



# wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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

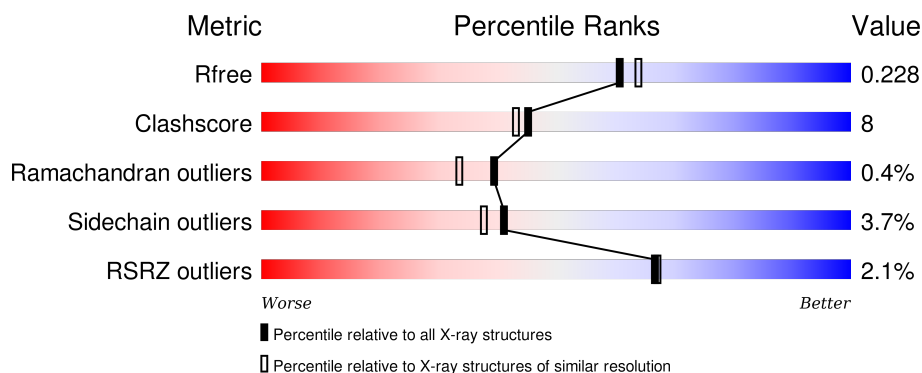
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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  $\geq 3$ , 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>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

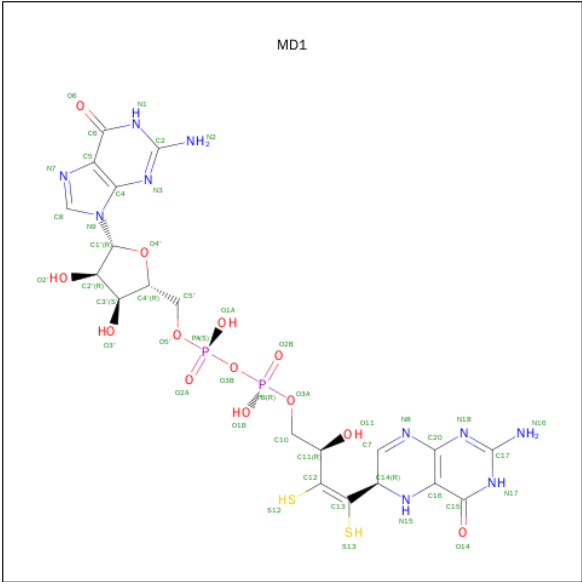
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

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: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).

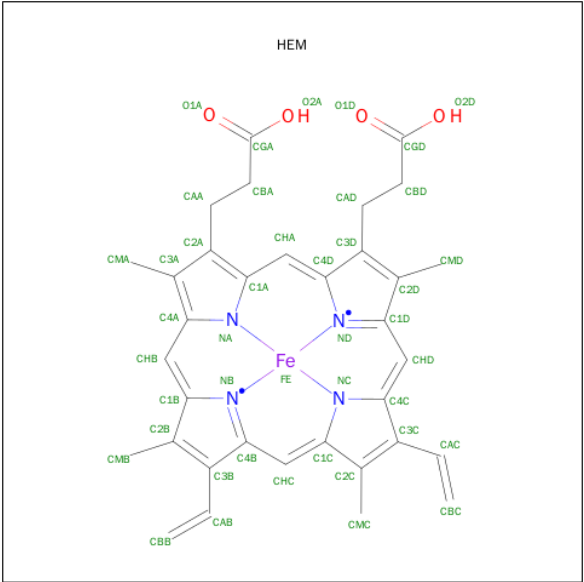


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

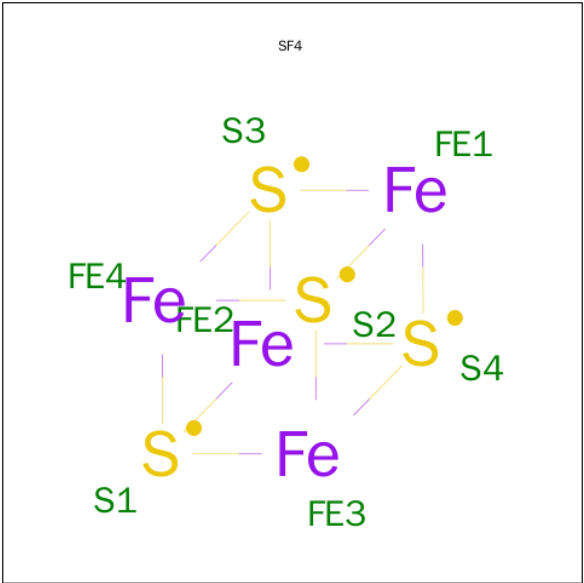
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

- 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: Fe<sub>4</sub>S<sub>4</sub>).



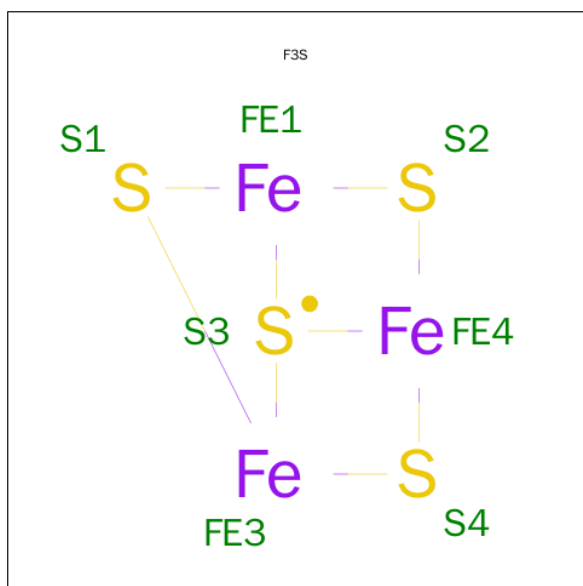
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

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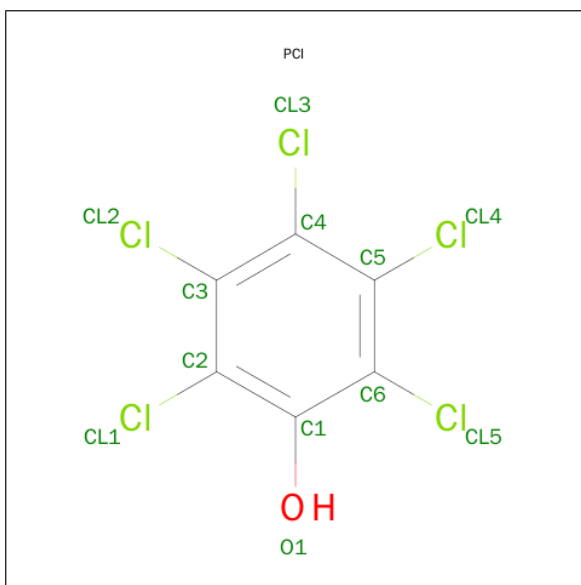
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

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



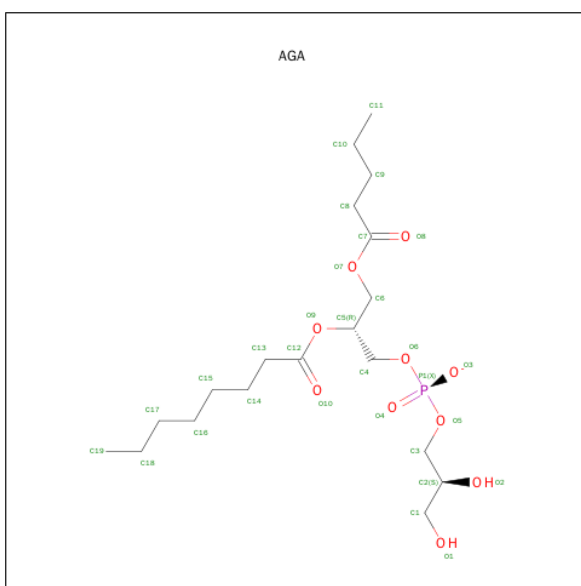
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	B	1	Total	Fe	S	0	0
			7	3	4		

- 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: C<sub>19</sub>H<sub>36</sub>O<sub>10</sub>P).



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

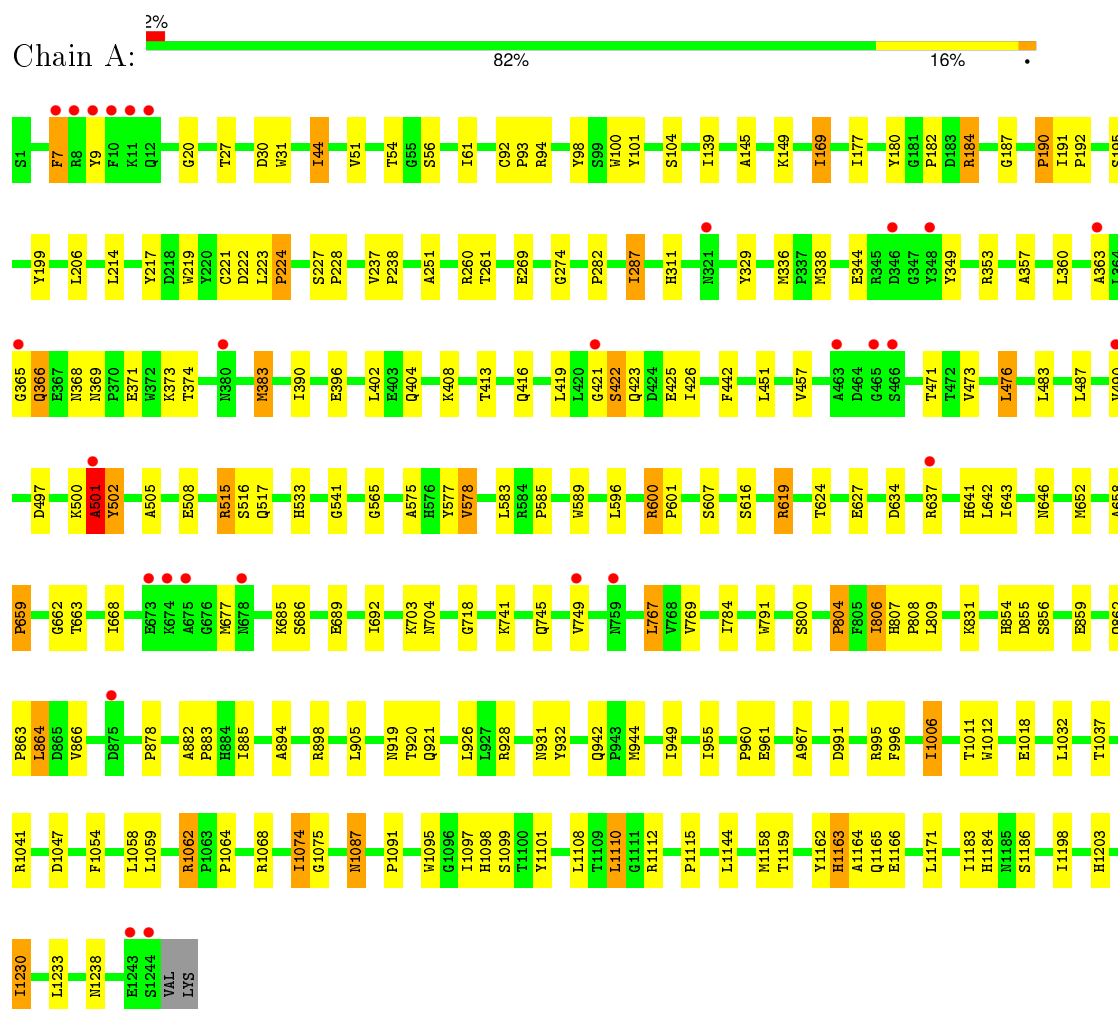
- Molecule 11 is water.

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

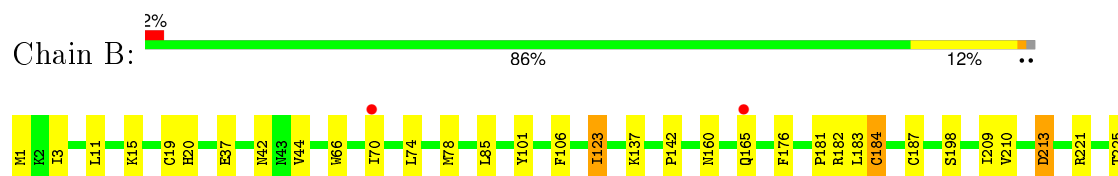
### 3 Residue-property plots

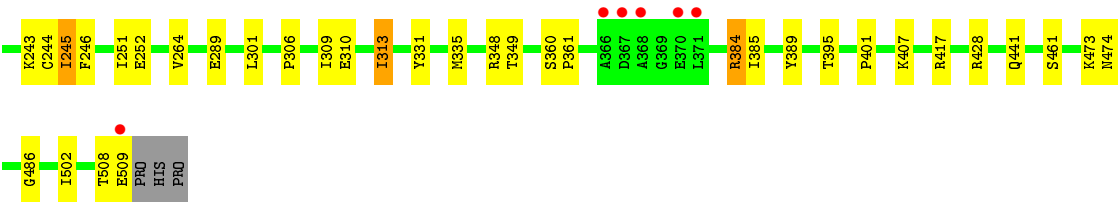
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Respiratory nitrate reductase 1 alpha chain

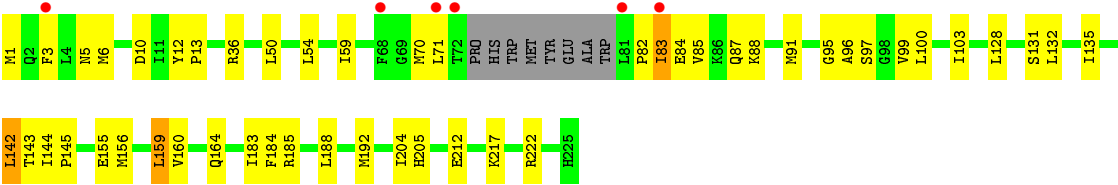


- Molecule 2: Respiratory nitrate reductase 1 beta chain





● Molecule 3: Respiratory nitrate reductase 1 gamma chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

<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 [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.

The worst 5 of 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

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 [i](#)

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.

The worst 5 of 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

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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

5 of 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

### 5.3.2 Protein sidechains [i](#)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	926	LEU
1	A	1062	ARG
3	C	83	ILE
1	A	944	MET
1	A	995	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	ASN
1	A	919	ASN
3	C	149	GLN
1	A	708	ASN
1	A	759	ASN

### 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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

The worst 5 of 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

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.17	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

The worst 5 of 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

### 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, 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	0.91	0.27	-	49,56,65,65	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	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 ⓘ

There are no such residues in this entry.