



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:09 am BST

PDB ID : 4UEW  
Title : Structure of H<sub>2</sub>-treated anaerobically purified D. fructosovorans NiFe- hydrogenase  
Authors : Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.  
Deposited on : 2014-12-20  
Resolution : 2.08 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

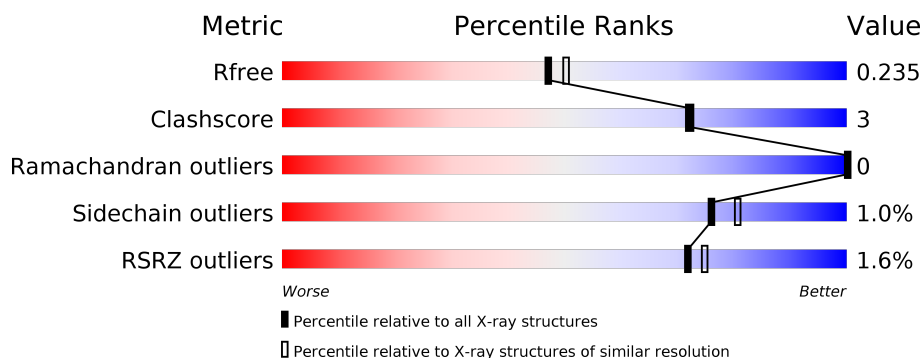
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div></div> <div>89% 9% .</div> </div>
1	B	264	<div> <div>3%</div> <div>91% 8% .</div> </div>
1	C	264	<div> <div></div> <div>91% 8% .</div> </div>
2	Q	549	<div> <div></div> <div>91% 8% .</div> </div>
2	R	549	<div> <div>%</div> <div>93% 6% .</div> </div>
2	S	549	<div> <div>5%</div> <div>91% 8% .</div> </div>

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	1564	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20352 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

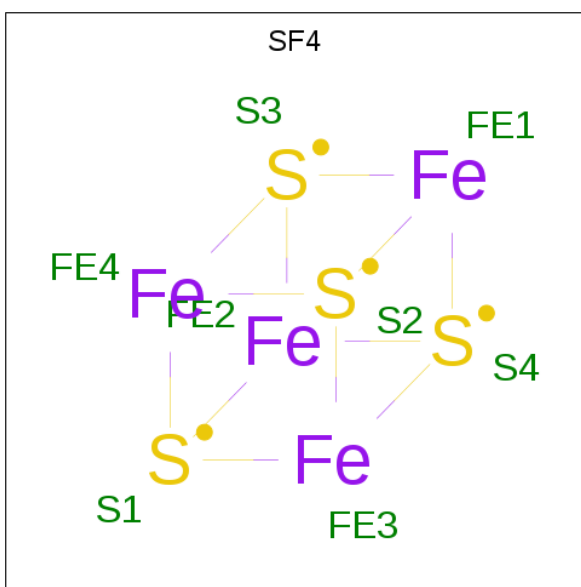
- Molecule 1 is a protein called PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1973	1256	330	372	15			
1	B	262	Total	C	N	O	S	0	2	0
			1980	1260	330	375	15			
1	C	260	Total	C	N	O	S	0	1	0
			1964	1251	328	370	15			

- Molecule 2 is a protein called PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT.

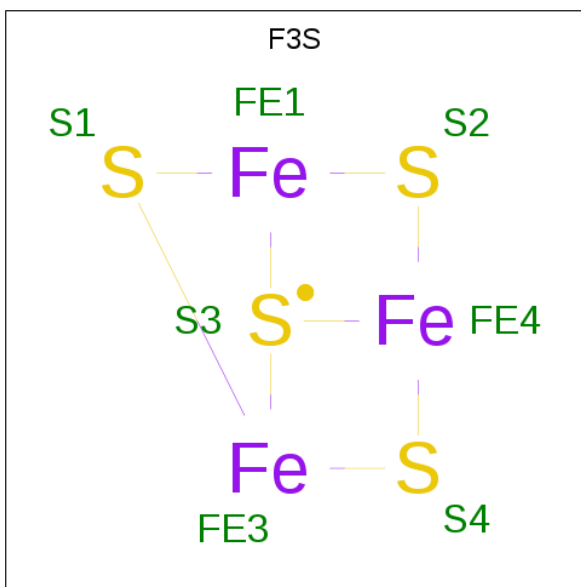
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	9	0
			4204	2680	728	774	22			
2	R	545	Total	C	N	O	S	0	3	0
			4181	2664	724	771	22			
2	S	544	Total	C	N	O	S	0	1	0
			4169	2654	724	769	22			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



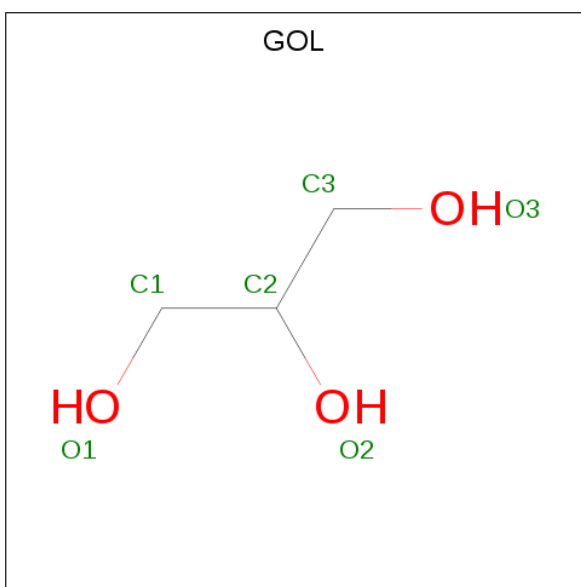
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



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 (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



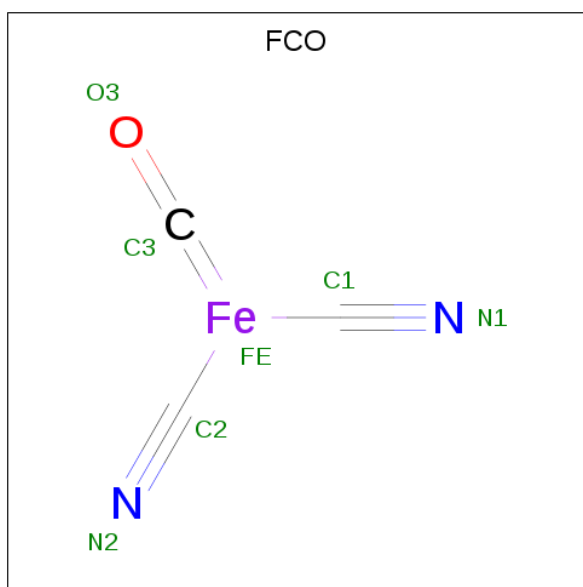
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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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	S	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: 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 (three-letter code: NI) (formula: Ni).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	R	1	Total	Mg	0	0
			1	1		
8	Q	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	310	Total 310	O 310	0	0
9	B	191	Total 191	O 191	0	0
9	C	216	Total 216	O 216	0	0
9	Q	405	Total 405	O 405	0	0
9	R	342	Total 342	O 342	0	0
9	S	237	Total 237	O 237	0	0

### 3 Residue-property plots [i](#)

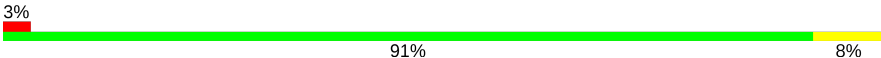
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT

Chain A: 



#### • Molecule 1: PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT

Chain B: 



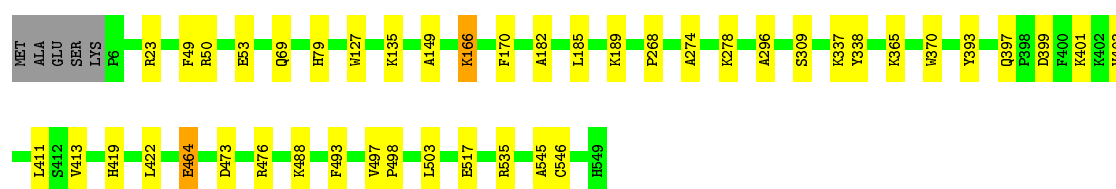
#### • Molecule 1: PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT

Chain C: 



#### • Molecule 2: PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT

Chain Q: 



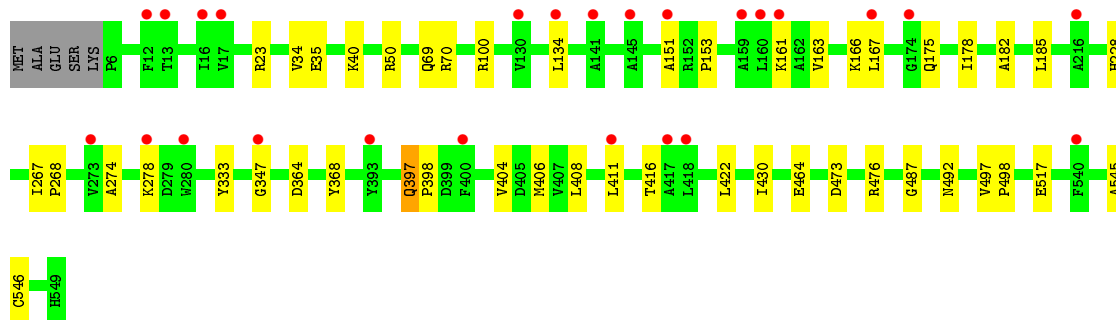
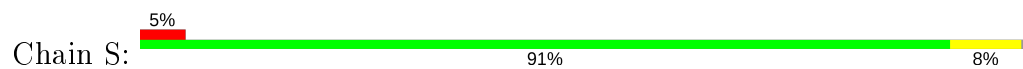
#### • Molecule 2: PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT

Chain R: 





• Molecule 2: PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.77Å 100.40Å 183.43Å 90.00° 91.55° 90.00°	Depositor
Resolution (Å)	21.98 – 2.08 21.98 – 2.08	Depositor EDS
% Data completeness (in resolution range)	87.6 (21.98-2.08) 87.7 (21.98-2.08)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.18 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.195 , 0.235 0.195 , 0.235	Depositor DCC
$R_{free}$ test set	6255 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, NI, SF4, MG, F3S, 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	0.74	4/2027 (0.2%)	0.75	4/2759 (0.1%)
1	B	0.53	1/2043 (0.0%)	0.61	0/2781
1	C	0.68	8/2023 (0.4%)	0.66	2/2754 (0.1%)
2	Q	0.58	2/4334 (0.0%)	0.68	3/5881 (0.1%)
2	R	0.50	2/4292 (0.0%)	0.64	3/5825 (0.1%)
2	S	0.43	1/4271 (0.0%)	0.60	3/5796 (0.1%)
All	All	0.56	18/18990 (0.1%)	0.65	15/25796 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	517	GLU	CD-OE2	-10.55	1.14	1.25
1	C	261	TYR	CE1-CZ	-10.53	1.24	1.38
2	Q	464	GLU	CD-OE1	-9.32	1.15	1.25
1	C	261	TYR	CG-CD2	-9.06	1.27	1.39
1	C	261	TYR	CG-CD1	-8.65	1.27	1.39
1	A	232	PHE	CG-CD2	-7.94	1.26	1.38
1	A	232	PHE	CG-CD1	-7.68	1.27	1.38
1	C	261	TYR	CE2-CZ	-7.40	1.28	1.38
1	C	224	TYR	CE1-CZ	-6.37	1.30	1.38
2	Q	517	GLU	CD-OE1	-6.26	1.18	1.25
1	A	215	GLU	CD-OE2	-6.19	1.18	1.25
1	C	215	GLU	CD-OE2	-5.72	1.19	1.25
1	C	224	TYR	CG-CD1	-5.71	1.31	1.39
1	C	224	TYR	CG-CD2	-5.60	1.31	1.39
2	R	517	GLU	CD-OE1	-5.52	1.19	1.25
1	A	261	TYR	CG-CD2	-5.50	1.32	1.39
2	S	517	GLU	CD-OE1	-5.49	1.19	1.25
1	B	261	TYR	CE1-CZ	-5.03	1.32	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	517	GLU	OE1-CD-OE2	-9.88	111.45	123.30
2	Q	464	GLU	OE1-CD-OE2	-7.94	113.77	123.30
2	S	161	LYS	CD-CE-NZ	7.87	129.79	111.70
1	A	203	ASP	CB-CG-OD2	7.55	125.09	118.30
1	C	215	GLU	OE1-CD-OE2	-7.03	114.86	123.30
2	Q	166	LYS	CD-CE-NZ	6.06	125.64	111.70
2	Q	517	GLU	OE1-CD-OE2	-6.04	116.06	123.30
2	S	517	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	215	GLU	OE1-CD-OE2	-5.70	116.46	123.30
2	R	166	LYS	CD-CE-NZ	5.53	124.42	111.70
2	R	517	GLU	CG-CD-OE1	5.50	129.31	118.30
2	S	166	LYS	CD-CE-NZ	5.39	124.09	111.70
1	A	171	GLU	CB-CA-C	-5.25	99.90	110.40
1	A	203	ASP	OD1-CG-OD2	-5.13	113.56	123.30
1	C	171	GLU	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1973	0	1911	13	0
1	B	1980	0	1918	21	0
1	C	1964	0	1906	19	0
2	Q	4204	0	4192	31	0
2	R	4181	0	4154	24	0
2	S	4169	0	4140	28	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	18	0	24	3	0
5	Q	24	0	32	5	0
5	R	36	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	6	0	8	0	0
6	Q	7	0	0	1	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	310	0	0	4	0
9	B	191	0	0	2	0
9	C	216	0	0	5	0
9	Q	405	0	0	2	0
9	R	342	0	0	4	0
9	S	237	0	0	5	0
All	All	20352	0	18333	124	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 (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PHE:CE2	2:R:233:VAL:HG11	1.83	1.13
1:B:202:PHE:CE1	1:B:216:LEU:HD13	1.87	1.09
1:B:202:PHE:CD2	2:R:233:VAL:HG11	1.95	1.00
9:C:2216:HOH:O	2:Q:189:LYS:HE3	1.73	0.88
2:Q:337:LYS:HE2	5:Q:1564:GOL:H2	1.56	0.85
1:B:202:PHE:HE1	1:B:216:LEU:HD13	1.37	0.85
2:Q:488:LYS:HE2	9:Q:2372:HOH:O	1.80	0.81
2:Q:337:LYS:HE2	5:Q:1564:GOL:C2	2.15	0.76
1:B:202:PHE:CE2	2:R:233:VAL:CG1	2.68	0.73
1:B:202:PHE:HE2	2:R:233:VAL:HG11	1.51	0.71
1:B:202:PHE:CD1	1:B:216:LEU:HD13	2.26	0.69
1:C:182:LEU:HG	1:C:224:TYR:HE1	1.57	0.69
5:A:1273:GOL:H11	2:Q:170:PHE:HA	1.74	0.68
1:C:182:LEU:CD2	1:C:224:TYR:CE1	2.77	0.67
1:B:99:LYS:HD2	1:B:137:LEU:HD22	1.80	0.64
1:C:182:LEU:CD2	1:C:224:TYR:HE1	2.12	0.63
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:274:ALA:HA	2:R:422[A]:LEU:HD11	1.81	0.62
1:B:14:ASN:ND2	1:B:94:MET:HB3	2.14	0.61
2:S:34:VAL:HG12	2:S:35:GLU:N	2.16	0.60
2:S:163:VAL:HG23	9:S:2085:HOH:O	2.01	0.60
5:A:1273:GOL:C1	2:Q:170:PHE:HA	2.31	0.60
1:B:14:ASN:HD22	1:B:94:MET:HB3	1.66	0.59
1:C:182:LEU:HD23	1:C:224:TYR:CE1	2.38	0.58
1:C:182:LEU:CG	1:C:224:TYR:HE1	2.16	0.58
2:Q:274:ALA:HA	2:Q:422[A]:LEU:HD11	1.86	0.58
1:A:104:LYS:HD2	9:A:2091:HOH:O	2.03	0.58
1:B:202:PHE:HE2	2:R:233:VAL:CG1	2.10	0.58
1:B:131:LYS:HB2	1:B:136:ALA:HB2	1.86	0.57
2:S:364:ASP:O	2:S:368:TYR:HB3	2.05	0.57
1:C:182:LEU:HD23	1:C:224:TYR:CD1	2.39	0.57
2:Q:278:LYS:NZ	2:Q:411:LEU:O	2.38	0.57
2:Q:419:HIS:O	5:Q:1563:GOL:H2	2.06	0.56
2:Q:393:TYR:O	2:Q:401[A]:LYS:NZ	2.27	0.56
1:C:262:GLU:OE2	2:Q:135:LYS:NZ	2.39	0.55
2:Q:497:VAL:HG11	2:Q:546:CYS:HB3	1.89	0.55
2:S:333:TYR:CD2	2:S:347:GLY:HA2	2.43	0.53
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.91	0.52
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.40	0.52
2:R:464:GLU:OE1	2:R:487:GLY:HA2	2.10	0.51
1:B:202:PHE:HD2	2:R:233:VAL:HG21	1.74	0.51
2:R:245:LYS:NZ	9:R:2171:HOH:O	2.43	0.51
2:S:404:VAL:HG22	2:S:430:ILE:HD13	1.92	0.50
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.41	0.50
2:S:274:ALA:HA	2:S:422:LEU:HD11	1.94	0.49
2:Q:182:ALA:HB3	2:Q:185:LEU:HG	1.94	0.49
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.94	0.49
1:B:145:PRO:HD2	1:B:179:TYR:CZ	2.46	0.49
2:Q:413:VAL:HG11	9:Q:2221:HOH:O	2.10	0.49
1:A:80:THR:HG21	1:A:131:LYS:HD2	1.94	0.49
2:S:34:VAL:HG12	2:S:35:GLU:H	1.78	0.49
1:A:264:GLY:HA3	9:A:2302:HOH:O	2.14	0.48
1:A:61:HIS:HE1	9:A:2085:HOH:O	1.95	0.48
1:A:112:GLY:HA2	1:A:149:PRO:HD3	1.94	0.48
5:R:1564:GOL:H11	9:R:2228:HOH:O	2.13	0.48
2:Q:399:ASP:O	2:Q:403:VAL:HG23	2.14	0.48
2:S:100:ARG:HD3	9:S:2056:HOH:O	2.14	0.48
2:S:182:ALA:HB3	2:S:185:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD22	1:A:95:ILE:HA	1.96	0.48
1:C:224:TYR:HE2	9:C:2050:HOH:O	1.97	0.47
2:S:492:ASN:ND2	9:S:2176:HOH:O	2.41	0.47
2:R:497:VAL:HG11	2:R:546:CYS:HB3	1.97	0.47
1:C:112:GLY:HA2	1:C:149:PRO:HD3	1.97	0.46
2:R:50:ARG:NH2	2:R:545:ALA:HB1	2.29	0.45
2:S:476:ARG:HD2	6:S:1550:FCO:C2	2.46	0.45
2:Q:338:TYR:CE2	5:Q:1564:GOL:H12	2.52	0.45
2:Q:69:GLN:HA	2:Q:79:HIS:HB2	1.99	0.45
2:S:278:LYS:NZ	2:S:411:LEU:O	2.44	0.45
1:B:80:THR:HG21	1:B:131:LYS:HD2	1.99	0.45
1:B:150:ASN:HB2	9:B:2132:HOH:O	2.16	0.45
2:Q:401[A]:LYS:HB2	2:Q:401[A]:LYS:HE2	1.74	0.45
2:S:497:VAL:HG11	2:S:546:CYS:HB3	1.99	0.45
1:C:30:PRO:HG3	9:C:2023:HOH:O	2.16	0.45
2:Q:50:ARG:NH2	2:Q:545:ALA:HB1	2.32	0.44
1:A:14:ASN:ND2	1:A:94:MET:HB3	2.32	0.44
1:C:26:ARG:NH2	9:C:2013:HOH:O	2.50	0.44
1:C:47:THR:O	2:S:23:ARG:HA	2.18	0.44
2:R:182:ALA:HB3	2:R:185:LEU:HG	1.99	0.44
2:S:397:GLN:HA	2:S:398:PRO:HD3	1.82	0.44
1:B:176:LYS:HE2	9:B:2063:HOH:O	2.17	0.44
2:R:53:GLU:HG2	2:R:493:PHE:O	2.18	0.43
1:A:98:THR:HG22	1:A:137:LEU:HD11	2.00	0.43
2:Q:149:ALA:HB2	2:Q:268:PRO:HB3	1.99	0.43
2:S:151:ALA:HA	9:S:2079:HOH:O	2.17	0.43
2:R:284:GLY:HA2	2:R:518:ALA:O	2.18	0.43
2:R:410:LYS:HD3	5:R:1562:GOL:H32	2.00	0.43
2:S:134:LEU:CD2	2:S:167:LEU:HD23	2.48	0.43
2:S:50:ARG:NH2	2:S:545:ALA:HB1	2.33	0.43
2:Q:296:ALA:HA	2:Q:309:SER:HA	2.00	0.43
2:S:153:PRO:HD2	9:S:2083:HOH:O	2.18	0.43
1:B:112:GLY:HA2	1:B:149:PRO:HD3	2.01	0.43
2:S:464:GLU:OE1	2:S:487:GLY:HA2	2.19	0.42
2:R:410:LYS:HD3	5:R:1562:GOL:H11	2.00	0.42
1:B:18:THR:HA	1:B:75:GLU:OE2	2.19	0.42
5:A:1273:GOL:H11	2:Q:170:PHE:CA	2.46	0.42
2:S:69:GLN:OE1	2:S:228:HIS:HA	2.19	0.42
1:A:228:PRO:HB3	1:A:237:TRP:CZ2	2.54	0.42
2:R:69:GLN:HA	2:R:79:HIS:HB2	1.99	0.42
1:B:47:THR:O	2:R:23:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:34:VAL:CG1	2:S:35:GLU:N	2.82	0.42
2:Q:476:ARG:HD2	6:Q:1550:FCO:C2	2.49	0.42
1:A:61:HIS:HD2	9:A:2097:HOH:O	2.01	0.42
1:C:42:LEU:HD21	1:C:45:GLN:HG3	2.01	0.42
1:A:47:THR:O	2:Q:23:ARG:HA	2.20	0.41
1:C:237:TRP:CZ2	1:C:239:VAL:HB	2.55	0.41
1:C:182:LEU:HG	1:C:224:TYR:CE1	2.45	0.41
1:A:35:LEU:HD12	1:A:39:THR:HB	2.01	0.41
1:B:6:ARG:NH2	2:R:175:GLN:HB2	2.35	0.41
1:C:95:ILE:O	1:C:99:LYS:HB2	2.20	0.41
2:Q:464:GLU:OE1	2:Q:464:GLU:HA	2.20	0.41
1:C:5:HIS:HA	2:S:175:GLN:OE1	2.21	0.41
2:R:401:LYS:NZ	9:R:2296:HOH:O	2.47	0.41
2:R:497:VAL:HG13	2:R:498:PRO:HD2	2.02	0.41
1:C:254:TRP:HH2	2:S:70:ARG:HD3	1.85	0.41
9:C:2027:HOH:O	2:S:178:ILE:HG12	2.20	0.41
1:A:145:PRO:HD2	1:A:179:TYR:CZ	2.56	0.41
2:Q:337:LYS:HE2	5:Q:1564:GOL:O2	2.19	0.41
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.56	0.41
2:R:410:LYS:HG2	9:R:2299:HOH:O	2.21	0.41
2:S:267:ILE:HB	2:S:268:PRO:HD3	2.03	0.41
2:Q:53:GLU:HG2	2:Q:493:PHE:O	2.21	0.40
2:R:126:ASP:HB3	2:R:535:ARG:HG2	2.02	0.40
2:Q:127:TRP:CZ3	2:Q:535:ARG:HD3	2.56	0.40
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	262/264 (99%)	254 (97%)	8 (3%)	0	100	100
1	C	259/264 (98%)	251 (97%)	8 (3%)	0	100	100
2	Q	550/549 (100%)	533 (97%)	17 (3%)	0	100	100
2	R	545/549 (99%)	534 (98%)	11 (2%)	0	100	100
2	S	542/549 (99%)	524 (97%)	18 (3%)	0	100	100
All	All	2418/2439 (99%)	2350 (97%)	68 (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%)	76	81
1	B	210/210 (100%)	209 (100%)	1 (0%)	88	92
1	C	208/210 (99%)	208 (100%)	0	100	100
2	Q	443/438 (101%)	438 (99%)	5 (1%)	73	78
2	R	437/438 (100%)	432 (99%)	5 (1%)	73	78
2	S	435/438 (99%)	429 (99%)	6 (1%)	67	72
All	All	1941/1944 (100%)	1922 (99%)	19 (1%)	76	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	A	171	GLU
1	B	171	GLU
2	Q	166	LYS
2	Q	365	LYS
2	Q	397	GLN
2	Q	473	ASP
2	Q	503	LEU

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Mol	Chain	Res	Type
2	R	92	LYS
2	R	397	GLN
2	R	473	ASP
2	R	500	THR
2	R	503	LEU
2	S	40	LYS
2	S	397	GLN
2	S	406	MET
2	S	408	LEU
2	S	416	THR
2	S	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	B	14	ASN
1	B	61	HIS
1	C	14	ASN
1	C	172	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	S	543	2,7	3,6,7	0.83	0	0,6,8	0.00	-
2	CSO	Q	543	2,7	3,6,7	0.54	0	0,6,8	0.00	-
2	CSO	R	543	2,7	3,6,7	0.66	0	0,6,8	0.00	-

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	S	543	2,7	-	1/1/5/7	-
2	CSO	Q	543	2,7	-	1/1/5/7	-
2	CSO	R	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	S	543	CSO	N-CA-CB-SG
2	Q	543	CSO	N-CA-CB-SG
2	R	543	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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	0.00	-	-		

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	0.00	-	-		
5	GOL	R	1565	-	5,5,5	0.32	0	5,5,5	0.20	0
5	GOL	R	1561	-	5,5,5	0.31	0	5,5,5	0.61	0
5	GOL	A	1271	-	5,5,5	0.30	0	5,5,5	0.55	0
5	GOL	Q	1561	-	5,5,5	0.26	0	5,5,5	0.18	0
3	SF4	C	1265	1	0,12,12	0.00	-	-		
6	FCO	R	1550	2,7	0,6,6	0.00	-	-		
5	GOL	A	1273	-	5,5,5	0.39	0	5,5,5	0.54	0
3	SF4	A	1267	1	0,12,12	0.00	-	-		
4	F3S	C	1266	1	0,9,9	0.00	-	-		
5	GOL	A	1272	-	5,5,5	0.33	0	5,5,5	0.42	0
6	FCO	S	1550	2,7	0,6,6	0.00	-	-		
3	SF4	C	1267	1	0,12,12	0.00	-	-		
5	GOL	Q	1564	-	5,5,5	0.34	0	5,5,5	0.46	0
5	GOL	Q	1563	-	5,5,5	0.27	0	5,5,5	0.26	0
5	GOL	R	1566	-	5,5,5	0.36	0	5,5,5	0.27	0
5	GOL	R	1564	-	5,5,5	0.33	0	5,5,5	0.18	0
5	GOL	Q	1562	-	5,5,5	0.20	0	5,5,5	0.30	0
6	FCO	Q	1550	2,7	0,6,6	0.00	-	-		
5	GOL	S	1561	-	5,5,5	0.38	0	5,5,5	0.24	0
5	GOL	R	1562	-	5,5,5	0.26	0	5,5,5	0.18	0
3	SF4	A	1265	1	0,12,12	0.00	-	-		
3	SF4	B	1265	1	0,12,12	0.00	-	-		
3	SF4	B	1267	1	0,12,12	0.00	-	-		
5	GOL	R	1563	-	5,5,5	0.26	0	5,5,5	0.43	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
4	F3S	B	1266	1	-	-	0/3/3/3
4	F3S	A	1266	1	-	-	0/3/3/3
5	GOL	R	1565	-	-	4/4/4/4	-
5	GOL	R	1561	-	-	1/4/4/4	-
5	GOL	A	1271	-	-	3/4/4/4	-
5	GOL	S	1561	-	-	0/4/4/4	-
3	SF4	C	1265	1	-	-	0/6/5/5
5	GOL	A	1273	-	-	2/4/4/4	-
3	SF4	A	1267	1	-	-	0/6/5/5
5	GOL	Q	1561	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F3S	C	1266	1	-	-	0/3/3/3
5	GOL	A	1272	-	-	2/4/4/4	-
3	SF4	C	1267	1	-	-	0/6/5/5
3	SF4	B	1265	1	-	-	0/6/5/5
5	GOL	Q	1563	-	-	0/4/4/4	-
5	GOL	R	1566	-	-	4/4/4/4	-
5	GOL	R	1564	-	-	2/4/4/4	-
3	SF4	B	1267	1	-	-	0/6/5/5
5	GOL	R	1562	-	-	4/4/4/4	-
3	SF4	A	1265	1	-	-	0/6/5/5
5	GOL	Q	1564	-	-	2/4/4/4	-
5	GOL	Q	1562	-	-	0/4/4/4	-
5	GOL	R	1563	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1271	GOL	C1-C2-C3-O3
5	R	1566	GOL	O1-C1-C2-O2
5	R	1566	GOL	O1-C1-C2-C3
5	R	1566	GOL	C1-C2-C3-O3
5	R	1562	GOL	O1-C1-C2-C3
5	R	1565	GOL	O1-C1-C2-C3
5	R	1565	GOL	C1-C2-C3-O3
5	A	1273	GOL	O1-C1-C2-C3
5	Q	1564	GOL	C1-C2-C3-O3
5	R	1564	GOL	O1-C1-C2-C3
5	R	1562	GOL	C1-C2-C3-O3
5	R	1562	GOL	O2-C2-C3-O3
5	A	1271	GOL	O2-C2-C3-O3
5	Q	1564	GOL	O2-C2-C3-O3
5	A	1271	GOL	O1-C1-C2-O2
5	A	1272	GOL	O1-C1-C2-O2
5	R	1562	GOL	O1-C1-C2-O2
5	A	1272	GOL	O1-C1-C2-C3
5	R	1565	GOL	O2-C2-C3-O3
5	A	1273	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	R	1566	GOL	O2-C2-C3-O3
5	R	1565	GOL	O1-C1-C2-O2
5	R	1561	GOL	O1-C1-C2-O2
5	R	1564	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1273	GOL	3	0
6	S	1550	FCO	1	0
5	Q	1564	GOL	4	0
5	Q	1563	GOL	1	0
5	R	1564	GOL	1	0
6	Q	1550	FCO	1	0
5	R	1562	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/264 (99%)	-0.56	0 100 100	9, 17, 27, 47	4 (1%)
1	B	262/264 (99%)	0.17	9 (3%) 45 50	21, 36, 57, 71	6 (2%)
1	C	260/264 (98%)	-0.05	0 100 100	19, 33, 56, 70	4 (1%)
2	Q	543/549 (98%)	-0.52	0 100 100	9, 19, 33, 42	7 (1%)
2	R	544/549 (99%)	-0.19	4 (0%) 87 89	16, 29, 47, 65	6 (1%)
2	S	543/549 (98%)	0.41	25 (4%) 32 36	20, 48, 77, 90	7 (1%)
All	All	2414/2439 (98%)	-0.12	38 (1%) 72 75	9, 29, 63, 90	34 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	GLY	5.5
2	S	400	PHE	4.2
2	S	280	TRP	3.9
2	S	160	LEU	3.9
2	S	134	LEU	3.6
1	B	193	PHE	3.6
1	B	202	PHE	3.4
2	S	141	ALA	3.4
2	S	12	PHE	3.2
1	B	158	VAL	3.1
2	S	411	LEU	3.0
2	S	347	GLY	3.0
2	S	145	ALA	2.9
2	S	159	ALA	2.8
1	B	4	LYS	2.8
2	S	161	LYS	2.7
2	S	167	LEU	2.6
1	B	3	ALA	2.6
2	S	151	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	S	16	ILE	2.6
2	S	417	ALA	2.5
1	B	239	VAL	2.5
2	S	130	VAL	2.5
2	R	418	LEU	2.4
2	S	273	VAL	2.4
1	B	177	LEU	2.3
2	R	403	VAL	2.3
2	S	418	LEU	2.3
1	B	133	VAL	2.3
2	S	13	THR	2.2
2	S	393	TYR	2.2
2	R	250	ASN	2.1
2	R	461	GLU	2.1
2	S	174	GLY	2.1
2	S	216	ALA	2.1
2	S	278	LYS	2.1
2	S	17	VAL	2.1
2	S	540	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CSO	S	543	7/8	0.97	0.09	29,31,32,33	1
2	CSO	Q	543	7/8	0.99	0.06	9,9,10,10	1
2	CSO	R	543	7/8	0.99	0.06	18,18,19,19	1

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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	1566	6/6	0.67	0.25	55,60,61,62	0
5	GOL	Q	1563	6/6	0.83	0.20	43,49,53,53	0
5	GOL	R	1562	6/6	0.83	0.19	49,50,52,53	0
5	GOL	S	1561	6/6	0.85	0.15	34,40,41,42	0
5	GOL	Q	1564	6/6	0.85	0.20	36,38,41,46	0
5	GOL	R	1563	6/6	0.89	0.15	34,36,38,39	0
5	GOL	R	1564	6/6	0.91	0.20	40,43,47,53	0
5	GOL	A	1273	6/6	0.91	0.17	43,43,46,47	0
5	GOL	R	1565	6/6	0.93	0.13	40,41,42,42	0
5	GOL	Q	1561	6/6	0.94	0.16	35,36,38,39	0
5	GOL	A	1272	6/6	0.95	0.16	39,39,42,46	0
8	MG	S	1553	1/1	0.95	0.05	34,34,34,34	0
5	GOL	R	1561	6/6	0.96	0.08	28,29,30,30	0
3	SF4	B	1265	8/8	0.96	0.07	45,47,48,50	0
5	GOL	A	1271	6/6	0.96	0.11	25,30,32,36	0
8	MG	R	1553	1/1	0.97	0.03	24,24,24,24	0
3	SF4	B	1267	8/8	0.98	0.06	24,25,26,26	0
5	GOL	Q	1562	6/6	0.98	0.11	20,22,23,25	0
7	NI	S	1551	1/1	0.99	0.08	27,27,27,27	0
4	F3S	A	1266	7/7	0.99	0.06	9,10,10,10	0
8	MG	Q	1553	1/1	0.99	0.06	9,9,9,9	0
3	SF4	A	1267	8/8	0.99	0.07	8,8,9,9	0
4	F3S	B	1266	7/7	0.99	0.04	32,32,34,34	0
4	F3S	C	1266	7/7	0.99	0.05	20,21,21,22	0
3	SF4	C	1265	8/8	0.99	0.07	19,21,21,22	0
6	FCO	S	1550	7/7	0.99	0.12	29,30,31,32	0
3	SF4	C	1267	8/8	0.99	0.07	23,23,24,25	0
6	FCO	R	1550	7/7	0.99	0.08	19,20,20,21	0
3	SF4	A	1265	8/8	1.00	0.06	13,14,15,15	0
6	FCO	Q	1550	7/7	1.00	0.07	9,9,9,9	0
7	NI	R	1551	1/1	1.00	0.06	20,20,20,20	0
7	NI	Q	1551	1/1	1.00	0.07	10,10,10,10	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.