Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 06:14 PM EDT

PDB ID	:	3CUS
Title	:	Structure of a double ILE/PHE mutant of NI-FE hydrogenase refined at 2.2 angstrom resolution
Authors	:	Volbeda, A.
Deposited on	:	2008-04-17
Resolution	:	2.20 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:

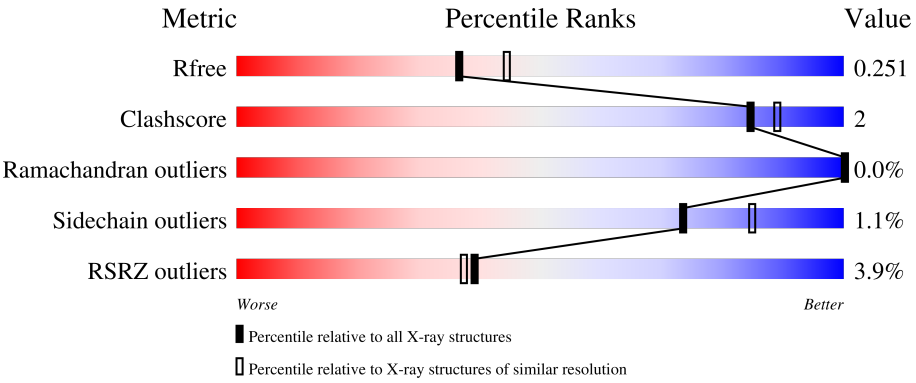
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	264	2% 93% 6%
1	B	264	18% 92% 7%
1	C	264	% 95%
2	Q	549	93% 6%
2	R	549	4% 95%

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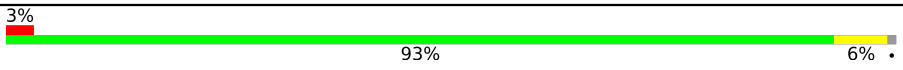
Mol	Chain	Length	Quality of chain
2	S	549	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19590 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 Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1973	1256	330	372	15			
1	B	262	Total	C	N	O	S	0	2	0
			1980	1260	330	375	15			
1	C	260	Total	C	N	O	S	0	1	0
			1965	1251	329	370	15			

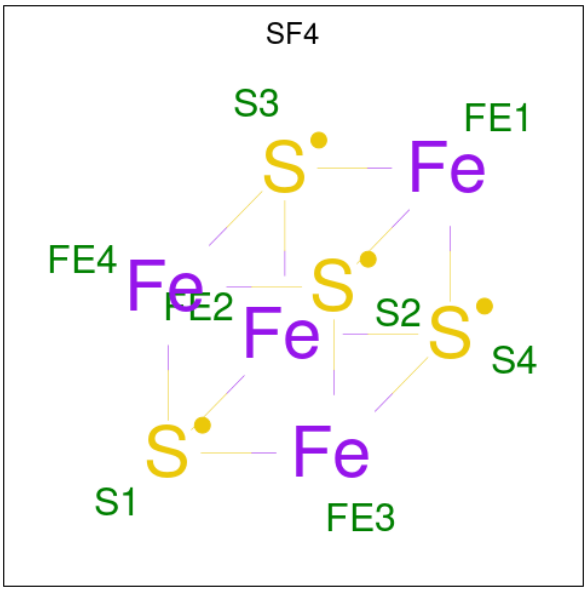
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	4	0
			4185	2668	724	770	23			
2	R	545	Total	C	N	O	S	0	1	0
			4178	2661	725	770	22			
2	S	544	Total	C	N	O	S	0	1	0
			4170	2657	724	767	22			

There are 6 discrepancies between the modelled and reference sequences:

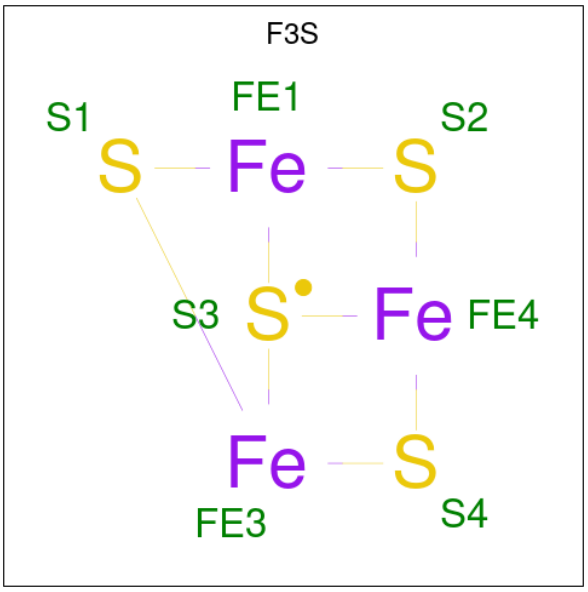
Chain	Residue	Modelled	Actual	Comment	Reference
Q	74	ILE	VAL	engineered mutation	UNP P18188
Q	122	PHE	LEU	engineered mutation	UNP P18188
R	74	ILE	VAL	engineered mutation	UNP P18188
R	122	PHE	LEU	engineered mutation	UNP P18188
S	74	ILE	VAL	engineered mutation	UNP P18188
S	122	PHE	LEU	engineered mutation	UNP P18188

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



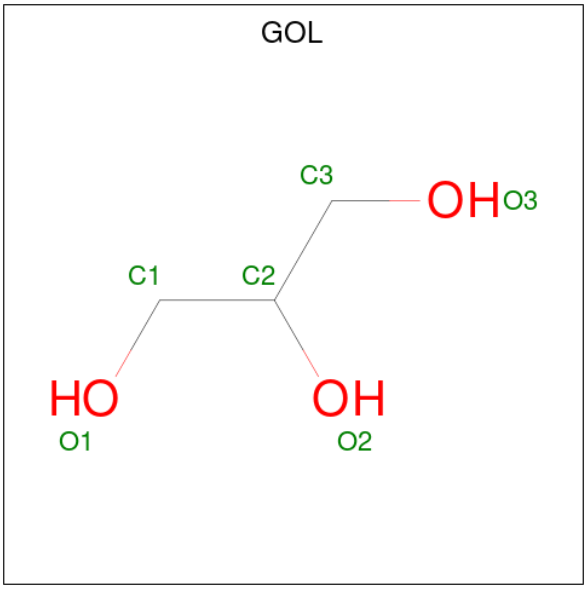
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	S	1	Total C O 6 3 3	0	0

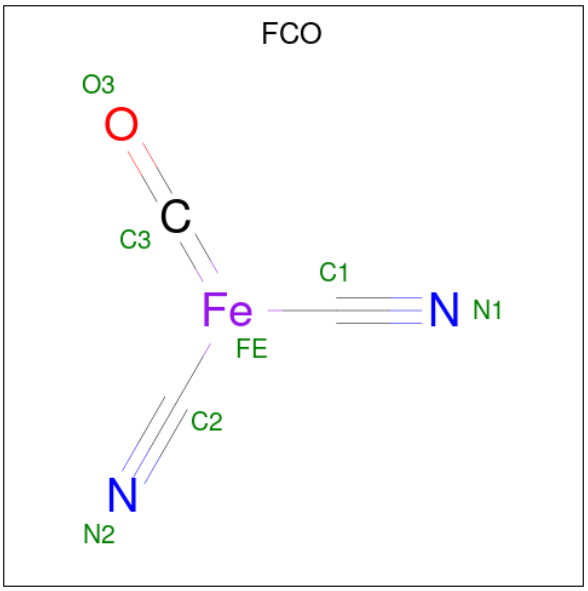
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Q	1	Total Ni 1 1	0	0
6	R	1	Total Ni 1 1	0	0
6	S	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	Q	1	Total Mg 1 1	0	0
7	R	1	Total Mg 1 1	0	0
7	S	1	Total Mg 1 1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	Q	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
8	R	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
8	S	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	134	Total	O	0	0
			134	134		
9	Q	245	Total	O	0	0
			245	245		
9	B	91	Total	O	0	0
			91	91		
9	R	215	Total	O	0	0
			215	215		
9	C	123	Total	O	0	0
			123	123		
9	S	205	Total	O	0	0
			205	205		

3 Residue-property plots (i)

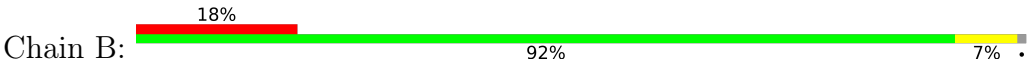
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

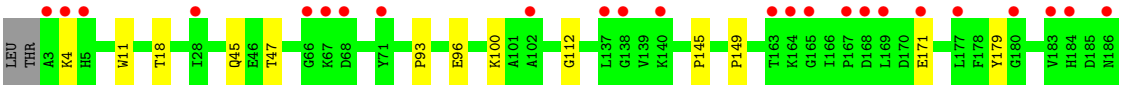
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

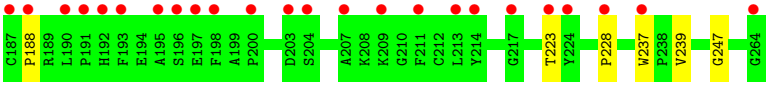
Chain A:

• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain B:

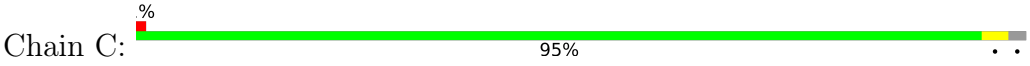


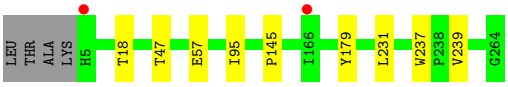




• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

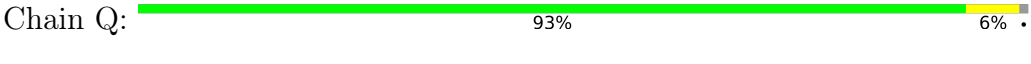
Chain C:

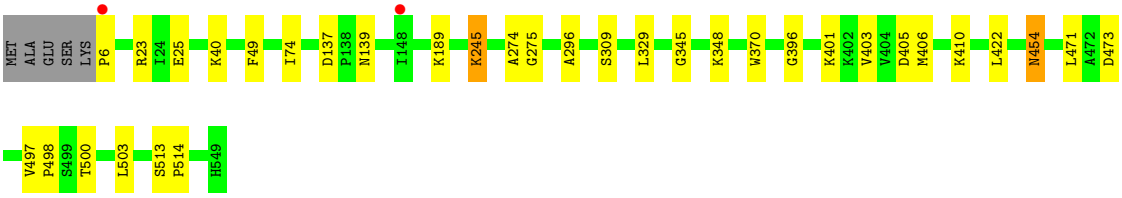




• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

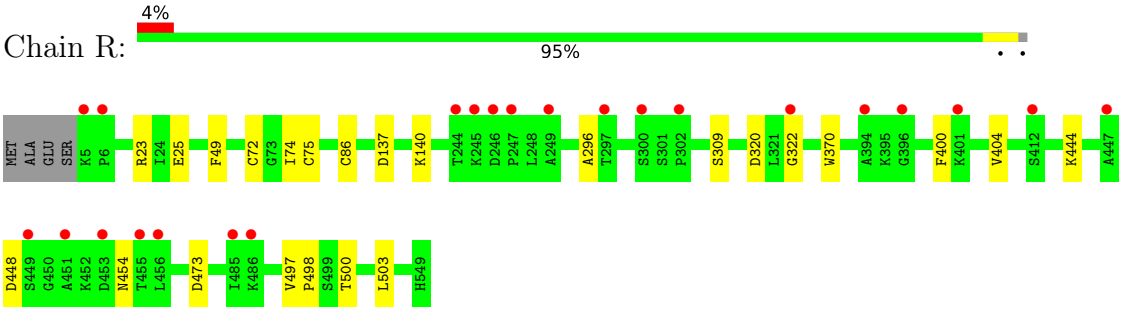
Chain Q:





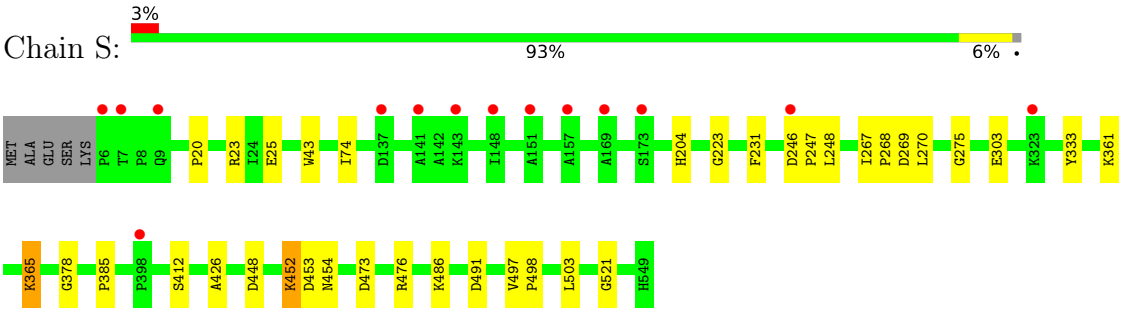
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain R:



• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.40Å 99.96Å 182.69Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.20) 94.2 (19.99-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.222 0.217 , 0.251	Depositor DCC
R_{free} test set	5404 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19590	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: GOL, F3S, NI, SF4, FCO, CSO, 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	A	0.62	0/2027	0.60	0/2759
1	B	0.50	0/2043	0.55	0/2781
1	C	0.54	0/2025	0.59	0/2758
2	Q	0.61	0/4302	0.65	0/5835
2	R	0.56	0/4281	0.60	0/5809
2	S	0.55	1/4273 (0.0%)	0.62	0/5798
All	All	0.57	1/18951 (0.0%)	0.61	0/25740

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	303	GLU	CB-CG	-5.21	1.42	1.52

There are no bond angle outliers.

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	1973	0	1911	11	0
1	B	1980	0	1918	11	0
1	C	1965	0	1900	5	0
2	Q	4185	0	4161	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	4178	0	4142	15	0
2	S	4170	0	4138	22	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
5	A	6	0	8	0	0
5	Q	12	0	16	0	0
5	R	6	0	8	0	0
5	S	6	0	8	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	Q	7	0	0	0	0
8	R	7	0	0	1	0
8	S	7	0	0	1	0
9	A	134	0	0	3	0
9	B	91	0	0	1	0
9	C	123	0	0	5	0
9	Q	245	0	0	4	0
9	R	215	0	0	4	0
9	S	205	0	0	4	0
All	All	19590	0	18210	83	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 2.

All (83) 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:R:322:GLY:HA3	9:R:721:HOH:O	1.71	0.89
9:C:341:HOH:O	2:S:361:LYS:HE3	1.81	0.81
1:C:57:GLU:HB2	9:C:390:HOH:O	1.84	0.78
2:S:385:PRO:HB2	9:S:614:HOH:O	1.86	0.75
1:A:215:GLU:HG3	9:A:373:HOH:O	1.88	0.72
2:Q:245:LYS:HD3	9:Q:785:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:412:SER:HB2	9:S:715:HOH:O	1.92	0.68
2:R:137:ASP:OD2	2:R:140:LYS:HG3	1.97	0.64
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.79	0.63
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.31	0.60
1:B:188:PRO:HA	9:B:331:HOH:O	2.02	0.60
1:B:47:THR:O	2:R:23:ARG:HA	2.01	0.59
2:S:25:GLU:HB2	2:S:74:ILE:HD12	1.86	0.56
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.38	0.53
2:Q:6:PRO:HG3	9:R:721:HOH:O	2.09	0.53
1:A:215:GLU:CG	9:A:373:HOH:O	2.52	0.53
2:Q:396:GLY:HA2	2:Q:401:LYS:HE3	1.91	0.52
2:Q:275:GLY:HA3	9:Q:653:HOH:O	2.11	0.50
2:Q:6:PRO:HG3	2:R:320:ASP:OD1	2.11	0.50
2:R:497:VAL:HG13	2:R:498:PRO:HD2	1.93	0.50
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.42	0.50
2:S:246:ASP:HB2	2:S:247:PRO:HD3	1.93	0.49
2:S:267:ILE:HB	2:S:268:PRO:HD3	1.94	0.49
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.48	0.49
2:Q:25:GLU:HB2	2:Q:74:ILE:HD12	1.93	0.49
2:S:270:LEU:HD21	2:S:426:ALA:HA	1.95	0.49
2:Q:403:VAL:HA	9:Q:736:HOH:O	2.12	0.49
2:Q:329:LEU:HD11	2:Q:471:LEU:HD11	1.95	0.49
9:C:390:HOH:O	2:S:20:PRO:CD	2.61	0.49
9:C:390:HOH:O	2:S:20:PRO:HD2	2.14	0.47
2:R:25:GLU:HB2	2:R:74:ILE:HD12	1.96	0.47
2:Q:245:LYS:O	2:Q:245:LYS:HE2	2.15	0.47
2:S:204:HIS:ND1	2:S:269:ASP:OD2	2.48	0.47
2:R:444:LYS:HG3	9:R:737:HOH:O	2.14	0.47
2:Q:454:ASN:H	2:Q:454:ASN:HD22	1.62	0.46
1:C:18:THR:HG22	1:C:18:THR:O	2.15	0.46
2:Q:405:ASP:HB2	9:Q:735:HOH:O	2.15	0.46
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.51	0.46
1:A:145:PRO:HD2	1:A:179:TYR:CZ	2.51	0.46
2:Q:274:ALA:HB1	2:Q:422:LEU:HD11	1.98	0.46
1:A:96:GLU:HB2	9:A:400:HOH:O	2.16	0.45
2:S:43:TRP:CE2	2:S:365:LYS:HE2	2.51	0.45
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.52	0.45
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.52	0.45
2:S:275:GLY:HA3	9:S:646:HOH:O	2.17	0.45
2:R:448:ASP:HB3	9:R:659:HOH:O	2.17	0.45
1:C:47:THR:O	2:S:23:ARG:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:HIS:HB2	1:A:220:GLY:C	2.36	0.44
2:Q:497:VAL:HG12	2:Q:498:PRO:HD2	1.98	0.44
1:A:33:ASP:O	1:A:37:LEU:HG	2.18	0.44
2:S:448:ASP:O	2:S:452:LYS:HE2	2.17	0.44
2:Q:137:ASP:OD2	2:Q:139:ASN:HB2	2.17	0.44
2:Q:274:ALA:CB	2:Q:422:LEU:HD11	2.47	0.44
1:B:223:THR:OG1	1:B:247:GLY:HA2	2.18	0.44
2:R:72:CYS:HB3	2:R:75:CYS:SG	2.57	0.44
2:S:476:ARG:HD2	8:S:550:FCO:C2	2.48	0.44
1:C:145:PRO:HD2	1:C:179:TYR:CZ	2.53	0.43
1:B:112:GLY:HA2	1:B:149:PRO:HD3	2.01	0.43
1:A:18:THR:HG22	1:A:18:THR:O	2.19	0.43
2:R:296:ALA:HA	2:R:309:SER:HA	2.02	0.42
1:A:47:THR:O	2:Q:23:ARG:HA	2.20	0.42
2:Q:189:LYS:HE2	9:C:299:HOH:O	2.19	0.42
2:Q:296:ALA:HA	2:Q:309:SER:HA	2.00	0.42
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.55	0.42
2:S:521:GLY:O	9:S:762:HOH:O	2.21	0.42
1:B:18:THR:HG22	1:B:18:THR:O	2.20	0.41
1:A:112:GLY:HA2	1:A:149:PRO:HD3	2.01	0.41
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.56	0.41
2:R:497:VAL:HG12	2:R:498:PRO:HD2	2.01	0.41
2:S:248:LEU:HD23	2:S:248:LEU:HA	1.79	0.41
1:B:93:PRO:HB2	1:B:96[B]:GLU:HG3	2.03	0.41
2:S:223:GLY:HA2	2:S:231:PHE:CD1	2.55	0.41
2:Q:513:SER:HB2	2:Q:514:PRO:HD2	2.02	0.41
2:R:400:PHE:O	2:R:404:VAL:HG23	2.20	0.41
2:S:453:ASP:C	2:S:453:ASP:OD1	2.59	0.41
2:S:486:LYS:HB3	2:S:491:ASP:HB2	2.03	0.41
2:Q:406[A]:MET:HG2	2:Q:410:LYS:HD2	2.03	0.41
1:B:145:PRO:HD2	1:B:179:TYR:CZ	2.56	0.40
2:Q:345:GLY:O	2:Q:348:LYS:HG2	2.21	0.40
1:B:11:TRP:HB3	1:B:45:GLN:HG2	2.03	0.40
2:S:333:TYR:OH	2:S:378:GLY:HA2	2.21	0.40
1:A:228:PRO:HB3	1:A:237:TRP:CZ2	2.56	0.40
2:R:75:CYS:CB	8:R:550:FCO:C2	2.99	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	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	B	262/264 (99%)	252 (96%)	10 (4%)	0	100	100
1	C	259/264 (98%)	252 (97%)	6 (2%)	1 (0%)	34	37
2	Q	545/549 (99%)	532 (98%)	13 (2%)	0	100	100
2	R	543/549 (99%)	529 (97%)	14 (3%)	0	100	100
2	S	542/549 (99%)	527 (97%)	15 (3%)	0	100	100
All	All	2411/2439 (99%)	2346 (97%)	64 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	231	LEU

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	A	208/210 (99%)	207 (100%)	1 (0%)	88	94
1	B	210/210 (100%)	207 (99%)	3 (1%)	67	80
1	C	208/210 (99%)	207 (100%)	1 (0%)	88	94
2	Q	438/438 (100%)	432 (99%)	6 (1%)	67	80
2	R	435/438 (99%)	430 (99%)	5 (1%)	73	85
2	S	434/438 (99%)	429 (99%)	5 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1933/1944 (99%)	1912 (99%)	21 (1%)	73 85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
2	Q	40	LYS
2	Q	245	LYS
2	Q	454	ASN
2	Q	473	ASP
2	Q	500	THR
2	Q	503	LEU
1	B	4	LYS
1	B	100	LYS
1	B	171	GLU
2	R	86	CYS
2	R	454	ASN
2	R	473	ASP
2	R	500	THR
2	R	503	LEU
1	C	95	ILE
2	S	365	LYS
2	S	452	LYS
2	S	454	ASN
2	S	473	ASP
2	S	503	LEU

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

Mol	Chain	Res	Type
1	A	14	ASN
1	A	61	HIS
2	Q	454	ASN
1	B	14	ASN
2	R	454	ASN
1	C	14	ASN
2	S	454	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	R	543	2,6	3,6,7	0.85	0	0,6,8	-	-
2	CSO	Q	543	2,6	3,6,7	0.80	0	0,6,8	-	-
2	CSO	S	543	2,6	3,6,7	0.97	0	0,6,8	-	-

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	R	543	2,6	-	1/1/5/7	-
2	CSO	Q	543	2,6	-	1/1/5/7	-
2	CSO	S	543	2,6	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	543	CSO	N-CA-CB-SG
2	R	543	CSO	N-CA-CB-SG
2	S	543	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
8	FCO	S	550	2	0,6,6	-	-	-		
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
5	GOL	R	563	-	5,5,5	0.42	0	5,5,5	0.39	0
3	SF4	C	267	1	0,12,12	-	-	-		
5	GOL	S	561	-	5,5,5	0.37	0	5,5,5	0.41	0
3	SF4	A	265	1	0,12,12	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	B	266	1	0,9,9	-	-	-		
8	FCO	Q	550	2	0,6,6	-	-	-		
5	GOL	Q	561	-	5,5,5	0.51	0	5,5,5	0.25	0
8	FCO	R	550	2	0,6,6	-	-	-		
3	SF4	B	265	1	0,12,12	-	-	-		
3	SF4	B	267	1	0,12,12	-	-	-		
5	GOL	Q	562	-	5,5,5	0.44	0	5,5,5	0.58	0
5	GOL	A	271	-	5,5,5	0.38	0	5,5,5	0.23	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
3	SF4	C	265	1	-	-	0/6/5/5
5	GOL	R	563	-	-	4/4/4/4	-
3	SF4	A	267	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
5	GOL	S	561	-	-	0/4/4/4	-
3	SF4	C	267	1	-	-	0/6/5/5
3	SF4	A	265	1	-	-	0/6/5/5
4	F3S	C	266	1	-	-	0/3/3/3
4	F3S	B	266	1	-	-	0/3/3/3
3	SF4	B	267	1	-	-	0/6/5/5
3	SF4	B	265	1	-	-	0/6/5/5
5	GOL	Q	561	-	-	0/4/4/4	-
5	GOL	Q	562	-	-	0/4/4/4	-
5	GOL	A	271	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	271	GOL	O1-C1-C2-C3
5	A	271	GOL	O1-C1-C2-O2
5	R	563	GOL	O1-C1-C2-C3
5	R	563	GOL	C1-C2-C3-O3
5	R	563	GOL	O1-C1-C2-O2
5	R	563	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	S	550	FCO	1	0
8	R	550	FCO	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

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	A	262/264 (99%)	0.09	5 (1%) 66 65	13, 15, 17, 26	8 (3%)
1	B	262/264 (99%)	0.89	48 (18%) 1 1	13, 15, 17, 23	9 (3%)
1	C	260/264 (98%)	-0.05	2 (0%) 86 85	13, 15, 17, 21	5 (1%)
2	Q	543/549 (98%)	0.02	2 (0%) 92 91	12, 14, 17, 23	12 (2%)
2	R	544/549 (99%)	0.28	23 (4%) 36 34	12, 15, 18, 22	13 (2%)
2	S	543/549 (98%)	0.11	14 (2%) 56 53	12, 15, 17, 22	15 (2%)
All	All	2414/2439 (98%)	0.19	94 (3%) 39 37	12, 15, 17, 26	62 (2%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	PHE	4.7
1	B	228	PRO	4.5
1	B	163	THR	4.4
2	R	453	ASP	4.2
1	B	168	ASP	4.2
1	B	3	ALA	4.0
2	R	451	ALA	3.9
2	S	157	ALA	3.9
2	R	249	ALA	3.7
1	B	191	PRO	3.7
1	B	140	LYS	3.7
1	B	264	GLY	3.7
1	B	190	LEU	3.7
1	B	213	LEU	3.7
1	C	5	HIS	3.7
1	B	183	VAL	3.6
1	B	188	PRO	3.6
2	R	447	ALA	3.6
1	B	180	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	S	6	PRO	3.5
1	B	164	LYS	3.4
2	R	246	ASP	3.4
2	R	247	PRO	3.3
1	B	197	GLU	3.3
1	B	195	ALA	3.3
2	R	322	GLY	3.3
1	B	169	LEU	3.3
1	B	67	LYS	3.2
1	B	184	HIS	3.2
2	R	449	SER	3.2
1	B	165	GLY	3.2
1	B	196	SER	3.1
2	S	398	PRO	3.1
1	A	3	ALA	3.0
1	B	171	GLU	3.0
2	R	6	PRO	2.9
2	S	151	ALA	2.9
2	Q	6	PRO	2.9
2	S	173	SER	2.9
2	R	455	THR	2.8
1	B	68	ASP	2.8
2	R	245	LYS	2.8
1	B	167	PRO	2.8
1	A	4	LYS	2.8
2	R	244	THR	2.8
2	R	5	LYS	2.7
1	B	198	PHE	2.7
1	B	5	HIS	2.7
1	B	237	TRP	2.6
1	B	4	LYS	2.6
2	R	297	THR	2.6
1	B	186	ASN	2.5
1	B	223	THR	2.5
2	S	141	ALA	2.5
1	B	137	LEU	2.5
1	B	203	ASP	2.5
2	S	9	GLN	2.5
1	B	71	TYR	2.4
2	S	7	THR	2.4
1	B	193	PHE	2.4
1	B	207	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	177	LEU	2.4
1	B	28	ILE	2.3
2	R	485	ILE	2.3
1	B	102	ALA	2.3
1	B	209	LYS	2.3
1	B	214	TYR	2.3
1	B	217	GLY	2.3
2	S	323	LYS	2.3
1	B	224	TYR	2.3
2	R	302	PRO	2.3
2	S	246	ASP	2.3
1	A	165	GLY	2.2
2	Q	148	ILE	2.2
2	S	137	ASP	2.2
1	B	200	PRO	2.2
1	A	67	LYS	2.2
2	R	412	SER	2.2
1	B	66	GLY	2.1
1	B	138	GLY	2.1
1	B	187	CYS	2.1
2	R	396	GLY	2.1
2	R	456	LEU	2.1
1	B	204	SER	2.1
1	B	192	HIS	2.1
2	R	394	ALA	2.1
2	R	401	LYS	2.1
2	S	143	LYS	2.1
1	C	166	ILE	2.1
2	S	148	ILE	2.0
1	A	164	LYS	2.0
2	R	486	LYS	2.0
2	S	169	ALA	2.0
2	R	300	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	CSO	Q	543	7/8	0.96	0.13	14,14,16,16	0
2	CSO	R	543	7/8	0.96	0.11	14,14,14,16	0
2	CSO	S	543	7/8	0.96	0.11	14,14,15,16	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	MG	R	553	1/1	0.78	0.10	13,13,13,13	0
7	MG	S	553	1/1	0.84	0.12	13,13,13,13	0
5	GOL	R	563	6/6	0.85	0.19	16,18,19,19	0
5	GOL	A	271	6/6	0.86	0.19	18,20,20,21	0
3	SF4	B	265	8/8	0.88	0.11	14,14,15,16	0
5	GOL	Q	562	6/6	0.89	0.19	13,16,16,16	0
4	F3S	B	266	7/7	0.90	0.11	13,14,15,15	0
5	GOL	S	561	6/6	0.91	0.14	13,14,14,15	0
5	GOL	Q	561	6/6	0.95	0.11	10,11,12,12	0
3	SF4	B	267	8/8	0.96	0.07	13,14,15,15	0
3	SF4	A	265	8/8	0.97	0.12	12,13,13,14	0
7	MG	Q	553	1/1	0.97	0.12	13,13,13,13	0
3	SF4	C	267	8/8	0.98	0.11	13,14,14,15	0
4	F3S	A	266	7/7	0.98	0.13	13,14,14,14	0
3	SF4	C	265	8/8	0.98	0.10	12,13,14,14	0
4	F3S	C	266	7/7	0.98	0.11	13,14,14,15	0
8	FCO	R	550	7/7	0.98	0.10	13,13,14,14	0
6	NI	Q	551	1/1	0.99	0.10	15,15,15,15	0
6	NI	R	551	1/1	0.99	0.04	15,15,15,15	0
8	FCO	Q	550	7/7	0.99	0.13	13,14,15,15	0
3	SF4	A	267	8/8	0.99	0.14	12,13,14,15	0
8	FCO	S	550	7/7	0.99	0.12	14,14,14,15	0
6	NI	S	551	1/1	1.00	0.09	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.