



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:02 AM GMT

PDB ID : 3IR7
Title : Crystal structure of NarGHI mutant NarG-R94S
Authors : Bertero, M.G.; Rothery, R.A.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2009-08-21
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

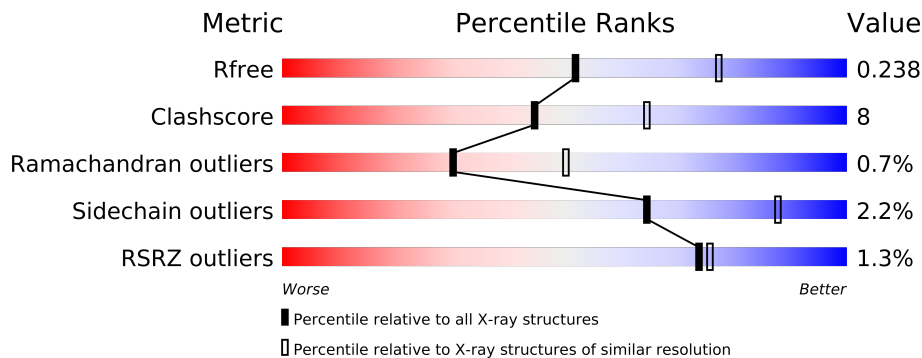
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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
6	6MO	A	1250	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16102 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	1242	Total	C	N	O	S	0	0	0
			9840	6214	1723	1855	48			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	SER	ARG	ENGINEERED	UNP P09152

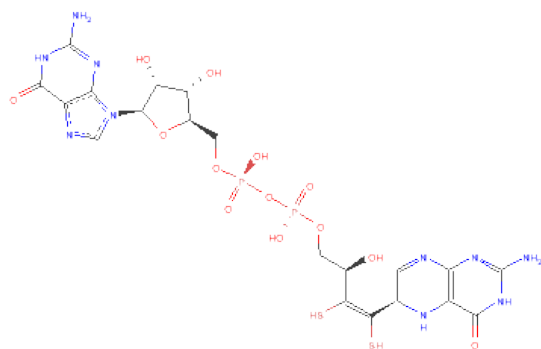
- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

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.

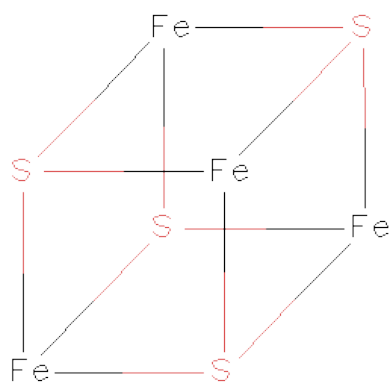
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	225	Total	C	N	O	S	0	0	0
			1791	1188	303	286	14			

- 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: C₂₀H₂₆N₁₀O₁₃P₂S₂).



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

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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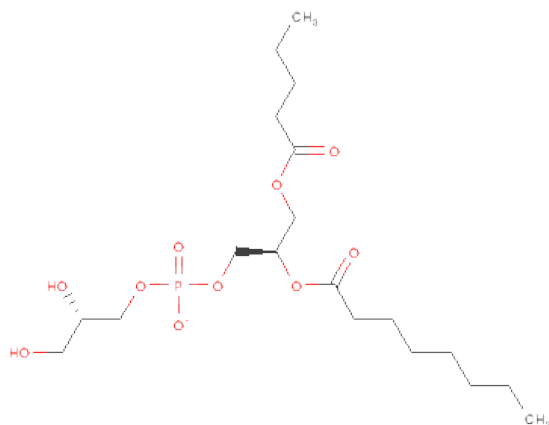
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

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

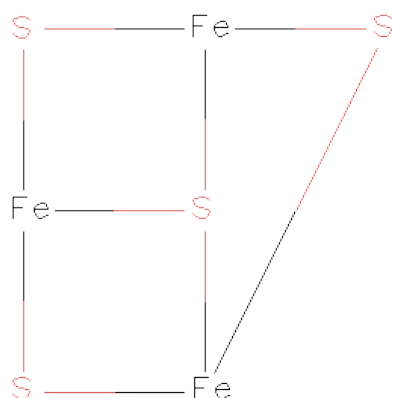
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		

- Molecule 7 is (1S)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYLOCTANOATE (three-letter code: AGA) (formula: C₁₉H₃₆O₁₀P).



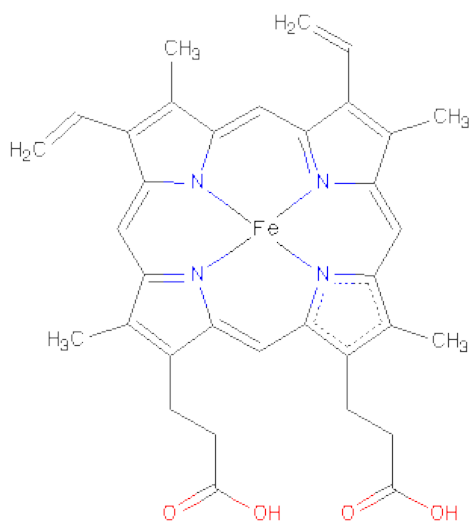
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			25	16	8	1		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



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

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



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

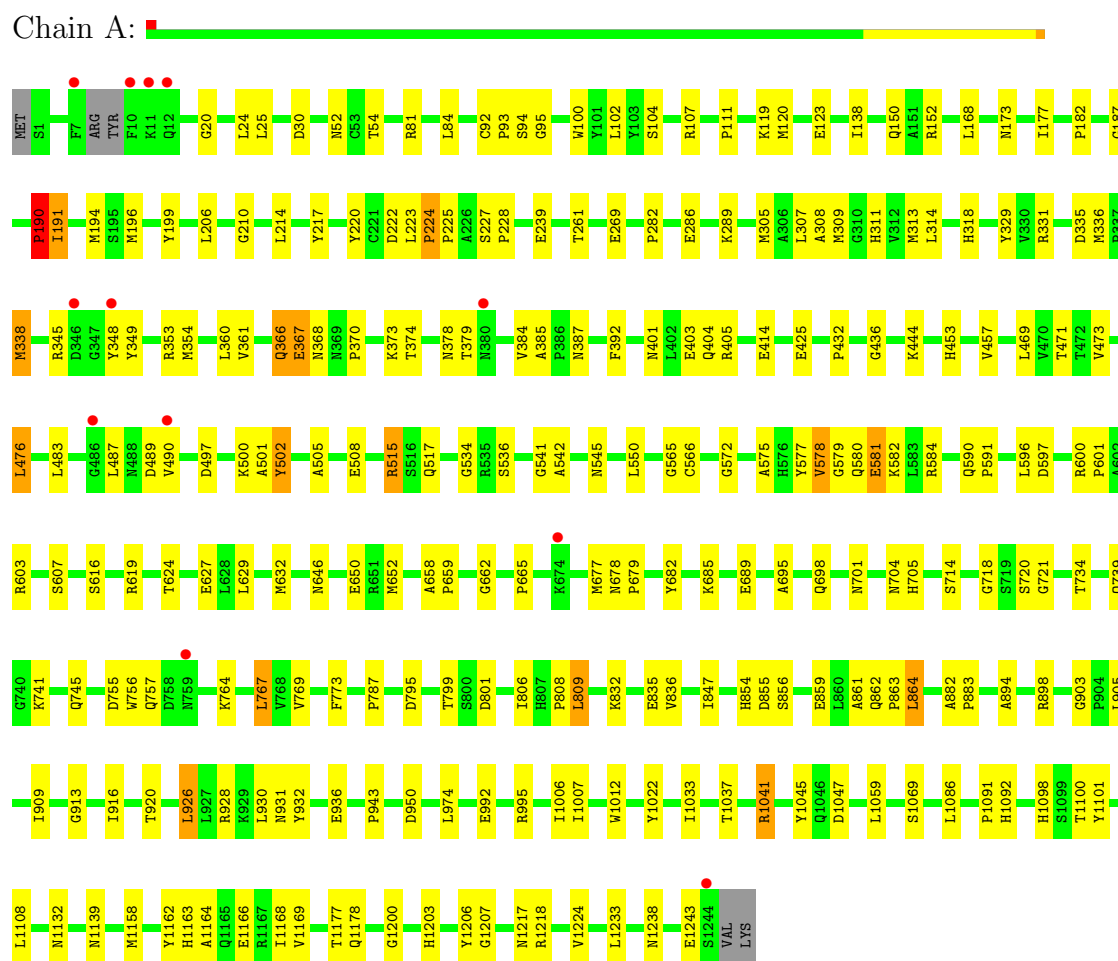
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	82	Total 82	O 82	0	0
10	A	86	Total 86	O 86	0	0
10	C	8	Total 8	O 8	0	0

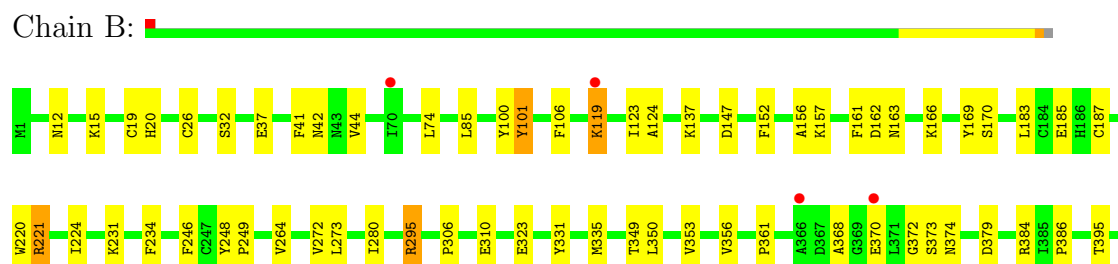
3 Residue-property plots

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



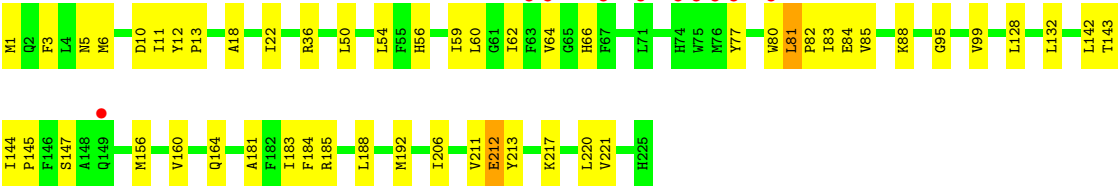
- Molecule 2: Respiratory nitrate reductase 1 beta chain





● Molecule 3: Respiratory nitrate reductase 1 gamma chain

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	153.85Å 241.15Å 139.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 2.50 24.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.96-2.50) 99.9 (24.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.243 0.199 , 0.238	Depositor DCC
R_{free} test set	7209 reflections (8.74%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 89737 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16102	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, 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	0.35	0/10097	0.62	2/13707 (0.0%)
2	B	0.37	0/4146	0.64	1/5609 (0.0%)
3	C	0.39	0/1833	0.55	0/2481
All	All	0.36	0/16076	0.62	3/21797 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	407	LYS	CB-CA-C	5.56	121.53	110.40
1	A	809	LEU	N-CA-C	-5.37	96.52	111.00
1	A	767	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

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	9840	0	9496	185	0
2	B	4050	0	3973	53	0
3	C	1791	0	1825	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	94	0	42	8	0
5	A	8	0	0	1	0
5	B	24	0	0	1	0
6	A	1	0	0	0	0
7	A	25	0	29	0	0
8	B	7	0	0	0	0
9	C	86	0	60	2	0
10	A	86	0	0	6	0
10	B	82	0	0	4	0
10	C	8	0	0	0	0
All	All	16102	0	15425	265	0

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 8.

All (265) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:508:GLU:OE1	1:A:515:ARG:HD2	1.75	0.86
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.62	0.81
1:A:584:ARG:HD3	1:A:1006:ILE:HD13	1.62	0.80
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.67	0.77
1:A:1218:ARG:HD2	10:A:1319:HOH:O	1.88	0.71
2:B:407:LYS:NZ	2:B:432:GLU:HG2	2.07	0.70
1:A:578:VAL:HG23	1:A:579:GLY:H	1.56	0.69
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.74	0.69
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.75	0.69
3:C:6:MET:O	3:C:10:ASP:HB2	1.94	0.68
1:A:1098:HIS:CE1	4:A:1251:MD1:S13	2.88	0.66
1:A:677:MET:HG3	1:A:682:TYR:HB2	1.77	0.66
1:A:1098:HIS:HE1	4:A:1251:MD1:S13	2.18	0.66
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.78	0.65
1:A:335:ASP:O	1:A:338:MET:HB2	1.96	0.65
1:A:387:ASN:ND2	1:A:405:ARG:HB2	2.11	0.65
1:A:225:PRO:O	1:A:228:PRO:HD2	1.97	0.65
3:C:95:GLY:O	3:C:99:VAL:HG23	1.96	0.64
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.79	0.63
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.35	0.62
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.64	0.62
1:A:168:LEU:O	1:A:168:LEU:HD23	2.00	0.62
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.82	0.62
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.80	0.61
1:A:336:MET:HA	1:A:473:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:187:CYS:HB3	2:B:349:THR:O	2.01	0.60
3:C:143:THR:HG22	3:C:183:ILE:HG13	1.84	0.59
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.18	0.59
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.83	0.59
1:A:1098:HIS:CE1	4:A:1247:MD1:S12	2.96	0.59
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.85	0.59
2:B:373:SER:HB3	2:B:428:ARG:NH1	2.19	0.58
2:B:508:THR:O	2:B:509:GLU:HB3	2.03	0.58
1:A:191:ILE:O	1:A:194:MET:HG2	2.04	0.57
1:A:345:ARG:HB2	1:A:348:TYR:O	2.04	0.57
3:C:84:GLU:O	3:C:88:LYS:HG2	2.04	0.57
1:A:1092:HIS:HA	1:A:1163:HIS:HB3	1.85	0.57
3:C:12:TYR:N	3:C:13:PRO:HD2	2.19	0.57
1:A:487:LEU:N	1:A:487:LEU:HD12	2.20	0.57
1:A:119:LYS:O	1:A:123:GLU:HG3	2.04	0.57
1:A:360:LEU:N	1:A:360:LEU:HD22	2.20	0.57
1:A:578:VAL:HG23	1:A:579:GLY:N	2.20	0.56
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.40	0.56
1:A:338:MET:HG3	1:A:374:THR:HB	1.87	0.56
2:B:407:LYS:HZ1	2:B:432:GLU:HG2	1.71	0.56
1:A:214:LEU:HB3	1:A:607:SER:OG	2.05	0.56
3:C:50:LEU:HD13	3:C:54:LEU:HD12	1.88	0.56
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.74	0.56
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.88	0.56
1:A:931:ASN:O	1:A:932:TYR:HB2	2.05	0.55
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.88	0.55
1:A:338:MET:HB3	1:A:354:MET:HE2	1.88	0.55
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.88	0.55
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.87	0.55
4:A:1247:MD1:H7	4:A:1247:MD1:C11	2.37	0.55
2:B:372:GLY:HA3	2:B:379:ASP:OD1	2.07	0.55
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.88	0.55
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.42	0.55
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.42	0.55
3:C:1:FME:O1	3:C:3:PHE:HB3	2.07	0.55
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.42	0.55
1:A:220:TYR:CE1	1:A:720:SER:HB2	2.42	0.55
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.88	0.54
1:A:220:TYR:CE2	4:A:1247:MD1:H101	2.43	0.54
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.07	0.54
1:A:309:MET:O	1:A:313:MET:HG3	2.06	0.54
3:C:128:LEU:O	3:C:132:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:581:GLU:OE2	1:A:801:ASP:OD2	2.25	0.54
1:A:662:GLY:HA2	1:A:704:ASN:OD1	2.07	0.54
3:C:83:ILE:HD11	3:C:156:MET:HG2	1.89	0.54
1:A:1132:ASN:ND2	2:B:137:LYS:HE3	2.22	0.54
2:B:370:GLU:HA	2:B:370:GLU:OE2	2.07	0.53
1:A:1086:LEU:HD12	1:A:1224:VAL:HG21	1.90	0.53
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.28	0.53
1:A:1006:ILE:CD1	10:A:1323:HOH:O	2.57	0.53
2:B:450:ALA:HB1	2:B:455:ARG:HD3	1.91	0.53
1:A:795:ASP:HA	1:A:809:LEU:O	2.10	0.52
1:A:223:LEU:O	1:A:225:PRO:HD3	2.09	0.52
1:A:453:HIS:HA	1:A:489:ASP:OD1	2.10	0.52
3:C:181:ALA:HB3	3:C:184:PHE:CD2	2.45	0.52
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.30	0.51
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.10	0.51
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.46	0.51
1:A:282:PRO:HB2	1:A:1158:MET:HE3	1.92	0.51
1:A:767:LEU:HD13	1:A:769:VAL:HG23	1.93	0.51
1:A:679:PRO:HB2	1:A:847:ILE:HD11	1.93	0.51
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.22	0.51
1:A:920:THR:HG23	1:A:920:THR:O	2.12	0.50
1:A:52:ASN:CG	1:A:191:ILE:HG13	2.32	0.50
1:A:856:SER:O	1:A:859:GLU:HG2	2.11	0.50
1:A:490:VAL:O	1:A:500:LYS:HE2	2.11	0.50
3:C:81:LEU:HD23	3:C:81:LEU:N	2.27	0.50
1:A:652:MET:CE	1:A:862:GLN:HE22	2.25	0.50
1:A:739:GLN:NE2	1:A:1177:THR:HG22	2.27	0.50
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.47	0.50
2:B:137:LYS:HA	10:B:585:HOH:O	2.11	0.50
2:B:119:LYS:HD2	2:B:119:LYS:N	2.26	0.50
1:A:473:VAL:HG13	1:A:1045:TYR:HB2	1.93	0.50
1:A:624:THR:O	1:A:627:GLU:HG2	2.12	0.50
1:A:269:GLU:HG3	2:B:15:LYS:HE3	1.94	0.50
2:B:185:GLU:OE1	2:B:353:VAL:HB	2.12	0.49
1:A:1218:ARG:HG3	10:A:1319:HOH:O	2.11	0.49
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.43	0.49
1:A:373:LYS:HD3	1:A:392:PHE:CZ	2.47	0.49
1:A:835:GLU:HG3	1:A:836:VAL:N	2.27	0.49
3:C:160:VAL:O	3:C:164:GLN:HG3	2.12	0.49
1:A:331:ARG:HH11	1:A:331:ARG:HG3	1.78	0.49
2:B:306:PRO:O	2:B:310:GLU:HG3	2.13	0.49
2:B:407:LYS:HZ3	2:B:432:GLU:HG2	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:ASN:O	1:A:373:LYS:HE3	2.13	0.49
2:B:137:LYS:HE2	10:B:591:HOH:O	2.12	0.49
3:C:18:ALA:O	3:C:22:ILE:HG22	2.13	0.49
1:A:107:ARG:HD2	1:A:773:PHE:O	2.12	0.49
1:A:378:ASN:HA	1:A:414:GLU:O	2.13	0.49
3:C:50:LEU:CD1	3:C:54:LEU:HD12	2.43	0.48
1:A:695:ALA:HB1	1:A:704:ASN:HB3	1.95	0.48
1:A:102:LEU:H	1:A:102:LEU:HD12	1.78	0.48
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.61	0.48
2:B:220:TRP:C	2:B:221:ARG:HG3	2.33	0.48
3:C:56:HIS:HA	3:C:59:ILE:HG22	1.94	0.48
1:A:974:LEU:HD21	1:A:1033:ILE:HD13	1.94	0.48
2:B:427:THR:O	2:B:431:GLU:HG3	2.13	0.48
1:A:534:GLY:O	1:A:572:GLY:HA3	2.12	0.48
1:A:497:ASP:HA	1:A:505:ALA:HB2	1.96	0.48
1:A:225:PRO:C	1:A:228:PRO:HD2	2.34	0.48
3:C:80:TRP:C	3:C:81:LEU:HD23	2.34	0.48
3:C:83:ILE:HG23	3:C:84:GLU:N	2.28	0.48
1:A:152:ARG:HB2	1:A:734:THR:CG2	2.43	0.48
1:A:926:LEU:HD22	1:A:930:LEU:CD1	2.44	0.48
1:A:436:GLY:O	1:A:444:LYS:HD3	2.13	0.48
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.96	0.48
4:A:1247:MD1:H7	4:A:1247:MD1:H11	1.94	0.47
1:A:864:LEU:HD22	1:A:864:LEU:N	2.29	0.47
2:B:404:ARG:O	2:B:408:ARG:HG3	2.14	0.47
1:A:387:ASN:HD22	1:A:405:ARG:HB2	1.77	0.47
2:B:331:TYR:CE2	2:B:335:MET:HG3	2.49	0.47
2:B:152:PHE:CE2	2:B:170:SER:HB3	2.49	0.47
1:A:894:ALA:O	1:A:898:ARG:HG3	2.14	0.47
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.50	0.47
1:A:373:LYS:HD3	1:A:392:PHE:CE1	2.49	0.47
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.29	0.47
1:A:1100:THR:O	1:A:1101:TYR:HB2	2.14	0.47
1:A:582:LYS:NZ	1:A:584:ARG:NH1	2.63	0.46
2:B:19:CYS:O	2:B:20:HIS:HB2	2.16	0.46
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.96	0.46
1:A:597:ASP:O	1:A:903:GLY:HA3	2.15	0.46
1:A:384:VAL:HG22	1:A:385:ALA:N	2.29	0.46
1:A:210:GLY:O	1:A:603:ARG:HD2	2.16	0.46
1:A:20:GLY:O	3:C:217:LYS:HD2	2.14	0.46
1:A:54:THR:HA	1:A:580:GLN:HG3	1.96	0.46
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:GLY:HA3	5:A:1248:SF4:S4	2.55	0.46
1:A:24:LEU:HD12	3:C:221:VAL:O	2.16	0.46
1:A:338:MET:HB3	1:A:354:MET:CE	2.45	0.46
1:A:366:GLN:O	1:A:370:PRO:HB3	2.16	0.46
1:A:100:TRP:O	1:A:104:SER:HB3	2.15	0.46
1:A:220:TYR:CE1	1:A:720:SER:CB	2.99	0.46
2:B:224:ILE:HD11	2:B:234:PHE:HB2	1.98	0.46
1:A:289:LYS:O	1:A:289:LYS:HD3	2.16	0.45
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.51	0.45
1:A:308:ALA:O	1:A:311:HIS:HB3	2.16	0.45
1:A:102:LEU:N	1:A:102:LEU:HD12	2.31	0.45
1:A:30:ASP:HB2	2:B:486:GLY:HA2	1.98	0.45
3:C:211:VAL:HG23	3:C:212:GLU:N	2.30	0.45
1:A:832:LYS:O	1:A:836:VAL:HG23	2.17	0.45
2:B:162:ASP:O	2:B:163:ASN:HB2	2.16	0.45
1:A:584:ARG:HD3	1:A:1006:ILE:CD1	2.39	0.45
2:B:26:CYS:SG	2:B:41:PHE:HB2	2.56	0.45
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.82	0.45
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.46	0.45
2:B:123:ILE:HG13	2:B:124:ALA:H	1.82	0.45
2:B:12:ASN:HA	2:B:356:VAL:HB	1.99	0.45
2:B:295:ARG:HA	2:B:295:ARG:HE	1.82	0.45
1:A:191:ILE:HG23	1:A:580:GLN:O	2.17	0.44
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.52	0.44
1:A:239:GLU:HG2	1:A:1022:TYR:HB3	1.98	0.44
1:A:120:MET:O	1:A:138:ILE:HD11	2.17	0.44
1:A:471:THR:HG21	1:A:476:LEU:HD13	1.99	0.44
1:A:81:ARG:CZ	1:A:84:LEU:HD11	2.47	0.44
2:B:482:ASP:OD1	2:B:499:ILE:HG13	2.17	0.44
1:A:349:TYR:CZ	1:A:469:LEU:HD12	2.52	0.44
2:B:156:ALA:HB1	2:B:166:LYS:HD2	1.99	0.44
1:A:1059:LEU:N	1:A:1059:LEU:HD23	2.33	0.44
1:A:578:VAL:CG2	1:A:579:GLY:H	2.21	0.44
1:A:1218:ARG:CD	10:A:1319:HOH:O	2.57	0.44
3:C:11:ILE:C	3:C:13:PRO:HD2	2.38	0.44
3:C:62:ILE:HG23	3:C:66:HIS:CE1	2.53	0.44
1:A:905:LEU:HD22	1:A:909:ILE:HD12	1.99	0.44
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.18	0.43
1:A:658:ALA:HA	1:A:659:PRO:C	2.38	0.43
1:A:94:SER:HB3	1:A:1101:TYR:CD1	2.53	0.43
1:A:425:GLU:O	1:A:457:VAL:HG22	2.18	0.43
1:A:582:LYS:HB2	1:A:801:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:913:GLY:O	1:A:916:ILE:HG12	2.19	0.43
1:A:168:LEU:C	1:A:168:LEU:HD23	2.39	0.43
1:A:1218:ARG:CG	10:A:1319:HOH:O	2.66	0.43
2:B:100:TYR:O	2:B:101:TYR:HB3	2.18	0.43
2:B:231:LYS:HD3	2:B:231:LYS:HA	1.82	0.43
2:B:123:ILE:HG13	2:B:124:ALA:N	2.34	0.43
1:A:854:HIS:O	1:A:855:ASP:HB2	2.18	0.43
1:A:926:LEU:HD22	1:A:930:LEU:HD11	2.00	0.42
1:A:314:LEU:O	1:A:318:HIS:HB2	2.19	0.42
2:B:169:TYR:OH	2:B:386:PRO:HB3	2.19	0.42
1:A:545:ASN:OD1	1:A:550:LEU:HD12	2.18	0.42
1:A:190:PRO:HD3	1:A:714:SER:HB2	2.01	0.42
1:A:541:GLY:HA3	4:A:1251:MD1:O1B	2.20	0.42
1:A:487:LEU:CD1	1:A:487:LEU:N	2.82	0.42
1:A:305:MET:O	1:A:309:MET:HG3	2.19	0.42
2:B:374:ASN:HA	2:B:414:HIS:CD2	2.55	0.42
2:B:508:THR:O	2:B:509:GLU:CB	2.67	0.42
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.34	0.42
1:A:432:PRO:HD3	1:A:632:MET:CE	2.50	0.42
1:A:367:GLU:HG3	1:A:368:ASN:N	2.35	0.42
3:C:212:GLU:HG3	3:C:213:TYR:N	2.35	0.42
1:A:196:MET:CE	1:A:799:THR:HG23	2.50	0.42
1:A:1177:THR:O	1:A:1178:GLN:HB2	2.19	0.42
1:A:861:ALA:HB3	1:A:1200:GLY:O	2.19	0.42
1:A:199:TYR:C	1:A:199:TYR:CD1	2.93	0.42
1:A:862:GLN:HA	1:A:863:PRO:HD2	1.93	0.41
1:A:54:THR:HA	1:A:580:GLN:CG	2.50	0.41
3:C:13:PRO:HB3	3:C:192:MET:SD	2.60	0.41
2:B:137:LYS:CE	10:B:591:HOH:O	2.66	0.41
1:A:701:ASN:ND2	1:A:704:ASN:ND2	2.68	0.41
3:C:188:LEU:HD22	9:C:807:HEM:HMB3	2.02	0.41
1:A:360:LEU:HD22	1:A:360:LEU:H	1.84	0.41
1:A:767:LEU:CD1	1:A:769:VAL:HG23	2.50	0.41
1:A:685:LYS:O	1:A:689:GLU:HG3	2.20	0.41
2:B:248:TYR:CG	2:B:249:PRO:HD3	2.55	0.41
1:A:992:GLU:HG2	1:A:1007:ILE:HD11	2.02	0.41
1:A:1059:LEU:HD23	1:A:1059:LEU:H	1.85	0.41
2:B:280:ILE:HG23	2:B:350:LEU:HD12	2.03	0.41
3:C:144:ILE:N	3:C:145:PRO:HD2	2.35	0.41
1:A:182:PRO:HD2	1:A:665:PRO:HG2	2.02	0.41
1:A:542:ALA:HB3	4:A:1251:MD1:O3B	2.21	0.41
1:A:806:ILE:O	1:A:806:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:764:LYS:CE	10:A:1328:HOH:O	2.67	0.41
1:A:329:TYR:CD1	1:A:565:GLY:HA2	2.55	0.41
3:C:184:PHE:O	3:C:188:LEU:HG	2.21	0.41
2:B:272:VAL:CG1	2:B:273:LEU:N	2.83	0.41
2:B:246:PHE:HA	5:B:803:SF4:S4	2.60	0.41
3:C:77:TYR:CB	3:C:81:LEU:HD21	2.51	0.41
1:A:289:LYS:C	1:A:289:LYS:HD3	2.41	0.41
1:A:756:TRP:CG	1:A:757:GLN:N	2.89	0.41
2:B:157:LYS:HB3	2:B:157:LYS:HE2	1.78	0.41
1:A:286:GLU:OE1	2:B:147:ASP:OD1	2.39	0.41
1:A:403:GLU:O	1:A:405:ARG:N	2.54	0.41
1:A:591:PRO:HA	1:A:596:LEU:HB2	2.01	0.41
1:A:590:GLN:N	1:A:591:PRO:HD2	2.36	0.41
3:C:60:LEU:O	3:C:64:VAL:HG23	2.21	0.41
1:A:227:SER:HB3	1:A:228:PRO:CD	2.46	0.41
1:A:536:SER:HB2	1:A:566:CYS:SG	2.61	0.41
1:A:992:GLU:CG	1:A:1007:ILE:HD11	2.50	0.40
1:A:111:PRO:HA	1:A:787:PRO:HD3	2.03	0.40
1:A:222:ASP:O	1:A:224:PRO:HD3	2.21	0.40
3:C:50:LEU:CD1	3:C:54:LEU:CD1	3.00	0.40
1:A:379:THR:HG21	1:A:414:GLU:OE2	2.21	0.40
2:B:32:SER:HB2	10:B:556:HOH:O	2.22	0.40
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.54	0.40
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.21	0.40
1:A:307:LEU:HD13	1:A:502:TYR:CD2	2.56	0.40
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.56	0.40
1:A:307:LEU:HD13	1:A:502:TYR:CE2	2.56	0.40
1:A:646:ASN:O	1:A:650:GLU:HG3	2.22	0.40
1:A:173:ASN:O	1:A:177:ILE:HG13	2.21	0.40
1:A:25:LEU:HD11	3:C:220:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

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	1238/1247 (99%)	1149 (93%)	78 (6%)	11 (1%)	25	42
2	B	507/512 (99%)	486 (96%)	19 (4%)	2 (0%)	43	66
3	C	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
All	All	1968/1984 (99%)	1845 (94%)	110 (6%)	13 (1%)	30	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	A	721	GLY
1	A	1166	GLU
1	A	578	VAL
2	B	101	TYR
1	A	190	PRO
1	A	224	PRO
1	A	361	VAL
1	A	502	TYR
1	A	718	GLY
1	A	1217	ASN
2	B	368	ALA
1	A	191	ILE

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	1037/1044 (99%)	1017 (98%)	20 (2%)	69	90
2	B	436/439 (99%)	425 (98%)	11 (2%)	60	85
3	C	184/186 (99%)	179 (97%)	5 (3%)	57	83
All	All	1657/1669 (99%)	1621 (98%)	36 (2%)	64	88

All (36) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	338	MET
1	A	366	GLN
1	A	367	GLU
1	A	476	LEU
1	A	515	ARG
1	A	581	GLU
1	A	600	ARG
1	A	601	PRO
1	A	629	LEU
1	A	808	PRO
1	A	864	LEU
1	A	926	LEU
1	A	936	GLU
1	A	995	ARG
1	A	1041	ARG
1	A	1233	LEU
1	A	1238	ASN
1	A	1243	GLU
2	B	37	GLU
2	B	42	ASN
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	295	ARG
2	B	323	GLU
2	B	428	ARG
3	C	36	ARG
3	C	81	LEU
3	C	142	LEU
3	C	147	SER
3	C	212	GLU

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	37	GLN
1	A	173	ASN
1	A	234	GLN

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Mol	Chain	Res	Type
1	A	387	ASN
1	A	461	GLN
1	A	517	GLN
1	A	559	ASN
1	A	599	GLN
1	A	704	ASN
1	A	708	ASN
1	A	759	ASN
1	A	946	ASN
1	A	1076	GLN
1	A	1082	GLN
1	A	1098	HIS
2	B	20	HIS
2	B	160	ASN
2	B	414	HIS
2	B	451	ASN
3	C	53	ASN
3	C	149	GLN
3	C	175	GLN
3	C	225	HIS

5.3.3 RNA ⓘ

There are no RNA 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	5.94	4 (44%)	6,9,11	1.61	1 (16%)

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	16.13	1.22	1.11
3	C	1	FME	CB-CA	-6.03	1.48	1.53
3	C	1	FME	CA-C	3.65	1.55	1.48
3	C	1	FME	CB-CG	2.15	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	2.89	127.75	122.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	1247	6	51,51,51	3.77	16 (31%)	64,78,78	2.73	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	A	1248	1	12,12,12	8.18	12 (100%)	0,24,24	0.00	-
7	AGA	A	1249	-	24,24,29	1.18	3 (12%)	29,29,35	1.49	3 (10%)
4	MD1	A	1251	6	51,51,51	3.55	18 (35%)	64,78,78	2.45	15 (23%)
5	SF4	B	802	2	12,12,12	7.74	12 (100%)	0,24,24	0.00	-
5	SF4	B	803	2	12,12,12	10.83	12 (100%)	0,24,24	0.00	-
5	SF4	B	804	2	12,12,12	7.09	12 (100%)	0,24,24	0.00	-
8	F3S	B	805	2	3,9,9	8.77	3 (100%)	0,15,15	0.00	-
9	HEM	C	806	3	49,50,50	4.33	20 (40%)	46,82,82	1.45	4 (8%)
9	HEM	C	807	3	49,50,50	4.53	23 (46%)	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	1247	6	-	0/22/59/59	0/1/5/5
5	SF4	A	1248	1	-	0/0/48/48	0/0/5/5
7	AGA	A	1249	-	-	0/26/26/34	0/0/0/0
4	MD1	A	1251	6	-	0/22/59/59	0/1/5/5
5	SF4	B	802	2	-	0/0/48/48	0/0/5/5
5	SF4	B	803	2	-	0/0/48/48	0/0/5/5
5	SF4	B	804	2	-	0/0/48/48	0/0/5/5
8	F3S	B	805	2	-	0/0/24/24	0/0/3/3
9	HEM	C	806	3	-	0/14/114/114	0/0/8/8
9	HEM	C	807	3	-	0/14/114/114	0/0/8/8

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1247	MD1	C7-N8	22.20	1.50	1.27
4	A	1251	MD1	C7-N8	20.99	1.49	1.27
9	C	807	HEM	C2D-C1D	18.56	1.49	1.44
9	C	806	HEM	C3D-C4D	17.68	1.49	1.44
5	B	803	SF4	S2-FE3	-16.82	2.21	2.33
9	C	807	HEM	C2B-C1B	14.35	1.48	1.44
9	C	806	HEM	C2D-C1D	13.64	1.48	1.44
5	B	803	SF4	S1-FE2	-13.51	2.24	2.33
5	B	803	SF4	S4-FE1	-12.75	2.24	2.33
9	C	807	HEM	C3D-C4D	12.60	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	SF4	S2-FE1	-12.38	2.24	2.33
5	B	803	SF4	S1-FE4	-12.38	2.24	2.33
9	C	806	HEM	C2B-C1B	12.32	1.47	1.44
5	B	802	SF4	S4-FE1	-12.19	2.25	2.33
5	B	803	SF4	S2-FE4	-12.15	2.25	2.33
5	B	804	SF4	S2-FE4	-11.30	2.25	2.33
8	B	805	F3S	S3-FE3	-10.88	2.25	2.33
5	B	802	SF4	S4-FE2	-10.78	2.26	2.33
5	A	1248	SF4	S2-FE1	-10.42	2.26	2.33
5	A	1248	SF4	S3-FE4	-10.07	2.26	2.33
5	B	802	SF4	S3-FE2	-9.59	2.26	2.33
5	A	1248	SF4	S2-FE3	-9.46	2.26	2.33
5	B	804	SF4	S2-FE1	-9.46	2.26	2.33
5	A	1248	SF4	S3-FE2	-9.23	2.27	2.33
5	B	804	SF4	S4-FE3	-9.01	2.27	2.33
5	B	803	SF4	S4-FE3	-8.92	2.27	2.33
5	B	803	SF4	S3-FE2	-8.88	2.27	2.33
5	B	802	SF4	S1-FE2	-8.80	2.27	2.33
5	B	804	SF4	S2-FE3	-8.74	2.27	2.33
5	A	1248	SF4	S4-FE1	-8.62	2.27	2.33
5	B	802	SF4	S4-FE3	-8.58	2.27	2.33
5	A	1248	SF4	S2-FE4	-8.22	2.27	2.33
5	B	804	SF4	S4-FE2	-7.99	2.27	2.33
8	B	805	F3S	S3-FE1	-7.95	2.27	2.33
4	A	1251	MD1	C11-C12	7.86	1.59	1.50
5	A	1248	SF4	S4-FE3	-7.81	2.28	2.33
5	A	1248	SF4	S3-FE1	-7.77	2.28	2.33
4	A	1247	MD1	C11-C12	7.65	1.59	1.50
5	B	804	SF4	S3-FE1	-7.65	2.28	2.33
5	B	803	SF4	S3-FE4	-7.38	2.28	2.33
5	A	1248	SF4	S1-FE2	-7.20	2.28	2.33
5	B	803	SF4	S4-FE2	-7.09	2.28	2.33
5	A	1248	SF4	S4-FE2	-7.04	2.28	2.33
8	B	805	F3S	S3-FE4	-7.00	2.28	2.33
5	B	802	SF4	S3-FE4	-6.82	2.28	2.33
5	B	803	SF4	S1-FE3	-6.73	2.28	2.33
5	B	802	SF4	S1-FE3	-6.25	2.29	2.33
9	C	807	HEM	C4A-C3A	6.24	1.48	1.40
5	A	1248	SF4	S1-FE3	-6.23	2.29	2.33
9	C	807	HEM	C3B-CAB	6.23	1.60	1.40
4	A	1247	MD1	C13-C12	6.09	1.43	1.34
5	B	802	SF4	S2-FE1	-6.06	2.29	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	804	SF4	S1-FE3	-5.84	2.29	2.33
9	C	806	HEM	C3B-CAB	5.79	1.58	1.40
5	B	802	SF4	S3-FE1	-5.40	2.29	2.33
9	C	806	HEM	C4A-C3A	5.34	1.46	1.40
9	C	806	HEM	C3C-CAC	5.31	1.57	1.40
9	C	807	HEM	C3C-CAC	5.17	1.56	1.40
4	A	1247	MD1	C16-C20	4.93	1.48	1.40
5	B	802	SF4	S1-FE4	-4.81	2.30	2.33
9	C	806	HEM	C3D-C2D	-4.76	1.35	1.43
9	C	806	HEM	C3C-C2C	-4.55	1.35	1.43
9	C	807	HEM	C3D-C2D	-4.51	1.35	1.43
5	B	802	SF4	S2-FE3	-4.48	2.30	2.33
5	B	804	SF4	S1-FE4	-4.35	2.30	2.33
9	C	807	HEM	C3C-C2C	-4.24	1.36	1.43
5	B	804	SF4	S1-FE2	-4.24	2.30	2.33
5	B	803	SF4	S3-FE1	-4.20	2.30	2.33
5	B	802	SF4	S2-FE4	-4.05	2.30	2.33
7	A	1249	AGA	P1-O5	3.96	1.58	1.51
5	A	1248	SF4	S1-FE4	-3.95	2.30	2.33
5	B	804	SF4	S4-FE1	-3.83	2.30	2.33
9	C	806	HEM	C3B-C2B	-3.82	1.37	1.43
5	B	804	SF4	S3-FE4	-3.64	2.30	2.33
4	A	1251	MD1	C6-N1	3.60	1.43	1.37
9	C	807	HEM	C3B-C2B	-3.59	1.37	1.43
9	C	807	HEM	CMC-C2C	3.40	1.58	1.47
4	A	1251	MD1	C13-C12	3.33	1.39	1.34
9	C	806	HEM	CMC-C2C	3.31	1.57	1.47
4	A	1251	MD1	C20-N18	3.22	1.40	1.35
9	C	807	HEM	CMB-C2B	3.15	1.57	1.47
4	A	1251	MD1	C15-N17	3.09	1.42	1.37
4	A	1247	MD1	C15-N17	3.07	1.42	1.37
9	C	806	HEM	CMD-C2D	3.05	1.56	1.47
9	C	807	HEM	CMD-C2D	3.01	1.56	1.47
9	C	807	HEM	CAA-C2A	3.01	1.57	1.52
4	A	1247	MD1	C20-N18	3.00	1.39	1.35
4	A	1247	MD1	C14-C13	2.95	1.55	1.51
4	A	1247	MD1	C6-N1	2.95	1.42	1.37
4	A	1247	MD1	C17-N17	2.94	1.41	1.36
9	C	806	HEM	CMB-C2B	2.93	1.56	1.47
4	A	1247	MD1	C4-N3	2.85	1.40	1.35
9	C	806	HEM	CHB-C1B	2.83	1.39	1.35
4	A	1251	MD1	C17-N18	2.77	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1251	MD1	C17-N17	2.77	1.41	1.36
9	C	806	HEM	CMA-C3A	2.70	1.57	1.51
9	C	806	HEM	CHA-C4D	2.69	1.39	1.35
9	C	807	HEM	CHB-C1B	2.68	1.39	1.35
4	A	1251	MD1	C8-N9	2.67	1.40	1.36
9	C	807	HEM	CHA-C4D	2.64	1.39	1.35
4	A	1251	MD1	C15-C16	2.63	1.46	1.41
4	A	1251	MD1	C16-C20	2.63	1.44	1.40
4	A	1247	MD1	C2-N1	2.60	1.40	1.36
9	C	807	HEM	CAD-CBD	2.59	1.59	1.52
4	A	1251	MD1	C20-N8	2.56	1.41	1.37
9	C	806	HEM	C3B-C4B	2.54	1.47	1.44
4	A	1251	MD1	C2-N1	2.53	1.40	1.36
4	A	1251	MD1	PA-O3B	-2.53	1.55	1.59
5	B	804	SF4	S3-FE2	-2.52	2.31	2.33
9	C	807	HEM	C3B-C4B	2.51	1.47	1.44
4	A	1247	MD1	C17-N18	2.50	1.36	1.33
7	A	1249	AGA	C8-C7	2.49	1.58	1.50
9	C	806	HEM	CAD-CBD	2.44	1.59	1.52
4	A	1251	MD1	O11-C11	2.38	1.48	1.42
9	C	807	HEM	FE-NC	2.38	2.06	1.97
4	A	1251	MD1	C6-C5	2.35	1.45	1.41
9	C	806	HEM	FE-NC	2.35	2.06	1.97
4	A	1247	MD1	C2-N3	2.32	1.36	1.33
4	A	1247	MD1	C10-C11	2.32	1.55	1.51
9	C	807	HEM	C1A-C2A	2.30	1.47	1.43
4	A	1247	MD1	C8-N9	2.30	1.40	1.36
9	C	807	HEM	C4C-NC	2.24	1.41	1.38
9	C	807	HEM	CBA-CGA	2.22	1.56	1.50
9	C	807	HEM	CMA-C3A	2.22	1.56	1.51
4	A	1251	MD1	C4-N3	2.15	1.39	1.35
4	A	1251	MD1	C2-N3	2.14	1.36	1.33
4	A	1247	MD1	C20-N8	2.13	1.41	1.37
9	C	806	HEM	CAA-C2A	2.07	1.55	1.52
9	C	807	HEM	CBD-CGD	2.06	1.55	1.50
9	C	806	HEM	C1A-C2A	2.03	1.47	1.43
7	A	1249	AGA	P1-O4	2.02	1.55	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1247	MD1	C6-C5-N7	-18.50	131.65	134.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1251	MD1	C6-C5-N7	-13.12	132.37	134.14
4	A	1251	MD1	C14-C7-N8	-8.39	104.71	124.80
9	C	806	HEM	C3B-C4B-NB	-5.46	110.09	114.00
9	C	807	HEM	C3B-C4B-NB	-5.18	110.30	114.00
7	A	1249	AGA	C9-C8-C7	4.79	132.28	113.51
4	A	1251	MD1	O4'-C1'-N9	4.69	112.81	108.44
7	A	1249	AGA	C14-C13-C12	4.58	131.45	113.51
4	A	1247	MD1	O4'-C1'-N9	-4.10	104.63	108.44
4	A	1247	MD1	C14-C7-N8	-3.88	115.50	124.80
4	A	1251	MD1	PA-O3B-PB	3.50	141.94	131.68
9	C	807	HEM	CMA-C3A-C4A	-3.34	123.49	128.62
4	A	1247	MD1	C6-N1-C2	3.22	125.15	119.51
4	A	1247	MD1	C8-N9-C4	-3.20	104.46	106.90
4	A	1251	MD1	C8-N9-C1'	3.15	132.59	126.38
9	C	806	HEM	CMA-C3A-C4A	-3.13	123.81	128.62
4	A	1251	MD1	C8-N9-C4	-3.06	104.56	106.90
4	A	1247	MD1	C8-N9-C1'	3.03	132.36	126.38
9	C	807	HEM	C2D-C1D-ND	-2.89	109.51	112.93
4	A	1247	MD1	O3A-C10-C11	-2.86	101.64	108.63
4	A	1251	MD1	C10-C11-C12	2.82	115.63	111.51
4	A	1251	MD1	N18-C20-N8	2.69	121.22	116.18
4	A	1251	MD1	N2-C2-N1	2.66	120.79	117.86
4	A	1251	MD1	N16-C17-N17	2.65	120.77	117.86
4	A	1247	MD1	C15-N17-C17	2.62	124.09	119.51
9	C	806	HEM	CMA-C3A-C2A	2.61	129.87	124.94
9	C	807	HEM	CAD-C3D-C4D	-2.61	119.84	124.53
9	C	807	HEM	CMA-C3A-C2A	2.59	129.83	124.94
4	A	1247	MD1	N17-C17-N18	-2.42	118.39	121.78
4	A	1251	MD1	C6-N1-C2	2.40	123.71	119.51
9	C	806	HEM	C2D-C1D-ND	-2.39	110.11	112.93
7	A	1249	AGA	O5-P1-O4	-2.38	107.26	112.73
4	A	1251	MD1	O3B-PB-O3A	-2.30	93.10	103.41
9	C	807	HEM	CAD-C3D-C2D	2.24	132.22	127.25
4	A	1251	MD1	C1'-N9-C4	-2.19	122.84	126.64
4	A	1251	MD1	C2-N3-C4	2.11	118.06	115.09
4	A	1251	MD1	C15-C16-C20	2.10	119.42	114.53
4	A	1247	MD1	N18-C20-N8	2.05	120.02	116.18
4	A	1247	MD1	C13-C14-N15	-2.00	104.24	111.53

There are no chirality outliers.

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, 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	1242/1247 (99%)	-0.34	12 (0%) 79 81	20, 36, 56, 73	0
2	B	509/512 (99%)	-0.56	4 (0%) 83 84	18, 30, 45, 68	0
3	C	225/225 (100%)	-0.10	10 (4%) 33 34	26, 41, 67, 87	0
All	All	1976/1984 (99%)	-0.37	26 (1%) 74 76	18, 35, 57, 87	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	75	TRP	7.5
3	C	80	TRP	5.2
1	A	10	PHE	5.1
3	C	76	MET	4.8
3	C	77	TYR	3.7
1	A	11	LYS	3.7
1	A	12	GLN	3.1
3	C	74	HIS	2.9
3	C	67	PHE	2.9
2	B	119	LYS	2.9
1	A	380	ASN	2.8
1	A	7	PHE	2.7
1	A	348	TYR	2.7
3	C	149	GLN	2.6
2	B	70	ILE	2.4
3	C	63	PHE	2.4
2	B	366	ALA	2.4
2	B	370	GLU	2.4
3	C	71	LEU	2.4
3	C	64	VAL	2.4
1	A	346	ASP	2.3
1	A	1244	SER	2.3
1	A	490	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	486	GLY	2.1
1	A	759	ASN	2.0
1	A	674	LYS	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FME	C	1	10/11	0.29	10.17	60,64,72,72	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	6MO	A	1250	1/1	0.20	3.23	67,67,67,67	0
9	HEM	C	806	43/43	0.13	1.18	26,31,35,43	0
7	AGA	A	1249	25/30	0.14	1.03	39,42,55,56	0
9	HEM	C	807	43/43	0.14	0.51	49,52,61,66	0
4	MD1	A	1251	47/47	0.12	0.24	31,47,60,63	0
5	SF4	B	803	8/8	0.10	-0.08	20,22,23,24	0
4	MD1	A	1247	47/47	0.12	-0.21	33,44,62,65	0
8	F3S	B	805	7/7	0.09	-0.91	25,26,28,30	0
5	SF4	B	804	8/8	0.08	-1.88	30,35,36,37	0
5	SF4	A	1248	8/8	0.06	-2.28	30,31,31,34	0
5	SF4	B	802	8/8	0.07	-2.50	25,26,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.