



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:23 PM UTC

PDB ID : 5JRD / pdb_00005jrd
Title : E. coli Hydrogenase-1 variant P508A
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Deposited on : 2016-05-06
Resolution : 1.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

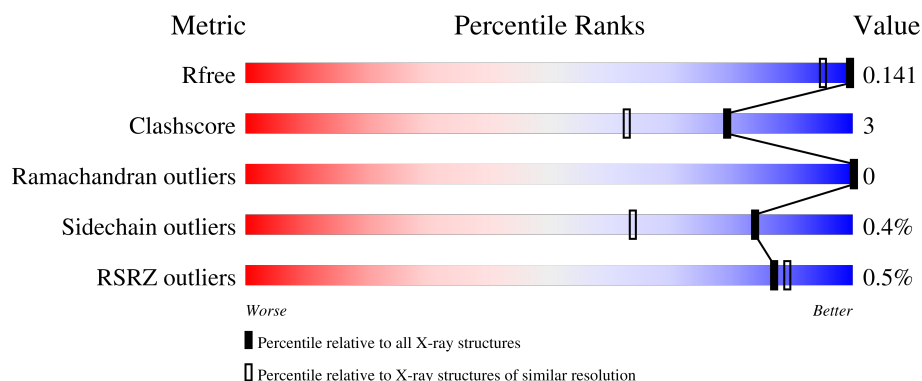
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S	335	
1	T	335	
2	L	582	
2	M	582	

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
10	SO4	M	604	-	X	-	-
2	CSO	L	79	-	-	X	-
2	CSO	M	79	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15068 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	S	264	Total	C	N	O	S	0	14	0
			2116	1353	357	385	21			
1	T	264	Total	C	N	O	S	0	13	0
			2112	1349	359	383	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	328	ARG	-	expression tag	UNP P69740
S	329	SER	-	expression tag	UNP P69740
S	330	HIS	-	expression tag	UNP P69740
S	331	HIS	-	expression tag	UNP P69740
S	332	HIS	-	expression tag	UNP P69740
S	333	HIS	-	expression tag	UNP P69740
S	334	HIS	-	expression tag	UNP P69740
S	335	HIS	-	expression tag	UNP P69740
T	328	ARG	-	expression tag	UNP P69740
T	329	SER	-	expression tag	UNP P69740
T	330	HIS	-	expression tag	UNP P69740
T	331	HIS	-	expression tag	UNP P69740
T	332	HIS	-	expression tag	UNP P69740
T	333	HIS	-	expression tag	UNP P69740
T	334	HIS	-	expression tag	UNP P69740
T	335	HIS	-	expression tag	UNP P69740

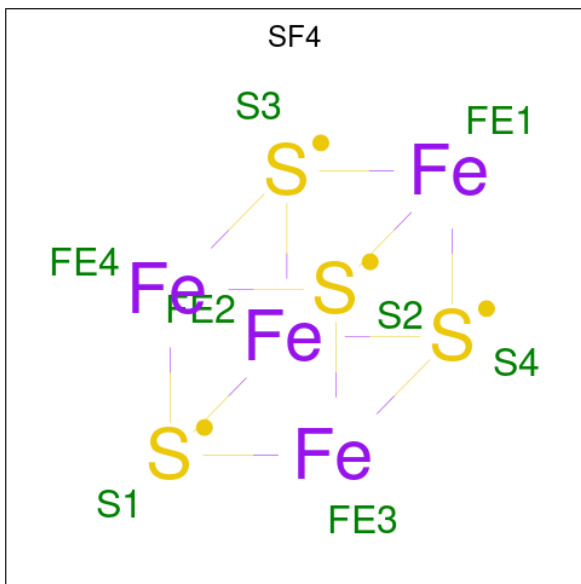
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	29	0
			4701	2989	819	862	31			
2	M	581	Total	C	N	O	S	0	27	0
			4685	2987	808	859	31			

There are 2 discrepancies between the modelled and reference sequences:

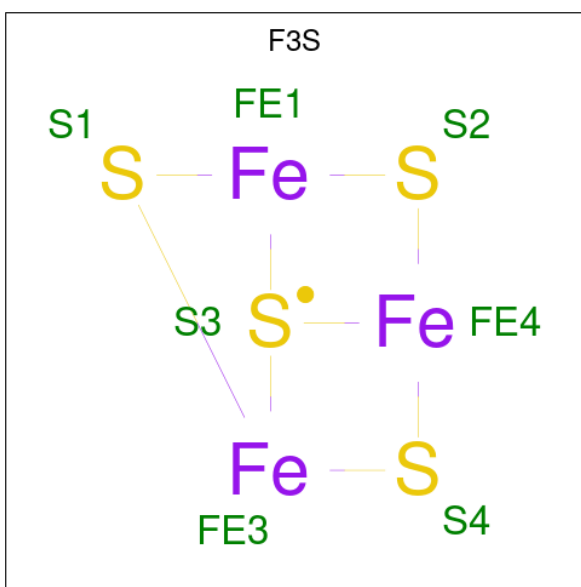
Chain	Residue	Modelled	Actual	Comment	Reference
L	508	ALA	PRO	conflict	UNP P0ACD8
M	508	ALA	PRO	conflict	UNP P0ACD8

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



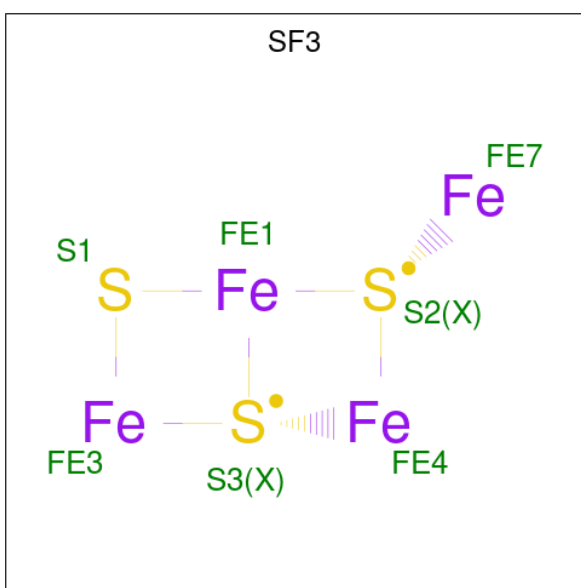
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

- Molecule 5 is FE4-S3 CLUSTER (CCD ID: SF3) (formula: Fe_4S_3).

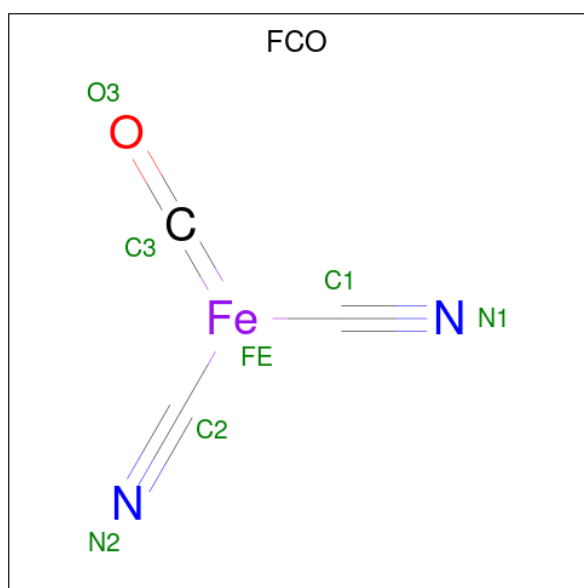


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	1
			8	5	3		
5	T	1	Total	Fe	S	0	1
			8	5	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C₃FeN₂O).



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

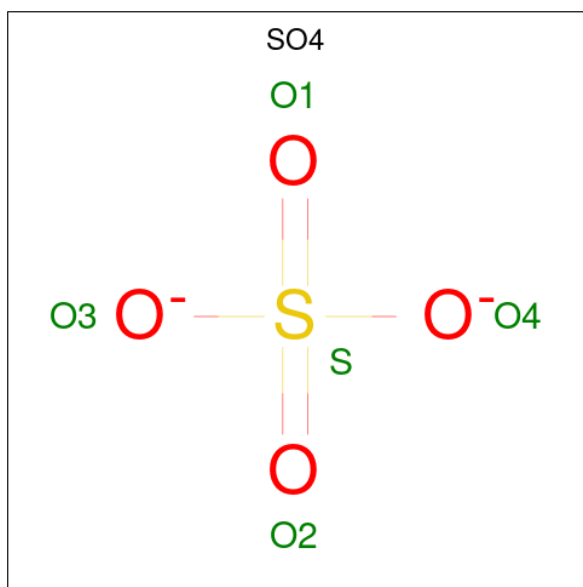
- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

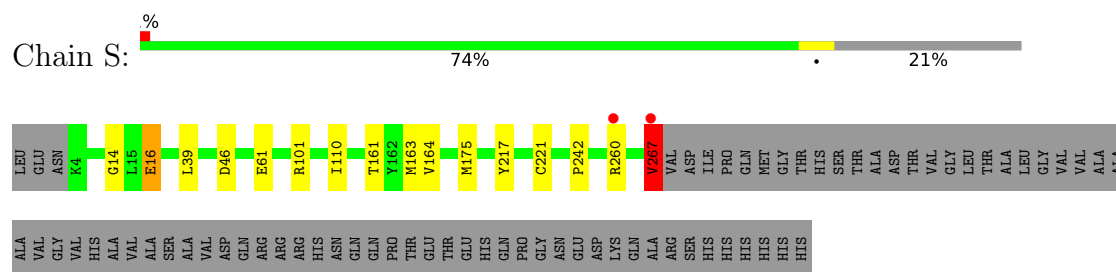
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	S	207	Total	O	0	0
			207	207		
11	L	474	Total	O	0	0
			474	474		
11	T	195	Total	O	0	0
			195	195		
11	M	495	Total	O	0	0
			495	495		

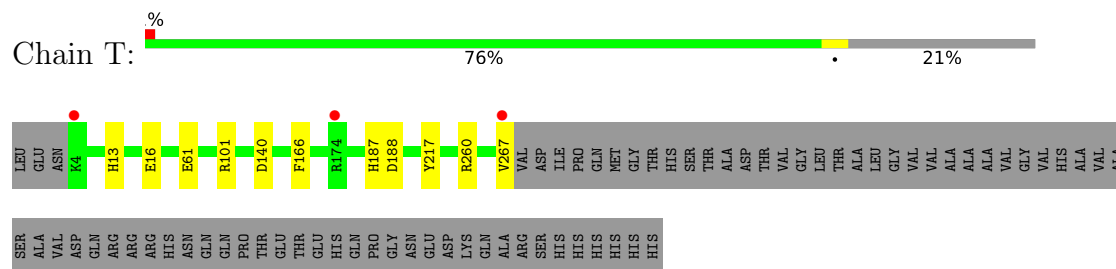
3 Residue-property plots [i](#)

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.

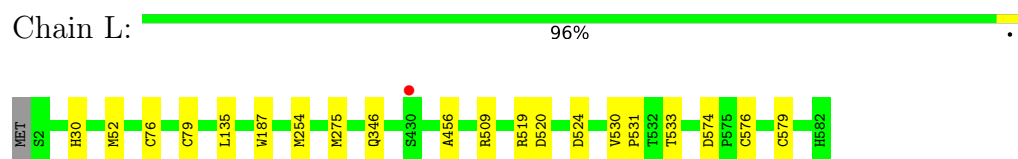
- Molecule 1: Hydrogenase-1 small chain



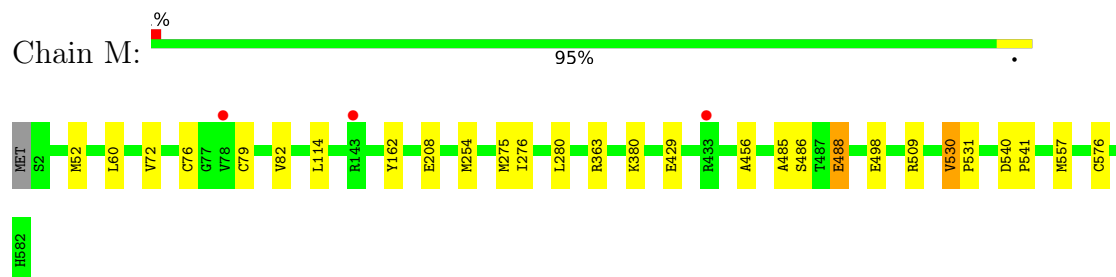
- Molecule 1: Hydrogenase-1 small chain



- Molecule 2: Hydrogenase-1 large chain



- Molecule 2: Hydrogenase-1 large chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.69Å 98.59Å 185.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.69 – 1.20 92.69 – 1.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.69-1.20) 100.0 (92.69-1.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.121 , 0.141 0.121 , 0.141	Depositor DCC
R_{free} test set	26714 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15068	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CSO, CL, F3S, FCO, SF4, NI, MG, SF3, SO4

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	S	1.15	2/2207 (0.1%)	0.92	1/2996 (0.0%)
1	T	1.18	3/2203 (0.1%)	0.90	1/2990 (0.0%)
2	L	1.12	1/4899 (0.0%)	0.87	0/6660
2	M	1.13	4/4879 (0.1%)	0.87	2/6630 (0.0%)
All	All	1.14	10/14188 (0.1%)	0.88	4/19276 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	276	ILE	CA-CB	7.71	1.58	1.54
2	M	498	GLU	CD-OE2	-5.97	1.14	1.25
1	T	260	ARG	CZ-NH1	5.84	1.41	1.32
2	M	485	ALA	N-CA	5.68	1.52	1.46
1	S	260	ARG	CZ-NH1	5.63	1.40	1.32
1	T	188	ASP	CG-OD2	-5.23	1.15	1.25
2	L	574	ASP	CA-CB	5.19	1.56	1.52
1	T	140	ASP	CG-OD2	-5.11	1.15	1.25
2	M	557	MET	N-CA	5.10	1.52	1.46
1	S	217	TYR	CZ-OH	-5.08	1.27	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	363	ARG	NE-CZ-NH2	7.18	125.66	119.20
2	M	530	VAL	N-CA-CB	-7.08	106.94	111.83
1	S	267	VAL	CA-CB-CG1	6.57	121.56	110.40
1	T	187	HIS	CA-CB-CG	5.10	118.90	113.80

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	S	2116	0	2097	15	0
1	T	2112	0	2093	9	0
2	L	4701	0	4645	24	0
2	M	4685	0	4647	26	0
3	S	8	0	0	0	0
3	T	8	0	0	0	0
4	S	7	0	0	0	0
4	T	7	0	0	0	0
5	S	8	0	0	0	0
5	T	8	0	0	0	0
6	S	2	0	0	0	0
6	T	2	0	0	0	0
7	L	7	0	0	0	0
7	M	7	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
10	L	10	0	0	0	0
10	M	5	0	0	0	0
11	L	474	0	0	3	0
11	M	495	0	0	4	0
11	S	207	0	0	7	0
11	T	195	0	0	3	0
All	All	15068	0	13482	72	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 3.

All (72) 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:L:79:CSO:OD	2:L:79:CSO:SG	1.95	1.24
2:M:79:CSO:SG	2:M:79:CSO:OD	1.94	1.23
1:S:61[B]:GLU:OE2	1:S:101[B]:ARG:NH1	1.76	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:509:ARG:NE	2:L:576[B]:CYS:SG	2.28	1.07
2:M:509:ARG:NE	2:M:576[B]:CYS:SG	2.31	1.04
2:L:76[B]:CYS:SG	2:L:79:CSO:OD	2.15	1.02
2:L:509:ARG:CD	2:L:576[B]:CYS:SG	2.56	0.93
2:M:76[B]:CYS:SG	2:M:79:CSO:OD	2.28	0.92
2:M:486[A]:SER:OG	2:M:488[A]:GLU:OE1	1.84	0.92
2:M:509:ARG:CD	2:M:576[B]:CYS:SG	2.59	0.89
1:S:267:VAL:HG23	11:S:560:HOH:O	1.76	0.84
2:L:346[A]:GLN:OE1	11:L:704:HOH:O	1.97	0.82
2:M:82[B]:VAL:HG13	2:M:114[B]:LEU:CD2	2.08	0.82
1:S:110[B]:ILE:HD11	1:S:163:MET:HE1	1.61	0.82
2:M:82[B]:VAL:HG13	2:M:114[B]:LEU:HD23	1.62	0.79
1:S:267:VAL:CG2	11:S:560:HOH:O	2.31	0.77
1:T:217:TYR:CE1	1:T:267:VAL:HG12	2.25	0.72
1:T:217:TYR:HE1	1:T:267:VAL:HG12	1.59	0.68
2:L:76[A]:CYS:HB3	2:L:79:CSO:OD	1.93	0.67
1:T:61[B]:GLU:HG2	11:T:591:HOH:O	1.94	0.65
1:S:175[B]:MET:HA	1:S:175[B]:MET:HE2	1.78	0.64
2:M:76[A]:CYS:HB3	2:M:79:CSO:OD	1.98	0.63
2:M:76[B]:CYS:HB2	2:M:79:CSO:OD	1.98	0.63
2:L:509:ARG:CZ	2:L:576[B]:CYS:SG	2.86	0.63
2:L:76[B]:CYS:CB	2:L:79:CSO:OD	2.43	0.62
2:M:509:ARG:CZ	2:M:576[B]:CYS:SG	2.87	0.62
1:S:61[B]:GLU:HG2	11:S:636:HOH:O	2.00	0.61
2:M:76[B]:CYS:CB	2:M:79:CSO:OD	2.47	0.61
2:L:76[B]:CYS:HB2	2:L:79:CSO:OD	2.01	0.60
2:M:82[B]:VAL:CG1	2:M:114[B]:LEU:HD23	2.29	0.60
1:S:221:CYS:O	1:S:267:VAL:CG2	2.49	0.60
2:M:275[B]:MET:HE2	2:M:456:ALA:HA	1.85	0.59
2:M:576[B]:CYS:SG	11:M:918:HOH:O	2.13	0.58
1:S:161[B]:THR:HG23	11:S:679:HOH:O	2.03	0.58
2:L:576[B]:CYS:SG	11:L:949:HOH:O	2.19	0.58
2:L:275[B]:MET:HE2	2:L:456:ALA:HA	1.86	0.56
2:L:509:ARG:HD3	2:L:576[B]:CYS:SG	2.46	0.56
2:M:429[B]:GLU:HG3	11:M:916:HOH:O	2.07	0.55
2:L:530[B]:VAL:HG21	2:L:579:CYS:O	2.08	0.54
2:M:280[A]:LEU:HG	11:M:1100:HOH:O	2.08	0.54
2:L:52:MET:HG2	11:L:964:HOH:O	2.09	0.53
1:T:16[B]:GLU:HG2	11:T:602:HOH:O	2.09	0.53
2:L:530[B]:VAL:HG21	2:L:579:CYS:C	2.34	0.53
2:L:519[B]:ARG:HG2	2:L:520:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:LEU:HD22	2:L:187:TRP:CD1	2.45	0.52
2:M:488[A]:GLU:H	2:M:488[A]:GLU:CD	2.18	0.52
1:S:16[B]:GLU:HG2	11:S:624:HOH:O	2.09	0.51
2:M:60[B]:LEU:HD11	2:M:72:VAL:CG1	2.40	0.51
1:T:217:TYR:HE1	1:T:267:VAL:CG1	2.22	0.51
2:M:79:CSO:OD	2:M:79:CSO:N	2.44	0.50
2:M:509:ARG:HD2	2:M:576[B]:CYS:SG	2.50	0.48
1:T:101:ARG:HH11	1:T:101:ARG:HG3	1.78	0.48
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.96	0.48
1:S:221:CYS:O	1:S:267:VAL:HG22	2.13	0.47
2:M:162:TYR:OH	2:M:208[B]:GLU:OE2	2.31	0.47
2:M:254[B]:MET:HE2	2:M:254[B]:MET:HA	1.96	0.47
2:M:52:MET:HG2	11:M:893:HOH:O	2.15	0.47
2:L:79:CSO:OD	2:L:79:CSO:N	2.49	0.46
1:S:221:CYS:O	1:S:267:VAL:HG21	2.15	0.46
2:L:509:ARG:HD2	2:L:576[B]:CYS:SG	2.50	0.46
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.47	0.45
2:L:254[B]:MET:HE1	1:T:166:PHE:HE1	1.81	0.44
1:S:14:GLY:O	2:L:30[B]:HIS:HE1	2.01	0.43
2:L:530[B]:VAL:HG22	2:L:533:THR:OG1	2.19	0.43
1:T:61[B]:GLU:OE1	1:T:101:ARG:NH2	2.43	0.42
1:T:13:HIS:HD2	11:T:570:HOH:O	2.02	0.42
1:S:39[B]:LEU:HG	1:S:164:VAL:HG21	2.01	0.42
2:L:530[A]:VAL:CG1	2:L:531:PRO:HD2	2.50	0.42
2:M:509:ARG:HD3	2:M:576[B]:CYS:SG	2.52	0.42
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.50	0.41
1:S:46:ASP:CG	11:S:549:HOH:O	2.64	0.41
1:S:267:VAL:HG22	11:S:560:HOH:O	2.11	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	S	276/335 (82%)	264 (96%)	12 (4%)	0	100	100
1	T	275/335 (82%)	262 (95%)	13 (5%)	0	100	100
2	L	607/582 (104%)	591 (97%)	16 (3%)	0	100	100
2	M	606/582 (104%)	591 (98%)	15 (2%)	0	100	100
All	All	1764/1834 (96%)	1708 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	S	231/274 (84%)	227 (98%)	4 (2%)	53	18
1	T	230/274 (84%)	230 (100%)	0	100	100
2	L	507/479 (106%)	506 (100%)	1 (0%)	87	67
2	M	506/479 (106%)	502 (99%)	4 (1%)	73	44
All	All	1474/1506 (98%)	1465 (99%)	9 (1%)	84	52

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

Mol	Chain	Res	Type
1	S	16[A]	GLU
1	S	16[B]	GLU
1	S	242	PRO
1	S	267	VAL
2	L	524	ASP
2	M	380[A]	LYS
2	M	380[B]	LYS
2	M	488[A]	GLU
2	M	488[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	68	ASN
2	L	392	GLN
1	T	255	ASN
2	M	4	GLN
2	M	122	HIS
2	M	213	GLN
2	M	392	GLN
2	M	460	GLN

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	$\# Z > 2$
2	CSO	M	79	8,2,7	3,6,7	0.60	0	1,6,8	0.90	0
2	CSO	L	79	8,2,7	3,6,7	0.91	0	1,6,8	0.41	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
2	CSO	M	79	8,2,7	-	0/1/5/7	-
2	CSO	L	79	8,2,7	-	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 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	79	CSO	6	0
2	L	79	CSO	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\# Z > 2$
4	F3S	T	402	1	0,9,9	-	-	-		
4	F3S	S	402	1	0,9,9	-	-	-		
10	SO4	L	604	-	4,4,4	0.54	0	6,6,6	0.56	0
7	FCO	M	601	11,2	0,6,6	-	-	-		
5	SF3	S	403[B]	11,1	0,8,8	-	-	-		
3	SF4	T	401	1	0,12,12	-	-	-		
10	SO4	L	605	-	4,4,4	0.39	0	6,6,6	0.26	0
5	SF3	T	403[C]	11,1	0,8,8	-	-	-		
7	FCO	L	601	11,2	0,6,6	-	-	-		
5	SF3	S	403[C]	11,1	0,8,8	-	-	-		
3	SF4	S	401	1	0,12,12	-	-	-		
5	SF3	T	403[B]	11,1	0,8,8	-	-	-		
10	SO4	M	604	-	4,4,4	4.31	2 (50%)	6,6,6	1.53	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F3S	T	402	1	-	-	0/3/3/3
4	F3S	S	402	1	-	-	0/3/3/3
5	SF3	S	403[B]	11,1	-	-	0/2/2/2
3	SF4	T	401	1	-	-	0/6/5/5
5	SF3	T	403[C]	11,1	-	-	0/2/2/2
5	SF3	S	403[C]	11,1	-	-	0/2/2/2
3	SF4	S	401	1	-	-	0/6/5/5
5	SF3	T	403[B]	11,1	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	604	SO4	O1-S	6.75	1.84	1.44
10	M	604	SO4	O4-S	4.73	1.86	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	604	SO4	O4-S-O3	2.66	123.18	108.54
10	M	604	SO4	O4-S-O1	-2.42	96.89	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	S	264/335 (78%)	-0.19	2 (0%) 82 86	6, 13, 22, 56	14 (5%)
1	T	264/335 (78%)	-0.09	3 (1%) 78 79	6, 13, 24, 60	13 (4%)
2	L	580/582 (99%)	-0.22	1 (0%) 91 92	6, 14, 25, 47	29 (5%)
2	M	580/582 (99%)	-0.25	3 (0%) 87 89	5, 14, 23, 39	27 (4%)
All	All	1688/1834 (92%)	-0.20	9 (0%) 87 89	5, 13, 24, 60	83 (4%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	267	VAL	6.1
1	T	267	VAL	5.5
1	T	4	LYS	3.3
1	T	174[A]	ARG	2.4
2	M	78	VAL	2.3
1	S	260	ARG	2.1
2	L	430	SER	2.1
2	M	143	ARG	2.1
2	M	433[A]	ARG	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. 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
2	CSO	L	79	7/8	0.98	0.10	12,16,17,19	0
2	CSO	M	79	7/8	0.98	0.09	12,16,18,20	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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
10	SO4	M	604	5/5	0.75	0.19	72,76,95,104	0
10	SO4	L	605	5/5	0.81	0.13	51,53,56,65	5
10	SO4	L	604	5/5	0.98	0.06	20,21,25,26	5
6	CL	T	405	1/1	0.99	0.14	26,26,26,26	0
6	CL	S	405	1/1	0.99	0.12	23,23,23,23	0
5	SF3	S	403[C]	7/7	1.00	0.03	11,13,13,15	1
5	SF3	T	403[B]	7/7	1.00	0.03	11,13,14,14	1
5	SF3	T	403[C]	7/7	1.00	0.03	11,13,14,17	1
6	CL	S	404	1/1	1.00	0.05	15,15,15,15	0
3	SF4	S	401	8/8	1.00	0.01	10,10,11,11	0
6	CL	T	404	1/1	1.00	0.06	16,16,16,16	0
3	SF4	T	401	8/8	1.00	0.01	10,10,11,11	0
7	FCO	L	601	7/7	1.00	0.02	11,11,12,12	0
7	FCO	M	601	7/7	1.00	0.02	10,11,12,12	0
8	NI	L	602	1/1	1.00	0.06	19,19,19,19	1
8	NI	M	602	1/1	1.00	0.06	21,21,21,21	1
9	MG	L	603	1/1	1.00	0.01	9,9,9,9	0
9	MG	M	603	1/1	1.00	0.01	9,9,9,9	0
4	F3S	S	402	7/7	1.00	0.04	10,10,11,11	0
4	F3S	T	402	7/7	1.00	0.03	10,10,11,11	0
5	SF3	S	403[B]	7/7	1.00	0.03	11,13,13,13	1

6.5 Other polymers ⓘ

There are no such residues in this entry.