C	-2.22	1.33	1.38
5	B	802	HEM	O1A-CGA	2.20	1.29	1.22
9	C	201	HEC	C3B-C2B	-2.04	1.32	1.36
5	B	801	HEM	CAC-C3C	2.03	1.52	1.47

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	HEM	CHC-C4B-NB	6.08	130.97	124.42
5	B	801	HEM	C3B-C4B-NB	-6.04	105.13	109.47
5	B	801	HEM	CHD-C4C-NC	5.41	130.34	124.45
5	B	802	HEM	CBA-CAA-C2A	-5.27	97.96	112.53
5	B	801	HEM	C4C-C3C-C2C	5.12	111.25	106.81
9	C	201	HEC	CAB-C3B-C4B	4.95	131.23	124.79
9	C	201	HEC	CHB-C1B-NB	4.57	129.34	124.42
5	B	801	HEM	C4B-C3B-C2B	4.47	111.39	107.28
9	C	201	HEC	CBD-CAD-C3D	-4.29	100.67	112.53
5	B	802	HEM	C4D-ND-C1D	4.12	110.08	105.21
5	B	801	HEM	C4D-ND-C1D	4.09	110.06	105.21
5	B	801	HEM	CAD-C3D-C4D	3.63	131.02	124.70
5	B	801	HEM	CMC-C2C-C1C	3.58	131.03	124.73
9	C	201	HEC	CAB-C3B-C2B	-3.55	121.04	127.56
5	B	802	HEM	CAD-C3D-C4D	3.31	130.47	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	201	HEC	CBA-CAA-C2A	-3.01	104.21	112.53
9	C	201	HEC	C1D-ND-C4D	2.95	108.70	105.21
5	B	801	HEM	CBC-CAC-C3C	-2.77	113.68	127.53
5	B	801	HEM	CBB-CAB-C3B	-2.75	113.80	127.53
5	B	801	HEM	CHC-C1C-C2C	2.67	131.04	125.49
5	B	801	HEM	CMD-C2D-C1D	2.65	129.17	125.03
5	B	801	HEM	CHC-C1C-NC	-2.61	121.61	124.45
5	B	802	HEM	C4D-C3D-C2D	-2.60	103.10	106.89
5	B	802	HEM	CAD-CBD-CGD	-2.59	106.78	113.67
5	B	801	HEM	CMB-C2B-C1B	2.58	129.07	125.03
5	B	801	HEM	CHB-C1B-NB	2.51	127.47	124.37
5	B	802	HEM	CHA-C1A-NA	2.48	128.35	123.86
5	B	801	HEM	O1D-CGD-CBD	-2.47	115.26	123.09
5	B	802	HEM	CHD-C4C-NC	2.45	127.12	124.45
5	B	801	HEM	CAD-CBD-CGD	2.41	120.05	113.67
5	B	801	HEM	C1C-CHC-C4B	-2.36	121.00	126.02
9	C	201	HEC	CHB-C1B-C2B	-2.32	121.37	125.03
9	C	201	HEC	O2A-CGA-O1A	-2.31	117.38	123.33
9	C	201	HEC	O2A-CGA-CBA	2.31	121.30	114.00
5	B	801	HEM	O2D-CGD-CBD	2.30	121.26	114.00
5	B	802	HEM	CAA-CBA-CGA	-2.27	107.64	113.67
5	B	801	HEM	CMC-C2C-C3C	-2.25	122.98	128.43
5	B	801	HEM	C4D-C3D-C2D	-2.22	103.66	106.89
5	B	801	HEM	C1B-NB-C4B	2.21	107.83	105.21
9	C	201	HEC	CAD-C3D-C4D	2.21	128.55	124.70
5	B	801	HEM	CBD-CAD-C3D	-2.15	106.58	112.53
9	C	201	HEC	C4D-C3D-C2D	-2.13	103.79	106.89
5	B	801	HEM	C4C-NC-C1C	2.12	109.27	105.82
9	C	201	HEC	CHD-C4C-NC	2.11	127.69	123.86
5	B	802	HEM	CHD-C1D-ND	2.06	126.64	124.42
9	C	201	HEC	C3B-C4B-NB	-2.05	107.93	110.17
9	C	201	HEC	CHC-C4B-C3B	2.03	128.97	125.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	C	201	HEC	NA

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	HEM	C2B-C3B-CAB-CBB

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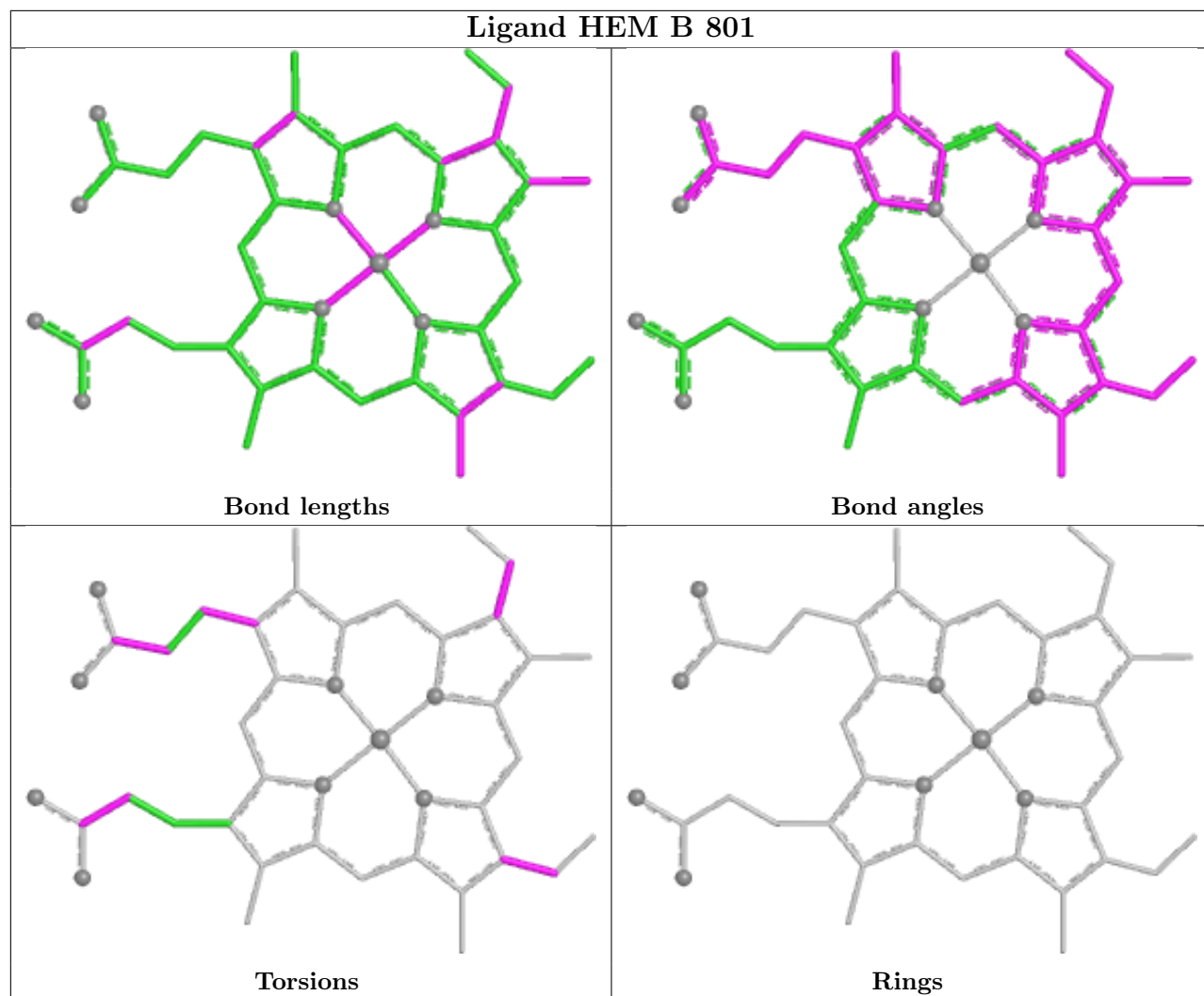
Mol	Chain	Res	Type	Atoms
5	B	801	HEM	C2C-C3C-CAC-CBC
5	B	801	HEM	C4C-C3C-CAC-CBC
5	B	801	HEM	C4B-C3B-CAB-CBB
5	B	802	HEM	CAA-CBA-CGA-O1A
5	B	801	HEM	CAA-CBA-CGA-O1A
5	B	802	HEM	CAA-CBA-CGA-O2A
9	C	201	HEC	CAD-CBD-CGD-O1D
5	B	801	HEM	C4D-C3D-CAD-CBD
9	C	201	HEC	CAD-CBD-CGD-O2D
5	B	801	HEM	CAA-CBA-CGA-O2A
5	B	802	HEM	C4B-C3B-CAB-CBB
5	B	802	HEM	C4C-C3C-CAC-CBC
5	B	801	HEM	CAD-CBD-CGD-O1D
5	B	801	HEM	CAD-CBD-CGD-O2D
5	B	802	HEM	C2B-C3B-CAB-CBB
5	B	802	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

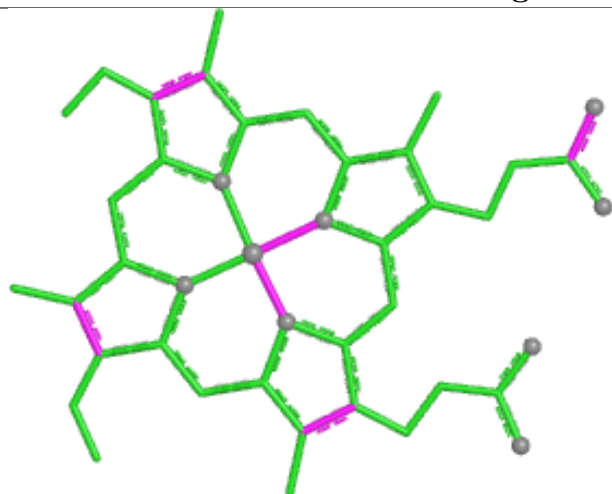
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	HEM	3	0
9	C	201	HEC	7	0
5	B	802	HEM	5	0

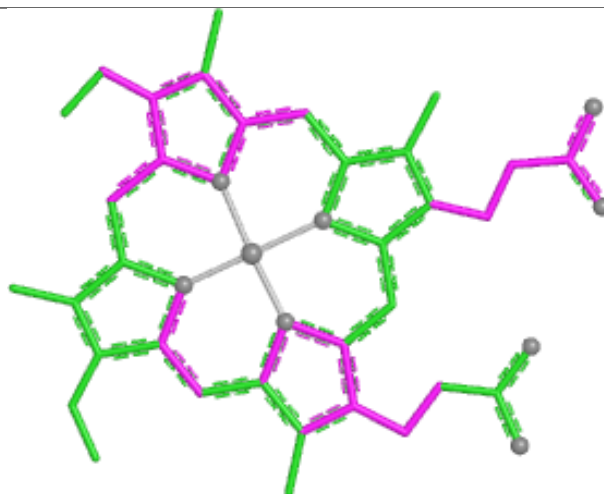
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



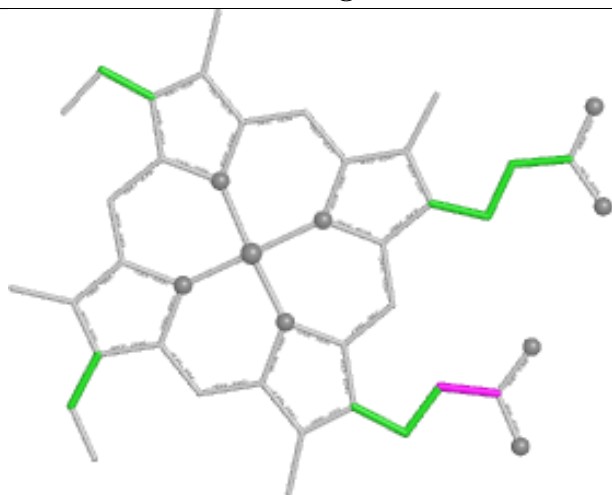
Ligand HEC C 201



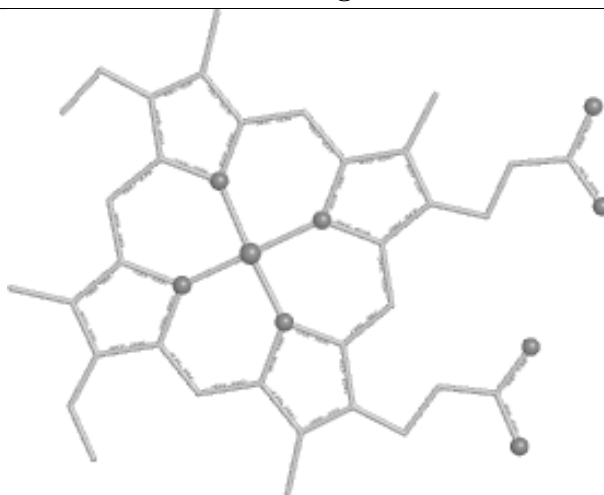
Bond lengths



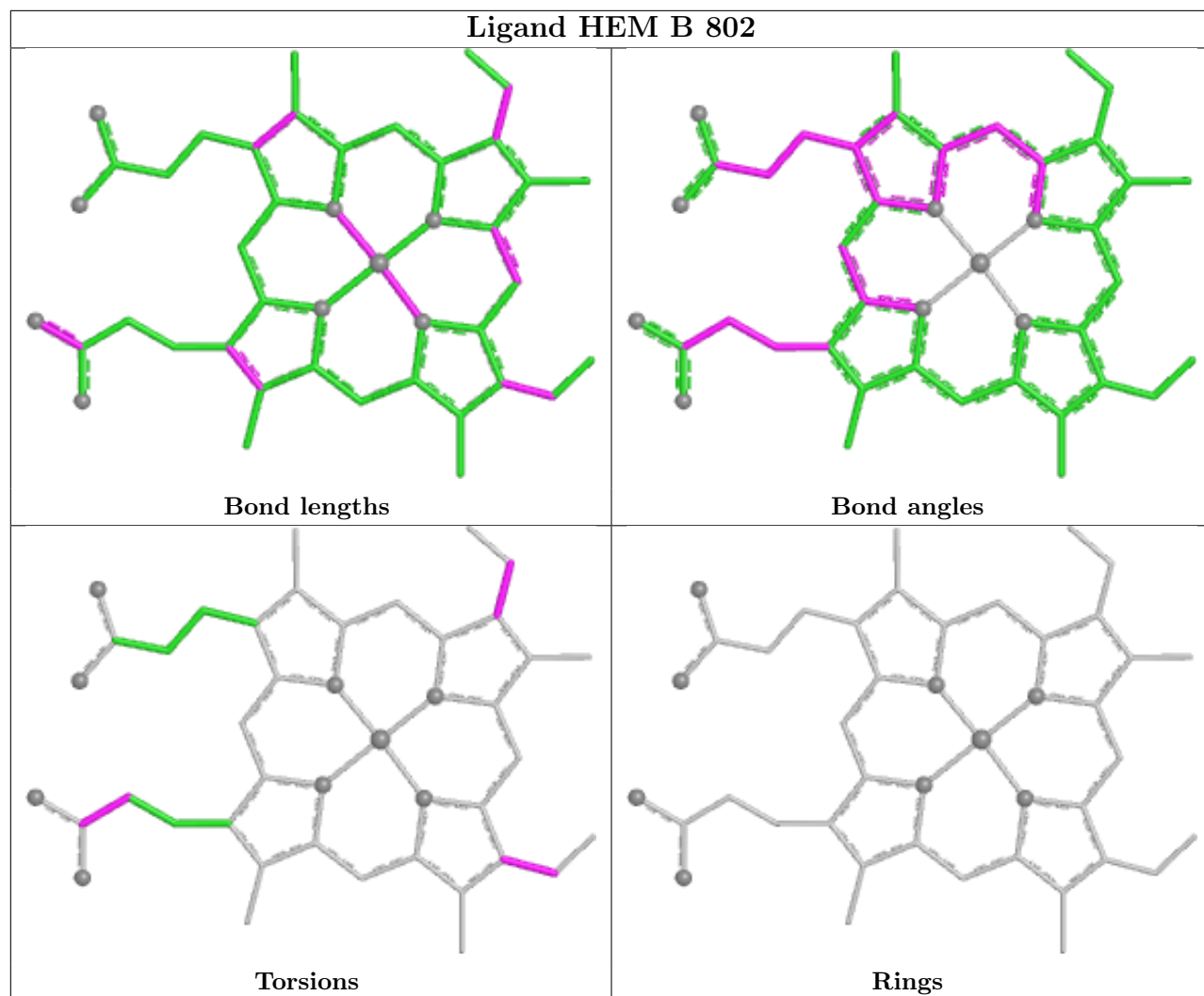
Bond angles



Torsions



Rings



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	L	213/213 (100%)	-0.71	0 100 100	48, 72, 99, 121	1 (0%)
2	H	225/225 (100%)	-0.54	4 (1%) 67 65	42, 70, 107, 134	3 (1%)
3	B	449/465 (96%)	-0.43	1 (0%) 91 90	57, 89, 141, 179	0
4	C	142/146 (97%)	-0.62	1 (0%) 84 83	49, 78, 114, 137	0
All	All	1029/1049 (98%)	-0.54	6 (0%) 85 85	42, 79, 129, 179	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	22	CYS	3.2
2	H	206	CYS	2.9
3	B	85	ASP	2.9
2	H	225	GLY	2.8
4	C	139	GLN	2.6
2	H	88	ASN	2.2

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,

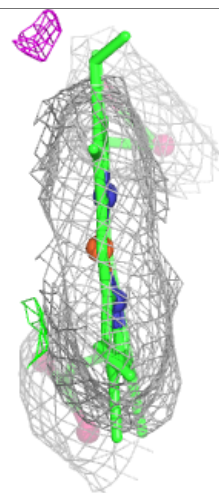
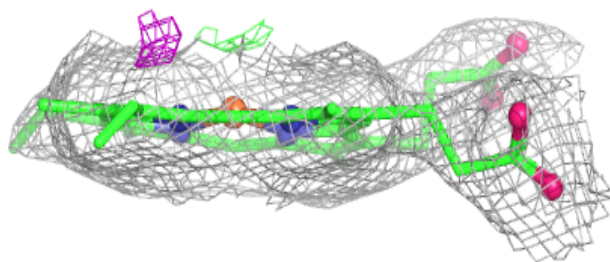
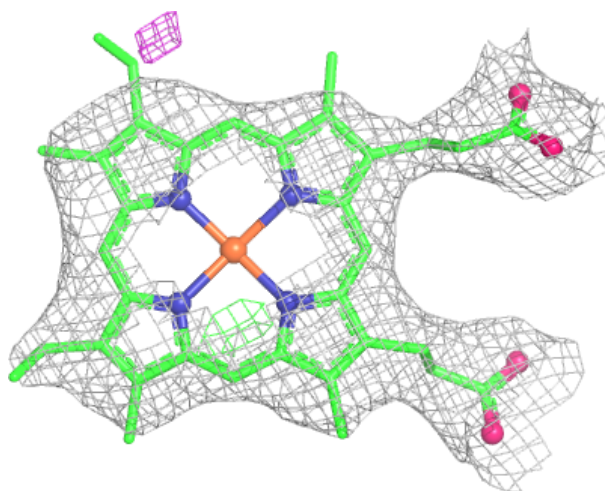
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	O	B	805	1/1	0.97	0.07	60,60,60,60	0
5	HEM	B	802	43/43	0.99	0.06	57,66,73,83	0
5	HEM	B	801	43/43	0.99	0.06	51,59,68,76	0
8	CA	C	804	1/1	0.99	0.03	60,60,60,60	0
9	HEC	C	201	43/43	0.99	0.06	50,58,64,70	0
6	FE	B	803	1/1	1.00	0.02	64,64,64,64	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.

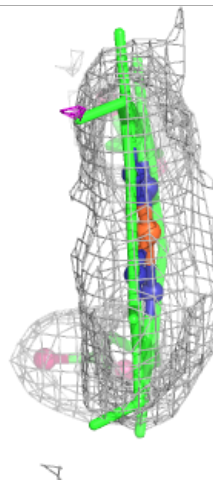
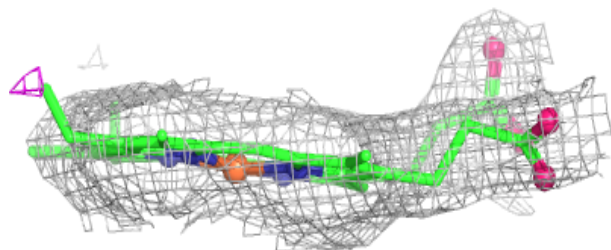
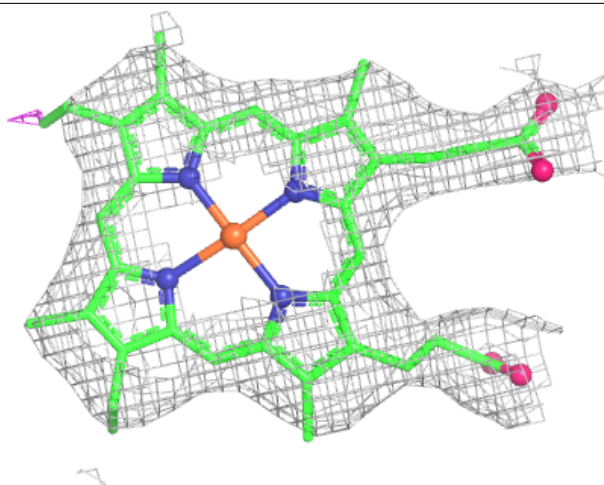
Electron density around HEM B 802:

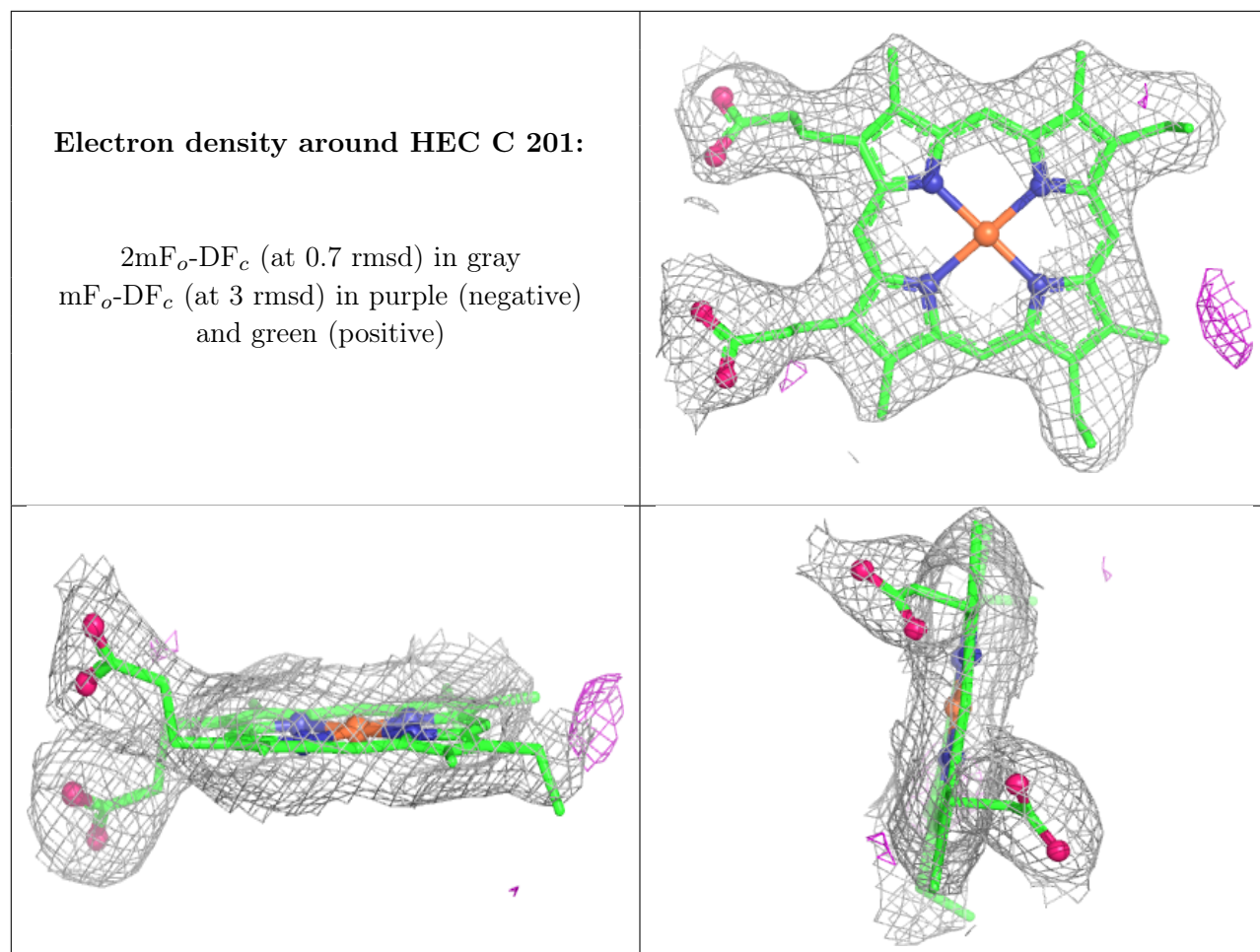
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 801:

$2mF_o-DF_c$ (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.