Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 11:08 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

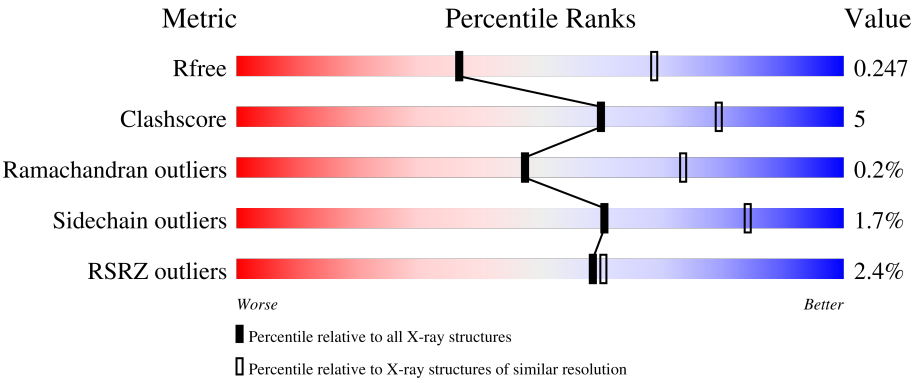
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	85% 14%
1	B	264	8% 88% 11%
1	C	264	85% 13%
2	Q	549	89% 10%
2	R	549	3% 88% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	S	549	2% 86% 13%

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	R	561	-	-	-	X

2 Entry composition (i)

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			

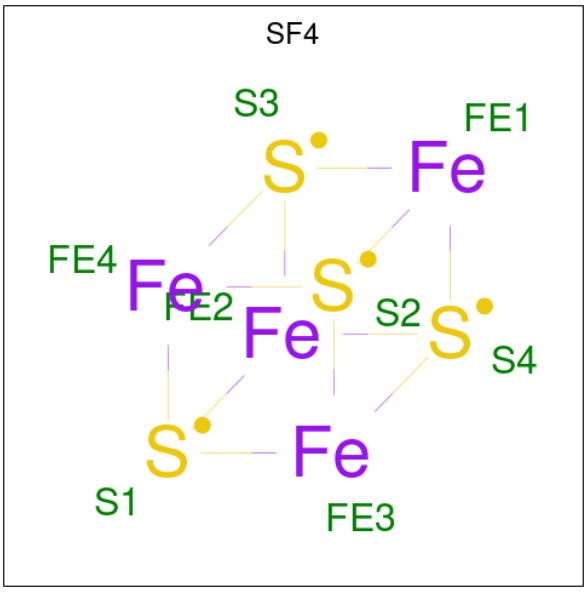
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

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:

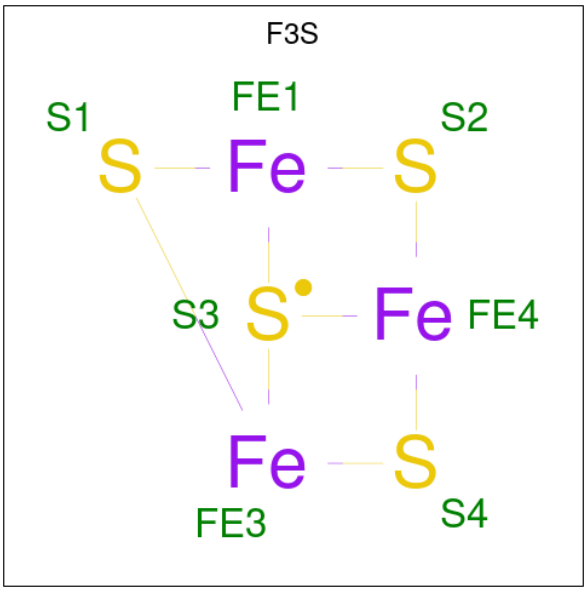
Chain	Residue	Modelled	Actual	Comment	Reference
Q	74	MET	VAL	engineered mutation	UNP P18188
R	74	MET	VAL	engineered mutation	UNP P18188
S	74	MET	VAL	engineered mutation	UNP P18188

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



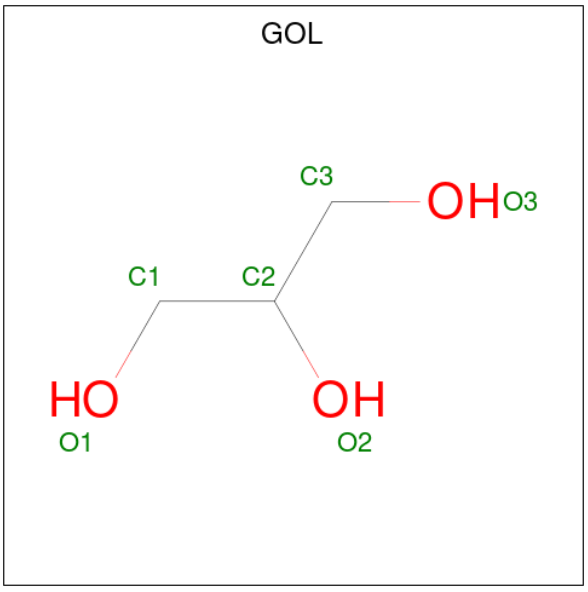
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



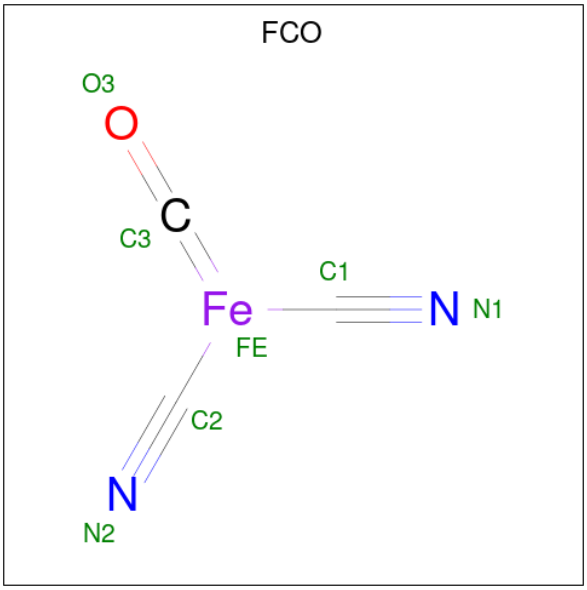
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



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

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 9 is water.

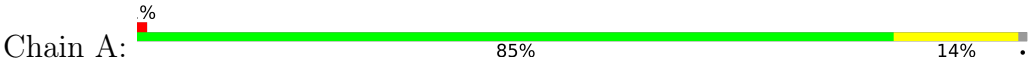
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	68	Total O 68 68	0	0
9	Q	144	Total O 144 144	0	0
9	B	58	Total O 58 58	0	0
9	R	133	Total O 133 133	0	0
9	C	65	Total O 65 65	0	0
9	S	94	Total O 94 94	0	0

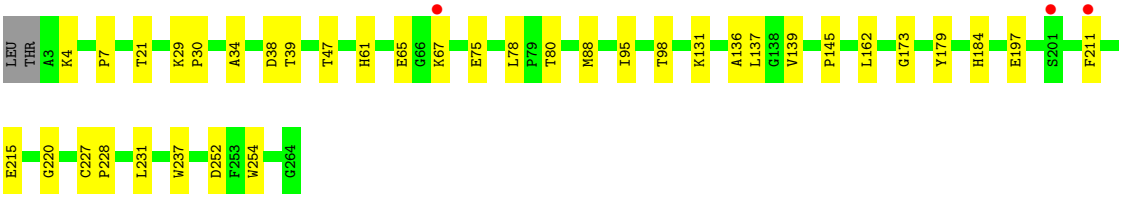
3 Residue-property plots (i)

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

• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

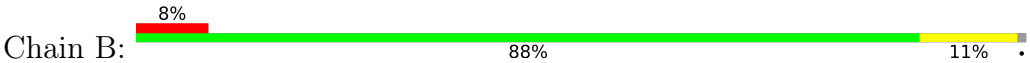
Chain A:

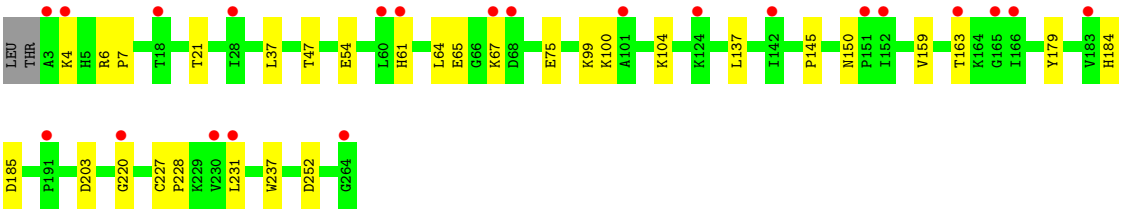




• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

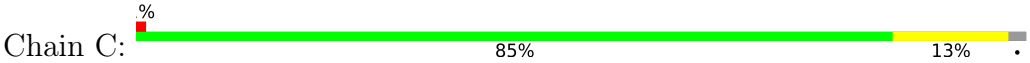
Chain B:

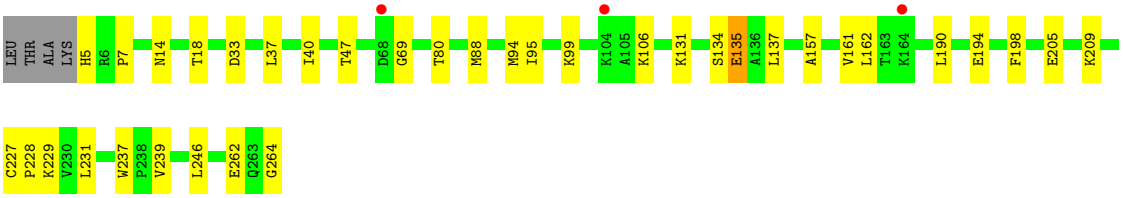




• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

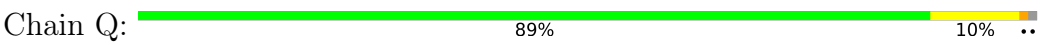
Chain C:

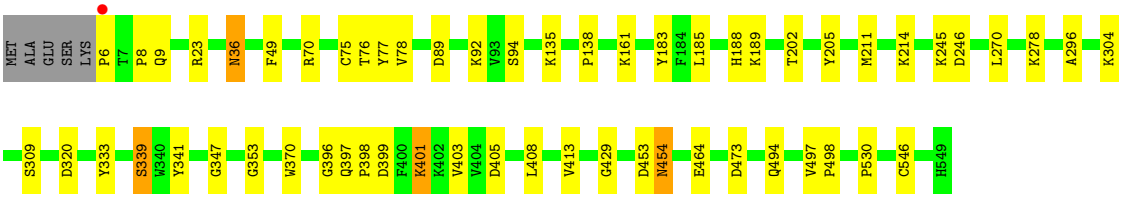




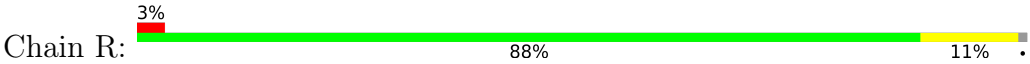
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

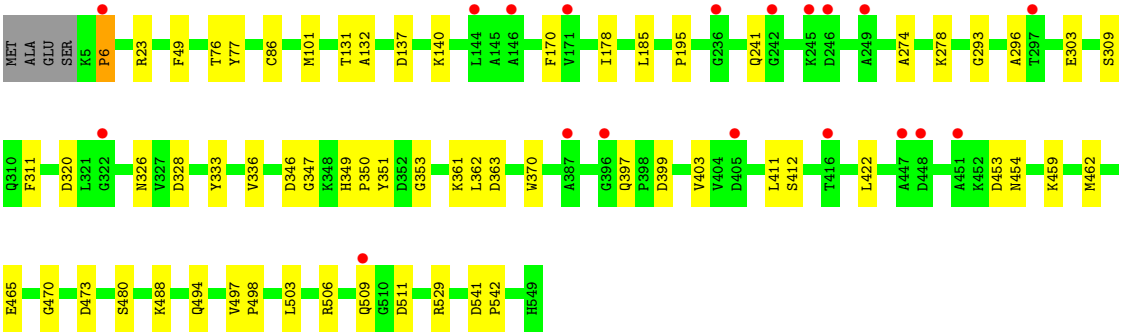
Chain Q:



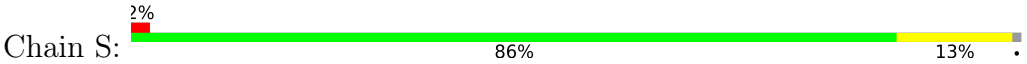


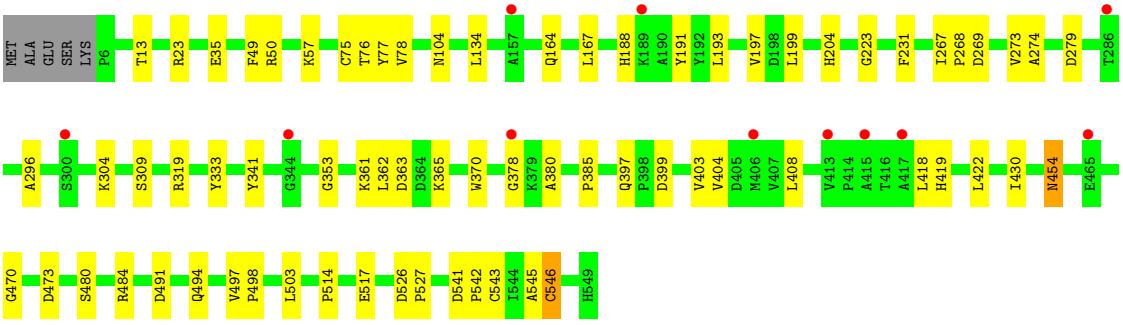
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit





• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.40Å 99.20Å 182.30Å 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
$< I/\sigma(I) >$ [1]	4.78 (at 2.71Å)	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 (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19100	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FCO, F3S, NI, MG, GOL, SF4

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:Q:6:PRO:HG3	2:R:320:ASP:HA	1.78	0.64
2:R:274:ALA:HA	2:R:422:LEU:HD11	1.79	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:R:462:MET:HG3	2:R:488:LYS:HG2	1.83	0.61
2:S:362:LEU:O	2:S:363:ASP:HB2	2.01	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:R:49:PHE:HB2	2:R:370:TRP:CD2	2.40	0.56
2:S:408:LEU:HD21	2:S:418:LEU:HD21	1.86	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
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.43	0.54
1:C:40:ILE:HG22	1:C:162:LEU:HD11	1.90	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:A:47:THR:O	2:Q:23:ARG:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:THR:O	2:S:23:ARG:HA	2.08	0.53
1:A:254:TRP:HH2	2:Q:70:ARG:HD3	1.73	0.53
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.39	0.53
2:Q:464:GLU:HA	2:Q:464:GLU:OE1	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:A:34:ALA:O	1:A:38:ASP:HB2	2.11	0.51
1:B:150:ASN:HB2	9:B:297:HOH:O	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
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.47	0.50
2:R:137:ASP:HB3	2:R:140:LYS:HD2	1.93	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:HD22	2:Q:454:ASN:N	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:R:328:ASP:OD2	1:C:134:SER:OG	2.26	0.47
2:S:76:THR:O	2:S:77:TYR:HB3	2.15	0.47
1:A:252:ASP:HA	9:A:282:HOH:O	2.15	0.47
2:S:484:ARG:NH2	9:S:641:HOH:O	2.46	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

Continued on next page...

Continued from previous page...

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:OD1	2:S:279:ASP:N	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:HD22	2:S:454:ASN:H	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
1:B:64:LEU:O	1:B:104:LYS:NZ	2.49	0.45
2:S:470:GLY:O	2:S:480:SER:HA	2.16	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:9:GLN:NE2	2:Q:36:ASN:O	2.50	0.44
2:Q:408:LEU:HD23	2:Q:408:LEU:HA	1.88	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
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
2:R:296:ALA:HA	2:R:309:SER:HA	2.00	0.44
1:A:184:HIS:HB2	1:A:220:GLY:C	2.39	0.43
1:B:227:CYS:HB2	1:B:228:PRO:HD3	1.98	0.43
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.99	0.43
2:Q:296:ALA:HA	2:Q:309:SER:HA	1.99	0.43
2:S:134:LEU:HD23	2:S:167:LEU:HD23	2.00	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
1:A:197:GLU:HB3	1:A:211:PHE:CE2	2.54	0.43
2:Q:304:LYS:HA	2:Q:304:LYS:HD3	1.85	0.43
1:C:95:ILE:HG22	9:C:285:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LEU:O	1:C:194:GLU:HG3	2.19	0.43
1:A:215:GLU:OE1	9:A:316:HOH:O	2.21	0.42
2:S:193:LEU:HD22	2:S:197:VAL:HG11	2.01	0.42
1:A:80:THR:HG21	1:A:131:LYS:HD2	2.01	0.42
1:A:95:ILE:HD12	1:A:136:ALA:HB1	2.02	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:S:497:VAL:HG12	2:S:498:PRO:HD2	2.00	0.42
2:R:336:VAL:N	2:R:346:ASP:OD1	2.37	0.42
2:R:351:TYR:HD1	2:R:351:TYR:HA	1.76	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
1:B:203:ASP:OD2	2:R:459:LYS:HE3	2.19	0.42
2:S:341:TYR:HB3	9:S:619:HOH:O	2.19	0.42
2:Q:339:SER:HB2	2:Q:341:TYR:HD2	1.85	0.41
1:B:184:HIS:HB2	1:B:220:GLY:C	2.40	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:470:GLY:O	2:R:480:SER:HA	2.20	0.41
2:R:497:VAL:HG13	2:R:498:PRO:HD2	2.03	0.41
2:Q:202:THR:O	2:Q:205:TYR:HB3	2.21	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:76:THR:O	2:Q:77:TYR:HB3	2.21	0.41
2:Q:397:GLN:HA	2:Q:398:PRO:HD3	1.91	0.41
2:R:101:MET:HA	9:R:641:HOH:O	2.20	0.40
2:R:293:GLY:HA2	2:R:311:PHE:O	2.21	0.40
2:R:326:ASN:HD22	1:C:135:GLU:CD	2.24	0.40
1:C:18:THR:HG22	1:C:18:THR:O	2.21	0.40
2:Q:188:HIS:N	1:C:264:GLY:HA2	2.36	0.40
2:R:326:ASN:HB2	1:C:135:GLU:CD	2.41	0.40
2:R:362:LEU:O	2:R:363:ASP:HB2	2.21	0.40
2:R:541:ASP:N	2:R:542:PRO:HD3	2.36	0.40
1:A:61:HIS:O	1:A:65:GLU:HG3	2.21	0.40
2:S:164:GLN:NE2	2:S:199:LEU:HD22	2.36	0.40
2:S:296:ALA:HA	2:S:309:SER:HA	2.01	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%)	34 60
1	B	260/264 (98%)	252 (97%)	7 (3%)	1 (0%)	34 60
1	C	258/264 (98%)	250 (97%)	7 (3%)	1 (0%)	34 60
2	Q	542/549 (99%)	522 (96%)	20 (4%)	0	100 100
2	R	543/549 (99%)	519 (96%)	23 (4%)	1 (0%)	47 73
2	S	542/549 (99%)	520 (96%)	22 (4%)	0	100 100
All	All	2405/2439 (99%)	2316 (96%)	85 (4%)	4 (0%)	47 73

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%)	67 86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	208/210 (99%)	205 (99%)	3 (1%)	67 86
1	C	207/210 (99%)	204 (99%)	3 (1%)	67 86
2	Q	434/439 (99%)	427 (98%)	7 (2%)	62 85
2	R	434/439 (99%)	425 (98%)	9 (2%)	53 80
2	S	434/439 (99%)	426 (98%)	8 (2%)	59 83
All	All	1925/1947 (99%)	1892 (98%)	33 (2%)	60 84

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

Continued on next page...

Continued from previous page...

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

Sometimes 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	F3S	C	266	1	0,9,9	-	-	-		
3	SF4	B	267	1	0,12,12	-	-	-		
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
5	GOL	S	561	-	5,5,5	0.54	0	5,5,5	0.40	0
5	GOL	Q	561	-	5,5,5	0.34	0	5,5,5	1.10	0
3	SF4	A	265	1	0,12,12	-	-	-		
5	GOL	A	271	-	5,5,5	0.30	0	5,5,5	0.55	0
5	GOL	R	563	-	5,5,5	0.37	0	5,5,5	0.36	0
5	GOL	R	562	-	5,5,5	0.50	0	5,5,5	0.52	0
3	SF4	C	267	1	0,12,12	-	-	-		
6	FCO	R	550	2	0,6,6	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
5	GOL	Q	562	-	5,5,5	0.41	0	5,5,5	0.89	0
4	F3S	B	266	1	0,9,9	-	-	-		
6	FCO	S	550	2	0,6,6	-	-	-		
3	SF4	B	265	1	0,12,12	-	-	-		
6	FCO	Q	550	2	0,6,6	-	-	-		
5	GOL	R	561	-	5,5,5	0.50	0	5,5,5	0.26	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
5	GOL	Q	561	-	-	0/4/4/4	-
3	SF4	C	267	1	-	-	0/6/5/5
4	F3S	C	266	1	-	-	0/3/3/3
3	SF4	A	267	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
5	GOL	A	271	-	-	0/4/4/4	-
5	GOL	Q	562	-	-	1/4/4/4	-
4	F3S	B	266	1	-	-	0/3/3/3
3	SF4	B	267	1	-	-	0/6/5/5
3	SF4	B	265	1	-	-	0/6/5/5
5	GOL	S	561	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	R	563	-	-	0/4/4/4	-
3	SF4	C	265	1	-	-	0/6/5/5
3	SF4	A	265	1	-	-	0/6/5/5
5	GOL	R	561	-	-	4/4/4/4	-
5	GOL	R	562	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	561	GOL	O1-C1-C2-C3
5	R	561	GOL	C1-C2-C3-O3
5	Q	562	GOL	O1-C1-C2-C3
5	R	562	GOL	O1-C1-C2-C3
5	R	562	GOL	C1-C2-C3-O3
5	S	561	GOL	C1-C2-C3-O3
5	R	561	GOL	O1-C1-C2-O2
5	R	561	GOL	O2-C2-C3-O3
5	S	561	GOL	O2-C2-C3-O3
5	R	562	GOL	O1-C1-C2-O2
5	R	562	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	561	GOL	2	0
5	Q	562	GOL	2	0
6	Q	550	FCO	1	0
5	R	561	GOL	2	0

5.7 Other polymers

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	262/264 (99%)	-0.23	3 (1%) 80 82	34, 36, 38, 46	8 (3%)
1	B	262/264 (99%)	0.61	22 (8%) 11 9	34, 36, 38, 41	10 (3%)
1	C	260/264 (98%)	-0.19	3 (1%) 79 80	32, 36, 38, 42	6 (2%)
2	Q	544/549 (99%)	-0.25	1 (0%) 95 96	33, 36, 39, 42	15 (2%)
2	R	545/549 (99%)	0.20	19 (3%) 44 44	31, 36, 38, 41	15 (2%)
2	S	544/549 (99%)	0.12	11 (2%) 65 67	32, 36, 38, 43	14 (2%)
All	All	2417/2439 (99%)	0.04	59 (2%) 59 60	31, 36, 38, 46	68 (2%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	415	ALA	5.8
1	B	4	LYS	5.5
1	B	142	ILE	5.2
2	S	344	GLY	4.3
2	R	416	THR	3.8
2	R	451	ALA	3.4
2	R	447	ALA	3.4
1	B	61	HIS	3.3
1	B	191	PRO	3.3
2	S	378	GLY	3.1
1	B	60	LEU	3.1
1	B	3	ALA	3.1
2	S	406	MET	3.0
2	R	396	GLY	3.0
1	B	101	ALA	3.0
2	R	242	GLY	3.0
2	R	6	PRO	3.0
2	S	157	ALA	2.9
1	B	183	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	S	413	VAL	2.9
2	R	405	ASP	2.9
1	B	264	GLY	2.8
1	B	152	ILE	2.7
1	B	163	THR	2.7
2	R	245	LYS	2.7
2	R	509	GLN	2.7
2	R	249	ALA	2.6
1	B	68	ASP	2.6
2	R	322	GLY	2.6
2	R	297	THR	2.5
1	A	201	SER	2.5
2	S	465	GLU	2.5
2	S	286	THR	2.5
2	R	146	ALA	2.4
2	S	189	LYS	2.4
1	B	230	VAL	2.4
2	R	144	LEU	2.4
1	B	18	THR	2.4
2	R	236	GLY	2.4
2	S	300	SER	2.4
1	B	165	GLY	2.3
1	B	67	LYS	2.3
1	A	211	PHE	2.3
2	R	246	ASP	2.2
1	B	220	GLY	2.2
1	B	166	ILE	2.1
1	B	151	PRO	2.1
1	B	28	ILE	2.1
1	C	104	LYS	2.1
1	C	164	LYS	2.1
1	A	67	LYS	2.1
2	R	448	ASP	2.1
2	S	417	ALA	2.1
1	C	68	ASP	2.1
2	Q	6	PRO	2.0
2	R	171	VAL	2.0
1	B	124	LYS	2.0
1	B	231	LEU	2.0
2	R	387	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	R	561	6/6	0.75	0.40	46,49,49,50	0
5	GOL	S	561	6/6	0.83	0.31	45,48,49,50	0
5	GOL	R	563	6/6	0.87	0.35	45,47,49,50	0
5	GOL	A	271	6/6	0.90	0.29	34,34,35,36	0
5	GOL	R	562	6/6	0.92	0.29	44,45,46,46	0
5	GOL	Q	562	6/6	0.93	0.16	35,36,37,39	0
7	NI	Q	551	1/1	0.93	0.07	39,39,39,39	0
5	GOL	Q	561	6/6	0.94	0.16	32,34,35,38	0
3	SF4	B	267	8/8	0.95	0.06	35,35,36,37	0
8	MG	S	553	1/1	0.95	0.07	33,33,33,33	0
4	F3S	B	266	7/7	0.96	0.12	36,38,39,42	0
3	SF4	B	265	8/8	0.96	0.10	30,32,33,34	0
3	SF4	A	267	8/8	0.97	0.08	36,37,39,39	0
7	NI	R	551	1/1	0.97	0.05	41,41,41,41	0
8	MG	Q	553	1/1	0.97	0.12	35,35,35,35	0
8	MG	R	553	1/1	0.97	0.09	34,34,34,34	0
6	FCO	S	550	7/7	0.97	0.18	35,37,40,40	0
3	SF4	C	267	8/8	0.98	0.05	36,37,37,38	0
7	NI	S	551	1/1	0.98	0.03	39,39,39,39	0
6	FCO	R	550	7/7	0.98	0.14	36,36,40,41	0
3	SF4	A	265	8/8	0.98	0.05	29,32,34,35	0
4	F3S	C	266	7/7	0.98	0.05	35,36,37,40	0
6	FCO	Q	550	7/7	0.99	0.12	34,35,37,37	0
4	F3S	A	266	7/7	0.99	0.05	32,34,34,35	0
3	SF4	C	265	8/8	0.99	0.06	33,34,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.