Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 10:08 PM EDT

PDB ID	:	1FRF
Title	:	CRYSTAL STRUCTURE OF THE NI-FE HYDROGENASE FROM DESULFOVIBRIO FRUCTOSOVORANS
Authors	:	Montet, Y.; Volbeda, A.; Piras, C.; Hatchikian, E.C.; Frey, M.; Fontecilla, J.C.
Deposited on	:	1998-07-21
Resolution	:	2.70 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:

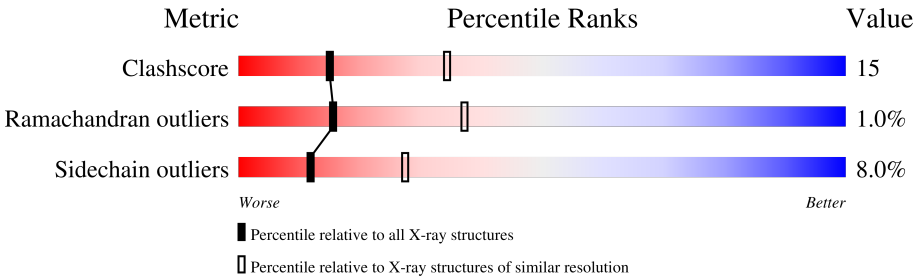
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	264	66% 30%
2	L	564	64% 28%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6296 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 [NI-FE] HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	261	Total	C	N	O	S	0	0	0
			1971	1254	328	373	16			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	62	GLU	GLN	conflict	UNP P18187
S	98	CYS	THR	conflict	UNP P18187
S	112	GLY	-	insertion	UNP P18187
S	113	THR	ARG	conflict	UNP P18187
S	114	CYS	HIS	conflict	UNP P18187
S	115	SER	LEU	conflict	UNP P18187
S	117	TYR	HIS	conflict	UNP P18187

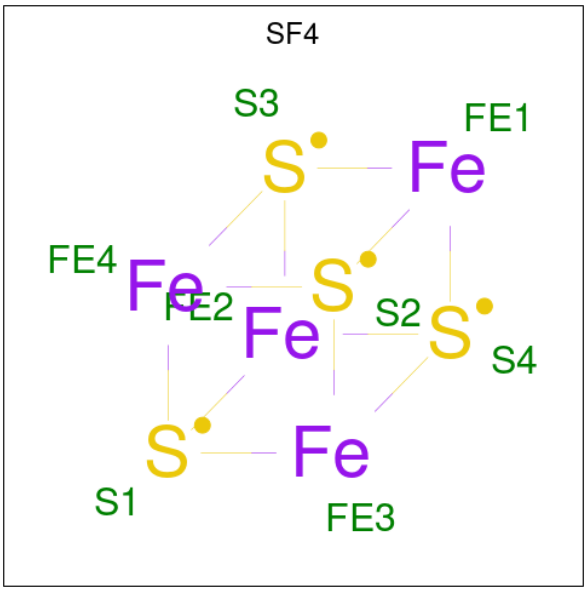
- Molecule 2 is a protein called [NI-FE] HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	543	Total	C	N	O	S	0	0	0
			4167	2651	723	771	22			

There is a discrepancy between the modelled and reference sequences:

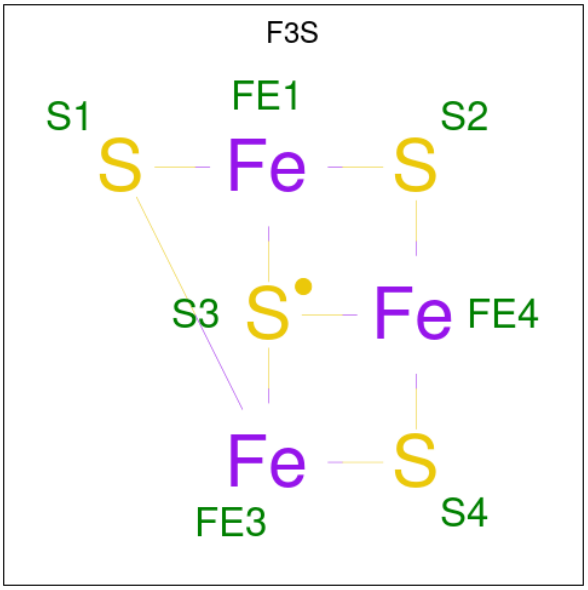
Chain	Residue	Modelled	Actual	Comment	Reference
L	353	GLY	CYS	conflict	UNP P18188

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



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

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Fe 1 1	0	0

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total Ni 1 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total Mg 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	S	54	Total O 54 54	0	0
8	L	78	Total O 78 78	0	0

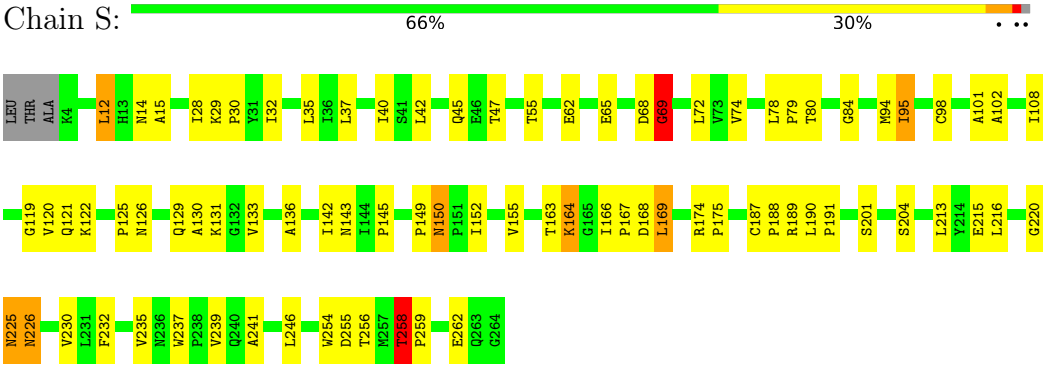
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

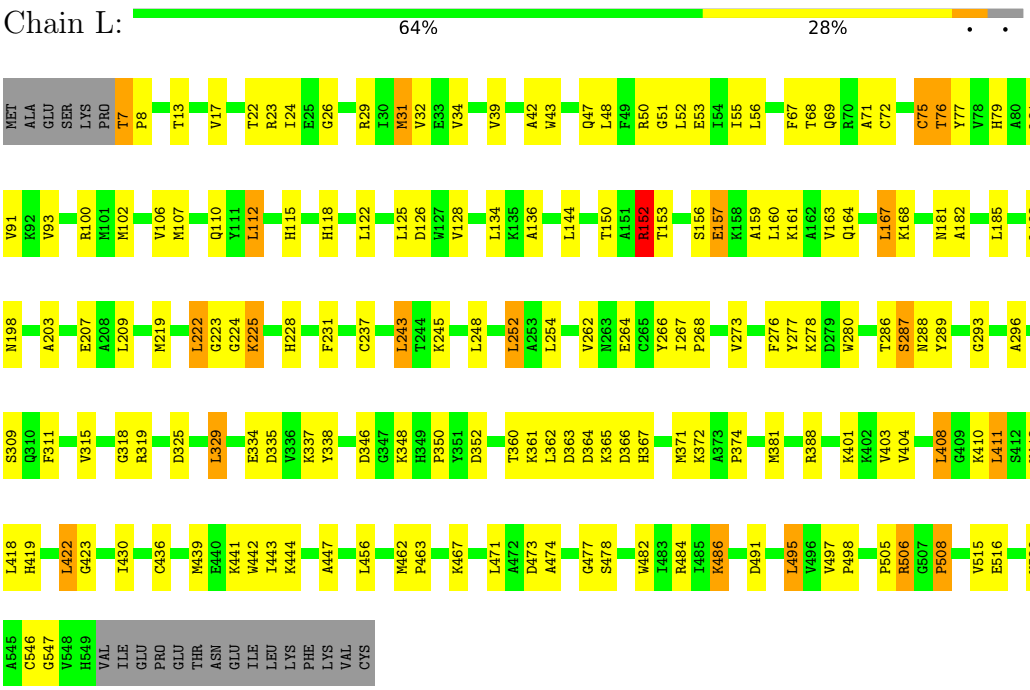
- Molecule 1: [NI-FE] HYDROGENASE

Chain S:



- Molecule 2: [NI-FE] HYDROGENASE

Chain L:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.61Å 99.77Å 184.51Å 90.00° 90.88° 90.00°	Depositor
Resolution (Å)	12.00 – 2.70	Depositor
% Data completeness (in resolution range)	66.7 (12.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6296	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, NI, SF4, FE, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	S	0.58	0/2025	0.81	3/2756 (0.1%)
2	L	0.57	1/4270 (0.0%)	0.83	4/5796 (0.1%)
All	All	0.57	1/6295 (0.0%)	0.82	7/8552 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	436	CYS	CB-SG	-5.12	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	318	GLY	N-CA-C	-7.04	95.49	113.10
1	S	28	ILE	N-CA-C	-5.96	94.90	111.00
1	S	69	GLY	N-CA-C	5.21	126.12	113.10
1	S	37	LEU	CA-CB-CG	5.17	127.19	115.30
2	L	47	GLN	N-CA-C	5.07	124.70	111.00
2	L	152	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	L	311	PHE	N-CA-C	-5.05	97.37	111.00

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	S	1971	0	1904	59	0
2	L	4167	0	4136	127	0
3	S	16	0	0	0	0
4	S	7	0	0	1	0
5	L	1	0	0	0	0
6	L	1	0	0	0	0
7	L	1	0	0	0	0
8	L	78	0	0	5	0
8	S	54	0	0	4	0
All	All	6296	0	6040	175	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 15.

All (175) 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)
1:S:80:THR:HB	1:S:129:GLN:O	1.66	0.94
1:S:55:THR:HG22	2:L:181:ASN:HB3	1.53	0.89
2:L:31:MET:HG3	2:L:43:TRP:HB2	1.56	0.84
2:L:408:LEU:HG	2:L:414:PRO:O	1.79	0.83
2:L:194:PRO:HG2	2:L:197:VAL:HG23	1.63	0.80
1:S:55:THR:CG2	2:L:181:ASN:HB3	2.13	0.79
2:L:152:ARG:HD2	2:L:264:GLU:HB3	1.62	0.79
2:L:335:ASP:CG	2:L:508:PRO:HD3	2.03	0.79
2:L:329:LEU:HD21	2:L:471:LEU:HD11	1.65	0.78
1:S:12:LEU:HD22	1:S:72:LEU:HD11	1.65	0.78
2:L:7:THR:HG22	2:L:8:PRO:HD3	1.66	0.77
2:L:76:THR:HG22	2:L:228:HIS:CD2	2.21	0.76
1:S:126:ASN:HD21	1:S:130:ALA:H	1.37	0.73
1:S:255:ASP:HA	1:S:258:THR:HG23	1.69	0.73
1:S:258:THR:OG1	1:S:259:PRO:HD3	1.91	0.70
2:L:7:THR:HG22	2:L:8:PRO:CD	2.22	0.68
2:L:414:PRO:HB2	2:L:416:THR:HG22	1.74	0.68
2:L:508:PRO:HD2	8:L:578:HOH:O	1.93	0.68
1:S:35:LEU:HD13	1:S:40:ILE:HG12	1.77	0.66
1:S:145:PRO:HG3	1:S:174:ARG:HD3	1.77	0.65
2:L:337:LYS:HD2	2:L:508:PRO:HA	1.78	0.65
2:L:252:LEU:HD23	2:L:443:ILE:HD12	1.77	0.65
2:L:486:LYS:HE3	2:L:491:ASP:HB2	1.79	0.65
2:L:497:VAL:HG13	2:L:498:PRO:HD2	1.80	0.64
2:L:128:VAL:HG13	2:L:198:ASN:HD22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:42:LEU:HD21	1:S:45:GLN:HG3	1.81	0.62
1:S:78:LEU:HD21	1:S:98:CYS:SG	2.40	0.62
1:S:32:ILE:HG21	2:L:209:LEU:HD22	1.82	0.61
1:S:55:THR:HG22	2:L:181:ASN:CB	2.29	0.61
1:S:259:PRO:HB3	8:S:299:HOH:O	1.99	0.61
2:L:335:ASP:OD1	2:L:508:PRO:HD3	2.01	0.61
1:S:68:ASP:HB2	8:S:304:HOH:O	2.00	0.60
2:L:43:TRP:CZ2	2:L:365:LYS:HE2	2.38	0.59
2:L:156:SER:O	2:L:160:LEU:HG	2.03	0.59
2:L:388:ARG:NH2	2:L:474:ALA:O	2.35	0.59
2:L:152:ARG:CD	2:L:264:GLU:HB3	2.33	0.58
2:L:418:LEU:O	2:L:423:GLY:HA3	2.04	0.58
2:L:486:LYS:HB3	2:L:491:ASP:HB2	1.84	0.58
2:L:115:HIS:HD2	8:L:624:HOH:O	1.87	0.58
2:L:69:GLN:HA	2:L:79:HIS:HB2	1.86	0.57
2:L:126:ASP:OD2	2:L:538:HIS:HD2	1.88	0.57
1:S:222:VAL:HG22	1:S:222:VAL:O	2.05	0.57
2:L:50:ARG:HH22	2:L:71:ALA:HA	1.70	0.57
1:S:47:THR:O	2:L:23:ARG:HA	2.06	0.56
2:L:497:VAL:CG1	2:L:498:PRO:HD2	2.35	0.56
1:S:15:ALA:HA	2:L:48:LEU:HD21	1.88	0.56
2:L:296:ALA:HA	2:L:309:SER:HA	1.87	0.56
2:L:364:ASP:O	2:L:365:LYS:HB2	2.04	0.56
1:S:78:LEU:HD22	1:S:95:ILE:HA	1.87	0.56
1:S:220:GLY:N	1:S:221:PRO:CD	2.69	0.56
2:L:87:VAL:O	2:L:91:VAL:HB	2.07	0.55
1:S:125:PRO:HD2	2:L:55:ILE:HA	1.87	0.54
2:L:24:ILE:HG23	2:L:538:HIS:CE1	2.42	0.54
2:L:278:LYS:HE2	2:L:411:LEU:O	2.08	0.54
1:S:79:PRO:O	1:S:84:GLY:HA2	2.08	0.54
2:L:337:LYS:CD	2:L:508:PRO:HA	2.38	0.54
2:L:422:LEU:HD12	8:L:570:HOH:O	2.07	0.54
2:L:364:ASP:HB3	2:L:367:HIS:O	2.08	0.53
1:S:32:ILE:CG2	2:L:209:LEU:HD22	2.38	0.53
2:L:439:MET:O	2:L:443:ILE:HG13	2.09	0.53
1:S:190:LEU:N	1:S:191:PRO:HD2	2.24	0.53
2:L:42:ALA:O	2:L:506:ARG:NH2	2.42	0.53
2:L:13:THR:HA	2:L:34:VAL:O	2.09	0.52
1:S:30:PRO:HD2	1:S:155:VAL:HG11	1.90	0.52
1:S:201:SER:OG	1:S:204:SER:HB3	2.09	0.52
2:L:102:MET:CE	2:L:243:LEU:HD13	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:441:LYS:HE3	2:L:442:TRP:CD1	2.44	0.52
2:L:76:THR:O	2:L:77:TYR:HB3	2.10	0.51
1:S:78:LEU:O	1:S:130:ALA:HA	2.11	0.51
2:L:76:THR:HG22	2:L:228:HIS:HD2	1.73	0.51
2:L:411:LEU:HB3	2:L:413:VAL:HG22	1.93	0.51
2:L:404:VAL:HG12	2:L:408:LEU:HD22	1.92	0.51
2:L:280:TRP:HB2	2:L:422:LEU:HD23	1.93	0.51
1:S:29:LYS:N	8:S:303:HOH:O	2.34	0.50
1:S:142:ILE:HD11	1:S:166:ILE:HD12	1.92	0.50
1:S:232:PHE:CB	2:L:225:LYS:HB2	2.41	0.50
1:S:102:ALA:HB1	1:S:108:ILE:HD11	1.94	0.50
2:L:110:GLN:HE21	2:L:219:MET:CE	2.25	0.50
2:L:24:ILE:HG23	2:L:538:HIS:HE1	1.76	0.50
2:L:286:THR:HG22	2:L:287:SER:N	2.26	0.50
2:L:248:LEU:CD1	2:L:447:ALA:HA	2.42	0.50
2:L:110:GLN:HB2	2:L:219:MET:HE3	1.94	0.49
2:L:372:LYS:O	2:L:374:PRO:HD3	2.12	0.49
2:L:56:LEU:HD11	2:L:68:THR:HG23	1.94	0.49
1:S:114:CYS:HA	1:S:119:GLY:CA	2.43	0.49
2:L:51:GLY:O	2:L:53:GLU:N	2.46	0.48
2:L:164:GLN:O	2:L:168:LYS:HB2	2.14	0.48
2:L:193:LEU:HD23	2:L:276:PHE:CD2	2.49	0.48
2:L:150:THR:HG22	8:L:643:HOH:O	2.12	0.48
1:S:112:GLY:HA2	1:S:149:PRO:HD3	1.95	0.48
2:L:223:GLY:HA2	2:L:231:PHE:CD2	2.47	0.48
2:L:31:MET:O	2:L:43:TRP:HE3	1.97	0.48
2:L:53:GLU:HB2	8:L:637:HOH:O	2.13	0.48
1:S:121:GLN:H	1:S:121:GLN:CD	2.16	0.47
2:L:515:VAL:HG13	2:L:516:GLU:N	2.29	0.47
1:S:150:ASN:HD22	1:S:152:ILE:H	1.61	0.47
1:S:232:PHE:HB2	2:L:225:LYS:HB2	1.96	0.47
2:L:203:ALA:O	2:L:207:GLU:HG3	2.13	0.47
1:S:167:PRO:O	1:S:169:LEU:HD13	2.15	0.47
2:L:88:ASP:HA	2:L:93:VAL:HG12	1.97	0.47
2:L:182:ALA:HB3	2:L:185:LEU:HG	1.96	0.46
2:L:273:VAL:O	2:L:277:TYR:HD1	1.97	0.46
2:L:364:ASP:OD2	2:L:366:ASP:HB2	2.16	0.46
1:S:213:LEU:HD12	1:S:239:VAL:HG13	1.96	0.46
1:S:120:VAL:HA	1:S:254:TRP:CD1	2.49	0.46
2:L:100:ARG:HD3	2:L:299:ASP:HB2	1.97	0.46
2:L:237:CYS:HB2	2:L:456:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:187:CYS:HA	1:S:188:PRO:HD2	1.80	0.46
2:L:315:VAL:HG13	2:L:325:ASP:HB2	1.96	0.46
2:L:194:PRO:HG2	2:L:197:VAL:CG2	2.41	0.46
1:S:14:ASN:ND2	1:S:94:MET:HB3	2.31	0.46
1:S:122:LYS:HA	1:S:126:ASN:ND2	2.31	0.46
8:S:273:HOH:O	2:L:225:LYS:HE3	2.15	0.46
2:L:157:GLU:O	2:L:161:LYS:HB2	2.15	0.46
2:L:350:PRO:HB3	2:L:482:TRP:CD1	2.51	0.45
2:L:262:VAL:HA	2:L:266:TYR:HB3	1.98	0.45
1:S:74:VAL:HG11	1:S:133:VAL:HG21	1.99	0.45
2:L:26:GLY:HA3	2:L:544:ILE:HB	1.98	0.45
2:L:106:VAL:HG21	2:L:231:PHE:CZ	2.51	0.45
2:L:134:LEU:HD23	2:L:134:LEU:HA	1.75	0.45
2:L:319:ARG:HB3	2:L:419:HIS:CE1	2.52	0.45
1:S:131:LYS:HG3	1:S:136:ALA:HB2	1.99	0.45
1:S:237:TRP:CZ2	1:S:239:VAL:HB	2.52	0.45
2:L:50:ARG:NH2	2:L:71:ALA:HA	2.30	0.45
2:L:72:CYS:SG	2:L:75:CYS:SG	3.15	0.45
2:L:102:MET:O	2:L:106:VAL:HG23	2.16	0.45
2:L:224:GLY:O	2:L:225:LYS:HB3	2.17	0.44
1:S:143:ASN:O	1:S:174:ARG:HA	2.16	0.44
1:S:78:LEU:HA	1:S:79:PRO:HD3	1.82	0.44
1:S:74:VAL:HG11	1:S:133:VAL:CG2	2.48	0.44
1:S:72:LEU:HD13	1:S:101:ALA:HB1	1.98	0.44
1:S:241:ALA:HB2	2:L:224:GLY:HA2	2.00	0.44
2:L:134:LEU:HG	2:L:167:LEU:HD13	2.00	0.44
2:L:118:HIS:HA	2:L:122:LEU:HB2	2.00	0.43
1:S:169:LEU:HD12	1:S:175:PRO:HA	1.99	0.43
2:L:462:MET:HA	2:L:463:PRO:HD3	1.69	0.43
2:L:288:ASN:HB3	2:L:381:MET:CE	2.48	0.43
2:L:477:GLY:C	2:L:498:PRO:HG3	2.38	0.43
2:L:22:THR:O	2:L:538:HIS:CE1	2.71	0.43
2:L:159:ALA:O	2:L:163:VAL:HG23	2.18	0.43
1:S:259:PRO:HB2	1:S:262:GLU:HB2	2.00	0.43
2:L:29:ARG:NH1	2:L:363:ASP:OD1	2.52	0.43
2:L:497:VAL:HG11	2:L:546:CYS:HB3	2.01	0.43
2:L:267:ILE:HB	2:L:268:PRO:HD3	2.00	0.43
1:S:68:ASP:O	1:S:69:GLY:O	2.37	0.43
2:L:56:LEU:HD21	2:L:67:PHE:HB2	2.00	0.42
2:L:112:LEU:HD12	2:L:112:LEU:HA	1.86	0.42
2:L:403:VAL:HG12	2:L:430:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:225:ASN:HD22	1:S:226:ASN:H	1.67	0.42
2:L:77:TYR:OH	2:L:81:LEU:HD13	2.20	0.42
2:L:150:THR:HB	2:L:264:GLU:HG2	2.00	0.42
2:L:76:THR:HG21	2:L:228:HIS:H	1.84	0.42
2:L:467:LYS:HD3	2:L:484:ARG:HH11	1.84	0.42
1:S:226:ASN:C	1:S:226:ASN:HD22	2.22	0.42
2:L:50:ARG:HH22	2:L:71:ALA:CA	2.30	0.42
2:L:280:TRP:C	2:L:422:LEU:HB2	2.40	0.42
2:L:319:ARG:HD3	2:L:419:HIS:CE1	2.55	0.42
2:L:495:LEU:HD23	2:L:495:LEU:N	2.35	0.42
2:L:350:PRO:HB2	2:L:482:TRP:CD2	2.55	0.41
1:S:163:THR:O	1:S:164:LYS:CB	2.68	0.41
2:L:337:LYS:HD3	2:L:338:TYR:CE2	2.56	0.41
1:S:95:ILE:H	1:S:95:ILE:HG13	1.57	0.41
1:S:223:THR:HG21	4:S:266:F3S:S3	2.60	0.41
2:L:289:TYR:O	2:L:315:VAL:HA	2.21	0.41
2:L:136:ALA:HB2	2:L:195:PRO:C	2.40	0.41
2:L:293:GLY:O	2:L:305:HIS:NE2	2.53	0.41
1:S:226:ASN:O	1:S:230:VAL:HB	2.20	0.41
2:L:338:TYR:HA	2:L:366:ASP:O	2.20	0.41
2:L:32:VAL:HB	2:L:39:VAL:HG13	2.02	0.41
2:L:107:MET:CE	2:L:474:ALA:HA	2.51	0.40
2:L:360:THR:OG1	2:L:361:LYS:N	2.52	0.40
2:L:348:LYS:HG2	2:L:352:ASP:O	2.22	0.40
2:L:371:MET:CE	2:L:547:GLY:HA3	2.51	0.40
2:L:486:LYS:HE3	2:L:486:LYS:HB3	1.89	0.40
2:L:102:MET:HG3	2:L:222:LEU:HG	2.04	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	S	259/264 (98%)	240 (93%)	16 (6%)	3 (1%)	13	32
2	L	541/564 (96%)	506 (94%)	30 (6%)	5 (1%)	17	40
All	All	800/828 (97%)	746 (93%)	46 (6%)	8 (1%)	15	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	69	GLY
2	L	52	LEU
2	L	414	PRO
1	S	164	LYS
1	S	258	THR
2	L	76	THR
2	L	415	ALA
2	L	505	PRO

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	S	210/213 (99%)	194 (92%)	16 (8%)	13	30
2	L	438/458 (96%)	402 (92%)	36 (8%)	11	26
All	All	648/671 (97%)	596 (92%)	52 (8%)	12	27

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	12	LEU
1	S	62	GLU
1	S	65	GLU
1	S	95	ILE
1	S	150	ASN
1	S	168	ASP
1	S	169	LEU
1	S	189	ARG

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Mol	Chain	Res	Type
1	S	215	GLU
1	S	216	LEU
1	S	225	ASN
1	S	226	ASN
1	S	235	VAL
1	S	246	LEU
1	S	256	THR
1	S	258	THR
2	L	7	THR
2	L	17	VAL
2	L	31	MET
2	L	75	CYS
2	L	112	LEU
2	L	125	LEU
2	L	144	LEU
2	L	152	ARG
2	L	153	THR
2	L	157	GLU
2	L	167	LEU
2	L	222	LEU
2	L	225	LYS
2	L	243	LEU
2	L	245	LYS
2	L	252	LEU
2	L	254	LEU
2	L	287	SER
2	L	299	ASP
2	L	329	LEU
2	L	334	GLU
2	L	346	ASP
2	L	362	LEU
2	L	401	LYS
2	L	408	LEU
2	L	410	LYS
2	L	411	LEU
2	L	422	LEU
2	L	444	LYS
2	L	473	ASP
2	L	478	SER
2	L	486	LYS
2	L	495	LEU
2	L	506	ARG

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Mol	Chain	Res	Type
2	L	508	PRO
2	L	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	14	ASN
1	S	85	GLN
1	S	126	ASN
1	S	150	ASN
1	S	225	ASN
1	S	226	ASN
1	S	263	GLN
2	L	47	GLN
2	L	104	ASN
2	L	110	GLN
2	L	115	HIS
2	L	121	HIS
2	L	155	ASN
2	L	198	ASN
2	L	230	GLN
2	L	538	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	S	266	1	0,9,9	-	-	-		
3	SF4	S	265	1	0,12,12	-	-	-		
3	SF4	S	267	1	0,12,12	-	-	-		

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	S	266	1	-	-	0/3/3/3
3	SF4	S	265	1	-	-	0/6/5/5
3	SF4	S	267	1	-	-	0/6/5/5

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
4	S	266	F3S	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.