



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:02 AM UTC

PDB ID : 1Y5L / pdb_00001y5l
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

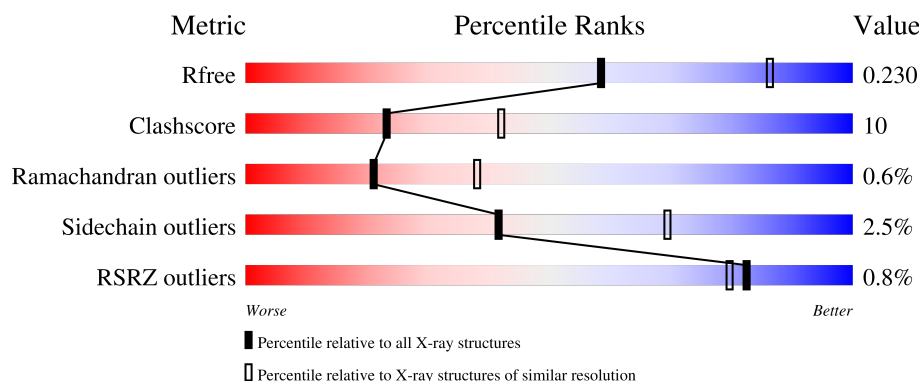
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	2% 75% 22% .
2	B	512	81% 17% ..
3	C	225	2% 66% 25% . 6%

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			

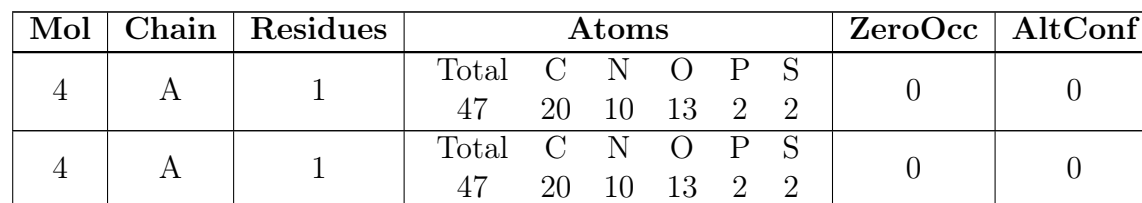
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

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 (CCD ID: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

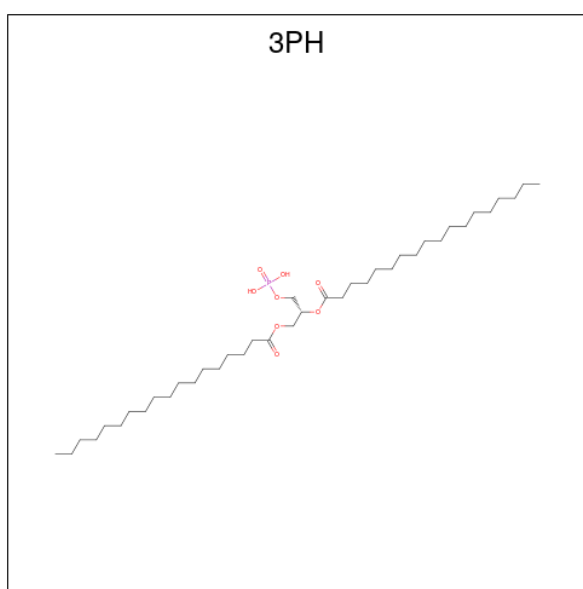


- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | A | 1 | Total Mo
1 1 | 0 | 0 |

-

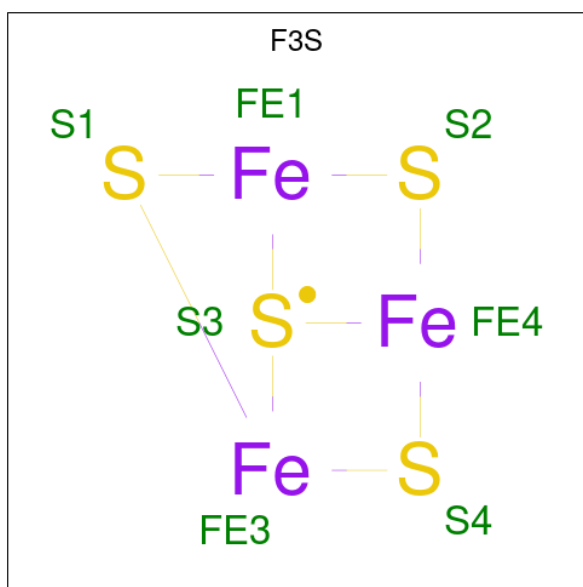
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



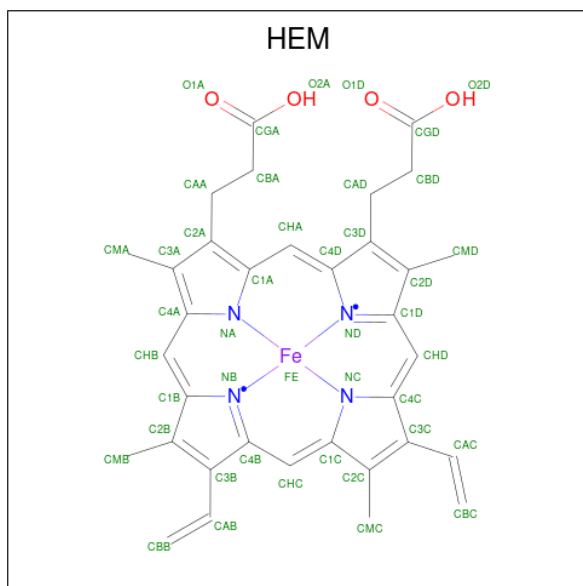
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			27	18	8	1		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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	

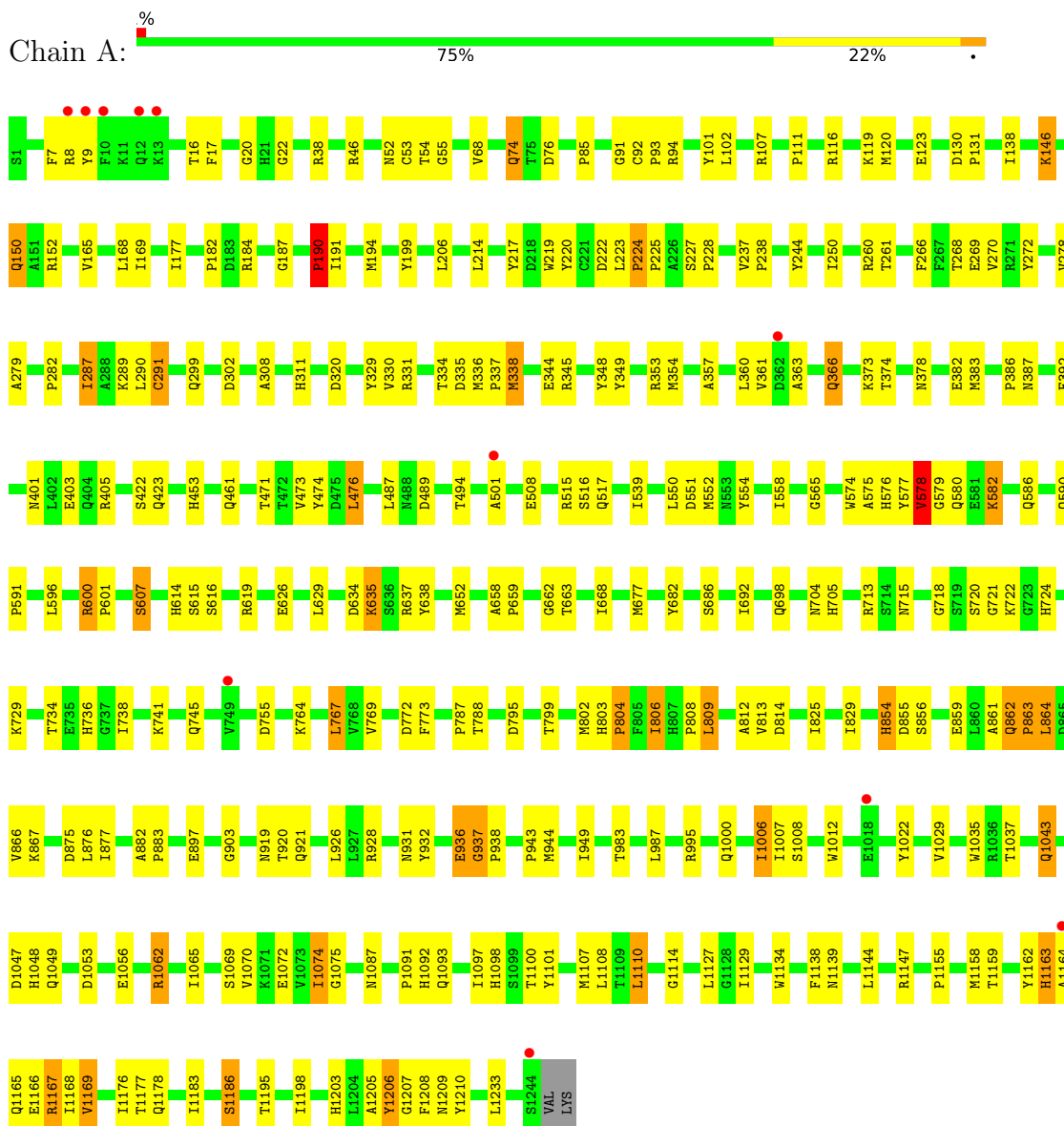
- Molecule 10 is water.

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

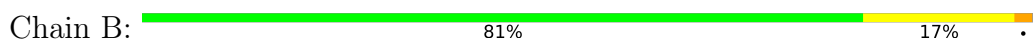
3 Residue-property plots

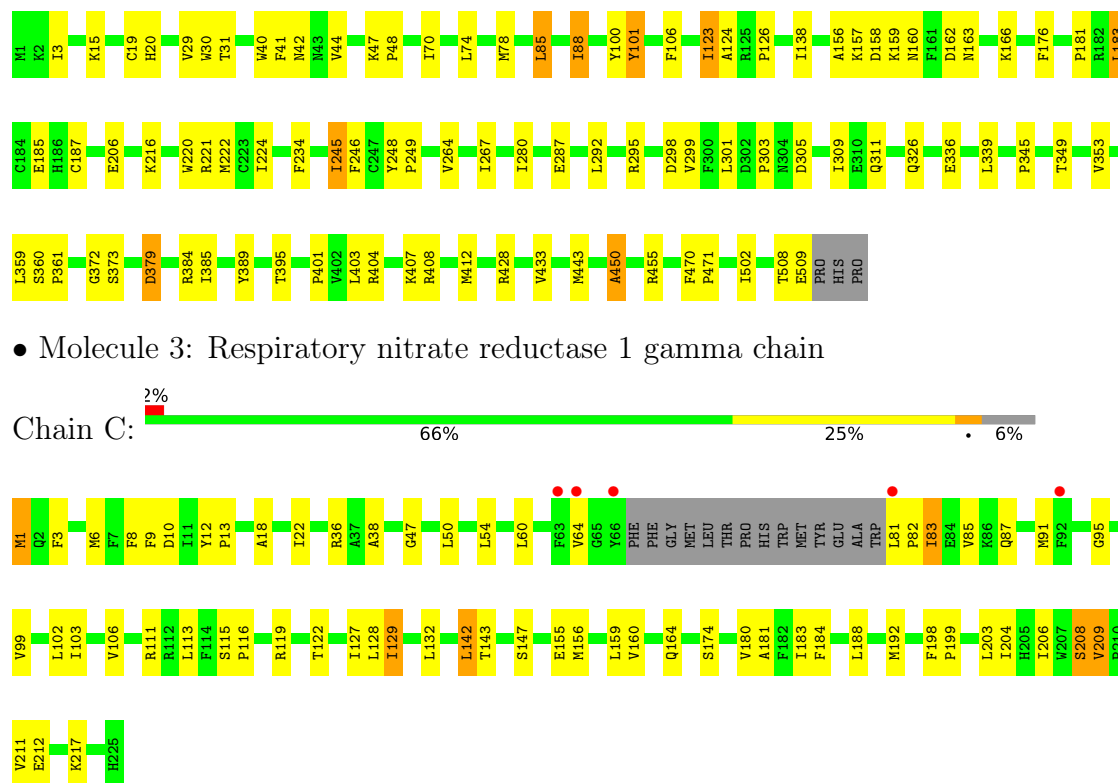
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	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) 99.4 (24.79-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.237 0.182 , 0.230	Depositor DCC
R_{free} test set	7209 reflections (8.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.999	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16150	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 6MO, 3PH, F3S, FME, MD1, 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	A	0.39	0/10128	0.93	43/13749 (0.3%)
2	B	0.41	0/4146	0.95	12/5609 (0.2%)
3	C	0.40	0/1709	0.89	3/2309 (0.1%)
All	All	0.40	0/15983	0.93	58/21667 (0.3%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	SER	N-CA-C	9.16	122.25	111.71
2	B	30	TRP	N-CA-C	7.65	122.74	113.41
1	A	1070	VAL	N-CA-C	7.64	118.67	111.48
1	A	1093	GLN	N-CA-C	7.54	119.68	110.41
1	A	1163	HIS	N-CA-C	7.41	121.42	110.30
1	A	809	LEU	N-CA-C	-7.40	97.68	109.59
1	A	1206	TYR	N-CA-C	7.23	119.90	110.43
1	A	862	GLN	CA-C-N	6.99	126.47	118.85
1	A	862	GLN	C-N-CA	6.99	126.47	118.85
3	C	209	VAL	CA-C-N	6.98	128.56	119.84
3	C	209	VAL	C-N-CA	6.98	128.56	119.84
1	A	863	PRO	N-CA-C	6.93	122.68	113.40
1	A	1165	GLN	N-CA-C	-6.80	104.66	114.12
2	B	280	ILE	N-CA-C	6.71	117.21	110.23
2	B	206	GLU	N-CA-C	6.68	119.57	111.82
1	A	1167	ARG	N-CA-C	6.60	121.17	111.87
1	A	361	VAL	N-CA-C	6.60	117.09	110.23
2	B	216	LYS	N-CA-C	6.43	119.28	111.82
1	A	615	SER	N-CA-C	-6.32	105.43	113.02
1	A	1035	TRP	N-CA-C	-6.27	99.42	109.96
1	A	8	ARG	N-CA-C	-6.27	105.91	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1097	ILE	N-CA-C	-6.12	96.99	106.72
1	A	1043	GLN	N-CA-C	6.00	117.97	108.67
1	A	101	TYR	N-CA-C	5.92	117.40	111.07
1	A	713	ARG	N-CA-C	-5.91	105.37	112.58
2	B	379	ASP	N-CA-C	-5.82	100.79	110.17
2	B	29	VAL	N-CA-C	5.76	116.41	110.82
1	A	1186	SER	N-CA-C	-5.74	106.23	113.18
2	B	359	LEU	N-CA-C	-5.67	101.58	110.36
1	A	74	GLN	N-CA-C	-5.60	102.19	110.48
2	B	222	MET	N-CA-C	-5.60	106.12	113.12
1	A	494	THR	N-CA-C	-5.55	106.68	113.50
1	A	291	CYS	N-CA-C	5.51	118.61	110.46
3	C	208	SER	N-CA-C	5.50	119.70	113.15
2	B	31	THR	N-CA-C	5.50	119.16	111.30
1	A	937	GLY	CA-C-N	5.48	125.31	119.28
1	A	937	GLY	C-N-CA	5.48	125.31	119.28
1	A	903	GLY	CA-C-N	5.47	125.56	119.87
1	A	903	GLY	C-N-CA	5.47	125.56	119.87
1	A	812	ALA	N-CA-C	-5.47	105.34	112.23
2	B	287	GLU	N-CA-C	5.46	117.68	111.02
1	A	802	MET	N-CA-C	5.42	117.19	111.28
1	A	16	THR	N-CA-C	-5.41	102.74	110.59
1	A	76	ASP	N-CA-C	5.41	118.71	112.97
1	A	854	HIS	N-CA-C	-5.39	102.90	110.50
1	A	1169	VAL	N-CA-C	5.36	116.19	108.48
1	A	1029	VAL	N-CA-C	5.28	116.05	110.72
1	A	1114	GLY	CA-C-N	5.23	126.37	119.84
1	A	1114	GLY	C-N-CA	5.23	126.37	119.84
1	A	715	ASN	N-CA-C	-5.19	104.24	110.88
1	A	614	HIS	N-CA-C	5.16	117.81	111.82
1	A	582	LYS	N-CA-C	5.16	117.71	108.17
1	A	302	ASP	N-CA-C	5.13	117.53	111.33
1	A	38	ARG	N-CA-C	-5.08	105.39	112.45
1	A	1000	GLN	N-CA-C	-5.07	105.94	111.82
1	A	320	ASP	N-CA-C	5.05	116.47	111.07
2	B	450	ALA	N-CA-C	5.01	118.23	111.17
2	B	157	LYS	N-CA-C	-5.01	107.00	113.01

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	A	9869	0	9527	218	0
2	B	4050	0	3973	61	0
3	C	1676	0	1726	46	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
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	321	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 10.

All (321) 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:652:MET:HE1	1:A:866:VAL:HG13	1.72	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:338:MET:HE1	1:A:386:PRO:HG3	1.81	0.63
1:A:116:ARG:NH1	1:A:119:LYS:HD3	2.15	0.62
1:A:360:LEU:HG	1:A:383:MET:HE3	1.80	0.61
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:338:MET:HB3	1:A:354:MET:HE2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:83:ILE:HD13	3:C:83:ILE:C	2.30	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:1098:HIS:C	1:A:1164:ALA:HB3	2.31	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
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:338:MET:HE2	1:A:374:THR:OG1	2.08	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
1:A:652:MET:HE3	1:A:867:LYS:O	2.08	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:338:MET:HE1	1:A:386:PRO:CG	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:19:CYS:O	2:B:20:HIS:HB2	2.10	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:921:GLN:HB2	10:A:3926:HOH:O	2.10	0.51
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.34	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
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
1:A:658:ALA:HA	1:A:659:PRO:C	2.36	0.50
2:B:162:ASP:O	2:B:163:ASN:HB2	2.12	0.50
1:A:225:PRO:C	1:A:228:PRO:HD2	2.37	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
2:B:220:TRP:C	2:B:221:ARG:HG3	2.37	0.49
1:A:93:PRO:HG2	1:A:94:ARG:HD3	1.94	0.49
3:C:8:PHE:O	3:C:192:MET:HE1	2.11	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
1:A:1107:MET:HA	1:A:1107:MET:HE2	1.93	0.49
3:C:143:THR:HB	3:C:184:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:7:PHE:C	1:A:9:TYR:H	2.19	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
1:A:652:MET:HE1	1:A:866:VAL:CG1	2.41	0.47
3:C:87:GLN:O	3:C:91:MET:HG3	2.14	0.47
1:A:552:MET:HE3	1:A:1056:GLU:CD	2.39	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:1074:ILE:HD13	1:A:1074:ILE:C	2.39	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: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
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:TYR:CD1	1:A:199:TYR:C	2.94	0.46
1:A:225:PRO:O	1:A:228:PRO:HD2	2.16	0.46
1:A:282:PRO:CG	1:A:1158:MET:HE1	2.46	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: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:168:LEU:HD23	1:A:168:LEU:C	2.42	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
1:A:638:TYR:OH	1:A:1053:ASP:OD2	2.31	0.45
1:A:287:ILE:HD13	1:A:287:ILE:C	2.42	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:176:PHE:CD1	2:B:176:PHE:C	2.94	0.45
2:B:185:GLU:OE1	2:B:353:VAL:HB	2.16	0.45
1:A:552:MET:HE3	1:A:1056:GLU:OE1	2.17	0.44
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
1:A:282:PRO:HB2	1:A:1158:MET:HE1	1.99	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:1168:ILE:O	2:B:123:ILE:HD13	2.18	0.44
2:B:156:ALA:C	2:B:158:ASP:N	2.75	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:272:TYR:HB3	2:B:412:MET:HE3	1.98	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:652:MET:HE2	1:A:862:GLN:HE22	1.82	0.44
1:A:772:ASP:C	1:A:788:THR:HG22	2.43	0.44
1:A:1138:PHE:CG	1:A:1176:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:100:TYR:O	2:B:101:TYR:HB3	2.17	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
2:B:40:TRP:O	2:B:41:PHE:C	2.61	0.43
2:B:156:ALA:C	2:B:158:ASP:H	2.26	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
2:B:339:LEU:HD11	2:B:443:MET:HE3	2.00	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:1110:LEU:HD12	1:A:1110:LEU:HA	1.89	0.43
2:B:47:LYS:HA	2:B:48:PRO:C	2.43	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:53:CYS:C	1:A:54:THR:HG23	2.43	0.43
1:A:289:LYS:HD3	1:A:289:LYS:C	2.44	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:1098:HIS:C	1:A:1164:ALA:CB	2.91	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:876:LEU:C	1:A:876:LEU:HD23	2.43	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
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
1:A:338:MET:HB3	1:A:354:MET:CE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:282:PRO:HB2	1:A:1158:MET:CE	2.49	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:423:GLN:CD	1:A:423:GLN:H	2.28	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:52:ASN:CG	1:A:191:ILE:HG12	2.46	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
3:C:208:SER:O	3:C:209:VAL:C	2.62	0.41
1:A:177:ILE:HG12	1:A:182:PRO:HA	2.02	0.41
1:A:299:GLN:CD	1:A:1158:MET:HE2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:TYR:CZ	1:A:565:GLY:HA2	2.55	0.41
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:1048:HIS:O	1:A:1049:GLN:C	2.64	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: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
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%)	16 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	507/512 (99%)	487 (96%)	19 (4%)	1 (0%)	43	63
3	C	207/225 (92%)	198 (96%)	9 (4%)	0	100	100
All	All	1956/1983 (99%)	1835 (94%)	110 (6%)	11 (1%)	21	38

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%)	1010 (97%)	29 (3%)	38	66
2	B	436/439 (99%)	428 (98%)	8 (2%)	51	77
3	C	174/186 (94%)	169 (97%)	5 (3%)	37	65
All	All	1649/1668 (99%)	1607 (98%)	42 (2%)	42	69

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LYS
1	A	150	GLN
1	A	190	PRO

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Mol	Chain	Res	Type
1	A	287	ILE
1	A	338	MET
1	A	366	GLN
1	A	461	GLN
1	A	476	LEU
1	A	578	VAL
1	A	582	LYS
1	A	586	GLN
1	A	600	ARG
1	A	601	PRO
1	A	629	LEU
1	A	767	LEU
1	A	804	PRO
1	A	806	ILE
1	A	808	PRO
1	A	864	LEU
1	A	926	LEU
1	A	936	GLU
1	A	944	MET
1	A	995	ARG
1	A	1006	ILE
1	A	1062	ARG
1	A	1072	GLU
1	A	1074	ILE
1	A	1110	LEU
1	A	1233	LEU
2	B	74	LEU
2	B	85	LEU
2	B	88	ILE
2	B	123	ILE
2	B	183	LEU
2	B	245	ILE
2	B	267	ILE
2	B	299	VAL
3	C	83	ILE
3	C	129	ILE
3	C	142	LEU
3	C	147	SER
3	C	204	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	26	ASN
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	369	ASN
1	A	387	ASN
1	A	461	GLN
1	A	480	ASN
1	A	517	GLN
1	A	559	ASN
1	A	604	HIS
1	A	704	ASN
1	A	708	ASN
1	A	884	HIS
1	A	919	ASN
1	A	942	GLN
1	A	946	ASN
1	A	1000	GLN
1	A	1023	ASN
1	A	1076	GLN
1	A	1082	GLN
1	A	1098	HIS
1	A	1179	GLN
1	A	1185	ASN
2	B	110	ASN
2	B	255	GLN
2	B	294	GLN
2	B	441	GLN
2	B	451	ASN
3	C	49	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	1.31	2 (25%)	8,9,11	1.60	2 (25%)

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-CG	2.25	1.60	1.51
3	C	1	FME	CB-CA	-2.08	1.48	1.53

All (2) 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
3	C	1	FME	CB-CA-N	2.01	114.17	110.52

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	C-CA-CB-CG
3	C	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
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 oligosaccharides 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	B	1804	2	0,12,12	-	-	-		
9	HEM	C	806	3	50,50,50	1.73	14 (28%)	67,82,82	0.89	2 (2%)
4	MD1	A	1800	5	47,51,51	2.87	7 (14%)	56,78,78	1.32	4 (7%)
4	MD1	A	2800	5	47,51,51	2.78	6 (12%)	56,78,78	1.42	4 (7%)
6	SF4	B	1802	2	0,12,12	-	-	-		
6	SF4	B	1803	2	0,12,12	-	-	-		
6	SF4	A	1801	1	0,12,12	-	-	-		
7	3PH	A	1309	-	26,26,47	0.78	1 (3%)	29,31,52	1.57	3 (10%)
8	F3S	B	1805	2	0,9,9	-	-	-		

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	HEM	C	806	3	-	8/14/54/54	-
6	SF4	B	1804	2	-	-	0/6/5/5
4	MD1	A	1800	5	-	7/22/59/59	0/5/5/5
4	MD1	A	2800	5	-	2/22/59/59	0/5/5/5
6	SF4	B	1802	2	-	-	0/6/5/5
6	SF4	B	1803	2	-	-	0/6/5/5
6	SF4	A	1801	1	-	-	0/6/5/5
7	3PH	A	1309	-	-	3/28/28/49	-
8	F3S	B	1805	2	-	-	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	MD1	C7-N8	17.45	1.50	1.28
4	A	2800	MD1	C7-N8	16.35	1.48	1.28
4	A	2800	MD1	PA-O3B	-5.30	1.53	1.59
9	C	806	HEM	CAB-C3B	4.09	1.58	1.47
4	A	1800	MD1	C14-C13	3.79	1.55	1.51
9	C	806	HEM	CAC-C3C	3.61	1.57	1.47
9	C	806	HEM	CMC-C2C	3.45	1.57	1.50
9	C	806	HEM	FE-NC	3.23	2.05	1.95
4	A	2800	MD1	C20-N8	3.17	1.41	1.36
4	A	1800	MD1	C16-C20	3.16	1.47	1.39
4	A	1800	MD1	C12-C13	2.93	1.43	1.34
9	C	806	HEM	CAD-C3D	2.82	1.58	1.51
9	C	806	HEM	CMA-C3A	2.82	1.56	1.50
9	C	806	HEM	CMD-C2D	2.73	1.56	1.50
9	C	806	HEM	CMB-C2B	2.71	1.56	1.50
4	A	1800	MD1	C4-N3	2.66	1.40	1.34
9	C	806	HEM	FE-NB	2.60	2.02	1.94
4	A	1800	MD1	C20-N8	2.50	1.40	1.36
7	A	1309	3PH	C32-C31	2.37	1.57	1.50
4	A	2800	MD1	C6-N1	2.26	1.43	1.38
9	C	806	HEM	CBD-CAD	2.12	1.59	1.51
9	C	806	HEM	C4D-C3D	2.11	1.48	1.45
4	A	2800	MD1	O11-C11	2.10	1.47	1.42
9	C	806	HEM	C1D-C2D	2.09	1.48	1.44
4	A	1800	MD1	C15-N17	2.08	1.42	1.38
4	A	2800	MD1	C4-N3	2.07	1.39	1.34
9	C	806	HEM	FE-ND	2.03	2.01	1.94
9	C	806	HEM	CBA-CAA	2.00	1.58	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1800	MD1	C17-N18-C20	5.85	122.31	114.20
4	A	2800	MD1	C17-N18-C20	5.73	122.14	114.20
7	A	1309	3PH	C23-C22-C21	5.22	132.84	113.69
7	A	1309	3PH	C33-C32-C31	4.63	130.68	113.69
4	A	2800	MD1	C2-N3-C4	3.32	118.02	112.30
4	A	1800	MD1	N17-C17-N18	-2.72	118.35	123.32
4	A	1800	MD1	O14-C15-C16	-2.54	121.14	127.26
9	C	806	HEM	CAD-C3D-C4D	-2.25	120.78	124.70
7	A	1309	3PH	C2-O21-C21	2.21	123.10	117.80
4	A	2800	MD1	N1-C2-N3	-2.19	119.32	123.32
9	C	806	HEM	O1D-CGD-CBD	-2.16	116.26	123.09
4	A	1800	MD1	C15-C16-N15	2.03	121.81	116.27
4	A	2800	MD1	C1'-N9-C8	2.01	132.44	126.73

There are no chirality outliers.

All (20) torsion outliers are listed below:

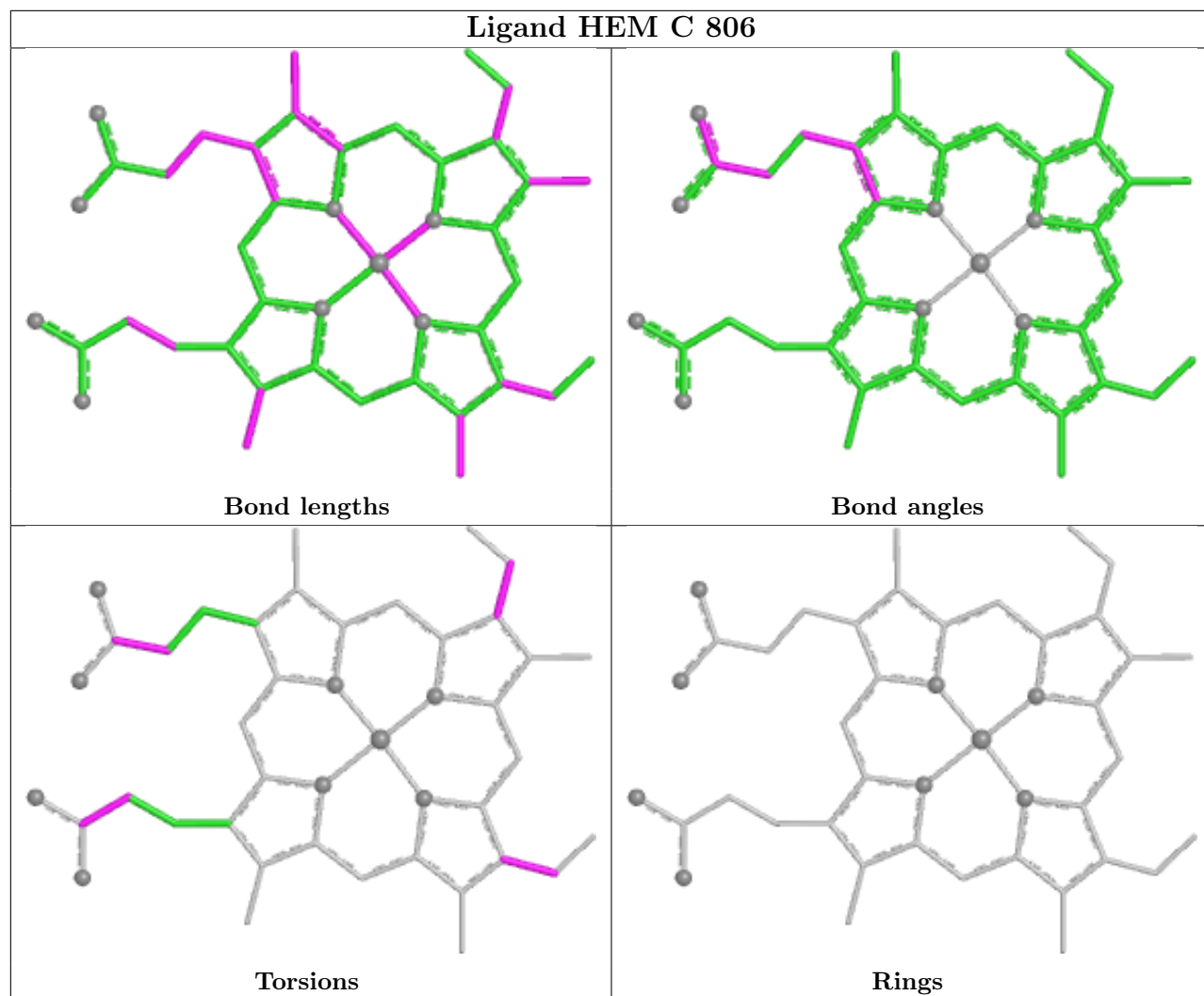
Mol	Chain	Res	Type	Atoms
4	A	1800	MD1	C5'-O5'-PA-O3B
4	A	1800	MD1	C5'-O5'-PA-O2A
9	C	806	HEM	C2C-C3C-CAC-CBC
4	A	1800	MD1	O4'-C4'-C5'-O5'
4	A	1800	MD1	C3'-C4'-C5'-O5'
9	C	806	HEM	C2B-C3B-CAB-CBB
9	C	806	HEM	C4B-C3B-CAB-CBB
9	C	806	HEM	C4C-C3C-CAC-CBC
7	A	1309	3PH	C32-C31-O31-C3
7	A	1309	3PH	O32-C31-O31-C3
4	A	1800	MD1	PA-O3B-PB-O2B
4	A	2800	MD1	PA-O3B-PB-O2B
4	A	1800	MD1	C5'-O5'-PA-O1A
9	C	806	HEM	CAA-CBA-CGA-O1A
9	C	806	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAD-CBD-CGD-O2D
9	C	806	HEM	CAA-CBA-CGA-O2A
7	A	1309	3PH	O31-C31-C32-C33
4	A	1800	MD1	PA-O3B-PB-O1B
4	A	2800	MD1	PA-O3B-PB-O1B

There are no ring outliers.

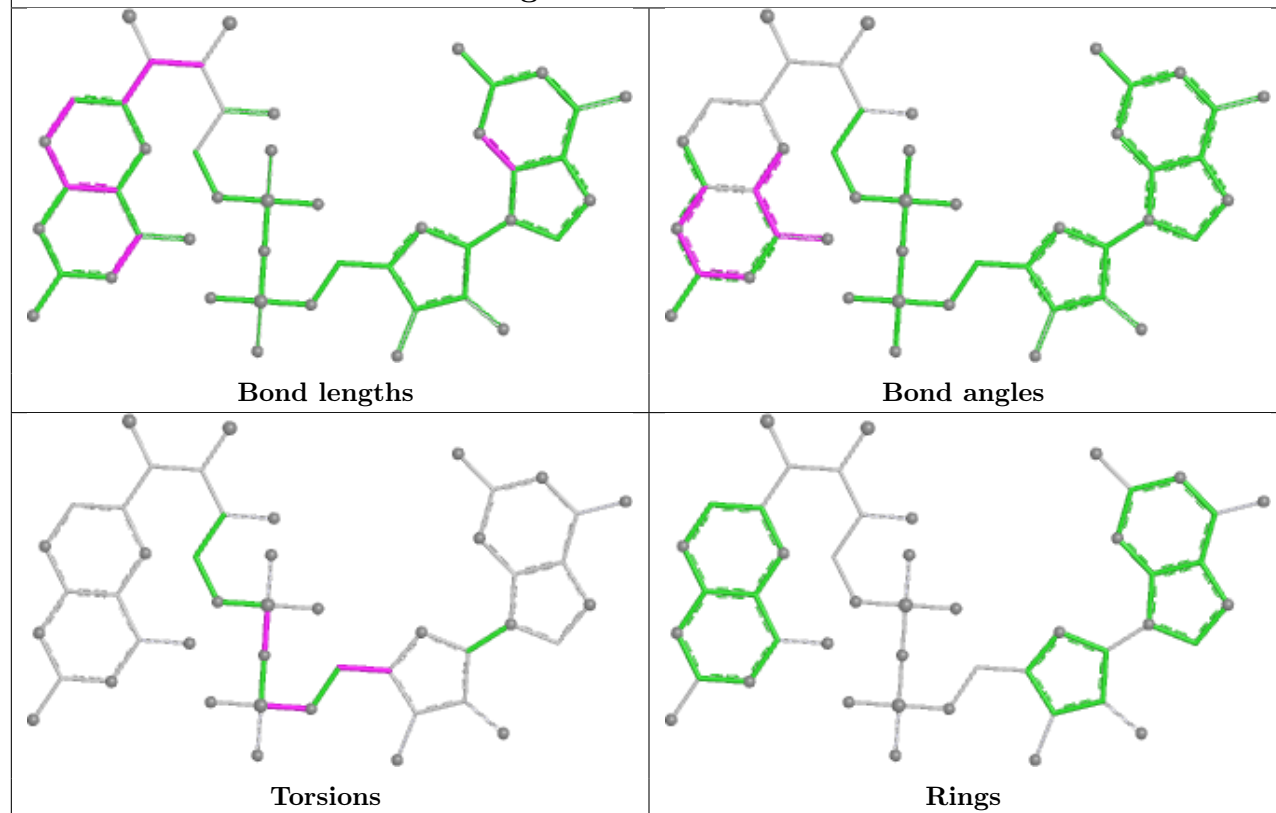
5 monomers are involved in 11 short contacts:

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

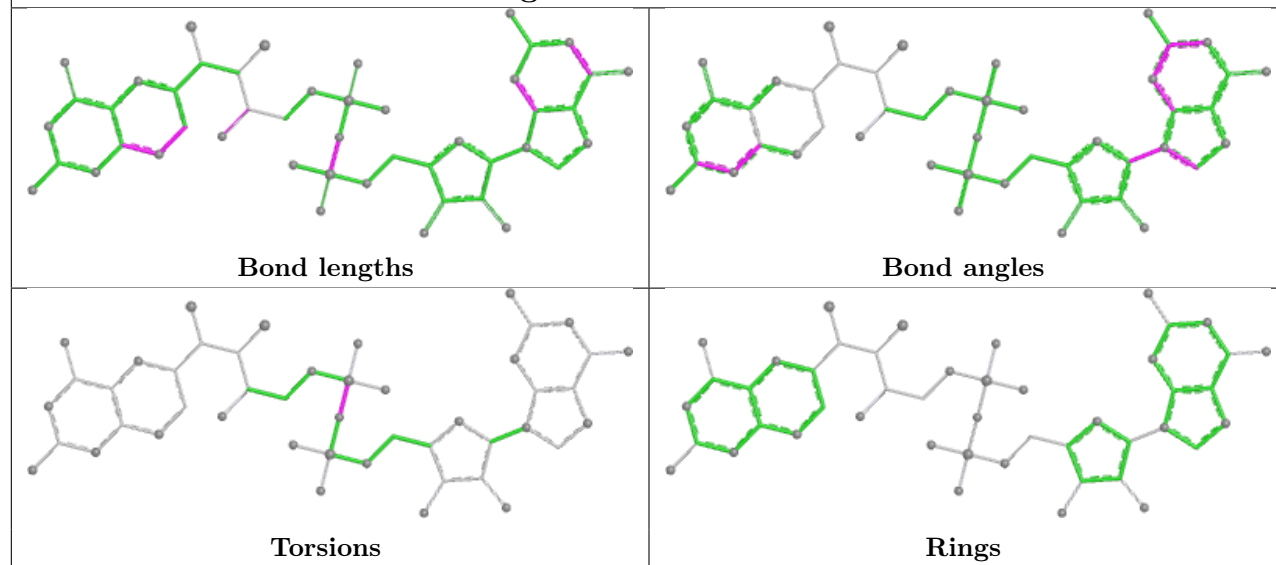
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

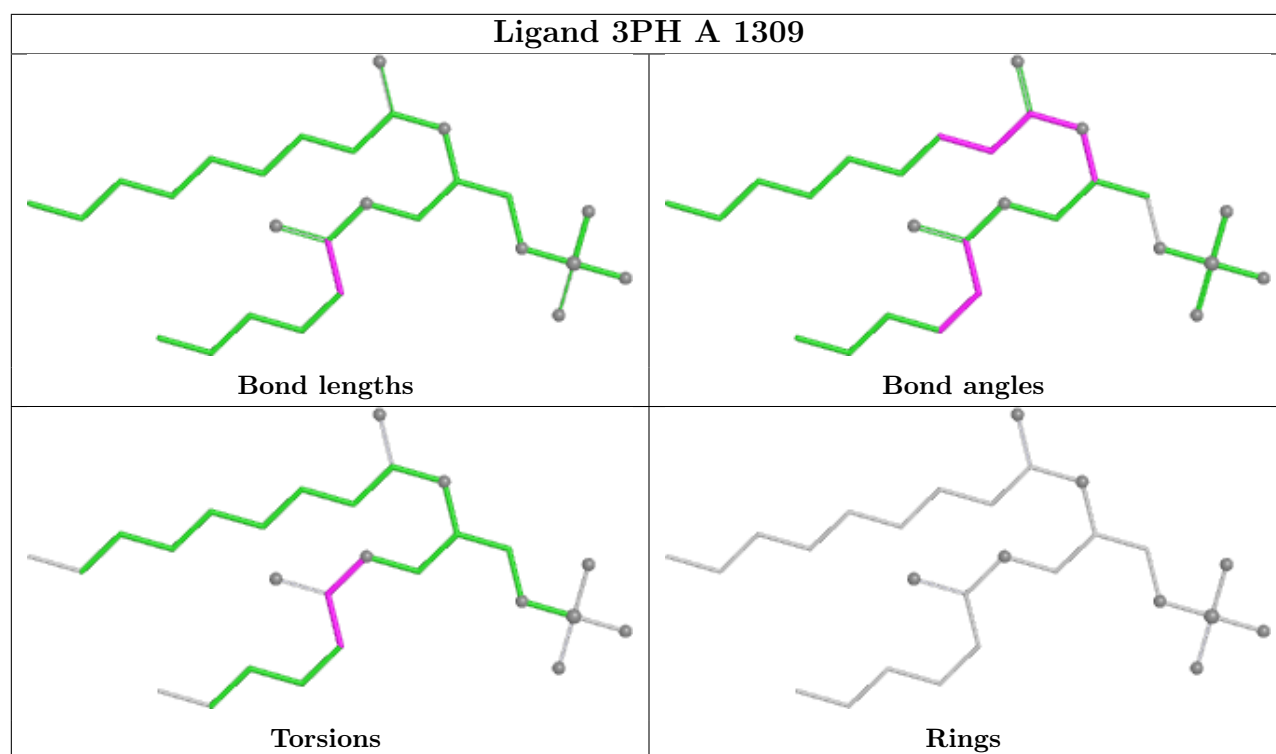


Ligand MD1 A 1800



Ligand MD1 A 2800





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	1244/1246 (99%)	-0.38	11 (0%) 81 78	13, 26, 46, 83	0
2	B	509/512 (99%)	-0.61	0 100 100	10, 21, 38, 63	0
3	C	210/225 (93%)	-0.00	5 (2%) 59 55	18, 33, 59, 65	0
All	All	1963/1983 (98%)	-0.40	16 (0%) 82 80	10, 25, 48, 83	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	5.7
1	A	10	PHE	4.7
3	C	81	LEU	4.2
3	C	92	PHE	3.2
1	A	1018	GLU	2.9
3	C	66	TYR	2.8
1	A	1164	ALA	2.8
1	A	501	ALA	2.7
3	C	63	PHE	2.6
1	A	1244	SER	2.6
3	C	64	VAL	2.5
1	A	362	ASP	2.2
1	A	12	GLN	2.1
1	A	749	VAL	2.1
1	A	8	ARG	2.1
1	A	13	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FME	C	1	10/11	0.86	0.12	54,60,75,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

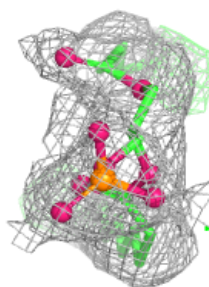
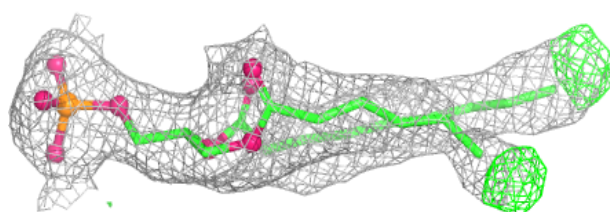
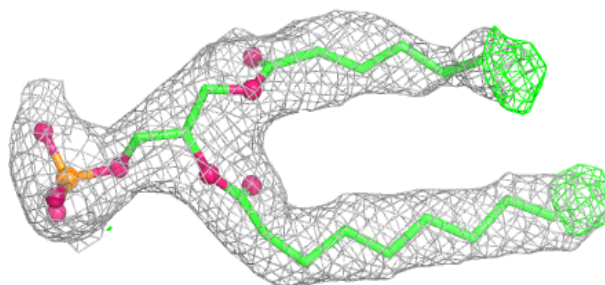
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	3PH	A	1309	27/48	0.93	0.11	20,28,50,54	0
4	MD1	A	1800	47/47	0.96	0.07	17,25,36,38	0
5	6MO	A	3800	1/1	0.97	0.07	38,38,38,38	0
4	MD1	A	2800	47/47	0.97	0.06	13,25,34,37	0
6	SF4	B	1804	8/8	0.98	0.03	19,21,25,25	0
6	SF4	B	1802	8/8	0.98	0.04	21,24,25,26	0
9	HEM	C	806	43/43	0.98	0.07	12,24,29,45	0
6	SF4	B	1803	8/8	0.99	0.03	15,17,18,18	0
8	F3S	B	1805	7/7	0.99	0.03	17,18,20,21	0
6	SF4	A	1801	8/8	0.99	0.04	20,21,25,33	0

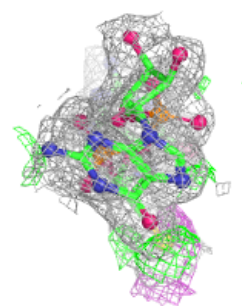
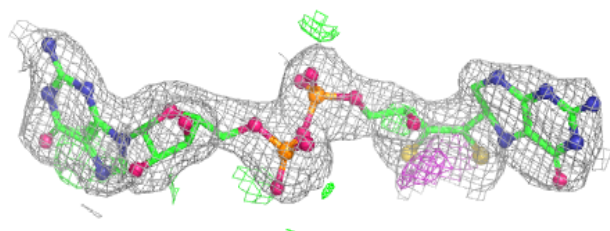
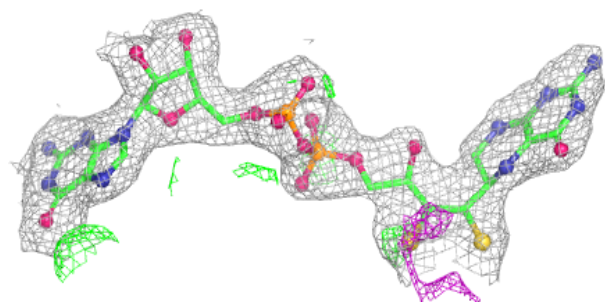
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

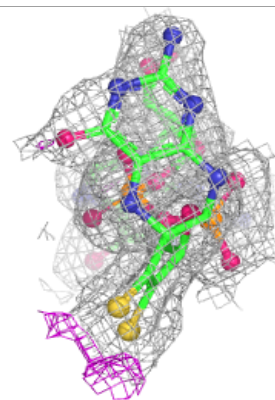
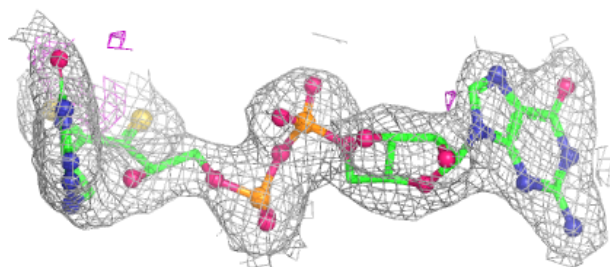
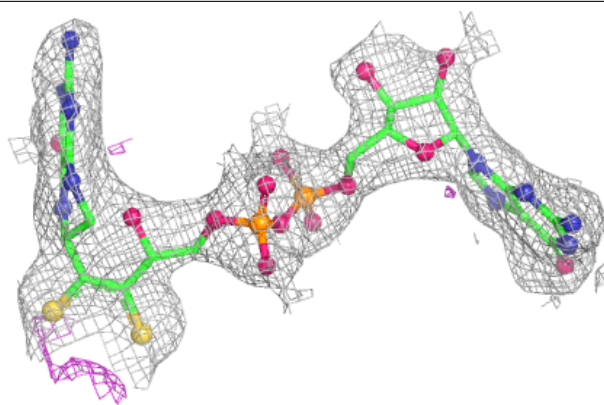
**Electron density around MD1 A 1800:**

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



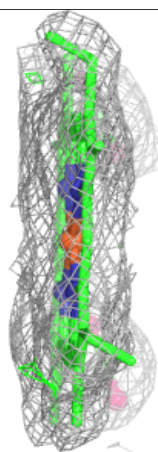
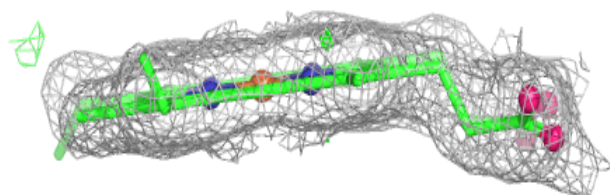
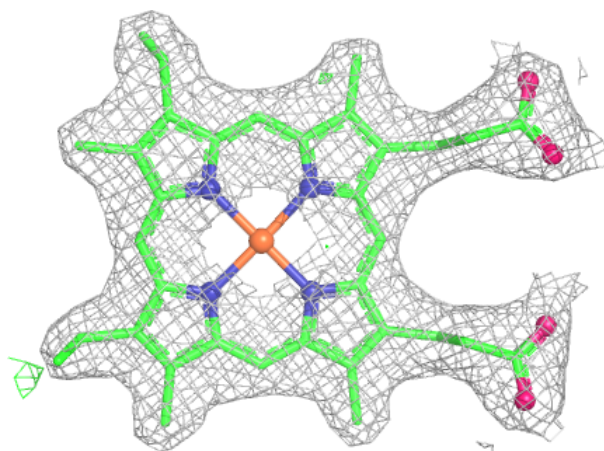
Electron density around MD1 A 2800:

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



Electron density around HEM C 806:

$2mF_o-DF_c$ (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.