



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:31 pm BST

PDB ID : 3CUR  
Title : Structure of a double methionine mutant of NI-FE hydrogenase  
Authors : Volbeda, A.  
Deposited on : 2008-04-17  
Resolution : 2.40 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

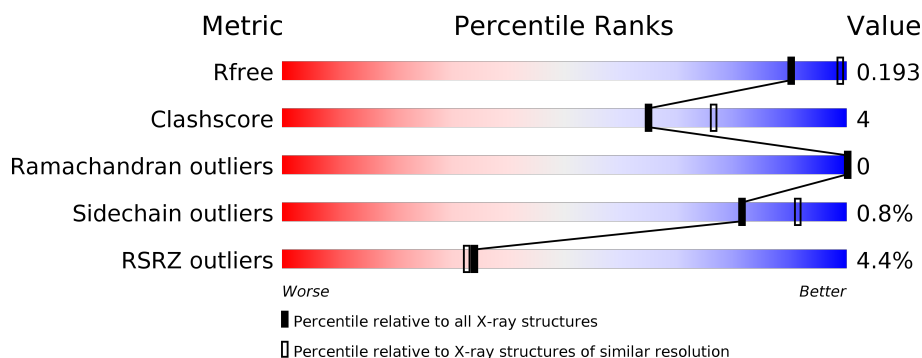
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>2%</div> <div>92%</div> <div>7%</div> </div>
1	B	264	<div> <div>11%</div> <div>88%</div> <div>11%</div> </div>
1	C	264	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
2	H	549	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
2	I	549	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
2	J	549	<div> <div>6%</div> <div>89%</div> <div>11%</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
8	PER	H	552	-	-	X	-
9	GOL	I	564	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19483 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	1	0
			1978	1259	332	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	3	0
			1972	1255	330	372	15			

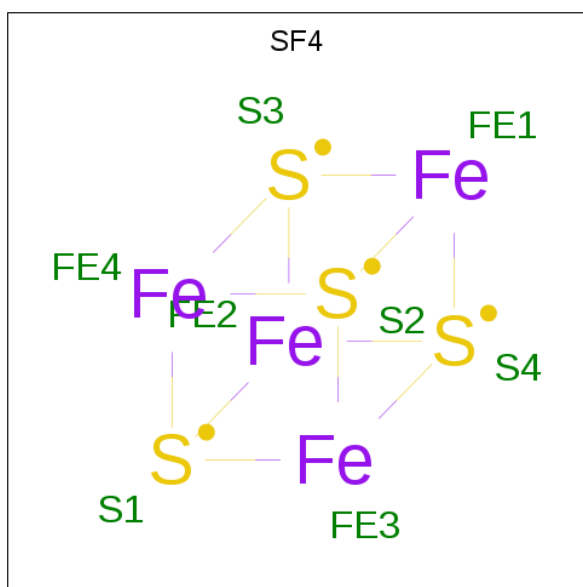
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	545	Total	C	N	O	S	0	9	0
			4199	2674	727	772	26			
2	I	545	Total	C	N	O	S	0	3	0
			4181	2660	726	770	25			
2	J	545	Total	C	N	O	S	0	3	0
			4179	2659	725	769	26			

There are 6 discrepancies between the modelled and reference sequences:

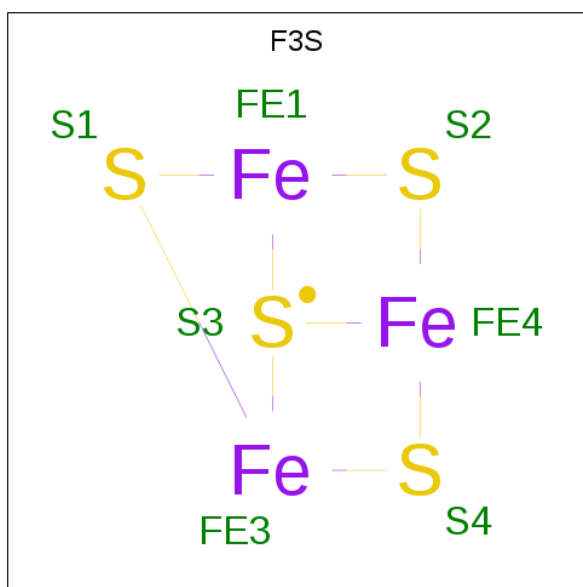
Chain	Residue	Modelled	Actual	Comment	Reference
H	74	MET	VAL	ENGINEERED MUTATION	UNP P18188
H	122	MET	LEU	ENGINEERED MUTATION	UNP P18188
I	74	MET	VAL	ENGINEERED MUTATION	UNP P18188
I	122	MET	LEU	ENGINEERED MUTATION	UNP P18188
J	74	MET	VAL	ENGINEERED MUTATION	UNP P18188
J	122	MET	LEU	ENGINEERED MUTATION	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		

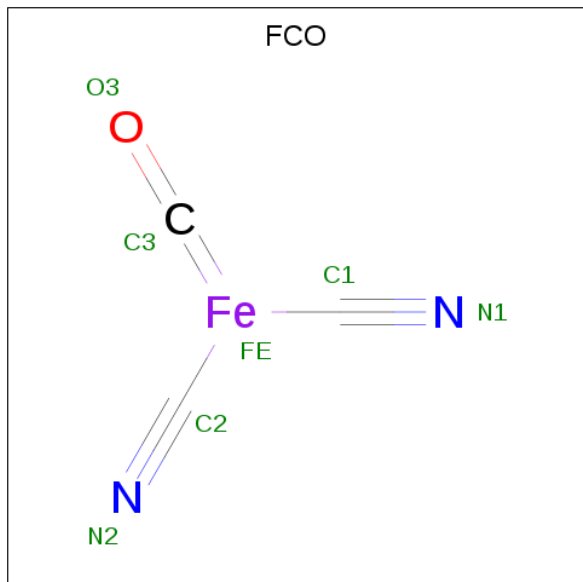
- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ni	0	0
			1	1		
5	J	1	Total	Ni	0	0
			1	1		
5	I	1	Total	Ni	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

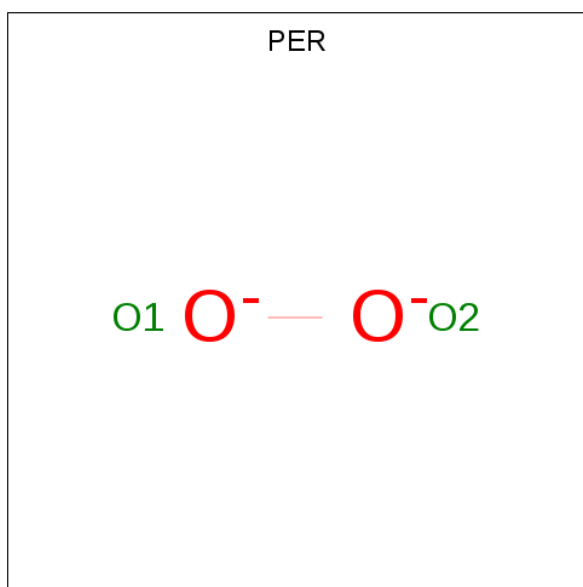
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula:  $\text{C}_3\text{FeN}_2\text{O}$ ).



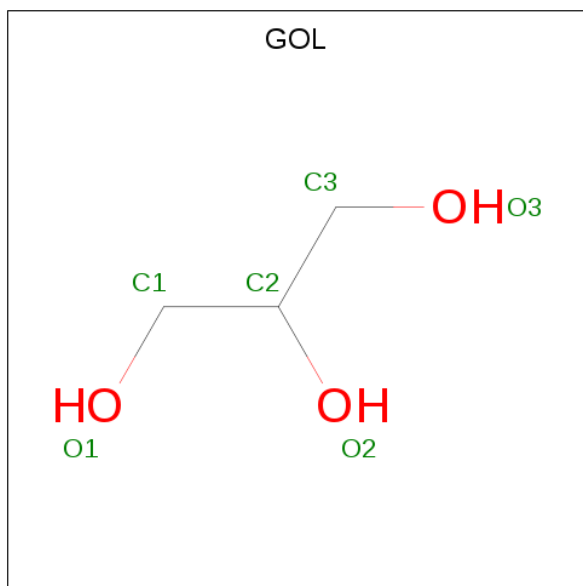
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	H	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	I	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 8 is PEROXIDE ION (three-letter code: PER) (formula:  $\text{O}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total O 2 2	0	0
8	I	1	Total O 2 2	0	0
8	J	1	Total O 2 2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total C O 6 3 3	0	0
9	H	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	0

- Molecule 10 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	121	Total 121	O 121	0	0
10	H	215	Total 215	O 215	0	0
10	B	81	Total 81	O 81	0	0
10	I	177	Total 177	O 177	0	0
10	C	100	Total 100	O 100	0	0
10	J	156	Total 156	O 156	0	0

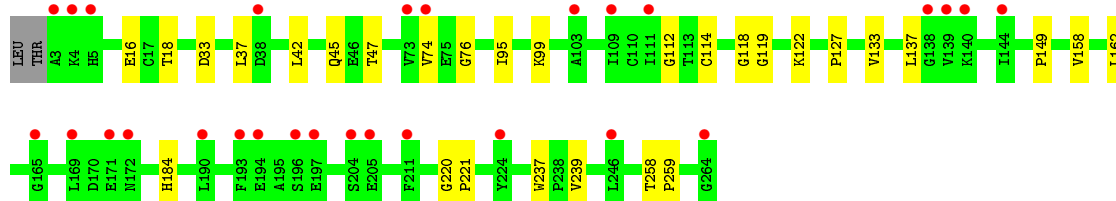
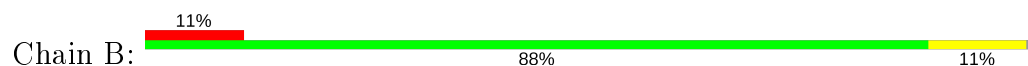
### 3 Residue-property plots [i](#)

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.

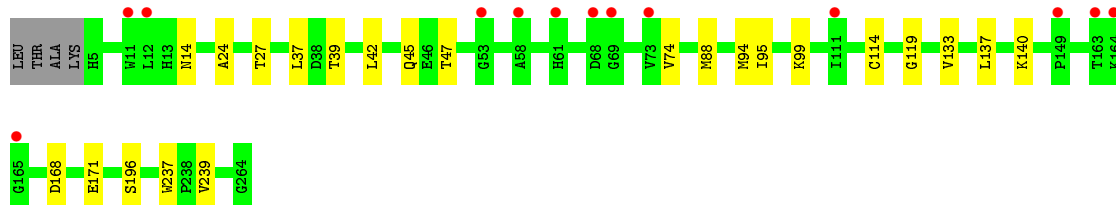
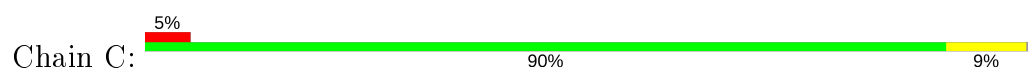
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



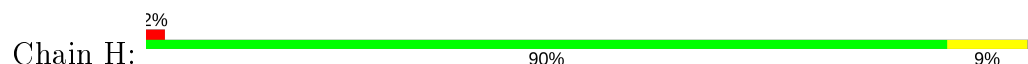
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

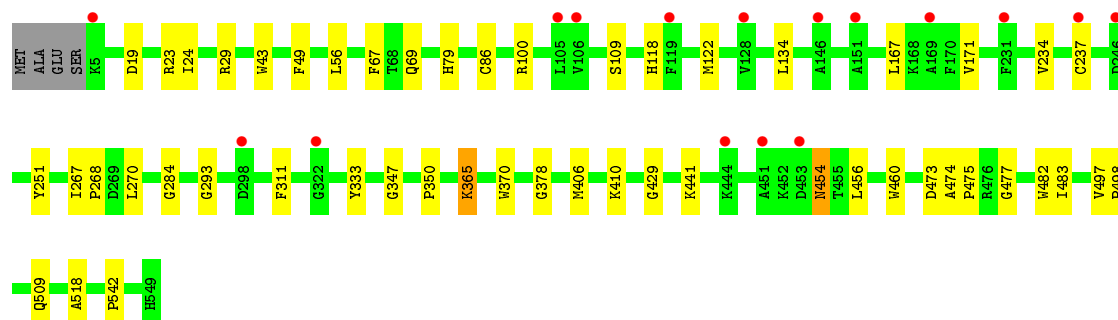
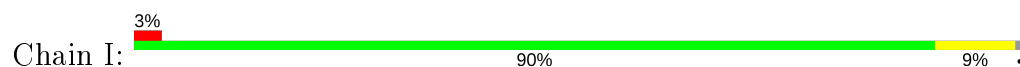


- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

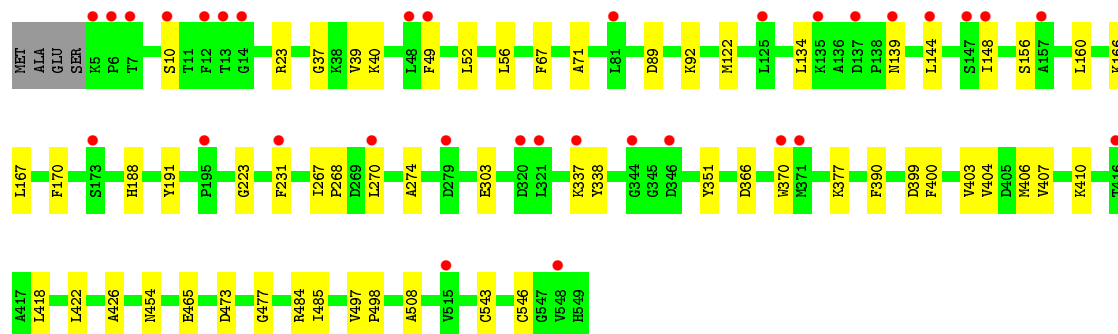




• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit



• 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, $\alpha$ , $\beta$ , $\gamma$	64.60 Å 99.90 Å 183.00 Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	24.99 – 2.40 24.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (24.99-2.40) 95.4 (24.99-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.42 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.150 , 0.194 0.151 , 0.193	Depositor DCC
$R_{free}$ test set	4350 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, MG, NI, SF4, PER, 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	0.57	0/2038	0.60	0/2774
1	B	0.50	0/2043	0.55	0/2781
1	C	0.49	0/2042	0.55	0/2780
2	H	0.55	0/4346	0.61	0/5894
2	I	0.50	0/4300	0.59	0/5834
2	J	0.49	1/4298 (0.0%)	0.57	0/5831
All	All	0.52	1/19067 (0.0%)	0.58	0/25894

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	139	ASN	C-N	6.13	1.48	1.34

There are no bond angle outliers.

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	1978	0	1914	13	0
1	B	1980	0	1918	17	0
1	C	1972	0	1905	14	0
2	H	4199	0	4179	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	4181	0	4147	40	0
2	J	4179	0	4142	37	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	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	H	7	0	0	0	0
7	I	7	0	0	0	0
7	J	7	0	0	0	0
8	H	2	0	0	2	0
8	I	2	0	0	0	0
8	J	2	0	0	1	0
9	H	12	0	16	0	0
9	I	18	0	24	6	0
9	J	12	0	16	0	0
10	A	121	0	0	2	0
10	B	81	0	0	0	0
10	C	100	0	0	2	0
10	H	215	0	0	5	0
10	I	177	0	0	1	0
10	J	156	0	0	1	0
All	All	19483	0	18261	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (151) 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:A:61[B]:HIS:NE2	1:A:65:GLU:OE2	1.65	1.26
1:A:61[B]:HIS:CD2	1:A:65:GLU:OE2	1.99	1.15
2:I:118:HIS:HA	2:I:122[B]:MET:CG	2.06	0.85
1:C:140:LYS:HE3	10:C:311:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:118:HIS:HA	2:I:122[B]:MET:HG3	1.61	0.80
2:H:497:VAL:CG1	2:H:498:PRO:HD2	2.18	0.74
1:C:37:LEU:HD23	2:J:170:PHE:CD1	2.21	0.74
1:A:61[B]:HIS:CE1	1:A:65:GLU:OE2	2.41	0.73
1:B:99:LYS:HG3	1:B:137:LEU:HD22	1.73	0.70
2:I:460:TRP:HE1	9:I:564:GOL:H31	1.57	0.68
2:H:497:VAL:HG12	2:H:498:PRO:HD2	1.76	0.67
2:I:497:VAL:CG1	2:I:498:PRO:HD2	2.26	0.66
2:I:460:TRP:NE1	9:I:564:GOL:H31	2.11	0.65
2:H:543[B]:CYS:SG	8:H:552:PER:O1	2.45	0.65
2:I:118:HIS:HA	2:I:122[B]:MET:HG2	1.78	0.64
2:J:39:VAL:O	2:J:40:LYS:HE2	1.98	0.63
2:H:117:VAL:HG12	2:H:122[A]:MET:CE	2.28	0.62
2:I:118:HIS:CD2	2:I:122[B]:MET:HG3	2.35	0.62
2:J:497:VAL:CG1	2:J:498:PRO:HD2	2.29	0.62
2:I:454:ASN:H	2:I:454:ASN:HD22	1.47	0.62
2:H:23:ARG:O	2:H:122[A]:MET:HG2	2.00	0.61
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.84	0.59
2:J:274:ALA:HA	2:J:422:LEU:HD11	1.84	0.59
2:I:234:VAL:HB	9:I:564:GOL:H31	1.85	0.57
2:I:497:VAL:HG12	2:I:498:PRO:HD2	1.86	0.56
2:H:543[B]:CYS:HB3	2:H:546:CYS:HB2	1.89	0.55
2:H:237:CYS:HB2	2:H:456:LEU:HG	1.88	0.55
2:H:267:ILE:HB	2:H:268:PRO:HD3	1.88	0.55
2:H:385:PRO:HB2	10:H:600:HOH:O	2.07	0.55
2:I:267:ILE:HB	2:I:268:PRO:HD3	1.90	0.54
2:H:440:GLU:HG3	10:H:752:HOH:O	2.07	0.54
2:H:497:VAL:HG13	2:H:498:PRO:HD2	1.89	0.54
1:C:42:LEU:HD21	1:C:45:GLN:HG3	1.91	0.53
2:H:117:VAL:HG12	2:H:122[A]:MET:HE3	1.90	0.53
2:J:89:ASP:O	2:J:92:LYS:HD3	2.09	0.53
2:J:543[B]:CYS:HB3	2:J:546:CYS:HB2	1.90	0.52
2:I:134:LEU:HD21	2:I:167:LEU:HG	1.91	0.52
2:I:333:TYR:CD1	2:I:347:GLY:HA2	2.45	0.52
2:I:406:MET:O	2:I:410:LYS:HG2	2.10	0.52
2:I:460:TRP:HE1	9:I:564:GOL:C3	2.23	0.52
2:J:377:LYS:HA	10:J:645:HOH:O	2.11	0.50
2:H:252:LEU:HG	2:H:256:LYS:HD2	1.94	0.50
1:B:158:VAL:O	1:B:162:LEU:HG	2.12	0.50
2:I:284:GLY:HA2	2:I:518:ALA:O	2.12	0.50
1:C:74:VAL:HG11	1:C:133:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:THR:O	2:J:23:ARG:HA	2.13	0.49
2:J:270:LEU:HD21	2:J:426:ALA:HA	1.94	0.49
2:J:497:VAL:HG12	2:J:498:PRO:HD2	1.94	0.49
2:J:465:GLU:HA	2:J:485:ILE:O	2.12	0.49
2:J:223:GLY:HA2	2:J:231:PHE:CD1	2.48	0.48
1:B:33:ASP:O	1:B:37:LEU:HG	2.12	0.48
2:I:24:ILE:HG22	2:I:542:PRO:HD2	1.95	0.48
2:J:497:VAL:HG13	2:J:498:PRO:HD2	1.94	0.48
2:I:100:ARG:HD2	9:I:563:GOL:O3	2.13	0.48
1:C:237:TRP:CZ2	1:C:239:VAL:HB	2.48	0.48
2:J:477:GLY:O	2:J:498:PRO:HG3	2.14	0.48
2:J:543[B]:CYS:SG	8:J:552:PER:O1	2.64	0.48
1:A:112:GLY:HA2	1:A:149:PRO:HD3	1.95	0.47
2:I:454:ASN:N	2:I:454:ASN:HD22	2.12	0.47
2:I:86:CYS:SG	2:I:483:ILE:HG22	2.55	0.47
1:B:118:GLY:HA3	1:B:122:LYS:HD2	1.96	0.47
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.96	0.47
2:H:350:PRO:HB2	2:H:482:TRP:CG	2.50	0.47
2:H:374:PRO:HD3	2:H:500:THR:HG22	1.96	0.47
2:I:497:VAL:HG13	2:I:498:PRO:HD2	1.95	0.47
2:J:400:PHE:O	2:J:404:VAL:HG23	2.15	0.47
2:H:543[B]:CYS:SG	8:H:552:PER:O2	1.95	0.47
2:I:237:CYS:HB2	2:I:456:LEU:HG	1.97	0.47
2:I:49:PHE:HB2	2:I:370:TRP:CD2	2.51	0.46
1:A:70:TYR:OH	1:A:101:ALA:O	2.21	0.46
2:J:337:LYS:HD2	2:J:508:ALA:HA	1.97	0.46
1:C:114:CYS:HA	1:C:119:GLY:HA3	1.97	0.46
2:H:353:GLY:HA3	2:H:494:GLN:HG3	1.97	0.46
2:H:56:LEU:HD21	2:H:67:PHE:HB2	1.98	0.46
2:I:109:SER:HG	2:I:251:TYR:HH	1.63	0.46
2:J:144:LEU:O	2:J:148:ILE:HG12	2.16	0.46
2:I:333:TYR:OH	2:I:378:GLY:HA2	2.15	0.46
2:J:497:VAL:HG11	2:J:546:CYS:HB3	1.98	0.46
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.51	0.45
2:J:351:TYR:O	2:J:484:ARG:NE	2.46	0.45
1:B:220:GLY:N	1:B:221:PRO:CD	2.80	0.45
2:H:477:GLY:O	2:H:498:PRO:HG3	2.16	0.45
2:H:464:GLU:OE2	2:H:487:GLY:HA2	2.16	0.45
2:H:144:LEU:O	2:H:148:ILE:HG12	2.16	0.45
2:H:89:ASP:O	2:H:92[B]:LYS:HD2	2.17	0.45
1:A:61[A]:HIS:HE1	10:A:355:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:267:ILE:HB	2:J:268:PRO:HD3	1.99	0.45
2:J:303:GLU:CD	2:J:303:GLU:H	2.20	0.44
1:A:57:GLU:CG	10:A:355:HOH:O	2.65	0.44
2:J:49:PHE:HB2	2:J:370:TRP:CD2	2.52	0.44
2:I:293:GLY:HA2	2:I:311:PHE:O	2.18	0.44
2:I:19:ASP:HB2	2:I:29:ARG:HG3	1.99	0.44
2:I:477:GLY:O	2:I:498:PRO:HG3	2.18	0.44
2:H:49:PHE:HB2	2:H:370:TRP:CD2	2.53	0.44
1:C:37:LEU:HD13	2:J:166:LYS:HD3	2.00	0.44
1:A:233:ASN:O	2:H:217[B]:SER:OG	2.34	0.44
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.52	0.44
1:B:18:THR:HG22	1:B:18:THR:O	2.18	0.44
2:J:406:MET:O	2:J:410:LYS:HG2	2.18	0.44
2:I:350:PRO:HB2	2:I:482:TRP:CD2	2.53	0.43
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.54	0.43
2:H:543[A]:CYS:HB3	2:H:546:CYS:HB2	2.00	0.43
1:C:95:ILE:O	1:C:99:LYS:HB2	2.19	0.43
2:H:397:GLN:HA	2:H:398:PRO:HD3	1.85	0.43
2:J:23:ARG:C	2:J:122[B]:MET:HE3	2.39	0.43
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.53	0.43
2:H:117:VAL:HG12	2:H:122[A]:MET:HE1	1.98	0.43
1:B:74:VAL:HG11	1:B:133:VAL:HG21	2.01	0.43
2:I:56:LEU:HD21	2:I:67:PHE:HB2	2.01	0.43
1:B:95:ILE:O	1:B:99:LYS:HB2	2.19	0.43
2:H:274:ALA:HA	2:H:422:LEU:HD11	2.00	0.43
2:H:168:LYS:HE3	10:H:778:HOH:O	2.19	0.42
2:J:134:LEU:CD2	2:J:167:LEU:HD23	2.49	0.42
1:B:184:HIS:HB2	1:B:220:GLY:C	2.40	0.42
2:J:156:SER:O	2:J:160:LEU:HG	2.19	0.42
1:C:99:LYS:HG3	1:C:137:LEU:HD22	2.00	0.42
1:C:14:ASN:ND2	1:C:94:MET:HB3	2.34	0.42
2:H:178:ILE:HG23	10:H:686:HOH:O	2.19	0.42
2:I:474:ALA:HB1	2:I:475:PRO:HD2	2.00	0.42
2:I:350:PRO:HB2	2:I:482:TRP:CG	2.54	0.42
2:H:338:TYR:HA	2:H:366:ASP:O	2.20	0.42
2:J:399:ASP:O	2:J:403:VAL:HG23	2.20	0.42
1:A:114:CYS:HA	1:A:119:GLY:HA3	2.02	0.42
1:A:118:GLY:HA3	1:A:122:LYS:HD2	2.02	0.41
2:H:204:HIS:CE1	10:H:646:HOH:O	2.73	0.41
2:H:69:GLN:HA	2:H:79:HIS:HB2	2.02	0.41
2:I:43:TRP:CE2	2:I:365:LYS:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:441:LYS:HE3	10:I:671:HOH:O	2.20	0.41
2:J:338:TYR:HA	2:J:366:ASP:O	2.20	0.41
1:A:18:THR:HG22	1:A:18:THR:O	2.19	0.41
2:H:167[B]:LEU:HD11	2:H:202:THR:HG21	2.02	0.41
2:I:134:LEU:HD11	2:I:171:VAL:HG21	2.02	0.41
2:I:270:LEU:CD2	2:I:429:GLY:HA3	2.51	0.41
2:H:29:ARG:NE	2:H:363:ASP:OD1	2.48	0.41
2:J:56:LEU:HD21	2:J:67:PHE:HB2	2.03	0.41
2:I:69:GLN:HA	2:I:79:HIS:HB2	2.02	0.41
2:J:10:SER:O	2:J:37:GLY:HA3	2.20	0.41
2:J:52:LEU:HD11	2:J:71:ALA:HA	2.03	0.41
1:B:16:GLU:HB3	1:B:76:GLY:CA	2.51	0.41
1:B:114:CYS:HA	1:B:119:GLY:HA3	2.03	0.41
1:C:171:GLU:HG2	10:C:332:HOH:O	2.21	0.41
2:J:188:HIS:HB3	2:J:191:TYR:HD1	1.86	0.41
2:J:403:VAL:O	2:J:407:VAL:HG23	2.21	0.41
1:C:24:ALA:O	1:C:27:THR:HG22	2.21	0.40
1:B:258:THR:HA	1:B:259:PRO:C	2.42	0.40
2:J:134:LEU:HD21	2:J:167:LEU:HD23	2.03	0.40
2:J:390:PHE:CZ	2:J:418:LEU:HB2	2.56	0.40
1:B:47:THR:O	2:I:23:ARG:HA	2.21	0.40
1:B:112:GLY:HA2	1:B:149:PRO:HD3	2.03	0.40
2:I:109:SER:OG	2:I:251:TYR:OH	2.33	0.40
2:I:234:VAL:HB	9:I:564:GOL:C3	2.48	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	261/264 (99%)	252 (97%)	9 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
1	C	261/264 (99%)	255 (98%)	6 (2%)	0	100	100
2	H	552/549 (100%)	539 (98%)	13 (2%)	0	100	100
2	I	546/549 (100%)	528 (97%)	18 (3%)	0	100	100
2	J	546/549 (100%)	529 (97%)	17 (3%)	0	100	100
All	All	2428/2439 (100%)	2358 (97%)	70 (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	209/210 (100%)	208 (100%)	1 (0%)	88	95
1	B	210/210 (100%)	209 (100%)	1 (0%)	88	95
1	C	210/210 (100%)	206 (98%)	4 (2%)	57	75
2	H	444/439 (101%)	440 (99%)	4 (1%)	78	90
2	I	438/439 (100%)	433 (99%)	5 (1%)	73	87
2	J	438/439 (100%)	436 (100%)	2 (0%)	88	95
All	All	1949/1947 (100%)	1932 (99%)	17 (1%)	81	90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	MET
2	H	454	ASN
2	H	473	ASP
2	H	509[A]	GLN
2	H	509[B]	GLN
1	B	127	PRO
2	I	365	LYS
2	I	454	ASN

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Mol	Chain	Res	Type
2	I	473	ASP
2	I	509[A]	GLN
2	I	509[B]	GLN
1	C	39	THR
1	C	88	MET
1	C	168	ASP
1	C	196	SER
2	J	454	ASN
2	J	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
2	H	454	ASN
1	B	14	ASN
2	I	454	ASN
1	C	14	ASN
2	J	123	HIS
2	J	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 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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	$\# Z  > 2$
9	GOL	H	561	-	5,5,5	0.53	0	5,5,5	0.26	0
9	GOL	J	565	-	5,5,5	0.50	0	5,5,5	0.35	0
4	F3S	C	266	1	0,9,9	0.00	-	-		
3	SF4	A	267	1	0,12,12	0.00	-	-		
7	FCO	I	550	8,2	0,6,6	0.00	-	-		
4	F3S	A	266	1	0,9,9	0.00	-	-		
3	SF4	A	265	1	0,12,12	0.00	-	-		
3	SF4	B	265	1	0,12,12	0.00	-	-		
9	GOL	J	564	-	5,5,5	0.41	0	5,5,5	0.31	0
9	GOL	H	562	-	5,5,5	0.42	0	5,5,5	0.24	0
3	SF4	B	267	1	0,12,12	0.00	-	-		
9	GOL	I	561	-	5,5,5	0.35	0	5,5,5	0.38	0
8	PER	J	552	5,7	0,1,1	0.00	-	-		
8	PER	H	552	5,7	0,1,1	0.00	-	-		
3	SF4	C	265	1	0,12,12	0.00	-	-		
7	FCO	H	550	8,2	0,6,6	0.00	-	-		
7	FCO	J	550	8,2	0,6,6	0.00	-	-		
9	GOL	I	564	-	5,5,5	0.29	0	5,5,5	0.31	0
3	SF4	C	267	1	0,12,12	0.00	-	-		
8	PER	I	552	5,7	0,1,1	0.00	-	-		
9	GOL	I	563	-	5,5,5	0.32	0	5,5,5	0.61	0
4	F3S	B	266	1	0,9,9	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
9	GOL	H	562	-	-	0/4/4/4	-
3	SF4	B	267	1	-	-	0/6/5/5
3	SF4	A	267	1	-	-	0/6/5/5
9	GOL	I	564	-	-	2/4/4/4	-
3	SF4	C	267	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
9	GOL	H	561	-	-	0/4/4/4	-
9	GOL	J	565	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	I	561	-	-	0/4/4/4	-
4	F3S	C	266	1	-	-	0/3/3/3
3	SF4	B	265	1	-	-	0/6/5/5
3	SF4	C	265	1	-	-	0/6/5/5
9	GOL	J	564	-	-	2/4/4/4	-
9	GOL	I	563	-	-	2/4/4/4	-
4	F3S	B	266	1	-	-	0/3/3/3
3	SF4	A	265	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	565	GOL	O1-C1-C2-C3
9	I	564	GOL	C1-C2-C3-O3
9	I	563	GOL	O1-C1-C2-C3
9	J	565	GOL	O1-C1-C2-O2
9	I	564	GOL	O2-C2-C3-O3
9	J	564	GOL	O1-C1-C2-C3
9	J	564	GOL	O1-C1-C2-O2
9	I	563	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	552	PER	1	0
8	H	552	PER	2	0
9	I	564	GOL	5	0
9	I	563	GOL	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	-0.04	6 (2%) 60 58	36, 41, 47, 57	9 (3%)
1	B	262/264 (99%)	0.53	28 (10%) 6 5	37, 41, 46, 58	6 (2%)
1	C	260/264 (98%)	0.34	13 (5%) 28 27	38, 41, 48, 58	7 (2%)
2	H	545/549 (99%)	0.01	11 (2%) 65 63	35, 41, 46, 56	7 (1%)
2	I	545/549 (99%)	0.15	16 (2%) 51 50	36, 41, 46, 59	7 (1%)
2	J	545/549 (99%)	0.34	33 (6%) 21 20	37, 41, 46, 50	11 (2%)
All	All	2419/2439 (99%)	0.20	107 (4%) 34 33	35, 41, 46, 59	47 (1%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	10.0
1	B	111	ILE	5.6
1	B	165	GLY	4.8
1	B	5	HIS	4.5
2	J	14	GLY	4.3
1	B	3	ALA	4.1
1	B	190	LEU	4.0
2	J	320	ASP	3.8
1	B	140	LYS	3.8
2	J	5	LYS	3.8
2	J	148	ILE	3.7
1	B	224	TYR	3.7
2	J	147	SER	3.7
2	J	6	PRO	3.7
1	B	109	ILE	3.6
1	B	144	ILE	3.6
2	J	144	LEU	3.4
1	A	163	THR	3.4
1	C	61[A]	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	163	THR	3.4
1	C	165	GLY	3.4
2	J	173	SER	3.3
2	J	7	THR	3.3
1	C	69	GLY	3.3
2	H	6	PRO	3.3
2	H	548	VAL	3.2
1	B	138	GLY	3.1
1	C	111	ILE	3.1
2	J	548	VAL	3.1
2	J	137	ASP	3.0
2	I	231	PHE	3.0
1	B	74	VAL	3.0
1	B	139	VAL	3.0
1	B	196	SER	2.9
1	C	164	LYS	2.9
2	J	344	GLY	2.9
1	A	4	LYS	2.9
2	H	412	SER	2.9
1	B	171	GLU	2.9
2	J	515	VAL	2.8
2	J	135	LYS	2.8
2	I	298	ASP	2.8
1	B	193	PHE	2.8
1	C	58	ALA	2.8
2	H	370	TRP	2.8
2	J	416	THR	2.8
1	B	38	ASP	2.7
1	B	204	SER	2.7
1	B	169	LEU	2.6
1	C	68	ASP	2.6
1	B	246	LEU	2.6
1	B	73	VAL	2.6
2	I	5	LYS	2.6
2	I	246	ASP	2.6
2	H	383	VAL	2.6
2	I	151	ALA	2.5
1	A	144	ILE	2.5
1	B	103	ALA	2.5
1	C	11	TRP	2.4
2	J	195	PRO	2.4
1	B	4	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	427	ALA	2.4
1	A	5	HIS	2.4
2	I	451	ALA	2.4
1	B	194	GLU	2.4
2	J	321	LEU	2.4
1	C	73	VAL	2.3
2	I	444	LYS	2.3
1	C	53	GLY	2.3
2	J	279	ASP	2.3
1	B	172	ASN	2.3
2	J	370	TRP	2.3
2	J	49	PHE	2.3
2	J	48	LEU	2.3
2	J	13	THR	2.3
2	J	10	SER	2.3
2	J	12	PHE	2.2
2	J	337	LYS	2.2
2	I	322	GLY	2.2
2	J	371	MET	2.2
2	I	119	PHE	2.2
2	I	105	LEU	2.2
2	J	270	LEU	2.2
2	H	153	PRO	2.2
2	J	346	ASP	2.2
1	C	149	PRO	2.2
1	B	205	GLU	2.2
2	I	146	ALA	2.2
1	B	264	GLY	2.2
2	I	106	VAL	2.1
1	A	191	PRO	2.1
2	I	128	VAL	2.1
2	H	35	GLU	2.1
2	J	231	PHE	2.1
2	J	139	ASN	2.1
2	H	344	GLY	2.1
2	I	169	ALA	2.1
2	H	270	LEU	2.1
1	B	197	GLU	2.1
2	I	453	ASP	2.1
1	B	211	PHE	2.1
2	I	237	CYS	2.1
2	H	48	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	125	LEU	2.0
2	J	157	ALA	2.0
1	C	12	LEU	2.0
2	J	81	LEU	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. 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
9	GOL	I	564	6/6	0.82	0.21	38,40,46,56	0
6	MG	I	553	1/1	0.90	0.13	38,38,38,38	0
9	GOL	I	563	6/6	0.90	0.20	41,44,49,49	0
9	GOL	H	562	6/6	0.92	0.17	32,38,42,50	0
9	GOL	H	561	6/6	0.94	0.15	34,39,40,42	0
9	GOL	J	564	6/6	0.94	0.27	55,65,68,69	0
9	GOL	I	561	6/6	0.94	0.15	35,42,46,46	0
9	GOL	J	565	6/6	0.95	0.20	43,47,49,49	0
6	MG	H	553	1/1	0.97	0.21	38,38,38,38	0
3	SF4	A	265	8/8	0.97	0.05	36,38,40,40	0
3	SF4	B	267	8/8	0.97	0.05	38,42,45,46	0
3	SF4	C	267	8/8	0.97	0.05	37,39,40,42	0
5	NI	H	551	1/1	0.97	0.04	48,48,48,48	0
5	NI	J	551	1/1	0.97	0.03	44,44,44,44	0
3	SF4	A	267	8/8	0.98	0.05	39,40,42,43	0
3	SF4	C	265	8/8	0.98	0.07	35,37,38,39	0
7	FCO	H	550	7/7	0.98	0.11	39,40,41,44	0
7	FCO	J	550	7/7	0.98	0.10	40,41,42,44	0
4	F3S	C	266	7/7	0.98	0.09	38,39,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	F3S	A	266	7/7	0.98	0.07	39,39,42,43	0
3	SF4	B	265	8/8	0.98	0.06	36,38,39,40	0
6	MG	J	553	1/1	0.98	0.10	37,37,37,37	0
8	PER	J	552	2/2	0.98	0.27	49,49,49,50	1
8	PER	H	552	2/2	0.98	0.44	49,49,49,49	1
4	F3S	B	266	7/7	0.98	0.06	37,39,42,42	0
7	FCO	I	550	7/7	0.99	0.09	39,40,43,43	0
8	PER	I	552	2/2	0.99	0.16	49,49,49,49	1
5	NI	I	551	1/1	0.99	0.03	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.