



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:39 PM GMT

PDB ID : 1Q16  
Title : Crystal structure of Nitrate Reductase A, NarGHI, from Escherichia coli  
Authors : Bertero, M.G.; Strynadka, N.C.J.  
Deposited on : 2003-07-18  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

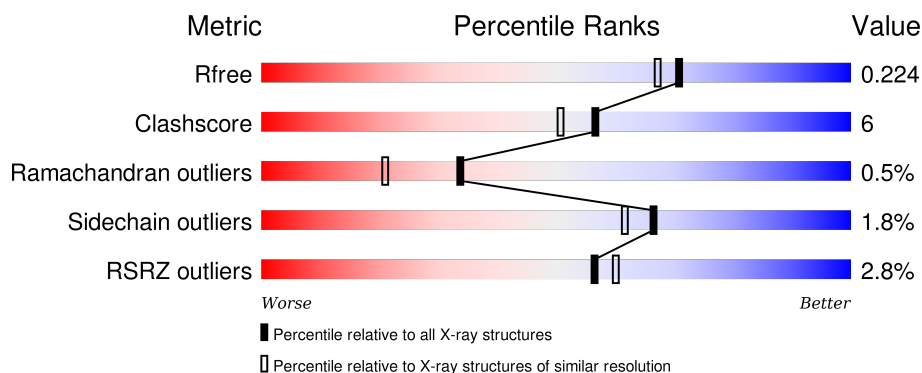
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1247	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	B	512	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
3	C	225	<div> <div>4%</div> <div>80%</div> <div>20%</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
10	3PH	B	1310	X	-	-	X
7	SF4	B	1403	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17199 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
			9878	6239	1731	1860	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			

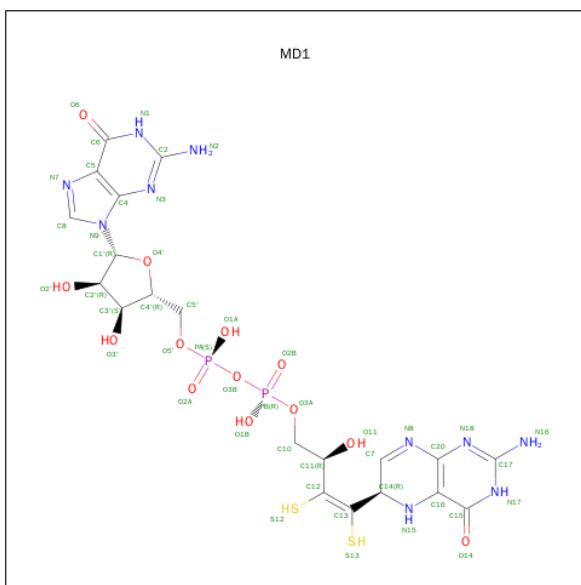
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	224	Total	C	N	O	S	0	0	0
			1790	1187	302	287	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	MET	MODIFIED RESIDUE	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>).

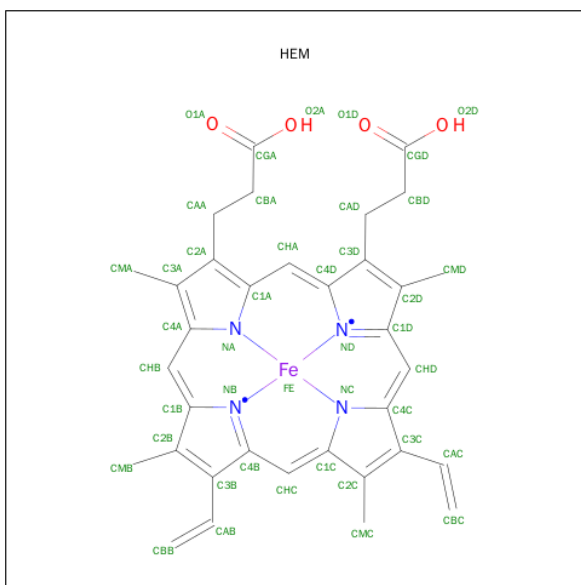


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

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

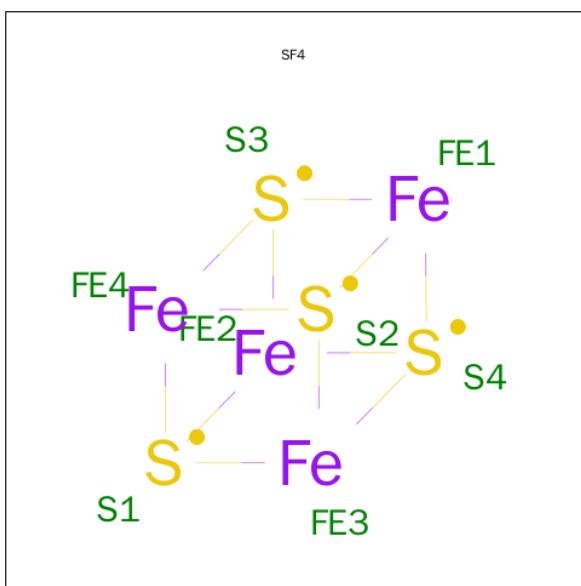
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mo 1 1	0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



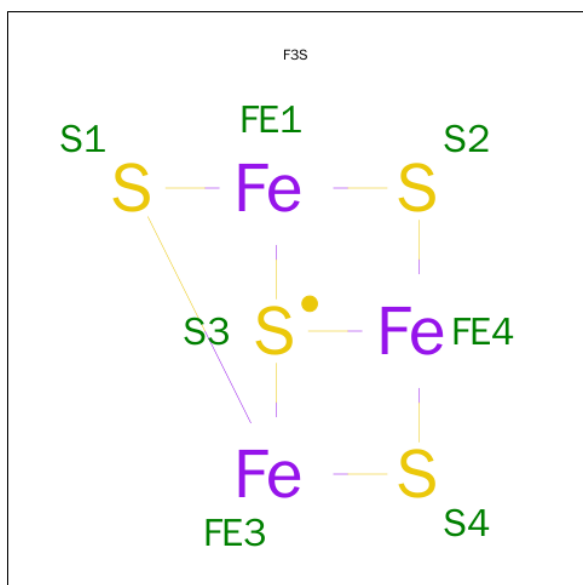
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 8	Fe 4	S 4	0	0
7	B	1	Total 8	Fe 4	S 4	0	0

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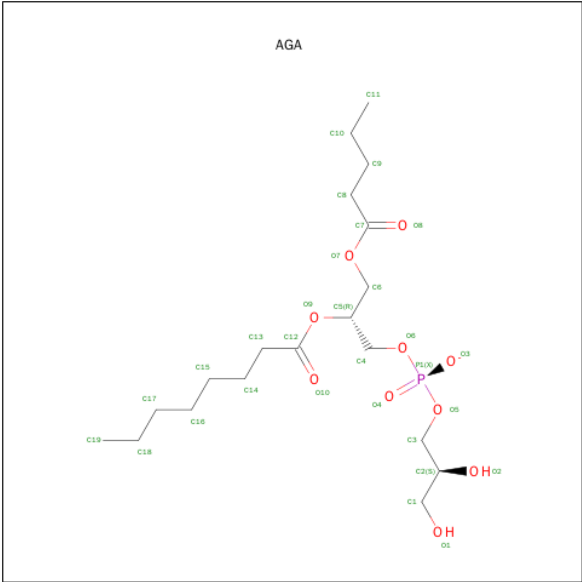
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



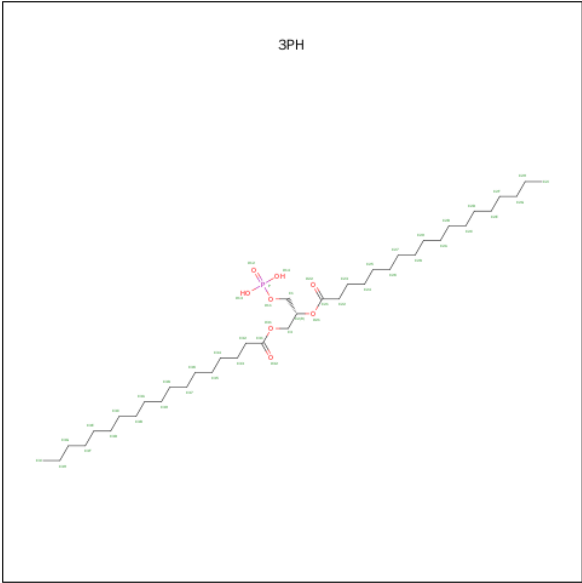
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is (1S)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula:  $\text{C}_{19}\text{H}_{36}\text{O}_{10}\text{P}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O	P	0	0
			30	19	10	1		

- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	O	P	0	0
			18	9	8	1		

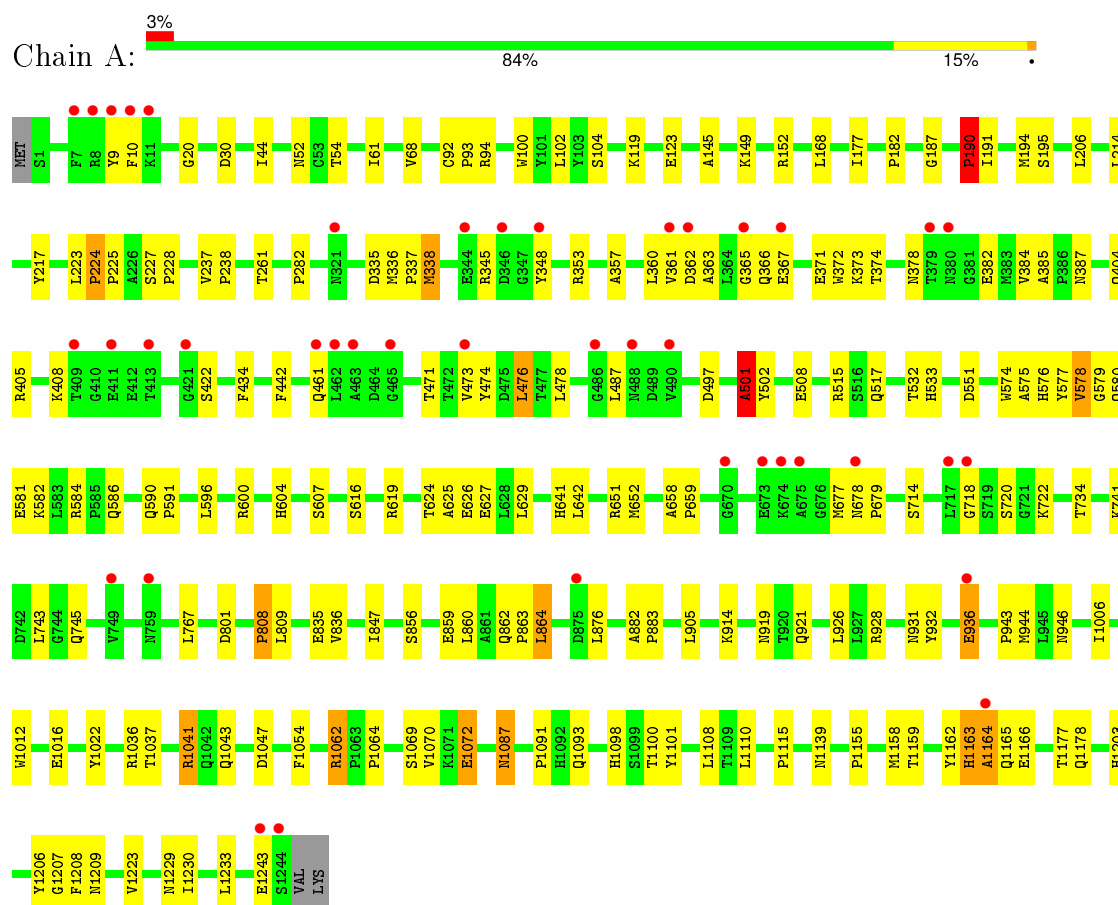
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	710	Total 710	O 710	0	0
11	B	427	Total 427	O 427	0	0
11	C	76	Total 76	O 76	0	0

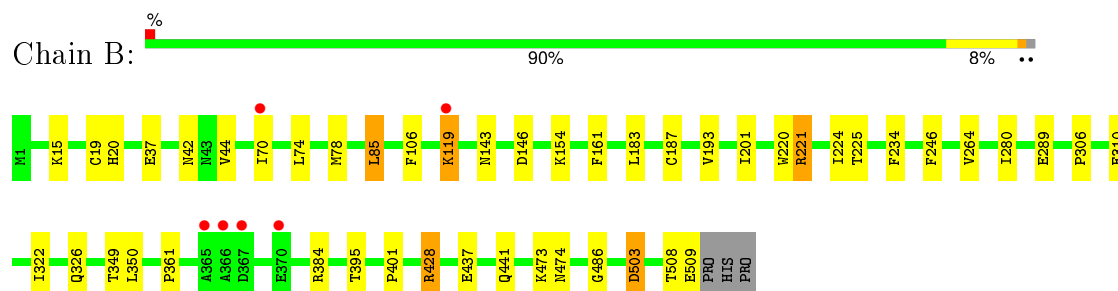
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

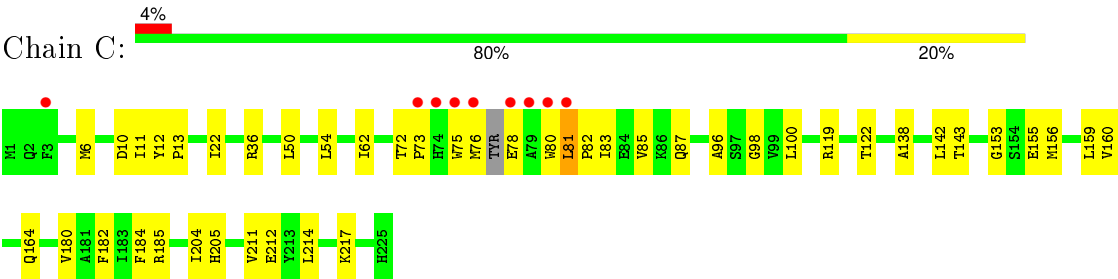
- Molecule 1: Respiratory nitrate reductase 1 alpha chain



- 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, $\alpha$ , $\beta$ , $\gamma$	154.18 Å   241.38 Å   139.49 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.68 – 1.90 29.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.68-1.90) 99.6 (29.67-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 1.91 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202   ,   0.230 0.195   ,   0.224	Depositor DCC
$R_{free}$ test set	10078 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 202288 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 6MO, FME, SF4, AGA, 3PH, F3S, HEM, MD1

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	0.31	0/10138	0.64	11/13762 (0.1%)
2	B	0.33	0/4146	0.61	0/5609
3	C	0.32	0/1831	0.53	0/2476
All	All	0.32	0/16115	0.62	11/21847 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	C-N-CA	13.34	155.04	121.70
1	A	502	TYR	CB-CG-CD1	-10.86	114.48	121.00
1	A	502	TYR	CB-CG-CD2	10.19	127.11	121.00
1	A	501	ALA	C-N-CA	10.11	146.96	121.70
1	A	1163	HIS	O-C-N	-8.48	109.13	122.70
1	A	502	TYR	CA-CB-CG	7.42	127.49	113.40
1	A	501	ALA	N-CA-CB	6.37	119.01	110.10
1	A	809	LEU	N-CA-C	-5.55	96.02	111.00
1	A	10	PHE	CB-CA-C	5.32	121.05	110.40
1	A	362	ASP	CB-CA-C	5.31	121.01	110.40
1	A	1164	ALA	N-CA-CB	5.28	117.49	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Peptide
1	A	501	ALA	Mainchain,Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9878	0	9534	133	0
2	B	4050	0	3973	31	0
3	C	1790	0	1826	31	0
4	A	94	0	42	5	0
5	A	1	0	0	0	0
6	C	86	0	60	0	0
7	A	8	0	0	0	0
7	B	24	0	0	2	0
8	B	7	0	0	0	0
9	A	30	0	36	0	0
10	B	18	0	10	0	0
11	A	710	0	0	10	1
11	B	427	0	0	6	0
11	C	76	0	0	2	0
All	All	17199	0	15481	192	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 6.

All (192) 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	1.18	1.00
1:A:378:ASN:ND2	1:A:382:GLU:HB2	1.93	0.84
3:C:73:PRO:HG2	3:C:76:MET:HG3	1.57	0.84
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.60	0.83
2:B:503:ASP:HB3	11:B:1830:HOH:O	1.82	0.80
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:THR:HG23	3:C:76:MET:HE2	1.69	0.74
1:A:586:GLN:HE21	1:A:590:GLN:HG3	1.55	0.70
1:A:1098:HIS:HE1	4:A:1301:MD1:S13	2.14	0.70
1:A:578:VAL:HG23	1:A:579:GLY:H	1.56	0.69
1:A:626:GLU:HA	1:A:629:LEU:HD23	1.74	0.69
1:A:365:GLY:HA3	1:A:408:LYS:HG3	1.74	0.68
1:A:586:GLN:HE21	1:A:590:GLN:CG	2.06	0.68
1:A:508:GLU:OE1	1:A:515:ARG:HD2	1.92	0.68
11:A:1958:HOH:O	3:C:212:GLU:HG3	1.94	0.68
1:A:1098:HIS:CE1	4:A:1301:MD1:S13	2.88	0.66
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.78	0.66
1:A:1098:HIS:CE1	4:A:1300:MD1:S12	2.89	0.66
1:A:20:GLY:O	3:C:217:LYS:HD2	1.97	0.65
1:A:596:LEU:O	1:A:600:ARG:HD2	1.98	0.64
1:A:722:LYS:H	1:A:722:LYS:HD2	1.62	0.64
1:A:720:SER:O	1:A:722:LYS:HD2	1.97	0.64
1:A:1062:ARG:HD2	11:A:1502:HOH:O	1.97	0.63
1:A:387:ASN:ND2	1:A:405:ARG:HB2	2.14	0.63
3:C:83:ILE:HD11	3:C:156:MET:HG2	1.80	0.63
1:A:497:ASP:HA	1:A:515:ARG:HH11	1.62	0.62
1:A:336:MET:HA	1:A:473:VAL:HB	1.82	0.62
1:A:619:ARG:O	1:A:743:LEU:HD13	2.00	0.62
3:C:138:ALA:O	3:C:142:LEU:HD13	2.00	0.61
1:A:335:ASP:O	1:A:338:MET:HB2	1.99	0.61
1:A:859:GLU:HG3	1:A:860:LEU:HD12	1.83	0.61
1:A:191:ILE:O	1:A:194:MET:HG2	2.01	0.61
1:A:584:ARG:HD3	1:A:1006:ILE:HG12	1.83	0.60
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.16	0.60
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.83	0.59
1:A:338:MET:HG3	1:A:374:THR:HB	1.84	0.59
3:C:12:TYR:N	3:C:13:PRO:HD2	2.18	0.58
1:A:471:THR:HG21	1:A:476:LEU:HD13	1.86	0.58
1:A:1037:THR:HB	1:A:1043:GLN:HG3	1.84	0.58
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.85	0.58
1:A:345:ARG:HD2	11:A:2082:HOH:O	2.04	0.57
3:C:96:ALA:O	3:C:100:LEU:HD13	2.04	0.57
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.87	0.57
3:C:160:VAL:O	3:C:164:GLN:HG3	2.04	0.57
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.86	0.57
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.53	0.56
1:A:578:VAL:HG23	1:A:579:GLY:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:TYR:O	1:A:478:LEU:HD13	2.06	0.56
1:A:619:ARG:NH1	11:A:1939:HOH:O	2.39	0.56
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.41	0.56
2:B:119:LYS:HD2	2:B:119:LYS:N	2.21	0.55
1:A:652:MET:HE3	1:A:862:GLN:HE22	1.71	0.55
1:A:931:ASN:O	1:A:932:TYR:HB2	2.05	0.55
3:C:159:LEU:HD21	3:C:180:VAL:HG21	1.87	0.55
1:A:119:LYS:O	1:A:123:GLU:HG3	2.07	0.55
1:A:679:PRO:HB2	1:A:847:ILE:HD11	1.89	0.55
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.28	0.54
1:A:191:ILE:HG23	1:A:580:GLN:O	2.08	0.54
1:A:582:LYS:HD2	11:A:2072:HOH:O	2.08	0.54
1:A:223:LEU:O	1:A:225:PRO:HD3	2.08	0.54
1:A:652:MET:CE	1:A:862:GLN:HE22	2.21	0.53
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.90	0.53
4:A:1300:MD1:C11	4:A:1300:MD1:H7	2.39	0.53
3:C:155:GLU:O	3:C:159:LEU:HD23	2.08	0.53
1:A:1087:ASN:O	1:A:1159:THR:HG22	2.08	0.53
2:B:508:THR:O	2:B:509:GLU:HB3	2.09	0.53
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.89	0.53
1:A:624:THR:O	1:A:627:GLU:HG2	2.10	0.52
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.91	0.52
2:B:246:PHE:HA	7:B:1403:SF4:S4	2.49	0.52
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.74	0.52
3:C:72:THR:HG23	3:C:76:MET:CE	2.38	0.51
1:A:856:SER:O	1:A:859:GLU:HG2	2.10	0.51
3:C:81:LEU:HD23	3:C:81:LEU:N	2.26	0.51
1:A:919:ASN:ND2	1:A:921:GLN:H	2.07	0.51
1:A:936:GLU:HB2	11:A:1590:HOH:O	2.10	0.51
1:A:677:MET:HB2	11:A:2095:HOH:O	2.11	0.51
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.91	0.51
3:C:204:ILE:HD12	3:C:205:HIS:N	2.25	0.50
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.75	0.50
2:B:187:CYS:HB3	2:B:349:THR:O	2.11	0.50
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.94	0.50
2:B:19:CYS:O	2:B:20:HIS:HB2	2.12	0.50
1:A:487:LEU:N	1:A:487:LEU:HD12	2.27	0.49
1:A:864:LEU:HD22	1:A:864:LEU:N	2.27	0.49
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.94	0.49
1:A:722:LYS:N	1:A:722:LYS:HD2	2.25	0.49
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:LYS:HD3	11:B:1747:HOH:O	2.13	0.49
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.48	0.48
1:A:282:PRO:HB2	1:A:1158:MET:HE3	1.94	0.48
3:C:80:TRP:HB2	3:C:81:LEU:HD23	1.96	0.48
1:A:1230:ILE:N	1:A:1230:ILE:HD12	2.28	0.48
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.29	0.48
3:C:76:MET:O	3:C:78:GLU:N	2.47	0.48
1:A:52:ASN:CG	1:A:191:ILE:HG13	2.34	0.48
3:C:6:MET:O	3:C:10:ASP:HB2	2.14	0.48
3:C:87:GLN:OE1	3:C:153:GLY:HA2	2.14	0.48
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.96	0.48
2:B:78:MET:HG3	11:B:1535:HOH:O	2.12	0.48
2:B:437:GLU:O	2:B:441:GLN:HG3	2.14	0.48
1:A:372:TRP:CE2	1:A:863:PRO:HB3	2.49	0.48
1:A:1006:ILE:HD13	1:A:1016:GLU:HG3	1.95	0.48
3:C:155:GLU:HB2	11:C:870:HOH:O	2.13	0.48
1:A:863:PRO:HG2	1:A:864:LEU:CD2	2.40	0.48
1:A:177:ILE:HG12	1:A:182:PRO:HA	1.96	0.48
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.14	0.47
2:B:322:ILE:O	2:B:326:GLN:HG3	2.15	0.47
3:C:211:VAL:HG23	3:C:212:GLU:N	2.29	0.47
1:A:360:LEU:N	1:A:360:LEU:HD22	2.30	0.47
3:C:83:ILE:HG22	11:C:879:HOH:O	2.15	0.47
1:A:944:MET:CE	1:A:946:ASN:HD21	2.28	0.47
2:B:154:LYS:HE3	11:B:1751:HOH:O	2.14	0.47
1:A:835:GLU:HG3	1:A:836:VAL:N	2.29	0.47
1:A:384:VAL:HG22	1:A:385:ALA:N	2.28	0.47
1:A:214:LEU:HB3	1:A:607:SER:OG	2.15	0.47
2:B:85:LEU:HD22	3:C:214:LEU:HD21	1.97	0.47
1:A:625:ALA:O	1:A:629:LEU:HD22	2.14	0.47
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.97	0.47
1:A:914:LYS:HE3	1:A:1036:ARG:NH1	2.30	0.46
2:B:220:TRP:C	2:B:221:ARG:HG3	2.36	0.46
3:C:143:THR:HB	3:C:184:PHE:CE1	2.50	0.46
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.15	0.46
1:A:1072:GLU:HB2	11:A:1888:HOH:O	2.16	0.46
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.84	0.46
2:B:428:ARG:HB3	2:B:428:ARG:NH2	2.30	0.46
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.16	0.46
1:A:1100:THR:O	1:A:1101:TYR:HB2	2.15	0.46
2:B:280:ILE:HG23	2:B:350:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.30	0.46
1:A:600:ARG:HD3	1:A:905:LEU:HD13	1.97	0.46
2:B:42:ASN:HB2	7:B:1403:SF4:S1	2.56	0.46
3:C:62:ILE:HD11	3:C:98:GLY:HA2	1.98	0.45
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.51	0.45
4:A:1300:MD1:H11	4:A:1300:MD1:H7	1.98	0.45
1:A:434:PHE:CD1	1:A:1062:ARG:HD3	2.51	0.45
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.98	0.45
1:A:336:MET:N	1:A:337:PRO:HD2	2.31	0.45
1:A:100:TRP:O	1:A:104:SER:HB3	2.17	0.45
1:A:30:ASP:HB2	2:B:486:GLY:HA2	1.99	0.45
2:B:70:ILE:HG13	11:B:1723:HOH:O	2.17	0.45
1:A:54:THR:HA	1:A:580:GLN:HG3	1.98	0.45
1:A:225:PRO:HB2	1:A:551:ASP:OD1	2.16	0.45
1:A:658:ALA:HA	1:A:659:PRO:C	2.36	0.45
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.99	0.45
2:B:78:MET:HG2	2:B:225:THR:HG22	1.98	0.45
1:A:581:GLU:OE2	1:A:801:ASP:OD2	2.35	0.45
1:A:371:GLU:HG2	1:A:372:TRP:CD1	2.53	0.44
1:A:1229:ASN:C	1:A:1230:ILE:HD12	2.38	0.44
1:A:1091:PRO:O	1:A:1162:TYR:HA	2.16	0.44
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.53	0.44
2:B:306:PRO:O	2:B:310:GLU:HG3	2.18	0.44
1:A:366:GLN:HG2	1:A:373:LYS:CD	2.48	0.44
3:C:182:PHE:O	3:C:185:ARG:HB2	2.17	0.44
1:A:168:LEU:C	1:A:168:LEU:HD23	2.38	0.44
3:C:11:ILE:C	3:C:13:PRO:HD2	2.37	0.44
1:A:357:ALA:O	1:A:363:ALA:HA	2.18	0.44
1:A:604:HIS:HB3	1:A:1208:PHE:CD2	2.52	0.43
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.18	0.43
1:A:578:VAL:CG2	1:A:579:GLY:H	2.23	0.43
2:B:428:ARG:CZ	2:B:428:ARG:HB3	2.49	0.43
1:A:876:LEU:HD23	1:A:876:LEU:C	2.39	0.43
1:A:223:LEU:HD12	1:A:224:PRO:HD2	2.00	0.43
2:B:289:GLU:HG2	11:B:1581:HOH:O	2.18	0.43
1:A:1093:GLN:HB3	1:A:1162:TYR:HB3	2.01	0.43
2:B:193:VAL:HG22	2:B:201:ILE:HG22	2.02	0.42
3:C:73:PRO:HB2	3:C:75:TRP:CD1	2.54	0.42
1:A:345:ARG:HB2	1:A:348:TYR:O	2.19	0.42
1:A:1208:PHE:O	1:A:1209:ASN:HB2	2.18	0.42
1:A:68:VAL:HB	1:A:102:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:HIS:ND1	1:A:642:LEU:N	2.67	0.42
1:A:190:PRO:HD3	1:A:714:SER:HB2	2.01	0.42
1:A:145:ALA:O	1:A:149:LYS:HG3	2.20	0.42
1:A:722:LYS:H	1:A:722:LYS:CD	2.31	0.42
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.55	0.42
3:C:119:ARG:O	3:C:122:THR:HG22	2.20	0.41
1:A:651:ARG:HD3	11:A:2064:HOH:O	2.20	0.41
1:A:1070:VAL:HG13	1:A:1223:VAL:CG2	2.51	0.41
1:A:476:LEU:HA	1:A:476:LEU:HD12	1.96	0.41
1:A:532:THR:O	1:A:533:HIS:HB2	2.20	0.41
3:C:50:LEU:HD13	3:C:54:LEU:HD12	2.01	0.41
1:A:384:VAL:HG23	11:A:2085:HOH:O	2.20	0.41
1:A:1177:THR:O	1:A:1178:GLN:HB2	2.20	0.41
1:A:590:GLN:N	1:A:591:PRO:HD2	2.36	0.41
1:A:44:ILE:HA	1:A:61:ILE:O	2.21	0.41
1:A:574:TRP:CZ2	1:A:576:HIS:HB2	2.55	0.41
3:C:22:ILE:HA	3:C:22:ILE:HD12	1.94	0.41
2:B:224:ILE:CD1	2:B:234:PHE:HB2	2.51	0.41
1:A:152:ARG:HB2	1:A:734:THR:CG2	2.51	0.41
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.54	0.41
1:A:625:ALA:O	1:A:629:LEU:CD2	2.68	0.40
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.33	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)
11:A:1448:HOH:O	11:A:1448:HOH:O[3_354]	0.98	1.22

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1242/1247 (100%)	1171 (94%)	61 (5%)	10 (1%)	24	11
2	B	507/512 (99%)	495 (98%)	12 (2%)	0	100	100
3	C	220/225 (98%)	216 (98%)	4 (2%)	0	100	100
All	All	1969/1984 (99%)	1882 (96%)	77 (4%)	10 (0%)	34	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL
1	A	1166	GLU
1	A	501	ALA
1	A	578	VAL
1	A	190	PRO
1	A	224	PRO
1	A	195	SER
1	A	422	SER
1	A	718	GLY
1	A	808	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	1041/1044 (100%)	1022 (98%)	19 (2%)	66	61
2	B	436/439 (99%)	427 (98%)	9 (2%)	61	55
3	C	185/186 (100%)	183 (99%)	2 (1%)	80	79
All	All	1662/1669 (100%)	1632 (98%)	30 (2%)	66	61

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	94	ARG
1	A	190	PRO

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Mol	Chain	Res	Type
1	A	338	MET
1	A	367	GLU
1	A	461	GLN
1	A	476	LEU
1	A	767	LEU
1	A	808	PRO
1	A	864	LEU
1	A	926	LEU
1	A	936	GLU
1	A	1041	ARG
1	A	1062	ARG
1	A	1072	GLU
1	A	1087	ASN
1	A	1110	LEU
1	A	1233	LEU
1	A	1243	GLU
2	B	37	GLU
2	B	74	LEU
2	B	85	LEU
2	B	119	LYS
2	B	161	PHE
2	B	183	LEU
2	B	221	ARG
2	B	428	ARG
2	B	503	ASP
3	C	36	ARG
3	C	81	LEU

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

Mol	Chain	Res	Type
1	A	12	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	404	GLN
1	A	461	GLN
1	A	517	GLN
1	A	586	GLN

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Mol	Chain	Res	Type
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	1098	HIS
2	B	160	ASN
2	B	451	ASN
3	C	53	ASN
3	C	149	GLN
3	C	175	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FME	C	1	3	8,9,10	1.41	2 (25%)	6,9,11	1.93	3 (50%)

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	-	0/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-2.88	1.48	1.53
3	C	1	FME	CB-CG	2.16	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	O1-CN-N	-2.96	120.50	124.76
3	C	1	FME	O-C-CA	-2.02	120.11	125.44
3	C	1	FME	CA-N-CN	2.89	127.27	122.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z  > 2$
4	MD1	A	1300	5	39,51,51	3.93	11 (28%)	37,78,78	2.37	10 (27%)
4	MD1	A	1301	5	39,51,51	3.68	10 (25%)	37,78,78	2.38	11 (29%)
9	AGA	A	1309	-	29,29,29	0.69	1 (3%)	30,35,35	1.46	3 (10%)
7	SF4	A	1401	1	0,12,12	0.00	-	0,24,24	0.00	-
10	3PH	B	1310	-	17,17,47	0.84	0	19,21,52	2.13	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SF4	B	1402	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1403	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1404	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	B	1405	2	0,9,9	0.00	-	0,15,15	0.00	-
6	HEM	C	806	3	30,50,50	2.32	10 (33%)	24,82,82	2.66	10 (41%)
6	HEM	C	807	3	30,50,50	2.44	12 (40%)	24,82,82	2.79	11 (45%)

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
4	MD1	A	1300	5	-	0/18/59/59	0/5/5/5
4	MD1	A	1301	5	-	0/18/59/59	0/5/5/5
9	AGA	A	1309	-	-	0/34/34/34	0/0/0/0
7	SF4	A	1401	1	-	0/0/48/48	0/6/5/5
10	3PH	B	1310	-	1/1/3/4	1/18/18/49	0/0/0/0
7	SF4	B	1402	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1403	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1404	2	-	0/0/48/48	0/6/5/5
8	F3S	B	1405	2	-	0/0/24/24	0/0/3/3
6	HEM	C	806	3	-	0/10/54/54	0/0/8/8
6	HEM	C	807	3	-	0/10/54/54	0/0/8/8

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	806	HEM	C2D-C3D	-6.25	1.35	1.54
6	C	807	HEM	C2D-C3D	-6.08	1.36	1.54
6	C	806	HEM	C3B-C4B	-5.27	1.47	1.51
6	C	807	HEM	C3B-C4B	-5.12	1.47	1.51
6	C	807	HEM	C3D-C4D	-3.34	1.47	1.51
6	C	807	HEM	C2C-C1C	-2.85	1.47	1.52
6	C	806	HEM	C3D-C4D	-2.77	1.48	1.51
6	C	806	HEM	C2C-C1C	-2.62	1.47	1.52
4	A	1301	MD1	C6-C5	2.10	1.45	1.41
9	A	1309	AGA	C8-C7	2.10	1.56	1.50
6	C	807	HEM	CAD-C3D	2.10	1.58	1.54
6	C	807	HEM	CMA-C3A	2.11	1.56	1.51
4	A	1301	MD1	O11-C11	2.14	1.48	1.42
6	C	806	HEM	C1C-NC	2.20	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	807	HEM	C1C-NC	2.36	1.38	1.36
4	A	1300	MD1	O4'-C1'	2.53	1.44	1.41
6	C	806	HEM	CMA-C3A	2.58	1.57	1.51
6	C	806	HEM	C4C-NC	2.69	1.39	1.36
6	C	806	HEM	FE-NC	2.69	2.06	1.95
6	C	807	HEM	FE-NC	2.73	2.06	1.95
4	A	1301	MD1	C2-N1	2.73	1.40	1.35
4	A	1300	MD1	C13-C12	2.74	1.43	1.34
4	A	1301	MD1	C16-C20	2.82	1.44	1.40
4	A	1300	MD1	C20-N18	2.89	1.39	1.35
6	C	807	HEM	C3C-CAC	2.93	1.56	1.51
4	A	1300	MD1	C2-N1	3.02	1.40	1.35
6	C	807	HEM	CAA-C2A	3.09	1.57	1.52
4	A	1301	MD1	C20-N18	3.19	1.39	1.35
4	A	1301	MD1	C14-N15	3.22	1.50	1.47
4	A	1300	MD1	C4-N3	3.35	1.41	1.35
4	A	1301	MD1	C17-N17	3.39	1.41	1.35
6	C	806	HEM	C3C-CAC	3.41	1.57	1.51
4	A	1300	MD1	C17-N17	3.43	1.41	1.35
6	C	807	HEM	C4C-NC	3.44	1.40	1.36
4	A	1300	MD1	C14-C13	3.55	1.55	1.50
6	C	806	HEM	C3B-CAB	3.89	1.58	1.51
6	C	807	HEM	C3B-CAB	4.55	1.59	1.51
4	A	1300	MD1	C6-N1	4.82	1.42	1.33
4	A	1301	MD1	C15-N17	4.86	1.42	1.33
4	A	1301	MD1	C6-N1	5.01	1.42	1.33
4	A	1300	MD1	C15-N17	5.23	1.42	1.33
4	A	1300	MD1	C16-C20	5.24	1.48	1.40
4	A	1301	MD1	C7-N8	19.77	1.49	1.27
4	A	1300	MD1	C7-N8	20.87	1.50	1.27

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1300	MD1	C5-C6-N1	-6.46	114.76	123.59
4	A	1301	MD1	C5-C6-N1	-5.70	115.79	123.59
4	A	1301	MD1	N3-C2-N1	-5.23	119.48	127.44
4	A	1301	MD1	O3B-PB-O3A	-4.41	91.23	102.94
4	A	1300	MD1	N17-C17-N18	-4.36	118.38	125.53
4	A	1300	MD1	N3-C2-N1	-4.13	121.15	127.44
6	C	807	HEM	C3C-CAC-CBC	-3.96	118.38	124.46
4	A	1301	MD1	N17-C17-N18	-3.60	119.64	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	MD1	C6-C5-C4	-3.32	116.93	120.90
6	C	806	HEM	C3C-CAC-CBC	-3.24	119.48	124.46
6	C	806	HEM	CAA-C2A-C1A	-3.19	123.55	127.01
6	C	807	HEM	CMA-C3A-C4A	-3.11	123.22	128.36
6	C	806	HEM	CMA-C3A-C4A	-3.00	123.40	128.36
4	A	1301	MD1	C1'-N9-C4	-2.92	122.53	126.94
4	A	1300	MD1	C6-C5-C4	-2.89	117.44	120.90
6	C	807	HEM	CAA-C2A-C1A	-2.60	124.19	127.01
4	A	1300	MD1	O3B-PA-O5'	-2.55	96.16	102.94
4	A	1300	MD1	C1'-N9-C4	-2.23	123.58	126.94
4	A	1301	MD1	O4'-C1'-N9	2.05	112.39	108.10
9	A	1309	AGA	C5-O9-C12	2.05	122.82	117.89
6	C	807	HEM	CAD-C3D-C4D	2.10	119.89	112.47
4	A	1300	MD1	N2-C2-N3	2.15	121.92	117.80
10	B	1310	3PH	O21-C2-C1	2.23	116.22	108.36
4	A	1301	MD1	N16-C17-N17	2.25	120.92	117.20
6	C	807	HEM	CMA-C3A-C2A	2.38	130.21	125.24
6	C	806	HEM	CAD-C3D-C4D	2.41	120.99	112.47
6	C	806	HEM	CMA-C3A-C2A	2.47	130.41	125.24
6	C	807	HEM	CAA-CBA-CGA	2.81	117.89	112.75
4	A	1300	MD1	N16-C17-N18	2.91	122.02	117.20
4	A	1301	MD1	PA-O3B-PB	3.13	141.52	132.73
6	C	807	HEM	CMD-C2D-C3D	3.17	128.38	114.35
6	C	806	HEM	CMD-C2D-C3D	3.20	128.52	114.35
10	B	1310	3PH	O21-C2-C3	3.53	120.80	108.36
6	C	806	HEM	C2D-C3D-C4D	3.74	107.84	101.50
6	C	807	HEM	C2D-C3D-C4D	3.80	107.94	101.50
10	B	1310	3PH	C2-O21-C21	3.85	123.80	117.29
10	B	1310	3PH	C33-C32-C31	4.29	130.47	113.59
9	A	1309	AGA	C9-C8-C7	4.56	131.52	113.59
10	B	1310	3PH	C3-C2-C1	4.66	122.98	112.07
4	A	1301	MD1	C15-N17-C17	4.94	122.80	115.94
6	C	807	HEM	CMC-C2C-C3C	5.01	129.04	116.53
6	C	806	HEM	CMC-C2C-C3C	5.09	129.22	116.53
9	A	1309	AGA	C14-C13-C12	5.09	133.61	113.59
6	C	806	HEM	CMB-C2B-C3B	5.33	129.85	116.53
4	A	1301	MD1	C6-N1-C2	5.57	123.67	115.94
6	C	807	HEM	CMB-C2B-C3B	5.61	130.53	116.53
4	A	1300	MD1	C15-N17-C17	5.84	124.05	115.94
6	C	806	HEM	CAD-C3D-C2D	6.24	131.17	113.22
4	A	1300	MD1	C6-N1-C2	6.50	124.96	115.94
6	C	807	HEM	CAD-C3D-C2D	6.59	132.17	113.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	1310	3PH	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1310	3PH	C2-O21-C21-O22

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1300	MD1	3	0
4	A	1301	MD1	2	0
7	B	1403	SF4	2	0

## 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	1244/1247 (99%)	0.12	41 (3%) 50 53	12, 24, 42, 59	0
2	B	509/512 (99%)	-0.28	6 (1%) 81 83	11, 18, 31, 51	0
3	C	223/225 (99%)	0.12	9 (4%) 42 46	13, 24, 41, 55	0
All	All	1976/1984 (99%)	0.02	56 (2%) 56 60	11, 22, 41, 59	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	PHE	12.3
3	C	75	TRP	10.9
1	A	9	TYR	9.4
3	C	80	TRP	7.0
1	A	362	ASP	6.3
3	C	76	MET	5.9
3	C	78	GLU	5.8
1	A	673	GLU	4.3
3	C	74	HIS	4.1
2	B	70	ILE	3.9
1	A	361	VAL	3.9
1	A	11	LYS	3.9
1	A	7	PHE	3.7
1	A	380	ASN	3.6
2	B	366	ALA	3.3
1	A	463	ALA	3.2
3	C	73	PRO	3.2
3	C	81	LEU	3.1
1	A	759	ASN	2.9
1	A	461	GLN	2.8
1	A	1243	GLU	2.8
1	A	1244	SER	2.7
3	C	79	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	674	LYS	2.6
2	B	119	LYS	2.6
1	A	486	GLY	2.6
1	A	421	GLY	2.6
1	A	348	TYR	2.5
1	A	365	GLY	2.5
1	A	473	VAL	2.5
1	A	8	ARG	2.5
1	A	749	VAL	2.4
1	A	367	GLU	2.4
1	A	344	GLU	2.4
1	A	465	GLY	2.4
1	A	411	GLU	2.4
1	A	321	ASN	2.4
1	A	413	THR	2.4
1	A	346	ASP	2.3
1	A	670	GLY	2.3
1	A	675	ALA	2.3
2	B	367	ASP	2.3
2	B	370	GLU	2.3
1	A	718	GLY	2.3
1	A	678	ASN	2.3
1	A	875	ASP	2.2
1	A	490	VAL	2.2
1	A	717	LEU	2.2
3	C	3	PHE	2.2
1	A	936	GLU	2.2
1	A	1164	ALA	2.1
1	A	379	THR	2.1
1	A	409	THR	2.1
1	A	462	LEU	2.1
1	A	488	ASN	2.1
2	B	365	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FME	C	1	10/11	0.91	0.22	-	37,44,53,54	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	3PH	B	1310	18/48	0.78	0.19	19.46	42,55,60,62	0
6	HEM	C	806	43/43	0.97	0.11	1.82	11,16,19,30	0
6	HEM	C	807	43/43	0.95	0.12	0.85	20,25,37,45	0
9	AGA	A	1309	30/30	0.93	0.13	0.09	19,23,55,60	0
4	MD1	A	1300	47/47	0.94	0.11	0.06	14,22,35,39	0
4	MD1	A	1301	47/47	0.95	0.09	-0.27	16,21,29,34	0
8	F3S	B	1405	7/7	0.99	0.07	-1.38	13,14,15,15	0
5	6MO	A	1302	1/1	0.92	0.10	-1.47	40,40,40,40	0
7	SF4	B	1403	8/8	0.99	0.05	-1.58	13,13,14,15	0
7	SF4	B	1402	8/8	0.98	0.05	-1.64	19,21,21,23	0
7	SF4	A	1401	8/8	0.98	0.05	-2.15	19,22,22,24	0
7	SF4	B	1404	8/8	0.99	0.06	-4.23	17,19,20,21	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.