Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:26 AM GMT

PDB ID	:	3IHE
Title	:	Crystal structure of mouse Bcl-xl mutant (F105A) at pH 6.0
Authors	:	Priyadarshi, A.; Hwang, K.Y.
Deposited on	:	2009-07-30
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

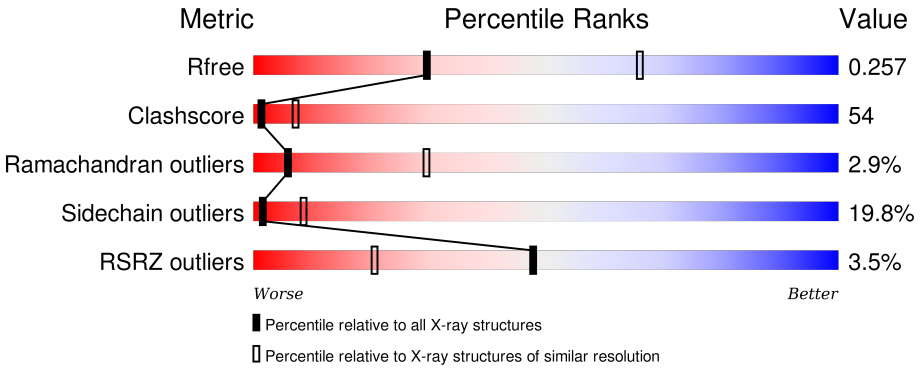
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	196	3% 22% 30% 18% • 28%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1148 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 Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1148	733	193	217	5			

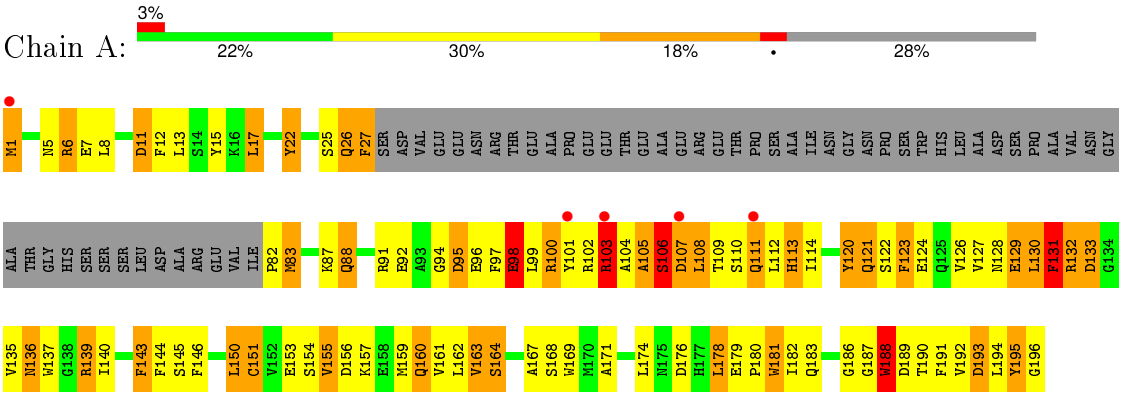
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	PHE	ENGINEERED	UNP Q64373

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

- Molecule 1: Bcl-2-like protein 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	63.15Å 63.15Å 110.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.56 – 3.00 41.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (41.56-3.00) 91.5 (41.54-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	4.81 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.239 0.221 , 0.257	Depositor DCC
R_{free} test set	204 reflections (4.60%)	DCC
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 4437 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	1148	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	2.00	28/1176 (2.4%)	1.74	22/1589 (1.4%)

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	A	0	4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CD-OE1	8.26	1.34	1.25
1	A	98	GLU	CD-OE2	7.95	1.34	1.25
1	A	131	PHE	CE1-CZ	7.68	1.51	1.37
1	A	120	TYR	CD1-CE1	7.46	1.50	1.39
1	A	143	PHE	CD2-CE2	7.16	1.53	1.39
1	A	153	GLU	CD-OE2	6.92	1.33	1.25
1	A	129	GLU	CD-OE1	6.69	1.33	1.25
1	A	123	PHE	CD1-CE1	6.52	1.52	1.39
1	A	153	GLU	CD-OE1	6.39	1.32	1.25
1	A	171	ALA	CA-CB	-6.17	1.39	1.52
1	A	27	PHE	CB-CG	6.14	1.61	1.51
1	A	124	GLU	CD-OE1	6.09	1.32	1.25
1	A	155	VAL	CB-CG1	-6.00	1.40	1.52
1	A	12	PHE	CD1-CE1	5.92	1.51	1.39
1	A	181	TRP	CE3-CZ3	5.84	1.48	1.38
1	A	144	PHE	CE2-CZ	5.83	1.48	1.37
1	A	195	TYR	CB-CG	-5.64	1.43	1.51
1	A	143	PHE	CG-CD2	5.54	1.47	1.38
1	A	107	ASP	CB-CG	5.50	1.63	1.51
1	A	189	ASP	CB-CG	5.49	1.63	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	PHE	CE1-CZ	5.44	1.47	1.37
1	A	188	TRP	CG-CD1	5.37	1.44	1.36
1	A	187	GLY	N-CA	5.32	1.54	1.46
1	A	11	ASP	N-CA	-5.22	1.35	1.46
1	A	160	GLN	CB-CG	-5.19	1.38	1.52
1	A	22	TYR	CD2-CE2	5.09	1.47	1.39
1	A	133	ASP	CA-C	-5.08	1.39	1.52
1	A	120	TYR	CD2-CE2	5.03	1.46	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	SER	N-CA-CB	-13.11	90.83	110.50
1	A	105	ALA	CB-CA-C	11.37	127.15	110.10
1	A	6	ARG	NE-CZ-NH2	9.09	124.84	120.30
1	A	17	LEU	CA-CB-CG	-8.23	96.38	115.30
1	A	156	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	A	95	ASP	N-CA-C	7.39	130.96	111.00
1	A	106	SER	N-CA-C	-7.15	91.70	111.00
1	A	139	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	13	LEU	CB-CG-CD2	6.92	122.77	111.00
1	A	13	LEU	CB-CG-CD1	-6.90	99.28	111.00
1	A	107	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	107	ASP	CB-CG-OD2	-6.63	112.34	118.30
1	A	168	SER	CB-CA-C	-6.33	98.07	110.10
1	A	95	ASP	CB-CA-C	-6.16	98.08	110.40
1	A	130	LEU	CB-CG-CD1	6.11	121.39	111.00
1	A	195	TYR	CB-CA-C	-5.59	99.22	110.40
1	A	151	CYS	CA-CB-SG	-5.42	104.25	114.00
1	A	108	LEU	CB-CG-CD1	5.35	120.10	111.00
1	A	160	GLN	N-CA-CB	-5.35	100.97	110.60
1	A	135	VAL	CB-CA-C	-5.33	101.27	111.40
1	A	8	LEU	CA-CB-CG	-5.26	103.19	115.30
1	A	145	SER	N-CA-CB	-5.20	102.69	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Peptide
1	A	106	SER	Peptide
1	A	186	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	82	PRO	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	1148	0	1093	120	0
All	All	1148	0	1093	120	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 54.

All (120) 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:105:ALA:O	1:A:108:LEU:HB2	1.37	1.24
1:A:107:ASP:O	1:A:111:GLN:HB2	1.40	1.21
1:A:106:SER:O	1:A:110:SER:HB3	1.44	1.15
1:A:103:ARG:O	1:A:103:ARG:HG3	1.46	1.15
1:A:104:ALA:C	1:A:106:SER:HB3	1.71	1.10
1:A:105:ALA:N	1:A:106:SER:HB3	1.70	1.05
1:A:95:ASP:O	1:A:99:LEU:HG	1.57	1.02
1:A:1:MET:O	1:A:1:MET:HG3	1.62	1.00
1:A:192:VAL:O	1:A:196:GLY:HA3	1.61	0.99
1:A:106:SER:H	1:A:108:LEU:H	1.05	0.99
1:A:105:ALA:N	1:A:106:SER:CA	2.26	0.97
1:A:136:ASN:ND2	1:A:139:ARG:H	1.62	0.97
1:A:83:MET:O	1:A:83:MET:HG3	1.62	0.96
1:A:106:SER:N	1:A:108:LEU:H	1.63	0.95
1:A:105:ALA:H	1:A:106:SER:HA	1.30	0.94
1:A:105:ALA:N	1:A:106:SER:CB	2.30	0.94
1:A:105:ALA:H	1:A:106:SER:CA	1.81	0.94
1:A:101:TYR:O	1:A:102:ARG:HB2	1.73	0.87
1:A:132:ARG:O	1:A:133:ASP:OD1	1.96	0.83
1:A:103:ARG:O	1:A:103:ARG:CG	2.30	0.79
1:A:104:ALA:C	1:A:106:SER:CB	2.52	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ALA:C	1:A:108:LEU:HB2	2.02	0.78
1:A:106:SER:O	1:A:110:SER:CB	2.30	0.77
1:A:1:MET:O	1:A:1:MET:CG	2.33	0.77
1:A:157:LYS:HD3	1:A:159:MET:CE	2.14	0.76
1:A:107:ASP:O	1:A:111:GLN:CB	2.30	0.75
1:A:101:TYR:HD1	1:A:103:ARG:HG2	1.52	0.73
1:A:192:VAL:O	1:A:196:GLY:CA	2.34	0.73
1:A:106:SER:HA	1:A:109:THR:OG1	1.89	0.72
1:A:136:ASN:HD21	1:A:139:ARG:H	1.37	0.71
1:A:95:ASP:O	1:A:99:LEU:CG	2.39	0.70
1:A:112:LEU:O	1:A:113:HIS:C	2.30	0.69
1:A:157:LYS:HD3	1:A:159:MET:HE1	1.74	0.69
1:A:160:GLN:O	1:A:163:VAL:HG13	1.95	0.67
1:A:5:ASN:HD21	1:A:188:TRP:HE1	1.40	0.66
1:A:106:SER:H	1:A:108:LEU:N	1.88	0.66
1:A:101:TYR:CD1	1:A:103:ARG:HG2	2.30	0.65
1:A:101:TYR:O	1:A:102:ARG:CB	2.41	0.65
1:A:108:LEU:HB3	1:A:146:PHE:HE1	1.60	0.65
1:A:25:SER:O	1:A:27:PHE:N	2.30	0.65
1:A:108:LEU:HB3	1:A:146:PHE:CE1	2.32	0.64
1:A:25:SER:C	1:A:27:PHE:H	2.01	0.64
1:A:106:SER:OG	1:A:107:ASP:N	2.24	0.63
1:A:137:TRP:O	1:A:140:ILE:HB	1.98	0.63
1:A:136:ASN:HD22	1:A:136:ASN:C	2.02	0.63
1:A:136:ASN:HD22	1:A:139:ARG:H	1.45	0.62
1:A:157:LYS:HD3	1:A:159:MET:HE2	1.81	0.62
1:A:105:ALA:HB1	1:A:146:PHE:HD1	1.66	0.61
1:A:15:TYR:CG	1:A:91:ARG:HG2	2.38	0.58
1:A:5:ASN:C	1:A:7:GLU:H	2.07	0.58
1:A:179:GLU:N	1:A:180:PRO:CD	2.66	0.58
1:A:109:THR:HG22	1:A:150:LEU:CD1	2.34	0.57
1:A:179:GLU:N	1:A:180:PRO:HD2	2.19	0.57
1:A:151:CYS:O	1:A:154:SER:HB2	2.04	0.57
1:A:107:ASP:OD1	1:A:107:ASP:O	2.23	0.57
1:A:132:ARG:O	1:A:132:ARG:HG3	2.03	0.57
1:A:136:ASN:HD21	1:A:139:ARG:HG3	1.71	0.56
1:A:112:LEU:O	1:A:112:LEU:HD12	2.06	0.55
1:A:5:ASN:C	1:A:7:GLU:N	2.59	0.54
1:A:96:GLU:HG3	1:A:97:PHE:N	2.22	0.54
1:A:26:GLN:H	1:A:26:GLN:CD	2.13	0.52
1:A:101:TYR:HD1	1:A:103:ARG:CG	2.19	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:OE1	1:A:179:GLU:HA	2.11	0.51
1:A:101:TYR:HE1	1:A:103:ARG:NE	2.07	0.51
1:A:94:GLY:O	1:A:98:GLU:HG3	2.11	0.51
1:A:132:ARG:HG2	1:A:132:ARG:NH2	2.26	0.51
1:A:182:ILE:HG22	1:A:183:GLN:HE21	1.76	0.50
1:A:112:LEU:O	1:A:114:ILE:N	2.45	0.50
1:A:126:VAL:O	1:A:129:GLU:HB2	2.12	0.50
1:A:136:ASN:HD21	1:A:139:ARG:N	2.09	0.50
1:A:100:ARG:HG2	1:A:101:TYR:N	2.28	0.49
1:A:123:PHE:CE2	1:A:169:TRP:HB3	2.49	0.48
1:A:105:ALA:CA	1:A:106:SER:HB3	2.41	0.48
1:A:164:SER:O	1:A:167:ALA:HB3	2.14	0.48
1:A:133:ASP:HB2	1:A:139:ARG:HH12	1.78	0.47
1:A:191:PHE:CE1	1:A:195:TYR:CD1	3.02	0.47
1:A:127:VAL:O	1:A:128:ASN:C	2.51	0.47
1:A:25:SER:C	1:A:27:PHE:N	2.67	0.47
1:A:191:PHE:O	1:A:195:TYR:HB2	2.15	0.47
1:A:136:ASN:HA	1:A:181:TRP:CH2	2.49	0.47
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.70	0.47
1:A:99:LEU:HD23	1:A:99:LEU:N	2.30	0.46
1:A:113:HIS:O	1:A:113:HIS:CG	2.69	0.46
1:A:105:ALA:N	1:A:106:SER:HA	2.04	0.46
1:A:106:SER:HA	1:A:109:THR:HG1	1.81	0.46
1:A:114:ILE:HG12	1:A:162:LEU:CD1	2.45	0.46
1:A:151:CYS:O	1:A:155:VAL:HG23	2.16	0.46
1:A:136:ASN:C	1:A:136:ASN:ND2	2.69	0.46
1:A:178:LEU:O	1:A:182:ILE:HD12	2.16	0.46
1:A:92:GLU:O	1:A:96:GLU:HB3	2.16	0.45
1:A:108:LEU:HD23	1:A:146:PHE:CE1	2.52	0.45
1:A:1:MET:HB2	1:A:1:MET:HE3	1.80	0.45
1:A:88:GLN:HA	1:A:91:ARG:HD2	1.98	0.45
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.82	0.44
1:A:123:PHE:HB2	1:A:169:TRP:CZ3	2.53	0.44
1:A:17:LEU:HD22	1:A:22:TYR:HB2	1.99	0.44
1:A:192:VAL:HG12	1:A:193:ASP:N	2.26	0.44
1:A:136:ASN:HA	1:A:181:TRP:CZ2	2.53	0.43
1:A:103:ARG:CG	1:A:103:ARG:HH11	2.30	0.43
1:A:132:ARG:CG	1:A:132:ARG:HH21	2.31	0.43
1:A:163:VAL:HG23	1:A:163:VAL:O	2.18	0.43
1:A:83:MET:CG	1:A:83:MET:O	2.48	0.43
1:A:132:ARG:HG2	1:A:132:ARG:HH21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:O	1:A:121:GLN:C	2.55	0.43
1:A:161:VAL:CG2	1:A:162:LEU:N	2.81	0.43
1:A:192:VAL:O	1:A:196:GLY:N	2.51	0.43
1:A:174:LEU:HD12	1:A:178:LEU:HB2	2.01	0.43
1:A:137:TRP:HA	1:A:140:ILE:HD12	2.01	0.43
1:A:136:ASN:ND2	1:A:139:ARG:HG3	2.33	0.42
1:A:178:LEU:C	1:A:180:PRO:HD2	2.39	0.42
1:A:95:ASP:O	1:A:99:LEU:CD2	2.68	0.42
1:A:104:ALA:HA	1:A:105:ALA:HA	1.63	0.42
1:A:22:TYR:N	1:A:22:TYR:CD2	2.87	0.42
1:A:127:VAL:HG12	1:A:131:PHE:HE2	1.85	0.42
1:A:123:PHE:CD1	1:A:169:TRP:HE3	2.38	0.41
1:A:107:ASP:C	1:A:111:GLN:HB2	2.30	0.40
1:A:101:TYR:CE1	1:A:103:ARG:NE	2.88	0.40
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.84	0.40
1:A:140:ILE:O	1:A:143:PHE:HB3	2.21	0.40
1:A:5:ASN:HA	1:A:5:ASN:HD22	1.74	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	138/196 (70%)	112 (81%)	22 (16%)	4 (3%)	6 29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	106	SER
1	A	113	HIS
1	A	188	TRP

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	121/165 (73%)	97 (80%)	24 (20%)	1 8

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ARG
1	A	11	ASP
1	A	83	MET
1	A	87	LYS
1	A	88	GLN
1	A	98	GLU
1	A	100	ARG
1	A	103	ARG
1	A	111	GLN
1	A	121	GLN
1	A	122	SER
1	A	130	LEU
1	A	131	PHE
1	A	132	ARG
1	A	136	ASN
1	A	150	LEU
1	A	163	VAL
1	A	164	SER
1	A	176	ASP
1	A	178	LEU
1	A	190	THR
1	A	193	ASP
1	A	194	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	26	GLN
1	A	88	GLN
1	A	125	GLN
1	A	136	ASN
1	A	160	GLN
1	A	175	ASN
1	A	183	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{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	142/196 (72%)	-0.41	5 (3%) 48 21	20, 43, 88, 113	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	ASP	3.6
1	A	101	TYR	2.7
1	A	111	GLN	2.7
1	A	1	MET	2.7
1	A	103	ARG	2.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.