WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 06:23 pm GMT

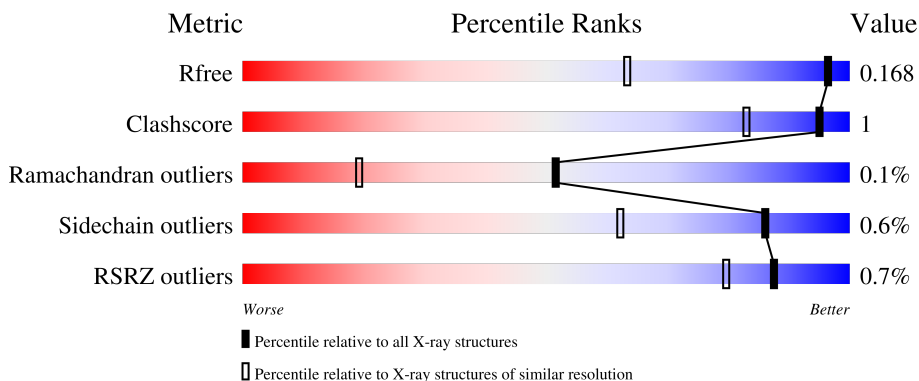|		
PDB ID	:	5A4F
Title	:	The mechanism of Hydrogen Activation by NiFe-hydrogenases.
Authors	:	Evans, R.M.; Brooke, E.J.; Wehlin, S.A.M.; Nomerotskaia, E.; Sargent, F.; Carr, S.B.; Phillips, S.E.V.; Armstrong, F.A.
Deposited on	:	2015-06-09
Resolution	:	1.25 Å(reported)

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 1.25 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}	130704	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	L	582	94% 5% •
1	M	582	95% 5%
2	S	335	73% 5% • 21%
2	T	335	74% • • 21%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14598 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 Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	581	Total 4707	C 2992	N 823	O 863	S 29	0	28	0
1	M	581	Total 4648	C 2957	N 808	O 855	S 28	0	19	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	118	ALA	ASP	engineered mutation	UNP P0ACD8
M	118	ALA	ASP	engineered mutation	UNP P0ACD8

- Molecule 2 is a protein called Hydrogenase-1 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	264	Total 2092	C 1328	N 359	O 384	S 21	0	9	0
2	T	264	Total 2100	C 1334	N 362	O 383	S 21	0	10	0

There are 16 discrepancies between the modelled and reference sequences:
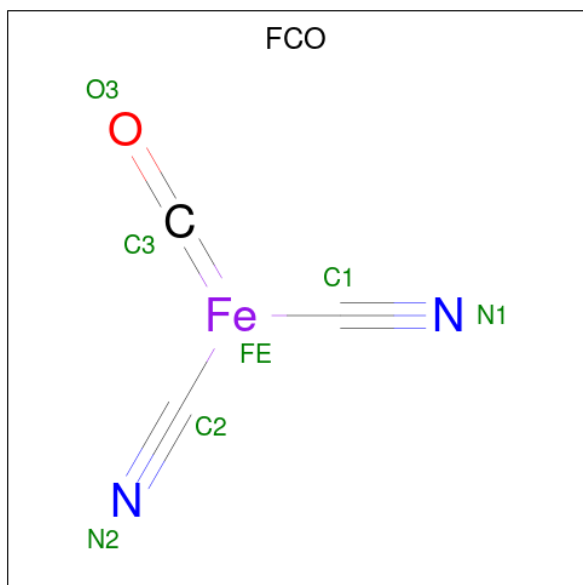
Chain	Residue	Modelled	Actual	Comment	Reference
S	328	ARG	-	expression tag	UNP P69739
S	329	SER	-	expression tag	UNP P69739
S	330	HIS	-	expression tag	UNP P69739
S	331	HIS	-	expression tag	UNP P69739
S	332	HIS	-	expression tag	UNP P69739
S	333	HIS	-	expression tag	UNP P69739
S	334	HIS	-	expression tag	UNP P69739
S	335	HIS	-	expression tag	UNP P69739
T	328	ARG	-	expression tag	UNP P69739
T	329	SER	-	expression tag	UNP P69739

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Chain	Residue	Modelled	Actual	Comment	Reference
T	330	HIS	-	expression tag	UNP P69739
T	331	HIS	-	expression tag	UNP P69739
T	332	HIS	-	expression tag	UNP P69739
T	333	HIS	-	expression tag	UNP P69739
T	334	HIS	-	expression tag	UNP P69739
T	335	HIS	-	expression tag	UNP P69739

- Molecule 3 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
3	M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Ni	0	0
			1	1		
4	M	1	Total	Ni	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total 1	Mg 1	0	0
5	M	1	Total 1	Mg 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total 5	O 4	S 1	0	0
6	S	1	Total 5	O 4	S 1	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

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

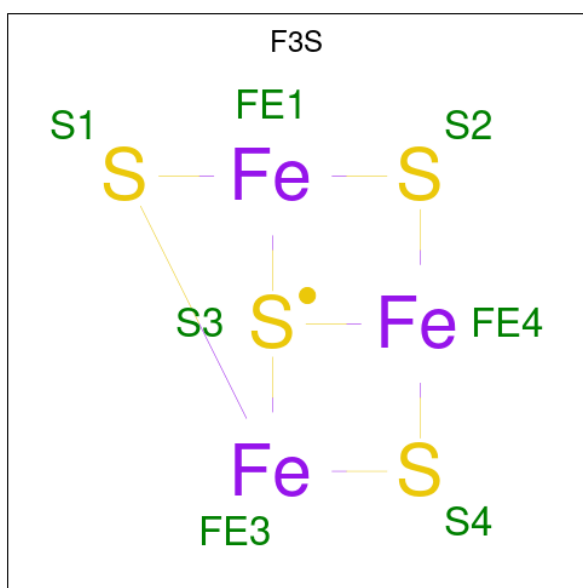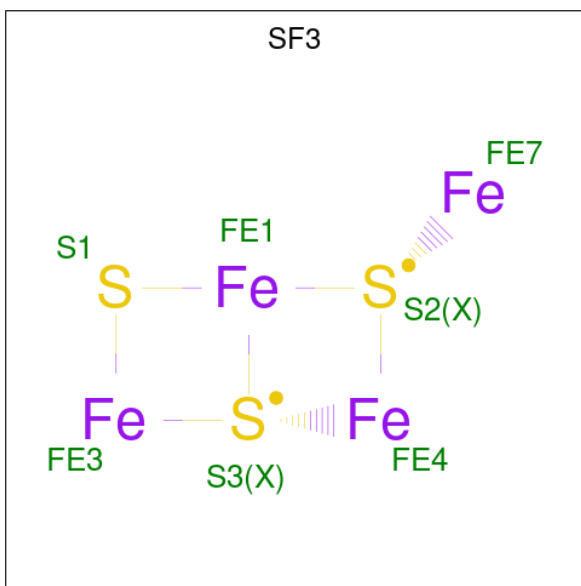- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

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

- Molecule 9 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe_4S_3).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	S	1	Total 8	Fe 5	S 3	0	1
9	T	1	Total 8	Fe 5	S 3	0	1

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

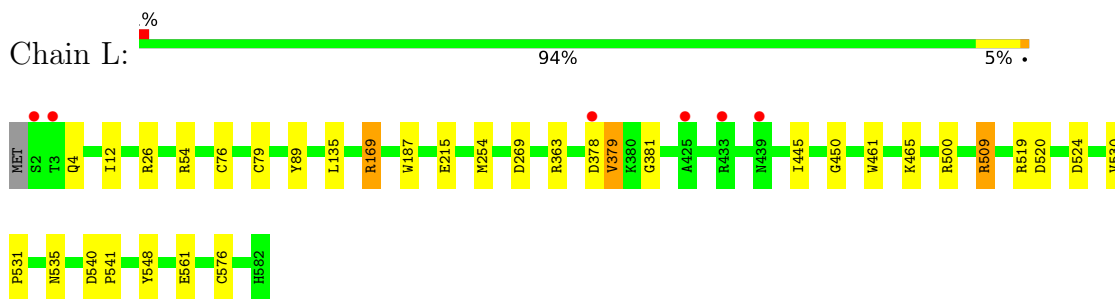| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	S	2	Total 2	Cl 2	0	0
10	T	2	Total 2	Cl 2	0	0

- Molecule 11 is water.

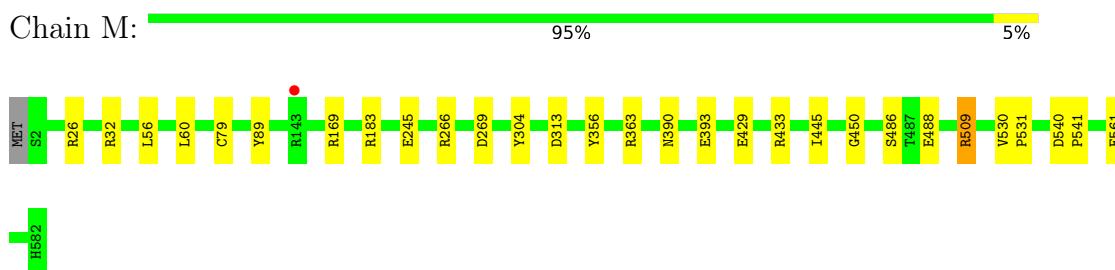| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	361	Total 361	O 361	0	0
11	M	381	Total 381	O 381	0	0
11	S	127	Total 127	O 127	0	0
11	T	104	Total 104	O 104	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.
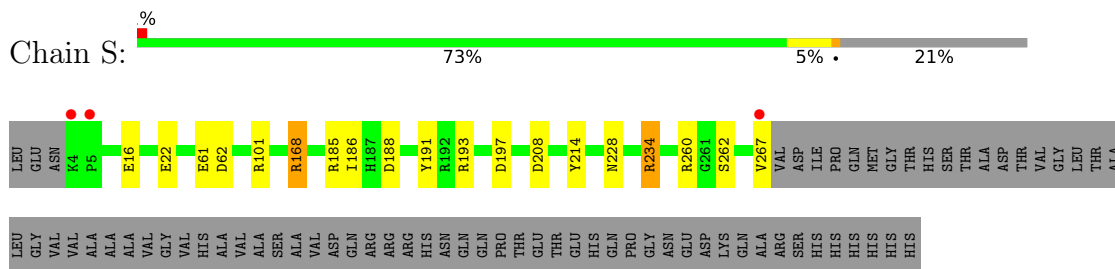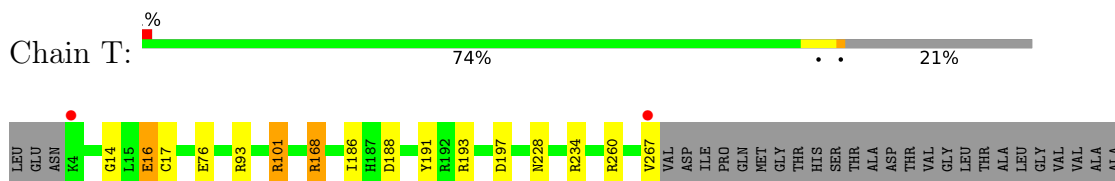
- Molecule 1: Hydrogenase-1 large chain

- Molecule 1: Hydrogenase-1 large chain

- Molecule 2: Hydrogenase-1 small chain

- Molecule 2: Hydrogenase-1 small chain

ALA VAL GLY VAL HIS ALA VAL ALA SER ALA VAL ASP GLN ARG ARG ARG HIS ASN GLN GLN PRO THR GLU THR GLU HIS GLN PRO GLY ASN GLU ASP LYS GLN ALA ARG SER HIS HIS HIS HIS HIS HIS

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.76Å 97.77Å 183.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.64 – 1.25 45.82 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (91.64-1.25) 99.8 (45.82-1.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.128 , 0.157 0.143 , 0.168	Depositor DCC
R_{free} test set	22969 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	10.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	14598	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, CL, FCO, F3S, NI, SF3, SF4, CSO, MG

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	L	0.78	2/4893 (0.0%)	0.91	18/6649 (0.3%)
1	M	0.78	2/4816 (0.0%)	0.91	18/6546 (0.3%)
2	S	0.87	3/2171 (0.1%)	1.04	17/2945 (0.6%)
2	T	0.82	1/2182 (0.0%)	1.02	9/2959 (0.3%)
All	All	0.80	8/14062 (0.1%)	0.95	62/19099 (0.3%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	260	ARG	CZ-NH1	9.21	1.45	1.33
2	T	260	ARG	CZ-NH1	8.37	1.44	1.33
2	S	262	SER	CB-OG	6.43	1.50	1.42
1	M	561	GLU	CD-OE1	6.39	1.32	1.25
1	L	561	GLU	CD-OE1	6.12	1.32	1.25

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	260	ARG	NE-CZ-NH2	-14.86	112.87	120.30
2	S	260	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	M	363	ARG	NE-CZ-NH1	11.88	126.24	120.30
2	S	197	ASP	CB-CG-OD1	10.89	128.10	118.30
2	T	260	ARG	NE-CZ-NH1	10.51	125.55	120.30

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	L	4707	0	4650	16	0
1	M	4648	0	4578	9	0
2	S	2092	0	2041	3	0
2	T	2100	0	2058	6	0
3	L	7	0	0	1	0
3	M	7	0	0	1	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
6	M	5	0	0	0	0
6	S	5	0	0	0	0
7	S	8	0	0	0	0
7	T	8	0	0	0	0
8	S	7	0	0	0	0
8	T	7	0	0	0	0
9	S	8	0	0	0	0
9	T	8	0	0	0	0
10	S	2	0	0	0	0
10	T	2	0	0	0	0
11	L	361	0	0	2	0
11	M	381	0	0	1	0
11	S	127	0	0	0	0
11	T	104	0	0	1	0
All	All	14598	0	13327	33	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 1.

The worst 5 of 33 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)
2:S:61[B]:GLU:OE2	2:S:101[B]:ARG:NH1	1.68	1.26
2:S:234[A]:ARG:HD3	2:T:234[A]:ARG:NH1	1.98	0.78
1:L:378:ASP:OD1	1:L:379[A]:VAL:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:254[B]:MET:HA	1:L:254[B]:MET:HE2	1.75	0.69
1:M:486[A]:SER:OG	1:M:488[A]:GLU:OE2	2.09	0.69

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	L	606/582 (104%)	591 (98%)	13 (2%)	2 (0%)	41	16
1	M	597/582 (103%)	582 (98%)	15 (2%)	0	100	100
2	S	271/335 (81%)	258 (95%)	13 (5%)	0	100	100
2	T	272/335 (81%)	259 (95%)	13 (5%)	0	100	100
All	All	1746/1834 (95%)	1690 (97%)	54 (3%)	2 (0%)	51	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	381[A]	GLY
1	L	381[B]	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	L	505/479 (105%)	503 (100%)	2 (0%)	91	77
1	M	497/479 (104%)	497 (100%)	0	100	100
2	S	226/274 (82%)	222 (98%)	4 (2%)	59	21
2	T	227/274 (83%)	222 (98%)	5 (2%)	52	14
All	All	1455/1506 (97%)	1444 (99%)	11 (1%)	86	53

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	16[B]	GLU
2	T	17	CYS
2	T	267	VAL
2	T	191	TYR
2	S	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	328	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	CSO	M	79	4,3,1	3,6,7	0.43	0	0,6,8	-	-
1	CSO	L	79	4,3,1	3,6,7	0.80	0	0,6,8	-	-

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	CSO	M	79	4,3,1	-	0/1/5/7	-
1	CSO	L	79	4,3,1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	79	CSO	1	0
1	L	79	CSO	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 8 are 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	#$|Z| > 2$
6	SO4	M	604	-	4,4,4	0.60	0	6,6,6	0.65	0
9	SF3	S	403[B]	11,2,9	0,8,8	-	-	-		
7	SF4	T	401	2	0,12,12	-	-	-		
9	SF3	S	403[C]	11,2,9	0,8,8	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles		
					Counts	RMSZ	#|Z| > 2		Counts	RMSZ	#|Z| > 2
8	F3S	T	402	2	0,9,9	-	-		-		
7	SF4	S	401	2	0,12,12	-	-		-		
9	SF3	T	403[B]	11,2,9	0,8,8	-	-		-		
6	SO4	S	407	-	4,4,4	0.63	0		6,6,6	1.10	1 (16%)
3	FCO	M	601	11,4,1	0,6,6	-	-		-		
3	FCO	L	601	11,4,1	0,6,6	-	-		-		
8	F3S	S	402	2	0,9,9	-	-		-		
9	SF3	T	403[C]	11,2,9	0,8,8	-	-		-		

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
9	SF3	S	403[B]	11,2,9	-	-	0/2/2/2
7	SF4	T	401	2	-	-	0/6/5/5
9	SF3	S	403[C]	11,2,9	-	-	0/2/2/2
8	F3S	T	402	2	-	-	0/3/3/3
7	SF4	S	401	2	-	-	0/6/5/5
9	SF3	T	403[B]	11,2,9	-	-	0/2/2/2
8	F3S	S	402	2	-	-	0/3/3/3
9	SF3	T	403[C]	11,2,9	-	-	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	407	SO4	O4-S-O3	2.18	118.38	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	601	FCO	1	0
3	L	601	FCO	1	0

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(Å²)	Q<0.9
1	L	580/582 (99%)	-0.54	6 (1%)	82	73	7, 12, 25, 53	0
1	M	580/582 (99%)	-0.60	1 (0%)	95	92	7, 12, 22, 36	0
2	S	264/335 (78%)	-0.55	3 (1%)	80	71	7, 11, 19, 53	0
2	T	264/335 (78%)	-0.48	2 (0%)	86	79	8, 12, 21, 55	0
All	All	1688/1834 (92%)	-0.55	12 (0%)	87	79	7, 12, 23, 55	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	267	VAL	4.5
2	T	4	LYS	4.0
2	S	4	LYS	3.5
2	S	267	VAL	3.2
1	M	143	ARG	2.7

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. 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	B-factors(Å²)	Q<0.9
1	CSO	L	79	7/8	0.98	0.07	11,11,14,21	0
1	CSO	M	79	7/8	0.99	0.06	11,11,14,21	0

6.3   Carbohydrates ⓘ

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
6	SO4	M	604	5/5	0.92	0.24	41,42,49,61	0
6	SO4	S	407	5/5	0.97	0.19	20,21,25,26	0
4	NI	L	602	1/1	1.00	0.02	15,15,15,15	0
4	NI	M	602	1/1	1.00	0.02	15,15,15,15	0
5	MG	L	603	1/1	1.00	0.06	6,6,6,6	0
5	MG	M	603	1/1	1.00	0.09	7,7,7,7	0
3	FCO	L	601	7/7	1.00	0.04	8,9,10,10	0
3	FCO	M	601	7/7	1.00	0.05	9,9,10,10	0
7	SF4	S	401	8/8	1.00	0.03	8,8,9,9	0
7	SF4	T	401	8/8	1.00	0.03	8,8,9,9	0
8	F3S	S	402	7/7	1.00	0.03	8,8,8,9	0
8	F3S	T	402	7/7	1.00	0.03	8,8,9,9	0
9	SF3	S	403[B]	7/7	1.00	0.03	8,10,11,12	1
9	SF3	S	403[C]	7/7	1.00	0.03	8,10,12,21	1
9	SF3	T	403[B]	7/7	1.00	0.03	8,10,11,12	1
9	SF3	T	403[C]	7/7	1.00	0.03	9,10,12,26	1
10	CL	S	405	1/1	1.00	0.03	13,13,13,13	0
10	CL	S	406	1/1	1.00	0.03	17,17,17,17	0
10	CL	T	405	1/1	1.00	0.03	14,14,14,14	0
10	CL	T	406	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.