Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:28 am BST

PDB ID	:	4UE3
Title	:	The Mechanism of Hydrogen Activation by NiFe-hydrogenases and the Importance of the active site Arginine
Authors	:	Evans, R.M.; Wehlin, S.A.M.; Nomerotskaia, E.; Sargent, F.; Carr, S.B.; Phillips, S.E.V.; Armstrong, F.A.
Deposited on	:	2014-12-15
Resolution	:	1.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

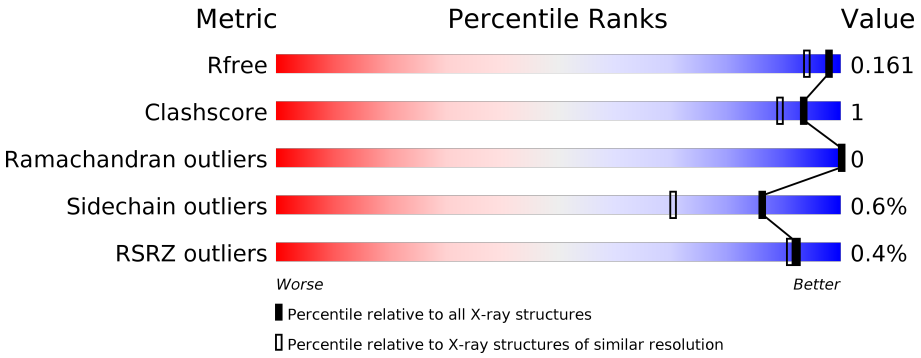
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

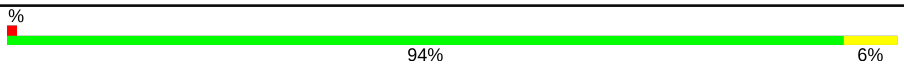
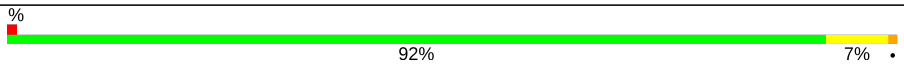
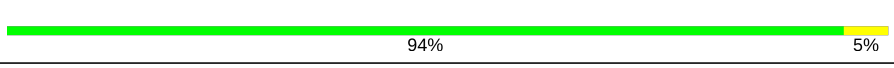
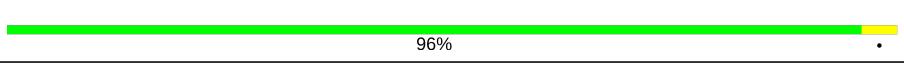
The reported resolution of this entry is 1.40 Å.

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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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	SSS	264	
1	TTT	264	
2	LLL	581	
2	MMM	581	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14815 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 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	SSS	264	Total	C	N	O	S	0	6	0
			2073	1318	354	381	20			
1	TTT	264	Total	C	N	O	S	0	7	0
			2075	1317	352	385	21			

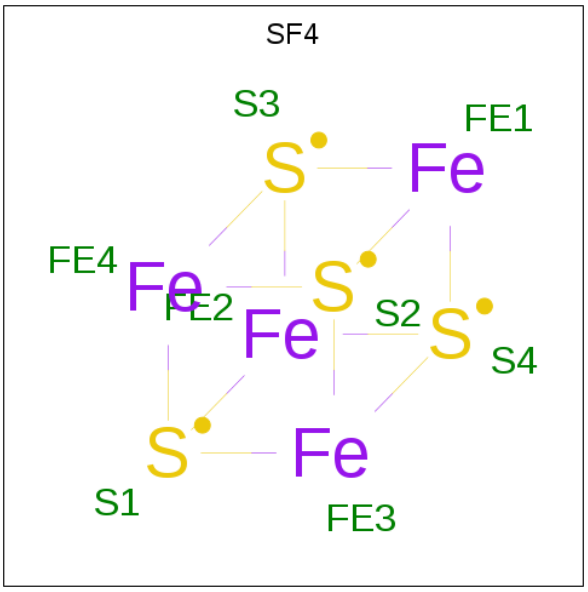
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	LLL	581	Total	C	N	O	S	0	17	0
			4647	2952	817	851	27			
2	MMM	581	Total	C	N	O	S	0	9	0
			4591	2916	802	846	27			

There are 2 discrepancies between the modelled and reference sequences:

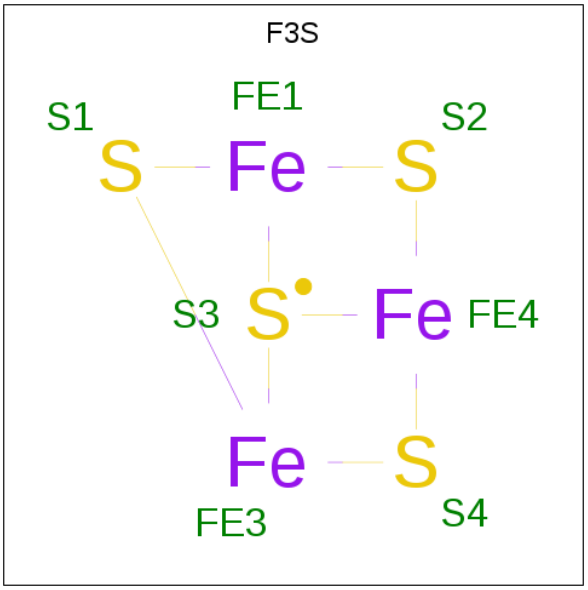
Chain	Residue	Modelled	Actual	Comment	Reference
LLL	509	LYS	ARG	engineered mutation	UNP P0ACD8
MMM	509	LYS	ARG	engineered mutation	UNP P0ACD8

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



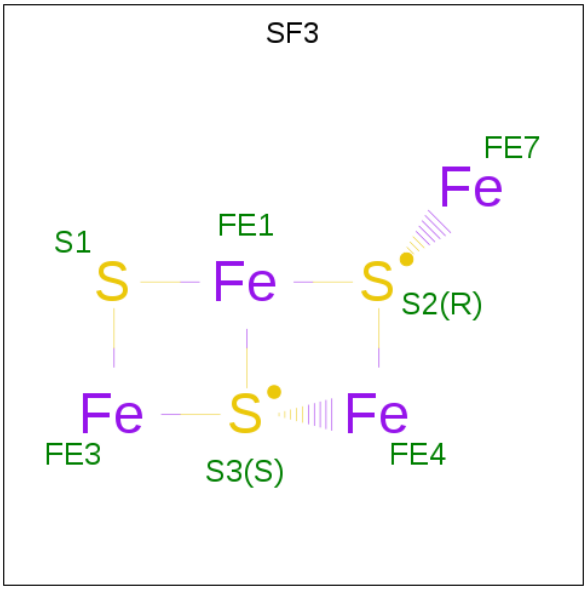
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	SSS	1	Total Fe S 8 4 4	0	0
3	TTT	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	SSS	1	Total Fe S 7 3 4	0	0
4	TTT	1	Total Fe S 7 3 4	0	0

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe_4S_3).

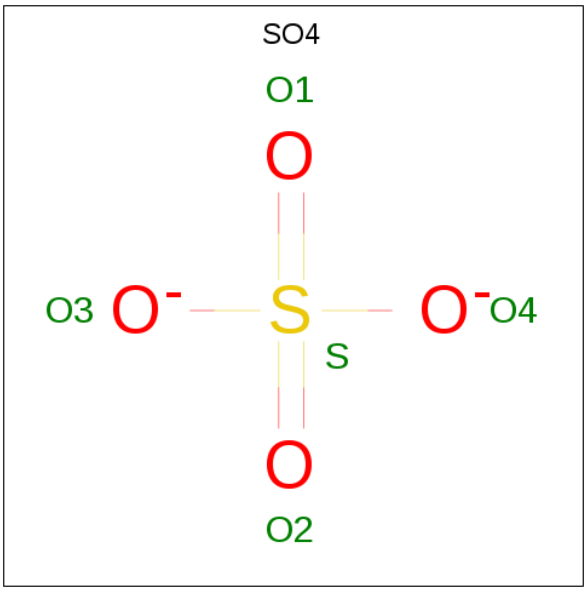


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	SSS	1	Total Fe S 8 5 3	0	1
5	TTT	1	Total Fe S 8 5 3	0	1

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

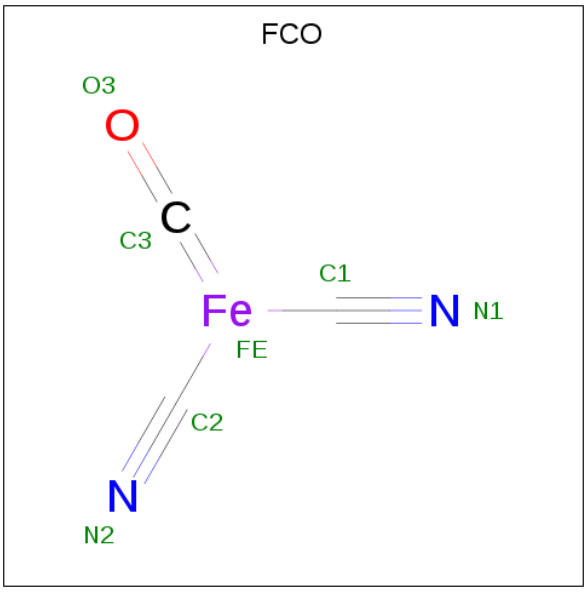
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	SSS	2	Total Cl 2 2	0	0
6	TTT	2	Total Cl 2 2	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	LLL	1	Total O S 5 4 1	0	0
7	TTT	1	Total O S 5 4 1	0	0
7	MMM	1	Total O S 5 4 1	0	0
7	MMM	1	Total O S 5 4 1	0	0

- Molecule 8 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	LLL	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
8	MMM	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 9 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	MMM	1	Total	Ni	0	0
			1	1		
9	LLL	1	Total	Ni	0	0
			1	1		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	MMM	1	Total	Mg	0	0
			1	1		
10	LLL	1	Total	Mg	0	0
			1	1		

- Molecule 11 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	MMM	1	Total	Li	0	0
			1	1		

- Molecule 12 is water.

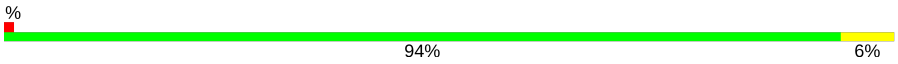
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	SSS	196	Total	O	0	0
			196	196		
12	LLL	455	Total	O	0	0
			455	455		
12	TTT	184	Total	O	0	0
			184	184		
12	MMM	505	Total	O	0	0
			505	505		

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 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.

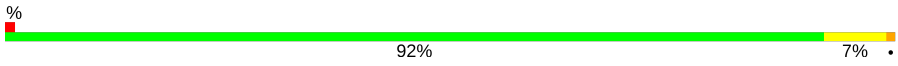
- Molecule 1: Hydrogenase-1 small chain

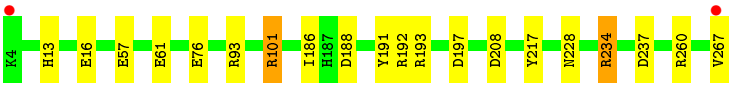
Chain SSS:



- Molecule 1: Hydrogenase-1 small chain

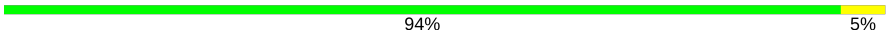
Chain TTT:

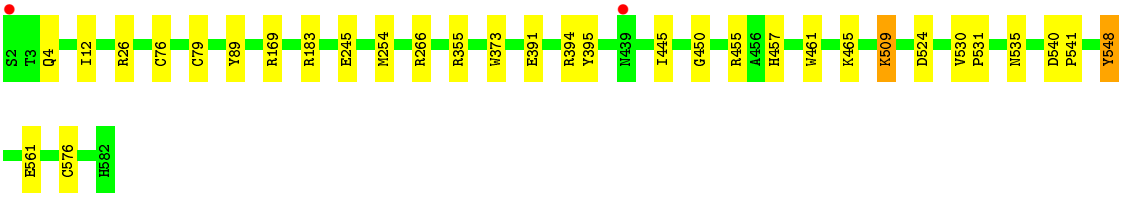




- Molecule 2: Hydrogenase-1 large chain

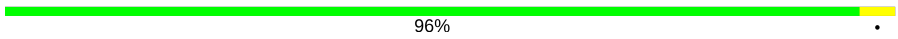
Chain LLL:

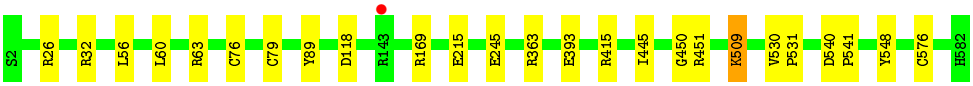




- Molecule 2: Hydrogenase-1 large chain

Chain MMM:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.52Å 97.41Å 183.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 1.40 48.70 – 1.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.75-1.40) 96.8 (48.70-1.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.140 , 0.160 0.140 , 0.161	Depositor DCC
R_{free} test set	15658 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	11.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14815	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 6.43% 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, 0.333 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: NI, CSO, CL, SF4, MG, SF3, F3S, SO4, LI, 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	SSS	0.82	3/2143 (0.1%)	1.04	10/2909 (0.3%)
1	TTT	0.81	2/2148 (0.1%)	1.07	13/2916 (0.4%)
2	LLL	0.78	2/4809 (0.0%)	0.95	11/6536 (0.2%)
2	MMM	0.80	3/4729 (0.1%)	0.96	12/6433 (0.2%)
All	All	0.80	10/13829 (0.1%)	0.99	46/18794 (0.2%)

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	SSS	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	LLL	245	GLU	CD-OE1	7.62	1.34	1.25
2	MMM	393	GLU	CD-OE1	6.66	1.32	1.25
1	SSS	97	GLU	CD-OE1	-6.46	1.18	1.25
2	MMM	245	GLU	CD-OE1	6.44	1.32	1.25
1	TTT	57	GLU	CD-OE2	-6.43	1.18	1.25
2	LLL	561	GLU	CD-OE1	6.07	1.32	1.25
1	TTT	188	ASP	CG-OD2	-5.67	1.12	1.25
2	MMM	215	GLU	CD-OE1	-5.65	1.19	1.25
1	SSS	107	SER	CA-CB	-5.19	1.45	1.52
1	SSS	97	GLU	CD-OE2	-5.19	1.20	1.25

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SSS	260	ARG	NE-CZ-NH2	-13.05	113.77	120.30
1	TTT	260	ARG	NE-CZ-NH2	-11.01	114.80	120.30
2	MMM	169	ARG	NE-CZ-NH2	-10.61	114.99	120.30
2	LLL	254	MET	CG-SD-CE	9.66	115.65	100.20
2	LLL	89	TYR	CB-CG-CD1	8.74	126.24	121.00
1	TTT	260	ARG	NE-CZ-NH1	8.24	124.42	120.30
2	LLL	26	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	SSS	237	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	SSS	234	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	SSS	260	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	LLL	26	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	TTT	197	ASP	CB-CG-OD1	7.07	124.67	118.30
2	MMM	363	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	TTT	193	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	TTT	93	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	LLL	169	ARG	NE-CZ-NH2	-6.37	117.12	120.30
2	LLL	89	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	SSS	197	ASP	CB-CG-OD1	6.31	123.98	118.30
2	LLL	266	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	SSS	193	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	TTT	237	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	TTT	193	ARG	CG-CD-NE	-6.08	99.03	111.80
2	MMM	26	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	MMM	451	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	MMM	415	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	MMM	63	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	TTT	193	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	MMM	89	TYR	CB-CG-CD1	5.76	124.46	121.00
2	MMM	548	TYR	CB-CG-CD2	-5.70	117.58	121.00
2	LLL	394	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	SSS	197	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	LLL	548	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	TTT	234	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	MMM	118	ASP	CB-CG-OD1	-5.54	113.31	118.30
2	LLL	455	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	TTT	197	ASP	CB-CG-OD2	-5.47	113.37	118.30
2	MMM	32	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	MMM	548	TYR	CB-CG-CD1	5.45	124.27	121.00
1	TTT	217	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	SSS	260	ARG	CG-CD-NE	-5.32	100.64	111.80
1	SSS	193	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	MMM	169	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	TTT	192	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	LLL	548	TYR	CB-CG-CD1	5.17	124.10	121.00
1	SSS	234	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	TTT	208	ASP	CB-CG-OD2	-5.07	113.74	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	SSS	26	ARG	Sidechain

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	SSS	2073	0	2022	5	0
1	TTT	2075	0	2014	9	0
2	LLL	4647	0	4576	16	0
2	MMM	4591	0	4493	7	0
3	SSS	8	0	0	0	0
3	TTT	8	0	0	0	0
4	SSS	7	0	0	0	0
4	TTT	7	0	0	0	0
5	SSS	8	0	0	0	0
5	TTT	8	0	0	0	0
6	SSS	2	0	0	0	0
6	TTT	2	0	0	0	0
7	LLL	5	0	0	0	0
7	MMM	10	0	0	1	0
7	TTT	5	0	0	0	0
8	LLL	7	0	0	0	0
8	MMM	7	0	0	0	0
9	LLL	1	0	0	0	0
9	MMM	1	0	0	0	0
10	LLL	1	0	0	0	0
10	MMM	1	0	0	0	0
11	MMM	1	0	0	0	0
12	LLL	455	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	MMM	505	0	0	1	0
12	SSS	196	0	0	2	0
12	TTT	184	0	0	3	0
All	All	14815	0	13105	37	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 (37) 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:LLL:183[B]:ARG:NH1	12:LLL:704:HOH:O	1.83	1.12
1:TTT:61[B]:GLU:HG2	12:TTT:506:HOH:O	1.80	0.82
1:TTT:101:ARG:HH11	1:TTT:101:ARG:HG3	1.60	0.66
1:TTT:76[B]:GLU:HG3	12:TTT:513:HOH:O	2.00	0.60
1:TTT:16[B]:GLU:HG2	12:TTT:538:HOH:O	2.00	0.60
2:LLL:79:CSO:OD	2:LLL:79:CSO:N	2.35	0.59
2:MMM:79:CSO:N	2:MMM:79:CSO:OD	2.38	0.57
1:SSS:16[B]:GLU:HG2	12:SSS:593:HOH:O	2.04	0.56
2:LLL:183[B]:ARG:NH2	12:LLL:701:HOH:O	0.70	0.55
1:TTT:61[B]:GLU:OE1	1:TTT:101:ARG:NH2	2.41	0.53
2:LLL:530:VAL:CG1	2:LLL:531:PRO:HD2	2.40	0.51
2:MMM:530:VAL:CG1	2:MMM:531:PRO:HD2	2.41	0.51
2:MMM:76:CYS:CB	2:MMM:79:CSO:OD	2.53	0.49
2:LLL:445:ILE:O	2:LLL:450:GLY:HA3	2.13	0.47
2:LLL:457:HIS:HB2	12:LLL:1106:HOH:O	2.14	0.47
2:MMM:56:LEU:O	2:MMM:60:LEU:HD23	2.15	0.47
1:TTT:186:ILE:HD11	1:TTT:228:ASN:HB3	1.97	0.47
2:LLL:183[B]:ARG:CZ	12:LLL:704:HOH:O	2.45	0.46
2:MMM:540:ASP:HB2	2:MMM:541:PRO:CD	2.45	0.46
2:LLL:4:GLN:HA	2:LLL:12:ILE:O	2.15	0.46
1:SSS:186:ILE:HD11	1:SSS:228:ASN:HB3	1.99	0.45
2:LLL:540:ASP:HB2	2:LLL:541:PRO:CD	2.46	0.45
2:LLL:355[A]:ARG:HG3	2:LLL:373:TRP:HB2	1.99	0.44
2:MMM:445:ILE:O	2:MMM:450:GLY:HA3	2.17	0.44
1:TTT:101:ARG:NH1	1:TTT:101:ARG:HG3	2.26	0.44
2:MMM:509:LYS:HE2	2:MMM:576:CYS:HB2	2.00	0.43
1:SSS:13:HIS:HD1	1:SSS:16[B]:GLU:CD	2.22	0.43
2:LLL:530:VAL:HG12	2:LLL:531:PRO:HD2	2.01	0.42
7:MMM:601:SO4:O3	12:MMM:701:HOH:O	2.21	0.42
1:TTT:13:HIS:HD1	1:TTT:16[B]:GLU:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:535:ASN:HB3	2:LLL:548:TYR:CE1	2.55	0.41
2:LLL:461:TRP:CZ2	2:LLL:465:LYS:HE2	2.55	0.41
1:SSS:234:ARG:NH1	1:TTT:234:ARG:HE	2.19	0.41
1:SSS:76[B]:GLU:HG3	12:SSS:582:HOH:O	2.20	0.41
2:LLL:509:LYS:HE2	2:LLL:576:CYS:HB2	2.02	0.41
2:LLL:391:GLU:HA	2:LLL:395:TYR:CD2	2.56	0.41
2:LLL:76:CYS:CB	2:LLL:79:CSO:OD	2.57	0.40

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	SSS	268/264 (102%)	257 (96%)	11 (4%)	0	100	100
1	TTT	269/264 (102%)	257 (96%)	12 (4%)	0	100	100
2	LLL	595/581 (102%)	581 (98%)	14 (2%)	0	100	100
2	MMM	587/581 (101%)	572 (97%)	15 (3%)	0	100	100
All	All	1719/1690 (102%)	1667 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	SSS	223/217 (103%)	220 (99%)	3 (1%)	69 42
1	TTT	224/217 (103%)	221 (99%)	3 (1%)	69 42
2	LLL	496/479 (104%)	494 (100%)	2 (0%)	91 78
2	MMM	488/479 (102%)	487 (100%)	1 (0%)	93 82
All	All	1431/1392 (103%)	1422 (99%)	9 (1%)	86 70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SSS	168	ARG
1	SSS	191	TYR
1	SSS	267	VAL
2	LLL	509	LYS
2	LLL	524	ASP
1	TTT	101	ARG
1	TTT	191	TYR
1	TTT	267	VAL
2	MMM	509	LYS

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 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	$\#\|Z\| > 2$
2	CSO	MMM	79	9,8,2	3,6,7	0.85	0	0,6,8	0.00	-
2	CSO	LLL	79	9,8,2	3,6,7	0.66	0	0,6,8	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
2	CSO	MMM	79	9,8,2	-	0/1/5/7	-
2	CSO	LLL	79	9,8,2	-	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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	MMM	79	CSO	2	0
2	LLL	79	CSO	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
5	SF3	TTT	403[C]	1,12	0,8,8	0.00	-	-		
7	SO4	MMM	605	-	4,4,4	0.22	0	6,6,6	0.24	0
5	SF3	TTT	403[B]	1,12	0,8,8	0.00	-	-		
3	SF4	TTT	401	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SF3	SSS	403[B]	1,12	0,8,8	0.00	-	-		
3	SF4	SSS	401	1	0,12,12	0.00	-	-		
5	SF3	SSS	403[C]	1,12	0,8,8	0.00	-	-		
8	FCO	MMM	602	12,2	0,6,6	0.00	-	-		
7	SO4	TTT	406	-	4,4,4	0.37	0	6,6,6	0.11	0
8	FCO	LLL	602	12,2	0,6,6	0.00	-	-		
4	F3S	SSS	402	1	0,9,9	0.00	-	-		
4	F3S	TTT	402	1	0,9,9	0.00	-	-		
7	SO4	MMM	601	-	4,4,4	0.32	0	6,6,6	0.10	0
7	SO4	LLL	601	-	4,4,4	0.32	0	6,6,6	0.42	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
5	SF3	TTT	403[C]	1,12	-	-	0/2/2/2
5	SF3	TTT	403[B]	1,12	-	-	0/2/2/2
3	SF4	TTT	401	1	-	-	0/6/5/5
5	SF3	SSS	403[B]	1,12	-	-	0/2/2/2
3	SF4	SSS	401	1	-	-	0/6/5/5
5	SF3	SSS	403[C]	1,12	-	-	0/2/2/2
4	F3S	SSS	402	1	-	-	0/3/3/3
4	F3S	TTT	402	1	-	-	0/3/3/3

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	MMM	601	SO4	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	SSS	264/264 (100%)	-0.39	2 (0%)	86	84	7, 10, 20, 53	0
1	TTT	264/264 (100%)	-0.35	2 (0%)	86	84	7, 11, 22, 54	0
2	LLL	580/581 (99%)	-0.44	2 (0%)	94	93	6, 12, 23, 51	0
2	MMM	580/581 (99%)	-0.50	1 (0%)	95	93	7, 11, 21, 36	0
All	All	1688/1690 (99%)	-0.44	7 (0%)	92	91	6, 11, 22, 54	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	TTT	267	VAL	5.2
1	SSS	267	VAL	4.6
1	TTT	4	LYS	3.6
2	LLL	2	SER	2.4
1	SSS	4	LYS	2.4
2	MMM	143	ARG	2.4
2	LLL	439	ASN	2.2

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, 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	B-factors(Å^2)	Q<0.9
2	CSO	MMM	79	7/8	0.98	0.06	7,11,12,12	1
2	CSO	LLL	79	7/8	0.98	0.07	7,11,12,12	1

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. 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	B-factors(Å^2)	Q<0.9
7	SO4	MMM	601	5/5	0.74	0.40	56,63,82,84	0
7	SO4	TTT	406	5/5	0.83	0.30	69,70,77,82	0
7	SO4	MMM	605	5/5	0.90	0.24	44,47,49,50	0
7	SO4	LLL	601	5/5	0.94	0.21	20,23,24,25	0
11	LI	MMM	606	1/1	0.97	0.11	14,14,14,14	0
6	CL	TTT	405	1/1	0.98	0.04	21,21,21,21	0
9	NI	MMM	603	1/1	0.98	0.09	19,19,19,19	0
5	SF3	SSS	403[B]	7/7	0.99	0.05	9,11,12,13	1
6	CL	TTT	404	1/1	0.99	0.04	13,13,13,13	0
9	NI	LLL	603	1/1	0.99	0.11	19,19,19,19	0
5	SF3	SSS	403[C]	7/7	0.99	0.05	9,11,13,14	1
5	SF3	TTT	403[B]	7/7	0.99	0.04	9,11,13,13	1
6	CL	SSS	405	1/1	0.99	0.05	20,20,20,20	0
6	CL	SSS	404	1/1	0.99	0.04	13,13,13,13	0
5	SF3	TTT	403[C]	7/7	0.99	0.04	10,11,13,19	1
8	FCO	LLL	602	7/7	1.00	0.05	9,9,10,11	0
10	MG	MMM	604	1/1	1.00	0.06	7,7,7,7	0
4	F3S	TTT	402	7/7	1.00	0.04	8,9,9,9	0
10	MG	LLL	604	1/1	1.00	0.05	7,7,7,7	0
3	SF4	TTT	401	8/8	1.00	0.04	8,9,9,10	0
3	SF4	SSS	401	8/8	1.00	0.04	8,9,9,10	0
4	F3S	SSS	402	7/7	1.00	0.04	8,8,9,9	0
8	FCO	MMM	602	7/7	1.00	0.05	9,9,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.