



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 07:06 PM EDT

PDB ID : 1Y5L  
Title : The crystal structure of the NarGHI mutant NarI-H66Y  
Authors : Bertero, M.G.; Rothery, R.A.; Boroumand, N.; Palak, M.; Blasco, F.; Ginet, N.; Weiner, J.H.; Strynadka, N.C.J.  
Deposited on : 2004-12-02  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.23.2  
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) : 2.23.2

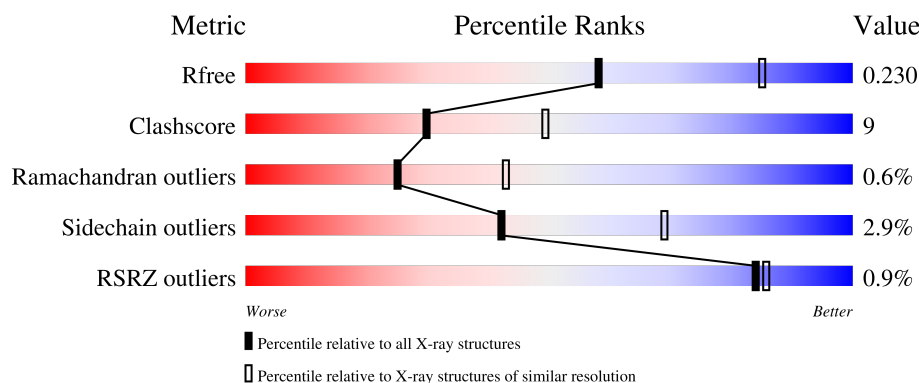
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1246	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 18%, green 79%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>79%</span> <span>19%</span> </div> </div>
2	B	512	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 14%, green 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>84%</span> <span>14%</span> </div> </div>
3	C	225	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 25%, green 67%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>67%</span> <span>25%</span> <span>6%</span> </div> </div>

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	SF4	A	1801	-	-	X	-
6	SF4	B	1803	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16150 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 Respiratory nitrate reductase 1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1244	Total	C	N	O	S	0	0	0
			9869	6232	1731	1858	48			

- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	509	Total	C	N	O	S	0	0	0
			4050	2562	701	755	32			

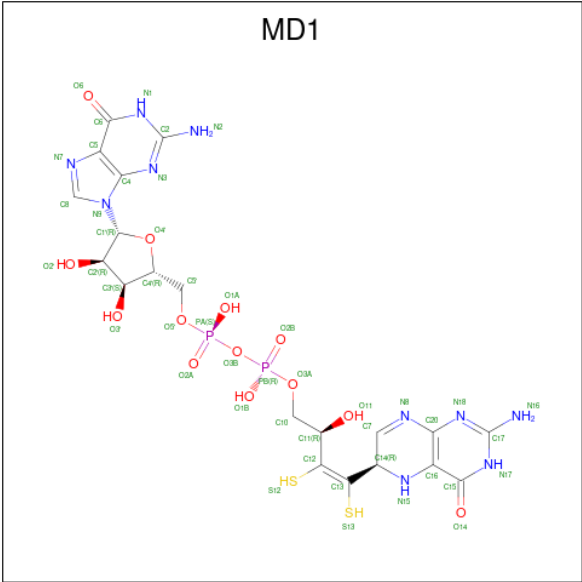
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1676	1109	283	272	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	MET	modified residue	UNP P11350
C	66	TYR	HIS	engineered mutation	UNP P11350

- Molecule 4 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (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>).

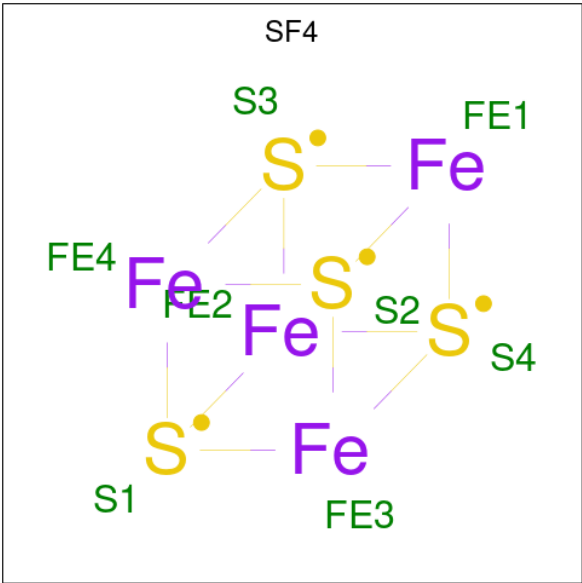


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 5 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

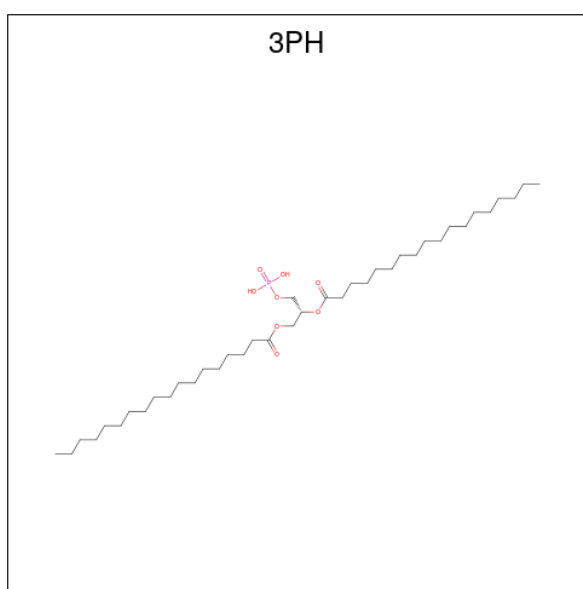
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



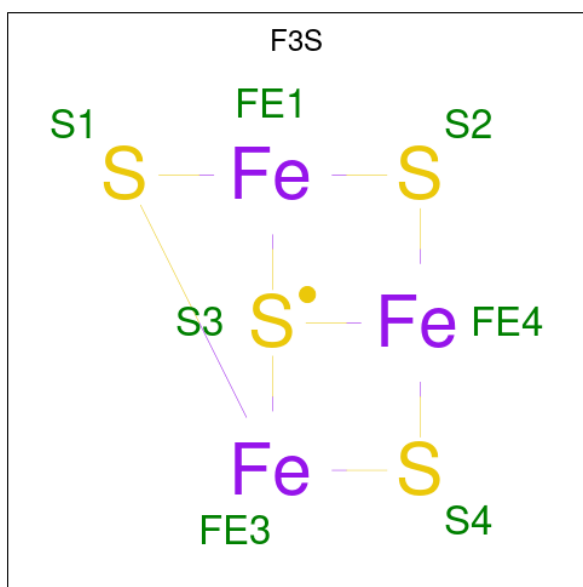
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



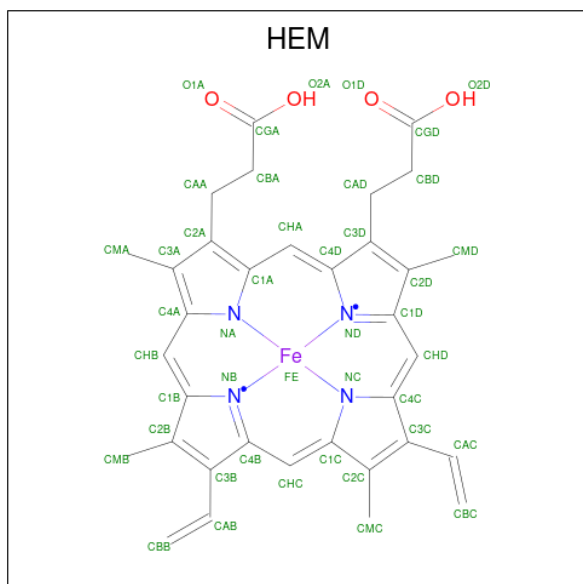
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			27	18	8	1		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	174	Total 174	O 174	0	0
10	B	145	Total 145	O 145	0	0
10	C	32	Total 32	O 32	0	0



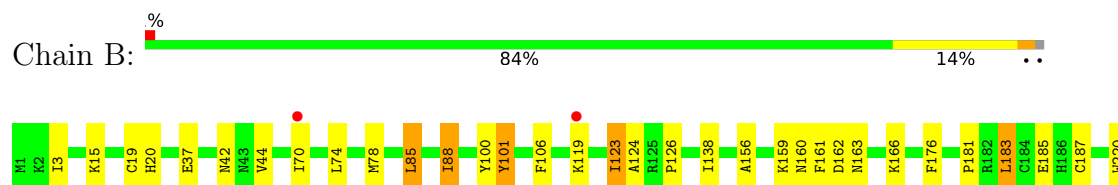
### 3 Residue-property plots

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: Respiratory nitrate reductase 1 alpha chain

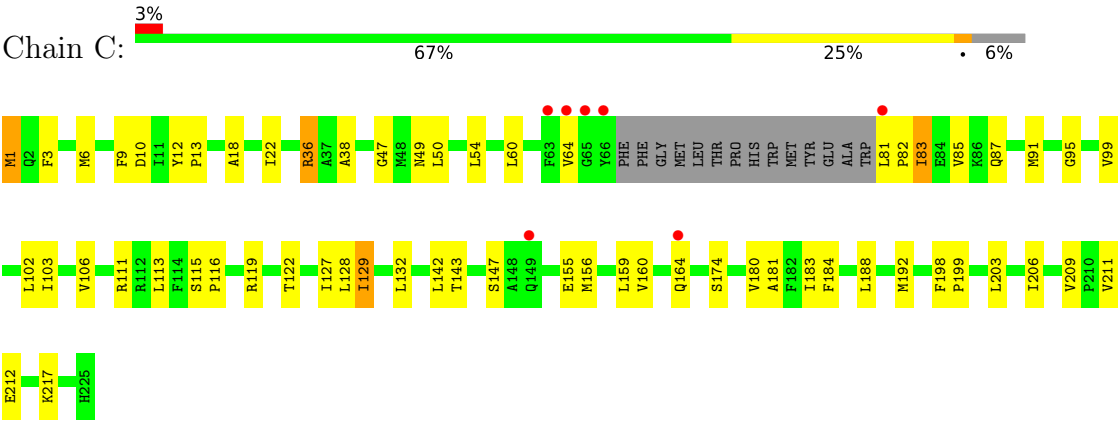


- Molecule 2: Respiratory nitrate reductase 1 beta chain





● Molecule 3: Respiratory nitrate reductase 1 gamma chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.16Å 241.90Å 139.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.79 – 2.50 24.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.79-2.50) 99.5 (24.79-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.188 , 0.237 0.183 , 0.230	Depositor DCC
$R_{free}$ test set	7209 reflections (8.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.999	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: F3S, MD1, 6MO, FME, 3PH, HEM, SF4

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	0.33	0/10128	0.61	1/13749 (0.0%)
2	B	0.36	0/4146	0.62	0/5609
3	C	0.37	0/1709	0.54	0/2309
All	All	0.34	0/15983	0.61	1/21667 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1097	ILE	N-CA-C	-5.19	96.99	111.00

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	9869	0	9527	197	0
2	B	4050	0	3973	55	0
3	C	1676	0	1726	44	0
4	A	94	0	42	6	0
5	A	1	0	0	0	0
6	A	8	0	0	2	0
6	B	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	27	0	27	0	0
8	B	7	0	0	0	0
9	C	43	0	30	1	0
10	A	174	0	0	2	1
10	B	145	0	0	4	0
10	C	32	0	0	3	0
All	All	16150	0	15325	293	1

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 9.

All (293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:HD21	1:A:382:GLU:HB2	1.34	0.92
3:C:129:ILE:HD11	3:C:203:LEU:HD11	1.50	0.91
2:B:123:ILE:HD13	2:B:124:ALA:H	1.36	0.89
1:A:165:VAL:O	1:A:169:ILE:HG12	1.83	0.78
1:A:250:ILE:HD13	1:A:278:VAL:HB	1.64	0.78
1:A:508:GLU:OE1	1:A:515:ARG:HD2	1.83	0.78
1:A:1098:HIS:HE1	4:A:2800:MD1:S13	2.07	0.77
1:A:663:THR:HG21	1:A:692:ILE:HD12	1.66	0.77
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.53	0.73
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.72	0.72
1:A:626:GLU:OE1	1:A:635:LYS:HE3	1.91	0.70
1:A:1098:HIS:CE1	4:A:2800:MD1:S13	2.84	0.70
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.72	0.69
2:B:123:ILE:HD13	2:B:124:ALA:N	2.07	0.69
1:A:116:ARG:HH11	1:A:119:LYS:HD3	1.57	0.69
1:A:282:PRO:HB2	1:A:1158:MET:HE3	1.72	0.69
2:B:3:ILE:HD12	2:B:301:LEU:CD1	2.24	0.68
1:A:146:LYS:HD3	1:A:150:GLN:HE22	1.58	0.67
1:A:378:ASN:ND2	1:A:382:GLU:HB2	2.07	0.67
2:B:303:PRO:O	2:B:309:ILE:HD11	1.94	0.67
1:A:387:ASN:HD22	1:A:405:ARG:HB2	1.61	0.65
3:C:155:GLU:HB2	10:C:837:HOH:O	1.95	0.65
1:A:578:VAL:HG23	1:A:579:GLY:H	1.61	0.65
3:C:6:MET:O	3:C:10:ASP:HB2	1.96	0.65
1:A:1092:HIS:HA	1:A:1163:HIS:HB3	1.79	0.64
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.80	0.64
1:A:223:LEU:O	1:A:225:PRO:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:HG3	2:B:15:LYS:HE3	1.80	0.64
3:C:83:ILE:HD13	3:C:83:ILE:O	1.98	0.63
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.79	0.63
1:A:116:ARG:NH1	1:A:119:LYS:HD3	2.15	0.62
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.82	0.61
2:B:373:SER:HB3	2:B:428:ARG:NH1	2.15	0.61
2:B:156:ALA:HB1	2:B:166:LYS:HD2	1.83	0.61
1:A:120:MET:HB3	1:A:138:ILE:HD12	1.83	0.60
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.83	0.60
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.84	0.60
1:A:931:ASN:O	1:A:932:TYR:HB2	2.00	0.60
2:B:508:THR:O	2:B:509:GLU:HB3	2.01	0.59
1:A:1074:ILE:HD13	1:A:1075:GLY:N	2.16	0.59
2:B:245:ILE:HD13	2:B:245:ILE:H	1.66	0.59
1:A:169:ILE:HD12	1:A:769:VAL:HG21	1.84	0.59
1:A:287:ILE:HD13	1:A:287:ILE:O	2.02	0.59
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.67	0.59
1:A:191:ILE:H	1:A:191:ILE:HD12	1.68	0.59
1:A:345:ARG:HB2	1:A:348:TYR:O	2.03	0.58
1:A:1098:HIS:CE1	4:A:1800:MD1:S12	2.97	0.58
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.84	0.58
1:A:825:ILE:O	1:A:829:ILE:HG12	2.04	0.58
1:A:335:ASP:O	1:A:338:MET:HB2	2.03	0.58
1:A:686:SER:HB3	1:A:692:ILE:HG12	1.85	0.58
1:A:799:THR:CG2	1:A:806:ILE:HG12	2.34	0.58
1:A:662:GLY:HA2	1:A:704:ASN:ND2	2.19	0.57
1:A:722:LYS:HD2	1:A:722:LYS:H	1.69	0.57
1:A:487:LEU:HD12	1:A:487:LEU:N	2.19	0.57
1:A:191:ILE:O	1:A:194:MET:HG2	2.05	0.56
3:C:81:LEU:N	3:C:81:LEU:HD23	2.20	0.56
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.87	0.56
3:C:160:VAL:O	3:C:164:GLN:HG3	2.05	0.56
1:A:191:ILE:O	1:A:191:ILE:HG22	2.06	0.56
4:A:1800:MD1:H7	4:A:1800:MD1:C11	2.36	0.55
3:C:181:ALA:HB3	3:C:184:PHE:CD2	2.41	0.55
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.88	0.55
1:A:308:ALA:O	1:A:311:HIS:HB3	2.07	0.55
1:A:634:ASP:OD1	1:A:637:ARG:HG3	2.07	0.55
1:A:453:HIS:HA	1:A:489:ASP:OD1	2.07	0.55
1:A:767:LEU:HD13	1:A:769:VAL:HG23	1.89	0.55
1:A:1127:LEU:HB2	1:A:1129:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:LEU:HG	3:C:81:LEU:O	2.06	0.55
1:A:336:MET:HA	1:A:473:VAL:HB	1.89	0.55
2:B:88:ILE:HD13	2:B:88:ILE:O	2.06	0.54
1:A:102:LEU:HD12	1:A:102:LEU:H	1.72	0.54
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.89	0.54
1:A:920:THR:O	1:A:920:THR:HG23	2.07	0.54
1:A:875:ASP:HB3	1:A:877:ILE:HD11	1.88	0.54
3:C:119:ARG:O	3:C:122:THR:HG22	2.08	0.54
1:A:720:SER:O	1:A:722:LYS:HD2	2.08	0.54
1:A:360:LEU:N	1:A:360:LEU:HD22	2.23	0.54
3:C:12:TYR:N	3:C:13:PRO:HD2	2.23	0.54
1:A:591:PRO:HA	1:A:596:LEU:HB2	1.89	0.53
3:C:142:LEU:HB3	3:C:183:ILE:HD11	1.88	0.53
1:A:214:LEU:HB3	1:A:607:SER:OG	2.08	0.53
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.89	0.53
2:B:78:MET:HG3	10:B:1911:HOH:O	2.09	0.53
1:A:1127:LEU:CB	1:A:1129:ILE:HD13	2.38	0.53
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.91	0.53
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.44	0.53
1:A:191:ILE:HD12	1:A:191:ILE:N	2.24	0.52
1:A:387:ASN:ND2	1:A:405:ARG:HB2	2.24	0.52
3:C:129:ILE:CD1	3:C:203:LEU:HD11	2.33	0.52
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.08	0.52
2:B:70:ILE:HG13	10:B:1928:HOH:O	2.09	0.52
2:B:88:ILE:HD11	2:B:220:TRP:CE3	2.44	0.52
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.92	0.52
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.91	0.52
1:A:360:LEU:HG	1:A:383:MET:HE3	1.91	0.52
2:B:19:CYS:O	2:B:20:HIS:HB2	2.10	0.52
3:C:83:ILE:HD13	3:C:83:ILE:C	2.30	0.52
3:C:99:VAL:O	3:C:103:ILE:HG12	2.09	0.52
1:A:168:LEU:HD23	1:A:168:LEU:O	2.10	0.52
1:A:338:MET:HG3	1:A:374:THR:HB	1.90	0.52
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.92	0.52
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.31	0.52
1:A:921:GLN:HB2	10:A:3926:HOH:O	2.10	0.51
1:A:517:GLN:HA	1:A:517:GLN:NE2	2.25	0.51
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.92	0.51
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.78	0.51
1:A:279:ALA:HB2	1:A:291:CYS:SG	2.51	0.51
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:O	1:A:123:GLU:HG3	2.10	0.51
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.46	0.51
1:A:190:PRO:HB2	1:A:191:ILE:HD12	1.93	0.50
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.41	0.50
1:A:111:PRO:HA	1:A:787:PRO:HD3	1.92	0.50
2:B:162:ASP:O	2:B:163:ASN:HB2	2.12	0.50
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.42	0.50
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.46	0.50
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.94	0.50
2:B:183:LEU:HD23	2:B:183:LEU:N	2.26	0.50
3:C:60:LEU:O	3:C:64:VAL:HG23	2.12	0.50
3:C:159:LEU:HD21	3:C:180:VAL:HG21	1.94	0.50
4:A:1800:MD1:H7	4:A:1800:MD1:H11	1.93	0.50
1:A:93:PRO:HG2	1:A:94:ARG:HD3	1.94	0.49
1:A:471:THR:HG21	1:A:476:LEU:HD13	1.95	0.49
3:C:211:VAL:HG23	3:C:212:GLU:N	2.27	0.49
3:C:143:THR:HB	3:C:184:PHE:CE1	2.48	0.49
2:B:224:ILE:CD1	2:B:234:PHE:HB2	2.43	0.49
2:B:176:PHE:CD1	2:B:385:ILE:HD12	2.47	0.48
1:A:54:THR:HG21	1:A:260:ARG:NH2	2.28	0.48
1:A:52:ASN:HB3	1:A:1098:HIS:HE2	1.78	0.48
3:C:95:GLY:O	3:C:99:VAL:HG23	2.14	0.48
3:C:142:LEU:HB3	3:C:183:ILE:CD1	2.43	0.48
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.14	0.48
3:C:129:ILE:HD11	3:C:203:LEU:CD1	2.33	0.48
1:A:222:ASP:HB3	1:A:578:VAL:HG21	1.96	0.47
3:C:87:GLN:O	3:C:91:MET:HG3	2.14	0.47
1:A:663:THR:CG2	1:A:668:ILE:HD11	2.44	0.47
2:B:336:GLU:HB3	10:B:1833:HOH:O	2.13	0.47
1:A:1006:ILE:HD13	1:A:1006:ILE:H	1.79	0.47
1:A:373:LYS:HD3	1:A:392:PHE:CZ	2.48	0.47
1:A:795:ASP:OD2	1:A:949:ILE:HD11	2.13	0.47
1:A:289:LYS:O	1:A:289:LYS:HD3	2.14	0.47
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.50	0.47
1:A:152:ARG:HB2	1:A:734:THR:CG2	2.44	0.47
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.80	0.47
1:A:250:ILE:CD1	1:A:278:VAL:HB	2.41	0.47
1:A:936:GLU:HG2	1:A:937:GLY:N	2.28	0.47
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.15	0.47
3:C:13:PRO:HB3	3:C:192:MET:SD	2.55	0.47
1:A:554:TYR:O	1:A:558:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.26	0.47
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.34	0.47
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.97	0.46
2:B:3:ILE:HD12	2:B:301:LEU:HD13	1.98	0.46
1:A:803:HIS:HB2	1:A:804:PRO:HD2	1.96	0.46
1:A:1062:ARG:HD2	10:A:3971:HOH:O	2.14	0.46
2:B:450:ALA:HB1	2:B:455:ARG:HD3	1.97	0.46
1:A:268:THR:HG22	1:A:290:LEU:HD22	1.98	0.46
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.30	0.46
3:C:113:LEU:CD2	3:C:127:ILE:HD12	2.45	0.46
1:A:919:ASN:ND2	1:A:921:GLN:H	2.14	0.46
2:B:295:ARG:NH1	2:B:298:ASP:OD1	2.49	0.46
1:A:338:MET:HB3	1:A:354:MET:HE2	1.97	0.46
1:A:373:LYS:HD3	1:A:392:PHE:CE1	2.51	0.46
1:A:729:LYS:HD2	1:A:736:HIS:CD2	2.50	0.46
2:B:404:ARG:O	2:B:408:ARG:HG3	2.15	0.46
1:A:854:HIS:HB2	1:A:1205:ALA:HB3	1.97	0.46
1:A:949:ILE:HD12	1:A:949:ILE:H	1.81	0.46
2:B:3:ILE:HG12	2:B:311:GLN:HG3	1.98	0.46
1:A:102:LEU:HD12	1:A:102:LEU:N	2.31	0.46
1:A:225:PRO:O	1:A:228:PRO:HD2	2.16	0.46
1:A:658:ALA:HA	1:A:659:PRO:C	2.36	0.46
1:A:736:HIS:CE1	1:A:738:ILE:HB	2.51	0.45
1:A:1087:ASN:O	1:A:1159:THR:HG22	2.16	0.45
1:A:225:PRO:C	1:A:228:PRO:HD2	2.37	0.45
1:A:677:MET:HG3	1:A:682:TYR:HB2	1.99	0.45
2:B:187:CYS:HB3	2:B:349:THR:O	2.16	0.45
3:C:82:PRO:HG2	3:C:85:VAL:CG2	2.45	0.45
1:A:596:LEU:O	1:A:600:ARG:HD2	2.17	0.45
1:A:68:VAL:HB	1:A:102:LEU:HD22	1.99	0.45
1:A:336:MET:HB3	1:A:474:TYR:HB2	1.98	0.45
2:B:220:TRP:C	2:B:221:ARG:HG3	2.37	0.45
1:A:107:ARG:HD2	1:A:773:PHE:O	2.16	0.45
1:A:487:LEU:N	1:A:487:LEU:CD1	2.80	0.45
2:B:224:ILE:HD11	2:B:234:PHE:HB2	1.97	0.45
3:C:18:ALA:O	3:C:22:ILE:HG22	2.16	0.45
2:B:185:GLU:OE1	2:B:353:VAL:HB	2.16	0.45
2:B:508:THR:O	2:B:509:GLU:CB	2.64	0.44
1:A:55:GLY:HA3	6:A:1801:SF4:S3	2.56	0.44
1:A:949:ILE:HD12	1:A:949:ILE:N	2.31	0.44
3:C:128:LEU:O	3:C:132:LEU:HG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:TYR:O	2:B:101:TYR:HB3	2.17	0.44
3:C:181:ALA:HB3	3:C:184:PHE:CE2	2.53	0.44
1:A:244:TYR:HA	1:A:270:VAL:CG2	2.48	0.44
1:A:7:PHE:C	1:A:9:TYR:H	2.19	0.44
1:A:1168:ILE:O	2:B:123:ILE:HD13	2.18	0.44
2:B:292:LEU:HD13	2:B:345:PRO:O	2.18	0.44
1:A:46:ARG:HG3	1:A:74:GLN:NE2	2.32	0.44
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.18	0.44
1:A:854:HIS:O	1:A:855:ASP:HB2	2.17	0.44
1:A:1138:PHE:CG	1:A:1176:ILE:HD13	2.53	0.44
1:A:1195:THR:HA	1:A:1198:ILE:CD1	2.47	0.44
1:A:983:THR:O	1:A:987:LEU:HG	2.18	0.44
3:C:198:PHE:HB3	3:C:199:PRO:CD	2.48	0.43
1:A:20:GLY:O	3:C:217:LYS:HD2	2.18	0.43
1:A:91:GLY:HA2	6:A:1801:SF4:S4	2.58	0.43
1:A:220:TYR:CE2	4:A:1800:MD1:H101	2.53	0.43
1:A:515:ARG:HG2	1:A:516:SER:N	2.34	0.43
1:A:1037:THR:HB	1:A:1043:GLN:HG3	1.99	0.43
1:A:1183:ILE:O	1:A:1186:SER:HB2	2.18	0.43
3:C:9:PHE:HB2	3:C:174:SER:HB3	2.00	0.43
1:A:856:SER:O	1:A:859:GLU:HG2	2.18	0.43
1:A:7:PHE:CD1	1:A:7:PHE:N	2.86	0.43
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.54	0.43
3:C:1:FME:O1	3:C:3:PHE:HB3	2.19	0.43
1:A:360:LEU:CD1	1:A:383:MET:HE1	2.49	0.43
1:A:1110:LEU:HD12	1:A:1110:LEU:HA	1.89	0.43
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.54	0.43
2:B:471:PRO:HB3	2:B:502:ILE:CD1	2.49	0.43
1:A:338:MET:HB3	1:A:354:MET:CE	2.48	0.43
1:A:795:ASP:HA	1:A:809:LEU:O	2.18	0.43
2:B:44:VAL:HA	2:B:181:PRO:HA	2.01	0.43
1:A:225:PRO:HB2	1:A:551:ASP:OD1	2.19	0.43
1:A:722:LYS:HD2	1:A:722:LYS:N	2.32	0.43
1:A:1127:LEU:HB3	1:A:1129:ILE:CD1	2.49	0.43
2:B:246:PHE:HA	6:B:1803:SF4:S4	2.58	0.43
3:C:102:LEU:O	3:C:106:VAL:HG23	2.19	0.43
1:A:1074:ILE:HD13	1:A:1074:ILE:C	2.39	0.42
2:B:360:SER:CB	2:B:385:ILE:HG12	2.48	0.42
3:C:50:LEU:HD11	3:C:54:LEU:HD11	2.01	0.42
1:A:330:VAL:HA	1:A:334:THR:HG23	2.02	0.42
2:B:407:LYS:HD3	2:B:433:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:O	1:A:224:PRO:HD3	2.19	0.42
2:B:373:SER:HB3	2:B:428:ARG:HH12	1.85	0.42
1:A:120:MET:O	1:A:138:ILE:HD11	2.20	0.42
2:B:85:LEU:HD12	2:B:85:LEU:HA	1.90	0.42
1:A:1195:THR:O	1:A:1198:ILE:HD13	2.19	0.42
2:B:159:LYS:HG3	10:B:1869:HOH:O	2.18	0.42
3:C:184:PHE:O	3:C:188:LEU:HG	2.20	0.42
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.85	0.42
1:A:590:GLN:N	1:A:591:PRO:HD2	2.35	0.42
1:A:550:LEU:H	1:A:550:LEU:HD23	1.84	0.42
1:A:1208:PHE:O	1:A:1209:ASN:HB2	2.20	0.42
1:A:550:LEU:HD23	1:A:550:LEU:N	2.35	0.42
1:A:862:GLN:HA	1:A:863:PRO:HD2	1.90	0.42
1:A:191:ILE:HG23	1:A:580:GLN:O	2.19	0.42
1:A:574:TRP:CZ2	1:A:576:HIS:HB2	2.55	0.42
1:A:1100:THR:HG22	1:A:1101:TYR:CD1	2.54	0.42
1:A:219:TRP:HB2	1:A:607:SER:HB2	2.02	0.41
1:A:52:ASN:OD1	1:A:191:ILE:HG12	2.20	0.41
1:A:357:ALA:O	1:A:363:ALA:HA	2.19	0.41
1:A:578:VAL:HG23	1:A:579:GLY:N	2.29	0.41
3:C:47:GLY:HA2	10:C:830:HOH:O	2.20	0.41
2:B:309:ILE:HD11	2:B:326:GLN:HE21	1.84	0.41
3:C:155:GLU:O	3:C:159:LEU:HD23	2.21	0.41
3:C:156:MET:O	3:C:160:VAL:HG23	2.21	0.41
1:A:1007:ILE:HG22	1:A:1008:SER:O	2.21	0.41
1:A:1167:ARG:HB2	1:A:1183:ILE:CG2	2.49	0.41
1:A:199:TYR:CD1	1:A:199:TYR:C	2.94	0.41
3:C:36:ARG:HG2	3:C:38:ALA:H	1.85	0.41
3:C:115:SER:HA	3:C:116:PRO:HD2	1.85	0.41
1:A:344:GLU:HG2	1:A:349:TYR:CE1	2.55	0.41
1:A:1134:TRP:CZ3	1:A:1147:ARG:HG3	2.56	0.41
1:A:177:ILE:HG12	1:A:182:PRO:HA	2.02	0.41
1:A:336:MET:N	1:A:337:PRO:HD2	2.35	0.41
1:A:1065:ILE:O	1:A:1065:ILE:HD12	2.21	0.41
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.56	0.41
2:B:42:ASN:HB2	6:B:1803:SF4:S1	2.61	0.41
2:B:160:ASN:HB2	2:B:389:TYR:CE2	2.56	0.41
2:B:305:ASP:O	2:B:309:ILE:HG12	2.21	0.41
2:B:372:GLY:HA3	2:B:379:ASP:OD1	2.21	0.41
2:B:403:LEU:O	2:B:407:LYS:HB2	2.20	0.41
1:A:329:TYR:CZ	1:A:565:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:THR:HG23	1:A:668:ILE:HD11	2.03	0.41
1:A:875:ASP:HB3	1:A:877:ILE:CD1	2.50	0.41
1:A:17:PHE:CZ	1:A:22:GLY:HA3	2.56	0.40
1:A:1177:THR:O	1:A:1178:GLN:HB2	2.20	0.40
3:C:209:VAL:HG13	3:C:209:VAL:O	2.21	0.40
1:A:168:LEU:HD23	1:A:168:LEU:C	2.42	0.40
1:A:1207:GLY:HA3	1:A:1210:TYR:HB3	2.02	0.40
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.48	0.40
1:A:130:ASP:HA	1:A:131:PRO:HD2	1.95	0.40
1:A:184:ARG:NH2	1:A:704:ASN:HD22	2.20	0.40
1:A:813:VAL:HG12	1:A:814:ASP:N	2.36	0.40
2:B:335:MET:HE2	2:B:335:MET:HB3	1.94	0.40
1:A:184:ARG:HH21	1:A:704:ASN:HD22	1.68	0.40
1:A:864:LEU:HD22	1:A:864:LEU:N	2.36	0.40
2:B:126:PRO:CB	2:B:138:ILE:HD11	2.51	0.40
1:A:539:ILE:HD13	1:A:575:ALA:HB3	2.03	0.40
1:A:724:HIS:NE2	1:A:1167:ARG:NH1	2.69	0.40
1:A:897:GLU:HG3	1:A:938:PRO:HD2	2.04	0.40
2:B:248:TYR:CG	2:B:249:PRO:HD3	2.56	0.40
3:C:111:ARG:NH2	10:C:833:HOH:O	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:3889:HOH:O	10:A:3889:HOH:O[3_354]	1.70	0.50

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1242/1246 (100%)	1150 (93%)	82 (7%)	10 (1%)	19 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	507/512 (99%)	487 (96%)	19 (4%)	1 (0%)	47	68
3	C	207/225 (92%)	198 (96%)	9 (4%)	0	100	100
All	All	1956/1983 (99%)	1835 (94%)	110 (6%)	11 (1%)	25	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	A	422	SER
1	A	1166	GLU
2	B	101	TYR
1	A	718	GLY
1	A	190	PRO
1	A	635	LYS
1	A	721	GLY
1	A	861	ALA
1	A	578	VAL
1	A	224	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	1039/1043 (100%)	1008 (97%)	31 (3%)	41	68
2	B	436/439 (99%)	425 (98%)	11 (2%)	47	73
3	C	174/186 (94%)	169 (97%)	5 (3%)	42	69
All	All	1649/1668 (99%)	1602 (97%)	47 (3%)	42	69

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	94	ARG
1	A	150	GLN

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Mol	Chain	Res	Type
1	A	190	PRO
1	A	287	ILE
1	A	338	MET
1	A	366	GLN
1	A	367	GLU
1	A	461	GLN
1	A	476	LEU
1	A	515	ARG
1	A	582	LYS
1	A	600	ARG
1	A	601	PRO
1	A	767	LEU
1	A	804	PRO
1	A	806	ILE
1	A	808	PRO
1	A	837	CYS
1	A	864	LEU
1	A	926	LEU
1	A	936	GLU
1	A	995	ARG
1	A	1006	ILE
1	A	1041	ARG
1	A	1062	ARG
1	A	1072	GLU
1	A	1074	ILE
1	A	1087	ASN
1	A	1110	LEU
1	A	1233	LEU
2	B	37	GLU
2	B	74	LEU
2	B	85	LEU
2	B	88	ILE
2	B	119	LYS
2	B	123	ILE
2	B	161	PHE
2	B	183	LEU
2	B	221	ARG
2	B	245	ILE
2	B	428	ARG
3	C	36	ARG
3	C	49	ASN
3	C	83	ILE

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Mol	Chain	Res	Type
3	C	129	ILE
3	C	147	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	37	GLN
1	A	150	GLN
1	A	173	ASN
1	A	179	ASN
1	A	234	GLN
1	A	258	GLN
1	A	387	ASN
1	A	461	GLN
1	A	517	GLN
1	A	559	ASN
1	A	604	HIS
1	A	704	ASN
1	A	708	ASN
1	A	919	ASN
1	A	942	GLN
1	A	946	ASN
1	A	1076	GLN
1	A	1082	GLN
1	A	1098	HIS
2	B	160	ASN
2	B	451	ASN
3	C	49	ASN
3	C	53	ASN
3	C	149	GLN
3	C	175	GLN
3	C	225	HIS

### 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	$\# Z  > 2$
3	FME	C	1	3	8,9,10	1.47	2 (25%)	7,9,11	1.53	1 (14%)

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	FME	C	1	3	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-2.80	1.48	1.53
3	C	1	FME	CB-CG	2.33	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	2.99	127.42	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	O1-CN-N-CA
3	C	1	FME	N-CA-CB-CG
3	C	1	FME	CB-CG-SD-CE
3	C	1	FME	C-CA-CB-CG
3	C	1	FME	CB-CA-N-CN



There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	SF4	A	1801	1	0,12,12	-	-	-		
7	3PH	A	1309	-	26,26,47	0.76	1 (3%)	30,31,52	1.57	3 (10%)
4	MD1	A	2800	5	38,51,51	3.71	10 (26%)	35,78,78	1.89	8 (22%)
4	MD1	A	1800	5	38,51,51	3.89	9 (23%)	35,78,78	2.11	9 (25%)
9	HEM	C	806	3	27,50,50	2.29	13 (48%)	17,82,82	1.74	5 (29%)
8	F3S	B	1805	2	0,9,9	-	-	-		
6	SF4	B	1804	2	0,12,12	-	-	-		
6	SF4	B	1803	2	0,12,12	-	-	-		
6	SF4	B	1802	2	0,12,12	-	-	-		

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
7	3PH	A	1309	-	-	3/28/28/49	-
6	SF4	A	1801	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MD1	A	2800	5	-	2/21/59/59	0/5/5/5
4	MD1	A	1800	5	-	7/21/59/59	0/5/5/5
6	SF4	B	1802	2	-	-	0/6/5/5
8	F3S	B	1805	2	-	-	0/3/3/3
6	SF4	B	1804	2	-	-	0/6/5/5
6	SF4	B	1803	2	-	-	0/6/5/5
9	HEM	C	806	3	-	0/6/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	MD1	C7-N8	19.08	1.50	1.27
4	A	2800	MD1	C7-N8	17.89	1.48	1.27
4	A	1800	MD1	C4-N9	-7.33	1.38	1.47
4	A	2800	MD1	C4-N9	-7.05	1.38	1.47
4	A	2800	MD1	C6-N1	6.11	1.43	1.33
4	A	1800	MD1	C15-N17	5.57	1.42	1.33
4	A	1800	MD1	C5-C6	-5.40	1.43	1.52
9	C	806	HEM	C3B-CAB	5.09	1.58	1.47
4	A	1800	MD1	C6-N1	5.01	1.41	1.33
4	A	2800	MD1	C15-N17	4.98	1.41	1.33
9	C	806	HEM	C3C-CAC	4.49	1.57	1.47
4	A	2800	MD1	C5-C6	-4.48	1.45	1.52
4	A	2800	MD1	C15-C16	3.95	1.46	1.41
9	C	806	HEM	CAD-C3D	3.63	1.58	1.52
4	A	1800	MD1	C14-C13	3.62	1.55	1.51
4	A	1800	MD1	C20-N18	3.45	1.39	1.34
4	A	2800	MD1	C20-N18	3.41	1.39	1.34
9	C	806	HEM	C3C-C2C	-3.36	1.35	1.40
4	A	1800	MD1	C17-N17	3.28	1.41	1.35
4	A	2800	MD1	C17-N17	3.10	1.40	1.35
4	A	1800	MD1	C13-C12	2.93	1.43	1.34
9	C	806	HEM	C3B-C2B	-2.77	1.36	1.40
9	C	806	HEM	C4D-C3D	2.67	1.48	1.42
9	C	806	HEM	CMC-C2C	2.63	1.57	1.51
4	A	2800	MD1	C5-C4	-2.50	1.37	1.53
9	C	806	HEM	CMA-C3A	2.36	1.56	1.51
7	A	1309	3PH	C32-C31	2.35	1.57	1.50
9	C	806	HEM	CMD-C2D	2.27	1.56	1.51
9	C	806	HEM	CAA-C2A	2.25	1.55	1.52
9	C	806	HEM	C1D-ND	2.16	1.40	1.36
4	A	2800	MD1	O11-C11	2.16	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	806	HEM	C1B-C2B	2.10	1.47	1.42
9	C	806	HEM	C1C-C2C	2.04	1.47	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1800	MD1	C4-C5-N7	6.41	110.96	102.46
4	A	2800	MD1	C4-C5-N7	6.02	110.44	102.46
7	A	1309	3PH	C23-C22-C21	5.28	132.84	113.62
4	A	1800	MD1	C15-N17-C17	5.04	123.94	115.93
7	A	1309	3PH	C33-C32-C31	4.69	130.68	113.62
4	A	1800	MD1	N17-C17-N18	-4.51	118.35	125.42
4	A	2800	MD1	C15-N17-C17	4.31	122.77	115.93
4	A	2800	MD1	N17-C17-N18	-3.64	119.71	125.42
4	A	1800	MD1	N16-C17-N18	3.23	122.28	117.25
4	A	1800	MD1	C15-C16-N15	3.21	121.81	119.12
9	C	806	HEM	CMA-C3A-C4A	-3.19	123.56	128.46
4	A	1800	MD1	C5-C6-N1	-2.95	114.55	118.19
4	A	2800	MD1	C15-C16-N15	2.83	121.50	119.12
9	C	806	HEM	CMB-C2B-C3B	2.73	129.78	124.68
4	A	2800	MD1	C16-C15-N17	-2.62	116.55	124.01
9	C	806	HEM	CMA-C3A-C2A	2.60	129.84	124.94
4	A	2800	MD1	PA-O3B-PB	2.58	141.68	132.83
4	A	1800	MD1	C16-C15-N17	-2.43	117.10	124.01
4	A	1800	MD1	O4'-C1'-N9	-2.41	105.46	109.04
9	C	806	HEM	CAA-CBA-CGA	2.34	116.60	112.67
4	A	2800	MD1	N16-C17-N17	2.29	120.81	117.25
7	A	1309	3PH	C2-O21-C21	2.15	123.10	117.79
4	A	1800	MD1	O6-C6-C5	2.12	124.19	119.86
9	C	806	HEM	CMC-C2C-C3C	2.10	128.60	124.68
4	A	2800	MD1	N18-C20-N8	2.04	120.91	116.00

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1800	MD1	C5'-O5'-PA-O2A
4	A	2800	MD1	C2'-C1'-N9-C8
4	A	1800	MD1	O4'-C4'-C5'-O5'
4	A	1800	MD1	C3'-C4'-C5'-O5'
7	A	1309	3PH	C32-C31-O31-C3
7	A	1309	3PH	O32-C31-O31-C3

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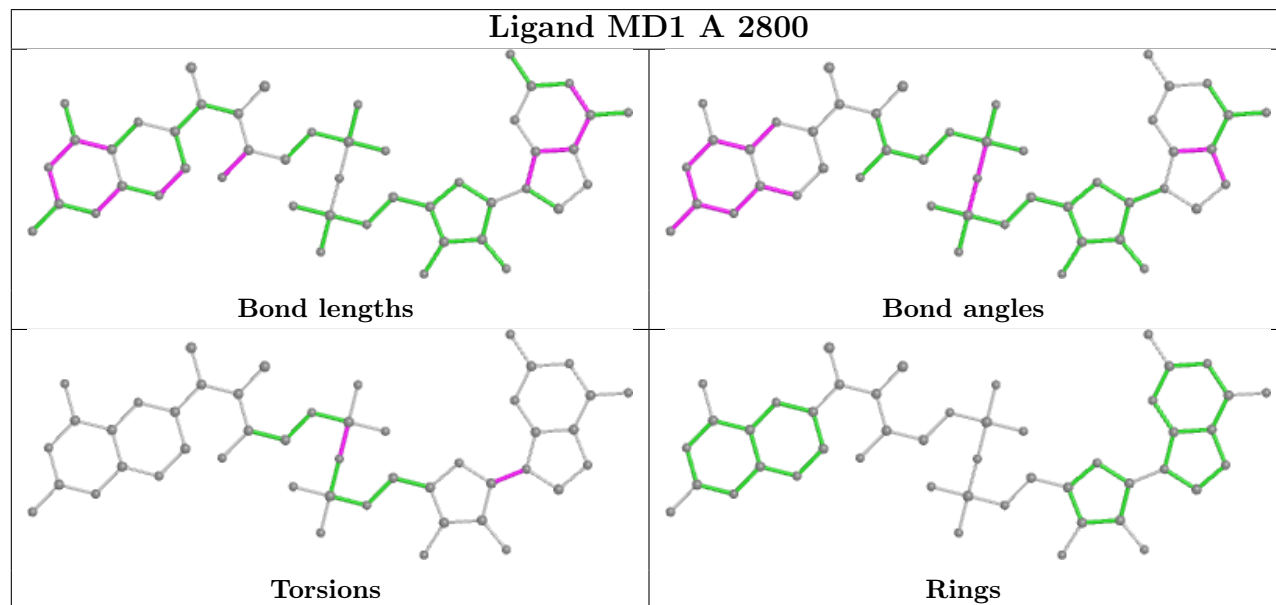
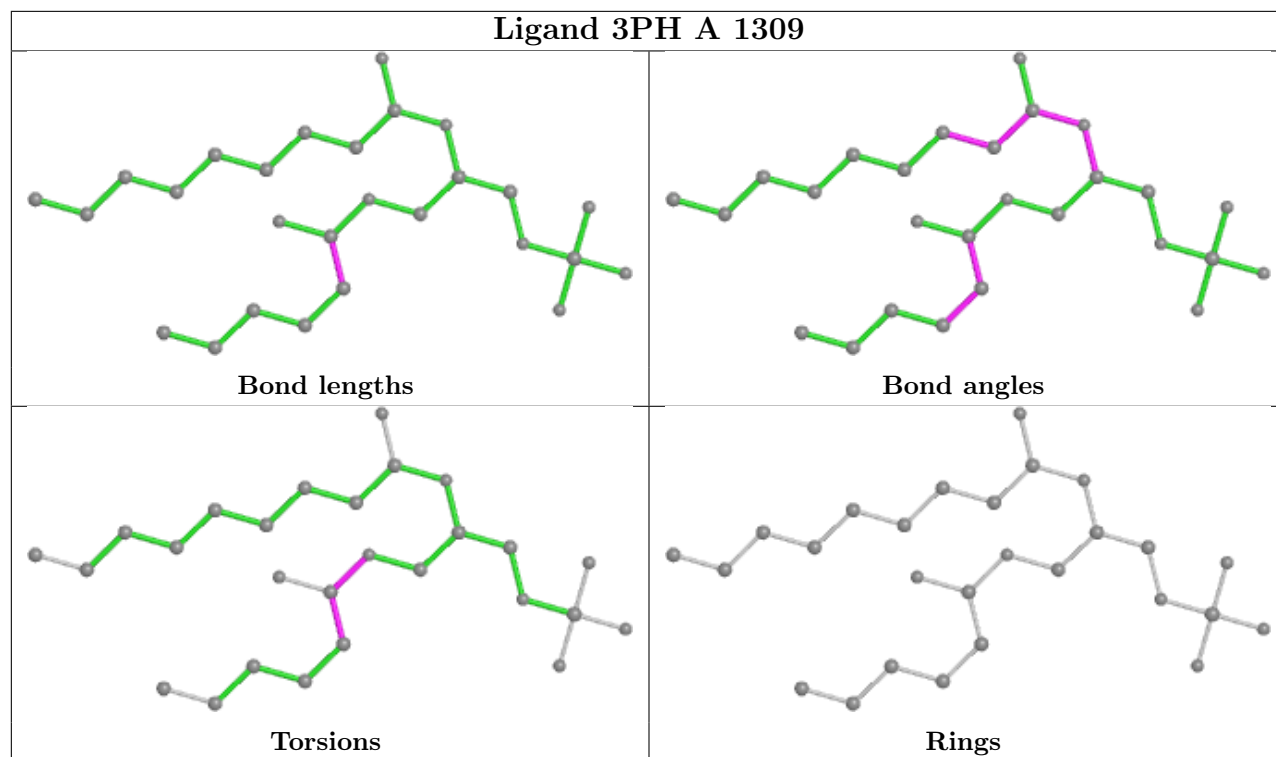
Mol	Chain	Res	Type	Atoms
4	A	1800	MD1	PA-O3B-PB-O2B
4	A	2800	MD1	PA-O3B-PB-O2B
4	A	1800	MD1	C5'-O5'-PA-O1A
4	A	1800	MD1	C5'-O5'-PA-O3B
4	A	1800	MD1	C2'-C1'-N9-C4
7	A	1309	3PH	O31-C31-C32-C33

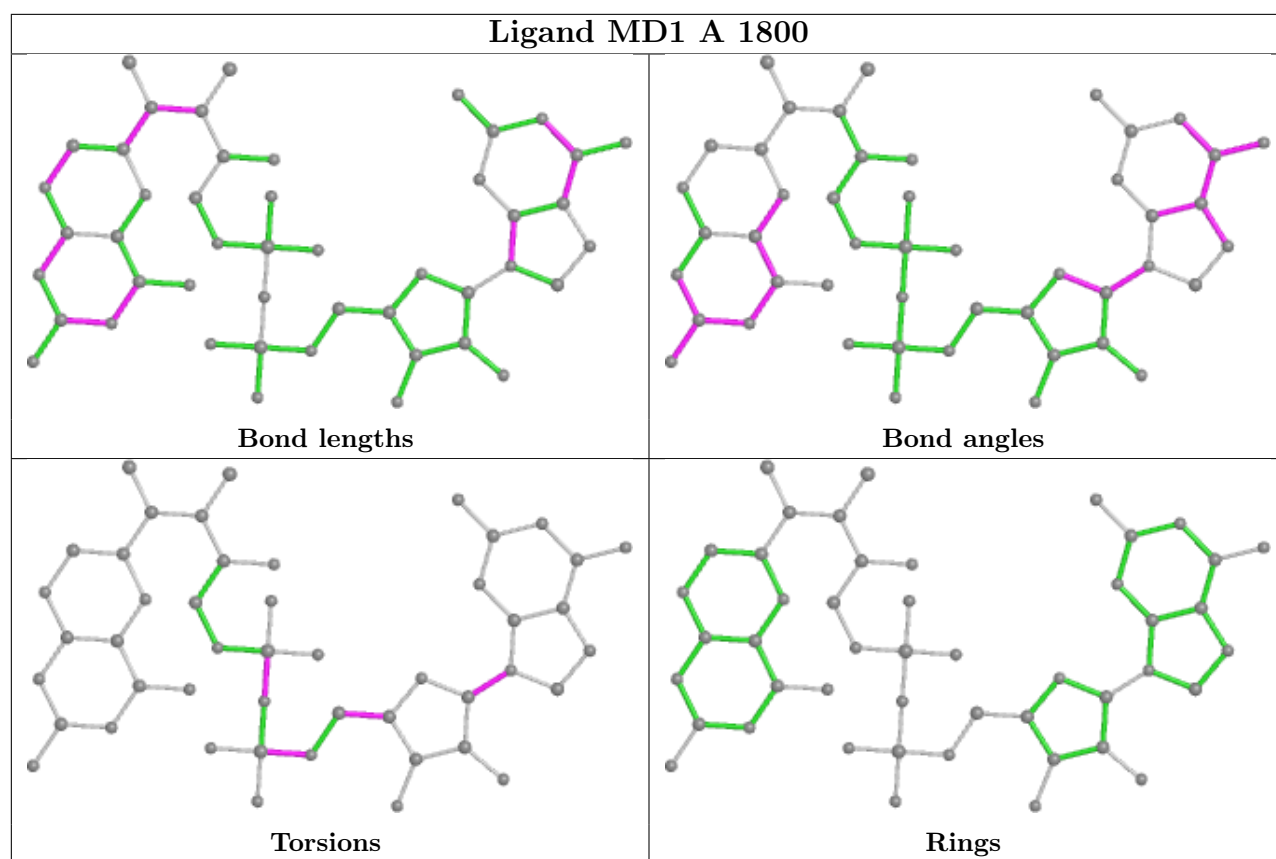
There are no ring outliers.

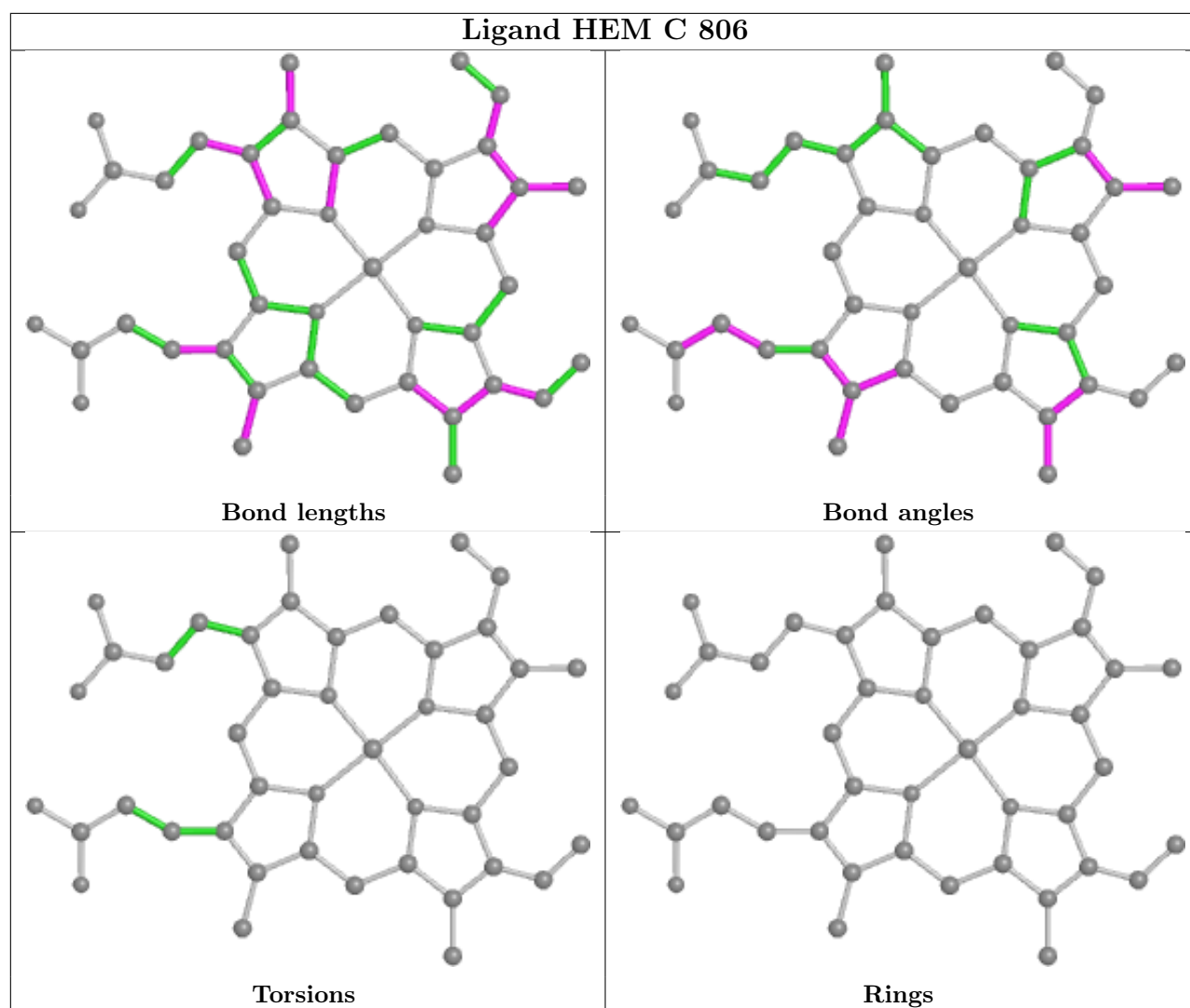
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1801	SF4	2	0
4	A	2800	MD1	2	0
4	A	1800	MD1	4	0
9	C	806	HEM	1	0
6	B	1803	SF4	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.







## 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

### 6.1 Protein, DNA and RNA chains

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	1244/1246 (99%)	-0.59	8 (0%)	89 90	13, 26, 46, 83	0
2	B	509/512 (99%)	-0.78	3 (0%)	89 90	10, 21, 38, 63	0
3	C	210/225 (93%)	-0.32	7 (3%)	46 50	18, 33, 59, 65	0
All	All	1963/1983 (98%)	-0.61	18 (0%)	84 86	10, 25, 48, 83	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	8.1
1	A	10	PHE	7.4
3	C	64	VAL	4.3
1	A	11	LYS	3.5
3	C	66	TYR	3.3
3	C	81	LEU	3.3
1	A	8	ARG	3.3
3	C	65	GLY	3.1
3	C	149	GLN	2.9
2	B	119	LYS	2.6
1	A	463	ALA	2.6
1	A	13	LYS	2.6
1	A	12	GLN	2.5
2	B	70	ILE	2.4
3	C	63	PHE	2.4
3	C	164	GLN	2.4
2	B	366	ALA	2.1
1	A	461	GLN	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
3	FME	C	1	10/11	0.89	0.28	54,60,75,76	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

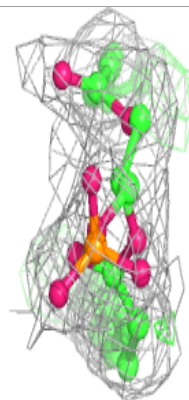
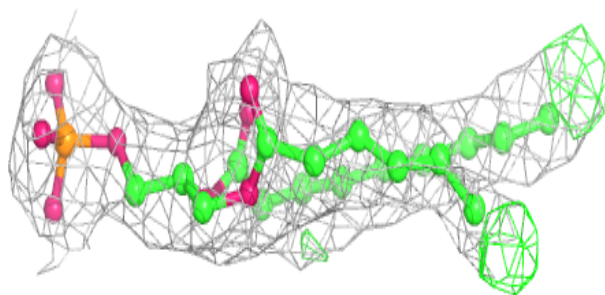
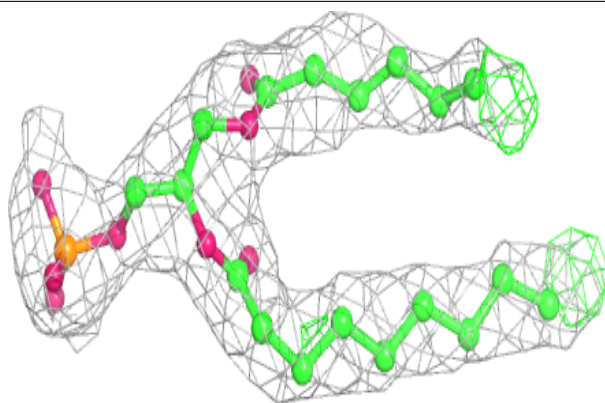
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	3PH	A	1309	27/48	0.95	0.13	20,28,50,54	0
4	MD1	A	2800	47/47	0.97	0.10	13,25,34,37	0
4	MD1	A	1800	47/47	0.97	0.09	17,25,36,38	0
9	HEM	C	806	43/43	0.97	0.12	12,24,29,45	0
6	SF4	B	1802	8/8	0.98	0.06	21,24,25,26	0
6	SF4	B	1804	8/8	0.98	0.06	19,21,25,25	0
5	6MO	A	3800	1/1	0.98	0.07	38,38,38,38	0
6	SF4	A	1801	8/8	0.98	0.04	20,21,25,33	0
8	F3S	B	1805	7/7	0.99	0.08	17,18,20,21	0
6	SF4	B	1803	8/8	0.99	0.07	15,17,18,18	0

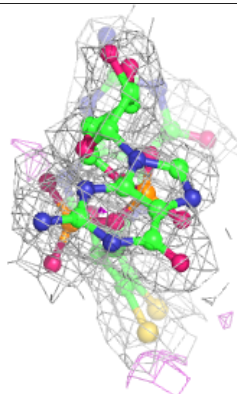
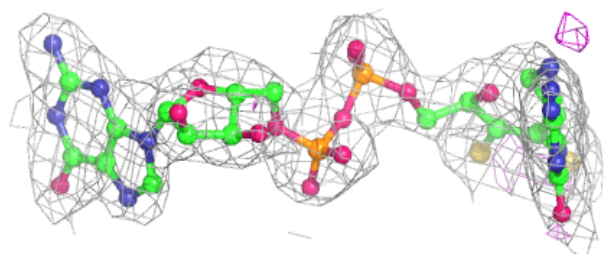
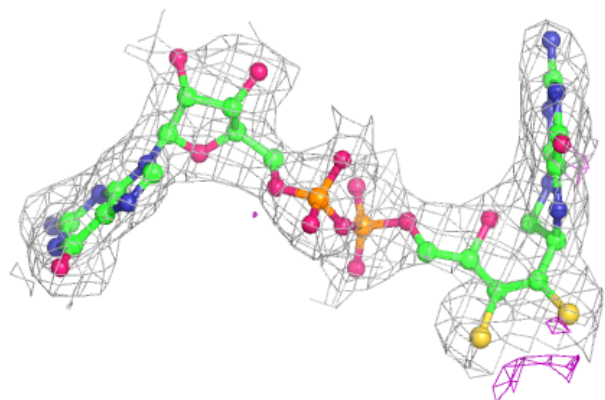
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 3PH A 1309:**

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

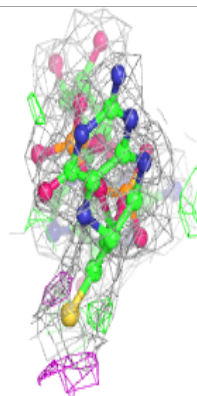
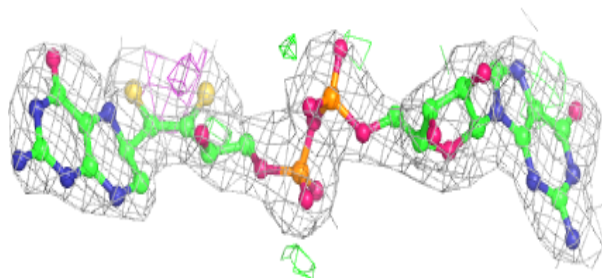
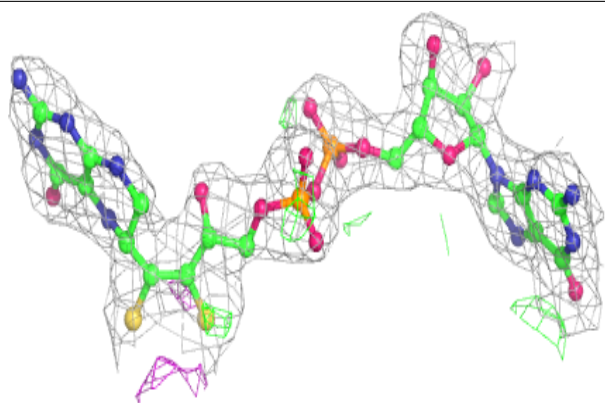
**Electron density around MD1 A 2800:**

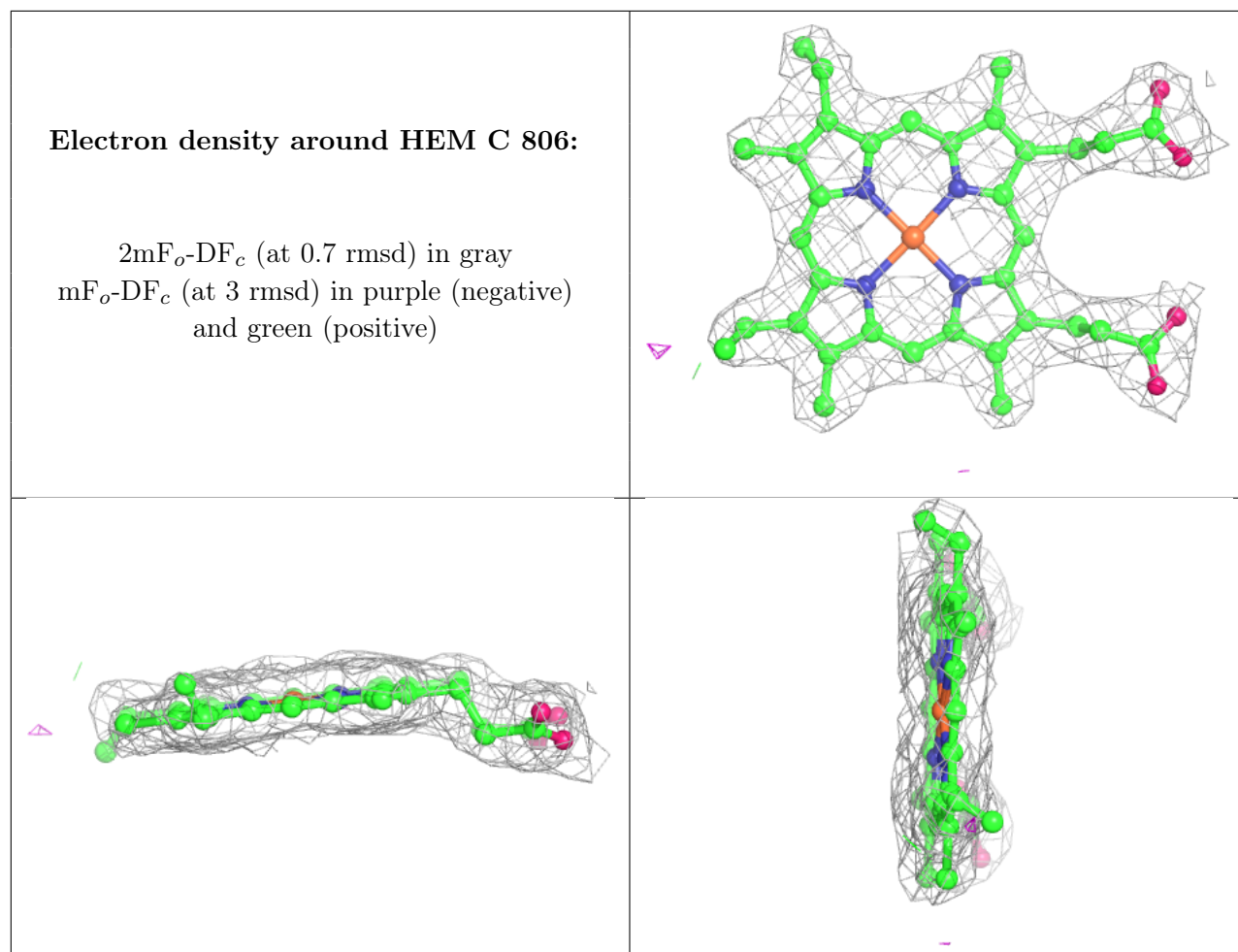
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MD1 A 1800:**

$2mF_o-DF_c$  (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.