



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:39 PM GMT

PDB ID : 1Y4Z
Title : The crystal structure of Nitrate Reductase A, NarGHI, in complex with the Q-site inhibitor 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 : 2004-12-01
Resolution : 2.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

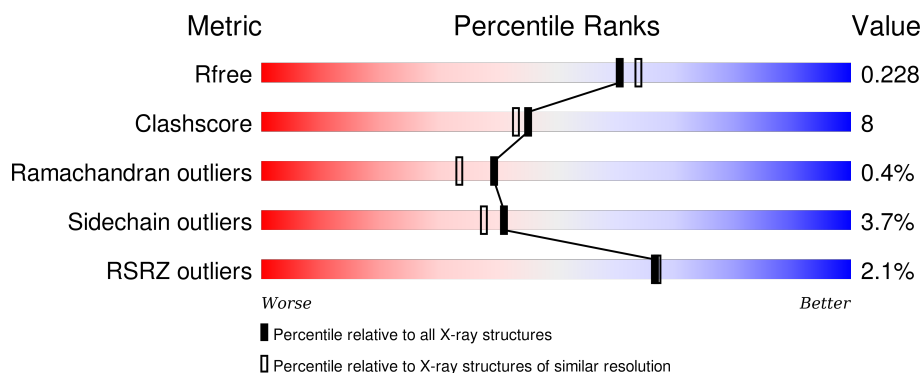
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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>2%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	B	512	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
3	C	225	<div> <div>3%</div> <div>75%</div> <div>20%</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
5	6MO	A	3800	-	-	-	X
8	F3S	B	1803	-	-	X	-
9	PCI	C	1808	-	X	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16919 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
			9871	6236	1731	1856	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
			4049	2562	701	755	31			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ALA	CYS	ENGINEERED	UNP P11349

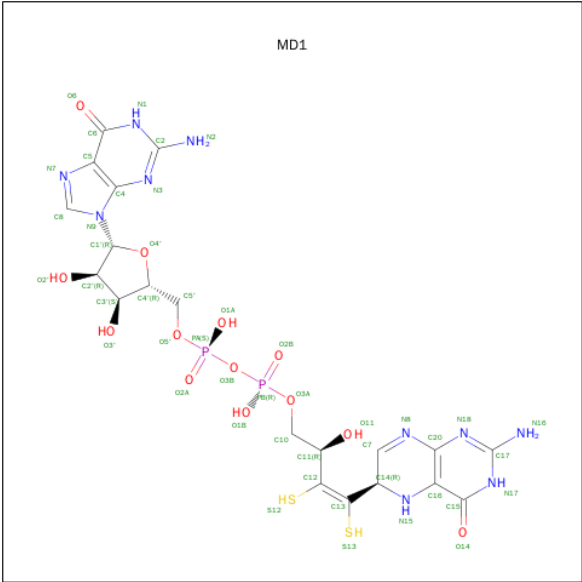
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1723	1141	291	278	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	MET	MODIFIED RESIDUE	UNP P11350

- Molecule 4 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

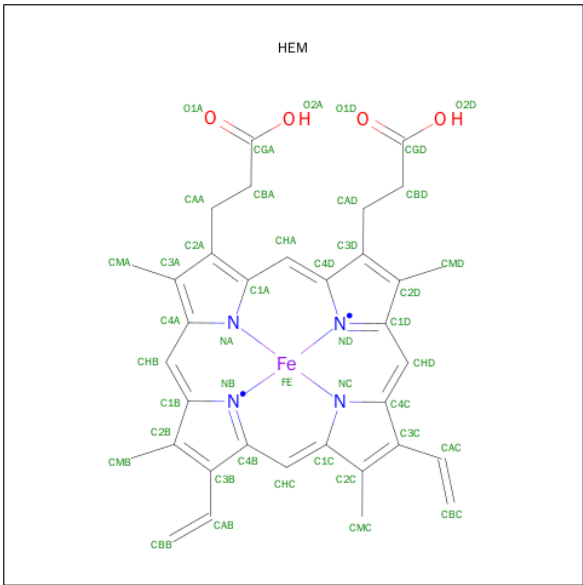


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

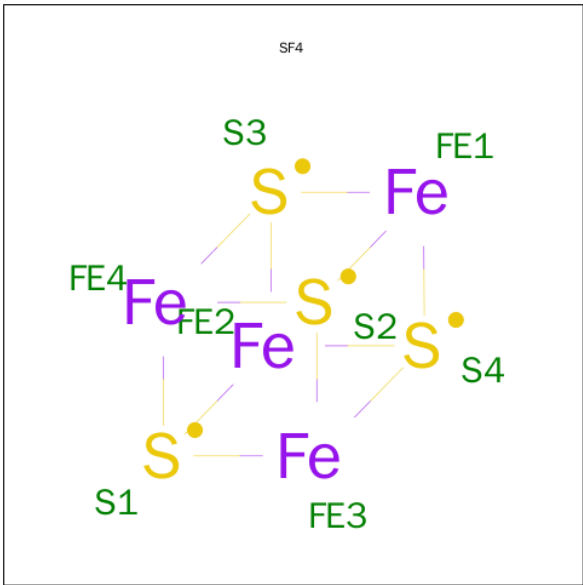
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



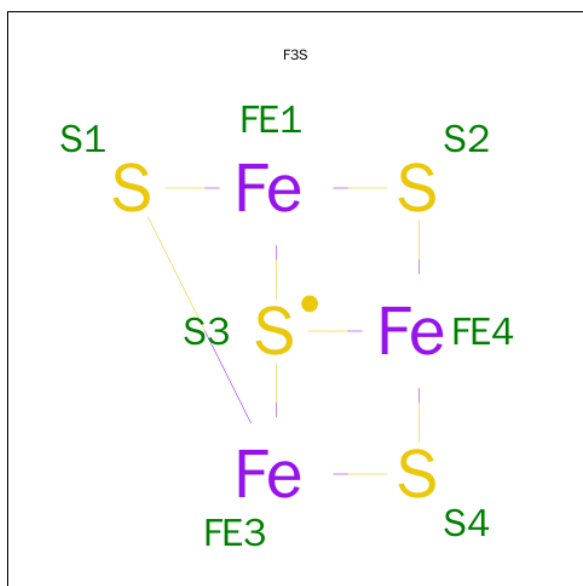
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

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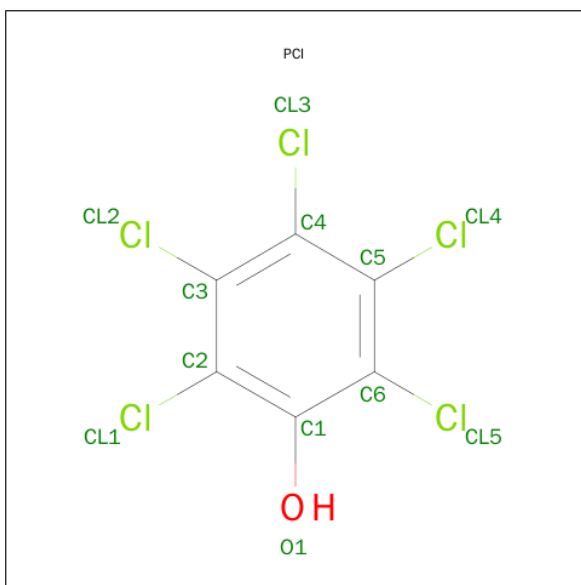
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



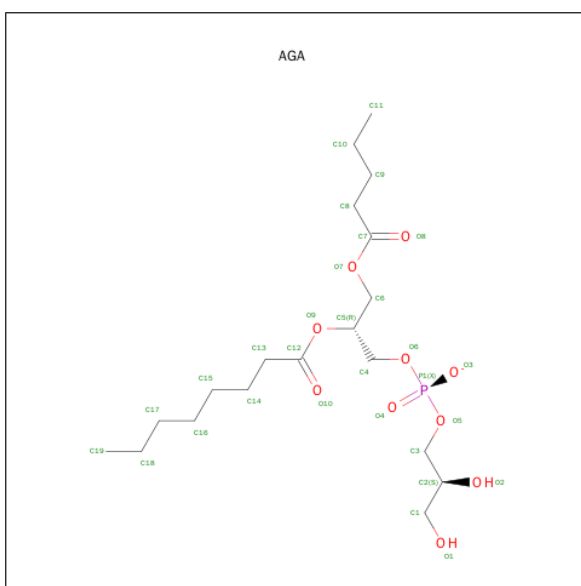
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is PENTACHLOROPHENOL (three-letter code: PCI) (formula: $\text{C}_6\text{HCl}_5\text{O}$).



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

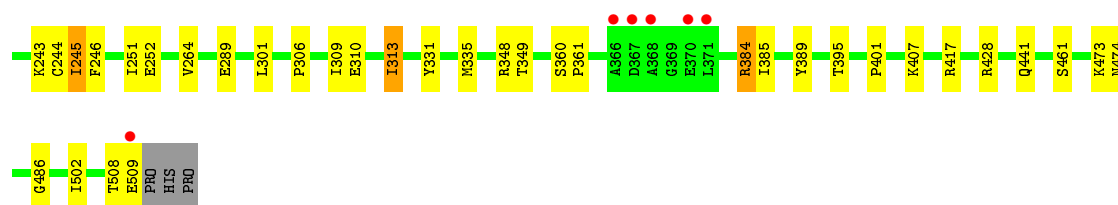
- Molecule 10 is (1S)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula: C₁₉H₃₆O₁₀P).



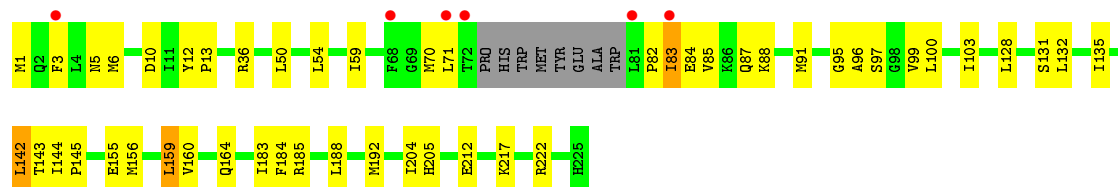
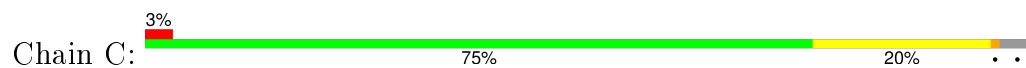
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	P	0	0
			25	16	8	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	595	Total 595	O 595	0	0
11	B	368	Total 368	O 368	0	0
11	C	57	Total 57	O 57	0	0



• Molecule 3: Respiratory nitrate reductase 1 gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.46Å 241.34Å 140.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.00 29.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.75-2.00) 92.1 (29.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.233 0.185 , 0.228	Depositor DCC
R_{free} test set	9703 reflections (6.40%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 161410 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16919	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, FME, SF4, AGA, 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	0.72	0/10131	0.87	13/13753 (0.1%)
2	B	0.77	0/4145	0.85	3/5608 (0.1%)
3	C	0.70	0/1758	0.74	0/2374
All	All	0.73	0/16034	0.85	16/21735 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	TYR	CB-CG-CD1	13.28	128.97	121.00
1	A	1163	HIS	C-N-CA	11.98	151.66	121.70
1	A	501	ALA	C-N-CA	10.56	148.10	121.70
1	A	501	ALA	N-CA-CB	9.32	123.14	110.10
1	A	502	TYR	CB-CG-CD2	-8.75	115.75	121.00
2	B	213	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	1097	ILE	N-CA-C	-5.68	95.68	111.00
1	A	1230	ILE	CG1-CB-CG2	-5.54	99.20	111.40
1	A	809	LEU	N-CA-C	-5.50	96.15	111.00
1	A	184	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	B	313	ILE	CG1-CB-CG2	-5.44	99.43	111.40
1	A	619	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	502	TYR	CG-CD2-CE2	5.14	125.41	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	384	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	600	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	583	LEU	N-CA-C	-5.02	97.45	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	501	ALA	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Mainchain,Peptide
1	A	501	ALA	Mainchain,Peptide
1	A	502	TYR	Mainchain

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	9871	0	9528	162	0
2	B	4049	0	3974	60	0
3	C	1723	0	1772	30	0
4	A	94	0	42	7	0
5	A	1	0	0	0	0
6	C	86	0	60	1	0
7	A	8	0	0	0	0
7	B	16	0	0	0	0
8	B	14	0	0	3	0
9	C	12	0	1	0	0
10	A	25	0	29	0	0
11	A	595	0	0	5	1
11	B	368	0	0	8	0
11	C	57	0	0	1	0
All	All	16919	0	15406	244	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (244) 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:641:HIS:HD2	1:A:643:ILE:H	1.14	0.93
2:B:3:ILE:HD12	2:B:301:LEU:CD1	2.06	0.86
2:B:361:PRO:HG2	2:B:384:ARG:HD3	1.59	0.84
1:A:663:THR:HG21	1:A:692:ILE:HD12	1.60	0.81
2:B:245:ILE:HD13	8:B:1803:F3S:S2	2.22	0.80
1:A:338:MET:HE2	1:A:374:THR:HB	1.65	0.78
1:A:589:TRP:HA	1:A:955:ILE:HD12	1.67	0.77
1:A:641:HIS:CD2	1:A:643:ILE:H	2.03	0.76
3:C:96:ALA:O	3:C:100:LEU:HD13	1.86	0.75
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.33	0.75
1:A:686:SER:HB3	1:A:692:ILE:HG12	1.71	0.72
1:A:1074:ILE:HD13	1:A:1075:GLY:N	2.05	0.71
1:A:508:GLU:OE1	1:A:515:ARG:HD2	1.90	0.71
1:A:596:LEU:O	1:A:600:ARG:HD2	1.92	0.70
2:B:165:GLN:HE21	2:B:165:GLN:HA	1.58	0.69
2:B:165:GLN:NE2	2:B:165:GLN:HA	2.07	0.68
2:B:176:PHE:CD1	2:B:385:ILE:HD12	2.28	0.68
1:A:1098:HIS:CE1	4:A:2800:MD1:S13	2.87	0.67
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.78	0.66
1:A:619:ARG:NH1	11:A:4214:HOH:O	2.29	0.64
1:A:490:VAL:O	1:A:500:LYS:HE3	1.97	0.63
1:A:589:TRP:HA	1:A:955:ILE:CD1	2.30	0.62
1:A:27:THR:HG23	3:C:222:ARG:HD3	1.81	0.62
1:A:1098:HIS:HE1	4:A:2800:MD1:S13	2.22	0.62
2:B:309:ILE:O	2:B:313:ILE:HD13	2.00	0.61
1:A:20:GLY:O	3:C:217:LYS:HD2	2.00	0.61
1:A:1171:LEU:H	2:B:123:ILE:HD12	1.64	0.61
3:C:160:VAL:O	3:C:164:GLN:HG3	2.01	0.60
2:B:246:PHE:CD2	2:B:251:ILE:CD1	2.85	0.60
1:A:169:ILE:N	1:A:169:ILE:HD13	2.16	0.60
4:A:1800:MD1:H7	4:A:1800:MD1:C11	2.32	0.59
1:A:749:VAL:HG12	11:A:4122:HOH:O	2.01	0.59
2:B:3:ILE:CD1	2:B:301:LEU:CD1	2.80	0.58
4:A:1800:MD1:H7	4:A:1800:MD1:O11	2.03	0.58
2:B:246:PHE:HD2	2:B:251:ILE:CD1	2.17	0.58
1:A:368:ASN:ND2	1:A:396:GLU:HG2	2.18	0.58
1:A:1006:ILE:HD12	1:A:1006:ILE:H	1.68	0.58
2:B:176:PHE:HB2	2:B:385:ILE:CD1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:HG13	11:B:2066:HOH:O	2.03	0.57
3:C:99:VAL:O	3:C:103:ILE:HG12	2.05	0.57
2:B:361:PRO:HG2	2:B:384:ARG:CD	2.33	0.57
2:B:508:THR:O	2:B:509:GLU:HB3	2.04	0.57
1:A:426:ILE:HD12	1:A:426:ILE:N	2.20	0.57
3:C:131:SER:O	3:C:135:ILE:HG12	2.04	0.57
1:A:338:MET:HE2	1:A:374:THR:CB	2.34	0.56
3:C:159:LEU:HG	6:C:807:HEM:HMA3	1.88	0.56
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.88	0.56
1:A:282:PRO:HB2	1:A:1158:MET:HE3	1.88	0.55
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.89	0.55
1:A:878:PRO:HB3	1:A:885:ILE:HG12	1.89	0.55
1:A:190:PRO:HB2	1:A:191:ILE:CD1	2.37	0.55
2:B:441:GLN:HG2	11:B:1912:HOH:O	2.06	0.55
1:A:686:SER:CB	1:A:692:ILE:HG12	2.36	0.55
1:A:371:GLU:N	1:A:371:GLU:OE1	2.22	0.55
1:A:919:ASN:ND2	1:A:921:GLN:H	2.04	0.55
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.38	0.55
1:A:191:ILE:H	1:A:191:ILE:HD12	1.71	0.54
2:B:198:SER:HB3	11:B:1950:HOH:O	2.07	0.54
2:B:78:MET:CG	2:B:225:THR:HG22	2.36	0.54
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.07	0.54
3:C:82:PRO:HG2	3:C:85:VAL:CG2	2.38	0.54
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.73	0.54
2:B:245:ILE:HD13	2:B:245:ILE:H	1.71	0.54
1:A:1074:ILE:C	1:A:1074:ILE:HD13	2.28	0.54
1:A:169:ILE:HD11	1:A:784:ILE:HD12	1.88	0.54
2:B:246:PHE:O	2:B:251:ILE:HD12	2.08	0.53
1:A:360:LEU:N	1:A:360:LEU:HD22	2.24	0.53
1:A:360:LEU:HG	1:A:383:MET:HE3	1.90	0.53
1:A:191:ILE:N	1:A:191:ILE:HD12	2.24	0.53
2:B:78:MET:HG2	2:B:225:THR:HG22	1.91	0.53
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.44	0.53
1:A:949:ILE:HD12	1:A:996:PHE:CD2	2.44	0.53
2:B:246:PHE:CD2	2:B:251:ILE:HD11	2.44	0.53
1:A:190:PRO:HB2	1:A:191:ILE:HD13	1.91	0.52
1:A:366:GLN:HG3	1:A:373:LYS:HD2	1.91	0.52
1:A:56:SER:HB2	1:A:800:SER:HB2	1.90	0.52
3:C:50:LEU:HD13	3:C:54:LEU:HD12	1.91	0.52
2:B:19:CYS:O	2:B:20:HIS:HB2	2.09	0.52
3:C:143:THR:HB	3:C:184:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:TRP:CA	1:A:955:ILE:HD12	2.38	0.52
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.92	0.52
1:A:1171:LEU:H	2:B:123:ILE:CD1	2.22	0.52
1:A:685:LYS:O	1:A:689:GLU:HG3	2.10	0.51
4:A:1800:MD1:C7	4:A:1800:MD1:O11	2.59	0.51
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.10	0.51
1:A:600:ARG:HD3	1:A:905:LEU:HD13	1.92	0.51
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.46	0.51
1:A:652:MET:HE2	1:A:862:GLN:HE22	1.76	0.51
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.11	0.51
1:A:251:ALA:HB3	1:A:287:ILE:HD11	1.92	0.51
2:B:137:LYS:HA	11:B:2048:HOH:O	2.10	0.51
1:A:804:PRO:O	1:A:1006:ILE:HD12	2.09	0.51
1:A:1098:HIS:CE1	4:A:1800:MD1:S12	3.04	0.51
2:B:245:ILE:CD1	8:B:1803:F3S:S2	2.95	0.50
3:C:142:LEU:HB3	3:C:183:ILE:HD11	1.94	0.50
1:A:100:TRP:O	1:A:104:SER:HB3	2.11	0.50
1:A:641:HIS:CD2	1:A:643:ILE:HG22	2.47	0.50
1:A:344:GLU:HG3	1:A:349:TYR:CE1	2.47	0.50
2:B:1:MET:SD	2:B:3:ILE:HD11	2.51	0.50
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.93	0.50
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.93	0.50
1:A:27:THR:CG2	3:C:222:ARG:HD3	2.42	0.49
3:C:142:LEU:HB3	3:C:183:ILE:CD1	2.42	0.49
1:A:864:LEU:N	1:A:864:LEU:HD22	2.28	0.49
1:A:191:ILE:O	1:A:191:ILE:HG22	2.12	0.49
1:A:357:ALA:O	1:A:363:ALA:HA	2.12	0.49
2:B:78:MET:HG2	2:B:225:THR:CG2	2.42	0.49
1:A:931:ASN:O	1:A:932:TYR:HB2	2.11	0.49
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.45	0.49
1:A:1006:ILE:CD1	1:A:1006:ILE:H	2.25	0.49
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.27	0.48
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.77	0.48
2:B:78:MET:HG3	11:B:1962:HOH:O	2.12	0.48
3:C:1:FME:O1	3:C:3:PHE:HB3	2.14	0.48
1:A:7:PHE:N	1:A:7:PHE:CD1	2.82	0.48
2:B:3:ILE:HD12	2:B:301:LEU:HD11	1.90	0.48
1:A:169:ILE:CD1	1:A:169:ILE:N	2.77	0.48
1:A:949:ILE:HD12	1:A:996:PHE:CE2	2.49	0.48
1:A:344:GLU:HG3	1:A:349:TYR:HE1	1.77	0.48
2:B:360:SER:HB3	2:B:385:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.48	0.47
2:B:187:CYS:HB3	2:B:349:THR:O	2.15	0.47
2:B:502:ILE:HD12	11:B:2149:HOH:O	2.14	0.47
1:A:451:LEU:CD1	1:A:501:ALA:HB3	2.44	0.47
1:A:624:THR:O	1:A:627:GLU:HG2	2.15	0.47
1:A:1062:ARG:HD3	11:A:4082:HOH:O	2.15	0.47
1:A:169:ILE:HD12	1:A:767:LEU:HD11	1.97	0.46
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.98	0.46
2:B:209:ILE:HD12	2:B:246:PHE:CB	2.45	0.46
1:A:749:VAL:O	1:A:749:VAL:HG23	2.16	0.46
1:A:920:THR:O	1:A:920:THR:HG23	2.16	0.46
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.97	0.46
3:C:13:PRO:HB3	3:C:192:MET:SD	2.56	0.46
1:A:421:GLY:O	1:A:422:SER:HB3	2.15	0.46
3:C:84:GLU:O	3:C:88:LYS:HG3	2.16	0.46
1:A:658:ALA:HA	1:A:659:PRO:C	2.36	0.45
1:A:139:ILE:HA	1:A:139:ILE:HD12	1.76	0.45
1:A:1062:ARG:CD	11:A:4082:HOH:O	2.65	0.45
1:A:7:PHE:N	1:A:7:PHE:HD1	2.14	0.45
1:A:471:THR:HG21	1:A:476:LEU:HD13	1.98	0.45
3:C:6:MET:O	3:C:10:ASP:HB2	2.16	0.45
1:A:663:THR:CG2	1:A:692:ILE:HD12	2.40	0.45
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.45
1:A:854:HIS:O	1:A:855:ASP:HB2	2.17	0.45
2:B:209:ILE:HD12	2:B:246:PHE:HB3	1.99	0.45
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.52	0.45
1:A:1006:ILE:N	1:A:1006:ILE:CD1	2.80	0.45
2:B:210:VAL:O	2:B:243:LYS:NZ	2.43	0.45
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.51	0.45
1:A:627:GLU:OE2	1:A:1068:ARG:NH1	2.46	0.45
1:A:274:GLY:HA3	2:B:417:ARG:HB2	1.99	0.44
1:A:425:GLU:C	1:A:426:ILE:HD12	2.38	0.44
1:A:214:LEU:HB3	1:A:607:SER:OG	2.17	0.44
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.98	0.44
3:C:204:ILE:HD12	3:C:205:HIS:N	2.32	0.44
3:C:184:PHE:O	3:C:188:LEU:HG	2.18	0.44
2:B:184:CYS:HB3	2:B:244:CYS:HB3	1.99	0.44
2:B:331:TYR:CE2	2:B:335:MET:HG3	2.52	0.44
2:B:306:PRO:O	2:B:310:GLU:HG3	2.18	0.44
1:A:31:TRP:CE2	2:B:213:ASP:HA	2.53	0.44
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ILE:HD12	2:B:301:LEU:HD12	1.93	0.44
1:A:1087:ASN:O	1:A:1159:THR:HG22	2.18	0.43
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.71	0.43
1:A:217:TYR:CD1	1:A:222:ASP:HB2	2.54	0.43
1:A:497:ASP:HA	1:A:505:ALA:HB2	2.00	0.43
1:A:261:THR:HG22	2:B:264:VAL:HG11	2.00	0.43
1:A:515:ARG:HG2	1:A:516:SER:N	2.33	0.43
1:A:767:LEU:HD13	1:A:769:VAL:HG23	1.99	0.43
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.54	0.43
1:A:44:ILE:HA	1:A:61:ILE:O	2.18	0.43
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.52	0.43
2:B:289:GLU:HG2	11:B:2119:HOH:O	2.19	0.43
1:A:336:MET:HA	1:A:473:VAL:HB	2.01	0.43
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.53	0.43
1:A:30:ASP:HB2	2:B:486:GLY:HA2	2.01	0.43
1:A:338:MET:HE1	1:A:374:THR:OG1	2.18	0.43
1:A:366:GLN:HG2	1:A:373:LYS:HD2	2.01	0.43
1:A:187:GLY:HA3	1:A:206:LEU:CD1	2.49	0.43
1:A:1183:ILE:O	1:A:1186:SER:HB2	2.19	0.43
2:B:11:LEU:HD22	2:B:181:PRO:HG2	2.01	0.43
1:A:192:PRO:HB3	1:A:199:TYR:CG	2.54	0.43
1:A:856:SER:O	1:A:859:GLU:HG2	2.19	0.42
1:A:145:ALA:O	1:A:149:LYS:HG3	2.19	0.42
1:A:423:GLN:HB2	1:A:457:VAL:O	2.18	0.42
1:A:928:ARG:HH11	1:A:942:GLN:NE2	2.17	0.42
1:A:541:GLY:HA3	4:A:2800:MD1:O1B	2.20	0.42
2:B:160:ASN:HB2	2:B:389:TYR:CE2	2.54	0.42
1:A:652:MET:CE	1:A:866:VAL:HG13	2.50	0.42
1:A:219:TRP:HB2	1:A:607:SER:HB2	2.01	0.42
1:A:1230:ILE:N	1:A:1230:ILE:HD12	2.35	0.42
2:B:246:PHE:HA	8:B:1803:F3S:S4	2.60	0.42
1:A:1037:THR:HA	1:A:1203:HIS:HB3	2.02	0.42
3:C:83:ILE:HD11	3:C:156:MET:HG2	2.01	0.42
1:A:98:TYR:CD1	1:A:791:TRP:CZ3	3.08	0.42
1:A:269:GLU:HG3	2:B:15:LYS:HE3	2.01	0.42
1:A:169:ILE:HD11	1:A:784:ILE:CD1	2.49	0.42
1:A:685:LYS:HD3	11:A:4360:HOH:O	2.20	0.42
1:A:180:TYR:HB3	1:A:184:ARG:HG2	2.01	0.42
2:B:335:MET:HA	2:B:335:MET:HE3	2.02	0.41
1:A:1095:TRP:CZ3	1:A:1110:LEU:HB3	2.55	0.41
1:A:1099:SER:HA	1:A:1164:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLY:HA2	1:A:704:ASN:ND2	2.35	0.41
2:B:335:MET:HE2	2:B:335:MET:HB3	1.86	0.41
1:A:260:ARG:HA	1:A:260:ARG:HD3	1.93	0.41
1:A:1058:LEU:HD23	1:A:1058:LEU:HA	1.95	0.41
3:C:12:TYR:N	3:C:13:PRO:HD2	2.35	0.41
1:A:634:ASP:OD1	1:A:637:ARG:HG3	2.20	0.41
1:A:223:LEU:HD12	1:A:224:PRO:HD2	2.01	0.41
1:A:703:LYS:HE3	1:A:703:LYS:HB2	1.84	0.41
1:A:177:ILE:HG12	1:A:182:PRO:HA	2.02	0.41
2:B:165:GLN:HB2	11:B:2062:HOH:O	2.20	0.41
3:C:95:GLY:O	3:C:99:VAL:HG23	2.21	0.41
1:A:369:ASN:O	1:A:373:LYS:HG3	2.21	0.41
1:A:960:PRO:O	1:A:967:ALA:HB2	2.20	0.41
1:A:51:VAL:HB	1:A:791:TRP:CH2	2.56	0.41
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.40	0.41
1:A:487:LEU:CD1	1:A:487:LEU:N	2.83	0.41
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.55	0.41
3:C:128:LEU:O	3:C:132:LEU:HG	2.21	0.41
1:A:641:HIS:CD2	1:A:642:LEU:N	2.89	0.41
1:A:101:TYR:OH	1:A:1101:TYR:HA	2.21	0.41
2:B:165:GLN:CA	2:B:165:GLN:HE21	2.22	0.41
1:A:949:ILE:CD1	1:A:996:PHE:CE2	3.04	0.41
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.55	0.41
2:B:252:GLU:HA	2:B:461:SER:HB2	2.03	0.41
1:A:668:ILE:N	1:A:668:ILE:HD13	2.36	0.41
1:A:1011:THR:HG22	1:A:1012:TRP:CE2	2.56	0.41
1:A:1112:ARG:HH11	1:A:1112:ARG:HD2	1.75	0.41
2:B:66:TRP:HB2	2:B:348:ARG:HB2	2.02	0.41
1:A:365:GLY:HA3	1:A:408:LYS:HG3	2.02	0.41
3:C:155:GLU:HB2	11:C:1851:HOH:O	2.20	0.41
1:A:426:ILE:CD1	1:A:426:ILE:N	2.83	0.40
1:A:363:ALA:O	1:A:366:GLN:HB2	2.21	0.40
1:A:1059:LEU:O	1:A:1059:LEU:HD23	2.21	0.40
3:C:87:GLN:O	3:C:91:MET:HG3	2.21	0.40
1:A:741:LYS:HB3	1:A:745:GLN:HB2	2.04	0.40
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.56	0.40
3:C:70:MET:O	3:C:71:LEU:HD23	2.21	0.40
3:C:143:THR:HG22	3:C:183:ILE:HG12	2.03	0.40
1:A:390:ILE:HA	1:A:390:ILE:HD12	1.83	0.40
1:A:806:ILE:HD13	1:A:807:HIS:N	2.37	0.40
1:A:54:THR:HG21	1:A:260:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ALA:O	1:A:898:ARG:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:4064:HOH:O	11:A:4064:HOH:O[3_354]	1.00	1.20

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%)	1174 (94%)	61 (5%)	7 (1%)	30	22
2	B	507/512 (99%)	495 (98%)	12 (2%)	0	100	100
3	C	213/225 (95%)	207 (97%)	6 (3%)	0	100	100
All	All	1962/1983 (99%)	1876 (96%)	79 (4%)	7 (0%)	39	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	501	ALA
1	A	578	VAL
1	A	1166	GLU
1	A	195	SER
1	A	224	PRO
1	A	718	GLY

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%)	997 (96%)	42 (4%)	38	33
2	B	435/438 (99%)	423 (97%)	12 (3%)	51	50
3	C	179/186 (96%)	172 (96%)	7 (4%)	39	35
All	All	1653/1667 (99%)	1592 (96%)	61 (4%)	41	38

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	9	TYR
1	A	44	ILE
1	A	94	ARG
1	A	169	ILE
1	A	190	PRO
1	A	221	CYS
1	A	287	ILE
1	A	366	GLN
1	A	383	MET
1	A	402	LEU
1	A	413	THR
1	A	416	GLN
1	A	476	LEU
1	A	515	ARG
1	A	533	HIS
1	A	578	VAL
1	A	601	PRO
1	A	646	ASN
1	A	659	PRO
1	A	677	MET
1	A	767	LEU
1	A	804	PRO
1	A	806	ILE
1	A	808	PRO
1	A	831	LYS

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Mol	Chain	Res	Type
1	A	864	LEU
1	A	926	LEU
1	A	944	MET
1	A	991	ASP
1	A	995	ARG
1	A	1006	ILE
1	A	1018	GLU
1	A	1032	LEU
1	A	1062	ARG
1	A	1074	ILE
1	A	1087	ASN
1	A	1110	LEU
1	A	1184	HIS
1	A	1198	ILE
1	A	1233	LEU
1	A	1238	ASN
2	B	37	GLU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU
2	B	123	ILE
2	B	182	ARG
2	B	183	LEU
2	B	184	CYS
2	B	221	ARG
2	B	245	ILE
2	B	407	LYS
2	B	428	ARG
3	C	36	ARG
3	C	59	ILE
3	C	83	ILE
3	C	97	SER
3	C	142	LEU
3	C	159	LEU
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	173	ASN
1	A	234	GLN

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Mol	Chain	Res	Type
1	A	258	GLN
1	A	366	GLN
1	A	404	GLN
1	A	517	GLN
1	A	559	ASN
1	A	604	HIS
1	A	641	HIS
1	A	704	ASN
1	A	708	ASN
1	A	759	ASN
1	A	919	ASN
1	A	942	GLN
1	A	946	ASN
1	A	1076	GLN
1	A	1098	HIS
1	A	1238	ASN
2	B	160	ASN
2	B	165	GLN
2	B	451	ASN
3	C	149	GLN
3	C	175	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FME	C	1	3	8,9,10	1.28	2 (25%)	6,9,11	1.98	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	-	0/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-2.63	1.48	1.53
3	C	1	FME	CB-CG	2.07	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	O1-CN-N	-2.57	121.06	124.76
3	C	1	FME	CA-N-CN	3.59	128.34	122.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	AGA	A	1309	-	24,24,29	0.92	1 (4%)	28,29,35	1.52	3 (10%)
4	MD1	A	1800	5	39,51,51	3.81	11 (28%)	37,78,78	2.25	8 (21%)
7	SF4	A	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MD1	A	2800	5	39,51,51	3.50	10 (25%)	37,78,78	2.51	12 (32%)
7	SF4	B	1802	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	B	1803	2	0,9,9	0.00	-	0,15,15	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	-
9	PCI	C	1808	-	12,12,12	9.39	11 (91%)	18,18,18	1.60	2 (11%)
6	HEM	C	806	3	30,50,50	2.42	11 (36%)	24,82,82	2.72	10 (41%)
6	HEM	C	807	3	30,50,50	2.48	13 (43%)	24,82,82	2.75	10 (41%)

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
10	AGA	A	1309	-	-	0/26/26/34	0/0/0/0
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
8	F3S	B	1803	2	-	0/0/24/24	0/0/3/3
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
9	PCI	C	1808	-	-	0/0/0/0	0/1/1/1
6	HEM	C	806	3	-	0/10/54/54	0/0/8/8
6	HEM	C	807	3	-	0/10/54/54	0/0/8/8

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1808	PCI	C6-CL5	-14.32	1.42	1.72
9	C	1808	PCI	C4-CL3	-13.80	1.43	1.72
9	C	1808	PCI	C2-CL1	-13.61	1.44	1.72
9	C	1808	PCI	C3-CL2	-13.58	1.44	1.72
9	C	1808	PCI	C5-CL4	-13.33	1.44	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	806	HEM	C3B-C4B	-6.94	1.45	1.51
6	C	806	HEM	C2D-C3D	-6.31	1.35	1.54
6	C	807	HEM	C2D-C3D	-5.83	1.37	1.54
6	C	807	HEM	C3B-C4B	-4.88	1.47	1.51
6	C	806	HEM	C2C-C1C	-3.19	1.46	1.52
6	C	806	HEM	C3D-C4D	-3.17	1.47	1.51
6	C	807	HEM	C3D-C4D	-3.13	1.47	1.51
4	A	1800	MD1	C8-N7	-2.31	1.30	1.34
6	C	807	HEM	C2C-C1C	-2.23	1.48	1.52
6	C	806	HEM	C2D-C1D	-2.15	1.44	1.51
4	A	1800	MD1	PB-O2B	-2.01	1.43	1.51
6	C	807	HEM	CAD-C3D	2.11	1.58	1.54
6	C	807	HEM	CAA-C2A	2.13	1.55	1.52
6	C	807	HEM	CMC-C2C	2.23	1.58	1.53
6	C	807	HEM	CMA-C3A	2.29	1.56	1.51
6	C	806	HEM	CMB-C2B	2.30	1.58	1.53
4	A	2800	MD1	C20-N18	2.33	1.38	1.35
6	C	806	HEM	CMC-C2C	2.33	1.58	1.53
6	C	806	HEM	CMA-C3A	2.39	1.56	1.51
6	C	806	HEM	FE-NC	2.46	2.05	1.95
4	A	2800	MD1	C14-N15	2.53	1.49	1.47
4	A	2800	MD1	C17-N17	2.64	1.40	1.35
4	A	2800	MD1	C6-C5	2.65	1.46	1.41
6	C	806	HEM	C3B-CAB	2.65	1.56	1.51
4	A	1800	MD1	C13-C12	2.79	1.43	1.34
4	A	2800	MD1	C4-N3	2.91	1.40	1.35
4	A	2800	MD1	C2-N1	3.07	1.40	1.35
6	C	807	HEM	C1C-NC	3.12	1.39	1.36
10	A	1309	AGA	C8-C7	3.14	1.60	1.50
4	A	1800	MD1	C2-N1	3.15	1.41	1.35
9	C	1808	PCI	C1-C2	3.15	1.45	1.39
4	A	1800	MD1	O4'-C1'	3.22	1.45	1.41
6	C	807	HEM	C3C-CAC	3.30	1.57	1.51
4	A	1800	MD1	C4-N3	3.31	1.40	1.35
4	A	2800	MD1	C16-C20	3.33	1.45	1.40
6	C	806	HEM	C3C-CAC	3.40	1.57	1.51
6	C	807	HEM	FE-NC	3.65	2.10	1.95
9	C	1808	PCI	C6-C5	3.68	1.48	1.39
9	C	1808	PCI	C3-C2	4.23	1.49	1.39
4	A	1800	MD1	C17-N17	4.30	1.43	1.35
6	C	807	HEM	C4C-NC	4.42	1.41	1.36
6	C	807	HEM	C3B-CAB	4.59	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1808	PCI	C5-C4	4.67	1.50	1.39
4	A	2800	MD1	C6-N1	4.75	1.41	1.33
9	C	1808	PCI	C4-C3	4.87	1.51	1.39
9	C	1808	PCI	C1-C6	5.02	1.48	1.39
4	A	2800	MD1	C15-N17	5.14	1.42	1.33
4	A	1800	MD1	C6-N1	5.56	1.43	1.33
4	A	1800	MD1	C15-N17	6.39	1.45	1.33
4	A	1800	MD1	C16-C20	6.84	1.50	1.40
4	A	2800	MD1	C7-N8	18.51	1.48	1.27
4	A	1800	MD1	C7-N8	18.80	1.48	1.27

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1800	MD1	C5-C6-N1	-6.36	114.89	123.59
4	A	2800	MD1	C5-C6-N1	-5.49	116.08	123.59
4	A	2800	MD1	N3-C2-N1	-5.43	119.17	127.44
4	A	2800	MD1	O3B-PB-O3A	-4.80	90.19	102.94
4	A	1800	MD1	N17-C17-N18	-4.18	118.67	125.53
4	A	1800	MD1	N3-C2-N1	-4.18	121.08	127.44
6	C	807	HEM	C3C-CAC-CBC	-4.17	118.05	124.46
6	C	806	HEM	C3C-CAC-CBC	-3.89	118.50	124.46
4	A	2800	MD1	N17-C17-N18	-3.83	119.25	125.53
6	C	806	HEM	CAA-C2A-C1A	-3.63	123.07	127.01
4	A	2800	MD1	C6-C5-C4	-3.18	117.09	120.90
6	C	806	HEM	CMA-C3A-C4A	-3.14	123.16	128.36
6	C	807	HEM	CAA-C2A-C1A	-3.12	123.62	127.01
6	C	807	HEM	CMA-C3A-C4A	-3.05	123.32	128.36
4	A	2800	MD1	C1'-N9-C4	-2.85	122.65	126.94
4	A	1800	MD1	C6-C5-C4	-2.76	117.60	120.90
4	A	1800	MD1	O3B-PA-O5'	-2.64	95.92	102.94
9	C	1808	PCI	C1-C2-C3	-2.27	119.24	121.21
6	C	807	HEM	CAD-C3D-C4D	2.13	119.98	112.47
10	A	1309	AGA	C6-O7-C7	2.13	122.81	116.85
4	A	2800	MD1	O1B-PB-O2B	2.20	124.44	112.53
4	A	2800	MD1	O3B-PA-O5'	2.23	108.85	102.94
4	A	1800	MD1	N16-C17-N17	2.35	121.08	117.20
6	C	807	HEM	CMA-C3A-C2A	2.49	130.44	125.24
6	C	806	HEM	CAD-C3D-C4D	2.65	121.82	112.47
4	A	2800	MD1	N16-C17-N17	2.72	121.71	117.20
6	C	806	HEM	CMA-C3A-C2A	2.76	131.01	125.24
6	C	807	HEM	CMD-C2D-C3D	3.15	128.30	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	806	HEM	CMD-C2D-C3D	3.17	128.36	114.35
4	A	2800	MD1	PA-O3B-PB	3.45	142.41	132.73
6	C	806	HEM	C2D-C3D-C4D	3.78	107.90	101.50
6	C	807	HEM	C2D-C3D-C4D	3.92	108.14	101.50
10	A	1309	AGA	C14-C13-C12	4.45	131.09	113.59
6	C	807	HEM	CMC-C2C-C3C	5.13	129.34	116.53
10	A	1309	AGA	C9-C8-C7	5.16	133.86	113.59
6	C	806	HEM	CMB-C2B-C3B	5.19	129.49	116.53
4	A	1800	MD1	C15-N17-C17	5.37	123.39	115.94
9	C	1808	PCI	C6-C1-C2	5.39	122.86	117.64
4	A	2800	MD1	C15-N17-C17	5.48	123.55	115.94
6	C	806	HEM	CMC-C2C-C3C	5.51	130.29	116.53
6	C	807	HEM	CMB-C2B-C3B	5.54	130.35	116.53
4	A	1800	MD1	C6-N1-C2	5.76	123.93	115.94
6	C	806	HEM	CAD-C3D-C2D	5.93	130.28	113.22
4	A	2800	MD1	C6-N1-C2	6.07	124.36	115.94
6	C	807	HEM	CAD-C3D-C2D	6.49	131.88	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1800	MD1	4	0
4	A	2800	MD1	3	0
8	B	1803	F3S	3	0
6	C	807	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, 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	1244/1246 (99%)	-0.17	28 (2%) 64 64	14, 26, 47, 69	0
2	B	509/512 (99%)	-0.44	8 (1%) 74 75	14, 21, 33, 61	0
3	C	216/225 (96%)	-0.04	6 (2%) 56 57	15, 31, 51, 57	0
All	All	1969/1983 (99%)	-0.23	42 (2%) 67 67	14, 25, 46, 69	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	PHE	8.9
1	A	9	TYR	7.9
1	A	7	PHE	4.1
2	B	70	ILE	4.0
1	A	673	GLU	4.0
1	A	8	ARG	3.7
1	A	11	LYS	3.7
3	C	81	LEU	3.4
1	A	1244	SER	3.4
3	C	68	PHE	3.3
1	A	674	LYS	3.2
1	A	380	ASN	3.1
2	B	370	GLU	3.0
2	B	371	LEU	3.0
1	A	363	ALA	3.0
3	C	3	PHE	2.9
1	A	1243	GLU	2.9
1	A	749	VAL	2.7
1	A	463	ALA	2.6
1	A	759	ASN	2.6
1	A	675	ALA	2.5
3	C	83	ILE	2.5
1	A	12	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	72	THR	2.5
1	A	678	ASN	2.5
2	B	165	GLN	2.4
3	C	71	LEU	2.4
1	A	321	ASN	2.4
2	B	368	ALA	2.3
1	A	421	GLY	2.3
1	A	348	TYR	2.3
1	A	365	GLY	2.3
1	A	875	ASP	2.2
1	A	346	ASP	2.2
1	A	501	ALA	2.1
2	B	366	ALA	2.1
1	A	490	VAL	2.1
1	A	466	SER	2.1
1	A	637	ARG	2.1
2	B	509	GLU	2.1
2	B	367	ASP	2.0
1	A	465	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FME	C	1	10/11	0.91	0.27	-	49,56,65,65	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	PCI	C	1808	12/12	0.75	0.35	5.84	33,38,40,40	0
5	6MO	A	3800	1/1	0.95	0.18	2.50	52,52,52,52	0
6	HEM	C	807	43/43	0.94	0.12	0.25	35,39,45,50	0
10	AGA	A	1309	25/30	0.96	0.10	0.19	22,27,42,44	0
6	HEM	C	806	43/43	0.98	0.09	0.19	16,22,25,32	0
4	MD1	A	2800	47/47	0.96	0.09	-0.27	19,24,33,39	0
4	MD1	A	1800	47/47	0.97	0.08	-0.74	14,23,36,40	0
8	F3S	B	1805	7/7	0.99	0.06	-2.19	18,19,20,21	0
7	SF4	B	1802	8/8	0.99	0.04	-2.36	21,23,24,25	0
7	SF4	B	1804	8/8	0.96	0.07	-2.38	25,29,31,33	0
8	F3S	B	1803	7/7	0.99	0.03	-2.44	19,21,22,23	0
7	SF4	A	1801	8/8	0.98	0.05	-2.77	21,22,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.