



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2026 – 02:09 am BST

PDB ID : 4UD6 / pdb_00004ud6
Title : Structure of methylviologen-treated anaerobically purified D. fructosovorans
NiFe-hydrogenase
Authors : Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.
Deposited on : 2014-12-08
Resolution : 2.12 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

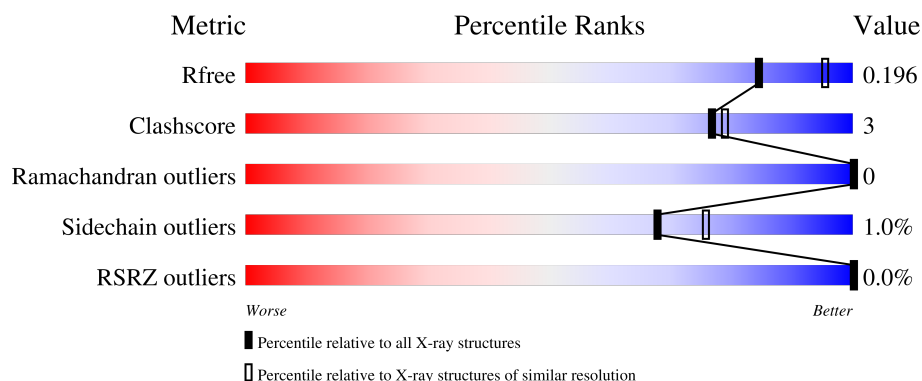
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

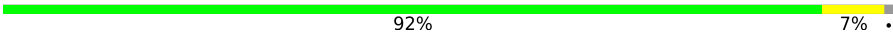
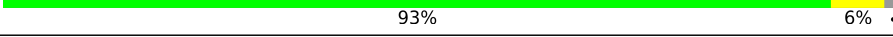
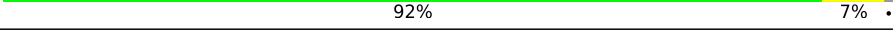
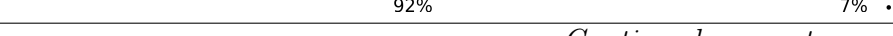
The reported resolution of this entry is 2.12 Å.

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.



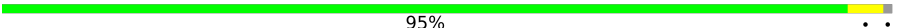
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	
1	C	264	
2	Q	549	
2	R	549	

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Mol	Chain	Length	Quality of chain
2	S	549	 95%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	Q	1563	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20531 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.

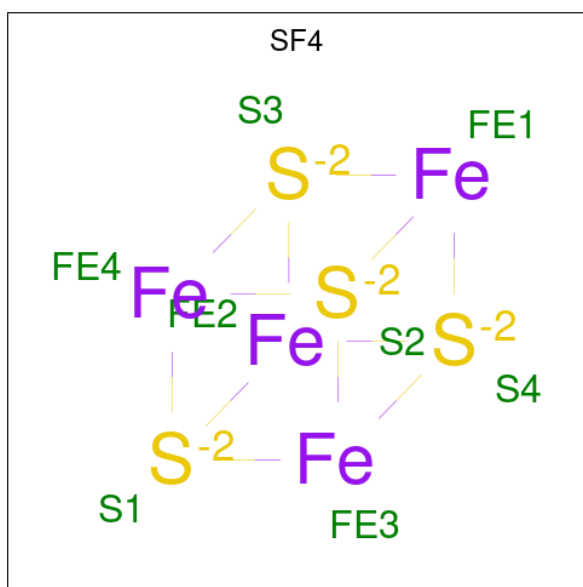
- Molecule 1 is a protein called HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1964	1251	328	370	15			

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

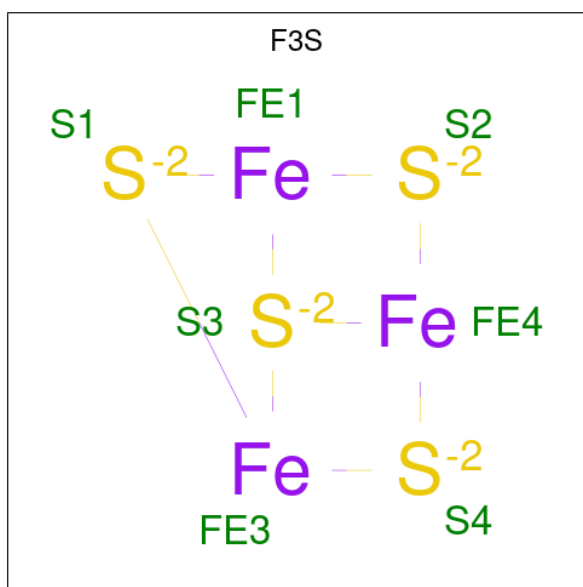
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	9	0
			4195	2676	728	769	22			
2	R	545	Total	C	N	O	S	0	3	0
			4178	2663	724	769	22			
2	S	544	Total	C	N	O	S	0	1	0
			4166	2653	724	767	22			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



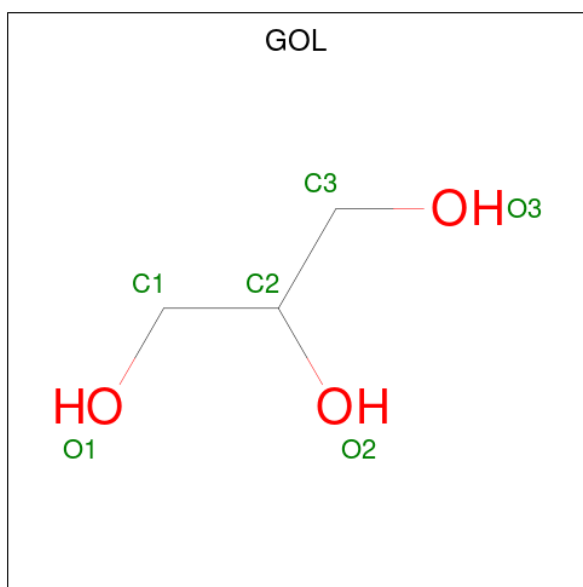
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



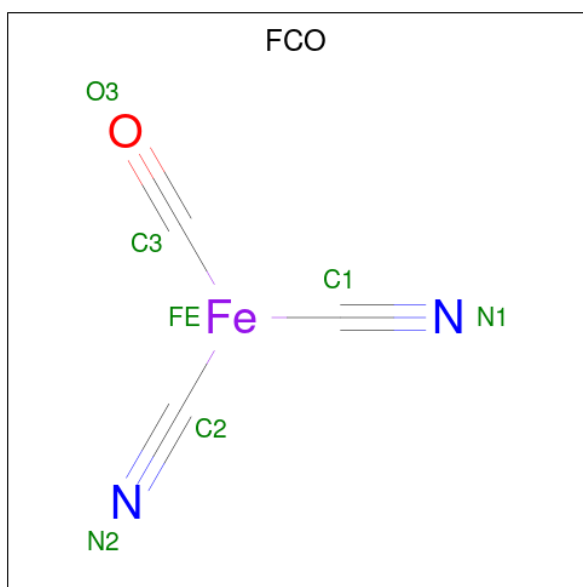
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



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

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	325	Total 325	O 325	0	0
9	B	210	Total 210	O 210	0	0
9	C	242	Total 242	O 242	0	0
9	Q	444	Total 444	O 444	0	0
9	R	389	Total 389	O 389	0	0
9	S	279	Total 279	O 279	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: 

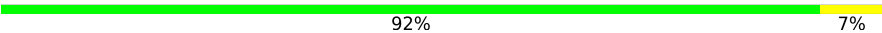


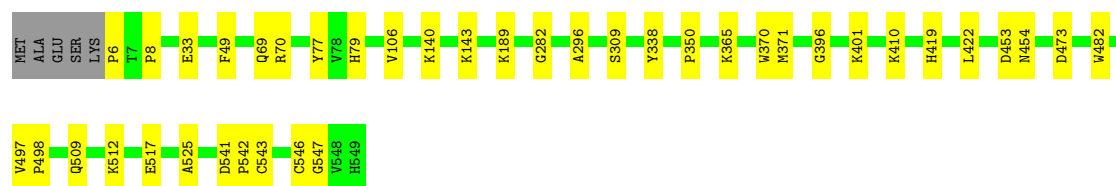
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain C: 



- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

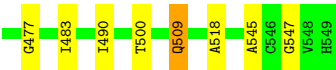
Chain Q: 



- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

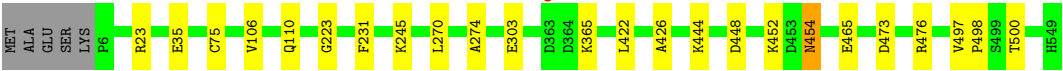
Chain R: 





● Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain S: 95% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.94Å 99.56Å 183.94Å 90.00° 91.31° 90.00°	Depositor
Resolution (Å)	19.99 – 2.12 19.99 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.99-2.12) 99.1 (19.99-2.12)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.13Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.152 , 0.196 0.153 , 0.196	Depositor DCC
R_{free} test set	6657 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20531	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CSO, MG, F3S, NI, SF4, GOL, FCO

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	0.76	0/2027	0.88	1/2759 (0.0%)
1	B	0.68	0/2043	0.86	1/2781 (0.0%)
1	C	0.67	0/2023	0.85	0/2754
2	Q	0.72	0/4335	0.84	0/5880
2	R	0.69	0/4289	0.88	1/5821 (0.0%)
2	S	0.63	0/4268	0.85	1/5792 (0.0%)
All	All	0.69	0/18985	0.86	4/25787 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	GLY	N-CA-C	-7.34	104.98	111.95
2	R	477	GLY	N-CA-C	5.27	118.30	110.60
2	S	245	LYS	N-CA-C	5.17	116.60	110.97
1	A	120	VAL	N-CA-C	5.07	116.39	110.62

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	1973	0	1911	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1980	0	1918	12	0
1	C	1964	0	1906	9	0
2	Q	4195	0	4192	24	0
2	R	4178	0	4152	29	0
2	S	4166	0	4138	14	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	1	0
4	A	7	0	0	0	0
4	B	7	0	0	1	0
4	C	7	0	0	0	0
5	A	18	0	24	1	0
5	Q	24	0	32	5	0
5	R	42	0	56	6	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	1	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	325	0	0	5	0
9	B	210	0	0	2	0
9	C	242	0	0	2	0
9	Q	444	0	0	10	0
9	R	389	0	0	10	0
9	S	279	0	0	2	0
All	All	20531	0	18337	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (107) 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)
9:Q:2291:HOH:O	2:R:6:PRO:HB3	1.75	0.86
5:R:1001:GOL:H11	9:R:2259:HOH:O	1.76	0.84
2:R:196:GLU:HG2	9:R:2172:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLU:HG3	9:B:2074:HOH:O	1.82	0.79
1:A:61:HIS:HE1	9:A:2093:HOH:O	1.70	0.74
9:Q:2290:HOH:O	2:R:6:PRO:HG3	1.92	0.69
9:C:2241:HOH:O	2:Q:189:LYS:HE3	1.92	0.68
2:Q:282:GLY:HA2	5:Q:1563:GOL:H12	1.77	0.65
2:S:448:ASP:O	2:S:452:LYS:HE2	1.97	0.65
2:R:363:ASP:HB2	9:R:2311:HOH:O	1.97	0.64
5:Q:1563:GOL:C3	9:Q:2443:HOH:O	2.47	0.62
5:Q:1563:GOL:H31	9:Q:2443:HOH:O	2.00	0.62
9:C:2149:HOH:O	2:R:509:GLN:HG2	2.00	0.61
2:Q:338:TYR:CE2	5:Q:1564:GOL:H12	2.36	0.60
2:Q:509:GLN:NE2	9:Q:2351:HOH:O	2.34	0.60
2:Q:419:HIS:O	5:Q:1563:GOL:H2	2.05	0.57
2:Q:371:MET:HE2	2:Q:547:GLY:HA3	1.87	0.56
1:A:14:ASN:ND2	1:A:94:MET:HB3	2.20	0.56
2:R:419:HIS:O	5:R:1001:GOL:H32	2.07	0.55
1:C:237:TRP:CZ2	1:C:239:VAL:HB	2.42	0.55
2:R:275:GLY:O	2:R:278:LYS:HG3	2.07	0.54
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.43	0.54
2:S:303:GLU:CG	9:S:2083:HOH:O	2.55	0.54
1:C:47:THR:O	2:S:23:ARG:HA	2.09	0.53
1:A:82:ASP:CG	9:A:2129:HOH:O	2.52	0.53
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.45	0.51
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.40	0.51
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.94	0.50
2:Q:33:GLU:HG3	9:Q:2029:HOH:O	2.10	0.50
2:Q:543:CSO:HB2	2:Q:546:CYS:HB2	1.92	0.50
2:R:50:ARG:NH2	2:R:545:ALA:HB1	2.26	0.50
2:Q:350:PRO:HB2	2:Q:482:TRP:CG	2.47	0.50
2:Q:365:LYS:HE3	9:Q:2342:HOH:O	2.11	0.50
4:B:1266:F3S:S2	2:R:225:LYS:HE2	2.52	0.50
1:B:96[B]:GLU:HG3	9:B:2096:HOH:O	2.12	0.49
2:R:410:LYS:HD3	5:R:1562:GOL:H32	1.93	0.49
2:S:223:GLY:HA2	2:S:231:PHE:CD1	2.48	0.49
2:S:476:ARG:HD2	6:S:1550:FCO:C2	2.42	0.49
2:R:454:ASN:H	2:R:454:ASN:HD22	1.61	0.48
1:A:229:LYS:HD3	9:A:2285:HOH:O	2.13	0.48
2:R:467:LYS:HG2	5:R:1004:GOL:H12	1.94	0.48
2:R:284:GLY:HA2	2:R:518:ALA:O	2.13	0.48
2:Q:396:GLY:HA2	2:Q:401[A]:LYS:HE3	1.95	0.47
2:R:223:GLY:HA2	2:R:231:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:410:LYS:HG2	9:R:2336:HOH:O	2.15	0.47
2:Q:69:GLN:HA	2:Q:79:HIS:HB2	1.97	0.47
2:R:483:ILE:HD11	2:R:490:ILE:HG12	1.97	0.47
2:Q:77:TYR:CD2	2:Q:106:VAL:HG12	2.50	0.47
2:R:31:MET:HB3	9:R:2027:HOH:O	2.14	0.47
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.50	0.47
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.45	0.46
1:C:78:LEU:HD22	1:C:95:ILE:HA	1.97	0.46
1:A:80:THR:HG21	1:A:131:LYS:HD2	1.97	0.46
1:A:259:PRO:HG3	9:Q:2423:HOH:O	2.16	0.46
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.50	0.46
1:C:258:THR:HA	1:C:259:PRO:C	2.41	0.46
2:R:274:ALA:HA	2:R:422[A]:LEU:HD11	1.97	0.46
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.98	0.46
2:S:444:LYS:HE3	9:S:2252:HOH:O	2.14	0.46
2:Q:6:PRO:N	9:Q:2002:HOH:O	2.48	0.46
2:S:454:ASN:N	2:S:454:ASN:HD22	2.13	0.45
2:S:274:ALA:HA	2:S:422:LEU:HD11	1.99	0.45
1:A:258:THR:HA	1:A:259:PRO:C	2.42	0.44
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.52	0.44
2:S:106:VAL:HG21	2:S:231:PHE:CZ	2.52	0.44
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.99	0.44
1:B:223:THR:OG1	1:B:247:GLY:HA2	2.17	0.44
5:A:1271:GOL:H11	9:A:2323:HOH:O	2.17	0.44
2:R:365:LYS:NZ	9:R:2029:HOH:O	2.50	0.44
1:A:145:PRO:HD2	1:A:179:TYR:CZ	2.53	0.44
1:C:42:LEU:HD21	1:C:45:GLN:HG3	1.99	0.44
2:R:81:LEU:HD23	2:R:107:MET:HE2	1.99	0.44
1:B:47:THR:O	2:R:23:ARG:HA	2.18	0.44
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.98	0.43
1:C:184:HIS:HA	3:C:1265:SF4:S2	2.59	0.43
2:S:454:ASN:HD22	2:S:454:ASN:H	1.65	0.43
2:Q:512[A]:LYS:HE2	2:Q:517[A]:GLU:OE1	2.18	0.43
2:S:270:LEU:HD21	2:S:426:ALA:HA	2.00	0.43
2:R:168:LYS:HD3	9:R:2122:HOH:O	2.18	0.43
1:B:18:THR:HG22	1:B:18:THR:O	2.19	0.43
1:A:254:TRP:HH2	2:Q:70:ARG:HD3	1.83	0.43
2:Q:296:ALA:HA	2:Q:309:SER:HA	2.00	0.43
5:R:1001:GOL:C1	9:R:2259:HOH:O	2.49	0.43
1:A:82:ASP:CB	9:A:2129:HOH:O	2.67	0.43
2:R:362:LEU:HD12	2:R:362:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:371:MET:HE2	2:R:547:GLY:HA3	2.01	0.42
2:Q:140:LYS:HB3	9:Q:2140:HOH:O	2.18	0.42
2:Q:541:ASP:N	2:Q:542:PRO:HD3	2.35	0.42
1:A:18:THR:HG22	1:A:18:THR:O	2.20	0.42
1:A:78:LEU:O	1:A:130:ALA:HA	2.19	0.42
1:A:114:CYS:HA	1:A:119:GLY:HA3	2.02	0.42
2:R:374:PRO:HD3	2:R:500:THR:HG22	2.01	0.42
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.55	0.42
1:B:145:PRO:HD2	1:B:179:TYR:CZ	2.54	0.41
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.55	0.41
1:C:80:THR:HG21	1:C:131:LYS:HD2	2.01	0.41
2:R:296:ALA:HA	2:R:309:SER:HA	2.02	0.41
2:Q:497:VAL:HG12	2:Q:498:PRO:HD2	2.02	0.41
2:R:196:GLU:CG	9:R:2172:HOH:O	2.56	0.41
2:S:75:CYS:HA	2:S:110:GLN:NE2	2.36	0.41
1:A:80:THR:HG22	1:A:95:ILE:HD12	2.03	0.40
1:B:111:ILE:HG23	1:B:111:ILE:O	2.21	0.40
1:A:98:THR:HG22	1:A:137:LEU:HD11	2.03	0.40
1:B:91:GLY:HA2	2:R:362:LEU:HD21	2.03	0.40
2:Q:8:PRO:HB2	2:Q:525:ALA:HB2	2.03	0.40
5:R:1004:GOL:H31	9:R:2366: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	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	B	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
1	C	259/264 (98%)	251 (97%)	8 (3%)	0	100	100
2	Q	550/549 (100%)	538 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	545/549 (99%)	531 (97%)	14 (3%)	0	100	100
2	S	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
All	All	2418/2439 (99%)	2354 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	206 (99%)	2 (1%)	68	76
1	B	210/210 (100%)	207 (99%)	3 (1%)	59	67
1	C	208/210 (99%)	207 (100%)	1 (0%)	81	87
2	Q	442/438 (101%)	437 (99%)	5 (1%)	65	74
2	R	436/438 (100%)	433 (99%)	3 (1%)	76	83
2	S	434/438 (99%)	428 (99%)	6 (1%)	59	67
All	All	1938/1944 (100%)	1918 (99%)	20 (1%)	68	76

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

Mol	Chain	Res	Type
1	A	67	LYS
1	A	88	MET
1	B	4	LYS
1	B	88	MET
1	B	104	LYS
1	C	100	LYS
2	Q	143	LYS
2	Q	410	LYS
2	Q	453	ASP
2	Q	454	ASN
2	Q	473	ASP
2	R	454	ASN

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Mol	Chain	Res	Type
2	R	473	ASP
2	R	509	GLN
2	S	35	GLU
2	S	365	LYS
2	S	454	ASN
2	S	465	GLU
2	S	473	ASP
2	S	500	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	61	HIS
1	A	240	GLN
1	B	172	ASN
1	B	234	GLN
1	B	240	GLN
1	C	14	ASN
1	C	62	GLN
1	C	240	GLN
2	Q	241	GLN
2	Q	263	ASN
2	Q	326	ASN
2	Q	454	ASN
2	Q	509	GLN
2	R	36	ASN
2	R	47	GLN
2	R	139	ASN
2	R	241	GLN
2	R	250	ASN
2	R	263	ASN
2	R	454	ASN
2	S	241	GLN
2	S	454	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	2,7	3,6,7	0.95	0	0,6,8	-	-
2	CSO	Q	543	2,7	3,6,7	0.85	0	0,6,8	-	-
2	CSO	S	543	2,7	3,6,7	0.72	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	2,7	-	1/1/5/7	-
2	CSO	Q	543	2,7	-	1/1/5/7	-
2	CSO	S	543	2,7	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	543	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 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	$\# Z > 2$
5	GOL	Q	1563	-	5,5,5	0.26	0	5,5,5	0.27	0
5	GOL	R	1002	-	5,5,5	0.25	0	5,5,5	0.39	0
4	F3S	B	1266	1	0,9,9	-	-	-		
6	FCO	R	1550	2	1,6,6	1.73	0	-		
5	GOL	R	1562	-	5,5,5	0.29	0	5,5,5	0.16	0
5	GOL	R	1003	-	5,5,5	0.39	0	5,5,5	0.21	0
5	GOL	R	1563	-	5,5,5	0.44	0	5,5,5	0.40	0
5	GOL	R	1001	-	5,5,5	0.37	0	5,5,5	0.24	0
6	FCO	S	1550	2	1,6,6	2.08	1 (100%)	-		
3	SF4	C	1265	1	0,12,12	-	-	-		
5	GOL	R	1004	-	5,5,5	0.41	0	5,5,5	0.58	0
5	GOL	A	1273	-	5,5,5	0.59	0	5,5,5	0.85	0
3	SF4	A	1267	1	0,12,12	-	-	-		
3	SF4	C	1267	1	0,12,12	-	-	-		
4	F3S	C	1266	1	0,9,9	-	-	-		
5	GOL	S	1561	-	5,5,5	0.49	0	5,5,5	0.29	0
3	SF4	A	1265	1	0,12,12	-	-	-		
4	F3S	A	1266	1	0,9,9	-	-	-		
6	FCO	Q	1550	2	1,6,6	1.59	0	-		
5	GOL	Q	1564	-	5,5,5	0.43	0	5,5,5	0.45	0
5	GOL	Q	1562	-	5,5,5	0.30	0	5,5,5	0.28	0
3	SF4	B	1267	1	0,12,12	-	-	-		
5	GOL	Q	1561	-	5,5,5	0.21	0	5,5,5	0.32	0
5	GOL	A	1272	-	5,5,5	0.54	0	5,5,5	0.72	0
5	GOL	R	1561	-	5,5,5	0.37	0	5,5,5	0.44	0
5	GOL	A	1271	-	5,5,5	0.27	0	5,5,5	0.63	0
3	SF4	B	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
5	GOL	Q	1563	-	-	0/4/4/4	-
5	GOL	R	1002	-	-	0/4/4/4	-
4	F3S	B	1266	1	-	-	0/3/3/3
5	GOL	R	1562	-	-	2/4/4/4	-
5	GOL	R	1003	-	-	2/4/4/4	-
5	GOL	R	1563	-	-	0/4/4/4	-
5	GOL	R	1001	-	-	2/4/4/4	-
3	SF4	C	1265	1	-	-	0/6/5/5
5	GOL	R	1004	-	-	1/4/4/4	-
5	GOL	A	1273	-	-	2/4/4/4	-
3	SF4	A	1267	1	-	-	0/6/5/5
3	SF4	C	1267	1	-	-	0/6/5/5
5	GOL	S	1561	-	-	0/4/4/4	-
4	F3S	C	1266	1	-	-	0/3/3/3
3	SF4	A	1265	1	-	-	0/6/5/5
4	F3S	A	1266	1	-	-	0/3/3/3
5	GOL	Q	1564	-	-	1/4/4/4	-
5	GOL	Q	1562	-	-	0/4/4/4	-
3	SF4	B	1267	1	-	-	0/6/5/5
5	GOL	Q	1561	-	-	0/4/4/4	-
5	GOL	A	1272	-	-	2/4/4/4	-
5	GOL	R	1561	-	-	0/4/4/4	-
5	GOL	A	1271	-	-	0/4/4/4	-
3	SF4	B	1265	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	1550	FCO	O3-C3	-2.08	1.13	1.16

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	1003	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	R	1003	GOL	O1-C1-C2-C3
5	R	1562	GOL	O2-C2-C3-O3
5	A	1272	GOL	C1-C2-C3-O3
5	A	1273	GOL	O1-C1-C2-C3
5	R	1001	GOL	O1-C1-C2-C3
5	R	1004	GOL	C1-C2-C3-O3
5	R	1562	GOL	C1-C2-C3-O3
5	R	1001	GOL	O1-C1-C2-O2
5	A	1273	GOL	O1-C1-C2-O2
5	A	1272	GOL	O2-C2-C3-O3
5	Q	1564	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	1563	GOL	4	0
4	B	1266	F3S	1	0
5	R	1562	GOL	1	0
5	R	1001	GOL	3	0
6	S	1550	FCO	1	0
3	C	1265	SF4	1	0
5	R	1004	GOL	2	0
5	Q	1564	GOL	1	0
5	A	1271	GOL	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 [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(Å²)	Q<0.9	
1	A	262/264 (99%)	-0.78	0	100	100	14, 20, 31, 55	4 (1%)
1	B	262/264 (99%)	-0.49	0	100	100	20, 30, 47, 63	8 (3%)
1	C	260/264 (98%)	-0.57	0	100	100	19, 27, 44, 58	5 (1%)
2	Q	543/549 (98%)	-0.74	0	100	100	13, 22, 35, 47	15 (2%)
2	R	544/549 (99%)	-0.65	0	100	100	14, 25, 38, 52	8 (1%)
2	S	543/549 (98%)	-0.42	1 (0%)	91	92	19, 34, 52, 68	7 (1%)
All	All	2414/2439 (98%)	-0.61	1 (0%)	100	100	13, 26, 46, 68	47 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	363	ASP	2.3

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	CSO	Q	543	7/8	0.98	0.05	16,18,19,22	1
2	CSO	R	543	7/8	0.99	0.05	20,21,23,23	1
2	CSO	S	543	7/8	0.99	0.04	23,23,24,25	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
5	GOL	R	1562	6/6	0.79	0.11	62,67,69,72	0
5	GOL	A	1273	6/6	0.80	0.16	51,58,58,59	0
5	GOL	R	1002	6/6	0.82	0.15	51,55,56,58	0
5	GOL	Q	1563	6/6	0.83	0.13	48,49,51,58	0
5	GOL	R	1004	6/6	0.84	0.12	49,58,61,65	0
5	GOL	A	1272	6/6	0.86	0.17	46,47,48,50	0
5	GOL	R	1003	6/6	0.86	0.12	52,55,58,65	0
5	GOL	Q	1564	6/6	0.86	0.11	37,49,49,50	0
5	GOL	R	1001	6/6	0.86	0.12	39,47,50,51	0
5	GOL	A	1271	6/6	0.90	0.10	42,46,51,55	0
5	GOL	S	1561	6/6	0.93	0.06	24,25,27,28	0
8	MG	Q	1553	1/1	0.94	0.04	15,15,15,15	0
5	GOL	R	1563	6/6	0.95	0.07	26,27,28,29	0
5	GOL	Q	1562	6/6	0.95	0.06	22,27,28,29	0
5	GOL	Q	1561	6/6	0.95	0.07	23,24,25,28	0
8	MG	S	1553	1/1	0.97	0.03	25,25,25,25	0
5	GOL	R	1561	6/6	0.98	0.03	23,24,24,25	0
3	SF4	C	1265	8/8	0.99	0.02	20,21,22,22	0
3	SF4	C	1267	8/8	0.99	0.02	17,19,19,20	0
4	F3S	B	1266	7/7	0.99	0.02	28,30,30,31	0
4	F3S	C	1266	7/7	0.99	0.03	18,20,21,22	0
3	SF4	A	1265	8/8	0.99	0.02	17,18,18,20	0
3	SF4	B	1265	8/8	0.99	0.03	35,37,38,40	0
8	MG	R	1553	1/1	0.99	0.03	19,19,19,19	0
3	SF4	B	1267	8/8	0.99	0.02	22,23,24,24	0
6	FCO	R	1550	7/7	1.00	0.02	16,17,18,18	0
6	FCO	S	1550	7/7	1.00	0.03	22,22,23,24	0
7	NI	Q	1551	1/1	1.00	0.01	18,18,18,18	0
7	NI	R	1551	1/1	1.00	0.01	20,20,20,20	0
7	NI	S	1551	1/1	1.00	0.01	21,21,21,21	0
4	F3S	A	1266	7/7	1.00	0.02	15,15,16,17	0
3	SF4	A	1267	8/8	1.00	0.02	14,14,14,15	0
6	FCO	Q	1550	7/7	1.00	0.03	15,16,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.