



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 11:10 PM GMT

PDB ID : 4JYD
Title : X-ray snapshots of possible intermediates in the time course of synthesis and degradation of protein-bound Fe₄S₄ clusters.
Authors : Nicolet, Y.; Rohac, R.; Martin, L.; Fontecilla-Camps, J.C.
Deposited on : 2013-03-29
Resolution : 1.71 Å (reported)

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

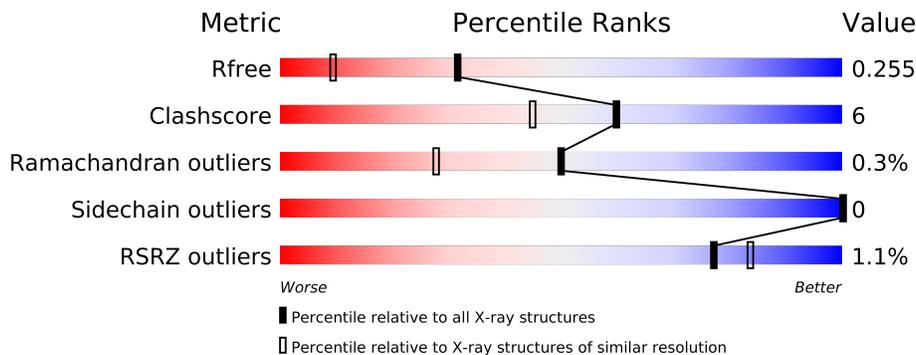
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2979 (1.74-1.70)
Clashscore	79885	3506 (1.74-1.70)
Ramachandran outliers	78287	3449 (1.74-1.70)
Sidechain outliers	78261	3449 (1.74-1.70)
RSRZ outliers	66119	2979 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	348	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	1N7	A	406	-	X
5	1N7	A	407	-	X
6	FE	A	408	-	X
7	H2S	A	409	-	X
7	H2S	A	410	-	X

2 Entry composition (i)

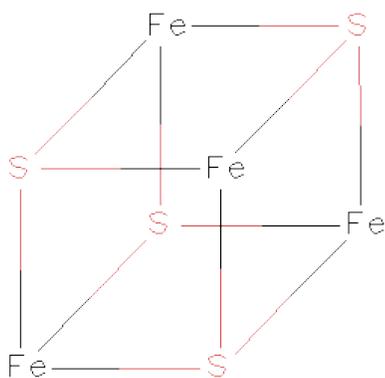
There are 9 unique types of molecules in this entry. The entry contains 3359 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called FEFE-HYDROGENASE MATURASE.

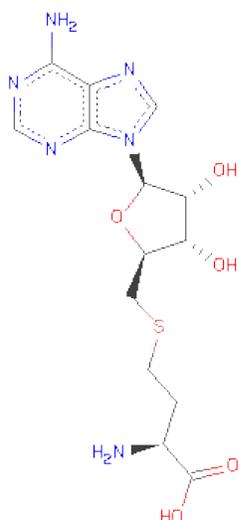
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2795	1794	476	503	22	0	15	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



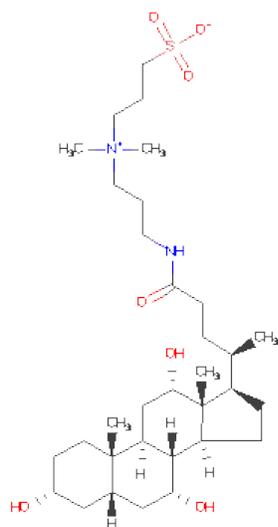
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	26	14	6	5	1	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	42	32	2	7	1	0	0

- Molecule 5 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total S 1 1	0	0
7	A	1	Total S 1 1	0	0

- Molecule 8 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total Br 4 4	0	0

- Molecule 9 is water.

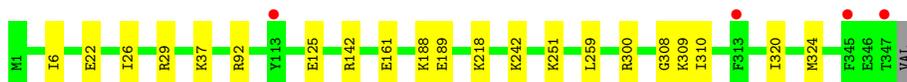
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	368	Total O 369 369	0	1

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: FEFE-HYDROGENASE MATURASE

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.60Å 78.70Å 85.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.60 – 1.71 42.98 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.60-1.71) 98.2 (42.98-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.71Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.251 0.194 , 0.255	Depositor DCC
R_{free} test set	1879 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	19.4	Xtrriage
Anisotropy	0.292	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Outliers	0 of 37102 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3359	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: SAH, SF4, H2S, OTY, 1N7, FE, BR, CPS

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	0.74	0/2887	0.80	2/3902 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	300	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2795	0	0	14	0
2	A	8	0	0	0	0
3	A	26	0	0	1	0
4	A	42	0	0	1	0
5	A	112	0	0	2	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	4	0	0	1	0
9	A	369	0	0	9	0
All	All	3359	0	0	18	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (18) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:407:1N7:C1	9:A:785:HOH:O	2.35	0.74
1:A:142[A]:ARG:NH1	1:A:189:GLU:OE1	2.34	0.60
1:A:218:LYS:NZ	1:A:259:LEU:O	2.37	0.58
8:A:411:BR:BR	9:A:585:HOH:O	2.72	0.57
1:A:29:ARG:NE	9:A:603:HOH:O	2.37	0.56
1:A:188[B]:LYS:CG	9:A:810:HOH:O	2.54	0.55
1:A:308:GLY:O	1:A:309:LYS:C	2.46	0.52
1:A:125:GLU:OE1	9:A:713:HOH:O	2.19	0.52
1:A:6:ILE:CD1	1:A:22:GLU:CG	2.93	0.47
1:A:320:ILE:CG2	1:A:324[A]:MET:CE	2.93	0.47
1:A:37:LYS:CD	9:A:841:HOH:O	2.62	0.47
1:A:242:LYS:N	9:A:655:HOH:O	2.48	0.45
1:A:161:GLU:OE2	3:A:402:SAH:O3'	2.34	0.45
1:A:308:GLY:N	9:A:821:HOH:O	2.50	0.45
5:A:407:1N7:C21	9:A:695:HOH:O	2.65	0.45
1:A:26:ILE:O	1:A:251:LYS:NZ	2.54	0.41
4:A:403:CPS:C24	4:A:403:CPS:C21	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	358/348 (103%)	345 (96%)	12 (3%)	1 (0%)	50 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	ILE

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	298/303 (98%)	298 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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
1	OTY	A	114	1	13,13,14	4.53	1 (7%)	15,17,19	1.17	1 (6%)

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
1	OTY	A	114	1	-	0/4/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	OTY	O-C	16.22	1.22	1.11

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	OTY	C-CA-N	3.10	116.92	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are modelled with single atom and 5 are monoatomic - leaving 7 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
2	SF4	A	401	1,3	12,12,12	3.67	8 (66%)	0,24,24	0.00	-
3	SAH	A	402	2	28,28,28	1.00	2 (7%)	40,40,40	2.30	8 (20%)
4	CPS	A	403	-	45,45,45	1.32	2 (4%)	70,70,70	1.14	7 (10%)
5	1N7	A	404	-	36,38,46	2.90	3 (8%)	55,59,72	1.40	8 (14%)
5	1N7	A	405	-	31,32,46	0.71	0	49,51,72	1.36	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1N7	A	406	-	27,28,46	0.76	0	44,46,72	1.03	2 (4%)
5	1N7	A	407	-	22,24,46	1.18	1 (4%)	33,40,72	1.52	5 (15%)

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
2	SF4	A	401	1,3	-	0/0/48/48	0/0/5/5
3	SAH	A	402	2	-	0/15/31/31	0/1/3/3
4	CPS	A	403	-	-	0/25/90/90	0/0/4/4
5	1N7	A	404	-	-	0/12/78/92	0/0/4/4
5	1N7	A	405	-	-	0/9/74/92	0/0/4/4
5	1N7	A	406	-	-	0/4/69/92	0/0/4/4
5	1N7	A	407	-	-	0/4/59/92	0/0/3/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	1N7	O5-C31	16.48	1.43	1.25
2	A	401	SF4	S4-FE3	-7.98	2.27	2.33
4	A	403	CPS	C32-S	-6.92	1.66	1.78
2	A	401	SF4	S3-FE2	-6.17	2.29	2.33
5	A	407	1N7	C2-C15	-4.28	1.53	1.56
2	A	401	SF4	S1-FE3	3.64	2.35	2.33
2	A	401	SF4	S2-FE4	-3.17	2.31	2.33
2	A	401	SF4	S1-FE4	-3.06	2.31	2.33
5	A	404	1N7	C32-S1	-3.03	1.67	1.76
3	A	402	SAH	C2-N1	2.93	1.39	1.33
2	A	401	SF4	S4-FE2	2.80	2.35	2.33
2	A	401	SF4	S2-FE3	-2.74	2.31	2.33
3	A	402	SAH	C2-N3	2.57	1.37	1.32
2	A	401	SF4	S2-FE1	-2.31	2.31	2.33
4	A	403	CPS	C5-C4	-2.08	1.51	1.54
5	A	404	1N7	C5-C6	-2.00	1.52	1.55

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	SAH	N3-C2-N1	-11.35	119.22	128.71
5	A	405	1N7	C6-C5-C9	3.72	103.87	100.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	1N7	O7-S1-C32	3.40	113.16	106.64
5	A	405	1N7	C10-C5-C9	-3.40	105.83	111.22
5	A	404	1N7	C16-C17-C18	-3.33	107.98	111.51
3	A	402	SAH	N3-C4-N9	3.10	131.03	125.43
5	A	407	1N7	C16-C17-C18	3.05	114.74	111.51
5	A	405	1N7	O4-C4-C5	3.05	116.15	111.13
5	A	407	1N7	C9-C5-C4	2.99	120.43	117.67
5	A	407	1N7	C19-C3-C4	-2.97	110.48	114.35
5	A	404	1N7	C11-C2-C1	-2.85	103.33	108.17
4	A	403	CPS	C29-N2-C30	2.79	116.72	109.38
5	A	405	1N7	C11-C2-C19	-2.70	107.68	111.17
3	A	402	SAH	C4'-O4'-C1'	-2.65	106.87	109.75
3	A	402	SAH	OXT-C-O	-2.60	118.18	124.07
5	A	407	1N7	C10-C5-C9	-2.59	107.10	111.22
3	A	402	SAH	C2'-C1'-N9	-2.58	106.64	113.27
3	A	402	SAH	CG-CB-CA	2.52	117.45	113.22
5	A	404	1N7	C3-C4-C5	2.51	113.78	111.21
4	A	403	CPS	C28-N2-C30	-2.49	102.84	109.38
3	A	402	SAH	C2-N1-C6	2.47	123.24	118.77
5	A	405	1N7	C8-C9-C5	-2.40	101.18	103.58
5	A	404	1N7	O8-S1-C32	2.36	108.68	105.64
3	A	402	SAH	C5'-SD-CG	-2.35	95.39	102.42
4	A	403	CPS	C9-C5-C4	2.33	119.82	117.67
5	A	406	1N7	O3-C17-C18	2.32	114.14	109.23
5	A	404	1N7	C5-C6-C18	-2.31	112.18	114.81
5	A	406	1N7	C9-C5-C4	2.26	119.75	117.67
4	A	403	CPS	C8-C9-C5	-2.22	101.36	103.58
4	A	403	CPS	O1S-S-C32	2.21	113.18	106.36
5	A	405	1N7	C22-C23-C24	-2.16	106.80	112.90
5	A	407	1N7	C3-C4-C5	-2.13	109.02	111.21
5	A	405	1N7	C16-C15-C14	-2.11	108.63	111.14
4	A	403	CPS	C3-C4-C5	-2.10	109.05	111.21
5	A	404	1N7	C23-C22-C20	-2.06	111.20	114.46
4	A	403	CPS	C1-C2-C15	2.05	110.05	107.79
5	A	404	1N7	C21-C20-C9	-2.03	109.40	112.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	347/348 (99%)	-0.13	4 (1%) 75 82	10, 19, 32, 38	9 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	PHE	2.6
1	A	313	PHE	2.6
1	A	113	TYR	2.4
1	A	347	THR	2.3

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OTY	A	114	13/14	0.10	0.47	19,20,20,22	1

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	1N7	A	407	22/43	0.18	5.51	25,34,35,37	0
7	H2S	A	410	1/1	0.21	4.23	32,32,32,32	1
7	H2S	A	409	1/1	0.19	4.21	21,21,21,21	1
6	FE	A	408	1/1	0.14	2.14	23,23,23,23	1
5	1N7	A	406	25/43	0.13	2.13	19,23,27,30	0
4	CPS	A	403	42/42	0.10	0.91	10,15,27,28	5
5	1N7	A	404	36/43	0.12	0.84	15,19,25,26	10
5	1N7	A	405	29/43	0.08	-0.27	11,15,32,35	0
3	SAH	A	402	26/26	0.07	-0.75	16,18,22,26	0
8	BR	A	411	1/1	0.04	-1.82	29,29,29,29	1
8	BR	A	413	1/1	0.04	-3.52	28,28,28,28	1
8	BR	A	414	1/1	0.03	-3.59	27,27,27,27	1
2	SF4	A	401	8/8	0.03	-3.81	19,20,22,22	0
8	BR	A	412	1/1	0.01	-4.39	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.