



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:39 PM GMT

PDB ID : 1Y5N  
Title : The crystal structure of the NarGHI mutant NarI-K86A in complex with pentachlorophenol  
Authors : Bertero, M.G.; Rothery, R.A.; Boroumand, N.; Palak, M.; Blasco, F.; Ginet, N.; Weiner, J.H.; Strynadka, N.C.J.  
Deposited on : 2004-12-02  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

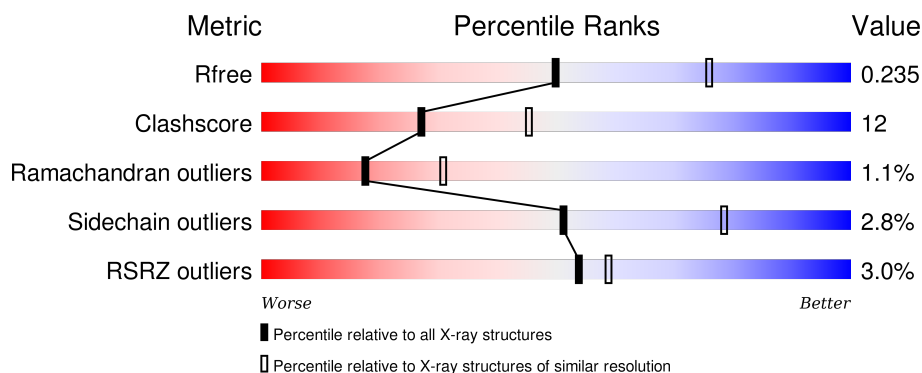
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1246	<div> <div>4%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	B	512	<div> <div>2%</div> <div>83%</div> <div>16%</div> <div>..</div> </div>
3	C	225	<div> <div>3%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	3PH	B	1806	X	-	-	X
11	PCI	C	808	-	-	-	X
7	SF4	A	1801	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15972 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1244	Total	C	N	O	S	0	0	0
			9869	6232	1731	1858	48			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	509	Total	C	N	O	S	0	0	0
			4050	2562	701	755	32			

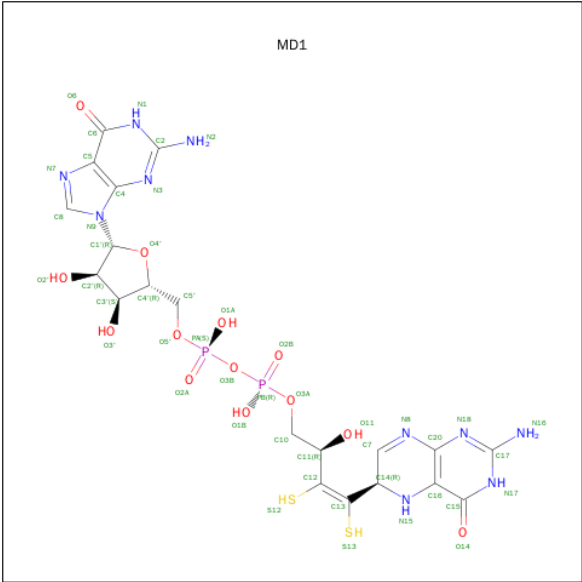
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1719	1138	290	278	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	MET	MODIFIED RESIDUE	UNP P11350
C	86	ALA	LYS	ENGINEERED	UNP P11350

- Molecule 4 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).

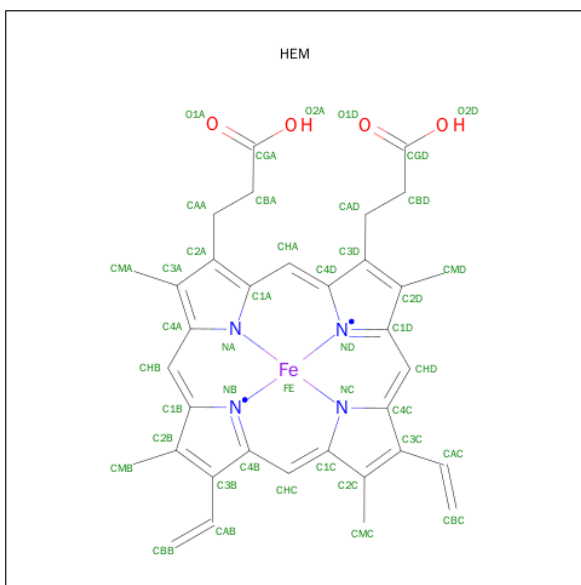


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

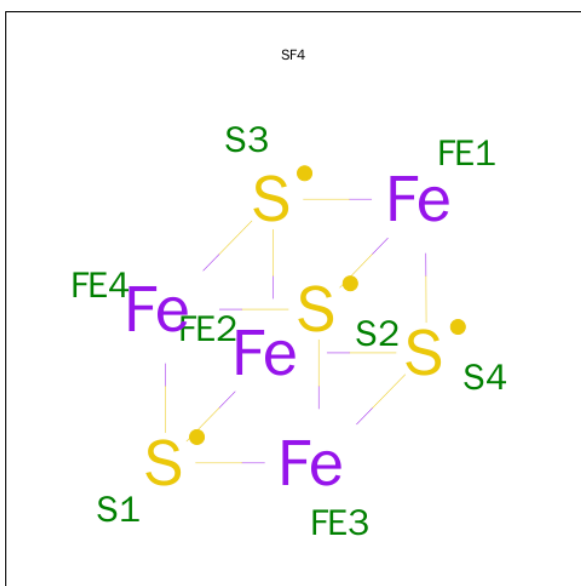
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

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



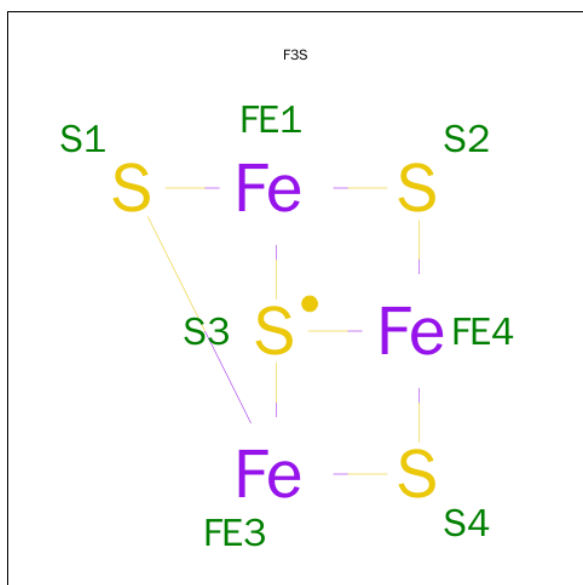
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 8	Fe 4	S 4	0	0
7	B	1	Total 8	Fe 4	S 4	0	0

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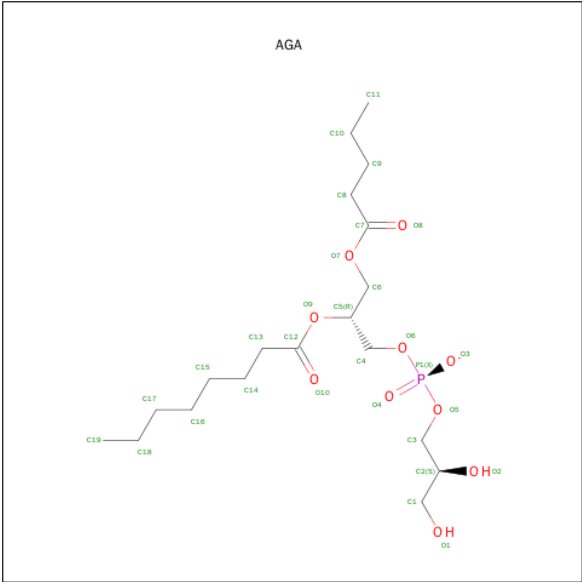
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



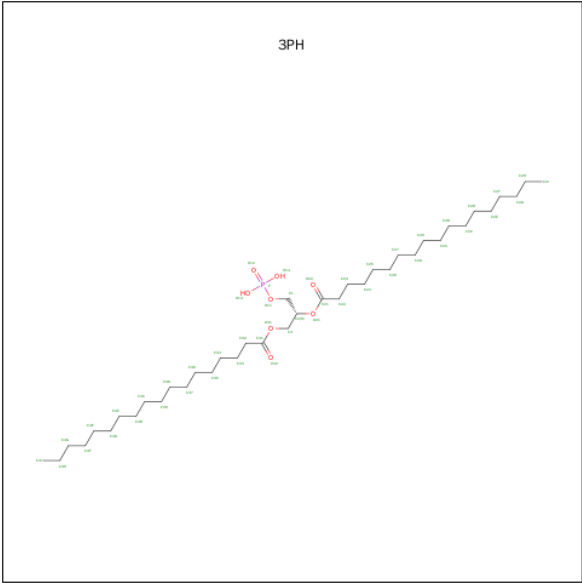
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

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



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

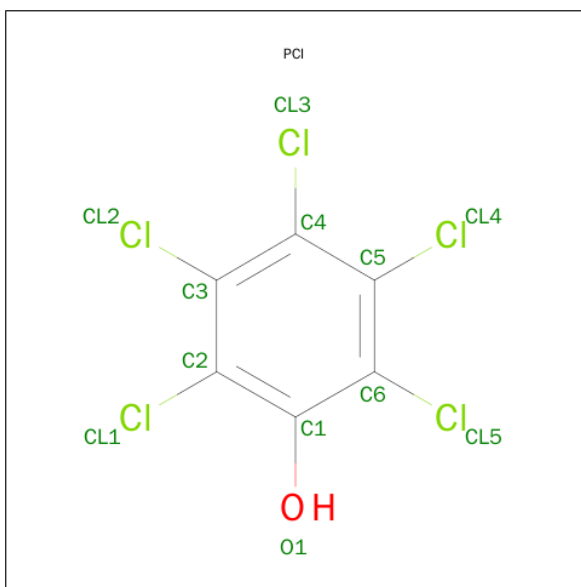
- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



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

- Molecule 11 is PENTACHLOROPHENOL (three-letter code: PCI) (formula: C<sub>6</sub>HCl<sub>5</sub>O).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Cl	O	0	0
			12	6	5	1		

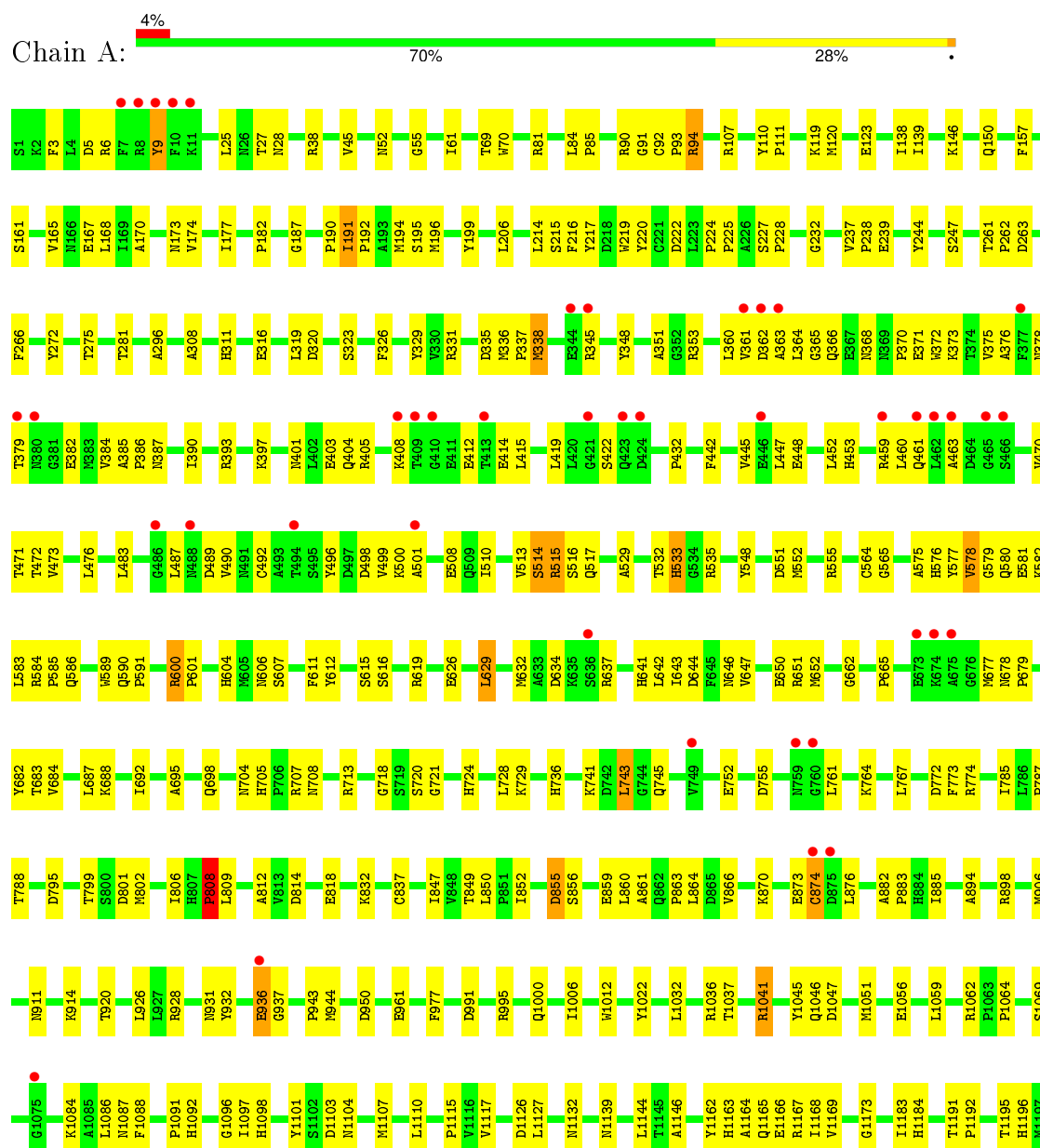
- Molecule 12 is water.

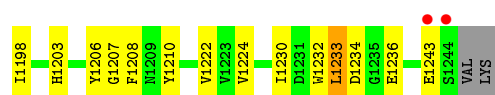
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	23	Total	O	0	0
			23	23		
12	B	29	Total	O	0	0
			29	29		
12	C	2	Total	O	0	0
			2	2		

### 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 ( $\text{RSRZ} > 2$ ). 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.

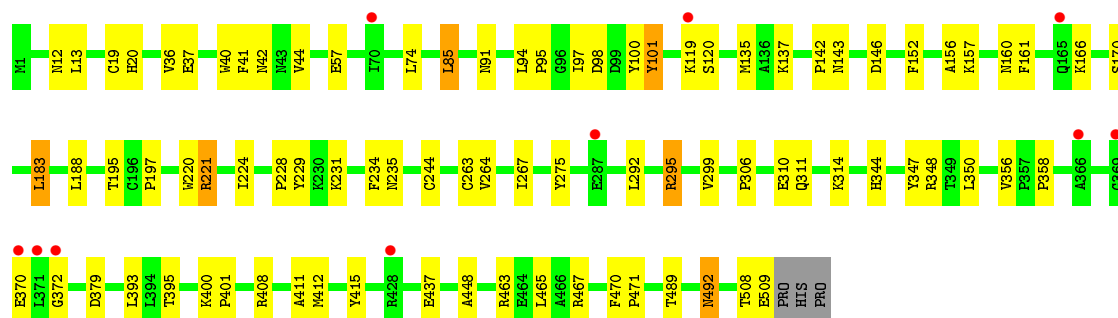
- Molecule 1: Respiratory nitrate reductase 1 alpha chain





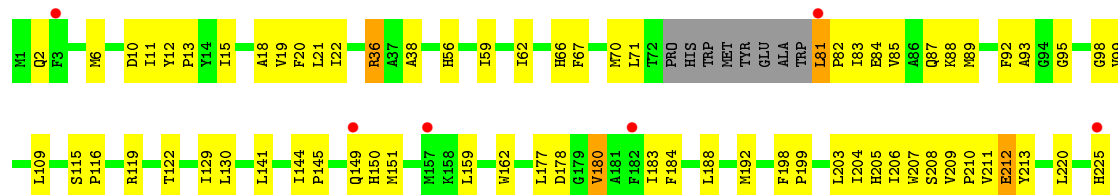
- Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B: 2% 83% 16% ..



- Molecule 3: Respiratory nitrate reductase 1 gamma chain

Chain C: 3% 65% 30% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.26 Å   241.96 Å   140.12 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	24.84 – 2.50 24.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.4 (24.84-2.50) 81.5 (24.84-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.50 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190   ,   0.238 0.189   ,   0.235	Depositor DCC
$R_{free}$ test set	6007 reflections (8.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 73659 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, FME, SF4, AGA, 3PH, F3S, PCI, 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	0.36	0/10128	0.62	0/13749
2	B	0.39	0/4146	0.65	0/5609
3	C	0.39	0/1754	0.58	0/2370
All	All	0.37	0/16028	0.62	0/21728

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9869	0	9527	277	0
2	B	4050	0	3973	60	0
3	C	1719	0	1764	47	0
4	A	94	0	42	8	0
5	A	1	0	0	0	0
6	C	86	0	60	1	0
7	A	8	0	0	2	0
7	B	24	0	0	0	0
8	B	7	0	0	0	0
9	C	30	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	18	0	10	0	0
11	C	12	0	1	0	0
12	A	23	0	0	0	0
12	B	29	0	0	0	0
12	C	2	0	0	0	0
All	All	15972	0	15413	375	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.62	0.81
1:A:578:VAL:HG23	1:A:579:GLY:H	1.46	0.80
1:A:1086:LEU:HD12	1:A:1224:VAL:HG21	1.67	0.77
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.68	0.75
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	1.86	0.73
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.04	0.73
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.71	0.72
3:C:81:LEU:HD23	3:C:81:LEU:N	2.03	0.72
1:A:471:THR:HG23	1:A:476:LEU:HD11	1.70	0.72
1:A:387:ASN:ND2	1:A:405:ARG:HB2	2.05	0.72
1:A:378:ASN:HD21	1:A:382:GLU:HB2	1.54	0.71
1:A:225:PRO:HB2	1:A:551:ASP:OD1	1.91	0.70
1:A:371:GLU:N	1:A:371:GLU:OE1	2.25	0.69
3:C:95:GLY:O	3:C:99:VAL:HG23	1.93	0.69
2:B:91:ASN:HB3	2:B:94:LEU:HB2	1.76	0.67
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.79	0.64
2:B:157:LYS:NZ	2:B:157:LYS:HB3	2.12	0.64
3:C:6:MET:O	3:C:10:ASP:HB2	1.98	0.64
1:A:196:MET:CE	1:A:799:THR:HG23	2.29	0.63
1:A:52:ASN:CG	1:A:191:ILE:HG13	2.19	0.63
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.18	0.63
1:A:1069:SER:O	1:A:1139:ASN:HB2	1.99	0.63
1:A:110:TYR:HD1	1:A:818:GLU:HG3	1.64	0.62
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.81	0.62
1:A:578:VAL:HG23	1:A:579:GLY:N	2.15	0.62
1:A:774:ARG:HH11	4:A:1800:MD1:H3'	1.64	0.61
1:A:1098:HIS:CE1	4:A:1800:MD1:S12	2.93	0.61
2:B:94:LEU:HD12	2:B:95:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:PRO:HB2	2:B:347:TYR:CD2	2.35	0.61
1:A:93:PRO:HG2	1:A:94:ARG:HD3	1.83	0.61
1:A:1163:HIS:HD2	1:A:1184:HIS:NE2	1.98	0.61
1:A:168:LEU:O	1:A:168:LEU:HD23	2.01	0.61
1:A:906:MET:HE3	1:A:911:ASN:HB2	1.81	0.61
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.82	0.60
3:C:12:TYR:N	3:C:13:PRO:HD2	2.16	0.60
1:A:25:LEU:HD11	3:C:220:LEU:HD22	1.84	0.60
1:A:584:ARG:HD3	1:A:1006:ILE:HD13	1.84	0.60
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.01	0.60
1:A:272:TYR:HB3	2:B:412:MET:CE	2.32	0.60
1:A:508:GLU:OE1	1:A:515:ARG:HD2	2.00	0.60
3:C:159:LEU:HD21	3:C:180:VAL:HG21	1.84	0.59
1:A:894:ALA:O	1:A:898:ARG:HG3	2.02	0.59
1:A:1059:LEU:HD23	1:A:1059:LEU:H	1.67	0.59
1:A:1084:LYS:HB2	1:A:1127:LEU:HD21	1.84	0.59
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.83	0.59
1:A:384:VAL:HG22	1:A:385:ALA:N	2.17	0.59
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.82	0.59
1:A:27:THR:HG22	1:A:28:ASN:N	2.17	0.59
1:A:5:ASP:OD2	2:B:489:THR:HG23	2.02	0.59
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.84	0.59
1:A:366:GLN:O	1:A:370:PRO:HB3	2.02	0.59
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.68	0.59
1:A:361:VAL:HA	1:A:463:ALA:HB2	1.85	0.58
1:A:3:PHE:CE1	9:C:309:AGA:H161	2.39	0.58
1:A:360:LEU:N	1:A:360:LEU:HD22	2.19	0.58
1:A:490:VAL:O	1:A:500:LYS:HE2	2.03	0.58
1:A:432:PRO:HD3	1:A:632:MET:HE1	1.86	0.58
1:A:107:ARG:HD2	1:A:773:PHE:O	2.04	0.58
2:B:220:TRP:O	2:B:221:ARG:NH1	2.36	0.58
1:A:684:VAL:HG13	1:A:876:LEU:HD22	1.86	0.58
1:A:110:TYR:CD1	1:A:818:GLU:HG3	2.38	0.58
1:A:498:ASP:OD1	1:A:500:LYS:HG2	2.02	0.58
1:A:353:ARG:CZ	1:A:864:LEU:HD12	2.34	0.57
3:C:204:ILE:HD12	3:C:205:HIS:N	2.18	0.57
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.86	0.57
1:A:772:ASP:C	1:A:788:THR:HG22	2.24	0.57
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.04	0.57
3:C:109:LEU:HD13	3:C:130:LEU:HD23	1.85	0.57
1:A:365:GLY:HA3	1:A:408:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:ILE:O	1:A:647:VAL:HG23	2.03	0.57
1:A:336:MET:HA	1:A:473:VAL:HB	1.86	0.57
1:A:225:PRO:O	1:A:228:PRO:HD2	2.05	0.57
1:A:859:GLU:HG3	1:A:860:LEU:HD12	1.86	0.57
1:A:219:TRP:HB2	1:A:607:SER:HB2	1.87	0.57
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.87	0.56
1:A:471:THR:CG2	1:A:476:LEU:HD11	2.34	0.56
1:A:360:LEU:C	1:A:463:ALA:HB2	2.26	0.56
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.53	0.56
1:A:61:ILE:N	1:A:61:ILE:HD12	2.19	0.56
1:A:366:GLN:HG3	1:A:373:LYS:HZ3	1.69	0.56
4:A:1800:MD1:H7	4:A:1800:MD1:C11	2.36	0.56
1:A:1098:HIS:CE1	4:A:2800:MD1:S13	2.99	0.56
1:A:191:ILE:HD13	1:A:216:PHE:CE1	2.41	0.55
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.41	0.55
1:A:646:ASN:O	1:A:650:GLU:HG3	2.06	0.55
1:A:487:LEU:N	1:A:487:LEU:HD12	2.20	0.55
1:A:345:ARG:HB2	1:A:348:TYR:O	2.06	0.55
1:A:1056:GLU:HG3	1:A:1195:THR:HG21	1.89	0.55
3:C:67:PHE:CE2	3:C:71:LEU:HD12	2.41	0.55
1:A:247:SER:C	1:A:275:THR:HG23	2.27	0.55
1:A:860:LEU:HD12	1:A:860:LEU:N	2.22	0.54
3:C:206:ILE:HD11	6:C:806:HEM:HBC2	1.88	0.54
1:A:931:ASN:O	1:A:932:TYR:HB2	2.07	0.54
1:A:806:ILE:O	1:A:806:ILE:HG23	2.06	0.54
3:C:83:ILE:HG23	3:C:84:GLU:N	2.22	0.54
1:A:873:GLU:O	1:A:874:CYS:HB3	2.07	0.54
1:A:634:ASP:HB3	1:A:637:ARG:HD3	1.90	0.54
3:C:198:PHE:HB3	3:C:199:PRO:CD	2.37	0.54
3:C:62:ILE:HG23	3:C:66:HIS:CE1	2.43	0.54
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.42	0.54
1:A:272:TYR:HB3	2:B:412:MET:HE3	1.89	0.54
1:A:489:ASP:HB3	1:A:492:CYS:HB2	1.89	0.54
1:A:453:HIS:HA	1:A:489:ASP:OD1	2.08	0.54
1:A:460:LEU:HD12	1:A:470:VAL:HG11	1.89	0.54
2:B:465:LEU:O	2:B:467:ARG:HG3	2.08	0.54
1:A:331:ARG:HH11	1:A:331:ARG:HG3	1.72	0.53
3:C:198:PHE:CE1	3:C:203:LEU:HB3	2.43	0.53
3:C:119:ARG:O	3:C:122:THR:HG22	2.07	0.53
1:A:856:SER:O	1:A:859:GLU:HG2	2.07	0.53
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASP:O	1:A:338:MET:HB2	2.08	0.53
1:A:146:LYS:O	1:A:150:GLN:HG3	2.08	0.53
1:A:936:GLU:HG2	1:A:937:GLY:N	2.23	0.53
1:A:351:ALA:HB1	1:A:1045:TYR:OH	2.09	0.53
1:A:170:ALA:O	1:A:174:VAL:HG23	2.09	0.53
1:A:687:LEU:HD23	1:A:692:ILE:O	2.09	0.53
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.09	0.52
1:A:191:ILE:HG23	1:A:580:GLN:O	2.09	0.52
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.73	0.52
1:A:419:LEU:HD11	1:A:471:THR:HA	1.91	0.52
1:A:432:PRO:HD3	1:A:632:MET:CE	2.38	0.52
2:B:292:LEU:HD11	2:B:348:ARG:HG2	1.90	0.52
2:B:19:CYS:O	2:B:20:HIS:HB2	2.08	0.52
1:A:1101:TYR:HB3	1:A:1107:MET:HG3	1.91	0.52
1:A:662:GLY:HA2	1:A:704:ASN:ND2	2.25	0.52
3:C:20:PHE:CD2	3:C:21:LEU:HD23	2.45	0.52
1:A:601:PRO:HG3	1:A:850:LEU:HD22	1.92	0.52
1:A:190:PRO:HD2	1:A:713:ARG:O	2.08	0.52
3:C:198:PHE:HB3	3:C:199:PRO:HD3	1.91	0.52
1:A:1230:ILE:HD12	1:A:1230:ILE:N	2.24	0.52
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.90	0.52
1:A:626:GLU:HA	1:A:629:LEU:HD23	1.92	0.52
1:A:447:LEU:O	1:A:448:GLU:HG2	2.08	0.52
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.92	0.52
3:C:70:MET:O	3:C:71:LEU:HD23	2.09	0.51
1:A:724:HIS:NE2	1:A:1167:ARG:NH1	2.57	0.51
1:A:119:LYS:O	1:A:123:GLU:HG3	2.10	0.51
1:A:239:GLU:HG2	1:A:1022:TYR:HB3	1.92	0.51
2:B:40:TRP:O	2:B:41:PHE:C	2.48	0.51
1:A:387:ASN:HD22	1:A:405:ARG:HB2	1.72	0.51
1:A:360:LEU:HD22	1:A:360:LEU:H	1.75	0.51
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.91	0.51
1:A:552:MET:HE2	1:A:555:ARG:HD3	1.93	0.51
2:B:12:ASN:HA	2:B:356:VAL:HB	1.93	0.51
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.76	0.51
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.92	0.51
1:A:1088:PHE:HB2	1:A:1222:VAL:HG22	1.93	0.51
3:C:56:HIS:HA	3:C:59:ILE:HG22	1.92	0.51
1:A:445:VAL:HG23	1:A:510:ILE:HD11	1.93	0.51
2:B:94:LEU:HD22	2:B:221:ARG:HD3	1.93	0.50
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG22	1:A:70:TRP:HE3	1.77	0.50
1:A:582:LYS:HD3	1:A:801:ASP:HA	1.93	0.50
2:B:57:GLU:OE2	2:B:344:HIS:NE2	2.41	0.50
1:A:191:ILE:O	1:A:194:MET:HG2	2.11	0.50
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.47	0.50
2:B:160:ASN:OD1	2:B:393:LEU:HD13	2.11	0.50
1:A:906:MET:CE	1:A:911:ASN:HB2	2.42	0.50
1:A:361:VAL:HA	1:A:463:ALA:CB	2.41	0.50
2:B:275:TYR:HB2	2:B:299:VAL:HG12	1.94	0.50
2:B:306:PRO:O	2:B:310:GLU:HG3	2.12	0.50
1:A:1059:LEU:N	1:A:1059:LEU:HD23	2.27	0.50
2:B:228:PRO:HG2	2:B:229:TYR:CD1	2.47	0.49
1:A:551:ASP:OD2	1:A:1196:HIS:NE2	2.38	0.49
1:A:45:VAL:HG21	1:A:812:ALA:HA	1.94	0.49
3:C:183:ILE:HG23	3:C:184:PHE:N	2.27	0.49
3:C:56:HIS:O	3:C:59:ILE:HG22	2.13	0.49
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.43	0.49
2:B:415:TYR:CE2	2:B:437:GLU:HG2	2.47	0.49
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.48	0.49
3:C:83:ILE:HG23	3:C:84:GLU:H	1.78	0.49
1:A:729:LYS:HB2	1:A:736:HIS:CG	2.48	0.49
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.95	0.48
1:A:157:PHE:CZ	1:A:785:ILE:HD11	2.48	0.48
1:A:1098:HIS:C	1:A:1164:ALA:CB	2.82	0.48
3:C:13:PRO:HB3	3:C:192:MET:SD	2.52	0.48
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.48	0.48
1:A:168:LEU:C	1:A:168:LEU:HD23	2.34	0.48
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.82	0.48
1:A:28:ASN:HA	3:C:225:HIS:CD2	2.48	0.48
1:A:69:THR:HG22	1:A:70:TRP:CE3	2.49	0.48
1:A:263:ASP:OD2	1:A:802:MET:HG3	2.13	0.48
3:C:2:GLN:O	3:C:6:MET:HG3	2.12	0.48
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.34	0.48
1:A:1167:ARG:HB2	1:A:1183:ILE:CG2	2.44	0.48
1:A:196:MET:HE1	1:A:799:THR:HG23	1.96	0.47
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.49	0.47
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.95	0.47
1:A:225:PRO:C	1:A:228:PRO:HD2	2.34	0.47
1:A:476:LEU:N	1:A:476:LEU:HD12	2.29	0.47
1:A:308:ALA:O	1:A:311:HIS:HB3	2.14	0.47
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:LEU:O	1:A:764:LYS:HE3	2.14	0.47
2:B:157:LYS:HB3	2:B:157:LYS:HZ3	1.79	0.47
3:C:89:MET:O	3:C:93:ALA:N	2.47	0.47
1:A:55:GLY:HA3	7:A:1801:SF4:S3	2.54	0.47
4:A:1800:MD1:H11	4:A:1800:MD1:H7	1.95	0.47
1:A:372:TRP:NE1	1:A:860:LEU:HB3	2.30	0.47
1:A:487:LEU:CD1	1:A:487:LEU:N	2.77	0.47
1:A:707:ARG:C	1:A:708:ASN:HD22	2.18	0.47
2:B:183:LEU:N	2:B:183:LEU:HD23	2.30	0.47
1:A:419:LEU:CD1	1:A:471:THR:HA	2.44	0.47
1:A:372:TRP:CE2	1:A:863:PRO:HB3	2.50	0.47
3:C:11:ILE:C	3:C:13:PRO:HD2	2.35	0.46
1:A:515:ARG:HG2	1:A:516:SER:N	2.29	0.46
1:A:214:LEU:HB3	1:A:607:SER:OG	2.15	0.46
2:B:370:GLU:HA	2:B:370:GLU:OE2	2.14	0.46
2:B:508:THR:O	2:B:509:GLU:HB3	2.15	0.46
1:A:384:VAL:CG2	1:A:385:ALA:N	2.78	0.46
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.50	0.46
1:A:405:ARG:HH12	1:A:412:GLU:HG3	1.80	0.46
2:B:220:TRP:C	2:B:221:ARG:HG3	2.35	0.46
1:A:61:ILE:N	1:A:61:ILE:CD1	2.78	0.46
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.80	0.46
1:A:323:SER:HB3	1:A:326:PHE:HB2	1.98	0.46
1:A:677:MET:HG3	1:A:682:TYR:HB2	1.97	0.46
1:A:220:TYR:CE2	4:A:1800:MD1:H101	2.51	0.46
1:A:876:LEU:HD23	1:A:876:LEU:C	2.34	0.46
1:A:473:VAL:HG13	1:A:1045:TYR:HB2	1.96	0.46
1:A:679:PRO:HB2	1:A:847:ILE:HD11	1.96	0.46
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.51	0.46
1:A:991:ASP:O	1:A:991:ASP:CG	2.54	0.46
1:A:1097:ILE:O	1:A:1098:HIS:HB2	2.16	0.46
1:A:173:ASN:O	1:A:177:ILE:HG13	2.15	0.46
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.31	0.46
1:A:795:ASP:HA	1:A:809:LEU:O	2.16	0.46
1:A:215:SER:OG	1:A:606:ASN:HA	2.16	0.46
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.30	0.46
1:A:1051:MET:HG2	1:A:1198:ILE:CD1	2.46	0.46
1:A:232:GLY:HA2	1:A:1210:TYR:OH	2.17	0.46
1:A:1041:ARG:HH21	1:A:1041:ARG:HG2	1.80	0.45
2:B:492:ASN:HD22	2:B:492:ASN:N	2.14	0.45
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:HIS:HE1	4:A:2800:MD1:S13	2.39	0.45
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.97	0.45
1:A:120:MET:O	1:A:138:ILE:HD11	2.16	0.45
1:A:27:THR:CG2	1:A:28:ASN:N	2.79	0.45
1:A:472:THR:O	1:A:476:LEU:HD13	2.16	0.45
1:A:261:THR:HB	1:A:262:PRO:CD	2.46	0.45
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.51	0.45
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.45
1:A:651:ARG:NH1	1:A:870:LYS:HD3	2.32	0.45
2:B:311:GLN:NE2	2:B:314:LYS:HE2	2.32	0.45
3:C:211:VAL:HG23	3:C:212:GLU:N	2.32	0.45
1:A:641:HIS:ND1	1:A:642:LEU:N	2.65	0.45
1:A:928:ARG:CG	1:A:943:PRO:HG3	2.41	0.45
3:C:177:LEU:O	3:C:178:ASP:C	2.55	0.45
1:A:774:ARG:HH11	4:A:1800:MD1:C3'	2.29	0.44
1:A:91:GLY:HA2	7:A:1801:SF4:S4	2.57	0.44
1:A:644:ASP:OD1	1:A:752:GLU:HG2	2.17	0.44
3:C:15:ILE:O	3:C:19:VAL:HG23	2.17	0.44
2:B:395:THR:HG21	2:B:401:PRO:CG	2.44	0.44
1:A:1092:HIS:HA	1:A:1163:HIS:HB3	1.98	0.44
3:C:198:PHE:HE2	3:C:207:TRP:NE1	2.15	0.44
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.47	0.44
1:A:90:ARG:HG2	1:A:90:ARG:HH11	1.81	0.44
1:A:513:VAL:O	1:A:514:SER:C	2.53	0.44
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.38	0.44
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.31	0.44
2:B:101:TYR:CD2	2:B:142:PRO:HD3	2.53	0.44
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.18	0.44
1:A:182:PRO:HD2	1:A:665:PRO:HG2	2.00	0.44
1:A:139:ILE:HA	1:A:139:ILE:HD12	1.81	0.44
1:A:6:ARG:HH21	1:A:6:ARG:HG2	1.83	0.44
1:A:316:GLU:HG3	1:A:496:TYR:OH	2.18	0.44
1:A:582:LYS:HB2	1:A:801:ASP:OD2	2.18	0.43
1:A:338:MET:HE1	1:A:386:PRO:CG	2.48	0.43
1:A:81:ARG:NH2	1:A:84:LEU:HD11	2.32	0.43
1:A:611:PHE:O	1:A:615:SER:HB3	2.19	0.43
1:A:364:LEU:HD13	1:A:385:ALA:HB2	2.00	0.43
1:A:688:LYS:HE3	1:A:876:LEU:HB3	2.00	0.43
1:A:220:TYR:CE1	1:A:720:SER:HB2	2.54	0.43
1:A:629:LEU:HD13	1:A:629:LEU:HA	1.86	0.43
1:A:743:LEU:H	1:A:743:LEU:HD13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:GLN:NE2	3:C:151:MET:HA	2.33	0.43
1:A:401:ASN:CG	1:A:403:GLU:HG3	2.39	0.43
2:B:195:THR:O	2:B:197:PRO:HD3	2.19	0.43
1:A:914:LYS:HG2	1:A:914:LYS:O	2.18	0.43
3:C:115:SER:HA	3:C:116:PRO:HD2	1.83	0.43
1:A:1132:ASN:ND2	2:B:137:LYS:HE3	2.33	0.43
1:A:403:GLU:HG2	1:A:1032:LEU:HD23	1.99	0.43
1:A:272:TYR:HB3	2:B:412:MET:HE1	1.98	0.43
1:A:353:ARG:NE	1:A:864:LEU:HD12	2.33	0.43
1:A:362:ASP:O	1:A:363:ALA:HB3	2.18	0.43
1:A:393:ARG:NH1	1:A:855:ASP:HA	2.33	0.43
1:A:1144:LEU:HD22	1:A:1184:HIS:HA	2.00	0.43
1:A:199:TYR:CE1	1:A:589:TRP:HZ2	2.36	0.43
1:A:393:ARG:HH12	1:A:855:ASP:HA	1.84	0.43
1:A:199:TYR:CD1	1:A:589:TRP:HZ2	2.36	0.43
1:A:548:TYR:HE2	1:A:1191:THR:HG22	1.82	0.43
2:B:400:LYS:HB3	2:B:401:PRO:HD3	2.01	0.43
2:B:157:LYS:CB	2:B:157:LYS:NZ	2.81	0.43
1:A:1041:ARG:HG2	1:A:1041:ARG:NH2	2.33	0.43
1:A:379:THR:HG21	1:A:414:GLU:CD	2.39	0.43
1:A:499:VAL:HG12	1:A:499:VAL:O	2.19	0.43
1:A:532:THR:OG1	1:A:535:ARG:HB2	2.19	0.43
1:A:611:PHE:O	1:A:615:SER:CB	2.67	0.42
1:A:590:GLN:N	1:A:591:PRO:HD2	2.34	0.42
3:C:208:SER:O	3:C:209:VAL:C	2.58	0.42
1:A:1233:LEU:HB3	2:B:120:SER:OG	2.19	0.42
2:B:263:CYS:SG	2:B:267:ILE:HG12	2.59	0.42
1:A:220:TYR:CE1	1:A:720:SER:CB	3.02	0.42
1:A:626:GLU:O	1:A:629:LEU:HB2	2.19	0.42
2:B:224:ILE:HD11	2:B:234:PHE:HB2	2.01	0.42
2:B:156:ALA:HB1	2:B:166:LYS:HD2	2.00	0.42
1:A:529:ALA:CB	1:A:564:CYS:HB3	2.49	0.42
1:A:161:SER:O	1:A:165:VAL:HG22	2.18	0.42
2:B:463:ARG:O	2:B:467:ARG:HD3	2.19	0.42
1:A:167:GLU:HG3	1:A:832:LYS:CE	2.50	0.42
1:A:683:THR:CG2	1:A:885:ILE:HD13	2.49	0.42
2:B:36:VAL:HG13	2:B:235:ASN:ND2	2.34	0.42
1:A:375:VAL:HG12	1:A:376:ALA:N	2.34	0.42
1:A:852:ILE:HD12	1:A:852:ILE:H	1.83	0.42
1:A:612:TYR:CE1	1:A:1192:PRO:HG3	2.55	0.42
1:A:331:ARG:NH1	1:A:415:LEU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:LEU:HB2	2:B:350:LEU:HB2	2.02	0.42
1:A:459:ARG:HH11	1:A:459:ARG:HG3	1.85	0.42
1:A:329:TYR:CZ	1:A:565:GLY:HA2	2.55	0.42
1:A:192:PRO:HB2	1:A:583:LEU:HD12	2.01	0.42
3:C:18:ALA:O	3:C:22:ILE:HG22	2.19	0.42
1:A:920:THR:O	1:A:920:THR:HG23	2.20	0.42
3:C:12:TYR:N	3:C:13:PRO:CD	2.82	0.41
2:B:231:LYS:HE2	2:B:231:LYS:HA	2.01	0.41
2:B:295:ARG:HH21	2:B:295:ARG:CG	2.32	0.41
1:A:774:ARG:NH2	1:A:1103:ASP:OD1	2.52	0.41
1:A:192:PRO:HG2	1:A:583:LEU:HD12	2.02	0.41
1:A:729:LYS:HB2	1:A:736:HIS:CD2	2.55	0.41
1:A:1232:TRP:O	1:A:1233:LEU:HB2	2.19	0.41
2:B:224:ILE:CD1	2:B:234:PHE:HB2	2.49	0.41
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.85	0.41
3:C:88:LYS:O	3:C:92:PHE:HD1	2.02	0.41
2:B:100:TYR:O	2:B:101:TYR:HB3	2.20	0.41
1:A:600:ARG:HA	1:A:601:PRO:HA	1.88	0.41
3:C:89:MET:O	3:C:93:ALA:HB3	2.19	0.41
1:A:336:MET:N	1:A:337:PRO:HD2	2.35	0.41
1:A:338:MET:HE1	1:A:386:PRO:HG3	2.02	0.41
1:A:532:THR:O	1:A:533:HIS:HB2	2.20	0.41
1:A:167:GLU:HG3	1:A:832:LYS:HE2	2.03	0.41
2:B:408:ARG:O	2:B:411:ALA:HB3	2.21	0.41
1:A:695:ALA:HB1	1:A:704:ASN:HB3	2.02	0.41
1:A:1101:TYR:O	1:A:1104:ASN:HB3	2.20	0.41
1:A:677:MET:CE	1:A:682:TYR:HA	2.51	0.41
1:A:1117:VAL:HG23	1:A:1146:ALA:HB3	2.02	0.41
3:C:36:ARG:HG2	3:C:38:ALA:H	1.85	0.41
1:A:808:PRO:HG3	1:A:1000:GLN:HA	2.01	0.41
1:A:705:HIS:HD2	1:A:764:LYS:HB3	1.84	0.41
1:A:1046:GLN:HG3	1:A:1051:MET:CE	2.51	0.41
3:C:149:GLN:HB2	3:C:150:HIS:HD2	1.86	0.41
1:A:368:ASN:O	1:A:373:LYS:HE3	2.21	0.41
3:C:81:LEU:N	3:C:81:LEU:CD2	2.75	0.41
1:A:52:ASN:ND2	1:A:191:ILE:HG13	2.35	0.41
2:B:13:LEU:HB2	2:B:356:VAL:O	2.21	0.41
1:A:90:ARG:HG2	1:A:90:ARG:NH1	2.35	0.41
2:B:372:GLY:HA3	2:B:379:ASP:OD1	2.21	0.41
1:A:578:VAL:CG2	1:A:579:GLY:N	2.81	0.41
3:C:162:TRP:CZ3	3:C:188:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TYR:OH	2:B:448:ALA:HB1	2.21	0.41
1:A:237:VAL:HG11	1:A:576:HIS:H	1.86	0.40
1:A:111:PRO:HA	1:A:787:PRO:HD3	2.03	0.40
1:A:1144:LEU:CD2	1:A:1184:HIS:HA	2.51	0.40
1:A:1096:GLY:HA2	1:A:1101:TYR:HB2	2.03	0.40
1:A:604:HIS:HB3	1:A:1208:PHE:CD2	2.56	0.40
2:B:97:ILE:HG23	2:B:98:ASP:N	2.36	0.40
3:C:82:PRO:HG2	3:C:85:VAL:CG2	2.50	0.40
2:B:152:PHE:CE2	2:B:170:SER:HB3	2.57	0.40
1:A:583:LEU:HD23	1:A:585:PRO:HD2	2.03	0.40
1:A:445:VAL:HG23	1:A:510:ILE:CD1	2.50	0.40
1:A:1173:GLY:HA3	1:A:1233:LEU:HD22	2.01	0.40
1:A:397:LYS:HE3	1:A:977:PHE:CE1	2.56	0.40
1:A:995:ARG:HA	1:A:995:ARG:HD3	1.89	0.40
1:A:38:ARG:O	1:A:38:ARG:HD2	2.21	0.40
1:A:1234:ASP:OD1	1:A:1236:GLU:HB2	2.21	0.40
1:A:1167:ARG:O	1:A:1167:ARG:HG2	2.21	0.40
3:C:98:GLY:HA3	3:C:141:LEU:HD21	2.03	0.40
1:A:281:THR:O	1:A:296:ALA:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1242/1246 (100%)	1127 (91%)	97 (8%)	18 (1%)	14	24
2	B	507/512 (99%)	483 (95%)	23 (4%)	1 (0%)	52	75
3	C	213/225 (95%)	193 (91%)	18 (8%)	2 (1%)	21	37
All	All	1962/1983 (99%)	1803 (92%)	138 (7%)	21 (1%)	17	31

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	1166	GLU
1	A	195	SER
1	A	320	ASP
1	A	501	ALA
1	A	586	GLN
1	A	578	VAL
1	A	718	GLY
1	A	855	ASP
1	A	861	ALA
1	A	874	CYS
1	A	9	TYR
1	A	191	ILE
1	A	1036	ARG
2	B	101	TYR
1	A	224	PRO
1	A	721	GLY
3	C	180	VAL
1	A	390	ILE
1	A	808	PRO
3	C	210	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1039/1043 (100%)	1010 (97%)	29 (3%)	51	78
2	B	436/439 (99%)	423 (97%)	13 (3%)	48	76
3	C	178/185 (96%)	174 (98%)	4 (2%)	60	84
All	All	1653/1667 (99%)	1607 (97%)	46 (3%)	51	78

All (46) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	319	LEU
1	A	338	MET
1	A	452	LEU
1	A	461	GLN
1	A	514	SER
1	A	515	ARG
1	A	533	HIS
1	A	581	GLU
1	A	600	ARG
1	A	629	LEU
1	A	728	LEU
1	A	743	LEU
1	A	767	LEU
1	A	808	PRO
1	A	814	ASP
1	A	837	CYS
1	A	849	THR
1	A	926	LEU
1	A	936	GLU
1	A	944	MET
1	A	1041	ARG
1	A	1062	ARG
1	A	1087	ASN
1	A	1110	LEU
1	A	1126	ASP
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	119	LYS
2	B	135	MET
2	B	161	PHE
2	B	183	LEU
2	B	221	ARG
2	B	244	CYS
2	B	295	ARG
2	B	358	PRO
2	B	492	ASN
3	C	36	ARG
3	C	81	LEU

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Mol	Chain	Res	Type
3	C	129	ILE
3	C	212	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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
1	A	245	ASN
1	A	258	GLN
1	A	311	HIS
1	A	369	ASN
1	A	387	ASN
1	A	461	GLN
1	A	517	GLN
1	A	599	GLN
1	A	704	ASN
1	A	705	HIS
1	A	708	ASN
1	A	946	ASN
1	A	1049	GLN
1	A	1076	GLN
1	A	1082	GLN
1	A	1087	ASN
1	A	1098	HIS
1	A	1163	HIS
2	B	20	HIS
2	B	110	ASN
2	B	143	ASN
2	B	160	ASN
2	B	311	GLN
2	B	414	HIS
2	B	451	ASN
3	C	149	GLN
3	C	164	GLN
3	C	175	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FME	C	1	3	8,9,10	1.52	1 (12%)	6,9,11	2.03	3 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FME	C	1	3	-	1/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-3.28	1.47	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	O1-CN-N	-2.95	120.51	124.76
3	C	1	FME	O-C-CA	-2.05	120.04	125.44
3	C	1	FME	CA-N-CN	3.16	127.69	122.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	1800	5	39,51,51	3.87	10 (25%)	37,78,78	2.36	10 (27%)
7	SF4	A	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MD1	A	2800	5	39,51,51	3.59	9 (23%)	37,78,78	2.35	12 (32%)
7	SF4	B	1802	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1803	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1804	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	B	1805	2	0,9,9	0.00	-	0,15,15	0.00	-
10	3PH	B	1806	-	17,17,47	0.97	1 (5%)	19,21,52	2.08	5 (26%)
9	AGA	C	309	-	29,29,29	0.77	1 (3%)	30,35,35	1.55	3 (10%)
6	HEM	C	806	3	30,50,50	2.31	10 (33%)	24,82,82	2.67	10 (41%)
6	HEM	C	807	3	30,50,50	2.47	11 (36%)	24,82,82	2.73	11 (45%)
11	PCI	C	808	-	12,12,12	9.72	11 (91%)	18,18,18	1.22	1 (5%)

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	1800	5	-	0/18/59/59	0/5/5/5
7	SF4	A	1801	1	-	0/0/48/48	0/6/5/5
4	MD1	A	2800	5	-	0/18/59/59	0/5/5/5
7	SF4	B	1802	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1803	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1804	2	-	0/0/48/48	0/6/5/5
8	F3S	B	1805	2	-	0/0/24/24	0/0/3/3
10	3PH	B	1806	-	1/1/3/4	1/18/18/49	0/0/0/0
9	AGA	C	309	-	-	0/34/34/34	0/0/0/0
6	HEM	C	806	3	-	0/10/54/54	0/0/8/8
6	HEM	C	807	3	-	0/10/54/54	0/0/8/8
11	PCI	C	808	-	-	0/0/0/0	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	808	PCI	C2-CL1	-15.59	1.40	1.72
11	C	808	PCI	C6-CL5	-14.95	1.41	1.72
11	C	808	PCI	C5-CL4	-14.31	1.42	1.72
11	C	808	PCI	C4-CL3	-14.00	1.43	1.72
11	C	808	PCI	C3-CL2	-13.81	1.43	1.72
6	C	806	HEM	C2D-C3D	-6.26	1.35	1.54
6	C	807	HEM	C2D-C3D	-6.04	1.36	1.54
6	C	807	HEM	C3B-C4B	-5.15	1.47	1.51
6	C	806	HEM	C3B-C4B	-4.80	1.47	1.51
6	C	807	HEM	C3D-C4D	-3.21	1.47	1.51
6	C	807	HEM	C2C-C1C	-2.92	1.47	1.52
6	C	806	HEM	C2C-C1C	-2.70	1.47	1.52
6	C	806	HEM	C3D-C4D	-2.36	1.48	1.51
10	B	1806	3PH	C32-C31	2.05	1.56	1.50
4	A	2800	MD1	C6-C5	2.05	1.45	1.41
6	C	807	HEM	CMA-C3A	2.28	1.56	1.51
9	C	309	AGA	C8-C7	2.30	1.57	1.50
6	C	806	HEM	C1C-NC	2.38	1.38	1.36
4	A	1800	MD1	C13-C12	2.56	1.42	1.34
6	C	806	HEM	CMA-C3A	2.62	1.57	1.51
11	C	808	PCI	C1-C6	2.68	1.44	1.39
6	C	807	HEM	C3C-CAC	2.69	1.56	1.51
6	C	807	HEM	FE-NC	2.72	2.06	1.95
4	A	2800	MD1	C14-N15	2.75	1.49	1.47
6	C	806	HEM	FE-NC	2.78	2.06	1.95
4	A	2800	MD1	C16-C20	2.80	1.44	1.40
4	A	1800	MD1	C2-N1	2.82	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	808	PCI	C1-C2	2.92	1.44	1.39
4	A	2800	MD1	C20-N18	2.96	1.39	1.35
6	C	806	HEM	C3C-CAC	3.05	1.57	1.51
4	A	2800	MD1	C17-N17	3.10	1.40	1.35
4	A	1800	MD1	C4-N3	3.15	1.40	1.35
4	A	2800	MD1	C2-N1	3.20	1.41	1.35
4	A	1800	MD1	C14-C13	3.21	1.54	1.50
6	C	807	HEM	CAA-C2A	3.22	1.57	1.52
6	C	806	HEM	C4C-NC	3.36	1.40	1.36
4	A	1800	MD1	C20-N18	3.40	1.40	1.35
6	C	807	HEM	C1C-NC	3.47	1.40	1.36
11	C	808	PCI	C3-C2	3.54	1.48	1.39
11	C	808	PCI	C6-C5	3.61	1.48	1.39
6	C	807	HEM	C4C-NC	3.88	1.40	1.36
11	C	808	PCI	C4-C3	3.88	1.48	1.39
4	A	1800	MD1	C17-N17	3.91	1.42	1.35
11	C	808	PCI	C5-C4	4.00	1.49	1.39
6	C	806	HEM	C3B-CAB	4.24	1.59	1.51
6	C	807	HEM	C3B-CAB	4.29	1.59	1.51
4	A	1800	MD1	C6-N1	4.49	1.41	1.33
4	A	2800	MD1	C15-N17	4.99	1.42	1.33
4	A	1800	MD1	C16-C20	5.03	1.47	1.40
4	A	1800	MD1	C15-N17	5.35	1.43	1.33
4	A	2800	MD1	C6-N1	5.50	1.43	1.33
4	A	2800	MD1	C7-N8	19.03	1.48	1.27
4	A	1800	MD1	C7-N8	20.62	1.50	1.27

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1800	MD1	C5-C6-N1	-6.26	115.02	123.59
4	A	2800	MD1	C5-C6-N1	-5.66	115.85	123.59
4	A	2800	MD1	N3-C2-N1	-5.30	119.37	127.44
4	A	1800	MD1	N17-C17-N18	-4.50	118.15	125.53
6	C	807	HEM	C3C-CAC-CBC	-4.27	117.90	124.46
4	A	1800	MD1	N3-C2-N1	-4.17	121.09	127.44
6	C	806	HEM	C3C-CAC-CBC	-4.04	118.26	124.46
4	A	2800	MD1	O3B-PB-O3A	-3.98	92.37	102.94
4	A	2800	MD1	N17-C17-N18	-3.53	119.75	125.53
4	A	2800	MD1	C6-C5-C4	-3.23	117.04	120.90
4	A	1800	MD1	C6-C5-C4	-3.13	117.16	120.90
6	C	807	HEM	CMA-C3A-C4A	-2.98	123.44	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	806	HEM	CAA-C2A-C1A	-2.78	123.99	127.01
6	C	806	HEM	CMA-C3A-C4A	-2.72	123.86	128.36
4	A	2800	MD1	C1'-N9-C4	-2.66	122.93	126.94
6	C	807	HEM	CAA-C2A-C1A	-2.62	124.17	127.01
4	A	1800	MD1	C1'-N9-C4	-2.47	123.21	126.94
4	A	1800	MD1	O3B-PA-O5'	-2.15	97.24	102.94
6	C	807	HEM	CAD-C3D-C4D	2.14	120.01	112.47
6	C	806	HEM	CMA-C3A-C2A	2.16	129.75	125.24
4	A	2800	MD1	N16-C17-N17	2.17	120.79	117.20
10	B	1806	3PH	O21-C2-C1	2.20	116.11	108.36
6	C	807	HEM	CMA-C3A-C2A	2.20	129.84	125.24
4	A	1800	MD1	N2-C2-N3	2.24	122.09	117.80
6	C	806	HEM	CAD-C3D-C4D	2.25	120.39	112.47
4	A	2800	MD1	N2-C2-N1	2.25	120.93	117.20
9	C	309	AGA	C5-O9-C12	2.55	124.01	117.89
4	A	2800	MD1	O4'-C1'-N9	2.58	113.51	108.10
6	C	807	HEM	CAA-CBA-CGA	2.63	117.57	112.75
4	A	1800	MD1	N16-C17-N18	3.00	122.17	117.20
4	A	2800	MD1	PA-O3B-PB	3.11	141.46	132.73
6	C	807	HEM	CMD-C2D-C3D	3.18	128.40	114.35
6	C	806	HEM	CMD-C2D-C3D	3.26	128.76	114.35
10	B	1806	3PH	O21-C2-C3	3.59	121.01	108.36
10	B	1806	3PH	C2-O21-C21	3.64	123.44	117.29
6	C	807	HEM	C2D-C3D-C4D	3.78	107.90	101.50
6	C	806	HEM	C2D-C3D-C4D	3.83	107.99	101.50
11	C	808	PCI	C6-C1-C2	4.23	121.74	117.64
10	B	1806	3PH	C33-C32-C31	4.31	130.53	113.59
9	C	309	AGA	C9-C8-C7	4.57	131.55	113.59
10	B	1806	3PH	C3-C2-C1	4.62	122.87	112.07
6	C	806	HEM	CMC-C2C-C3C	4.69	128.25	116.53
6	C	807	HEM	CMC-C2C-C3C	4.84	128.61	116.53
4	A	2800	MD1	C15-N17-C17	4.97	122.84	115.94
6	C	807	HEM	CMB-C2B-C3B	5.27	129.69	116.53
4	A	2800	MD1	C6-N1-C2	5.31	123.30	115.94
6	C	806	HEM	CMB-C2B-C3B	5.41	130.03	116.53
9	C	309	AGA	C14-C13-C12	5.55	135.43	113.59
4	A	1800	MD1	C15-N17-C17	5.74	123.91	115.94
6	C	806	HEM	CAD-C3D-C2D	6.40	131.62	113.22
4	A	1800	MD1	C6-N1-C2	6.48	124.93	115.94
6	C	807	HEM	CAD-C3D-C2D	6.56	132.08	113.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	1806	3PH	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1806	3PH	C2-O21-C21-O22

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1800	MD1	6	0
7	A	1801	SF4	2	0
4	A	2800	MD1	2	0
9	C	309	AGA	1	0
6	C	806	HEM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1244/1246 (99%)	-0.14	44 (3%) 48 53	25, 51, 80, 107	0
2	B	509/512 (99%)	-0.38	10 (1%) 68 72	23, 41, 66, 97	0
3	C	216/225 (96%)	-0.18	6 (2%) 56 61	32, 57, 83, 95	0
All	All	1969/1983 (99%)	-0.21	60 (3%) 54 59	23, 48, 78, 107	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	7.2
1	A	10	PHE	5.3
2	B	371	LEU	4.5
1	A	8	ARG	3.8
1	A	1244	SER	3.4
3	C	157	MET	3.4
1	A	421	GLY	3.3
2	B	372	GLY	3.2
2	B	70	ILE	3.2
1	A	11	LYS	3.2
1	A	361	VAL	3.2
1	A	1243	GLU	3.1
1	A	380	ASN	3.1
1	A	463	ALA	3.0
1	A	936	GLU	2.9
1	A	424	ASP	2.9
1	A	446	GLU	2.9
2	B	370	GLU	2.9
1	A	462	LEU	2.9
1	A	488	ASN	2.8
1	A	486	GLY	2.7
1	A	675	ALA	2.7
1	A	749	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	674	LYS	2.6
1	A	673	GLU	2.6
1	A	465	GLY	2.5
1	A	759	ASN	2.5
1	A	461	GLN	2.5
1	A	466	SER	2.5
2	B	119	LYS	2.5
1	A	760	GLY	2.5
1	A	363	ALA	2.5
3	C	149	GLN	2.4
1	A	379	THR	2.4
1	A	408	LYS	2.4
2	B	165	GLN	2.4
2	B	366	ALA	2.4
1	A	7	PHE	2.4
1	A	377	PHE	2.4
1	A	413	THR	2.3
1	A	1075	GLY	2.3
3	C	3	PHE	2.3
1	A	344	GLU	2.3
3	C	81	LEU	2.3
1	A	410	GLY	2.3
1	A	345	ARG	2.3
2	B	369	GLY	2.2
1	A	874	CYS	2.2
1	A	362	ASP	2.2
1	A	501	ALA	2.2
3	C	182	PHE	2.2
3	C	225	HIS	2.1
1	A	636	SER	2.1
1	A	875	ASP	2.1
2	B	287	GLU	2.1
2	B	428	ARG	2.1
1	A	409	THR	2.1
1	A	494	THR	2.1
1	A	423	GLN	2.0
1	A	459	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FME	C	1	10/11	0.90	0.29	-	82,84,96,98	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	PCI	C	808	12/12	0.71	0.39	6.52	59,69,74,76	0
10	3PH	B	1806	18/48	0.84	0.28	2.38	59,82,111,111	0
6	HEM	C	807	43/43	0.97	0.16	0.91	60,68,89,92	0
6	HEM	C	806	43/43	0.98	0.13	0.51	27,40,51,55	0
9	AGA	C	309	30/30	0.95	0.15	-0.12	30,54,85,95	0
4	MD1	A	2800	47/47	0.96	0.12	-0.22	32,45,61,64	0
7	SF4	B	1803	8/8	0.99	0.10	-0.60	22,27,30,33	0
4	MD1	A	1800	47/47	0.97	0.11	-0.69	35,50,66,71	0
7	SF4	B	1804	8/8	0.99	0.10	-1.40	31,38,38,39	0
8	F3S	B	1805	7/7	0.99	0.10	-1.51	30,33,34,37	0
7	SF4	B	1802	8/8	0.98	0.09	-1.58	37,40,43,44	0
7	SF4	A	1801	8/8	0.99	0.05	-3.20	34,39,46,47	0
5	6MO	A	3800	1/1	0.98	0.05	-5.53	72,72,72,72	0

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

There are no such residues in this entry.