



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:07 PM GMT

PDB ID : 1E3D  
Title : [NIFE] HYDROGENASE FROM DESULFOVIBRIO DESULFURICANS  
ATCC 27774  
Authors : Matias, P.M.; Soares, C.M.; Saraiva, L.M.; Coelho, R.; Morais, J.; Le Gall, J.;  
Carrondo, M.A.  
Deposited on : 2000-06-14  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

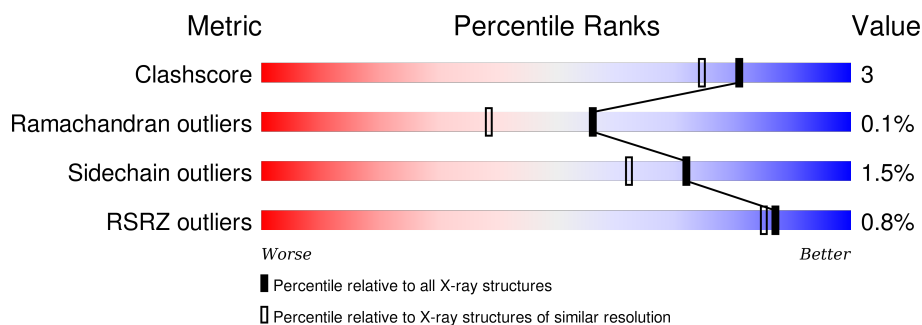
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	266	<div> <div>%</div> <div>89% 9% .</div> </div>
1	C	266	<div> <div>2%</div> <div>94% . . .</div> </div>
2	B	542	<div> <div>89% 10% .</div> </div>
2	D	542	<div> <div>%</div> <div>89% 9% ..</div> </div>

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
7	FNE	B	543	-	-	X	-
7	FNE	D	543	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 25871 atoms, of which 12026 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.

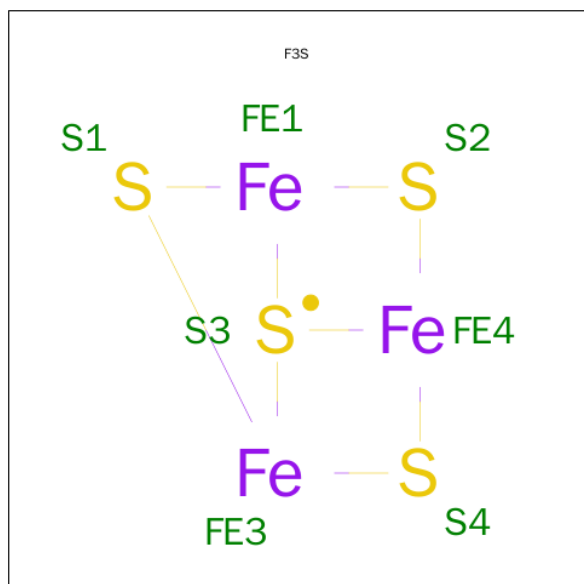
- Molecule 1 is a protein called [NIFE] HYDROGENASE SMALL SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	262	Total	C	H	N	O	S	13	0	0
			3878	1257	1895	329	377	20			
1	C	262	Total	C	H	N	O	S	27	0	0
			3878	1257	1895	329	377	20			

- Molecule 2 is a protein called [NIFE] HYDROGENASE LARGE SUBUNIT.

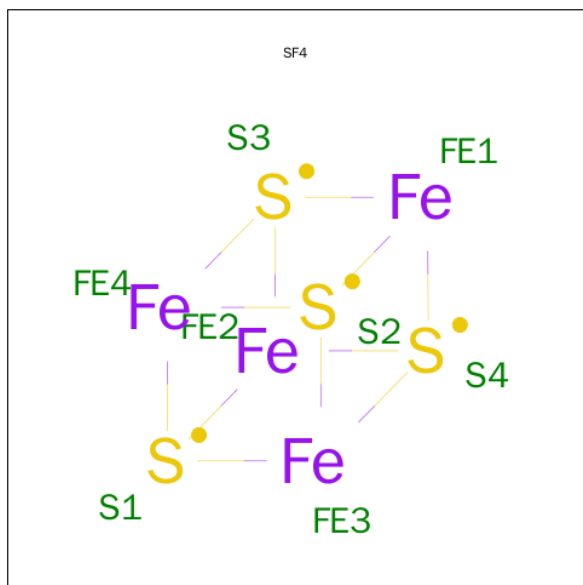
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	537	Total	C	H	N	O	S	84	4	0
			8332	2677	4125	734	775	21			
2	D	537	Total	C	H	N	O	S	42	2	0
			8310	2671	4111	734	775	19			

- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



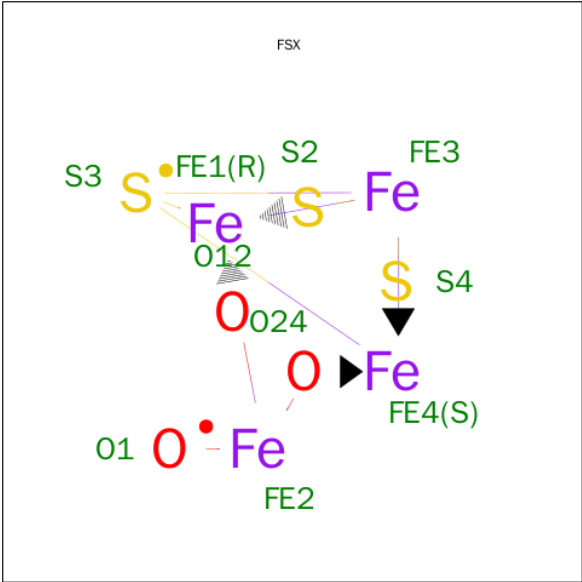
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		
3	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



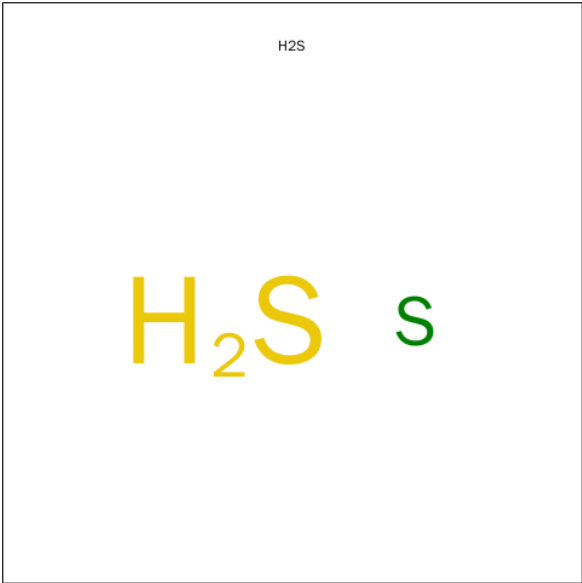
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is BIS-(MU-2-OXO),[(MU-3--SULFIDO)-BIS(MU-2--SULFIDO)-TRIS(CYS-S)-TRI-IRON] (AQUA)(GLU-O)IRON(II) (three-letter code: FSX) (formula: Fe<sub>4</sub>O<sub>3</sub>S<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	O	S	0	0
			10	4	3	3		
5	C	1	Total	Fe	O	S	0	0
			10	4	3	3		

- Molecule 6 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



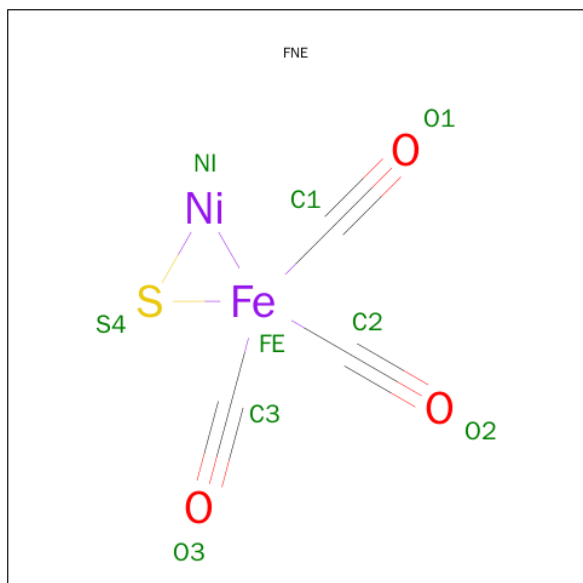
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	S	0	0
			1	1		
6	B	1	Total	S	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total S 1 1	0	0
6	D	1	Total S 1 1	0	0

- Molecule 7 is (MU-SULPHIDO)-BIS(MU-CYS,S)-[TRICARBONYLIRON-DI-(CYS,S)NICKEL(II)](FE-NI) (three-letter code: FNE) (formula:  $\text{C}_3\text{FeNiO}_3\text{S}$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	B	1	Total 9	C 3	Fe 1	Ni 1	O 3	S 1	0	0
7	D	1	Total 9	C 3	Fe 1	Ni 1	O 3	S 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0

- Molecule 9 is water.

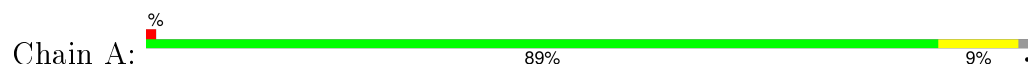
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	248	Total 248	O 248	0	0
9	B	512	Total 512	O 512	0	0
9	C	226	Total 226	O 226	0	0
9	D	413	Total 413	O 413	0	0



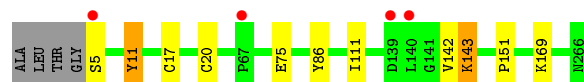
### 3 Residue-property plots [i](#)

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.

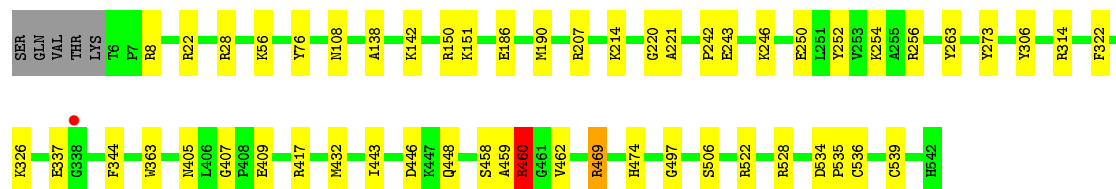
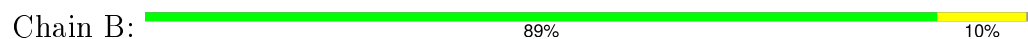
- Molecule 1: [NIFE] HYDROGENASE SMALL SUBUNIT



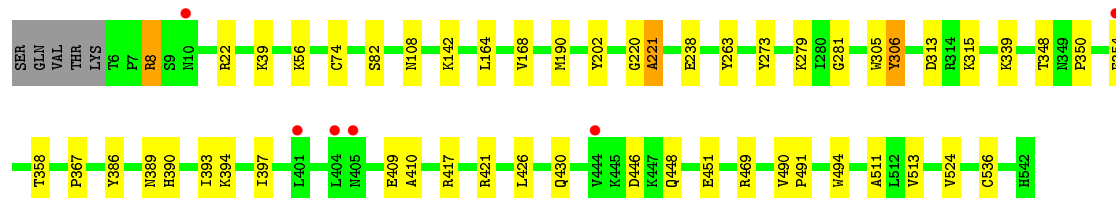
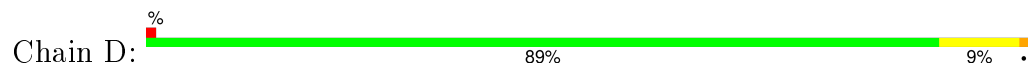
- Molecule 1: [NIFE] HYDROGENASE SMALL SUBUNIT



- Molecule 2: [NIFE] HYDROGENASE LARGE SUBUNIT



- Molecule 2: [NIFE] HYDROGENASE LARGE SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.09Å 169.98Å 72.62Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 25.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (25.00-1.80) 89.9 (25.00-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.167 , 0.223 0.168 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 77.5	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 128681 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MG, SF4, H2S, FNE, F3S, FSX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.37	0/2035	0.96	7/2770 (0.3%)
1	C	0.37	0/2035	0.96	1/2770 (0.0%)
2	B	0.38	0/4337	1.08	20/5896 (0.3%)
2	D	0.37	0/4321	1.01	8/5876 (0.1%)
All	All	0.37	0/12728	1.02	36/17312 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	528	ARG	NE-CZ-NH2	-9.86	115.37	120.30
2	D	263	TYR	CB-CG-CD1	8.29	125.97	121.00
2	D	421	ARG	NE-CZ-NH2	-8.10	116.25	120.30
2	B	322	PHE	C-N-CA	7.97	141.62	121.70
2	B	460	ARG	NE-CZ-NH1	7.59	124.09	120.30
2	B	469	ARG	NE-CZ-NH1	7.53	124.06	120.30
2	B	263	TYR	CB-CG-CD1	7.10	125.26	121.00
2	B	207	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	B	417	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	B	314	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	26	ARG	NE-CZ-NH2	-6.67	116.97	120.30
2	D	417	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	B	28	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	148	PRO	C-N-CA	6.30	135.54	122.30
2	B	22	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	D	446	ASP	CB-CG-OD1	6.12	123.81	118.30
2	B	417	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	D	22	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	D	306	TYR	CA-CB-CG	5.87	124.55	113.40
2	D	202	TYR	CA-CB-CG	5.87	124.55	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	26	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	11	TYR	CB-CG-CD1	5.71	124.43	121.00
2	B	522	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	363	TRP	O-C-N	-5.54	113.83	122.70
2	B	306	TYR	CA-CB-CG	5.43	123.72	113.40
2	B	76	TYR	CB-CG-CD1	5.38	124.23	121.00
2	B	522	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	227	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	6	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	6	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	D	417	ARG	CD-NE-CZ	5.20	130.88	123.60
2	B	460	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	B	256	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	B	528	ARG	CD-NE-CZ	5.05	130.67	123.60
1	C	11	TYR	CB-CG-CD1	5.04	124.03	121.00

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	A	1983	1895	1897	13	0
1	C	1983	1895	1897	7	0
2	B	4207	4125	4120	31	0
2	D	4199	4111	4111	31	0
3	A	7	0	0	0	0
3	C	7	0	0	0	0
4	A	8	0	0	0	0
4	C	8	0	0	0	0
5	A	10	0	0	0	0
5	C	10	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
7	B	9	0	0	6	0
7	D	9	0	0	5	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	248	0	0	6	0
9	B	512	0	0	9	0
9	C	226	0	0	1	0
9	D	413	0	0	11	0
All	All	13845	12026	12025	81	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 (81) 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:D:536[B]:CYS:SG	7:D:543:FNE:S4	2.48	0.90
2:B:536[C]:CYS:SG	7:B:543:FNE:C3	2.63	0.86
2:B:536[B]:CYS:SG	7:B:543:FNE:S4	2.59	0.85
2:B:186:GLU:HG3	9:B:2227:HOH:O	1.84	0.78
2:B:344:PHE:HB2	9:B:2372:HOH:O	1.89	0.72
2:D:426:LEU:O	2:D:430:GLN:HG3	1.89	0.72
2:D:56:LYS:HE3	9:D:2386:HOH:O	1.91	0.70
2:B:254:LYS:HE2	9:B:2286:HOH:O	1.94	0.68
2:D:315:LYS:HD2	9:D:2285:HOH:O	1.94	0.67
2:D:305:TRP:O	2:D:390:HIS:HE1	1.79	0.65
2:B:469:ARG:HD2	7:B:543:FNE:S4	2.37	0.64
2:B:242:PRO:HD2	2:B:243:GLU:OE2	1.97	0.64
2:D:238:GLU:HG3	9:D:2229:HOH:O	1.97	0.63
2:D:469:ARG:HD2	7:D:543:FNE:S4	2.41	0.60
2:B:536[C]:CYS:SG	2:B:539:CYS:HB2	2.41	0.60
2:D:358:THR:HG23	9:D:2330:HOH:O	2.03	0.59
2:B:536[A]:CYS:CB	7:B:543:FNE:S4	2.91	0.58
1:A:143:LYS:HD2	9:A:2143:HOH:O	2.04	0.57
1:C:11:TYR:CZ	1:C:111:ILE:HD11	2.40	0.56
2:D:390:HIS:CD2	2:D:393:ILE:HD12	2.41	0.55
2:B:138:ALA:O	2:B:142:LYS:HG3	2.06	0.55
2:B:56:LYS:HE2	9:B:2069:HOH:O	2.05	0.55
2:D:393:ILE:O	2:D:397:ILE:HG13	2.07	0.55
1:C:142:VAL:O	1:C:143:LYS:HE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:LYS:HE2	9:D:2196:HOH:O	2.07	0.54
2:D:281:GLY:HA2	2:D:511:ALA:O	2.08	0.53
2:D:348:THR:O	2:D:350:PRO:HD3	2.09	0.53
2:D:367:PRO:HB2	2:D:494:TRP:CE3	2.44	0.53
1:A:167:GLY:HA2	9:A:2154:HOH:O	2.07	0.53
2:B:536[B]:CYS:CB	7:B:543:FNE:S4	2.96	0.52
2:B:458:SER:O	2:B:459:ALA:HB2	2.12	0.50
2:D:8:ARG:NH1	9:D:2004:HOH:O	2.45	0.49
2:B:246:LYS:O	2:B:250:GLU:HG3	2.12	0.49
1:C:86:TYR:HB2	9:C:2065:HOH:O	2.12	0.49
2:D:536[A]:CYS:CB	7:D:543:FNE:S4	3.00	0.49
2:B:150:ARG:HD2	9:B:2243:HOH:O	2.12	0.48
2:B:190:MET:HG2	2:B:273:TYR:CG	2.48	0.48
2:D:513:VAL:HG12	9:D:2395:HOH:O	2.14	0.47
2:D:536[C]:CYS:SG	7:D:543:FNE:C3	3.03	0.47
2:B:8:ARG:NH2	9:B:2005:HOH:O	2.47	0.46
1:A:28:TYR:CZ	1:A:237:GLU:HG2	2.51	0.46
2:B:462:VAL:HA	2:B:474:HIS:O	2.17	0.45
1:C:11:TYR:OH	1:C:111:ILE:HD11	2.16	0.45
1:A:200:GLU:HB3	1:A:214:TRP:CD2	2.52	0.45
2:D:354:PHE:HA	9:D:2323:HOH:O	2.15	0.45
1:C:20:CYS:HB2	1:C:75:GLU:CD	2.37	0.45
1:A:11:TYR:CZ	1:A:111:ILE:HD11	2.52	0.45
1:A:231:PRO:HG3	1:A:240:TRP:CH2	2.52	0.45
2:D:279:LYS:NZ	9:D:2255:HOH:O	2.48	0.45
2:B:407:GLY:HA3	2:B:409:GLU:OE2	2.16	0.45
1:A:5:SER:N	9:A:2001:HOH:O	2.50	0.45
2:B:220:GLY:O	2:B:221:ALA:HB3	2.18	0.44
2:D:448:GLN:NE2	2:D:451:GLU:HG2	2.32	0.44
1:A:20:CYS:HB2	1:A:75:GLU:CD	2.37	0.44
2:B:326:LYS:NZ	9:B:2352:HOH:O	2.50	0.44
2:D:409:GLU:HG2	2:D:410:ALA:N	2.33	0.44
1:A:5:SER:N	9:A:2002:HOH:O	2.49	0.44
2:D:220:GLY:O	2:D:221:ALA:HB3	2.18	0.44
1:A:232:LYS:NZ	9:A:2215:HOH:O	2.47	0.43
2:D:490:VAL:HG12	2:D:491:PRO:HD2	2.01	0.42
1:C:142:VAL:C	1:C:143:LYS:HE2	2.40	0.42
2:D:313:ASP:HB3	9:D:2280:HOH:O	2.18	0.42
1:A:11:TYR:CE2	1:A:111:ILE:HD11	2.54	0.42
2:B:150:ARG:HD3	9:B:2242:HOH:O	2.20	0.42
2:D:386:TYR:CE2	2:D:394:LYS:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:LEU:O	2:D:168:VAL:HG23	2.20	0.42
2:D:339:LYS:NZ	9:D:2310:HOH:O	2.49	0.42
1:C:11:TYR:CE2	1:C:111:ILE:HD11	2.54	0.41
2:B:536[B]:CYS:HB2	7:B:543:FNE:S4	2.59	0.41
1:A:236:ASN:O	2:B:214:LYS:HE2	2.21	0.41
2:D:190:MET:HG2	2:D:273:TYR:CG	2.56	0.41
2:B:534:ASP:N	2:B:535:PRO:HD3	2.36	0.41
2:D:367:PRO:HB2	2:D:494:TRP:CD2	2.56	0.40
2:B:497:GLY:O	2:B:506:SER:HB2	2.20	0.40
2:D:74:CYS:CB	7:D:543:FNE:C1	2.99	0.40
2:B:344:PHE:CZ	2:B:460:ARG:HG3	2.56	0.40
1:A:163:ALA:O	1:A:168:GLN:HB2	2.22	0.40
2:B:151:LYS:NZ	9:B:2187:HOH:O	2.51	0.40
2:B:443:ILE:HA	2:B:446:ASP:O	2.22	0.40
2:B:252:TYR:CE1	2:B:432[B]:MET:HB2	2.57	0.40
9:A:2088:HOH:O	2:B:448:GLN:HB2	2.21	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	A	260/266 (98%)	246 (95%)	13 (5%)	1 (0%)	39	23
1	C	260/266 (98%)	252 (97%)	8 (3%)	0	100	100
2	B	540/542 (100%)	524 (97%)	16 (3%)	0	100	100
2	D	538/542 (99%)	519 (96%)	18 (3%)	1 (0%)	52	35
All	All	1598/1616 (99%)	1541 (96%)	55 (3%)	2 (0%)	56	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	221	ALA
1	A	67	PRO

### 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	A	210/212 (99%)	206 (98%)	4 (2%)	65	52
1	C	210/212 (99%)	205 (98%)	5 (2%)	57	41
2	B	444/444 (100%)	440 (99%)	4 (1%)	84	80
2	D	442/444 (100%)	435 (98%)	7 (2%)	70	59
All	All	1306/1312 (100%)	1286 (98%)	20 (2%)	72	62

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	CYS
1	A	169	LYS
1	A	174	GLU
1	A	225	GLU
2	B	108	ASN
2	B	337	GLU
2	B	405	ASN
2	B	460	ARG
1	C	5	SER
1	C	17	CYS
1	C	143	LYS
1	C	151	PRO
1	C	169	LYS
2	D	8	ARG
2	D	82	SER
2	D	108	ASN
2	D	142	LYS
2	D	306	TYR
2	D	389	ASN
2	D	524	VAL



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	GLN
1	C	168	GLN
2	D	204	GLN
2	D	349	ASN
2	D	390	HIS
2	D	405	ASN
2	D	448	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic and 4 are modelled with single atom - leaving 8 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	F3S	A	267	1	0,9,9	0.00	-	0,15,15	0.00	-
4	SF4	A	268	1	0,12,12	0.00	-	0,24,24	0.00	-
5	FSX	A	269	1	0,14,14	0.00	-	0,32,32	0.00	-
7	FNE	B	543	2	3,9,9	1.39	1 (33%)	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	F3S	C	267	1	0,9,9	0.00	-	0,15,15	0.00	-
4	SF4	C	268	1	0,12,12	0.00	-	0,24,24	0.00	-
5	FSX	C	269	1	0,14,14	0.00	-	0,32,32	0.00	-
7	FNE	D	543	2	3,9,9	1.06	0	0,15,15	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	F3S	A	267	1	-	0/0/24/24	0/0/3/3
4	SF4	A	268	1	-	0/0/48/48	0/6/5/5
5	FSX	A	269	1	-	0/0/56/56	0/0/5/5
7	FNE	B	543	2	-	0/0/18/18	0/0/1/1
3	F3S	C	267	1	-	0/0/24/24	0/0/3/3
4	SF4	C	268	1	-	0/0/48/48	0/6/5/5
5	FSX	C	269	1	-	0/0/56/56	0/0/5/5
7	FNE	D	543	2	-	0/0/18/18	0/0/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	543	FNE	O2-C2	-2.09	1.09	1.15

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 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	543	FNE	6	0
7	D	543	FNE	5	0

## 5.7 Other polymers [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/266 (98%)	-0.21	2 (0%) 87 85	12, 21, 36, 53	4 (1%)
1	C	262/266 (98%)	-0.20	4 (1%) 76 72	13, 21, 35, 54	6 (2%)
2	B	537/542 (99%)	-0.42	1 (0%) 95 93	12, 19, 30, 45	9 (1%)
2	D	537/542 (99%)	-0.28	6 (1%) 82 80	13, 22, 38, 50	7 (1%)
All	All	1598/1616 (98%)	-0.30	13 (0%) 87 85	12, 21, 35, 54	26 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	LEU	4.2
2	D	401	LEU	3.7
2	D	405	ASN	3.5
1	A	67	PRO	3.3
1	C	139	ASP	3.3
1	C	5	SER	2.4
2	B	338	GLY	2.3
2	D	354	PHE	2.2
2	D	444	VAL	2.1
2	D	10	ASN	2.1
1	A	214	TRP	2.1
2	D	404	LEU	2.0
1	C	67	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	H2S	B	904	1/1	0.97	0.13	1.80	18,18,18,18	1
6	H2S	D	904	1/1	0.98	0.10	1.53	19,19,19,19	1
8	MG	D	901	1/1	0.99	0.12	0.77	17,17,17,17	0
8	MG	B	901	1/1	1.00	0.08	0.29	15,15,15,15	0
6	H2S	A	904	1/1	0.99	0.08	-0.41	22,22,22,22	0
4	SF4	C	268	8/8	0.98	0.07	-0.52	16,18,19,20	0
3	F3S	C	267	7/7	0.99	0.07	-0.54	14,15,16,16	0
3	F3S	A	267	7/7	0.99	0.08	-0.88	15,17,18,18	0
5	FSX	A	269	10/10	1.00	0.07	-0.94	9,16,21,22	0
7	FNE	D	543	9/9	0.99	0.06	-0.96	15,16,19,23	1
5	FSX	C	269	10/10	0.99	0.06	-1.12	15,16,26,26	0
4	SF4	A	268	8/8	1.00	0.05	-1.12	19,21,22,24	0
7	FNE	B	543	9/9	0.99	0.06	-1.13	13,16,21,22	1
6	H2S	C	904	1/1	0.99	0.06	-1.20	23,23,23,23	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.