



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:23 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 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/ValidationPDFNotes.html>

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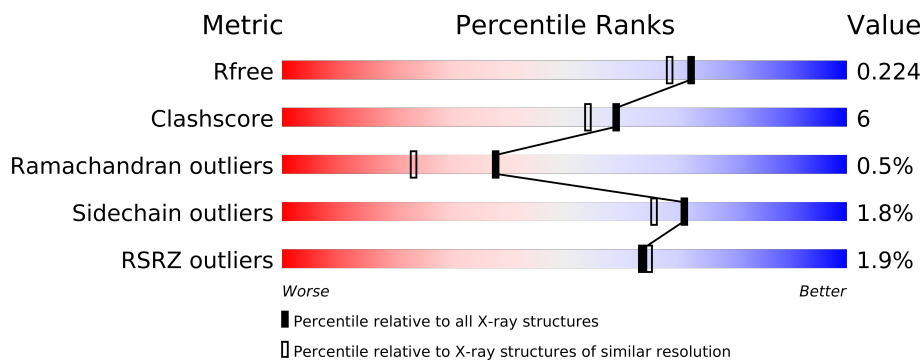
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1247	
2	B	512	
3	C	225	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	3PH	B	1310	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17199 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

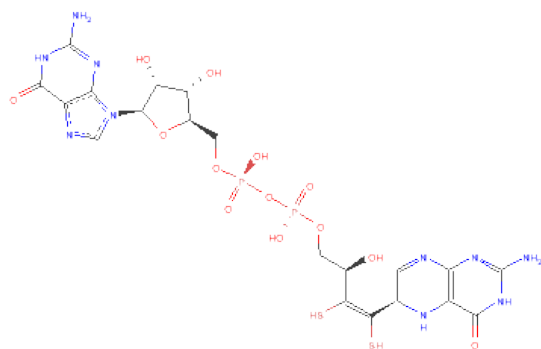
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

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-YLESTER 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>).

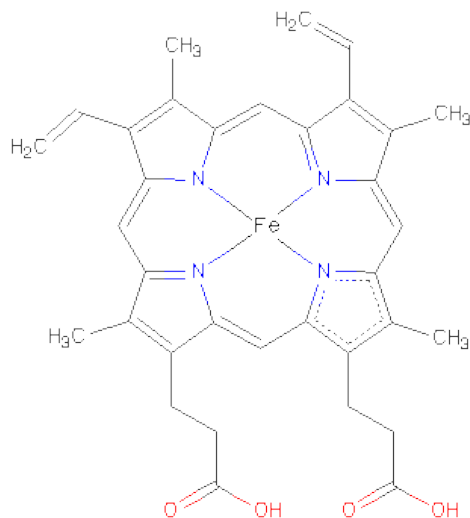


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

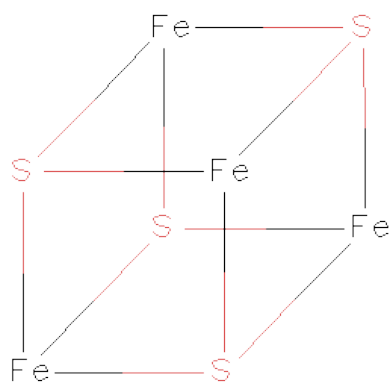
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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:  $\text{Fe}_4\text{S}_4$ ).



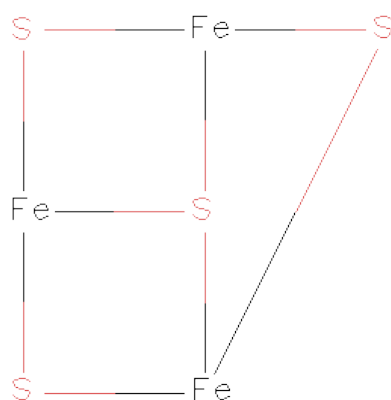
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

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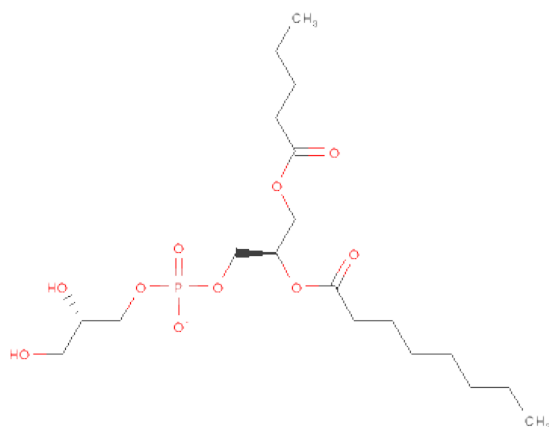
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

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



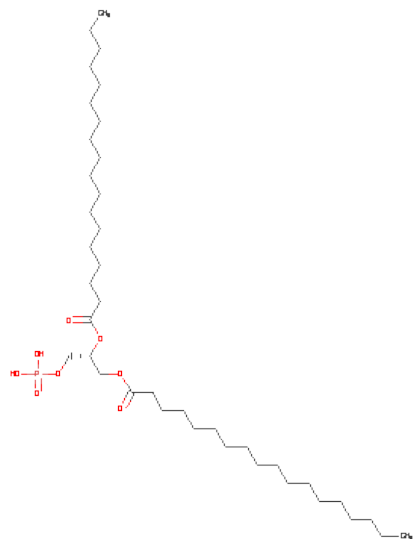
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is (1S)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYLOCTANOATE (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

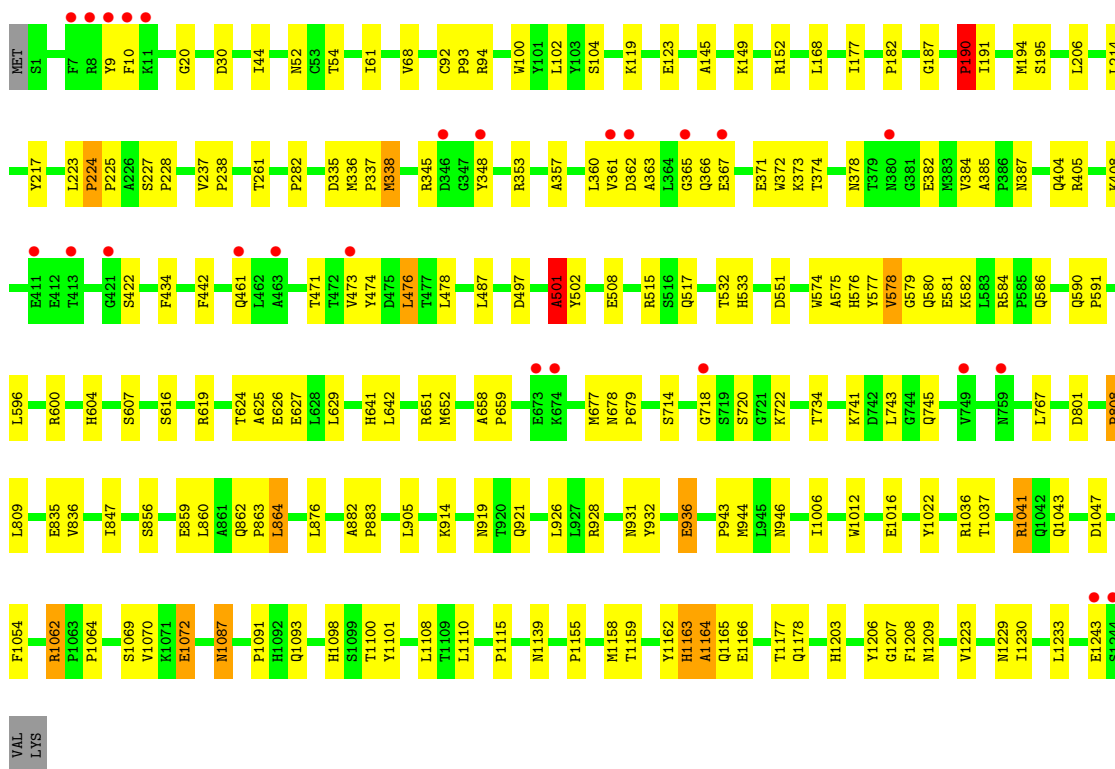


### 3 Residue-property plots


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.

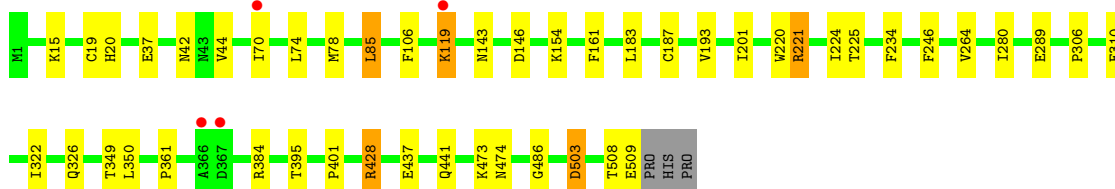
- Molecule 1: Respiratory nitrate reductase 1 alpha chain

Chain A: 



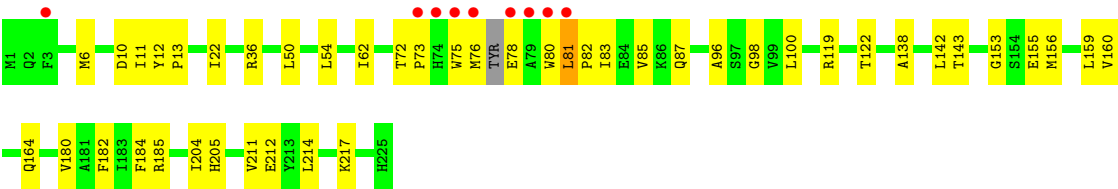
- Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B: 



- Molecule 3: Respiratory nitrate reductase 1 gamma chain

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.18Å 241.38Å 139.49Å 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 1.91Å)	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 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (192) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
3:C:72:THR:HG23	3:C:76:MET:HE2	1.69	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(Å)
11:A:1448:HOH:O	11:A:1448:HOH:O[3_354]	0.98	1.22

## 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	1242/1247 (100%)	1171 (94%)	61 (5%)	10 (1%)	27	12
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%)	38	23

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%)	71	66
2	B	436/439 (99%)	427 (98%)	9 (2%)	66	59
3	C	185/186 (100%)	183 (99%)	2 (1%)	84	82
All	All	1662/1669 (100%)	1632 (98%)	30 (2%)	71	66

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
3	C	149	GLN
3	C	175	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	9,9,10	5.66	4 (44%)	6,9,11	1.55	2 (33%)

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	-	0/7/9/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	O-C	15.13	1.21	1.11
3	C	1	FME	CB-CA	-6.23	1.48	1.53
3	C	1	FME	CA-C	3.54	1.55	1.48
3	C	1	FME	CB-CG	2.18	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	2.60	127.27	122.97
3	C	1	FME	CB-CA-N	2.03	114.79	111.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	51,51,51	3.78	16 (31%)	64,78,78	2.78	10 (15%)
4	MD1	A	1301	5	51,51,51	3.51	17 (33%)	64,78,78	2.21	14 (21%)
9	AGA	A	1309	-	29,29,29	0.93	2 (6%)	35,35,35	1.45	3 (8%)
7	SF4	A	1401	1	12,12,12	8.50	12 (100%)	0,24,24	0.00	-
10	3PH	B	1310	-	16,17,47	2.11	1 (6%)	19,21,52	1.95	4 (21%)
7	SF4	B	1402	2	12,12,12	7.28	12 (100%)	0,24,24	0.00	-
7	SF4	B	1403	2	12,12,12	9.09	12 (100%)	0,24,24	0.00	-
7	SF4	B	1404	2	12,12,12	7.88	12 (100%)	0,24,24	0.00	-
8	F3S	B	1405	2	3,9,9	7.39	3 (100%)	0,15,15	0.00	-
6	HEM	C	806	3	49,50,50	3.64	18 (36%)	46,82,82	1.45	5 (10%)
6	HEM	C	807	3	49,50,50	4.13	21 (42%)	46,82,82	1.51	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MD1	A	1300	5	-	0/22/59/59	0/1/5/5
4	MD1	A	1301	5	-	0/22/59/59	0/1/5/5
9	AGA	A	1309	-	-	0/34/34/34	0/0/0/0
7	SF4	A	1401	1	-	0/0/48/48	0/0/5/5
10	3PH	B	1310	-	1/1/3/4	0/17/18/49	0/0/0/0
7	SF4	B	1402	2	-	0/0/48/48	0/0/5/5
7	SF4	B	1403	2	-	0/0/48/48	0/0/5/5
7	SF4	B	1404	2	-	0/0/48/48	0/0/5/5
8	F3S	B	1405	2	-	0/0/24/24	0/0/3/3
6	HEM	C	806	3	-	0/14/114/114	0/0/8/8
6	HEM	C	807	3	-	0/14/114/114	0/0/8/8

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1300	MD1	C7-N8	22.11	1.50	1.27
4	A	1301	MD1	C7-N8	20.95	1.49	1.27
6	C	807	HEM	C2D-C1D	17.07	1.48	1.44
7	B	1403	SF4	S2-FE3	-14.28	2.23	2.33
6	C	806	HEM	C3D-C4D	13.91	1.48	1.44
6	C	807	HEM	C2B-C1B	11.88	1.47	1.44
7	B	1402	SF4	S4-FE1	-11.48	2.25	2.33
7	B	1403	SF4	S1-FE4	-10.98	2.25	2.33
6	C	807	HEM	C3D-C4D	10.95	1.47	1.44
7	B	1403	SF4	S2-FE1	-10.71	2.26	2.33
7	B	1403	SF4	S1-FE2	-10.55	2.26	2.33
7	B	1404	SF4	S2-FE1	-10.30	2.26	2.33
7	B	1403	SF4	S4-FE1	-10.28	2.26	2.33
6	C	806	HEM	C2B-C1B	10.21	1.47	1.44
7	B	1403	SF4	S2-FE4	-10.15	2.26	2.33
7	A	1401	SF4	S2-FE4	-10.09	2.26	2.33
7	B	1404	SF4	S2-FE3	-10.05	2.26	2.33
7	B	1404	SF4	S2-FE4	-9.93	2.26	2.33
6	C	806	HEM	C2D-C1D	9.89	1.47	1.44
7	A	1401	SF4	S3-FE1	-9.73	2.26	2.33
7	B	1404	SF4	S4-FE3	-9.49	2.26	2.33
7	A	1401	SF4	S3-FE4	-9.41	2.26	2.33
8	B	1405	F3S	S3-FE4	-9.39	2.26	2.33
7	B	1402	SF4	S4-FE2	-9.24	2.27	2.33
7	B	1403	SF4	S4-FE3	-9.10	2.27	2.33
7	A	1401	SF4	S3-FE2	-8.99	2.27	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1401	SF4	S2-FE3	-8.98	2.27	2.33
7	B	1402	SF4	S4-FE3	-8.84	2.27	2.33
7	A	1401	SF4	S4-FE3	-8.82	2.27	2.33
7	B	1402	SF4	S1-FE2	-8.64	2.27	2.33
7	B	1402	SF4	S3-FE2	-8.19	2.27	2.33
7	B	1404	SF4	S4-FE1	-8.04	2.27	2.33
4	A	1300	MD1	C11-C12	8.02	1.59	1.50
7	A	1401	SF4	S2-FE1	-7.97	2.27	2.33
10	B	1310	3PH	C35-C34	-7.88	1.52	1.55
7	B	1404	SF4	S4-FE2	-7.73	2.28	2.33
7	B	1404	SF4	S3-FE4	-7.69	2.28	2.33
7	A	1401	SF4	S1-FE4	-7.67	2.28	2.33
7	A	1401	SF4	S1-FE2	-7.66	2.28	2.33
7	A	1401	SF4	S4-FE2	-7.61	2.28	2.33
7	B	1402	SF4	S1-FE3	-7.55	2.28	2.33
7	B	1403	SF4	S4-FE2	-7.39	2.28	2.33
7	B	1404	SF4	S3-FE1	-7.38	2.28	2.33
7	B	1402	SF4	S1-FE4	-7.37	2.28	2.33
7	A	1401	SF4	S4-FE1	-7.28	2.28	2.33
7	A	1401	SF4	S1-FE3	-7.16	2.28	2.33
4	A	1301	MD1	C11-C12	7.13	1.58	1.50
8	B	1405	F3S	S3-FE3	-6.78	2.28	2.33
7	B	1403	SF4	S1-FE3	-6.27	2.29	2.33
7	B	1404	SF4	S1-FE3	-6.21	2.29	2.33
6	C	807	HEM	C3B-CAB	6.15	1.59	1.40
6	C	807	HEM	C4A-C3A	6.08	1.47	1.40
4	A	1300	MD1	C13-C12	6.03	1.43	1.34
7	B	1404	SF4	S1-FE4	-5.99	2.29	2.33
7	B	1402	SF4	S3-FE1	-5.87	2.29	2.33
6	C	806	HEM	C3B-CAB	5.76	1.58	1.40
6	C	806	HEM	C3C-CAC	5.48	1.57	1.40
8	B	1405	F3S	S3-FE1	-5.44	2.29	2.33
6	C	807	HEM	C3C-CAC	5.20	1.56	1.40
6	C	806	HEM	C4A-C3A	5.11	1.46	1.40
7	B	1404	SF4	S3-FE2	-5.08	2.29	2.33
4	A	1300	MD1	C16-C20	4.80	1.48	1.40
7	B	1403	SF4	S3-FE2	-4.71	2.30	2.33
6	C	806	HEM	C3D-C2D	-4.57	1.35	1.43
6	C	806	HEM	C3C-C2C	-4.50	1.35	1.43
7	B	1403	SF4	S3-FE4	-4.38	2.30	2.33
6	C	807	HEM	C3C-C2C	-4.33	1.36	1.43
6	C	807	HEM	C3D-C2D	-4.28	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1402	SF4	S3-FE4	-4.12	2.30	2.33
6	C	806	HEM	C3B-C2B	-4.09	1.36	1.43
7	B	1402	SF4	S2-FE3	-4.02	2.30	2.33
6	C	807	HEM	C3B-C2B	-3.76	1.37	1.43
7	B	1403	SF4	S3-FE1	-3.67	2.30	2.33
4	A	1301	MD1	C13-C12	3.60	1.39	1.34
7	B	1404	SF4	S1-FE2	-3.41	2.31	2.33
4	A	1300	MD1	C15-N17	3.34	1.42	1.37
7	B	1402	SF4	S2-FE4	-3.34	2.31	2.33
6	C	807	HEM	CMC-C2C	3.33	1.57	1.47
4	A	1301	MD1	PA-O3B	-3.33	1.53	1.59
6	C	806	HEM	CMC-C2C	3.33	1.57	1.47
4	A	1301	MD1	C20-N18	3.12	1.39	1.35
4	A	1301	MD1	C6-N1	3.10	1.42	1.37
4	A	1300	MD1	C4-N3	3.09	1.41	1.35
9	A	1309	AGA	P1-O4	3.07	1.56	1.48
6	C	807	HEM	CMB-C2B	3.06	1.56	1.47
6	C	806	HEM	CMD-C2D	3.04	1.56	1.47
6	C	807	HEM	CAA-C2A	3.01	1.57	1.52
4	A	1300	MD1	C17-N17	2.96	1.41	1.36
7	B	1402	SF4	S2-FE1	-2.95	2.31	2.33
6	C	806	HEM	CMB-C2B	2.94	1.56	1.47
4	A	1301	MD1	C15-N17	2.93	1.42	1.37
4	A	1300	MD1	C14-C13	2.93	1.55	1.51
4	A	1301	MD1	C17-N17	2.92	1.41	1.36
4	A	1300	MD1	C6-N1	2.88	1.42	1.37
6	C	807	HEM	CMD-C2D	2.87	1.56	1.47
6	C	806	HEM	CHA-C4D	2.85	1.39	1.35
4	A	1300	MD1	C20-N18	2.83	1.39	1.35
6	C	807	HEM	CHB-C1B	2.79	1.39	1.35
6	C	807	HEM	CHA-C4D	2.75	1.39	1.35
4	A	1301	MD1	C16-C20	2.65	1.44	1.40
4	A	1301	MD1	C6-C5	2.58	1.45	1.41
6	C	807	HEM	CAD-CBD	2.57	1.59	1.52
4	A	1300	MD1	C2-N3	2.54	1.36	1.33
6	C	806	HEM	CMA-C3A	2.54	1.57	1.51
4	A	1301	MD1	C17-N18	2.53	1.36	1.33
4	A	1301	MD1	C8-N9	2.53	1.40	1.36
4	A	1300	MD1	C2-N1	2.51	1.40	1.36
6	C	807	HEM	C1A-C2A	2.51	1.47	1.43
4	A	1301	MD1	C15-C16	2.43	1.45	1.41
6	C	807	HEM	C3B-C4B	2.41	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	806	HEM	CAD-CBD	2.40	1.59	1.52
4	A	1300	MD1	C17-N18	2.36	1.36	1.33
6	C	806	HEM	CHB-C1B	2.34	1.39	1.35
4	A	1300	MD1	C10-C11	2.33	1.55	1.51
6	C	807	HEM	FE-NC	2.33	2.06	1.97
4	A	1301	MD1	C20-N8	2.31	1.41	1.37
6	C	806	HEM	C3B-C4B	2.30	1.47	1.44
6	C	806	HEM	FE-NC	2.29	2.06	1.97
4	A	1301	MD1	C2-N3	2.26	1.36	1.33
4	A	1301	MD1	C2-N1	2.19	1.40	1.36
4	A	1301	MD1	O11-C11	2.17	1.48	1.42
4	A	1300	MD1	C8-N9	2.09	1.39	1.36
4	A	1300	MD1	C20-N8	2.07	1.41	1.37
6	C	807	HEM	CMA-C3A	2.07	1.56	1.51
9	A	1309	AGA	C8-C7	2.05	1.56	1.50
6	C	807	HEM	CBA-CGA	2.02	1.55	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1300	MD1	C6-C5-N7	-18.99	131.58	134.14
4	A	1301	MD1	C6-C5-N7	-10.27	132.76	134.14
4	A	1301	MD1	C14-C7-N8	-8.44	104.58	124.80
6	C	806	HEM	C3B-C4B-NB	-5.24	110.25	114.00
9	A	1309	AGA	C14-C13-C12	5.13	133.61	113.51
6	C	807	HEM	C3B-C4B-NB	-5.08	110.36	114.00
10	B	1310	3PH	C3-C2-C1	4.88	122.98	111.86
9	A	1309	AGA	C9-C8-C7	4.59	131.52	113.51
10	B	1310	3PH	C33-C32-C31	4.33	130.47	113.51
4	A	1301	MD1	O4'-C1'-N9	4.25	112.39	108.44
4	A	1300	MD1	O4'-C1'-N9	-3.96	104.75	108.44
4	A	1300	MD1	C14-C7-N8	-3.66	116.03	124.80
6	C	807	HEM	CMA-C3A-C4A	-3.51	123.22	128.62
4	A	1300	MD1	C8-N9-C4	-3.47	104.25	106.90
6	C	806	HEM	CMA-C3A-C4A	-3.40	123.40	128.62
10	B	1310	3PH	O21-C2-C3	3.37	120.80	108.44
4	A	1301	MD1	PA-O3B-PB	3.36	141.52	131.68
4	A	1301	MD1	C8-N9-C1'	3.27	132.83	126.38
4	A	1300	MD1	C6-N1-C2	3.12	124.96	119.51
4	A	1301	MD1	C8-N9-C4	-2.96	104.64	106.90
4	A	1300	MD1	C8-N9-C1'	2.94	132.17	126.38
6	C	807	HEM	C2D-C1D-ND	-2.91	109.49	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	806	HEM	CMA-C3A-C2A	2.90	130.41	124.94
6	C	807	HEM	CMA-C3A-C2A	2.79	130.21	124.94
4	A	1301	MD1	N16-C17-N17	2.78	120.92	117.86
4	A	1301	MD1	O3B-PB-O3A	-2.72	91.23	103.41
4	A	1301	MD1	C10-C11-C12	2.68	115.42	111.51
4	A	1300	MD1	O3A-C10-C11	-2.62	102.21	108.63
4	A	1300	MD1	C15-N17-C17	2.59	124.05	119.51
6	C	807	HEM	CAD-C3D-C4D	-2.58	119.89	124.53
4	A	1301	MD1	N18-C20-N8	2.55	120.95	116.18
9	A	1309	AGA	O5-C3-C2	2.43	116.26	108.62
4	A	1300	MD1	N17-C17-N18	-2.43	118.38	121.78
4	A	1300	MD1	C13-C14-N15	-2.40	102.81	111.53
4	A	1301	MD1	C6-N1-C2	2.38	123.67	119.51
4	A	1301	MD1	C1'-N9-C4	-2.37	122.53	126.64
6	C	806	HEM	C2D-C1D-ND	-2.37	110.13	112.93
4	A	1301	MD1	N2-C2-N1	2.26	120.35	117.86
6	C	807	HEM	CAD-C3D-C2D	2.21	132.17	127.25
10	B	1310	3PH	O21-C2-C1	2.12	116.22	108.44
4	A	1301	MD1	C15-C16-C20	2.04	119.28	114.53
6	C	806	HEM	O1D-CGD-CBD	-2.01	116.11	123.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	1310	3PH	C2

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	0.08	25 (2%) 62 63	12, 24, 42, 59	0
2	B	509/512 (99%)	-0.27	4 (0%) 83 85	11, 18, 31, 51	0
3	C	224/225 (99%)	0.09	9 (4%) 36 37	13, 24, 41, 55	0
All	All	1977/1984 (99%)	-0.01	38 (1%) 64 65	11, 22, 41, 59	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	PHE	10.5
3	C	75	TRP	9.2
1	A	9	TYR	8.9
3	C	80	TRP	6.0
1	A	362	ASP	5.8
3	C	78	GLU	5.7
3	C	76	MET	5.1
3	C	74	HIS	4.2
1	A	11	LYS	3.8
1	A	673	GLU	3.7
2	B	70	ILE	3.6
1	A	361	VAL	3.6
2	B	366	ALA	3.4
1	A	380	ASN	3.3
1	A	7	PHE	3.3
1	A	463	ALA	3.0
1	A	759	ASN	3.0
3	C	79	ALA	2.8
1	A	1243	GLU	2.7
3	C	81	LEU	2.7
2	B	119	LYS	2.6
3	C	73	PRO	2.6
1	A	421	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	413	THR	2.5
1	A	1244	SER	2.5
1	A	365	GLY	2.4
1	A	473	VAL	2.4
1	A	674	LYS	2.3
3	C	3	PHE	2.3
1	A	8	ARG	2.2
1	A	411	GLU	2.2
1	A	461	GLN	2.2
1	A	718	GLY	2.2
1	A	346	ASP	2.1
1	A	348	TYR	2.1
1	A	749	VAL	2.1
1	A	367	GLU	2.1
2	B	367	ASP	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FME	C	1	10/11	0.22	1.88	37,44,53,54	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	3PH	B	1310	18/48	0.19	22.66	42,55,60,62	0
6	HEM	C	806	43/43	0.11	1.85	11,16,19,30	0
6	HEM	C	807	43/43	0.12	0.89	20,25,37,45	0
9	AGA	A	1309	30/30	0.13	0.11	19,23,55,60	0
4	MD1	A	1300	47/47	0.11	0.09	14,22,35,39	0
4	MD1	A	1301	47/47	0.09	-0.21	16,21,29,34	0
8	F3S	B	1405	7/7	0.08	-1.11	13,14,15,15	0
5	6MO	A	1302	1/1	0.10	-1.16	40,40,40,40	0
7	SF4	B	1403	8/8	0.06	-1.20	13,13,14,15	0
7	SF4	B	1402	8/8	0.05	-1.50	19,21,21,23	0
7	SF4	A	1401	8/8	0.05	-2.05	19,22,22,24	0
7	SF4	B	1404	8/8	0.06	-3.35	17,19,20,21	0

## 6.5 Other polymers

There are no such residues in this entry.