Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 01:47 am GMT

PDB ID	:	4UEQ
Title	:	Structure of the V74C large subunit mutant of D. fructosovorans NiFe- hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.
Deposited on	:	2014-12-18
Resolution	:	1.70 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 (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:

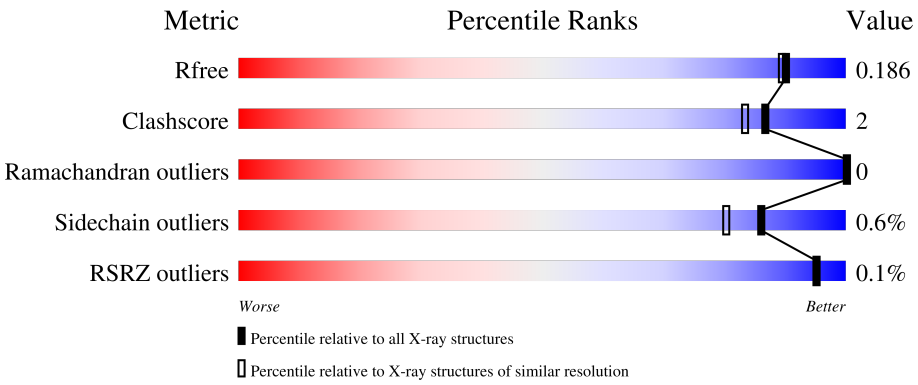
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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% 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	97%
1	B	264	93% 6%
1	C	264	91% 7%
1	D	264	% 94% 6%
1	E	264	94% 6%

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Mol	Chain	Length	Quality of chain
1	F	264	94% 5%
2	Q	564	92%
2	R	564	91% 5%
2	S	564	93%
2	T	564	93%
2	U	564	93%
2	V	564	93%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 40973 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	1982	1262	331	374	15	0	2	0
1	B	262	2007	1279	334	379	15	0	8	0
1	C	261	1977	1259	330	373	15	0	2	0
1	D	262	1978	1259	330	374	15	0	1	0
1	E	262	2001	1273	333	380	15	0	6	0
1	F	261	1988	1266	333	374	15	0	3	0

- 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	4238	2700	730	775	33	0	21	0
2	R	545	4220	2687	729	771	33	0	15	0
2	S	544	4205	2677	727	769	32	0	11	0
2	T	544	4248	2706	732	776	34	0	22	0
2	U	545	4221	2687	729	772	33	0	15	0
2	V	544	4211	2679	726	774	32	0	13	0

There are 102 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
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
Q	74	CYS	VAL	engineered mutation	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
R	74	CYS	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
S	74	CYS	VAL	engineered mutation	UNP E1K247
T	-13	ALA	-	expression tag	UNP E1K247
T	-12	SER	-	expression tag	UNP E1K247
T	-11	TRP	-	expression tag	UNP E1K247
T	-10	SER	-	expression tag	UNP E1K247
T	-9	HIS	-	expression tag	UNP E1K247
T	-8	PRO	-	expression tag	UNP E1K247
T	-7	GLN	-	expression tag	UNP E1K247
T	-6	PHE	-	expression tag	UNP E1K247
T	-5	GLU	-	expression tag	UNP E1K247
T	-4	LYS	-	expression tag	UNP E1K247
T	-3	GLY	-	expression tag	UNP E1K247
T	-2	ALA	-	expression tag	UNP E1K247
T	-1	SER	-	expression tag	UNP E1K247
T	0	GLY	-	expression tag	UNP E1K247
T	1	ALA	-	expression tag	UNP E1K247
T	74	CYS	VAL	engineered mutation	UNP E1K247
U	-13	ALA	-	expression tag	UNP E1K247
U	-12	SER	-	expression tag	UNP E1K247
U	-11	TRP	-	expression tag	UNP E1K247
U	-10	SER	-	expression tag	UNP E1K247
U	-9	HIS	-	expression tag	UNP E1K247
U	-8	PRO	-	expression tag	UNP E1K247
U	-7	GLN	-	expression tag	UNP E1K247
U	-6	PHE	-	expression tag	UNP E1K247
U	-5	GLU	-	expression tag	UNP E1K247
U	-4	LYS	-	expression tag	UNP E1K247
U	-3	GLY	-	expression tag	UNP E1K247
U	-2	ALA	-	expression tag	UNP E1K247
U	-1	SER	-	expression tag	UNP E1K247
U	0	GLY	-	expression tag	UNP E1K247
U	1	ALA	-	expression tag	UNP E1K247
U	74	CYS	VAL	engineered mutation	UNP E1K247
V	-13	ALA	-	expression tag	UNP E1K247
V	-12	SER	-	expression tag	UNP E1K247
V	-11	TRP	-	expression tag	UNP E1K247
V	-10	SER	-	expression tag	UNP E1K247
V	-9	HIS	-	expression tag	UNP E1K247

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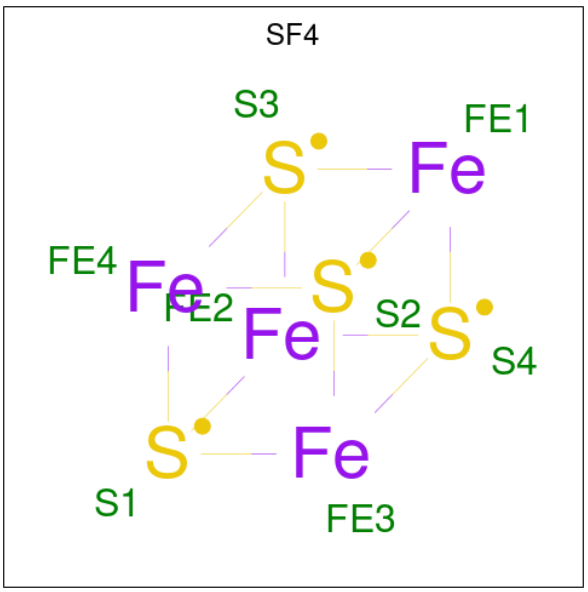
Chain	Residue	Modelled	Actual	Comment	Reference
V	-8	PRO	-	expression tag	UNP E1K247
V	-7	GLN	-	expression tag	UNP E1K247
V	-6	PHE	-	expression tag	UNP E1K247
V	-5	GLU	-	expression tag	UNP E1K247
V	-4	LYS	-	expression tag	UNP E1K247
V	-3	GLY	-	expression tag	UNP E1K247
V	-2	ALA	-	expression tag	UNP E1K247
V	-1	SER	-	expression tag	UNP E1K247
V	0	GLY	-	expression tag	UNP E1K247
V	1	ALA	-	expression tag	UNP E1K247
V	74	CYS	VAL	engineered mutation	UNP E1K247
Q	543	CSS	CYS	microheterogeneity	UNP E1K247
R	543	CSS	CYS	microheterogeneity	UNP E1K247
S	543	CSS	CYS	microheterogeneity	UNP E1K247
T	543	CSS	CYS	microheterogeneity	UNP E1K247
U	543	CSS	CYS	microheterogeneity	UNP E1K247
V	543	CSS	CYS	microheterogeneity	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

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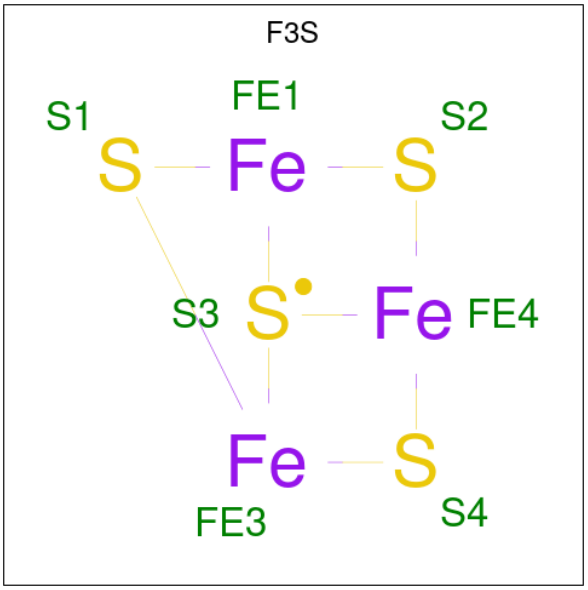
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	B	1	8	4	4	0	0
3	C	1	8	4	4	0	0
3	C	1	8	4	4	0	0
3	D	1	8	4	4	0	0
3	D	1	8	4	4	0	0
3	E	1	8	4	4	0	0
3	E	1	8	4	4	0	0
3	F	1	8	4	4	0	0
3	F	1	8	4	4	0	0

- 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

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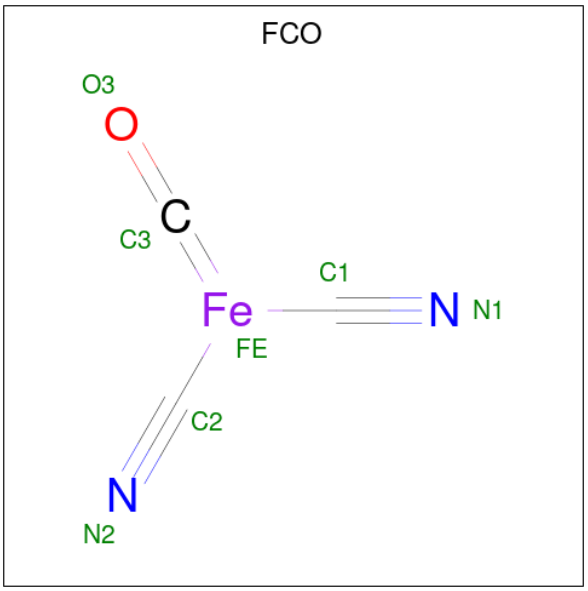
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	C	1	7	3	4	0	0
			Total	Fe	S		
4	D	1	7	3	4	0	0
			Total	Fe	S		
4	E	1	7	3	4	0	0
			Total	Fe	S		
4	F	1	7	3	4	0	0

- Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).

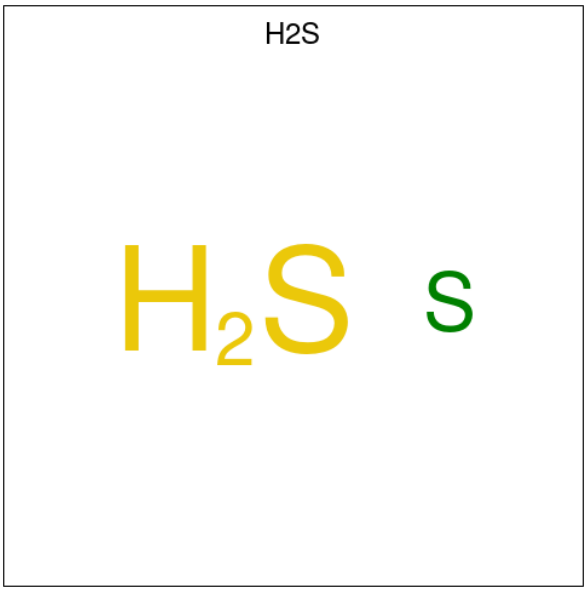


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	Q	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
5	R	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
5	S	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
5	T	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
5	U	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
5	V	1	7	3	1	2	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
6	Q	1	2	2	0	1
6	R	1	2	2	0	1
6	S	1	2	2	0	1
6	T	1	2	2	0	1
6	U	1	2	2	0	1
6	V	1	2	2	0	1

- Molecule 7 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	S		
7	Q	1	1	1	0	1
7	R	1	1	1	0	1
7	S	1	1	1	0	1
7	T	1	1	1	0	1
7	U	1	1	1	0	1
7	V	1	1	1	0	1

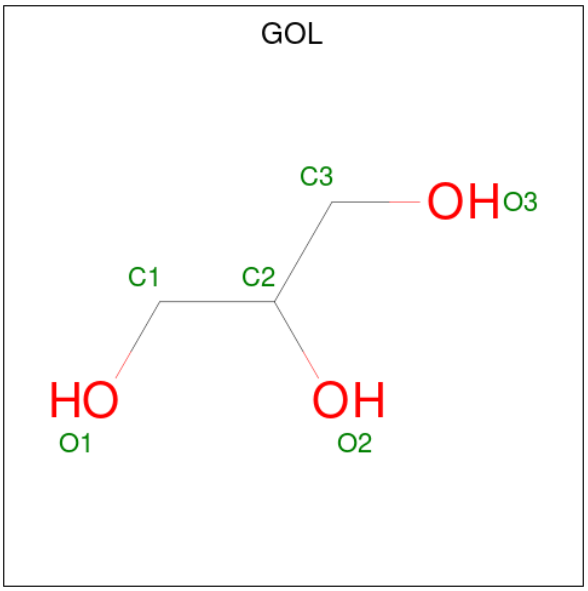
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Q	2	Total Mg 2 2	0	1
8	R	2	Total Mg 2 2	0	1
8	S	1	Total Mg 1 1	0	1
8	T	2	Total Mg 2 2	0	1
8	U	2	Total Mg 2 2	0	1
8	V	1	Total Mg 1 1	0	1

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

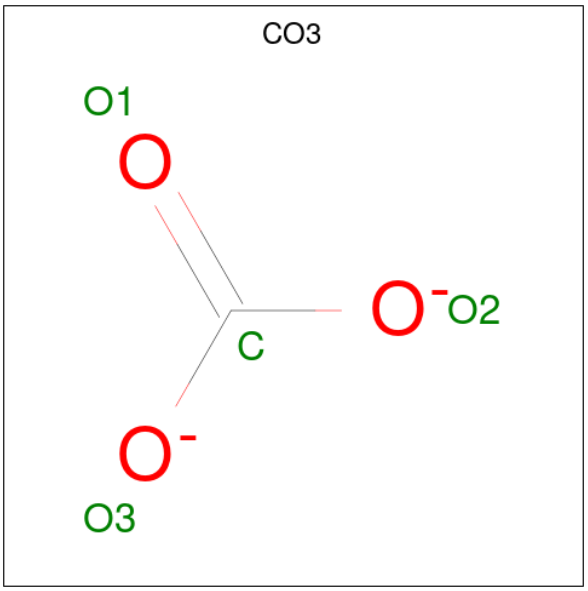
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Q	1	Total Ca 1 1	0	1
9	R	1	Total Ca 1 1	0	1
9	S	1	Total Ca 1 1	0	1
9	T	1	Total Ca 1 1	0	1
9	U	1	Total Ca 1 1	0	1
9	V	1	Total Ca 1 1	0	1

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	Q	1	6	3	3	0	0
			Total	C	O		
10	Q	1	6	3	3	0	0
			Total	C	O		
10	R	1	6	3	3	0	0
			Total	C	O		
10	R	1	6	3	3	0	0
			Total	C	O		
10	S	1	6	3	3	0	0
			Total	C	O		
10	T	1	6	3	3	0	0
			Total	C	O		
10	T	1	6	3	3	0	0
			Total	C	O		
10	U	1	6	3	3	0	0
			Total	C	O		
10	U	1	6	3	3	0	0
			Total	C	O		
10	V	1	6	3	3	0	0

- Molecule 11 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	V	1	4	1	3	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	298	301	301	0	7
12	B	198	198	198	0	0
12	C	226	226	226	0	2
12	D	297	299	299	0	7
12	E	204	204	204	0	2
12	F	209	209	209	0	0
12	Q	396	398	398	0	5
12	R	345	345	345	0	4
12	S	247	247	247	0	6
12	T	401	401	401	0	10
12	U	348	349	349	0	5

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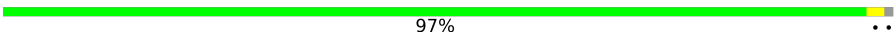
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	V	241	242	242	0	3

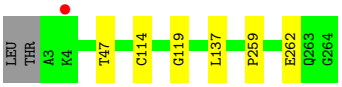
3 Residue-property plots (i)

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

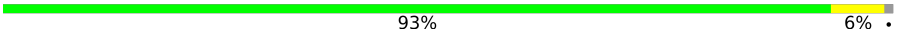
Chain A:

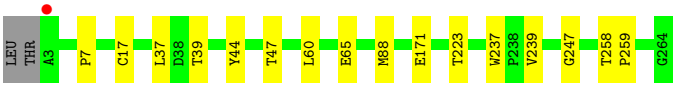




• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain B:



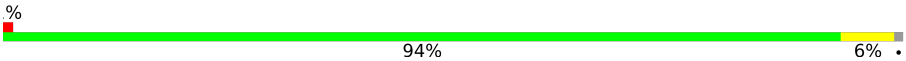


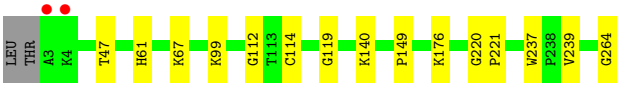
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain C:

• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

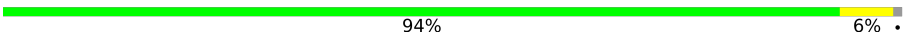
Chain D:





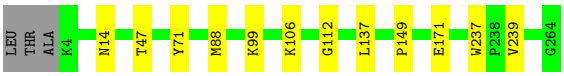
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain E:



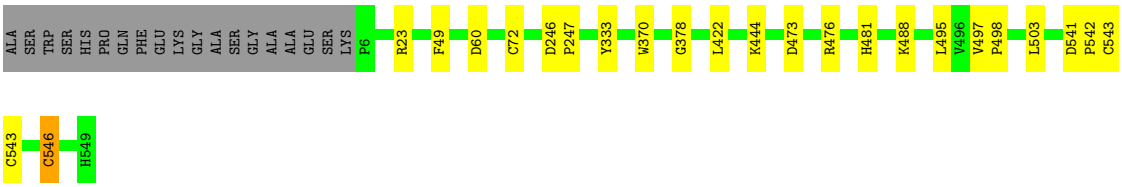
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain F: 94% 5%



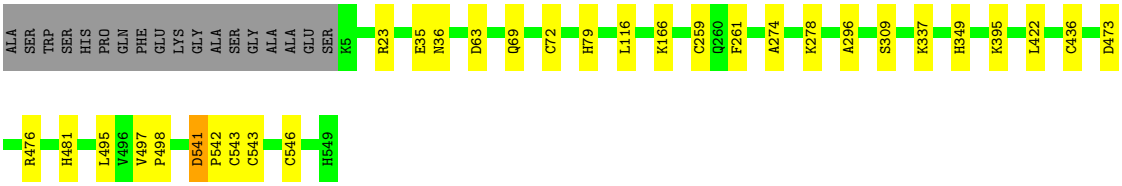
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain Q: 92%



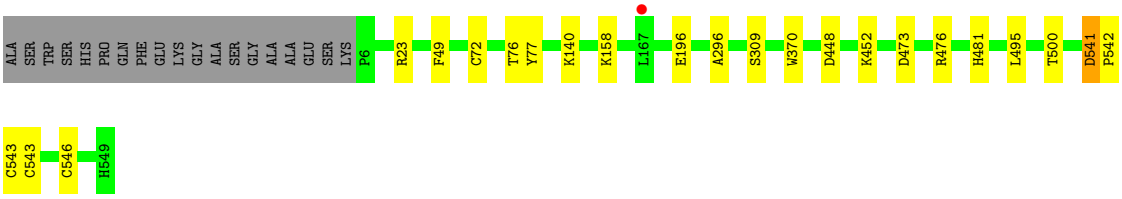
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain R: 91% 5%



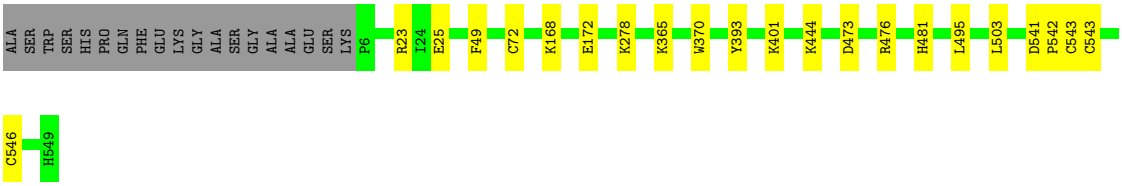
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain S: 93%



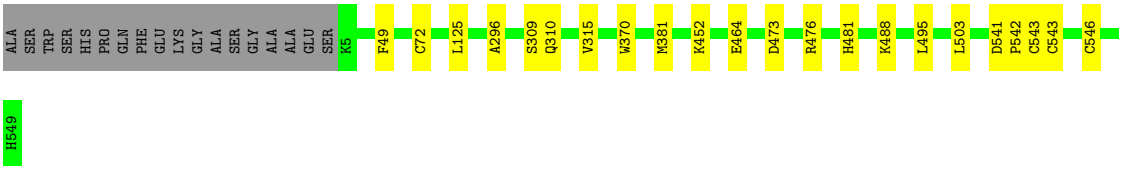
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain T: 93%

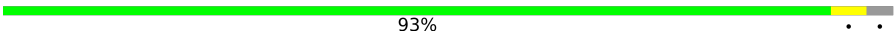


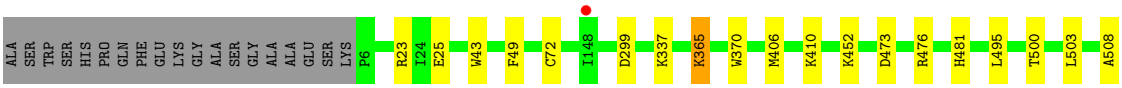
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

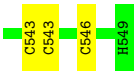
Chain U: 93%



• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain V: 





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.72Å 99.80Å 190.80Å 90.21° 98.61° 90.11°	Depositor
Resolution (Å)	20.00 – 1.70 29.99 – 1.70	Depositor EDS
% Data completeness (in resolution range)	85.0 (20.00-1.70) 84.2 (29.99-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.137 , 0.185 0.137 , 0.186	Depositor DCC
R_{free} test set	20976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-h-l 0.439 for -h,k,-l 0.054 for -h,-k,h+l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	40973	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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, CSS, CO3, GOL, F3S, H2S, FCO, CA, SF4, 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	0.64	0/2045	0.70	0/2782
1	B	0.55	0/2098	0.63	0/2853
1	C	0.61	0/2041	0.69	1/2777 (0.0%)
1	D	0.64	0/2036	0.71	0/2771
1	E	0.56	0/2087	0.64	0/2839
1	F	0.63	0/2052	0.65	0/2792
2	Q	0.61	0/4433	0.72	1/6010 (0.0%)
2	R	0.59	0/4387	0.71	1/5950 (0.0%)
2	S	0.54	0/4351	0.65	1/5901 (0.0%)
2	T	0.62	0/4437	0.71	0/6016
2	U	0.59	0/4387	0.71	0/5951
2	V	0.52	0/4367	0.65	0/5923
All	All	0.59	0/38721	0.68	4/52565 (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})
1	C	170	ASP	CB-CG-OD1	5.70	123.43	118.30
2	R	541	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	Q	60	ASP	CB-CG-OD1	5.28	123.05	118.30
2	S	541	ASP	CB-CG-OD1	5.14	122.92	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	1982	0	1922	3	0
1	B	2007	0	1950	12	0
1	C	1977	0	1921	18	0
1	D	1978	0	1913	10	0
1	E	2001	0	1937	10	0
1	F	1988	0	1927	11	0
2	Q	4238	0	4224	19	0
2	R	4220	0	4196	29	0
2	S	4205	0	4175	13	0
2	T	4248	0	4227	15	0
2	U	4221	0	4191	13	0
2	V	4211	0	4173	14	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
3	E	16	0	0	0	0
3	F	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
4	D	7	0	0	0	0
4	E	7	0	0	0	0
4	F	7	0	0	0	0
5	Q	7	0	0	0	0
5	R	7	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
5	U	7	0	0	0	0
5	V	7	0	0	0	0
6	Q	2	0	0	1	0
6	R	2	0	0	1	0
6	S	2	0	0	1	0
6	T	2	0	0	1	0
6	U	2	0	0	1	0
6	V	2	0	0	1	0
7	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
8	Q	2	0	0	0	0
8	R	2	0	0	0	0
8	S	1	0	0	0	0
8	T	2	0	0	0	0
8	U	2	0	0	0	0
8	V	1	0	0	0	0
9	Q	1	0	0	0	0
9	R	1	0	0	0	0
9	S	1	0	0	0	0
9	T	1	0	0	0	0
9	U	1	0	0	0	0
9	V	1	0	0	0	0
10	Q	12	0	16	0	0
10	R	12	0	16	0	0
10	S	6	0	8	0	0
10	T	12	0	16	0	0
10	U	12	0	16	0	0
10	V	6	0	8	0	0
11	V	4	0	0	0	0
12	A	301	0	0	0	0
12	B	198	0	0	0	0
12	C	226	0	0	7	0
12	D	299	0	0	5	0
12	E	204	0	0	1	0
12	F	209	0	0	3	0
12	Q	398	0	0	5	0
12	R	345	0	0	3	0
12	S	247	0	0	1	0
12	T	401	0	0	4	0
12	U	349	0	0	4	0
12	V	242	0	0	1	0
All	All	40973	0	36836	158	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 (158) 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:T:444:LYS:HG3	12:T:2360:HOH:O	1.39	1.21
1:C:171[A]:GLU:HG2	12:C:2144:HOH:O	1.58	1.01
2:R:259[B]:CYS:CB	2:R:436[B]:CYS:HG	1.75	0.99
1:E:96[B]:GLU:HG2	12:E:2100:HOH:O	1.67	0.94
2:S:543[A]:CSS:SD	6:S:1551[A]:NI:NI	1.40	0.93
1:C:171[A]:GLU:CG	12:C:2144:HOH:O	2.12	0.91
2:V:543[A]:CSS:SD	6:V:1551[A]:NI:NI	1.38	0.91
2:R:543[A]:CSS:SD	6:R:1551[A]:NI:NI	1.46	0.89
2:U:543[A]:CSS:SD	6:U:1551[A]:NI:NI	1.46	0.89
2:T:543[A]:CSS:SD	6:T:1551[A]:NI:NI	1.37	0.86
1:F:171[A]:GLU:HG2	12:F:2130:HOH:O	1.82	0.79
2:Q:543[A]:CSS:SD	6:Q:1551[A]:NI:NI	1.48	0.78
1:C:135:GLU:OE1	12:C:2095:HOH:O	2.03	0.76
2:Q:444[A]:LYS:HG2	12:Q:2351:HOH:O	1.87	0.74
2:Q:444[B]:LYS:HG3	12:Q:2348:HOH:O	1.87	0.74
2:U:310[B]:GLN:CD	12:U:2226:HOH:O	2.27	0.73
2:R:259[B]:CYS:CB	2:R:436[B]:CYS:SG	2.82	0.68
2:U:310[B]:GLN:NE2	12:U:2226:HOH:O	2.28	0.66
1:C:171[A]:GLU:CD	12:C:2144:HOH:O	2.29	0.65
2:S:140:LYS:HG2	2:S:196:GLU:HG2	1.79	0.64
1:C:171[A]:GLU:OE2	12:C:2144:HOH:O	2.15	0.64
2:V:43:TRP:CE2	2:V:365:LYS:HE2	2.37	0.59
2:T:72[D]:CYS:SG	2:T:546:CYS:SG	3.00	0.59
1:F:171[A]:GLU:CG	12:F:2130:HOH:O	2.46	0.59
1:B:37:LEU:HD13	2:R:166[B]:LYS:HD3	1.84	0.58
2:R:72[D]:CYS:SG	2:R:546:CYS:SG	3.03	0.57
2:V:543[A]:CSS:HB2	2:V:546:CYS:HB2	1.89	0.53
2:T:168:LYS:O	2:T:172:GLU:HG3	2.08	0.53
1:F:47:THR:O	2:V:23:ARG:HA	2.08	0.53
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.89	0.53
2:R:337:LYS:NZ	12:R:2255:HOH:O	2.39	0.51
2:R:476:ARG:NE	2:R:543[A]:CSS:SG	2.84	0.51
2:R:116[B]:LEU:HD11	2:R:261:PHE:CE2	2.46	0.51
2:R:481:HIS:CD2	2:R:495[B]:LEU:HG	2.46	0.50
2:S:543[A]:CSS:HB2	2:S:546:CYS:HB2	1.93	0.50
2:T:543[A]:CSS:HB2	2:T:546:CYS:HB2	1.94	0.50
1:F:71:TYR:CE1	1:F:106:LYS:HD2	2.46	0.50
2:V:72[D]:CYS:SG	2:V:546:CYS:SG	3.09	0.50
1:C:71:TYR:CE1	1:C:106:LYS:HD2	2.47	0.50
2:U:481:HIS:CD2	2:U:495[B]:LEU:HG	2.47	0.49
2:R:259[B]:CYS:HG	2:R:436[B]:CYS:CB	2.25	0.49
2:U:72[D]:CYS:SG	2:U:546:CYS:SG	3.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:543[A]:CSS:HB2	2:Q:546:CYS:HB2	1.95	0.49
2:Q:72[D]:CYS:SG	2:Q:546:CYS:SG	3.10	0.49
2:Q:444[B]:LYS:NZ	12:Q:2348:HOH:O	2.38	0.49
2:S:448:ASP:O	2:S:452:LYS:HG2	2.12	0.49
2:S:72[D]:CYS:SG	2:S:546:CYS:SG	3.11	0.48
1:E:258:THR:HA	1:E:259:PRO:C	2.34	0.48
2:V:476:ARG:NE	2:V:543[A]:CSS:SG	2.87	0.48
1:E:57:GLU:HG2	1:E:61[B]:HIS:CE1	2.49	0.48
2:R:543[A]:CSS:HB2	2:R:546:CYS:HB2	1.95	0.48
2:Q:476:ARG:NE	2:Q:543[A]:CSS:SG	2.87	0.48
2:Q:481:HIS:CD2	2:Q:495[B]:LEU:HG	2.49	0.48
2:V:481:HIS:CD2	2:V:495[B]:LEU:HG	2.49	0.48
1:D:176:LYS:NZ	12:D:2198:HOH:O	2.40	0.47
1:F:99:LYS:HG3	1:F:137:LEU:HD22	1.96	0.47
12:U:2131:HOH:O	2:V:452:LYS:HE2	2.14	0.47
1:C:47:THR:O	2:S:23:ARG:HA	2.13	0.47
2:T:481:HIS:CD2	2:T:495[B]:LEU:HG	2.48	0.47
1:E:171:GLU:H	1:E:171:GLU:CD	2.17	0.47
2:Q:444[B]:LYS:CG	12:Q:2348:HOH:O	2.56	0.47
2:R:259[B]:CYS:HB2	2:R:436[B]:CYS:SG	2.55	0.47
2:S:476:ARG:NE	2:S:543[A]:CSS:SG	2.88	0.47
2:U:541:ASP:N	2:U:542:PRO:HD3	2.30	0.47
1:D:140:LYS:HE3	12:D:2180:HOH:O	2.14	0.47
2:U:476:ARG:NE	2:U:543[A]:CSS:SG	2.88	0.47
1:C:140:LYS:HD2	2:R:349:HIS:HB2	1.97	0.47
2:R:116[B]:LEU:HD11	2:R:261:PHE:HE2	1.80	0.47
1:B:258:THR:HA	1:B:259:PRO:C	2.36	0.46
1:E:237:TRP:CZ2	1:E:239:VAL:HB	2.50	0.46
2:Q:246:ASP:HB2	2:Q:247:PRO:HD3	1.97	0.46
2:R:274:ALA:HA	2:R:422[A]:LEU:HD11	1.97	0.46
2:V:365:LYS:HD2	2:V:365:LYS:HA	1.74	0.46
1:B:37:LEU:CD1	2:R:166[B]:LYS:HD3	2.44	0.46
1:D:264:GLY:HA3	12:D:2293:HOH:O	2.14	0.46
1:C:100[A]:LYS:HG3	12:C:2085:HOH:O	2.14	0.46
2:Q:488:LYS:HE2	12:Q:2364:HOH:O	2.14	0.46
1:E:237:TRP:CH2	1:E:239:VAL:HB	2.51	0.46
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.45	0.46
2:S:49:PHE:HB2	2:S:370:TRP:CD2	2.50	0.46
2:R:541:ASP:N	2:R:542:PRO:HD3	2.31	0.46
2:R:278:LYS:HG2	12:R:2194:HOH:O	2.15	0.46
1:B:259:PRO:HA	2:R:63:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:HA	1:A:119:GLY:HA3	1.98	0.45
2:T:476:ARG:NE	2:T:543[A]:CSS:SG	2.88	0.45
2:R:395:LYS:HE3	12:R:2226:HOH:O	2.16	0.45
1:B:47:THR:O	2:R:23:ARG:HA	2.16	0.45
2:T:278:LYS:HG3	12:T:2225:HOH:O	2.17	0.45
1:D:47:THR:O	2:T:23:ARG:HA	2.17	0.45
1:D:61:HIS:HE1	12:D:2087:HOH:O	2.00	0.45
2:V:49:PHE:HB2	2:V:370:TRP:CD2	2.51	0.45
2:T:393:TYR:CE1	2:T:401[A]:LYS:HD3	2.52	0.45
1:E:142:ILE:HD11	1:E:166:ILE:HD12	1.99	0.44
1:E:223:THR:OG1	1:E:247:GLY:HA2	2.18	0.44
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.53	0.44
2:U:49:PHE:HB2	2:U:370:TRP:CD2	2.52	0.44
2:U:464:GLU:OE2	2:U:488:LYS:HE3	2.18	0.44
1:F:112:GLY:HA2	1:F:149:PRO:HD3	2.00	0.43
2:U:543[A]:CSS:HB2	2:U:546:CYS:HB2	2.00	0.43
1:B:223:THR:OG1	1:B:247:GLY:HA2	2.17	0.43
1:C:114:CYS:HA	1:C:119:GLY:HA3	2.00	0.43
2:S:481:HIS:CD2	2:S:495[B]:LEU:HG	2.53	0.43
2:Q:333:TYR:OH	2:Q:378:GLY:HA2	2.17	0.43
1:B:7:PRO:HD2	1:B:39:THR:O	2.18	0.43
2:R:259[B]:CYS:SG	2:R:436[B]:CYS:HB3	2.59	0.43
1:A:259:PRO:HG2	1:A:262:GLU:HB2	2.01	0.43
1:A:47:THR:O	2:Q:23:ARG:HA	2.18	0.43
2:V:337:LYS:HD2	2:V:508:ALA:O	2.18	0.43
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.49	0.42
2:T:49:PHE:HB2	2:T:370:TRP:CD2	2.54	0.42
2:T:365:LYS:HE3	12:T:2324:HOH:O	2.19	0.42
2:U:296:ALA:HA	2:U:309:SER:HA	2.01	0.42
1:C:40:ILE:HG22	1:C:162:LEU:CD1	2.50	0.42
2:S:296:ALA:HA	2:S:309:SER:HA	2.02	0.42
2:V:299:ASP:HB3	12:V:2161:HOH:O	2.19	0.42
2:V:25:GLU:HG3	2:V:72[A]:CYS:SG	2.60	0.42
1:C:112:GLY:HA2	1:C:149:PRO:HD3	2.02	0.42
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.54	0.42
1:D:114:CYS:HA	1:D:119:GLY:HA3	2.01	0.42
1:E:44:TYR:CD1	1:E:60:LEU:HB2	2.55	0.42
2:R:35:GLU:HG2	2:R:36[A]:ASN:ND2	2.35	0.42
1:D:220:GLY:N	1:D:221:PRO:CD	2.83	0.41
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.56	0.41
2:R:259[B]:CYS:SG	2:R:436[B]:CYS:CB	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:296:ALA:HA	2:R:309:SER:HA	2.02	0.41
2:S:541:ASP:N	2:S:542:PRO:HD3	2.35	0.41
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.55	0.41
1:C:67:LYS:HD2	1:C:67:LYS:N	2.35	0.41
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.55	0.41
2:S:476:ARG:HD2	12:S:2042[A]:HOH:O	2.20	0.41
2:T:25:GLU:HG3	2:T:72[A]:CYS:SG	2.61	0.41
1:D:99:LYS:HD2	12:D:2141:HOH:O	2.20	0.41
1:D:237:TRP:CZ2	1:D:239:VAL:HB	2.56	0.41
1:F:14:ASN:ND2	12:F:2011:HOH:O	2.44	0.41
1:F:237:TRP:CH2	1:F:239:VAL:HB	2.55	0.41
2:Q:541:ASP:N	2:Q:542:PRO:HD3	2.35	0.41
2:U:125:LEU:HG	12:U:2114:HOH:O	2.21	0.41
2:V:406:MET:O	2:V:410:LYS:HG2	2.20	0.41
1:F:237:TRP:CZ2	1:F:239:VAL:HB	2.56	0.40
2:R:69:GLN:HA	2:R:79:HIS:HB2	2.03	0.40
2:T:541:ASP:N	2:T:542:PRO:HD3	2.36	0.40
2:U:315:VAL:HG13	2:U:381[B]:MET:CE	2.51	0.40
1:D:112:GLY:HA2	1:D:149:PRO:HD3	2.03	0.40
1:E:229[A]:LYS:HE2	1:E:229[A]:LYS:HB3	1.87	0.40
2:T:476:ARG:HD2	12:T:2078[A]:HOH:O	2.21	0.40
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	2.03	0.40
1:B:44:TYR:CD1	1:B:60:LEU:HB2	2.57	0.40
2:S:76:THR:O	2:S:77:TYR:HB3	2.21	0.40
1:C:135:GLU:HG3	12:C:2117:HOH:O	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	262/264 (99%)	255 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	268/264 (102%)	260 (97%)	8 (3%)	0	100	100
1	C	261/264 (99%)	254 (97%)	7 (3%)	0	100	100
1	D	261/264 (99%)	254 (97%)	7 (3%)	0	100	100
1	E	267/264 (101%)	260 (97%)	7 (3%)	0	100	100
1	F	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
2	Q	563/564 (100%)	553 (98%)	10 (2%)	0	100	100
2	R	558/564 (99%)	546 (98%)	12 (2%)	0	100	100
2	S	553/564 (98%)	542 (98%)	11 (2%)	0	100	100
2	T	564/564 (100%)	553 (98%)	11 (2%)	0	100	100
2	U	558/564 (99%)	548 (98%)	10 (2%)	0	100	100
2	V	555/564 (98%)	545 (98%)	10 (2%)	0	100	100
All	All	4932/4968 (99%)	4825 (98%)	107 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	210/210 (100%)	209 (100%)	1 (0%)	88	83
1	B	216/210 (103%)	214 (99%)	2 (1%)	78	70
1	C	210/210 (100%)	209 (100%)	1 (0%)	88	83
1	D	209/210 (100%)	208 (100%)	1 (0%)	88	83
1	E	215/210 (102%)	215 (100%)	0	100	100
1	F	211/210 (100%)	210 (100%)	1 (0%)	88	83
2	Q	457/448 (102%)	454 (99%)	3 (1%)	84	77
2	R	451/448 (101%)	450 (100%)	1 (0%)	93	90
2	S	447/448 (100%)	444 (99%)	3 (1%)	84	77
2	T	457/448 (102%)	455 (100%)	2 (0%)	91	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	451/448 (101%)	448 (99%)	3 (1%)	84	77
2	V	449/448 (100%)	445 (99%)	4 (1%)	78	70
All	All	3983/3948 (101%)	3961 (99%)	22 (1%)	86	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	B	88	MET
1	B	171	GLU
1	C	67	LYS
1	D	67	LYS
1	F	88	MET
2	Q	473	ASP
2	Q	503	LEU
2	Q	546	CYS
2	R	473	ASP
2	S	158	LYS
2	S	473	ASP
2	S	500	THR
2	T	473	ASP
2	T	503	LEU
2	U	452	LYS
2	U	473	ASP
2	U	503	LEU
2	V	365	LYS
2	V	473	ASP
2	V	500	THR
2	V	503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	61	HIS
1	C	14	ASN
1	D	14	ASN
1	F	14	ASN
2	R	263	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)

6 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	CSS	V	543[A]	5,2	4,6,7	1.11	0	1,6,8	0.05	0
2	CSS	R	543[A]	5,2	4,6,7	1.07	0	1,6,8	0.01	0
2	CSS	S	543[A]	5,2	4,6,7	0.96	0	1,6,8	0.00	0
2	CSS	Q	543[A]	5,2	4,6,7	0.98	0	1,6,8	0.20	0
2	CSS	U	543[A]	5,2	4,6,7	1.00	0	1,6,8	0.10	0
2	CSS	T	543[A]	5,2	4,6,7	0.88	0	1,6,8	0.17	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	CSS	V	543[A]	5,2	-	0/1/5/7	-
2	CSS	R	543[A]	5,2	-	0/1/5/7	-
2	CSS	S	543[A]	5,2	-	0/1/5/7	-
2	CSS	Q	543[A]	5,2	-	0/1/5/7	-
2	CSS	U	543[A]	5,2	-	0/1/5/7	-
2	CSS	T	543[A]	5,2	-	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.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	543[A]	CSS	3	0
2	R	543[A]	CSS	3	0
2	S	543[A]	CSS	3	0
2	Q	543[A]	CSS	3	0
2	U	543[A]	CSS	3	0
2	T	543[A]	CSS	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 69 ligands modelled in this entry, 28 are monoatomic and 6 are modelled with single atom - leaving 35 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	$\#\|Z\| > 2$
10	GOL	Q	1562	-	5,5,5	0.40	0	5,5,5	0.27	0
10	GOL	T	1562	-	5,5,5	0.32	0	5,5,5	0.29	0
3	SF4	B	1265	1	0,12,12	-	-	-		
3	SF4	F	1265	1	0,12,12	-	-	-		
10	GOL	Q	1561	-	5,5,5	0.37	0	5,5,5	0.50	0
5	FCO	Q	1550	12,7,2	0,6,6	-	-	-		
11	CO3	V	1562	-	2,3,3	1.31	0	2,3,3	0.57	0
3	SF4	E	1267	1	0,12,12	-	-	-		
3	SF4	C	1265	1	0,12,12	-	-	-		
3	SF4	D	1267	1	0,12,12	-	-	-		
5	FCO	T	1550	12,7,2	0,6,6	-	-	-		
3	SF4	A	1267	1	0,12,12	-	-	-		
4	F3S	C	1266	1	0,9,9	-	-	-		
10	GOL	S	1561	-	5,5,5	0.29	0	5,5,5	0.53	0
3	SF4	E	1265	1	0,12,12	-	-	-		
5	FCO	R	1550	12,7,2	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	F3S	A	1266	1	0,9,9	-	-	-		
4	F3S	B	1266	1	0,9,9	-	-	-		
3	SF4	D	1265	1	0,12,12	-	-	-		
10	GOL	V	1561	-	5,5,5	0.27	0	5,5,5	0.44	0
4	F3S	F	1266	1	0,9,9	-	-	-		
5	FCO	V	1550	12,7,2	0,6,6	-	-	-		
10	GOL	U	1561	-	5,5,5	0.34	0	5,5,5	0.31	0
5	FCO	U	1550	12,7,2	0,6,6	-	-	-		
10	GOL	R	1561	-	5,5,5	0.27	0	5,5,5	0.50	0
10	GOL	T	1561	-	5,5,5	0.35	0	5,5,5	0.48	0
10	GOL	R	1563	-	5,5,5	0.43	0	5,5,5	0.63	0
3	SF4	B	1267	1	0,12,12	-	-	-		
5	FCO	S	1550	12,7,2	0,6,6	-	-	-		
10	GOL	U	1563	-	5,5,5	0.36	0	5,5,5	0.53	0
3	SF4	F	1267	1	0,12,12	-	-	-		
4	F3S	E	1266	1	0,9,9	-	-	-		
3	SF4	C	1267	1	0,12,12	-	-	-		
4	F3S	D	1266	1	0,9,9	-	-	-		
3	SF4	A	1265	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
10	GOL	Q	1562	-	-	0/4/4/4	-
10	GOL	T	1562	-	-	0/4/4/4	-
3	SF4	B	1265	1	-	-	0/6/5/5
3	SF4	F	1265	1	-	-	0/6/5/5
10	GOL	Q	1561	-	-	0/4/4/4	-
3	SF4	E	1267	1	-	-	0/6/5/5
3	SF4	C	1265	1	-	-	0/6/5/5
3	SF4	D	1267	1	-	-	0/6/5/5
3	SF4	A	1267	1	-	-	0/6/5/5
4	F3S	C	1266	1	-	-	0/3/3/3
10	GOL	S	1561	-	-	0/4/4/4	-
3	SF4	E	1265	1	-	-	0/6/5/5
10	GOL	V	1561	-	-	0/4/4/4	-
4	F3S	A	1266	1	-	-	0/3/3/3
4	F3S	B	1266	1	-	-	0/3/3/3
3	SF4	D	1265	1	-	-	0/6/5/5
4	F3S	F	1266	1	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	U	1561	-	-	0/4/4/4	-
10	GOL	R	1561	-	-	0/4/4/4	-
10	GOL	T	1561	-	-	2/4/4/4	-
10	GOL	R	1563	-	-	0/4/4/4	-
3	SF4	B	1267	1	-	-	0/6/5/5
10	GOL	U	1563	-	-	0/4/4/4	-
3	SF4	F	1267	1	-	-	0/6/5/5
4	F3S	E	1266	1	-	-	0/3/3/3
3	SF4	C	1267	1	-	-	0/6/5/5
4	F3S	D	1266	1	-	-	0/3/3/3
3	SF4	A	1265	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	T	1561	GOL	C1-C2-C3-O3
10	T	1561	GOL	O2-C2-C3-O3

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%)	-0.71	1 (0%)	92	93	9, 15, 28, 53	6 (2%)
1	B	262/264 (99%)	-0.51	1 (0%)	92	93	13, 22, 36, 54	4 (1%)
1	C	261/264 (98%)	-0.70	0	100	100	10, 17, 29, 45	8 (3%)
1	D	262/264 (99%)	-0.72	2 (0%)	86	88	9, 15, 27, 55	5 (1%)
1	E	262/264 (99%)	-0.57	1 (0%)	92	93	13, 21, 35, 49	8 (3%)
1	F	261/264 (98%)	-0.67	0	100	100	10, 17, 30, 44	5 (1%)
2	Q	543/564 (96%)	-0.70	0	100	100	9, 16, 30, 42	9 (1%)
2	R	544/564 (96%)	-0.69	0	100	100	9, 18, 32, 46	6 (1%)
2	S	543/564 (96%)	-0.56	1 (0%)	95	95	11, 23, 36, 45	8 (1%)
2	T	543/564 (96%)	-0.70	0	100	100	9, 16, 29, 39	9 (1%)
2	U	544/564 (96%)	-0.67	0	100	100	9, 17, 32, 44	9 (1%)
2	V	543/564 (96%)	-0.52	1 (0%)	95	95	11, 24, 37, 50	6 (1%)
All	All	4830/4968 (97%)	-0.64	7 (0%)	95	95	9, 19, 34, 55	83 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	6.9
2	S	167	LEU	3.0
1	E	3	ALA	2.9
2	V	148	ILE	2.6
1	D	4	LYS	2.3
1	D	3	ALA	2.2
1	A	4	LYS	2.1

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	CSS	S	543[A]	7/8	0.97	0.08	14,15,17,17	7
2	CSS	Q	543[A]	7/8	0.98	0.07	10,11,13,13	7
2	CSS	V	543[A]	7/8	0.98	0.09	15,15,17,18	7
2	CSS	T	543[A]	7/8	0.99	0.05	11,12,13,14	7
2	CSS	U	543[A]	7/8	0.99	0.06	10,12,13,15	7
2	CSS	R	543[A]	7/8	0.99	0.06	10,11,13,15	7

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
10	GOL	U	1563	6/6	0.94	0.08	15,18,18,22	6
11	CO3	V	1562	4/4	0.95	0.06	38,40,42,43	0
10	GOL	Q	1561	6/6	0.97	0.07	17,19,20,22	0
10	GOL	S	1561	6/6	0.97	0.06	19,22,22,24	0
10	GOL	T	1561	6/6	0.97	0.06	13,15,16,20	0
6	NI	V	1551[A]	1/1	0.97	0.06	20,20,20,20	1
10	GOL	V	1561	6/6	0.97	0.07	17,18,21,22	6
6	NI	V	1551[B]	1/1	0.97	0.06	17,17,17,17	1
10	GOL	U	1561	6/6	0.98	0.07	16,18,21,21	0
10	GOL	R	1563	6/6	0.98	0.05	16,19,21,22	0
10	GOL	Q	1562	6/6	0.98	0.06	10,12,12,12	6
10	GOL	R	1561	6/6	0.98	0.04	17,18,19,20	0
7	H2S	R	1552[B]	1/1	0.99	0.04	12,12,12,12	1
7	H2S	S	1552[B]	1/1	0.99	0.06	16,16,16,16	1
8	MG	R	1553[A]	1/1	0.99	0.04	12,12,12,12	1
8	MG	T	1553[A]	1/1	0.99	0.06	11,11,11,11	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	T	1560	1/1	0.99	0.06	16,16,16,16	1
8	MG	U	1560	1/1	0.99	0.11	13,13,13,13	1
9	CA	R	1554[D]	1/1	0.99	0.04	13,13,13,13	1
9	CA	T	1554[B]	1/1	0.99	0.06	11,11,11,11	1
5	FCO	S	1550	7/7	0.99	0.07	13,15,16,17	0
6	NI	Q	1551[A]	1/1	0.99	0.03	16,16,16,16	1
6	NI	Q	1551[B]	1/1	0.99	0.03	14,14,14,14	1
6	NI	R	1551[A]	1/1	0.99	0.03	18,18,18,18	1
6	NI	R	1551[B]	1/1	0.99	0.03	15,15,15,15	1
6	NI	S	1551[A]	1/1	0.99	0.06	21,21,21,21	1
10	GOL	T	1562	6/6	0.99	0.08	15,17,18,22	0
6	NI	S	1551[B]	1/1	0.99	0.06	17,17,17,17	1
3	SF4	B	1265	8/8	0.99	0.05	24,27,27,29	0
3	SF4	E	1265	8/8	0.99	0.06	23,24,26,28	0
7	H2S	Q	1552[B]	1/1	0.99	0.05	14,14,14,14	1
6	NI	T	1551[B]	1/1	1.00	0.04	13,13,13,13	1
6	NI	U	1551[A]	1/1	1.00	0.05	19,19,19,19	1
6	NI	U	1551[B]	1/1	1.00	0.05	15,15,15,15	1
3	SF4	E	1267	8/8	1.00	0.06	14,15,15,15	0
3	SF4	F	1265	8/8	1.00	0.06	10,12,13,13	0
3	SF4	F	1267	8/8	1.00	0.06	11,12,13,14	0
4	F3S	A	1266	7/7	1.00	0.06	10,11,12,12	0
4	F3S	B	1266	7/7	1.00	0.05	18,18,20,21	0
7	H2S	T	1552[B]	1/1	1.00	0.04	13,13,13,13	1
7	H2S	U	1552[B]	1/1	1.00	0.09	12,12,12,12	1
7	H2S	V	1552[B]	1/1	1.00	0.09	17,17,17,17	1
8	MG	Q	1553[A]	1/1	1.00	0.04	11,11,11,11	1
8	MG	Q	1560	1/1	1.00	0.04	9,9,9,9	1
4	F3S	C	1266	7/7	1.00	0.06	11,12,12,13	0
8	MG	R	1560	1/1	1.00	0.04	14,14,14,14	1
8	MG	S	1553[A]	1/1	1.00	0.04	15,15,15,15	1
4	F3S	D	1266	7/7	1.00	0.06	10,11,13,14	0
4	F3S	E	1266	7/7	1.00	0.05	17,18,19,19	0
8	MG	U	1553[A]	1/1	1.00	0.03	12,12,12,12	1
4	F3S	F	1266	7/7	1.00	0.05	12,12,12,13	0
8	MG	V	1553[A]	1/1	1.00	0.07	16,16,16,16	1
9	CA	Q	1554[B]	1/1	1.00	0.04	11,11,11,11	1
5	FCO	Q	1550	7/7	1.00	0.06	10,11,13,14	0
9	CA	S	1554[B]	1/1	1.00	0.04	16,16,16,16	1
5	FCO	R	1550	7/7	1.00	0.06	8,11,12,13	0
9	CA	U	1554[B]	1/1	1.00	0.03	12,12,12,12	1
9	CA	V	1554[B]	1/1	1.00	0.07	15,15,15,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SF4	A	1265	8/8	1.00	0.06	11,12,13,14	0
5	FCO	T	1550	7/7	1.00	0.06	10,11,12,14	0
5	FCO	U	1550	7/7	1.00	0.06	11,12,13,13	0
5	FCO	V	1550	7/7	1.00	0.06	13,16,17,18	0
3	SF4	B	1267	8/8	1.00	0.04	14,16,16,17	0
3	SF4	C	1265	8/8	1.00	0.06	11,12,13,13	0
3	SF4	C	1267	8/8	1.00	0.06	11,12,13,14	0
3	SF4	D	1265	8/8	1.00	0.06	12,12,14,14	0
3	SF4	D	1267	8/8	1.00	0.06	10,10,10,10	0
3	SF4	A	1267	8/8	1.00	0.06	9,10,11,11	0
6	NI	T	1551[A]	1/1	1.00	0.04	16,16,16,16	1

6.5 Other polymers (i)

There are no such residues in this entry.