



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:05 AM GMT

PDB ID : 3H3X  
Title : Structure of the V74M large subunit mutant of NI-FE hydrogenase in an oxidized state  
Authors : Volbeda, A.; Martinez, N.; Martin, L.; Fontecilla-Camps, J.C.  
Deposited on : 2009-04-17  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

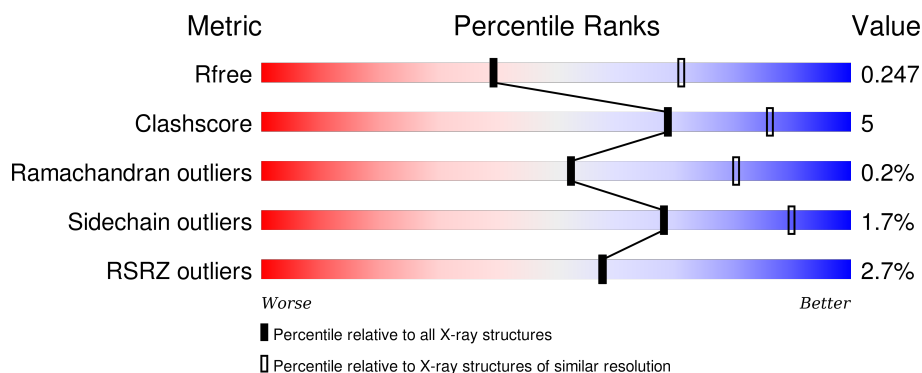
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	264	<div> <div>9%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	264	<div> <div></div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
2	Q	549	<div> <div></div> <div> <div></div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>
2	R	549	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	S	549	

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	A	271	-	-	-	X
5	GOL	R	561	-	-	-	X
5	GOL	R	562	-	-	-	X
5	GOL	S	561	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19100 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	0	0
			1974	1257	330	372	15			
1	C	260	Total	C	N	O	S	0	0	0
			1960	1248	327	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	0	0
			4163	2652	723	765	23			
2	R	545	Total	C	N	O	S	0	0	0
			4167	2654	724	766	23			
2	S	544	Total	C	N	O	S	0	0	0
			4163	2652	723	765	23			

There are 3 discrepancies between the modelled and reference sequences:

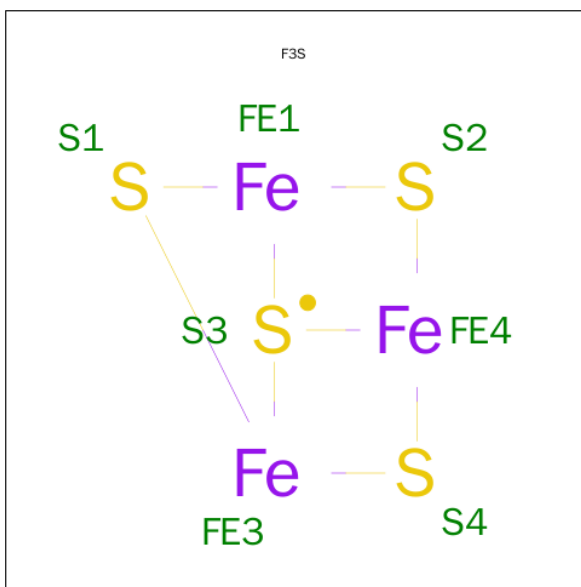
Chain	Residue	Modelled	Actual	Comment	Reference
Q	74	MET	VAL	ENGINEERED	UNP P18188
R	74	MET	VAL	ENGINEERED	UNP P18188
S	74	MET	VAL	ENGINEERED	UNP P18188

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



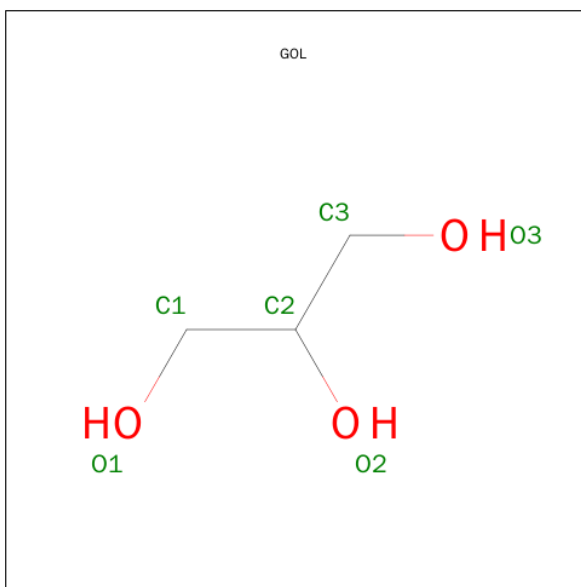
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



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:  $C_3H_8O_3$ ).



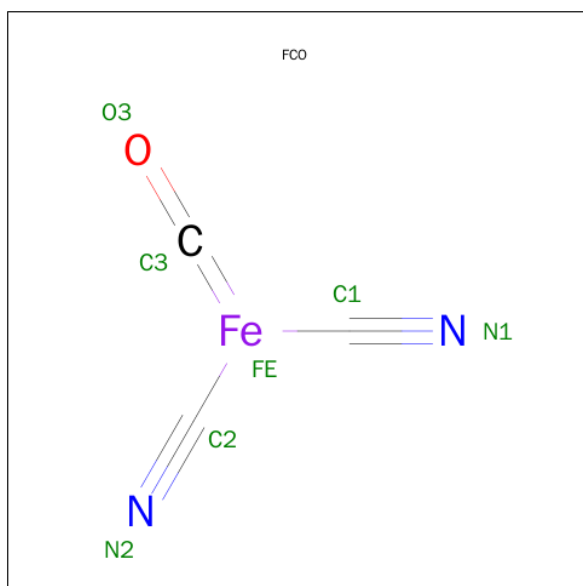
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	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	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 1 1	0	0
7	Q	1	Total Ni 1 1	0	0
7	S	1	Total Ni 1 1	0	0

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

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

- Molecule 9 is water.

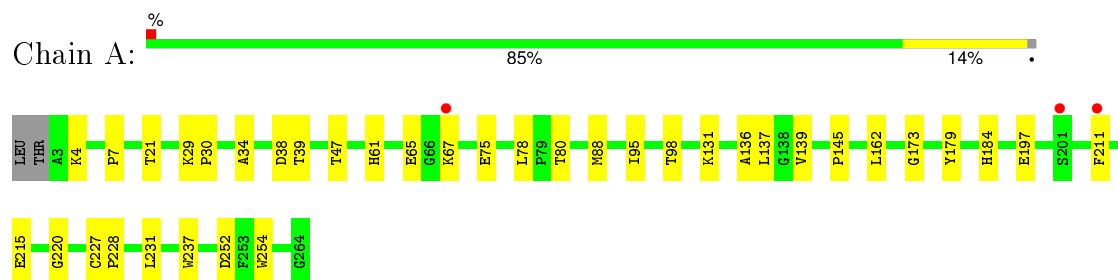
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	68	Total O 68 68	0	0
9	Q	144	Total O 144 144	0	0
9	B	58	Total O 58 58	0	0
9	R	133	Total O 133 133	0	0
9	C	65	Total O 65 65	0	0
9	S	94	Total O 94 94	0	0



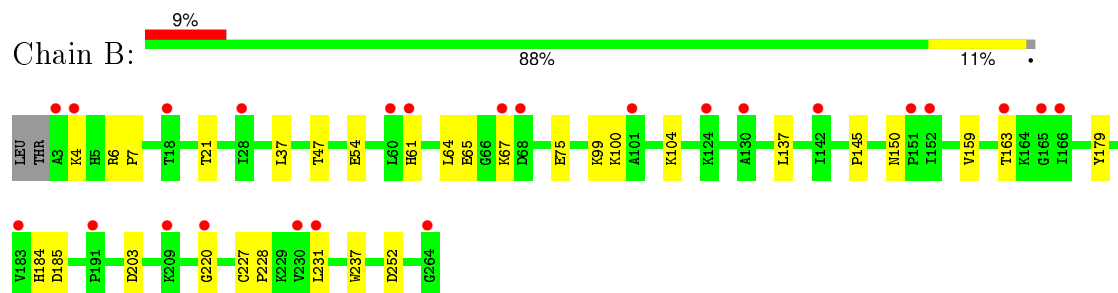
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

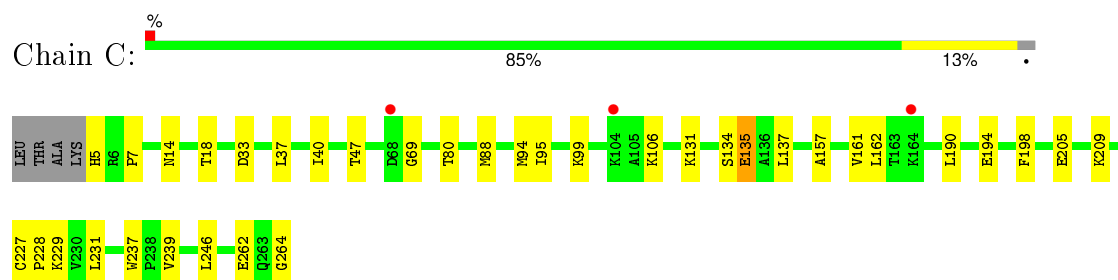
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



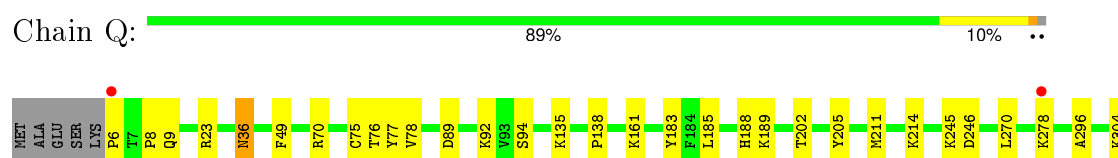
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

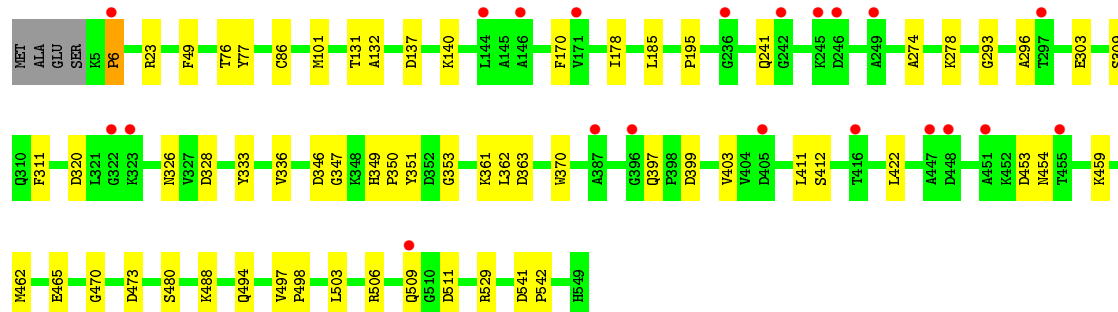
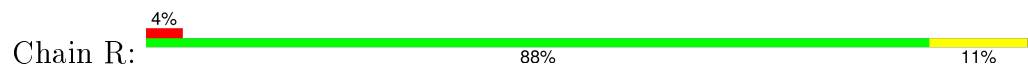


- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

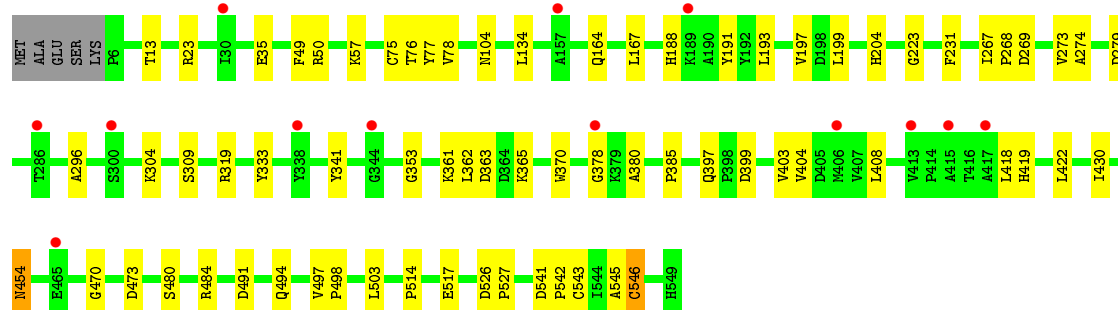
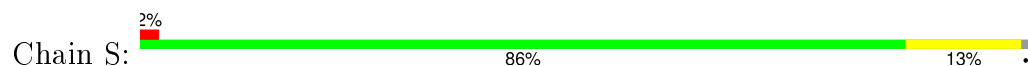




• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit



• 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, $\alpha$ , $\beta$ , $\gamma$	62.40 Å 99.20 Å 182.30 Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.70) 85.5 (19.90-2.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.78 (at 2.71 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.203 , 0.247 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	2935 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.0	EDS
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 60250 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, NI, SF4, 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	0.76	0/2027	0.73	0/2759
1	B	0.61	0/2028	0.63	0/2761
1	C	0.69	0/2014	0.68	0/2743
2	Q	0.74	1/4268 (0.0%)	0.74	0/5792
2	R	0.66	2/4272 (0.0%)	0.70	0/5798
2	S	0.61	0/4268	0.67	0/5792
All	All	0.68	3/18877 (0.0%)	0.70	0/25645

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	546	CYS	CB-SG	-5.63	1.72	1.81
2	R	303	GLU	CB-CG	-5.38	1.42	1.52
2	R	86	CYS	CB-SG	-5.28	1.73	1.81

There are no bond angle outliers.

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	21	0
1	B	1974	0	1915	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1960	0	1897	24	0
2	Q	4163	0	4136	40	0
2	R	4167	0	4136	38	0
2	S	4163	0	4136	40	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
5	A	6	0	8	0	0
5	Q	12	0	16	2	0
5	R	18	0	24	2	0
5	S	6	0	8	2	0
6	Q	7	0	0	1	0
6	R	7	0	0	0	0
6	S	7	0	0	0	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0
9	A	68	0	0	3	0
9	B	58	0	0	4	0
9	C	65	0	0	3	0
9	Q	144	0	0	1	0
9	R	133	0	0	5	0
9	S	94	0	0	3	0
All	All	19100	0	18187	168	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 5.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:104:ASN:HD22	5:S:561:GOL:H32	1.40	0.86
2:Q:89:ASP:O	2:Q:92:LYS:HE2	1.86	0.75
2:Q:320:ASP:HB2	2:R:6:PRO:HD3	1.70	0.74
2:Q:185:LEU:HB2	5:Q:562:GOL:H12	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:319:ARG:HG2	2:S:419:HIS:CE1	2.27	0.69
1:A:137:LEU:HB2	1:A:139:VAL:HG22	1.77	0.67
2:R:131:THR:HG21	2:R:185:LEU:CD2	2.27	0.65
2:R:274:ALA:HA	2:R:422:LEU:HD11	1.79	0.64
2:Q:6:PRO:HG3	2:R:320:ASP:HA	1.78	0.64
1:B:54:GLU:OE1	9:B:313:HOH:O	2.15	0.64
2:Q:454:ASN:H	2:Q:454:ASN:HD22	1.46	0.63
2:Q:138:PRO:HG2	2:Q:161:LYS:HD2	1.80	0.62
2:S:333:TYR:OH	2:S:378:GLY:HA2	1.99	0.62
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.30	0.61
2:S:362:LEU:O	2:S:363:ASP:HB2	2.01	0.61
2:R:462:MET:HG3	2:R:488:LYS:HG2	1.83	0.61
1:C:7:PRO:HD2	1:C:40:ILE:HA	1.84	0.60
2:Q:270:LEU:CD2	2:Q:429:GLY:HA3	2.31	0.60
1:C:5:HIS:N	9:C:316:HOH:O	2.34	0.60
1:B:185:ASP:HB3	9:B:319:HOH:O	2.01	0.59
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.85	0.58
2:S:13:THR:HG23	2:S:35:GLU:HG2	1.85	0.58
1:B:99:LYS:HG3	1:B:137:LEU:HD22	1.85	0.58
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.33	0.58
2:R:131:THR:HG21	2:R:185:LEU:HD23	1.86	0.57
2:S:408:LEU:HD21	2:S:418:LEU:HD21	1.86	0.56
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.40	0.56
2:R:278:LYS:NZ	2:R:411:LEU:O	2.39	0.56
2:R:349:HIS:ND1	2:R:350:PRO:HD2	2.20	0.56
2:S:274:ALA:HA	2:S:422:LEU:HD11	1.88	0.56
2:R:399:ASP:O	2:R:403:VAL:HG23	2.05	0.56
2:R:333:TYR:CD2	2:R:347:GLY:HA2	2.41	0.56
1:C:80:THR:HG21	1:C:131:LYS:HD2	1.87	0.56
2:Q:396:GLY:HA2	2:Q:401:LYS:HE3	1.88	0.56
5:R:561:GOL:O2	9:R:670:HOH:O	2.16	0.55
2:R:529:ARG:HD3	5:R:561:GOL:H31	1.87	0.55
1:B:159:VAL:O	1:B:163:THR:HG23	2.07	0.55
1:A:21:THR:OG1	1:A:75:GLU:OE1	2.25	0.54
2:R:178:ILE:HG12	9:R:639:HOH:O	2.06	0.54
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.90	0.54
1:C:40:ILE:HG22	1:C:162:LEU:HD11	1.90	0.54
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.43	0.54
2:R:349:HIS:CE1	2:R:350:PRO:HD2	2.43	0.54
2:S:267:ILE:HB	2:S:268:PRO:HD3	1.88	0.54
1:C:47:THR:O	2:S:23:ARG:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:O	2:Q:23:ARG:HA	2.08	0.53
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.39	0.53
1:A:254:TRP:HH2	2:Q:70:ARG:HD3	1.73	0.53
2:Q:464:GLU:OE1	2:Q:464:GLU:HA	2.08	0.53
1:C:33:ASP:O	1:C:37:LEU:HD12	2.08	0.53
2:Q:8:PRO:HG2	2:Q:189:LYS:O	2.08	0.52
2:Q:135:LYS:NZ	1:C:262:GLU:OE2	2.38	0.52
2:Q:399:ASP:O	2:Q:403:VAL:HG23	2.10	0.52
1:A:173:GLY:HA3	9:A:335:HOH:O	2.08	0.52
2:R:509:GLN:HB2	9:R:645:HOH:O	2.10	0.51
2:Q:183:TYR:CZ	2:Q:530:PRO:HD2	2.45	0.51
1:B:150:ASN:HB2	9:B:297:HOH:O	2.11	0.51
1:A:34:ALA:O	1:A:38:ASP:HB2	2.11	0.51
2:S:104:ASN:ND2	5:S:561:GOL:H32	2.19	0.51
2:R:137:ASP:OD2	2:R:140:LYS:HG3	2.11	0.51
2:Q:408:LEU:HD22	2:Q:413:VAL:O	2.10	0.51
2:S:543:CYS:SG	2:S:546:CYS:HB2	2.50	0.51
1:C:157:ALA:O	1:C:161:VAL:HG23	2.11	0.51
1:B:37:LEU:HD23	2:R:170:PHE:CD2	2.46	0.50
2:S:404:VAL:HG22	2:S:430:ILE:HD13	1.93	0.50
2:R:137:ASP:HB3	2:R:140:LYS:HD2	1.93	0.50
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.47	0.50
2:S:399:ASP:O	2:S:403:VAL:HG23	2.12	0.49
1:C:99:LYS:HG3	1:C:137:LEU:HD22	1.94	0.49
2:Q:454:ASN:N	2:Q:454:ASN:HD22	2.07	0.49
2:S:188:HIS:HB3	2:S:191:TYR:HD2	1.78	0.48
5:Q:562:GOL:H31	1:C:198:PHE:CE2	2.49	0.48
1:B:47:THR:O	2:R:23:ARG:HA	2.13	0.48
1:C:227:CYS:HB2	1:C:228:PRO:HD3	1.95	0.48
2:S:204:HIS:ND1	2:S:269:ASP:OD2	2.36	0.48
2:S:380:ALA:HB1	2:S:514:PRO:HD3	1.95	0.48
1:A:228:PRO:HB3	1:A:237:TRP:CZ2	2.49	0.48
2:Q:497:VAL:HG12	2:Q:498:PRO:HD2	1.96	0.47
2:R:353:GLY:HA3	2:R:494:GLN:HG3	1.96	0.47
1:C:14:ASN:ND2	1:C:94:MET:HB3	2.29	0.47
2:S:76:THR:O	2:S:77:TYR:HB3	2.15	0.47
2:R:328:ASP:OD2	1:C:134:SER:OG	2.26	0.47
2:S:484:ARG:NH2	9:S:641:HOH:O	2.46	0.47
1:A:252:ASP:HA	9:A:282:HOH:O	2.15	0.47
2:Q:75:CYS:CB	6:Q:550:FCO:C2	2.93	0.47
1:A:227:CYS:HB2	1:A:228:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.50	0.46
2:S:75:CYS:O	2:S:78:VAL:HG22	2.16	0.46
2:S:279:ASP:N	2:S:279:ASP:OD1	2.48	0.46
2:Q:75:CYS:O	2:Q:78:VAL:HG22	2.15	0.46
2:S:49:PHE:HB2	2:S:370:TRP:CD2	2.51	0.46
2:S:353:GLY:HA3	2:S:494:GLN:HG3	1.97	0.46
2:S:57:LYS:HE2	2:S:491:ASP:O	2.16	0.46
2:S:526:ASP:OD1	2:S:527:PRO:HD2	2.15	0.46
2:Q:245:LYS:HE2	2:Q:246:ASP:OD2	2.17	0.45
2:S:454:ASN:H	2:S:454:ASN:HD22	1.64	0.45
2:Q:333:TYR:CD1	2:Q:347:GLY:HA2	2.52	0.45
2:Q:353:GLY:HA3	2:Q:494:GLN:HG3	1.99	0.45
2:Q:183:TYR:CE2	2:Q:530:PRO:HD2	2.52	0.45
2:S:470:GLY:O	2:S:480:SER:HA	2.16	0.45
1:B:64:LEU:O	1:B:104:LYS:NZ	2.49	0.45
1:A:78:LEU:HD12	1:A:136:ALA:HB3	1.98	0.45
1:B:145:PRO:HD2	1:B:179:TYR:CZ	2.52	0.45
1:B:61:HIS:O	1:B:65:GLU:HG2	2.17	0.44
2:Q:408:LEU:HD23	2:Q:408:LEU:HA	1.88	0.44
2:Q:9:GLN:NE2	2:Q:36:ASN:O	2.50	0.44
1:C:246:LEU:HA	9:C:283:HOH:O	2.16	0.44
2:S:385:PRO:HB2	9:S:617:HOH:O	2.16	0.44
2:Q:405:ASP:HB2	9:Q:679:HOH:O	2.16	0.44
1:B:21:THR:OG1	1:B:75:GLU:OE1	2.32	0.44
2:R:296:ALA:HA	2:R:309:SER:HA	2.00	0.44
1:A:7:PRO:HG2	1:A:162:LEU:HD13	2.00	0.44
2:Q:211:MET:SD	2:Q:214:LYS:HD2	2.58	0.44
1:B:227:CYS:HB2	1:B:228:PRO:HD3	1.98	0.43
1:A:184:HIS:HB2	1:A:220:GLY:C	2.39	0.43
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.99	0.43
2:S:134:LEU:HD23	2:S:167:LEU:HD23	2.00	0.43
2:Q:296:ALA:HA	2:Q:309:SER:HA	1.99	0.43
2:R:6:PRO:HA	9:R:657:HOH:O	2.18	0.43
2:R:132:ALA:O	2:R:195:PRO:HB3	2.18	0.43
2:S:50:ARG:NH2	2:S:545:ALA:HB1	2.34	0.43
2:R:76:THR:O	2:R:77:TYR:HB3	2.18	0.43
2:S:193:LEU:HD11	2:S:273:VAL:HG22	2.01	0.43
1:B:6:ARG:HA	1:B:7:PRO:HD3	1.89	0.43
2:Q:304:LYS:HD3	2:Q:304:LYS:HA	1.85	0.43
1:C:190:LEU:O	1:C:194:GLU:HG3	2.19	0.43
1:A:197:GLU:HB3	1:A:211:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ILE:HG22	9:C:285:HOH:O	2.18	0.43
2:S:193:LEU:HD22	2:S:197:VAL:HG11	2.01	0.42
1:A:215:GLU:OE1	9:A:316:HOH:O	2.21	0.42
1:A:95:ILE:HD12	1:A:136:ALA:HB1	2.02	0.42
1:A:80:THR:HG21	1:A:131:LYS:HD2	2.01	0.42
2:S:497:VAL:HG12	2:S:498:PRO:HD2	2.00	0.42
2:R:506:ARG:HA	2:R:511:ASP:O	2.19	0.42
2:S:223:GLY:HA2	2:S:231:PHE:CD1	2.54	0.42
2:R:351:TYR:HD1	2:R:351:TYR:HA	1.76	0.42
2:R:336:VAL:N	2:R:346:ASP:OD1	2.37	0.42
1:A:7:PRO:HD2	1:A:39:THR:O	2.20	0.42
1:A:29:LYS:HA	1:A:30:PRO:HA	1.87	0.42
1:C:69:GLY:HA3	1:C:106:LYS:HE2	2.00	0.42
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.55	0.42
2:S:341:TYR:HB3	9:S:619:HOH:O	2.19	0.42
1:B:203:ASP:OD2	2:R:459:LYS:HE3	2.19	0.42
1:B:184:HIS:HB2	1:B:220:GLY:C	2.40	0.41
2:Q:339:SER:HB2	2:Q:341:TYR:HD2	1.85	0.41
2:S:541:ASP:N	2:S:542:PRO:HD3	2.35	0.41
1:A:145:PRO:HD2	1:A:179:TYR:CZ	2.55	0.41
2:Q:92:LYS:HD3	2:Q:92:LYS:HA	1.81	0.41
2:S:304:LYS:HD3	2:S:304:LYS:HA	1.85	0.41
1:C:205:GLU:O	1:C:209:LYS:HG3	2.20	0.41
2:R:497:VAL:HG13	2:R:498:PRO:HD2	2.03	0.41
2:R:470:GLY:O	2:R:480:SER:HA	2.20	0.41
2:Q:278:LYS:HE2	2:Q:413:VAL:HG12	2.03	0.41
1:B:252:ASP:HA	9:B:274:HOH:O	2.19	0.41
2:Q:202:THR:O	2:Q:205:TYR:HB3	2.21	0.41
2:Q:397:GLN:HA	2:Q:398:PRO:HD3	1.91	0.41
2:Q:76:THR:O	2:Q:77:TYR:HB3	2.21	0.41
2:R:293:GLY:HA2	2:R:311:PHE:O	2.21	0.40
1:C:18:THR:HG22	1:C:18:THR:O	2.21	0.40
2:R:326:ASN:HD22	1:C:135:GLU:CD	2.24	0.40
2:R:101:MET:HA	9:R:641:HOH:O	2.20	0.40
2:R:326:ASN:HB2	1:C:135:GLU:CD	2.41	0.40
2:Q:188:HIS:N	1:C:264:GLY:HA2	2.36	0.40
2:R:541:ASP:N	2:R:542:PRO:HD3	2.36	0.40
2:R:362:LEU:O	2:R:363:ASP:HB2	2.21	0.40
1:A:61:HIS:O	1:A:65:GLU:HG3	2.21	0.40
2:S:296:ALA:HA	2:S:309:SER:HA	2.01	0.40
2:S:164:GLN:NE2	2:S:199:LEU:HD22	2.36	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%)	253 (97%)	6 (2%)	1 (0%)	39	69
1	B	260/264 (98%)	252 (97%)	7 (3%)	1 (0%)	39	69
1	C	258/264 (98%)	250 (97%)	7 (3%)	1 (0%)	39	69
2	Q	542/549 (99%)	522 (96%)	20 (4%)	0	100	100
2	R	543/549 (99%)	519 (96%)	23 (4%)	1 (0%)	52	80
2	S	542/549 (99%)	520 (96%)	22 (4%)	0	100	100
All	All	2405/2439 (99%)	2316 (96%)	85 (4%)	4 (0%)	52	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	LEU
1	C	231	LEU
1	A	231	LEU
2	R	6	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	205 (99%)	3 (1%)	74	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	208/210 (99%)	205 (99%)	3 (1%)	74	92
1	C	207/210 (99%)	204 (99%)	3 (1%)	74	92
2	Q	434/439 (99%)	427 (98%)	7 (2%)	70	91
2	R	434/439 (99%)	425 (98%)	9 (2%)	61	87
2	S	434/439 (99%)	426 (98%)	8 (2%)	66	89
All	All	1925/1947 (99%)	1892 (98%)	33 (2%)	68	90

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	67	LYS
1	A	88	MET
2	Q	36	ASN
2	Q	94	SER
2	Q	339	SER
2	Q	401	LYS
2	Q	453	ASP
2	Q	454	ASN
2	Q	473	ASP
1	B	4	LYS
1	B	67	LYS
1	B	100	LYS
2	R	241	GLN
2	R	361	LYS
2	R	397	GLN
2	R	412	SER
2	R	453	ASP
2	R	454	ASN
2	R	465	GLU
2	R	473	ASP
2	R	503	LEU
1	C	88	MET
1	C	135	GLU
1	C	229	LYS
2	S	361	LYS
2	S	365	LYS
2	S	397	GLN
2	S	454	ASN
2	S	473	ASP

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Mol	Chain	Res	Type
2	S	503	LEU
2	S	517	GLU
2	S	546	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	172	ASN
1	A	234	GLN
2	Q	123	HIS
2	Q	210	HIS
2	Q	454	ASN
1	B	14	ASN
2	R	326	ASN
2	R	454	ASN
1	C	14	ASN
2	S	104	ASN
2	S	164	GLN
2	S	454	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 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	$\# Z  > 2$
3	SF4	A	265	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	A	266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	A	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	GOL	A	271	-	5,5,5	0.31	0	5,5,5	0.52	0
3	SF4	B	265	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	B	266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	B	267	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	C	265	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	C	266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	C	267	1	0,12,12	0.00	-	0,24,24	0.00	-
6	FCO	Q	550	2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	Q	561	-	5,5,5	0.36	0	5,5,5	1.07	0
5	GOL	Q	562	-	5,5,5	0.40	0	5,5,5	0.82	0
6	FCO	R	550	2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	R	561	-	5,5,5	0.47	0	5,5,5	0.28	0
5	GOL	R	562	-	5,5,5	0.48	0	5,5,5	0.53	0
5	GOL	R	563	-	5,5,5	0.33	0	5,5,5	0.36	0
6	FCO	S	550	2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	S	561	-	5,5,5	0.54	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	265	1	-	0/0/48/48	0/6/5/5
4	F3S	A	266	1	-	0/0/24/24	0/0/3/3
3	SF4	A	267	1	-	0/0/48/48	0/6/5/5
5	GOL	A	271	-	-	0/4/4/4	0/0/0/0
3	SF4	B	265	1	-	0/0/48/48	0/6/5/5
4	F3S	B	266	1	-	0/0/24/24	0/0/3/3
3	SF4	B	267	1	-	0/0/48/48	0/6/5/5
3	SF4	C	265	1	-	0/0/48/48	0/6/5/5
4	F3S	C	266	1	-	0/0/24/24	0/0/3/3
3	SF4	C	267	1	-	0/0/48/48	0/6/5/5
6	FCO	Q	550	2	-	0/0/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	Q	561	-	-	0/4/4/4	0/0/0/0
5	GOL	Q	562	-	-	0/4/4/4	0/0/0/0
6	FCO	R	550	2	-	0/0/6/6	0/0/0/0
5	GOL	R	561	-	-	0/4/4/4	0/0/0/0
5	GOL	R	562	-	-	0/4/4/4	0/0/0/0
5	GOL	R	563	-	-	0/4/4/4	0/0/0/0
6	FCO	S	550	2	-	0/0/6/6	0/0/0/0
5	GOL	S	561	-	-	0/4/4/4	0/0/0/0

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	550	FCO	1	0
5	Q	562	GOL	2	0
5	R	561	GOL	2	0
5	S	561	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%)	-0.20	3 (1%) 82 83	34, 36, 38, 46	8 (3%)
1	B	262/264 (99%)	0.66	24 (9%) 11 9	34, 36, 38, 41	10 (3%)
1	C	260/264 (98%)	-0.15	3 (1%) 81 81	32, 36, 38, 42	6 (2%)
2	Q	544/549 (99%)	-0.22	2 (0%) 93 94	33, 36, 39, 42	15 (2%)
2	R	545/549 (99%)	0.23	21 (3%) 43 43	31, 36, 38, 41	15 (2%)
2	S	544/549 (99%)	0.16	13 (2%) 62 62	32, 36, 38, 43	14 (2%)
All	All	2417/2439 (99%)	0.07	66 (2%) 58 58	31, 36, 38, 46	68 (2%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	415	ALA	5.9
1	B	4	LYS	5.6
1	B	142	ILE	5.2
2	S	344	GLY	4.4
2	R	416	THR	3.9
2	R	451	ALA	3.5
2	R	447	ALA	3.5
1	B	61	HIS	3.4
1	B	191	PRO	3.3
2	S	378	GLY	3.2
1	B	60	LEU	3.1
1	B	3	ALA	3.1
2	S	406	MET	3.1
1	B	101	ALA	3.0
2	R	396	GLY	3.0
2	R	242	GLY	3.0
2	S	157	ALA	3.0
2	R	6	PRO	3.0
2	R	405	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	183	VAL	3.0
2	S	413	VAL	3.0
1	B	264	GLY	2.8
2	R	245	LYS	2.8
1	B	163	THR	2.8
1	B	152	ILE	2.8
2	R	509	GLN	2.7
1	B	68	ASP	2.7
2	R	249	ALA	2.7
2	R	322	GLY	2.6
2	R	297	THR	2.6
1	A	201	SER	2.6
2	S	465	GLU	2.6
2	S	189	LYS	2.5
2	S	286	THR	2.5
2	R	146	ALA	2.5
1	B	230	VAL	2.5
1	B	18	THR	2.5
2	R	236	GLY	2.5
2	R	144	LEU	2.4
2	S	300	SER	2.4
1	B	165	GLY	2.4
1	B	67	LYS	2.4
1	A	211	PHE	2.3
2	R	246	ASP	2.3
1	B	220	GLY	2.3
2	R	448	ASP	2.2
1	B	166	ILE	2.2
1	C	104	LYS	2.2
1	B	151	PRO	2.2
1	A	67	LYS	2.2
1	C	164	LYS	2.2
1	C	68	ASP	2.2
1	B	28	ILE	2.1
2	S	417	ALA	2.1
1	B	124	LYS	2.1
2	R	171	VAL	2.1
2	Q	6	PRO	2.1
2	R	387	ALA	2.1
1	B	231	LEU	2.1
2	Q	278	LYS	2.1
1	B	130	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	R	455	THR	2.0
2	S	30	ILE	2.0
1	B	209	LYS	2.0
2	R	323	LYS	2.0
2	S	338	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	271	6/6	0.90	0.29	7.49	34,34,35,36	0
5	GOL	R	562	6/6	0.92	0.29	4.63	44,45,46,46	0
5	GOL	R	561	6/6	0.75	0.40	4.55	46,49,49,50	0
5	GOL	S	561	6/6	0.83	0.31	3.13	45,48,49,50	0
5	GOL	R	563	6/6	0.87	0.35	1.96	45,47,49,50	0
6	FCO	S	550	7/7	0.97	0.18	1.36	35,37,40,40	0
5	GOL	Q	562	6/6	0.93	0.17	0.15	35,36,37,39	0
5	GOL	Q	561	6/6	0.94	0.16	-0.19	32,34,35,38	0
6	FCO	R	550	7/7	0.98	0.14	-0.36	36,36,40,41	0
6	FCO	Q	550	7/7	0.99	0.12	-0.48	34,35,37,37	0
4	F3S	B	266	7/7	0.96	0.12	-1.27	36,38,39,42	0
8	MG	Q	553	1/1	0.97	0.12	-1.60	35,35,35,35	0
3	SF4	B	265	8/8	0.96	0.10	-1.85	30,32,33,34	0
7	NI	Q	551	1/1	0.93	0.07	-1.91	39,39,39,39	0
3	SF4	C	267	8/8	0.98	0.05	-2.16	36,37,37,38	0
3	SF4	B	267	8/8	0.95	0.06	-2.19	35,35,36,37	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SF4	A	267	8/8	0.97	0.08	-2.38	36,37,39,39	0
8	MG	R	553	1/1	0.97	0.09	-2.68	34,34,34,34	0
4	F3S	C	266	7/7	0.98	0.05	-2.78	35,36,37,40	0
4	F3S	A	266	7/7	0.99	0.05	-2.96	32,34,34,35	0
7	NI	S	551	1/1	0.98	0.03	-3.13	39,39,39,39	0
3	SF4	C	265	8/8	0.99	0.06	-3.30	33,34,35,36	0
8	MG	S	553	1/1	0.95	0.07	-3.39	33,33,33,33	0
7	NI	R	551	1/1	0.97	0.05	-3.58	41,41,41,41	0
3	SF4	A	265	8/8	0.98	0.05	-4.98	29,32,34,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.