



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:36 PM GMT

PDB ID : 3IR5
Title : Crystal structure of NarGHI mutant NarG-H49C
Authors : Bertero, M.G.; Rothery, R.A.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2009-08-21
Resolution : 2.30 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>

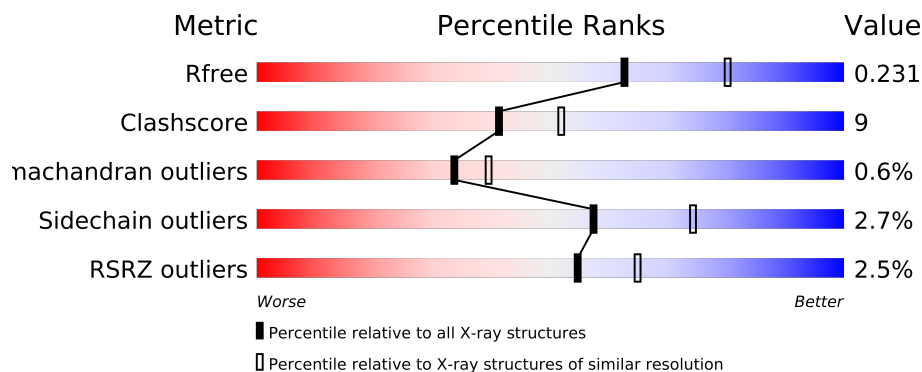
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16376 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
			9865	6229	1729	1858	49			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	CYS	HIS	ENGINEERED	UNP P09152

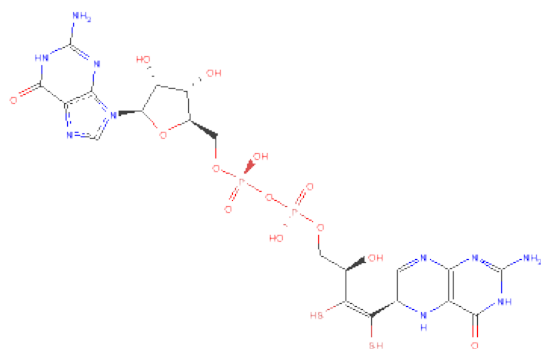
- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

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	220	Total	C	N	O	S	0	0	0
			1747	1158	295	281	13			

- 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).

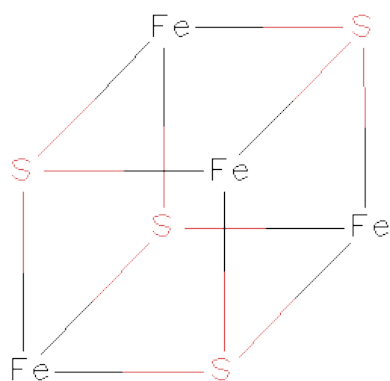


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

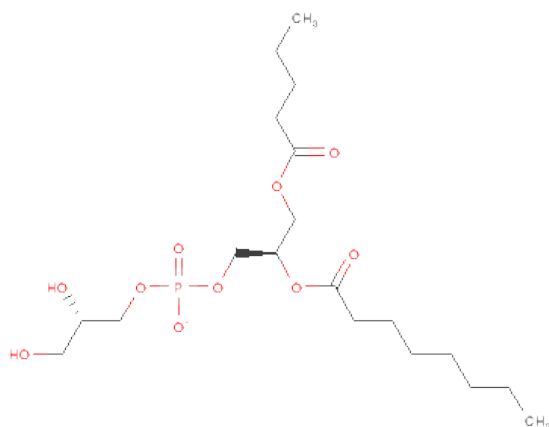
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



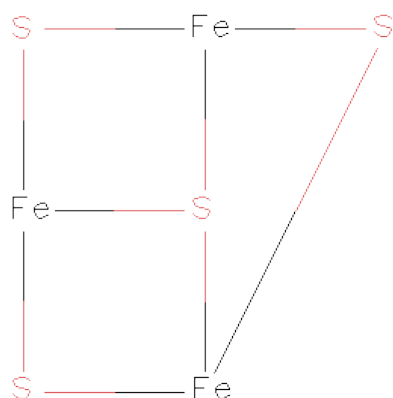
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

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



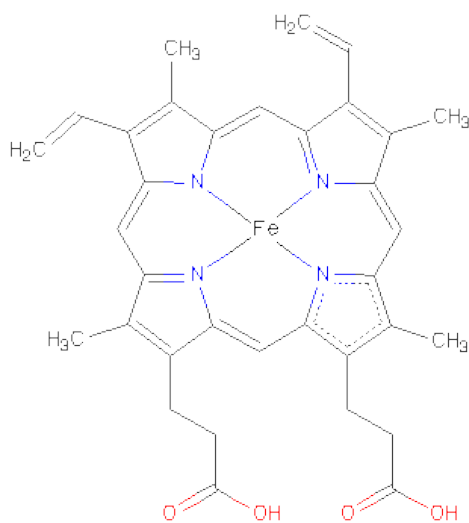
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			25	16	8	1		

- 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		

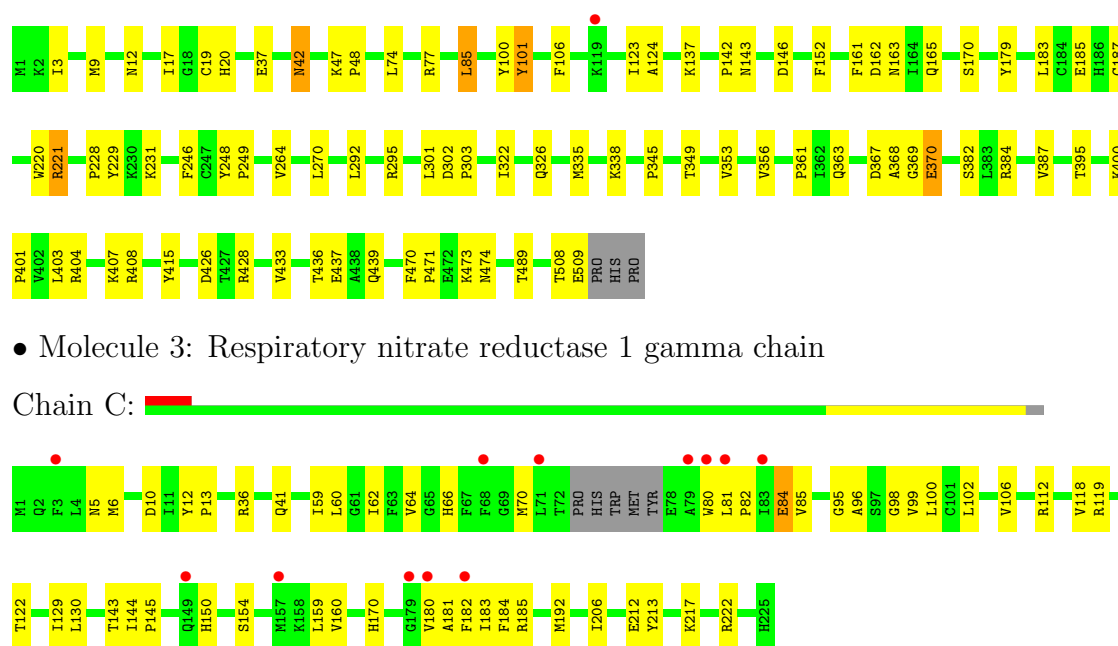
- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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	A	253	Total 253	O 253	0	0
10	B	182	Total 182	O 182	0	0
10	C	34	Total 34	O 34	0	0



- 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	153.45Å 240.69Å 139.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.30 49.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.61-2.30) 99.7 (49.84-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.237 0.196 , 0.231	Depositor DCC
R_{free} test set	6895 reflections (6.43%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.976	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 114166 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16376	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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	0.38	0/10123	0.66	6/13742 (0.0%)
2	B	0.36	0/4146	0.62	0/5609
3	C	0.42	0/1784	0.57	0/2411
All	All	0.38	0/16053	0.64	6/21762 (0.0%)

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	2	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	C-N-CA	12.74	153.56	121.70
1	A	501	ALA	C-N-CA	9.37	145.14	121.70
1	A	1163	HIS	CA-C-N	-6.47	102.95	117.20
1	A	501	ALA	N-CA-CB	6.20	118.78	110.10
1	A	809	LEU	N-CA-C	-5.50	96.15	111.00
1	A	720	SER	N-CA-C	5.13	124.84	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	501	ALA	CA
1	A	502	TYR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	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	9865	0	9522	205	0
2	B	4050	0	3973	56	0
3	C	1747	0	1789	33	0
4	A	94	0	42	11	0
5	A	1	0	0	0	0
6	A	8	0	0	1	0
6	B	24	0	0	2	0
7	A	25	0	29	0	0
8	B	7	0	0	0	0
9	C	86	0	60	3	0
10	A	253	0	0	5	2
10	B	182	0	0	4	0
10	C	34	0	0	0	0
All	All	16376	0	15415	287	2

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 9.

All (287) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:338:MET:HE2	1:A:374:THR:HB	1.58	0.85
1:A:360:LEU:HG	1:A:383:MET:HE3	1.59	0.81
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.66	0.78
1:A:715:ASN:O	1:A:718:GLY:O	2.02	0.77
1:A:345:ARG:HB2	1:A:348:TYR:O	1.86	0.75
2:B:426:ASP:OD2	2:B:428:ARG:HD3	1.88	0.74
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.70	0.72
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.70	0.71
2:B:407:LYS:HD2	10:B:693:HOH:O	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1098:HIS:CE1	4:A:1251:MD1:S13	2.85	0.69
1:A:401:ASN:HA	1:A:1034:PRO:HD3	1.77	0.67
1:A:402:LEU:HD13	1:A:1034:PRO:HB3	1.77	0.66
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.78	0.66
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.77	0.65
1:A:462:LEU:HD12	1:A:466:SER:OG	1.97	0.65
2:B:407:LYS:HG2	2:B:433:VAL:HG11	1.80	0.64
1:A:214:LEU:HB3	1:A:607:SER:OG	1.96	0.64
1:A:750:LYS:HD2	1:A:750:LYS:N	2.13	0.63
1:A:856:SER:O	1:A:859:GLU:HG2	1.98	0.63
1:A:578:VAL:HG23	1:A:579:GLY:H	1.64	0.63
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.15	0.62
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.80	0.62
1:A:282:PRO:HB2	1:A:1158:MET:HE3	1.80	0.61
1:A:1098:HIS:HE1	4:A:1251:MD1:S13	2.24	0.61
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.82	0.61
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.01	0.61
2:B:137:LYS:HA	10:B:667:HOH:O	2.00	0.61
1:A:191:ILE:HD12	1:A:191:ILE:H	1.65	0.60
2:B:370:GLU:HA	2:B:370:GLU:OE1	2.02	0.60
2:B:187:CYS:HB3	2:B:349:THR:O	2.02	0.60
1:A:223:LEU:O	1:A:225:PRO:HD3	2.00	0.60
1:A:1229:ASN:C	1:A:1230:ILE:HD12	2.22	0.60
2:B:407:LYS:HG2	2:B:433:VAL:CG1	2.31	0.59
1:A:49:CYS:HB3	1:A:791:TRP:CZ3	2.37	0.59
1:A:371:GLU:N	1:A:371:GLU:OE1	2.28	0.59
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.85	0.58
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.03	0.58
1:A:20:GLY:O	3:C:217:LYS:HD2	2.04	0.58
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.86	0.58
2:B:404:ARG:O	2:B:408:ARG:HG3	2.02	0.57
1:A:582:LYS:HD2	10:A:1497:HOH:O	2.04	0.57
1:A:190:PRO:HD3	1:A:714:SER:HB2	1.85	0.57
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.34	0.57
1:A:338:MET:CE	1:A:374:THR:HB	2.31	0.57
3:C:80:TRP:C	3:C:81:LEU:HG	2.24	0.57
1:A:719:SER:HB2	1:A:1099:SER:HB3	1.87	0.57
1:A:508:GLU:OE1	1:A:515:ARG:HD2	2.04	0.56
1:A:116:ARG:HE	1:A:147:SER:CB	2.19	0.56
3:C:6:MET:O	3:C:10:ASP:HB2	2.06	0.56
1:A:515:ARG:HG2	1:A:516:SER:N	2.20	0.56
3:C:96:ALA:O	3:C:100:LEU:HD13	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:362:ASP:C	1:A:364:LEU:N	2.58	0.56
1:A:336:MET:HA	1:A:473:VAL:HB	1.88	0.55
1:A:750:LYS:CD	1:A:750:LYS:N	2.69	0.55
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.40	0.55
2:B:367:ASP:C	2:B:369:GLY:H	2.10	0.55
3:C:180:VAL:HG22	3:C:184:PHE:CD2	2.42	0.55
1:A:220:TYR:HD1	10:A:1469:HOH:O	1.90	0.55
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.89	0.55
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.88	0.55
1:A:1098:HIS:CE1	4:A:1247:MD1:S12	3.00	0.54
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.27	0.54
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.90	0.54
1:A:974:LEU:HD21	1:A:1033:ILE:HD13	1.88	0.54
1:A:417:LEU:O	1:A:472:THR:HG21	2.06	0.54
1:A:500:LYS:O	1:A:502:TYR:N	2.41	0.54
1:A:225:PRO:HB2	1:A:551:ASP:OD1	2.07	0.54
4:A:1247:MD1:H7	4:A:1247:MD1:C11	2.38	0.54
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.90	0.54
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.88	0.54
3:C:13:PRO:HG3	3:C:192:MET:SD	2.48	0.53
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.77	0.53
1:A:299:GLN:NE2	1:A:1158:MET:HB3	2.24	0.53
1:A:499:VAL:O	1:A:500:LYS:HG2	2.07	0.53
1:A:457:VAL:HG21	1:A:469:LEU:HD22	1.90	0.53
1:A:402:LEU:CD1	1:A:1034:PRO:HB3	2.38	0.53
3:C:181:ALA:HB3	3:C:184:PHE:CD2	2.43	0.53
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.44	0.53
1:A:368:ASN:ND2	1:A:396:GLU:HG2	2.24	0.53
1:A:191:ILE:O	1:A:194:MET:HG2	2.07	0.53
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.42	0.53
3:C:60:LEU:O	3:C:64:VAL:HG23	2.09	0.53
2:B:246:PHE:HA	6:B:803:SF4:S4	2.48	0.52
1:A:457:VAL:CG2	1:A:469:LEU:HD22	2.39	0.52
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.90	0.52
3:C:181:ALA:HB3	3:C:184:PHE:CE2	2.44	0.52
1:A:54:THR:HA	1:A:580:GLN:HG3	1.91	0.52
1:A:68:VAL:HB	1:A:102:LEU:HD22	1.91	0.52
1:A:578:VAL:HG23	1:A:579:GLY:N	2.25	0.51
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.10	0.51
1:A:331:ARG:HH11	1:A:331:ARG:HG3	1.76	0.51
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.45	0.51
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:804:PRO:O	1:A:1006:ILE:HG13	2.11	0.51
2:B:19:CYS:O	2:B:20:HIS:HB2	2.10	0.51
1:A:119:LYS:O	1:A:123:GLU:HG3	2.10	0.51
1:A:360:LEU:CG	1:A:383:MET:HE3	2.36	0.51
1:A:1100:THR:O	1:A:1101:TYR:HB2	2.10	0.51
1:A:191:ILE:O	1:A:191:ILE:HG22	2.10	0.51
1:A:662:GLY:HA2	1:A:704:ASN:OD1	2.11	0.51
1:A:100:TRP:O	1:A:104:SER:HB3	2.10	0.51
1:A:864:LEU:N	1:A:864:LEU:HD22	2.25	0.50
1:A:914:LYS:O	1:A:914:LYS:HG2	2.11	0.50
1:A:338:MET:HE3	1:A:375:VAL:C	2.31	0.50
1:A:1243:GLU:O	1:A:1244:SER:O	2.29	0.50
1:A:371:GLU:H	1:A:371:GLU:CD	2.12	0.50
3:C:119:ARG:O	3:C:122:THR:HG22	2.11	0.50
4:A:1247:MD1:O11	4:A:1247:MD1:H7	2.12	0.50
1:A:400:TRP:CE2	1:A:1034:PRO:HG2	2.47	0.50
1:A:634:ASP:OD1	1:A:637:ARG:HG3	2.12	0.50
1:A:515:ARG:HG2	1:A:516:SER:H	1.77	0.50
1:A:49:CYS:HA	1:A:791:TRP:CE3	2.46	0.49
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.47	0.49
1:A:582:LYS:NZ	1:A:584:ARG:NH1	2.60	0.49
3:C:12:TYR:HB3	3:C:13:PRO:HD3	1.94	0.49
1:A:931:ASN:O	1:A:932:TYR:HB2	2.11	0.49
1:A:1093:GLN:HB3	1:A:1162:TYR:HB3	1.93	0.49
2:B:100:TYR:O	2:B:101:TYR:HB3	2.11	0.49
1:A:116:ARG:HE	1:A:147:SER:HB2	1.76	0.49
1:A:652:MET:CE	1:A:862:GLN:HE22	2.26	0.49
1:A:168:LEU:O	1:A:168:LEU:HD23	2.13	0.49
1:A:328:ASP:CG	1:A:332:ARG:HE	2.16	0.49
3:C:183:ILE:HG23	3:C:184:PHE:N	2.28	0.49
1:A:487:LEU:CD1	1:A:487:LEU:N	2.76	0.49
1:A:411:GLU:HG3	1:A:412:GLU:N	2.27	0.49
1:A:624:THR:O	1:A:627:GLU:HG2	2.12	0.48
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.95	0.48
3:C:102:LEU:O	3:C:106:VAL:HG23	2.14	0.48
1:A:220:TYR:CE1	4:A:1247:MD1:H101	2.49	0.48
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.96	0.48
1:A:490:VAL:O	1:A:500:LYS:HE2	2.14	0.48
2:B:363:GLN:HG2	2:B:382:SER:O	2.14	0.48
3:C:70:MET:HG2	3:C:160:VAL:HG22	1.96	0.48
1:A:1100:THR:OG1	4:A:1247:MD1:H5'1	2.14	0.47
3:C:59:ILE:HD13	9:C:806:HEM:HAC	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:220:TRP:C	2:B:221:ARG:HG3	2.34	0.47
1:A:695:ALA:HB1	1:A:704:ASN:HB3	1.96	0.47
1:A:1177:THR:O	1:A:1178:GLN:HB2	2.15	0.47
1:A:1132:ASN:ND2	2:B:137:LYS:HE2	2.28	0.47
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.15	0.47
1:A:378:ASN:OD1	1:A:382:GLU:HB2	2.15	0.47
3:C:84:GLU:HG3	3:C:85:VAL:N	2.29	0.47
1:A:1098:HIS:CE1	4:A:1251:MD1:H15	2.33	0.47
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.29	0.47
1:A:173:ASN:O	1:A:177:ILE:HG13	2.14	0.47
3:C:150:HIS:HB3	3:C:154:SER:HG	1.80	0.47
1:A:578:VAL:CG2	1:A:579:GLY:H	2.26	0.47
1:A:1062:ARG:HD2	10:A:1476:HOH:O	2.14	0.47
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.50	0.47
2:B:3:ILE:HG12	2:B:301:LEU:CD1	2.45	0.47
1:A:1070:VAL:HG13	1:A:1223:VAL:CG2	2.45	0.46
2:B:248:TYR:CG	2:B:249:PRO:HD3	2.50	0.46
1:A:1183:ILE:HG13	1:A:1185:ASN:H	1.79	0.46
1:A:33:ASP:O	1:A:37:GLN:HG3	2.16	0.46
2:B:335:MET:O	2:B:338:LYS:HE3	2.15	0.46
2:B:367:ASP:C	2:B:369:GLY:N	2.69	0.46
3:C:150:HIS:HB3	3:C:154:SER:OG	2.15	0.46
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.51	0.46
2:B:162:ASP:O	2:B:163:ASN:HB2	2.16	0.46
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.46	0.46
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.50	0.46
1:A:611:PHE:CD2	1:A:727:MET:HE1	2.51	0.46
1:A:279:ALA:HB2	1:A:291:CYS:SG	2.56	0.45
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.50	0.45
1:A:536:SER:HB2	1:A:566:CYS:SG	2.57	0.45
1:A:373:LYS:HD3	1:A:392:PHE:CE1	2.52	0.45
1:A:644:ASP:OD2	1:A:751:PRO:HB2	2.17	0.45
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.82	0.45
1:A:791:TRP:HZ3	1:A:1101:TYR:HH	1.62	0.45
1:A:1230:ILE:N	1:A:1230:ILE:HD12	2.32	0.45
3:C:182:PHE:O	3:C:185:ARG:N	2.50	0.45
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.37	0.45
2:B:295:ARG:HA	2:B:295:ARG:HD2	1.81	0.45
2:B:228:PRO:HG2	2:B:229:TYR:CD1	2.52	0.45
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.52	0.44
3:C:143:THR:HB	3:C:184:PHE:CE1	2.51	0.44
1:A:307:LEU:HD13	1:A:502:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.17	0.44
1:A:1084:LYS:HB2	1:A:1127:LEU:HD21	1.99	0.44
1:A:487:LEU:N	1:A:487:LEU:HD12	2.33	0.44
1:A:641:HIS:O	1:A:644:ASP:HB2	2.17	0.44
1:A:384:VAL:HG22	1:A:385:ALA:N	2.33	0.44
2:B:9:MET:HE2	2:B:270:LEU:HD21	2.00	0.44
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.44
1:A:1068:ARG:HG3	1:A:1068:ARG:HH21	1.82	0.44
1:A:362:ASP:C	1:A:364:LEU:H	2.20	0.44
1:A:425:GLU:O	1:A:457:VAL:HG22	2.18	0.44
1:A:336:MET:N	1:A:337:PRO:HD2	2.33	0.44
1:A:729:LYS:HD3	1:A:730:TYR:CE1	2.53	0.44
1:A:6:ARG:O	1:A:9:TYR:N	2.49	0.44
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.82	0.43
2:B:302:ASP:HA	2:B:303:PRO:HD2	1.88	0.43
1:A:894:ALA:O	1:A:898:ARG:HG3	2.16	0.43
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.47	0.43
1:A:1152:GLN:OE1	2:B:170:SER:HA	2.19	0.43
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.18	0.43
1:A:584:ARG:HD3	1:A:1006:ILE:HG12	1.99	0.43
1:A:876:LEU:HD23	1:A:876:LEU:C	2.39	0.43
1:A:56:SER:HB2	1:A:800:SER:HB2	1.99	0.43
1:A:338:MET:CE	1:A:374:THR:CB	2.97	0.43
1:A:582:LYS:HZ2	1:A:584:ARG:HG2	1.83	0.43
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.54	0.43
3:C:95:GLY:O	3:C:99:VAL:HG23	2.19	0.43
1:A:1028:ASN:HA	1:A:1033:ILE:O	2.18	0.43
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.83	0.43
2:B:42:ASN:HB2	6:B:803:SF4:S1	2.59	0.42
1:A:652:MET:HE3	1:A:862:GLN:HE22	1.83	0.42
1:A:286:GLU:HG2	2:B:179:TYR:OH	2.19	0.42
1:A:591:PRO:HA	1:A:596:LEU:HB2	2.00	0.42
1:A:308:ALA:HB2	1:A:507:ALA:HB2	2.00	0.42
1:A:155:GLY:HA2	10:B:619:HOH:O	2.18	0.42
1:A:26:ASN:HB3	10:A:1496:HOH:O	2.18	0.42
1:A:219:TRP:HB2	1:A:607:SER:HB2	2.01	0.42
1:A:268:THR:HA	1:A:271:ARG:HD3	2.00	0.42
2:B:12:ASN:HA	2:B:356:VAL:HB	2.01	0.42
1:A:772:ASP:C	1:A:788:THR:HG22	2.40	0.42
1:A:55:GLY:HA3	6:A:1249:SF4:S3	2.59	0.42
2:B:387:VAL:HG21	2:B:403:LEU:HG	2.01	0.42
2:B:508:THR:O	2:B:509:GLU:CB	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:41:GLN:HB2	9:C:806:HEM:O1A	2.20	0.42
1:A:1208:PHE:O	1:A:1209:ASN:HB2	2.19	0.42
1:A:5:ASP:OD2	2:B:489:THR:HG23	2.19	0.42
3:C:129:ILE:CG2	3:C:130:LEU:N	2.82	0.42
1:A:1006:ILE:CD1	1:A:1016:GLU:CD	2.88	0.42
1:A:525:PHE:CZ	1:A:536:SER:HB3	2.55	0.42
1:A:340:VAL:O	1:A:470:VAL:HA	2.19	0.42
1:A:1023:ASN:O	1:A:1026:TYR:HB2	2.20	0.42
1:A:862:GLN:HA	1:A:863:PRO:HD2	1.85	0.42
1:A:803:HIS:HB2	1:A:804:PRO:HD2	2.01	0.42
1:A:1037:THR:HA	1:A:1203:HIS:HB3	2.02	0.42
1:A:705:HIS:HD2	1:A:764:LYS:HB3	1.83	0.41
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.55	0.41
1:A:199:TYR:C	1:A:199:TYR:CD1	2.92	0.41
1:A:27:THR:HG23	3:C:222:ARG:HD3	2.01	0.41
1:A:116:ARG:HG3	1:A:120:MET:HE2	2.02	0.41
2:B:292:LEU:HD13	2:B:345:PRO:O	2.20	0.41
1:A:724:HIS:O	1:A:728:LEU:HD13	2.20	0.41
1:A:194:MET:HA	1:A:798:ASN:ND2	2.35	0.41
1:A:1006:ILE:HD13	1:A:1016:GLU:HG3	2.01	0.41
1:A:51:VAL:HB	1:A:791:TRP:CZ2	2.55	0.41
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.45	0.41
2:B:400:LYS:HB3	2:B:401:PRO:HD3	2.03	0.41
1:A:1091:PRO:O	1:A:1162:TYR:HA	2.20	0.41
1:A:54:THR:HA	1:A:580:GLN:CG	2.51	0.41
1:A:658:ALA:HA	1:A:659:PRO:C	2.40	0.41
1:A:934:LYS:HD3	1:A:944:MET:SD	2.60	0.41
1:A:1068:ARG:HG3	1:A:1068:ARG:NH2	2.35	0.41
2:B:185:GLU:OE1	2:B:353:VAL:HB	2.21	0.41
1:A:574:TRP:CZ2	1:A:576:HIS:HB2	2.55	0.41
1:A:489:ASP:HB3	1:A:492:CYS:SG	2.60	0.41
2:B:407:LYS:HG3	10:B:639:HOH:O	2.21	0.41
1:A:634:ASP:HB3	1:A:637:ARG:HG3	2.02	0.41
1:A:545:ASN:OD1	1:A:550:LEU:HD12	2.20	0.41
1:A:497:ASP:HA	1:A:505:ALA:HB2	2.03	0.41
2:B:77:ARG:HH11	2:B:77:ARG:HB2	1.86	0.41
2:B:123:ILE:HG13	2:B:124:ALA:H	1.85	0.41
2:B:415:TYR:CE2	2:B:437:GLU:HG2	2.55	0.41
4:A:1247:MD1:O11	4:A:1247:MD1:C7	2.69	0.41
1:A:336:MET:HB3	1:A:474:TYR:HB2	2.02	0.41
1:A:218:ASP:N	1:A:218:ASP:OD2	2.54	0.41
1:A:289:LYS:O	1:A:289:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1100:THR:HG1	4:A:1247:MD1:H5'1	1.85	0.41
1:A:261:THR:HG23	2:B:17:ILE:HD12	2.02	0.41
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.55	0.41
1:A:231:TRP:CD1	1:A:1042:GLN:HG2	2.56	0.41
3:C:159:LEU:H	3:C:159:LEU:HD22	1.86	0.41
2:B:101:TYR:CZ	2:B:142:PRO:HD3	2.56	0.40
1:A:378:ASN:OD1	1:A:382:GLU:N	2.54	0.40
2:B:508:THR:O	2:B:509:GLU:HB3	2.20	0.40
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.36	0.40
2:B:231:LYS:HD3	2:B:231:LYS:HA	1.73	0.40
1:A:152:ARG:HB2	1:A:734:THR:CG2	2.51	0.40
2:B:436:THR:OG1	2:B:439:GLN:HG3	2.21	0.40
3:C:12:TYR:N	3:C:13:PRO:CD	2.84	0.40
1:A:1048:HIS:O	1:A:1049:GLN:C	2.59	0.40
2:B:322:ILE:O	2:B:326:GLN:HG3	2.22	0.40
1:A:191:ILE:HA	1:A:192:PRO:HD2	1.97	0.40
1:A:37:GLN:HB3	10:A:1450:HOH:O	2.22	0.40
2:B:47:LYS:HA	2:B:48:PRO:C	2.41	0.40
1:A:806:ILE:HG23	1:A:806:ILE:O	2.21	0.40
3:C:112:ARG:HA	3:C:118:VAL:CG1	2.51	0.40
1:A:717:LEU:HG	1:A:778:THR:HG23	2.03	0.40
1:A:363:ALA:O	1:A:366:GLN:HB2	2.22	0.40
1:A:713:ARG:HA	4:A:1247:MD1:C4	2.51	0.40
1:A:307:LEU:HD13	1:A:502:TYR:CE2	2.56	0.40
1:A:696:ALA:O	1:A:699:PRO:HD3	2.22	0.40
3:C:62:ILE:HD11	3:C:98:GLY:HA2	2.03	0.40

All (2) 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)
10:A:1489:HOH:O	10:A:1489:HOH:O[3_354]	1.16	1.04
10:A:1450:HOH:O	10:A:1450:HOH:O[3_354]	1.59	0.61

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%)	1162 (94%)	71 (6%)	9 (1%)	30	34
2	B	507/512 (99%)	492 (97%)	13 (3%)	2 (0%)	43	52
3	C	216/225 (96%)	202 (94%)	14 (6%)	0	100	100
All	All	1965/1984 (99%)	1856 (94%)	98 (5%)	11 (1%)	33	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	A	502	TYR
1	A	1166	GLU
1	A	578	VAL
1	A	1164	ALA
1	A	720	SER
2	B	101	TYR
1	A	191	ILE
1	A	224	PRO
2	B	368	ALA
1	A	195	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1039/1044 (100%)	1009 (97%)	30 (3%)	55	71
2	B	436/439 (99%)	427 (98%)	9 (2%)	66	83
3	C	180/186 (97%)	175 (97%)	5 (3%)	56	73
All	All	1655/1669 (99%)	1611 (97%)	44 (3%)	57	74

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	94	ARG
1	A	371	GLU
1	A	383	MET

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Mol	Chain	Res	Type
1	A	402	LEU
1	A	461	GLN
1	A	467	THR
1	A	476	LEU
1	A	483	LEU
1	A	502	TYR
1	A	515	ARG
1	A	533	HIS
1	A	586	GLN
1	A	626	GLU
1	A	663	THR
1	A	673	GLU
1	A	717	LEU
1	A	727	MET
1	A	743	LEU
1	A	750	LYS
1	A	767	LEU
1	A	808	PRO
1	A	864	LEU
1	A	926	LEU
1	A	1006	ILE
1	A	1041	ARG
1	A	1087	ASN
1	A	1110	LEU
1	A	1233	LEU
1	A	1243	GLU
2	B	37	GLU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU
2	B	161	PHE
2	B	165	GLN
2	B	183	LEU
2	B	221	ARG
2	B	370	GLU
3	C	36	ARG
3	C	66	HIS
3	C	84	GLU
3	C	170	HIS
3	C	212	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	173	ASN
1	A	234	GLN
1	A	461	GLN
1	A	517	GLN
1	A	559	ASN
1	A	599	GLN
1	A	708	ASN
1	A	946	ASN
1	A	1098	HIS
2	B	143	ASN
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	6.23	4 (44%)	6,9,11	1.58	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	16.61	1.22	1.11
3	C	1	FME	CB-CA	-7.32	1.47	1.53
3	C	1	FME	CA-C	3.25	1.54	1.48
3	C	1	FME	CA-N	-2.27	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	2.24	126.68	122.97
3	C	1	FME	CB-CA-N	2.22	115.12	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 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	5	51,51,51	3.79	15 (29%)	64,78,78	2.75	11 (17%)
6	SF4	A	1249	1	12,12,12	8.09	12 (100%)	0,24,24	0.00	-
7	AGA	A	1250	-	24,24,29	0.92	2 (8%)	29,29,35	1.51	3 (10%)
4	MD1	A	1251	5	51,51,51	3.54	17 (33%)	64,78,78	2.54	11 (17%)
6	SF4	B	802	2	12,12,12	7.26	12 (100%)	0,24,24	0.00	-
6	SF4	B	803	2	12,12,12	8.71	12 (100%)	0,24,24	0.00	-
6	SF4	B	804	2	12,12,12	6.47	12 (100%)	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	F3S	B	805	2	3,9,9	7.97	3 (100%)	0,15,15	0.00	-
9	HEM	C	806	3	49,50,50	3.63	18 (36%)	46,82,82	1.47	6 (13%)
9	HEM	C	807	3	49,50,50	4.67	23 (46%)	46,82,82	1.52	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	5	-	0/22/59/59	0/1/5/5
6	SF4	A	1249	1	-	0/0/48/48	0/0/5/5
7	AGA	A	1250	-	-	0/26/26/34	0/0/0/0
4	MD1	A	1251	5	-	0/22/59/59	0/1/5/5
6	SF4	B	802	2	-	0/0/48/48	0/0/5/5
6	SF4	B	803	2	-	0/0/48/48	0/0/5/5
6	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 (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1247	MD1	C7-N8	22.05	1.50	1.27
4	A	1251	MD1	C7-N8	20.40	1.49	1.27
9	C	807	HEM	C2D-C1D	19.45	1.49	1.44
6	B	802	SF4	S4-FE1	-14.02	2.23	2.33
9	C	807	HEM	C3D-C4D	14.00	1.48	1.44
9	C	807	HEM	C2B-C1B	13.93	1.48	1.44
6	B	803	SF4	S2-FE3	-13.03	2.24	2.33
9	C	806	HEM	C3D-C4D	12.20	1.47	1.44
9	C	806	HEM	C2B-C1B	11.88	1.47	1.44
6	B	803	SF4	S2-FE4	-11.04	2.25	2.33
6	A	1249	SF4	S2-FE1	-10.85	2.26	2.33
6	B	803	SF4	S1-FE2	-10.66	2.26	2.33
6	B	804	SF4	S2-FE1	-10.39	2.26	2.33
6	B	803	SF4	S4-FE1	-10.28	2.26	2.33
9	C	806	HEM	C2D-C1D	10.07	1.47	1.44
6	B	804	SF4	S2-FE3	-9.77	2.26	2.33
6	A	1249	SF4	S2-FE4	-9.69	2.26	2.33
6	B	804	SF4	S2-FE4	-9.55	2.26	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1249	SF4	S2-FE3	-9.49	2.26	2.33
8	B	805	F3S	S3-FE4	-9.29	2.27	2.33
6	B	803	SF4	S2-FE1	-9.28	2.27	2.33
6	A	1249	SF4	S1-FE2	-9.23	2.27	2.33
4	A	1251	MD1	C11-C12	9.13	1.60	1.50
6	B	803	SF4	S1-FE4	-9.10	2.27	2.33
6	A	1249	SF4	S3-FE4	-8.97	2.27	2.33
6	A	1249	SF4	S4-FE1	-8.78	2.27	2.33
6	B	802	SF4	S1-FE2	-8.73	2.27	2.33
4	A	1247	MD1	C11-C12	8.34	1.59	1.50
6	B	802	SF4	S4-FE3	-8.15	2.27	2.33
6	B	804	SF4	S4-FE3	-7.97	2.27	2.33
6	B	802	SF4	S4-FE2	-7.91	2.27	2.33
6	B	802	SF4	S3-FE2	-7.79	2.28	2.33
6	A	1249	SF4	S3-FE2	-7.76	2.28	2.33
8	B	805	F3S	S3-FE3	-7.68	2.28	2.33
6	B	803	SF4	S4-FE3	-7.48	2.28	2.33
6	A	1249	SF4	S3-FE1	-7.42	2.28	2.33
6	B	803	SF4	S1-FE3	-7.30	2.28	2.33
6	A	1249	SF4	S4-FE3	-7.27	2.28	2.33
8	B	805	F3S	S3-FE1	-6.71	2.28	2.33
6	B	803	SF4	S4-FE2	-6.70	2.28	2.33
9	C	807	HEM	C4A-C3A	6.56	1.48	1.40
6	B	802	SF4	S1-FE3	-6.48	2.28	2.33
6	B	803	SF4	S3-FE4	-6.46	2.28	2.33
9	C	807	HEM	C3B-CAB	6.02	1.59	1.40
9	C	806	HEM	C3B-CAB	5.84	1.58	1.40
4	A	1247	MD1	C13-C12	5.75	1.42	1.34
6	A	1249	SF4	S1-FE4	-5.58	2.29	2.33
6	B	802	SF4	S3-FE1	-5.55	2.29	2.33
6	B	804	SF4	S4-FE2	-5.43	2.29	2.33
6	B	802	SF4	S2-FE3	-5.42	2.29	2.33
4	A	1247	MD1	C16-C20	5.25	1.48	1.40
9	C	806	HEM	C3C-CAC	5.17	1.56	1.40
9	C	807	HEM	C3C-CAC	5.16	1.56	1.40
9	C	806	HEM	C4A-C3A	5.11	1.46	1.40
9	C	806	HEM	C3C-C2C	-5.02	1.35	1.43
6	A	1249	SF4	S4-FE2	-5.00	2.29	2.33
6	B	802	SF4	S3-FE4	-4.80	2.30	2.33
9	C	806	HEM	C3D-C2D	-4.77	1.35	1.43
6	B	804	SF4	S4-FE1	-4.65	2.30	2.33
6	B	804	SF4	S1-FE4	-4.63	2.30	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	802	SF4	S1-FE4	-4.55	2.30	2.33
6	B	804	SF4	S3-FE1	-4.48	2.30	2.33
6	B	802	SF4	S2-FE1	-4.32	2.30	2.33
9	C	807	HEM	C3C-C2C	-4.28	1.36	1.43
6	B	803	SF4	S3-FE2	-4.24	2.30	2.33
9	C	807	HEM	C3D-C2D	-4.03	1.36	1.43
9	C	806	HEM	C3B-C2B	-4.02	1.36	1.43
6	B	804	SF4	S3-FE2	-4.01	2.30	2.33
6	B	803	SF4	S3-FE1	-4.00	2.30	2.33
6	A	1249	SF4	S1-FE3	-3.96	2.30	2.33
9	C	807	HEM	C3B-C2B	-3.95	1.36	1.43
6	B	804	SF4	S1-FE3	-3.79	2.30	2.33
6	B	804	SF4	S1-FE2	-3.76	2.30	2.33
4	A	1251	MD1	PA-O3B	-3.37	1.53	1.59
9	C	806	HEM	CMC-C2C	3.26	1.57	1.47
4	A	1251	MD1	C6-N1	3.24	1.42	1.37
4	A	1247	MD1	C15-N17	3.20	1.42	1.37
9	C	807	HEM	CMC-C2C	3.19	1.57	1.47
4	A	1251	MD1	C2-N3	3.18	1.37	1.33
9	C	807	HEM	CMD-C2D	3.16	1.57	1.47
9	C	807	HEM	CAA-C2A	3.16	1.57	1.52
4	A	1251	MD1	C15-N17	3.13	1.42	1.37
4	A	1247	MD1	C17-N17	3.06	1.41	1.36
4	A	1247	MD1	C4-N3	3.04	1.40	1.35
9	C	806	HEM	CMB-C2B	3.02	1.56	1.47
9	C	807	HEM	CMB-C2B	3.02	1.56	1.47
9	C	807	HEM	C3B-C4B	2.97	1.48	1.44
4	A	1247	MD1	C2-N3	2.95	1.37	1.33
9	C	806	HEM	CMD-C2D	2.95	1.56	1.47
4	A	1247	MD1	C20-N18	2.81	1.39	1.35
4	A	1251	MD1	C15-C16	2.79	1.46	1.41
9	C	807	HEM	CHB-C1B	2.79	1.39	1.35
4	A	1251	MD1	C13-C12	2.77	1.38	1.34
4	A	1251	MD1	C16-C20	2.77	1.45	1.40
4	A	1251	MD1	C20-N18	2.75	1.39	1.35
9	C	807	HEM	CAD-CBD	2.67	1.59	1.52
4	A	1247	MD1	C6-N1	2.67	1.41	1.37
9	C	806	HEM	C3B-C4B	2.64	1.47	1.44
4	A	1247	MD1	C2-N1	2.63	1.40	1.36
9	C	806	HEM	CHA-C4D	2.61	1.39	1.35
7	A	1250	AGA	P1-O5	2.57	1.56	1.51
9	C	807	HEM	C1A-C2A	2.55	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	804	SF4	S3-FE4	-2.52	2.31	2.33
9	C	806	HEM	CMA-C3A	2.46	1.56	1.51
4	A	1251	MD1	C8-N9	2.45	1.40	1.36
4	A	1247	MD1	C8-N9	2.45	1.40	1.36
6	B	802	SF4	S2-FE4	-2.44	2.31	2.33
4	A	1251	MD1	C6-C5	2.43	1.45	1.41
9	C	807	HEM	CHA-C4D	2.43	1.39	1.35
9	C	807	HEM	CMA-C3A	2.41	1.56	1.51
4	A	1251	MD1	C17-N17	2.41	1.40	1.36
4	A	1251	MD1	O11-C11	2.39	1.48	1.42
9	C	807	HEM	FE-NC	2.37	2.06	1.97
9	C	807	HEM	C4C-NC	2.37	1.41	1.38
7	A	1250	AGA	C8-C7	2.36	1.57	1.50
9	C	806	HEM	CHB-C1B	2.34	1.39	1.35
4	A	1251	MD1	C17-N18	2.28	1.36	1.33
4	A	1247	MD1	C17-N18	2.27	1.36	1.33
9	C	807	HEM	CBA-CGA	2.26	1.56	1.50
4	A	1247	MD1	C10-C11	2.23	1.55	1.51
4	A	1247	MD1	C20-N8	2.23	1.41	1.37
9	C	807	HEM	CBD-CGD	2.20	1.56	1.50
4	A	1251	MD1	C20-N8	2.18	1.41	1.37
9	C	806	HEM	CAD-CBD	2.14	1.58	1.52
4	A	1251	MD1	C4-N3	2.10	1.39	1.35
9	C	806	HEM	FE-NC	2.05	2.05	1.97

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1247	MD1	C6-C5-N7	-18.62	131.63	134.14
4	A	1251	MD1	C6-C5-N7	-14.42	132.20	134.14
4	A	1251	MD1	C14-C7-N8	-8.31	104.89	124.80
9	C	807	HEM	C3B-C4B-NB	-5.47	110.09	114.00
9	C	806	HEM	C3B-C4B-NB	-5.42	110.12	114.00
4	A	1251	MD1	O4'-C1'-N9	4.71	112.82	108.44
7	A	1250	AGA	C14-C13-C12	4.66	131.78	113.51
7	A	1250	AGA	C9-C8-C7	4.64	131.69	113.51
4	A	1247	MD1	C14-C7-N8	-3.96	115.33	124.80
4	A	1247	MD1	O4'-C1'-N9	-3.92	104.79	108.44
4	A	1251	MD1	PA-O3B-PB	3.63	142.33	131.68
9	C	807	HEM	CMA-C3A-C4A	-3.49	123.26	128.62
4	A	1251	MD1	C8-N9-C4	-3.33	104.36	106.90
4	A	1247	MD1	C8-N9-C4	-3.28	104.39	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1251	MD1	C10-C11-C12	3.20	116.18	111.51
9	C	806	HEM	CMA-C3A-C4A	-3.18	123.73	128.62
4	A	1247	MD1	C6-N1-C2	3.17	125.05	119.51
4	A	1247	MD1	C8-N9-C1'	3.09	132.48	126.38
4	A	1247	MD1	O3A-C10-C11	-3.08	101.09	108.63
9	C	807	HEM	C2D-C1D-ND	-2.89	109.52	112.93
9	C	807	HEM	CMA-C3A-C2A	2.87	130.36	124.94
4	A	1251	MD1	C8-N9-C1'	2.76	131.83	126.38
4	A	1251	MD1	N16-C17-N17	2.73	120.87	117.86
4	A	1247	MD1	C15-N17-C17	2.65	124.15	119.51
9	C	806	HEM	CMA-C3A-C2A	2.61	129.87	124.94
9	C	807	HEM	CAD-C3D-C4D	-2.57	119.90	124.53
9	C	806	HEM	C2D-C1D-ND	-2.42	110.07	112.93
4	A	1251	MD1	N18-C20-N8	2.38	120.64	116.18
4	A	1247	MD1	N17-C17-N18	-2.37	118.46	121.78
4	A	1251	MD1	O3B-PB-O3A	-2.33	92.97	103.41
4	A	1251	MD1	C6-N1-C2	2.28	123.49	119.51
4	A	1247	MD1	C13-C14-N15	-2.23	103.42	111.53
9	C	807	HEM	CAD-C3D-C2D	2.16	132.05	127.25
9	C	806	HEM	CAD-C3D-C4D	-2.15	120.66	124.53
7	A	1250	AGA	O5-P1-O4	-2.12	107.85	112.73
4	A	1247	MD1	C1'-N9-C4	-2.03	123.13	126.64
9	C	806	HEM	O1D-CGD-CBD	-2.01	116.12	123.03

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	1244/1247 (99%)	-0.11	37 (2%) 48 58	19, 34, 49, 58	0
2	B	509/512 (99%)	-0.47	1 (0%) 93 97	19, 28, 41, 57	0
3	C	220/225 (97%)	-0.06	12 (5%) 24 33	22, 39, 53, 58	0
All	All	1973/1984 (99%)	-0.20	50 (2%) 54 65	19, 33, 49, 58	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	80	TRP	6.6
1	A	10	PHE	6.1
1	A	9	TYR	6.0
3	C	79	ALA	4.2
1	A	460	LEU	3.6
1	A	348	TYR	3.6
3	C	71	LEU	3.5
2	B	119	LYS	3.5
1	A	221	CYS	3.5
3	C	182	PHE	3.4
1	A	7	PHE	3.3
1	A	461	GLN	3.2
3	C	81	LEU	3.1
1	A	11	LYS	3.0
1	A	717	LEU	2.9
1	A	223	LEU	2.8
1	A	462	LEU	2.8
1	A	346	ASP	2.8
1	A	759	ASN	2.8
3	C	180	VAL	2.7
1	A	679	PRO	2.7
3	C	179	GLY	2.6
3	C	83	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	3	PHE	2.5
1	A	347	GLY	2.5
1	A	8	ARG	2.5
1	A	486	GLY	2.4
1	A	225	PRO	2.4
1	A	220	TYR	2.4
1	A	465	GLY	2.4
1	A	875	ASP	2.3
1	A	1243	GLU	2.3
3	C	68	PHE	2.3
1	A	55	GLY	2.2
1	A	361	VAL	2.2
1	A	488	ASN	2.2
1	A	1215	GLY	2.2
3	C	149	GLN	2.1
1	A	349	TYR	2.1
1	A	719	SER	2.1
1	A	469	LEU	2.1
1	A	228	PRO	2.1
1	A	1244	SER	2.1
3	C	157	MET	2.1
1	A	578	VAL	2.1
1	A	676	GLY	2.1
1	A	674	LYS	2.1
1	A	459	ARG	2.0
1	A	467	THR	2.0
1	A	675	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, 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	0.28	1.52	53,57,63,64	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
7	AGA	A	1250	25/30	0.15	1.55	34,38,47,48	0
9	HEM	C	806	43/43	0.11	0.87	25,28,30,35	0
8	F3S	B	805	7/7	0.13	0.55	26,26,28,28	0
6	SF4	B	803	8/8	0.14	0.54	19,22,24,24	0
9	HEM	C	807	43/43	0.12	0.29	44,46,53,56	0
4	MD1	A	1247	47/47	0.14	-0.41	30,38,58,65	0
4	MD1	A	1251	47/47	0.15	-0.42	26,39,53,56	0
6	SF4	B	802	8/8	0.11	-0.84	26,28,30,32	0
5	6MO	A	1248	1/1	0.15	-0.88	61,61,61,61	0
6	SF4	B	804	8/8	0.09	-1.41	31,35,37,37	0
6	SF4	A	1249	8/8	0.07	-1.97	31,31,33,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.