Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 09:42 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)

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

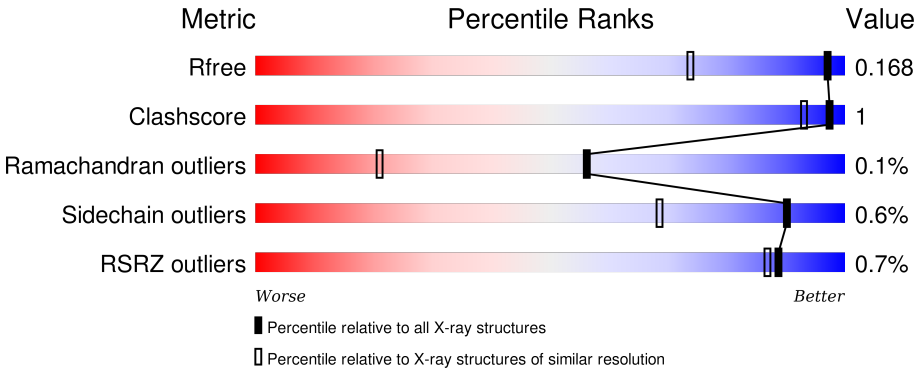
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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}	91344	1442 (1.30-1.22)
Clashscore	102246	1530 (1.30-1.22)
Ramachandran outliers	100387	1467 (1.30-1.22)
Sidechain outliers	100360	1465 (1.30-1.22)
RSRZ outliers	91569	1442 (1.30-1.22)

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 <=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%

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	MG	M	603	-	-	-	X
6	SO4	S	407	-	-	-	X

2 Entry composition

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	C	N	O	S	0	28	0
			4707	2992	823	863	29			
1	M	581	Total	C	N	O	S	0	19	0
			4648	2957	808	855	28			

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	C	N	O	S	0	9	0
			2092	1328	359	384	21			
2	T	264	Total	C	N	O	S	0	10	0
			2100	1334	362	383	21			

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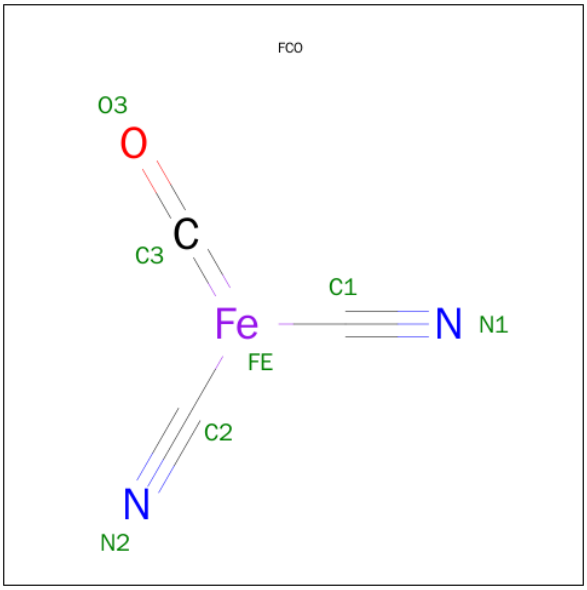
Chain	Residue	Modelled	Actual	Comment	Reference
T	330	HIS	-	EXPRESSION TAG	UNP P69739
T	331	HIS	-	EXPRESSION TAG	UNP P69739
T	332	HIS	-	EXPRESSION TAG	UNP P69739
T	333	HIS	-	EXPRESSION TAG	UNP P69739
T	334	HIS	-	EXPRESSION TAG	UNP P69739
T	335	HIS	-	EXPRESSION TAG	UNP P69739

- 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		

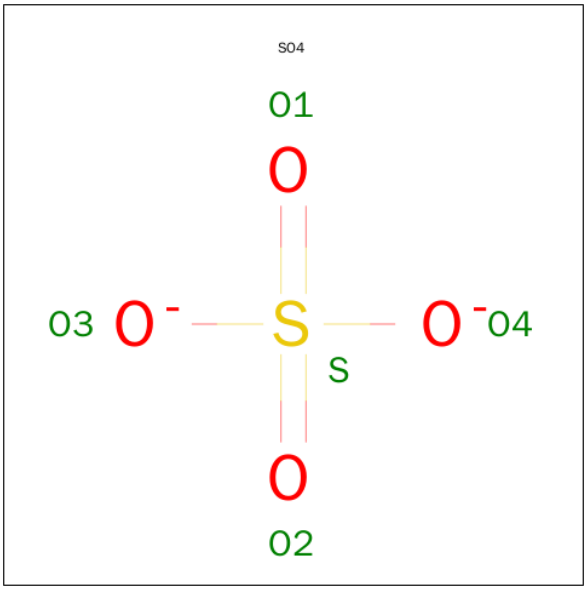
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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).

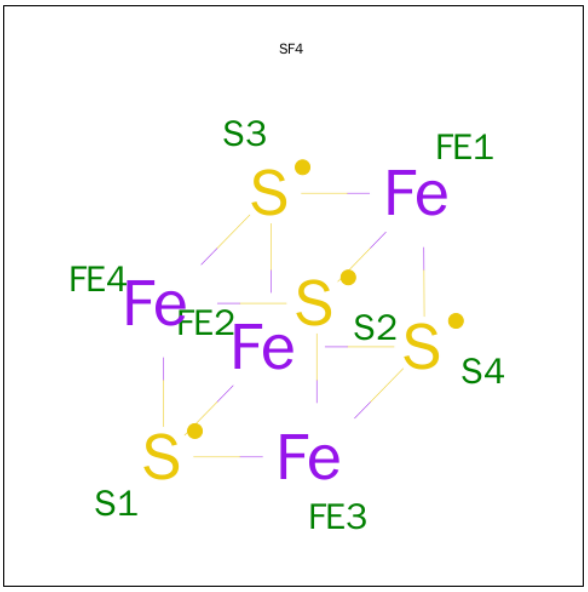
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Mg 1 1	0	0
5	M	1	Total Mg 1 1	0	0

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



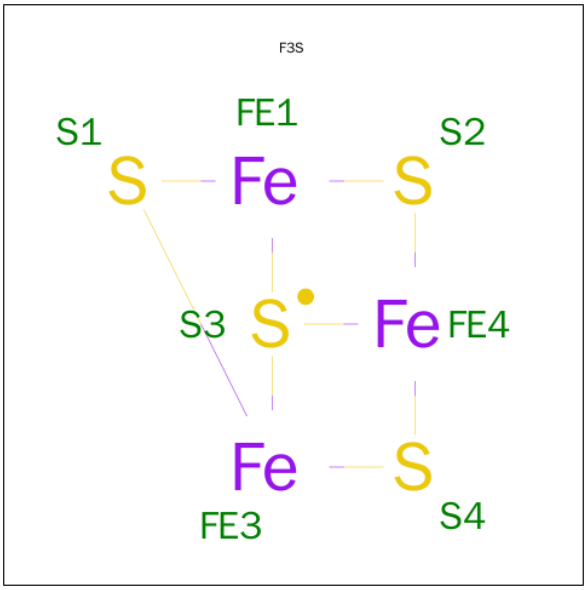
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total O S 5 4 1	0	0
6	S	1	Total O S 5 4 1	0	0

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



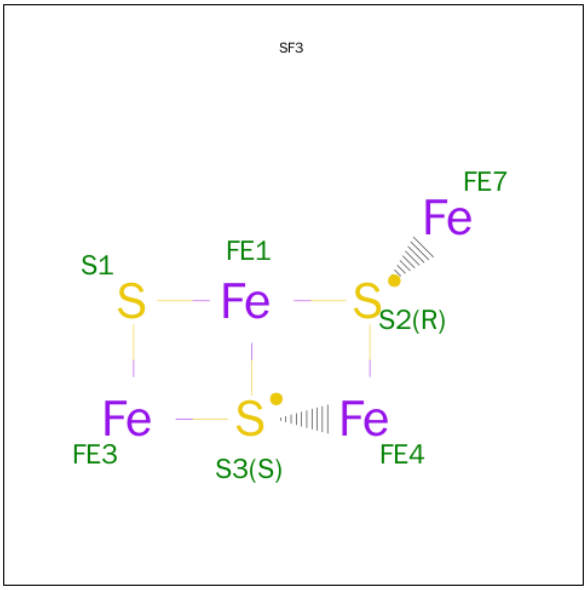
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	1	Total Fe S 8 4 4	0	0
7	T	1	Total Fe S 8 4 4	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	S	1	Total Fe S 7 3 4	0	0
8	T	1	Total Fe S 7 3 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 Fe S 8 5 3	0	1
9	T	1	Total Fe S 8 5 3	0	1

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

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

- Molecule 11 is water.

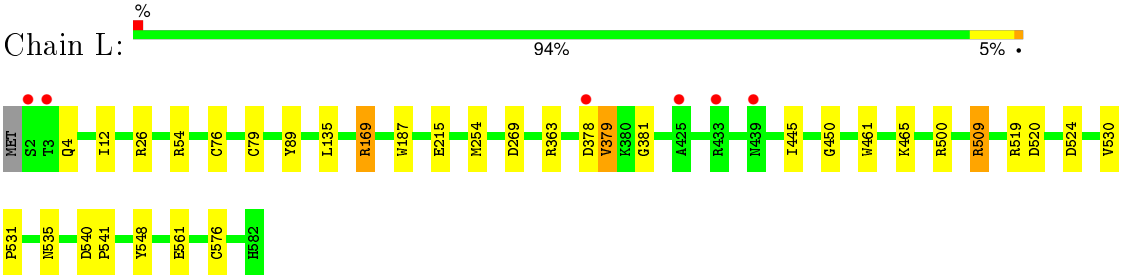
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	361	Total O 361 361	0	0
11	M	381	Total O 381 381	0	0
11	S	127	Total O 127 127	0	0
11	T	104	Total O 104 104	0	0

3 Residue-property plots (i)

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.

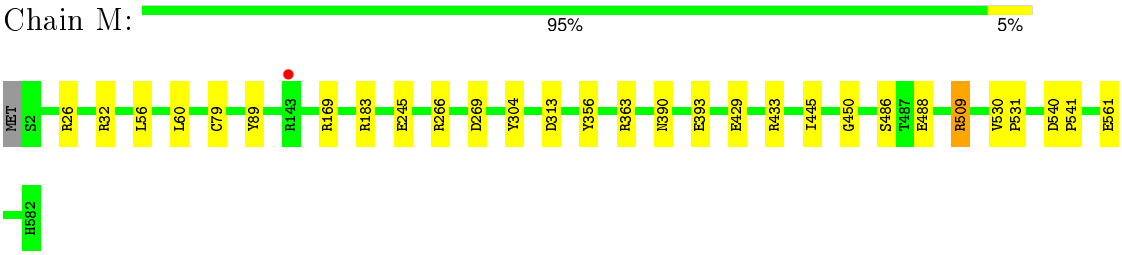
- Molecule 1: HYDROGENASE-1 LARGE CHAIN

Chain L:



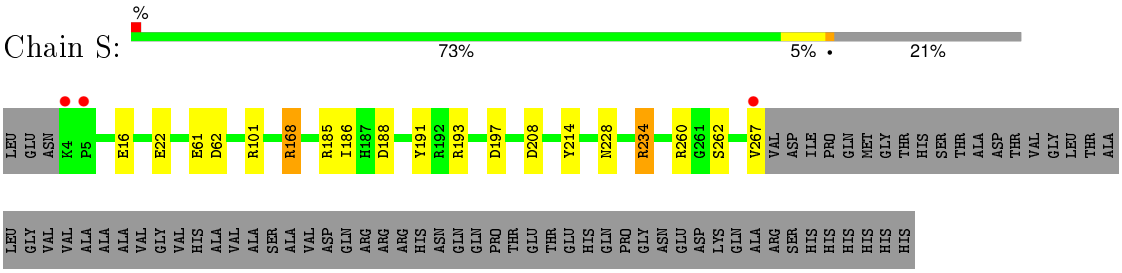
- Molecule 1: HYDROGENASE-1 LARGE CHAIN

Chain M:



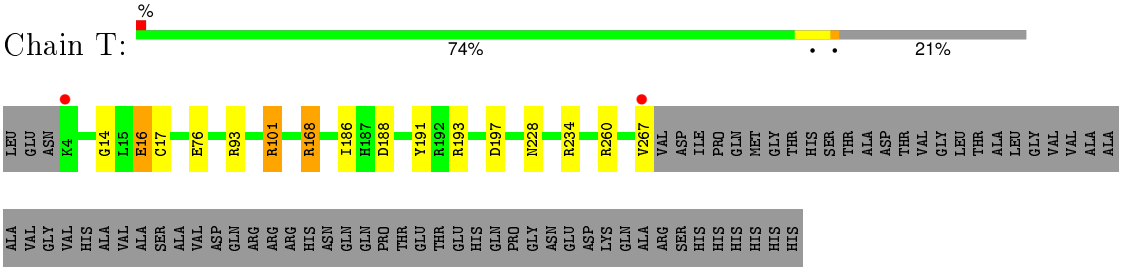
- Molecule 2: HYDROGENASE-1 SMALL CHAIN

Chain S:



- Molecule 2: HYDROGENASE-1 SMALL CHAIN

Chain T:



4 Data and refinement statistics (i)

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	23005 reflections (5.25%)	DCC
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
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 460770 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CSO, CL, SF4, MG, SF3, F3S, SO4, FCO

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%)

All (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
1	M	245	GLU	CD-OE2	5.54	1.31	1.25
1	L	561	GLU	CG-CD	5.15	1.59	1.51
2	S	188	ASP	CB-CG	5.15	1.62	1.51

All (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
2	S	260	ARG	NE-CZ-NH1	10.46	125.53	120.30
2	T	197	ASP	CB-CG-OD1	9.18	126.56	118.30
2	S	197	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	L	89	TYR	CB-CG-CD1	8.29	125.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	234[A]	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	S	234[B]	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	T	193	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	T	93	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	M	89	TYR	CB-CG-CD1	6.71	125.03	121.00
1	M	169	ARG	NE-CZ-NH1	6.71	123.65	120.30
2	S	185	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	M	169	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	M	269[A]	ASP	CB-CG-OD1	6.40	124.06	118.30
1	M	269[B]	ASP	CB-CG-OD1	6.40	124.06	118.30
1	L	89	TYR	CB-CG-CD2	-6.31	117.21	121.00
1	L	215	GLU	OE1-CD-OE2	-6.28	115.77	123.30
1	M	32	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	L	169	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	M	509	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	L	26	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	L	509	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	M	26	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	L	379[A]	VAL	N-CA-C	-5.80	95.35	111.00
1	L	379[B]	VAL	N-CA-C	-5.80	95.35	111.00
2	T	101	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	T	197	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	M	183	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	L	363[A]	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	L	363[B]	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	S	193	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	S	62	ASP	CB-CG-OD1	5.58	123.32	118.30
2	S	168	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	T	188	ASP	CB-CG-OD1	5.49	123.24	118.30
1	M	313	ASP	CB-CG-OD1	5.44	123.19	118.30
1	L	26	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	M	89	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	L	500	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	L	269[A]	ASP	CB-CG-OD1	5.30	123.07	118.30
1	L	269[B]	ASP	CB-CG-OD1	5.30	123.07	118.30
1	L	169	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	L	54	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	M	26	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	S	185	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	S	214	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	M	356	TYR	CB-CG-CD1	5.24	124.14	121.00
2	S	22	GLU	OE1-CD-OE2	-5.22	117.03	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	168	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	M	304	TYR	CB-CG-CD1	5.18	124.11	121.00
1	L	379[A]	VAL	CB-CA-C	5.14	121.17	111.40
1	L	379[B]	VAL	CB-CA-C	5.14	121.17	111.40
2	S	168	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	M	266	ARG	NE-CZ-NH2	-5.09	117.76	120.30
2	S	260	ARG	CG-CD-NE	-5.08	101.13	111.80
1	M	433[A]	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	M	433[B]	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	S	208	ASP	CB-CG-OD1	5.02	122.82	118.30
2	S	267	VAL	CG1-CB-CG2	-5.02	102.87	110.90

There are no chirality outliers.

There are no planarity outliers.

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:M:486[A]:SER:OG	1:M:488[A]:GLU:OE2	2.09	0.69
1:L:254[B]:MET:HA	1:L:254[B]:MET:HE2	1.75	0.69
1:L:135:LEU:HD22	1:L:187:TRP:CD1	2.46	0.50
1:M:429[B]:GLU:HG3	11:M:2322:HOH:O	2.12	0.50
11:L:2188:HOH:O	2:T:168:ARG:CZ	2.60	0.49
1:L:530:VAL:CG1	1:L:531:PRO:HD2	2.44	0.48
2:T:186:ILE:HD11	2:T:228:ASN:HB3	1.97	0.47
2:T:76[B]:GLU:HG3	11:T:2005:HOH:O	2.13	0.47
1:L:540:ASP:HB2	1:L:541:PRO:CD	2.45	0.46
1:L:76:CYS:CB	1:L:79:CSO:OD	2.56	0.46
1:M:390:ASN:ND2	1:M:393[B]:GLU:OE2	2.49	0.46
2:T:101:ARG:HH11	2:T:101:ARG:HG3	1.81	0.46
1:M:79:CSO:N	1:M:79:CSO:OD	2.50	0.44
1:L:530:VAL:HG12	1:L:531:PRO:HD2	1.99	0.44
1:L:576:CYS:CB	11:L:2071:HOH:O	2.66	0.44
2:T:14:GLY:O	2:T:16[A]:GLU:HG3	2.17	0.44
2:S:186:ILE:HD11	2:S:228:ASN:HB3	2.00	0.44
1:L:4:GLN:HA	1:L:12:ILE:O	2.18	0.43
1:L:79:CSO:N	1:L:79:CSO:OD	2.51	0.43
1:M:540:ASP:HB2	1:M:541:PRO:CD	2.47	0.43
1:L:254[B]:MET:HE2	1:L:254[B]:MET:CA	2.42	0.43
1:M:509:ARG:HD2	3:M:601:FCO:C2	2.49	0.43
1:L:445:ILE:O	1:L:450:GLY:HA3	2.18	0.43
1:L:509:ARG:HD2	3:L:601:FCO:C2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:530:VAL:CG1	1:M:531:PRO:HD2	2.49	0.42
1:M:56:LEU:O	1:M:60:LEU:HD23	2.20	0.42
1:M:445:ILE:O	1:M:450:GLY:HA3	2.19	0.42
1:L:535:ASN:HB3	1:L:548:TYR:CE1	2.55	0.42
1:L:461:TRP:CZ2	1:L:465:LYS:HE2	2.55	0.41
1:L:519[B]:ARG:HG2	1:L:520:ASP:OD2	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	606/582 (104%)	591 (98%)	13 (2%)	2 (0%)	46 17
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%)	56 21

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 (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	L	505/479 (105%)	503 (100%)	2 (0%)	93 77
1	M	497/479 (104%)	497 (100%)	0	100 100
2	S	226/274 (82%)	222 (98%)	4 (2%)	66 26
2	T	227/274 (83%)	222 (98%)	5 (2%)	60 18
All	All	1455/1506 (97%)	1444 (99%)	11 (1%)	90 61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	169	ARG
1	L	524	ASP
2	S	16[A]	GLU
2	S	16[B]	GLU
2	S	168	ARG
2	S	191	TYR
2	T	16[A]	GLU
2	T	16[B]	GLU
2	T	17	CYS
2	T	191	TYR
2	T	267	VAL

Some 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 (i)

There are no RNA molecules in this entry.

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

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	L	79	1,3,4	3,6,7	0.67	0	2,6,8	0.77	0
1	CSO	M	79	1,3,4	3,6,7	2.99	1 (33%)	2,6,8	1.24	0

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	79	CSO	CB-SG	-5.14	1.75	1.82

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	L	79	CSO	2	0
1	M	79	CSO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	FCO	L	601	1,11,4	0,6,6	0.00	-	0,6,6	0.00	-
3	FCO	M	601	1,11,4	0,6,6	0.00	-	0,6,6	0.00	-
6	SO4	M	604	-	4,4,4	0.96	0	6,6,6	0.57	0
7	SF4	S	401	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	S	402	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF3	S	403[B]	11,9,2	0,8,8	0.00	-	0,12,12	0.00	-
9	SF3	S	403[C]	11,9,2	0,8,8	0.00	-	0,12,12	0.00	-
6	SO4	S	407	-	4,4,4	1.00	0	6,6,6	1.08	1 (16%)
7	SF4	T	401	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	T	402	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF3	T	403[B]	11,9,2	0,8,8	0.00	-	0,12,12	0.00	-
9	SF3	T	403[C]	11,9,2	0,8,8	0.00	-	0,12,12	0.00	-

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	FCO	L	601	1,11,4	-	0/0/6/6	0/0/0/0
3	FCO	M	601	1,11,4	-	0/0/6/6	0/0/0/0
6	SO4	M	604	-	-	0/0/0/0	0/0/0/0
7	SF4	S	401	2	-	0/0/48/48	0/6/5/5
8	F3S	S	402	2	-	0/0/24/24	0/0/3/3
9	SF3	S	403[B]	11,9,2	-	0/0/17/17	0/2/2/2
9	SF3	S	403[C]	11,9,2	-	0/0/17/17	0/2/2/2
6	SO4	S	407	-	-	0/0/0/0	0/0/0/0
7	SF4	T	401	2	-	0/0/48/48	0/6/5/5
8	F3S	T	402	2	-	0/0/24/24	0/0/3/3
9	SF3	T	403[B]	11,9,2	-	0/0/17/17	0/2/2/2
9	SF3	T	403[C]	11,9,2	-	0/0/17/17	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	2.30	118.38	109.09

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	L	601	FCO	1	0
3	M	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, 95^{th} 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	L	580/582 (99%)	-0.53	6 (1%)	84	82	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%)	82	80	7, 11, 19, 53	0
2	T	264/335 (78%)	-0.47	2 (0%)	87	86	8, 12, 21, 55	0
All	All	1688/1834 (92%)	-0.55	12 (0%)	89	87	7, 12, 23, 55	0

All (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
2	S	5	PRO	2.3
1	L	2	SER	2.2
1	L	378	ASP	2.2
1	L	433	ARG	2.2
1	L	439[A]	ASN	2.1
1	L	425	ALA	2.1
1	L	3	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
1	CSO	M	79	7/8	0.99	0.06	-	11,11,14,21	0
1	CSO	L	79	7/8	0.98	0.07	-	11,11,14,21	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
6	SO4	S	407	5/5	0.97	0.19	5.38	20,21,25,26	0
5	MG	M	603	1/1	1.00	0.09	4.26	7,7,7,7	0
5	MG	L	603	1/1	1.00	0.06	0.12	6,6,6,6	0
8	F3S	S	402	7/7	1.00	0.03	-1.11	8,8,8,9	0
7	SF4	S	401	8/8	1.00	0.03	-1.46	8,8,9,9	0
3	FCO	M	601	7/7	1.00	0.05	-1.48	9,9,10,10	0
9	SF3	T	403[B]	7/7	1.00	0.03	-1.55	8,10,11,12	1
9	SF3	T	403[C]	7/7	1.00	0.03	-1.55	9,10,12,26	1
10	CL	S	405	1/1	1.00	0.03	-1.60	13,13,13,13	0
7	SF4	T	401	8/8	1.00	0.03	-1.61	8,8,9,9	0
10	CL	T	405	1/1	1.00	0.03	-1.70	14,14,14,14	0
9	SF3	S	403[B]	7/7	1.00	0.03	-1.83	8,10,11,12	1
9	SF3	S	403[C]	7/7	1.00	0.03	-1.83	8,10,12,21	1
8	F3S	T	402	7/7	1.00	0.03	-1.85	8,8,9,9	0
3	FCO	L	601	7/7	1.00	0.04	-1.93	8,9,10,10	0
10	CL	S	406	1/1	1.00	0.03	-2.03	17,17,17,17	0
10	CL	T	406	1/1	1.00	0.03	-2.43	18,18,18,18	0
6	SO4	M	604	5/5	0.91	0.24	-	41,42,49,61	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

6.5 Other polymers (i)

There are no such residues in this entry.