Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 08:49 PM EST

PDB ID	:	3QSI
Title	:	Nickel binding domain of NikR from Helicobacter pylori disclosing partial metal occupancy
Authors	:	Gonzalez, J.M.; Pozharski, E.
Deposited on	:	2011-02-21
Resolution	:	3.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

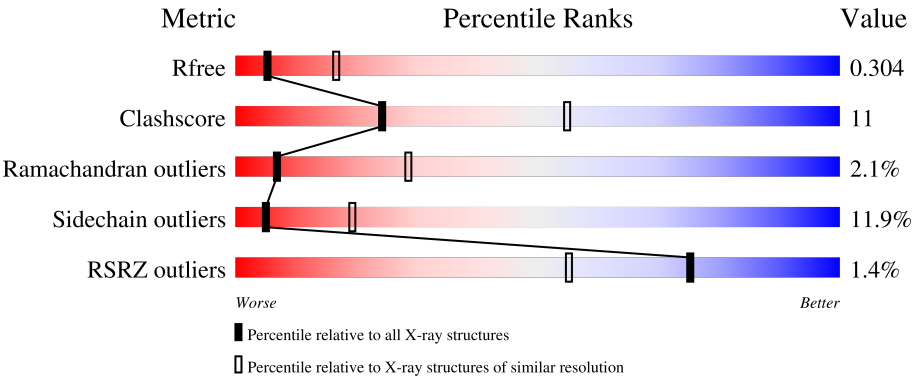
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



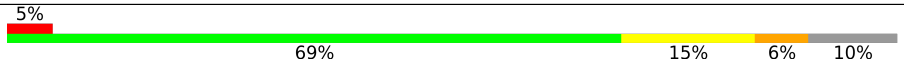
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	88	59% 30% 9%
1	B	88	75% 11% 6% 8%
1	C	88	53% 30% 7% 9%
1	D	88	67% 18% 5% 10%
1	E	88	58% 31% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	88	
1	G	88	
1	H	88	
1	I	88	
1	J	88	

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
3	SO4	C	5	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6138 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 NikR nickel-responsive regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	81	Total	C	N	O	S	0	0	0
			621	388	115	114	4			
1	C	80	Total	C	N	O	S	0	0	0
			637	399	119	115	4			
1	D	79	Total	C	N	O	S	0	0	0
			607	379	113	111	4			
1	A	80	Total	C	N	O	S	0	0	0
			602	377	111	110	4			
1	F	78	Total	C	N	O	S	0	0	0
			604	379	114	107	4			
1	G	79	Total	C	N	O	S	0	0	0
			599	379	107	109	4			
1	H	80	Total	C	N	O	S	0	0	0
			601	378	108	111	4			
1	E	80	Total	C	N	O	S	0	0	0
			622	391	116	111	4			
1	J	79	Total	C	N	O	S	0	0	0
			597	377	107	109	4			
1	I	79	Total	C	N	O	S	0	0	0
			614	387	115	108	4			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

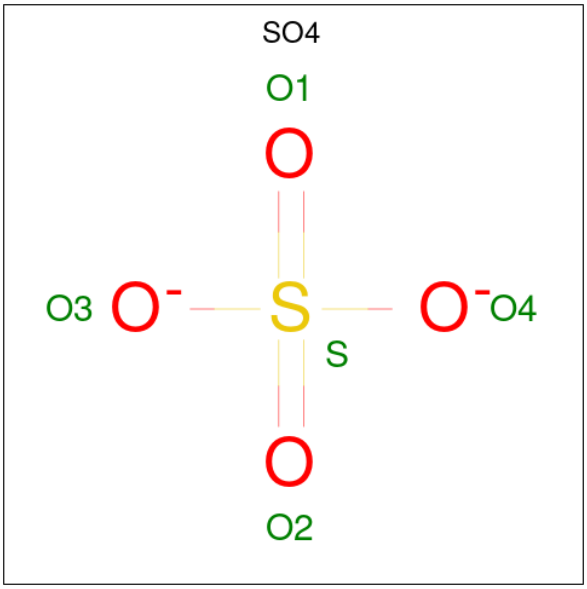
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		
2	D	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Ni 1 1	0	0
2	G	1	Total Ni 1 1	0	0
2	H	1	Total Ni 1 1	0	0
2	E	1	Total Ni 1 1	0	0
2	I	1	Total Ni 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



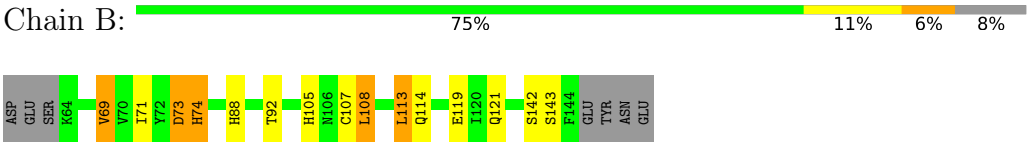
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

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.

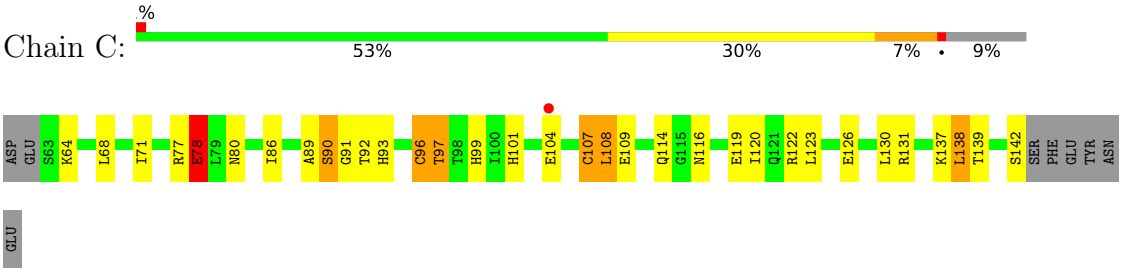
• Molecule 1: NikR nickel-responsive regulator

Chain B:



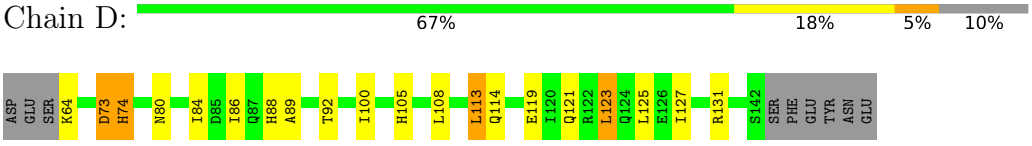
• Molecule 1: NikR nickel-responsive regulator

Chain C:



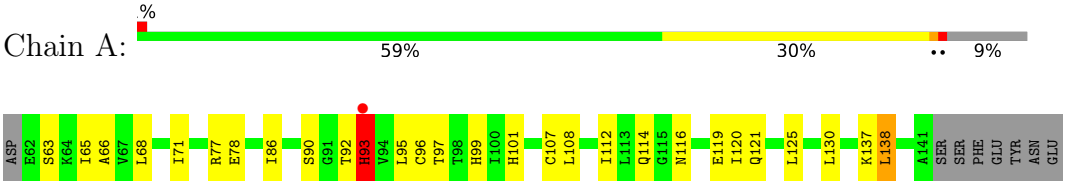
• Molecule 1: NikR nickel-responsive regulator

Chain D:



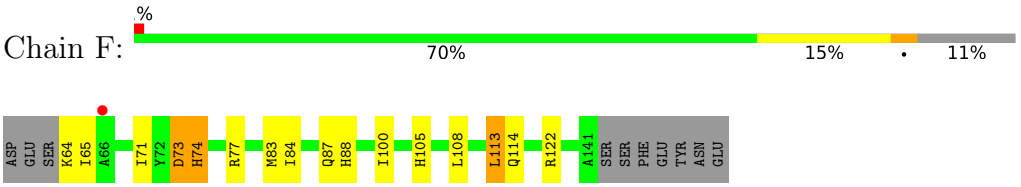
• Molecule 1: NikR nickel-responsive regulator

Chain A:



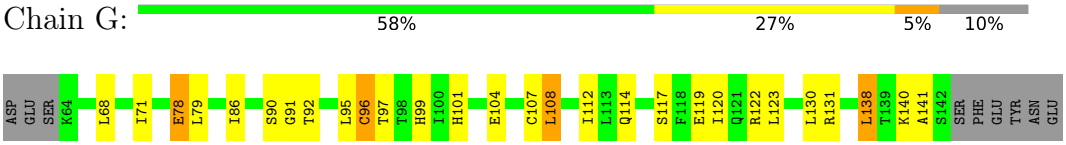
• Molecule 1: NikR nickel-responsive regulator

Chain F:



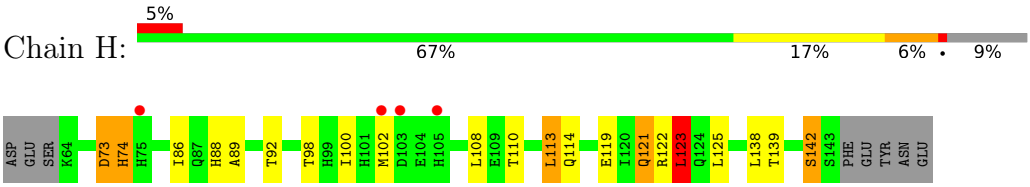
• Molecule 1: NikR nickel-responsive regulator

Chain G:



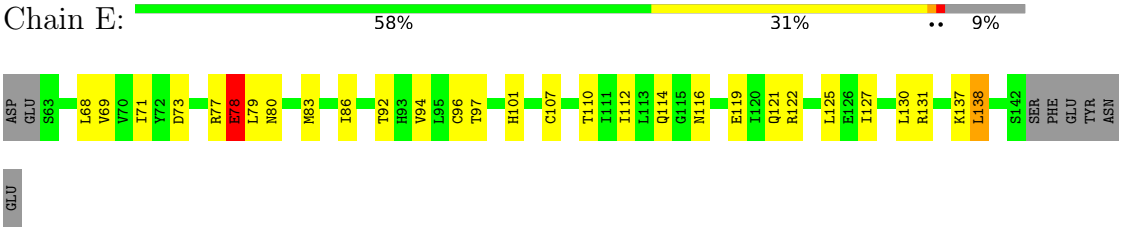
• Molecule 1: NikR nickel-responsive regulator

Chain H:



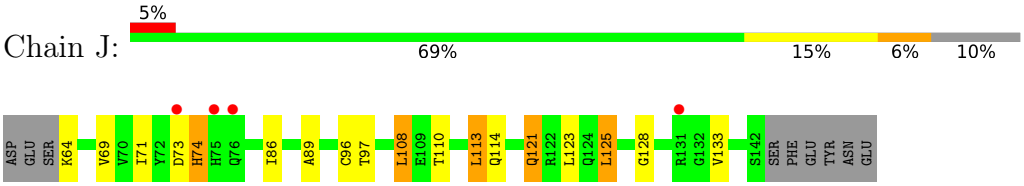
• Molecule 1: NikR nickel-responsive regulator

Chain E:



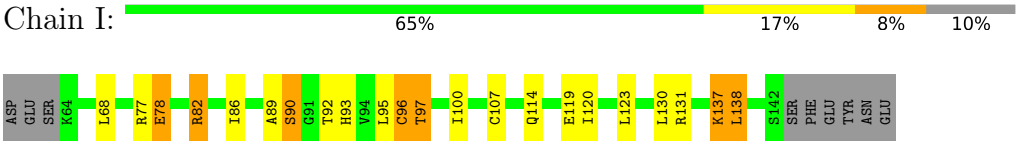
• Molecule 1: NikR nickel-responsive regulator

Chain J:



• Molecule 1: NikR nickel-responsive regulator

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.38Å 79.40Å 122.42Å 90.00° 122.28° 90.00°	Depositor
Resolution (Å)	103.50 – 3.08 40.80 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.5 (103.50-3.08) 95.6 (40.80-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.304 0.256 , 0.304	Depositor DCC
R_{free} test set	2164 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6138	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: SO4, NI

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	0.73	0/610	0.85	1/827 (0.1%)
1	B	0.76	1/630 (0.2%)	0.90	3/852 (0.4%)
1	C	0.83	3/646 (0.5%)	0.85	0/869
1	D	0.69	0/615	0.80	0/832
1	E	0.82	0/630	0.86	0/850
1	F	0.77	0/612	0.84	0/826
1	G	0.86	0/607	0.86	0/821
1	H	0.81	0/608	0.83	1/824 (0.1%)
1	I	0.93	3/623 (0.5%)	0.90	0/841
1	J	0.81	0/604	0.85	0/817
All	All	0.80	7/6185 (0.1%)	0.85	5/8359 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLU	CG-CD	6.38	1.61	1.51
1	B	107	CYS	CB-SG	-6.30	1.71	1.82
1	I	107	CYS	CB-SG	-6.23	1.71	1.82
1	I	78	GLU	CB-CG	5.76	1.63	1.52
1	C	107	CYS	CB-SG	-5.70	1.72	1.81
1	C	78	GLU	CB-CG	5.58	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	78	GLU	CG-CD	5.37	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	VAL	CG1-CB-CG2	7.93	123.58	110.90
1	A	93	HIS	CB-CA-C	6.36	123.13	110.40
1	B	108	LEU	CB-CG-CD1	6.05	121.28	111.00
1	H	123	LEU	CB-CG-CD2	5.69	120.67	111.00
1	B	108	LEU	CB-CG-CD2	5.02	119.53	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	SER	Peptide
1	G	91	GLY	Peptide

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	602	0	585	17	1
1	B	621	0	604	8	0
1	C	637	0	647	23	0
1	D	607	0	599	15	0
1	E	622	0	621	19	0
1	F	604	0	606	14	1
1	G	599	0	590	16	1
1	H	601	0	583	15	0
1	I	614	0	612	12	1
1	J	597	0	592	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
All	All	6138	0	6039	134	2

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 11.

All (134) 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:G:68:LEU:HD13	1:G:138:LEU:HD23	1.44	0.98
1:I:68:LEU:HD13	1:I:138:LEU:HD23	1.51	0.93
1:A:68:LEU:HD13	1:A:138:LEU:HD23	1.51	0.92
1:E:68:LEU:HD13	1:E:138:LEU:HD23	1.50	0.91
1:C:68:LEU:HD13	1:C:138:LEU:HD23	1.60	0.83
1:C:122:ARG:HG2	1:C:126:GLU:OE1	1.89	0.73
1:G:68:LEU:CD1	1:G:138:LEU:HD23	2.19	0.70
1:D:73:ASP:O	1:D:74:HIS:CB	2.39	0.68
1:G:71:ILE:HG12	1:G:108:LEU:HD22	1.76	0.68
1:B:73:ASP:O	1:B:74:HIS:CB	2.42	0.67
1:H:73:ASP:O	1:H:74:HIS:CB	2.43	0.66
1:F:73:ASP:O	1:F:74:HIS:CB	2.44	0.66
1:H:123:LEU:HD22	1:H:123:LEU:O	1.96	0.65
1:J:73:ASP:O	1:J:74:HIS:CB	2.43	0.65
1:D:73:ASP:O	1:D:74:HIS:HB2	1.97	0.65
1:F:113:LEU:HD23	1:F:113:LEU:N	2.12	0.64
1:D:123:LEU:HD22	1:D:123:LEU:O	1.97	0.64
1:J:73:ASP:O	1:J:74:HIS:HB2	1.97	0.64
1:H:142:SER:O	1:H:142:SER:OG	2.12	0.64
1:B:73:ASP:O	1:B:74:HIS:HB2	1.98	0.63
1:F:71:ILE:HD11	1:G:141:ALA:HB1	1.82	0.62
1:F:100:ILE:HD13	1:G:112:ILE:HG21	1.81	0.62
1:A:116:ASN:HD21	1:A:119:GLU:CG	2.13	0.62
1:J:113:LEU:HD23	1:J:113:LEU:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HD23	1:B:113:LEU:N	2.16	0.61
1:D:92:THR:HG23	1:D:119:GLU:HB3	1.83	0.61
1:H:73:ASP:O	1:H:74:HIS:HB2	2.01	0.61
1:F:73:ASP:O	1:F:74:HIS:HB2	2.02	0.60
1:H:113:LEU:N	1:H:113:LEU:HD23	2.18	0.59
1:D:113:LEU:N	1:D:113:LEU:HD23	2.18	0.59
1:F:88:HIS:CE1	1:E:101:HIS:HB3	2.38	0.59
1:C:71:ILE:HG12	1:C:108:LEU:HD22	1.86	0.58
1:I:120:ILE:CG2	1:I:138:LEU:HD11	2.34	0.57
1:D:121:GLN:O	1:D:125:LEU:HG	2.05	0.57
1:D:121:GLN:HE21	1:D:125:LEU:HD21	1.69	0.56
1:G:96:CYS:HB2	1:H:100:ILE:HG22	1.87	0.56
1:A:93:HIS:NE2	1:A:95:LEU:CD2	2.70	0.55
1:A:120:ILE:CG2	1:A:138:LEU:HD11	2.36	0.55
1:I:120:ILE:HG22	1:I:138:LEU:HD11	1.88	0.55
1:J:71:ILE:HG12	1:J:108:LEU:HD23	1.88	0.55
1:A:93:HIS:NE2	1:A:95:LEU:HD23	2.22	0.54
1:E:83:MET:HE2	1:E:127:ILE:HD12	1.89	0.54
1:A:120:ILE:HG22	1:A:138:LEU:HD11	1.89	0.54
1:I:86:ILE:CD1	1:I:130:LEU:HD11	2.38	0.54
1:A:116:ASN:HD21	1:A:119:GLU:HG2	1.71	0.54
1:E:83:MET:CE	1:E:127:ILE:HD12	2.38	0.54
1:F:84:ILE:CD1	1:E:80:ASN:ND2	2.71	0.54
1:E:86:ILE:CD1	1:E:130:LEU:HD11	2.39	0.53
1:H:92:THR:HG23	1:H:119:GLU:HB3	1.89	0.53
1:F:73:ASP:O	1:F:105:HIS:O	2.27	0.53
1:J:69:VAL:O	1:J:69:VAL:HG12	2.08	0.52
1:J:96:CYS:SG	1:I:100:ILE:HD11	2.49	0.52
1:E:116:ASN:HD21	1:E:119:GLU:CG	2.23	0.52
1:C:92:THR:HG23	1:C:119:GLU:HB3	1.92	0.52
1:C:116:ASN:HD21	1:C:119:GLU:CG	2.23	0.52
1:C:86:ILE:HD12	1:C:130:LEU:HD11	1.92	0.51
1:I:92:THR:HG23	1:I:119:GLU:HB3	1.93	0.51
1:F:71:ILE:HD11	1:G:141:ALA:CB	2.40	0.51
1:E:78:GLU:HG2	1:E:79:LEU:N	2.26	0.50
1:J:113:LEU:HD13	1:J:123:LEU:HD23	1.93	0.50
1:G:101:HIS:HB3	1:H:88:HIS:CE1	2.46	0.50
1:E:77:ARG:O	1:E:78:GLU:CB	2.59	0.50
1:J:121:GLN:O	1:J:125:LEU:HD23	2.12	0.49
1:E:77:ARG:O	1:E:78:GLU:HB3	2.13	0.49
1:J:86:ILE:O	1:J:89:ALA:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:ILE:CD1	1:G:141:ALA:HB1	2.43	0.48
1:D:100:ILE:HD13	1:A:112:ILE:HG21	1.95	0.48
1:I:96:CYS:SG	1:I:97:THR:N	2.87	0.48
1:C:71:ILE:HA	1:C:107:CYS:O	2.13	0.48
1:A:92:THR:HG23	1:A:119:GLU:HB3	1.96	0.48
1:E:86:ILE:HD12	1:E:130:LEU:HD11	1.96	0.48
1:E:92:THR:HG23	1:E:119:GLU:HB3	1.95	0.48
1:D:86:ILE:O	1:D:89:ALA:HB3	2.14	0.47
1:C:86:ILE:CD1	1:C:130:LEU:HD11	2.44	0.47
1:B:71:ILE:HG12	1:B:108:LEU:HD13	1.97	0.47
1:J:128:GLY:HA2	1:J:133:VAL:HG11	1.97	0.46
1:D:125:LEU:N	1:D:125:LEU:HD23	2.29	0.46
1:B:88:HIS:CE1	1:A:101:HIS:HB3	2.51	0.46
1:G:86:ILE:CD1	1:G:130:LEU:HD11	2.46	0.46
1:C:89:ALA:O	1:C:91:GLY:N	2.49	0.46
1:C:86:ILE:HG22	1:C:123:LEU:CD1	2.47	0.45
1:H:100:ILE:HD13	1:E:112:ILE:HG21	1.98	0.45
1:E:94:VAL:O	1:E:94:VAL:HG12	2.17	0.45
1:C:101:HIS:HB3	1:D:88:HIS:CE1	2.52	0.45
1:D:73:ASP:O	1:D:105:HIS:O	2.35	0.45
1:D:121:GLN:NE2	1:D:125:LEU:HD21	2.32	0.45
1:H:110:THR:O	1:H:110:THR:HG23	2.17	0.45
1:C:90:SER:HB2	1:C:123:LEU:HD13	1.99	0.44
1:A:77:ARG:O	1:A:78:GLU:CB	2.65	0.44
1:H:138:LEU:HD12	1:H:139:THR:N	2.32	0.44
1:C:80:ASN:ND2	1:D:84:ILE:CD1	2.80	0.44
1:G:86:ILE:HG22	1:G:123:LEU:CD1	2.48	0.44
1:G:71:ILE:HA	1:G:107:CYS:O	2.18	0.43
1:G:92:THR:HG23	1:G:119:GLU:HB3	2.00	0.43
1:C:77:ARG:O	1:C:78:GLU:HB2	2.19	0.43
1:B:73:ASP:O	1:B:105:HIS:O	2.36	0.43
1:F:113:LEU:HD23	1:F:113:LEU:H	1.80	0.43
1:I:86:ILE:HD12	1:I:130:LEU:HD11	2.00	0.43
1:H:98:THR:HB	1:H:110:THR:CG2	2.49	0.42
1:A:71:ILE:HA	1:A:107:CYS:O	2.19	0.42
1:G:78:GLU:O	1:G:79:LEU:C	2.58	0.42
1:C:120:ILE:HG22	1:C:138:LEU:HD11	2.01	0.42
1:F:65:ILE:O	1:F:65:ILE:HG23	2.19	0.42
1:C:99:HIS:CE1	1:C:107:CYS:SG	3.13	0.42
1:E:73:ASP:OD1	1:E:73:ASP:C	2.56	0.42
1:C:108:LEU:HD13	1:C:109:GLU:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:CG2	1:C:138:LEU:HD11	2.50	0.42
1:C:89:ALA:O	1:C:90:SER:C	2.58	0.42
1:H:86:ILE:O	1:H:89:ALA:HB3	2.20	0.42
1:I:89:ALA:O	1:I:90:SER:C	2.57	0.41
1:C:116:ASN:HD21	1:C:119:GLU:HG2	1.86	0.41
1:G:120:ILE:CG2	1:G:138:LEU:HD11	2.50	0.41
1:H:113:LEU:HD23	1:H:113:LEU:H	1.85	0.41
1:B:69:VAL:HG21	1:C:139:THR:HG21	2.02	0.41
1:D:123:LEU:HD22	1:D:127:ILE:HD12	2.01	0.41
1:H:121:GLN:OE1	1:H:125:LEU:HD11	2.21	0.41
1:B:92:THR:HG23	1:B:119:GLU:HB3	2.03	0.41
1:I:77:ARG:O	1:I:78:GLU:HB2	2.21	0.41
1:A:65:ILE:CG2	1:A:66:ALA:N	2.84	0.41
1:A:120:ILE:O	1:A:121:GLN:C	2.58	0.41
1:F:113:LEU:N	1:F:113:LEU:CD2	2.82	0.41
1:I:68:LEU:HD12	1:I:137:LYS:O	2.21	0.41
1:A:86:ILE:CD1	1:A:130:LEU:HD11	2.51	0.41
1:F:83:MET:O	1:F:87:GLN:HG3	2.20	0.41
1:E:71:ILE:HA	1:E:107:CYS:O	2.21	0.41
1:C:96:CYS:SG	1:C:97:THR:N	2.93	0.40
1:A:108:LEU:HD23	1:A:108:LEU:C	2.41	0.40
1:E:83:MET:HE2	1:E:83:MET:HB3	1.91	0.40
1:A:99:HIS:CE1	1:A:107:CYS:HB3	2.56	0.40
1:E:69:VAL:HG22	1:E:110:THR:HG22	2.04	0.40
1:C:77:ARG:O	1:C:78:GLU:CB	2.70	0.40
1:G:99:HIS:CE1	1:G:107:CYS:HB3	2.56	0.40
1:I:90:SER:HB2	1:I:123:LEU:HD13	2.03	0.40
1:E:122:ARG:O	1:E:125:LEU:HB3	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:O	1:I:82:ARG:NH1[3_445]	2.00	0.20
1:F:77:ARG:NH2	1:G:122:ARG:NH1[4_545]	2.08	0.12

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	78/88 (89%)	72 (92%)	5 (6%)	1 (1%)	12	40
1	B	79/88 (90%)	73 (92%)	4 (5%)	2 (2%)	5	25
1	C	78/88 (89%)	72 (92%)	4 (5%)	2 (3%)	5	24
1	D	77/88 (88%)	71 (92%)	4 (5%)	2 (3%)	5	24
1	E	78/88 (89%)	72 (92%)	5 (6%)	1 (1%)	12	40
1	F	76/88 (86%)	70 (92%)	4 (5%)	2 (3%)	5	24
1	G	77/88 (88%)	72 (94%)	3 (4%)	2 (3%)	5	24
1	H	78/88 (89%)	71 (91%)	5 (6%)	2 (3%)	5	24
1	I	77/88 (88%)	71 (92%)	5 (6%)	1 (1%)	12	40
1	J	77/88 (88%)	71 (92%)	5 (6%)	1 (1%)	12	40
All	All	775/880 (88%)	715 (92%)	44 (6%)	16 (2%)	7	28

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	HIS
1	H	74	HIS
1	J	74	HIS
1	D	74	HIS
1	F	74	HIS
1	C	90	SER
1	G	90	SER
1	E	78	GLU
1	C	78	GLU
1	D	73	ASP
1	A	90	SER
1	F	73	ASP
1	G	78	GLU
1	H	73	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	90	SER
1	B	73	ASP

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	63/79 (80%)	56 (89%)	7 (11%)	6 23
1	B	66/79 (84%)	62 (94%)	4 (6%)	18 48
1	C	71/79 (90%)	60 (84%)	11 (16%)	2 11
1	D	65/79 (82%)	58 (89%)	7 (11%)	6 24
1	E	66/79 (84%)	58 (88%)	8 (12%)	5 19
1	F	64/79 (81%)	59 (92%)	5 (8%)	12 39
1	G	63/79 (80%)	53 (84%)	10 (16%)	2 10
1	H	62/79 (78%)	54 (87%)	8 (13%)	4 17
1	I	65/79 (82%)	56 (86%)	9 (14%)	3 15
1	J	63/79 (80%)	55 (87%)	8 (13%)	4 17
All	All	648/790 (82%)	571 (88%)	77 (12%)	5 19

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	113	LEU
1	B	114	GLN
1	B	121	GLN
1	B	142	SER
1	C	64	LYS
1	C	93	HIS
1	C	96	CYS
1	C	97	THR
1	C	104	GLU
1	C	108	LEU
1	C	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	131	ARG
1	C	137	LYS
1	C	138	LEU
1	C	142	SER
1	D	64	LYS
1	D	80	ASN
1	D	108	LEU
1	D	113	LEU
1	D	114	GLN
1	D	123	LEU
1	D	131	ARG
1	A	63	SER
1	A	93	HIS
1	A	96	CYS
1	A	97	THR
1	A	114	GLN
1	A	137	LYS
1	A	138	LEU
1	F	64	LYS
1	F	108	LEU
1	F	113	LEU
1	F	114	GLN
1	F	122	ARG
1	G	95	LEU
1	G	96	CYS
1	G	97	THR
1	G	104	GLU
1	G	108	LEU
1	G	114	GLN
1	G	117	SER
1	G	131	ARG
1	G	138	LEU
1	G	140	LYS
1	H	102	MET
1	H	108	LEU
1	H	113	LEU
1	H	114	GLN
1	H	121	GLN
1	H	122	ARG
1	H	123	LEU
1	H	142	SER
1	E	78	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	96	CYS
1	E	97	THR
1	E	114	GLN
1	E	121	GLN
1	E	131	ARG
1	E	137	LYS
1	E	138	LEU
1	J	64	LYS
1	J	97	THR
1	J	108	LEU
1	J	110	THR
1	J	113	LEU
1	J	114	GLN
1	J	121	GLN
1	J	125	LEU
1	I	82	ARG
1	I	93	HIS
1	I	95	LEU
1	I	96	CYS
1	I	97	THR
1	I	114	GLN
1	I	131	ARG
1	I	137	LYS
1	I	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	GLN
1	C	74	HIS
1	C	80	ASN
1	C	116	ASN
1	D	81	GLN
1	D	121	GLN
1	A	74	HIS
1	A	80	ASN
1	A	116	ASN
1	F	75	HIS
1	F	80	ASN
1	F	81	GLN
1	F	105	HIS
1	G	74	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	80	ASN
1	H	81	GLN
1	E	80	ASN
1	E	116	ASN
1	J	114	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	SO4	F	2	-	4,4,4	0.13	0	6,6,6	0.23	0
3	SO4	E	3	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	C	5	-	4,4,4	0.10	0	6,6,6	0.29	0
3	SO4	B	4	-	4,4,4	0.14	0	6,6,6	0.20	0
3	SO4	G	1	2	4,4,4	0.17	0	6,6,6	0.34	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.

No monomer is involved in short contacts.

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^{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	80/88 (90%)	0.07	1 (1%) 77 58	42, 55, 74, 78	0
1	B	81/88 (92%)	0.07	0 100 100	43, 61, 88, 93	0
1	C	80/88 (90%)	-0.29	1 (1%) 77 58	41, 56, 77, 80	0
1	D	79/88 (89%)	0.03	0 100 100	43, 61, 87, 93	0
1	E	80/88 (90%)	-0.22	0 100 100	39, 54, 73, 76	0
1	F	78/88 (88%)	0.09	1 (1%) 77 58	41, 60, 88, 93	0
1	G	79/88 (89%)	-0.02	0 100 100	37, 61, 85, 92	0
1	H	80/88 (90%)	-0.01	4 (5%) 28 13	40, 58, 94, 111	0
1	I	79/88 (89%)	-0.05	0 100 100	39, 57, 77, 82	0
1	J	79/88 (89%)	0.20	4 (5%) 28 12	42, 57, 90, 102	0
All	All	795/880 (90%)	-0.01	11 (1%) 75 55	37, 58, 87, 111	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	75	HIS	5.0
1	J	76	GLN	4.1
1	C	104	GLU	3.2
1	J	73	ASP	3.0
1	H	103	ASP	2.9
1	H	102	MET	2.9
1	F	66	ALA	2.4
1	J	131	ARG	2.3
1	H	105	HIS	2.3
1	H	75	HIS	2.1
1	A	93	HIS	2.1

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
3	SO4	B	4	5/5	0.26	0.32	144,145,145,145	0
3	SO4	E	3	5/5	0.47	0.28	157,157,157,158	0
3	SO4	C	5	5/5	0.62	0.44	166,167,167,167	0
3	SO4	F	2	5/5	0.83	0.37	138,138,139,139	0
3	SO4	G	1	5/5	0.89	0.25	60,61,61,63	5
2	NI	H	9	1/1	0.91	0.06	73,73,73,73	0
2	NI	B	5	1/1	0.91	0.07	63,63,63,63	0
2	NI	D	7	1/1	0.94	0.11	68,68,68,68	0
2	NI	I	1	1/1	0.96	0.07	42,42,42,42	0
2	NI	F	6	1/1	0.96	0.06	64,64,64,64	0
2	NI	G	2	1/1	0.98	0.03	38,38,38,38	0
2	NI	A	3	1/1	0.99	0.05	43,43,43,43	0
2	NI	C	4	1/1	0.99	0.05	42,42,42,42	0
2	NI	E	8	1/1	0.99	0.03	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.