Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:24 PM EDT

PDB ID	:	4UCQ
Title	:	Structure of the T18D small subunit mutant of D. fructosovorans NiFe- hydrogenase
Authors	:	Abou-Hamdan, A.; Ceccaldi, P.; Lebrette, H.; Guttierez-Sanz, O.; Richaud, P.; Cournac, L.; Guigliarelli, B.; deLacey, A.L.; Leger, C.; Volbeda, A.; Burlat, B.; Dementin, S.
Deposited on	:	2014-12-04
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

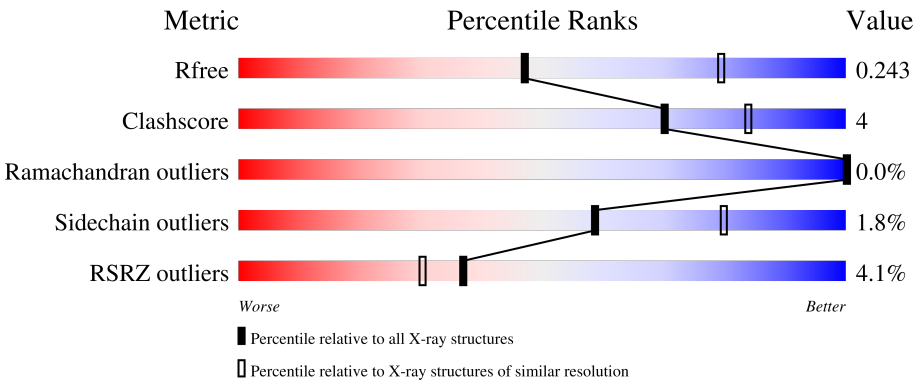
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	88% 11% •
1	B	264	91% 8% •
1	C	264	14% 88% 11% •
2	Q	563	% 89% 7% •

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Mol	Chain	Length	Quality of chain
2	R	563	% 89% 8%
2	S	563	8% 82% 13%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19027 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 (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	1975	1257	330	373	15	0	0	0
1	B	261	1976	1257	329	375	15	0	2	0
1	C	260	1961	1248	327	371	15	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ASP	THR	engineered mutation	UNP E1K248
B	18	ASP	THR	engineered mutation	UNP E1K248
C	18	ASP	THR	engineered mutation	UNP E1K248

- Molecule 2 is a protein called NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Q	544	4191	2671	727	771	22	0	7	0
2	R	545	4177	2662	724	769	22	0	2	0
2	S	544	4169	2654	724	769	22	0	1	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	expression tag	UNP E1K247
Q	-12	SER	-	expression tag	UNP E1K247
Q	-11	TRP	-	expression tag	UNP E1K247
Q	-10	SER	-	expression tag	UNP E1K247

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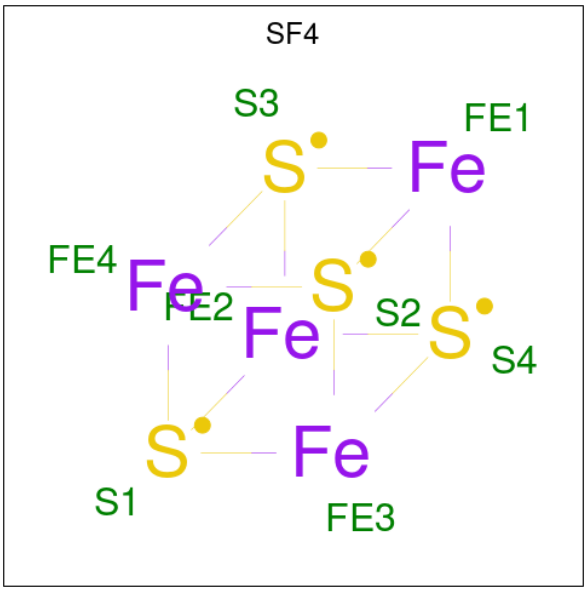
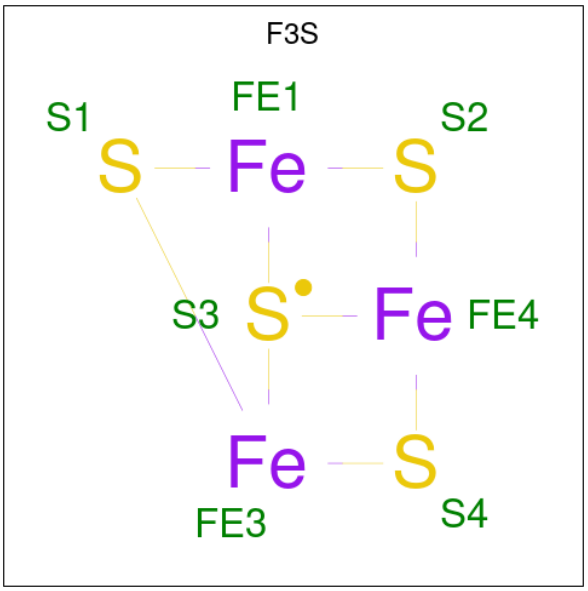
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-9	HIS	-	expression tag	UNP E1K247
Q	-8	PRO	-	expression tag	UNP E1K247
Q	-7	GLN	-	expression tag	UNP E1K247
Q	-6	PHE	-	expression tag	UNP E1K247
Q	-5	GLU	-	expression tag	UNP E1K247
Q	-4	LYS	-	expression tag	UNP E1K247
Q	-3	GLY	-	expression tag	UNP E1K247
Q	-2	ALA	-	expression tag	UNP E1K247
Q	-1	SER	-	expression tag	UNP E1K247
Q	0	GLY	-	expression tag	UNP E1K247
Q	1	ALA	-	expression tag	UNP E1K247
R	-13	ALA	-	expression tag	UNP E1K247
R	-12	SER	-	expression tag	UNP E1K247
R	-11	TRP	-	expression tag	UNP E1K247
R	-10	SER	-	expression tag	UNP E1K247
R	-9	HIS	-	expression tag	UNP E1K247
R	-8	PRO	-	expression tag	UNP E1K247
R	-7	GLN	-	expression tag	UNP E1K247
R	-6	PHE	-	expression tag	UNP E1K247
R	-5	GLU	-	expression tag	UNP E1K247
R	-4	LYS	-	expression tag	UNP E1K247
R	-3	GLY	-	expression tag	UNP E1K247
R	-2	ALA	-	expression tag	UNP E1K247
R	-1	SER	-	expression tag	UNP E1K247
R	0	GLY	-	expression tag	UNP E1K247
R	1	ALA	-	expression tag	UNP E1K247
S	-13	ALA	-	expression tag	UNP E1K247
S	-12	SER	-	expression tag	UNP E1K247
S	-11	TRP	-	expression tag	UNP E1K247
S	-10	SER	-	expression tag	UNP E1K247
S	-9	HIS	-	expression tag	UNP E1K247
S	-8	PRO	-	expression tag	UNP E1K247
S	-7	GLN	-	expression tag	UNP E1K247
S	-6	PHE	-	expression tag	UNP E1K247
S	-5	GLU	-	expression tag	UNP E1K247
S	-4	LYS	-	expression tag	UNP E1K247
S	-3	GLY	-	expression tag	UNP E1K247
S	-2	ALA	-	expression tag	UNP E1K247
S	-1	SER	-	expression tag	UNP E1K247
S	0	GLY	-	expression tag	UNP E1K247
S	1	ALA	-	expression tag	UNP E1K247

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



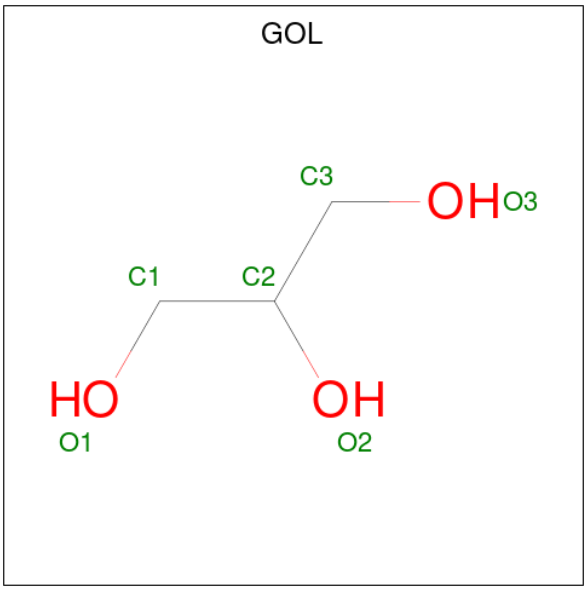
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0
			Total	Fe	S		
3	C	1	8	4	4	0	0
			Total	Fe	S		
3	C	1	8	4	4	0	0

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



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

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



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

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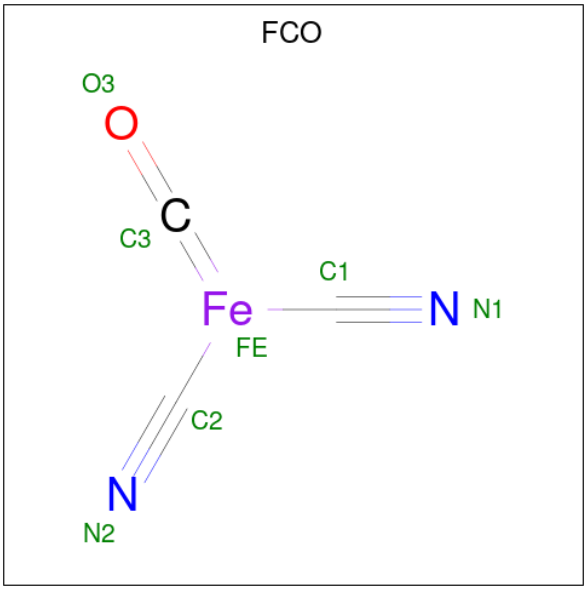
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	Q	1	6	3	3	0	0
			Total	C	O		
5	Q	1	6	3	3	0	0
			Total	C	O		
5	R	1	6	3	3	0	0
			Total	C	O		
5	R	1	6	3	3	0	0
			Total	C	O		
5	S	1	6	3	3	0	0

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



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

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
7	Q	1	1	1	0	0

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Q	1	Total Mg 1 1	0	0
8	R	1	Total Mg 1 1	0	0
8	S	1	Total Mg 1 1	0	0

- Molecule 9 is water.

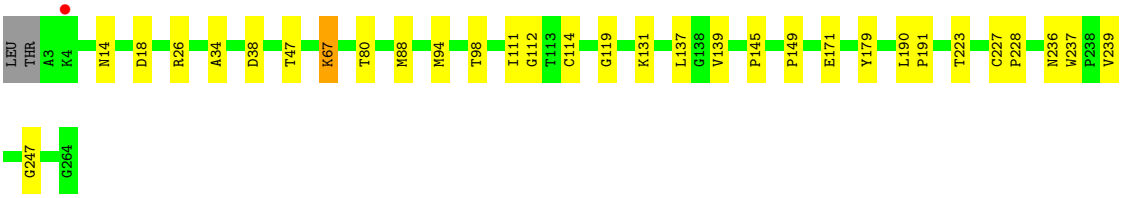
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	69	Total O 69 69	0	0
9	B	64	Total O 64 64	0	0
9	C	55	Total O 55 55	0	0
9	Q	98	Total O 98 98	0	0
9	R	90	Total O 90 90	0	0
9	S	70	Total O 70 70	0	0

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 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 (NIFE) SMALL SUBUNIT HYDA

Chain A:

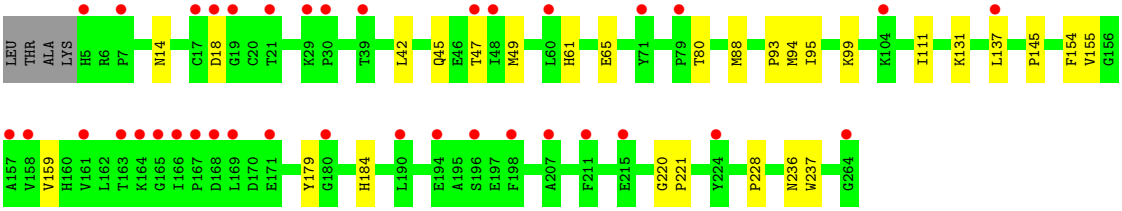


• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain B:

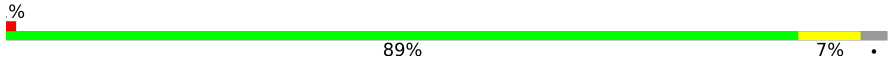
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

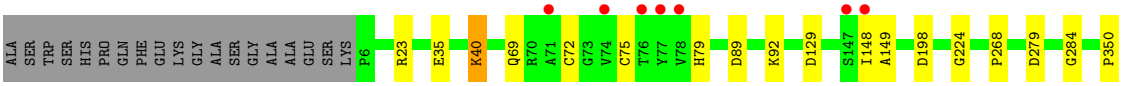
Chain C:

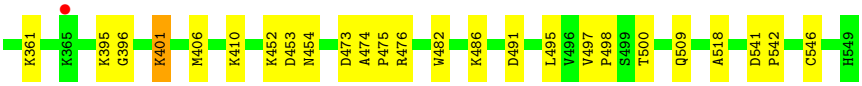


• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain Q:

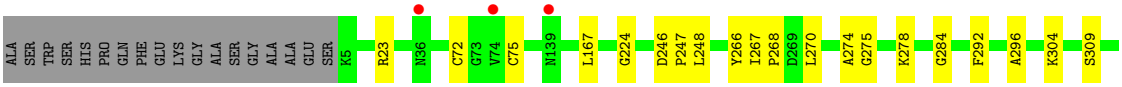






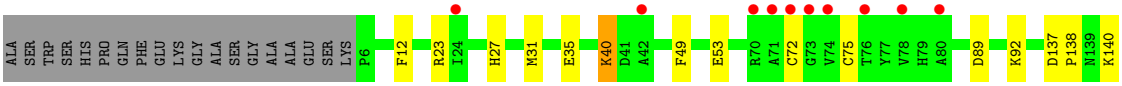
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

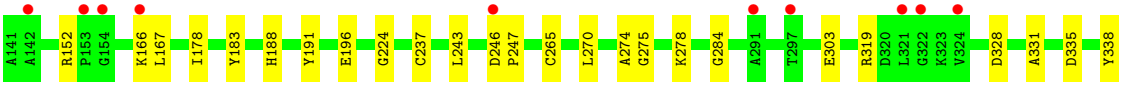
Chain R:

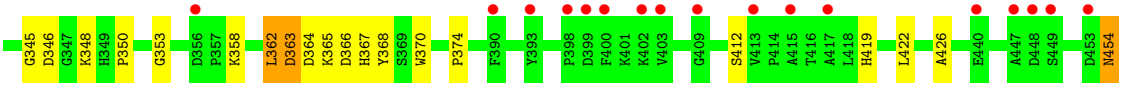


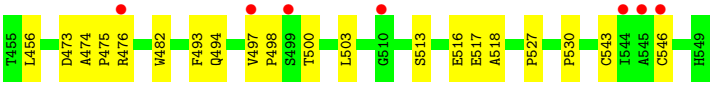
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

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	63.80Å 99.90Å 183.30Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 39.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.00-2.60) 99.2 (39.80-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.198 , 0.241 0.199 , 0.243	Depositor DCC
R_{free} test set	3464 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.917	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19027	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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 (i)

5.1 Standard geometry (i)

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

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	0.79	0/2029	0.81	0/2762
1	B	0.74	0/2039	0.77	1/2775 (0.0%)
1	C	0.72	0/2015	0.74	0/2744
2	Q	0.73	0/4321	0.80	3/5862 (0.1%)
2	R	0.73	0/4283	0.79	0/5813
2	S	0.75	0/4271	0.78	0/5796
All	All	0.74	0/18958	0.79	4/25752 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	279	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	252	ASP	CB-CG-OD1	5.84	123.56	118.30
2	Q	198	ASP	CB-CG-OD2	5.68	123.42	118.30
2	Q	129	ASP	CB-CG-OD1	5.67	123.41	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1975	0	1912	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1976	0	1910	11	0
1	C	1961	0	1894	17	0
2	Q	4191	0	4179	22	0
2	R	4177	0	4152	26	0
2	S	4169	0	4141	46	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	12	0	16	0	0
5	S	6	0	8	0	0
6	Q	7	0	0	0	0
6	R	7	0	0	0	0
6	S	7	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	1	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0
9	A	69	0	0	1	0
9	B	64	0	0	0	0
9	C	55	0	0	0	0
9	Q	98	0	0	3	0
9	R	90	0	0	1	0
9	S	70	0	0	3	0
All	All	19027	0	18236	133	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 4.

All (133) 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:S:362:LEU:O	2:S:363:ASP:HB2	1.73	0.88
2:Q:89:ASP:O	2:Q:92:LYS:HE2	1.77	0.84
2:S:72:CYS:HB3	2:S:75:CSX:OD	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:35:GLU:HB2	2:Q:40:LYS:HE2	1.78	0.66
2:S:275:GLY:O	2:S:278:LYS:HG3	1.97	0.65
2:R:464:GLU:OE2	2:R:488:LYS:HE3	1.98	0.63
2:S:338:TYR:HA	2:S:366:ASP:O	1.99	0.63
2:R:476:ARG:HD2	9:R:2023:HOH:O	1.99	0.62
2:R:246:ASP:HB2	2:R:247:PRO:HD3	1.81	0.60
2:S:303:GLU:HG2	9:S:2049:HOH:O	2.01	0.60
1:A:171:GLU:H	1:A:171:GLU:CD	2.05	0.59
2:R:72:CYS:HB3	2:R:75:CSX:OD	2.03	0.59
2:S:274:ALA:CB	2:S:422:LEU:HD11	2.32	0.58
2:Q:476:ARG:HD2	9:Q:2024:HOH:O	2.04	0.58
2:S:140:LYS:HG2	2:S:196:GLU:HG2	1.84	0.58
2:Q:72:CYS:HB3	2:Q:75:CSX:OD	2.04	0.57
1:C:14:ASN:ND2	1:C:94:MET:HB3	2.19	0.57
1:A:14:ASN:ND2	1:A:94:MET:HB3	2.21	0.55
1:A:236:ASN:HB3	2:Q:224:GLY:O	2.06	0.55
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.37	0.54
1:C:80:THR:HG21	1:C:131:LYS:HD2	1.89	0.54
1:C:111:ILE:HD12	1:C:154:PHE:CD1	2.42	0.54
2:R:275:GLY:O	2:R:278:LYS:HG3	2.08	0.54
1:A:228:PRO:HB3	1:A:237:TRP:CZ2	2.43	0.53
1:C:42:LEU:HD21	1:C:45:GLN:HG3	1.90	0.53
2:S:362:LEU:O	2:S:363:ASP:CB	2.51	0.53
2:S:350:PRO:HB2	2:S:482:TRP:CG	2.44	0.53
1:A:145:PRO:HD2	1:A:179:TYR:CZ	2.44	0.52
2:S:72:CYS:CB	2:S:75:CSX:OD	2.50	0.52
1:C:145:PRO:HD2	1:C:179:TYR:CZ	2.46	0.51
2:R:474:ALA:HB1	2:R:475:PRO:HD2	1.92	0.51
2:S:319:ARG:HG2	2:S:419:HIS:CE1	2.45	0.51
1:C:14:ASN:HD22	1:C:94:MET:HB3	1.74	0.50
2:S:476:ARG:HD2	9:S:2021:HOH:O	2.11	0.50
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.93	0.50
2:R:270:LEU:HD21	2:R:426:ALA:HA	1.94	0.49
2:R:274:ALA:HA	2:R:422[A]:LEU:HD11	1.95	0.49
2:S:284:GLY:HA2	2:S:518:ALA:O	2.13	0.49
1:C:61:HIS:O	1:C:65:GLU:HG2	2.13	0.49
2:Q:509:GLN:NE2	9:Q:2082:HOH:O	2.45	0.49
2:S:353:GLY:HA3	2:S:494:GLN:HG3	1.94	0.49
1:A:47:THR:O	2:Q:23:ARG:HA	2.13	0.48
2:S:35:GLU:HB2	2:S:40:LYS:HG2	1.94	0.48
1:A:137:LEU:HB2	1:A:139:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.43	0.48
1:C:184:HIS:CB	1:C:221:PRO:HA	2.44	0.48
2:S:53:GLU:HG2	2:S:493:PHE:O	2.14	0.48
1:A:67:LYS:HA	1:A:67:LYS:HD3	1.66	0.47
1:B:135:GLU:HA	2:S:328:ASP:CG	2.35	0.46
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.50	0.46
2:S:454:ASN:HD22	2:S:454:ASN:H	1.64	0.46
2:S:12:PHE:HB2	2:S:527:PRO:HG3	1.98	0.46
2:R:386:LEU:HD11	2:R:390:PHE:CE2	2.51	0.45
2:S:246:ASP:HB2	2:S:247:PRO:HD3	1.98	0.45
1:C:155:VAL:O	1:C:159:VAL:HG23	2.17	0.45
1:A:26:ARG:NH2	9:A:2008:HOH:O	2.47	0.45
2:R:296:ALA:HA	2:R:309:SER:HA	1.96	0.45
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.98	0.45
1:A:190:LEU:HB3	1:A:191:PRO:HD3	1.98	0.45
2:R:267:ILE:HB	2:R:268:PRO:HD3	1.97	0.45
1:A:80:THR:HG21	1:A:131:LYS:HD2	1.98	0.45
2:S:328:ASP:HB3	2:S:331:ALA:HB3	1.98	0.45
2:R:512:LYS:HB3	2:R:516:GLU:HB2	1.99	0.45
1:A:112:GLY:HA2	1:A:149:PRO:HD3	1.98	0.45
2:Q:495:LEU:HD12	2:Q:495:LEU:N	2.31	0.45
2:S:89:ASP:O	2:S:92:LYS:HE2	2.17	0.45
2:R:374:PRO:HD3	2:R:500:THR:HG22	1.99	0.44
1:B:258:THR:HA	1:B:259:PRO:C	2.37	0.44
1:C:99:LYS:HE3	1:C:137:LEU:HD22	1.99	0.44
2:Q:350:PRO:HB2	2:Q:482:TRP:CG	2.53	0.44
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.53	0.44
2:S:243:LEU:HD11	2:S:456:LEU:HD13	2.00	0.44
1:C:47:THR:O	2:S:23:ARG:HA	2.17	0.44
2:S:474:ALA:HB1	2:S:475:PRO:HD2	1.98	0.44
2:Q:69:GLN:HA	2:Q:79:HIS:HB2	1.99	0.44
2:S:137:ASP:HA	2:S:138:PRO:HD3	1.82	0.44
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.49	0.43
1:B:98:THR:HG22	1:B:137:LEU:HD11	2.00	0.43
2:S:364:ASP:HB3	2:S:367:HIS:O	2.17	0.43
1:B:14:ASN:ND2	1:B:94:MET:HB3	2.33	0.43
2:Q:72:CYS:CB	2:Q:75:CSX:OD	2.66	0.43
2:R:284:GLY:HA2	2:R:518:ALA:O	2.19	0.43
1:A:34:ALA:O	1:A:38:ASP:HB2	2.19	0.43
2:Q:396:GLY:HA2	2:Q:401:LYS:HE3	1.99	0.43
2:Q:486:LYS:HB3	2:Q:491:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:335:ASP:HA	2:S:346:ASP:HA	2.00	0.43
1:B:236:ASN:HB3	2:R:224:GLY:O	2.19	0.43
1:C:236:ASN:HB3	2:S:224:GLY:O	2.18	0.43
2:S:364:ASP:O	2:S:368:TYR:HB3	2.18	0.43
1:A:223:THR:OG1	1:A:247:GLY:HA2	2.18	0.43
1:B:47:THR:O	2:R:23:ARG:HA	2.19	0.43
1:B:95:ILE:O	1:B:99:LYS:HB2	2.18	0.43
1:B:223:THR:OG1	1:B:247:GLY:HA2	2.18	0.43
2:S:513:SER:OG	2:S:516:GLU:HG3	2.19	0.43
2:S:27:HIS:HA	9:S:2001:HOH:O	2.18	0.42
1:B:145:PRO:HD2	1:B:179:TYR:CZ	2.54	0.42
2:Q:497:VAL:HG11	2:Q:546:CYS:HB3	2.01	0.42
2:S:374:PRO:HD3	2:S:500:THR:HG22	2.01	0.42
2:R:72:CYS:CB	2:R:75:CSX:OD	2.65	0.42
2:S:152:ARG:CZ	2:S:265:CYS:SG	3.07	0.42
2:R:360:THR:OG1	2:R:361:LYS:N	2.52	0.42
2:R:248:LEU:HD23	2:R:248:LEU:HA	1.85	0.42
2:R:304:LYS:HD3	2:R:304:LYS:HA	1.89	0.42
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.55	0.42
2:Q:284:GLY:HA2	2:Q:518:ALA:O	2.20	0.42
2:Q:395:LYS:NZ	9:Q:2058:HOH:O	2.49	0.42
2:S:345:GLY:O	2:S:348:LYS:HG2	2.19	0.42
2:R:246:ASP:CB	2:R:247:PRO:HD3	2.48	0.42
1:C:49:MET:HA	2:S:178:ILE:HB	2.03	0.41
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	2.02	0.41
1:A:114:CYS:HA	1:A:119:GLY:HA3	2.01	0.41
2:Q:541:ASP:N	2:Q:542:PRO:HD3	2.36	0.41
2:S:40:LYS:HD3	2:S:40:LYS:HA	1.70	0.41
2:S:49:PHE:HB2	2:S:370:TRP:CD2	2.55	0.41
2:S:188:HIS:HB3	2:S:191:TYR:CD1	2.55	0.41
2:S:270:LEU:HD21	2:S:426:ALA:HA	2.03	0.41
2:S:543:CYS:SG	2:S:546:CYS:HB2	2.61	0.41
1:A:111:ILE:O	1:A:111:ILE:HG23	2.20	0.41
2:S:188:HIS:HB3	2:S:191:TYR:HD1	1.86	0.41
1:A:227:CYS:HB2	1:A:228:PRO:HD3	2.02	0.41
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.56	0.41
1:C:111:ILE:HD12	1:C:154:PHE:CG	2.55	0.41
2:R:397:GLN:HA	2:R:398:PRO:HD3	1.82	0.41
2:R:495:LEU:HD12	2:R:495:LEU:N	2.35	0.41
1:C:184:HIS:HB2	1:C:220:GLY:C	2.41	0.40
2:R:292:PHE:CD2	2:R:478:ALA:HB1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:474:ALA:HB1	2:Q:475:PRO:HD2	2.03	0.40
1:C:88:MET:HE1	1:C:93:PRO:HD3	2.04	0.40
2:Q:149:ALA:HB2	2:Q:268:PRO:HB3	2.04	0.40
2:R:418:LEU:O	2:R:423:GLY:HA3	2.22	0.40
2:S:183:TYR:CZ	2:S:530:PRO:HD2	2.56	0.40
2:Q:148:ILE:O	2:Q:268:PRO:HB3	2.21	0.40
2:S:237:CYS:HB2	2:S:456: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	A	260/264 (98%)	252 (97%)	8 (3%)	0	100	100
1	B	261/264 (99%)	253 (97%)	8 (3%)	0	100	100
1	C	258/264 (98%)	249 (96%)	9 (4%)	0	100	100
2	Q	548/563 (97%)	532 (97%)	16 (3%)	0	100	100
2	R	544/563 (97%)	522 (96%)	22 (4%)	0	100	100
2	S	542/563 (96%)	520 (96%)	21 (4%)	1 (0%)	47	71
All	All	2413/2481 (97%)	2328 (96%)	84 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	363	ASP

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%)	205 (99%)	3 (1%)	67	85
1	B	210/210 (100%)	208 (99%)	2 (1%)	76	90
1	C	207/210 (99%)	205 (99%)	2 (1%)	76	90
2	Q	441/447 (99%)	431 (98%)	10 (2%)	50	75
2	R	436/447 (98%)	431 (99%)	5 (1%)	73	88
2	S	435/447 (97%)	423 (97%)	12 (3%)	43	69
All	All	1937/1971 (98%)	1903 (98%)	34 (2%)	59	80

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	67	LYS
1	A	88	MET
1	B	100	LYS
1	B	164	LYS
1	C	18	ASP
1	C	95	ILE
2	Q	40	LYS
2	Q	361	LYS
2	Q	401	LYS
2	Q	406	MET
2	Q	410	LYS
2	Q	452	LYS
2	Q	453	ASP
2	Q	454	ASN
2	Q	473	ASP
2	Q	500	THR
2	R	167	LEU
2	R	266	TYR
2	R	397	GLN
2	R	454	ASN
2	R	473	ASP

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Mol	Chain	Res	Type
2	S	31	MET
2	S	40	LYS
2	S	166	LYS
2	S	167	LEU
2	S	358	LYS
2	S	362	LEU
2	S	365	LYS
2	S	412	SER
2	S	454	ASN
2	S	473	ASP
2	S	503	LEU
2	S	517	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	A	14	ASN
1	B	14	ASN
1	C	14	ASN
2	Q	454	ASN
2	Q	509	GLN
2	R	250	ASN
2	R	454	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	CSX	S	75	2,6,7	3,6,7	0.94	0	1,6,8	1.42	0
2	CSX	R	75	2,6,7	3,6,7	0.67	0	1,6,8	1.44	0
2	CSX	Q	75	2,6,7	3,6,7	0.69	0	1,6,8	1.89	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	CSX	S	75	2,6,7	-	0/1/5/7	-
2	CSX	R	75	2,6,7	-	0/1/5/7	-
2	CSX	Q	75	2,6,7	-	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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	75	CSX	2	0
2	R	75	CSX	2	0
2	Q	75	CSX	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	B	1266	1	0,9,9	-	-	-		
3	SF4	B	1265	1	0,12,12	-	-	-		
3	SF4	A	1267	1	0,12,12	-	-	-		
5	GOL	Q	1561	-	5,5,5	0.35	0	5,5,5	0.34	0
6	FCO	R	1550	2,9	0,6,6	-	-	-		
5	GOL	Q	1562	-	5,5,5	0.29	0	5,5,5	0.42	0
5	GOL	A	1271	-	5,5,5	0.49	0	5,5,5	0.99	0
5	GOL	R	1563	-	5,5,5	0.47	0	5,5,5	0.81	0
5	GOL	S	1561	-	5,5,5	0.41	0	5,5,5	0.67	0
3	SF4	B	1267	1	0,12,12	-	-	-		
5	GOL	R	1562	-	5,5,5	0.71	0	5,5,5	0.52	0
6	FCO	Q	1550	2,9	0,6,6	-	-	-		
4	F3S	A	1266	1	0,9,9	-	-	-		
3	SF4	A	1265	1	0,12,12	-	-	-		
6	FCO	S	1550	2,9	0,6,6	-	-	-		
3	SF4	C	1267	1	0,12,12	-	-	-		
3	SF4	C	1265	1	0,12,12	-	-	-		
4	F3S	C	1266	1	0,9,9	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	Q	1561	-	-	0/4/4/4	-
3	SF4	A	1267	1	-	-	0/6/5/5
3	SF4	B	1265	1	-	-	0/6/5/5
4	F3S	B	1266	1	-	-	0/3/3/3
5	GOL	Q	1562	-	-	0/4/4/4	-
5	GOL	R	1563	-	-	0/4/4/4	-
5	GOL	S	1561	-	-	1/4/4/4	-
5	GOL	R	1562	-	-	0/4/4/4	-
3	SF4	B	1267	1	-	-	0/6/5/5
3	SF4	C	1267	1	-	-	0/6/5/5
3	SF4	A	1265	1	-	-	0/6/5/5
4	F3S	A	1266	1	-	-	0/3/3/3
5	GOL	A	1271	-	-	2/4/4/4	-
3	SF4	C	1265	1	-	-	0/6/5/5
4	F3S	C	1266	1	-	-	0/3/3/3

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
5	A	1271	GOL	O1-C1-C2-O2
5	A	1271	GOL	O1-C1-C2-C3
5	S	1561	GOL	O1-C1-C2-C3

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A	262/264 (99%)	-0.37	1 (0%) 92 91	30, 39, 52, 60	8 (3%)
1	B	261/264 (98%)	-0.20	0 100 100	26, 43, 68, 82	9 (3%)
1	C	260/264 (98%)	0.85	37 (14%) 2 1	48, 66, 86, 102	6 (2%)
2	Q	543/563 (96%)	-0.14	8 (1%) 73 70	32, 45, 61, 71	12 (2%)
2	R	544/563 (96%)	-0.12	8 (1%) 73 70	23, 43, 70, 86	14 (2%)
2	S	543/563 (96%)	0.44	44 (8%) 12 8	35, 54, 73, 85	15 (2%)
All	All	2413/2481 (97%)	0.07	98 (4%) 37 30	23, 48, 73, 102	64 (2%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	322	GLY	4.8
1	C	207	ALA	4.6
1	C	47	THR	4.4
2	S	73	GLY	4.3
1	C	167	PRO	4.2
1	C	166	ILE	4.2
2	Q	74	VAL	4.0
1	C	164	LYS	3.9
2	S	398	PRO	3.8
2	S	415	ALA	3.7
2	S	74	VAL	3.7
2	S	42	ALA	3.7
1	C	165	GLY	3.6
1	C	171	GLU	3.5
2	S	417	ALA	3.5
1	C	264	GLY	3.4
2	S	545	ALA	3.4
2	S	154	GLY	3.4
1	C	224	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	158	VAL	3.3
1	C	71	TYR	3.3
1	C	19	GLY	3.2
1	C	198	PHE	3.1
2	R	74	VAL	3.1
1	C	215	GLU	3.1
2	S	393	TYR	3.0
1	C	18	ASP	3.0
1	C	163	THR	3.0
1	C	157	ALA	3.0
1	C	17	CYS	3.0
2	R	343	PRO	2.9
2	R	356	ASP	2.8
2	S	356	ASP	2.8
2	S	291	ALA	2.8
1	C	180	GLY	2.7
2	S	403	VAL	2.7
2	S	448	ASP	2.6
2	Q	76	THR	2.6
2	S	447	ALA	2.6
2	S	546	CYS	2.6
1	C	168	ASP	2.6
2	S	72	CYS	2.5
2	S	71	ALA	2.5
2	S	297	THR	2.5
2	S	80	ALA	2.5
1	C	161	VAL	2.5
2	S	78	VAL	2.5
1	C	79	PRO	2.5
2	S	76	THR	2.5
1	C	137	LEU	2.5
2	S	321	LEU	2.5
2	Q	78	VAL	2.5
2	S	453	ASP	2.4
2	S	497	VAL	2.4
2	R	36	ASN	2.4
2	S	399	ASP	2.4
1	C	60	LEU	2.4
2	R	415	ALA	2.4
2	S	324	VAL	2.4
2	S	510	GLY	2.4
2	S	402	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	30	PRO	2.4
2	S	390	PHE	2.4
1	C	194	GLU	2.4
1	C	29	LYS	2.3
1	C	39	THR	2.3
2	S	166	LYS	2.3
2	S	24	ILE	2.3
1	C	48	ILE	2.2
2	S	449	SER	2.2
2	S	499	SER	2.2
1	C	21	THR	2.2
1	C	190	LEU	2.2
2	Q	365	LYS	2.2
2	S	413	VAL	2.2
1	C	104	LYS	2.2
2	S	476	ARG	2.2
1	C	7	PRO	2.2
2	Q	71	ALA	2.2
2	S	409	GLY	2.2
1	A	4	LYS	2.2
1	C	211	PHE	2.2
2	R	139	ASN	2.1
2	S	544	ILE	2.1
1	C	5	HIS	2.1
2	Q	147	SER	2.1
2	R	499	SER	2.1
2	S	400	PHE	2.1
1	C	169	LEU	2.1
2	S	70	ARG	2.1
2	S	246	ASP	2.1
2	Q	148	ILE	2.1
1	C	196	SER	2.1
2	S	153	PRO	2.0
2	Q	77	TYR	2.0
2	S	142	ALA	2.0
2	S	440	GLU	2.0
2	R	322	GLY	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, 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	CSX	S	75	7/8	0.97	0.26	35,36,38,40	1
2	CSX	R	75	7/8	0.98	0.18	23,23,24,25	1
2	CSX	Q	75	7/8	0.99	0.24	33,34,35,35	1

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, 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
5	GOL	A	1271	6/6	0.80	0.29	57,59,62,63	0
5	GOL	R	1562	6/6	0.85	0.23	57,66,68,70	0
5	GOL	S	1561	6/6	0.88	0.20	53,57,60,60	0
5	GOL	R	1563	6/6	0.93	0.11	34,35,36,38	0
5	GOL	Q	1561	6/6	0.93	0.13	50,50,52,52	0
3	SF4	C	1267	8/8	0.94	0.11	49,51,53,54	0
5	GOL	Q	1562	6/6	0.95	0.16	38,40,42,44	0
8	MG	Q	1553	1/1	0.95	0.10	39,39,39,39	0
4	F3S	C	1266	7/7	0.96	0.07	58,59,63,64	0
7	NI	R	1551	1/1	0.96	0.11	25,25,25,25	0
3	SF4	C	1265	8/8	0.96	0.07	71,73,77,77	0
7	NI	Q	1551	1/1	0.97	0.13	34,34,34,34	0
8	MG	S	1553	1/1	0.97	0.05	47,47,47,47	0
8	MG	R	1553	1/1	0.98	0.09	38,38,38,38	0
3	SF4	B	1265	8/8	0.99	0.06	31,34,35,36	0
6	FCO	Q	1550	7/7	0.99	0.21	33,34,37,38	0
6	FCO	R	1550	7/7	0.99	0.18	23,24,26,28	0
6	FCO	S	1550	7/7	0.99	0.23	34,35,36,37	0
3	SF4	B	1267	8/8	0.99	0.11	27,29,30,31	0
3	SF4	A	1265	8/8	0.99	0.06	42,44,45,46	0
7	NI	S	1551	1/1	0.99	0.13	36,36,36,36	0
3	SF4	A	1267	8/8	0.99	0.12	30,31,31,31	0
4	F3S	A	1266	7/7	0.99	0.05	34,36,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	F3S	B	1266	7/7	0.99	0.08	28,30,31,33	0

6.5 Other polymers (i)

There are no such residues in this entry.