



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 PM UTC

PDB ID : 3IHE / pdb_00003ihe
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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

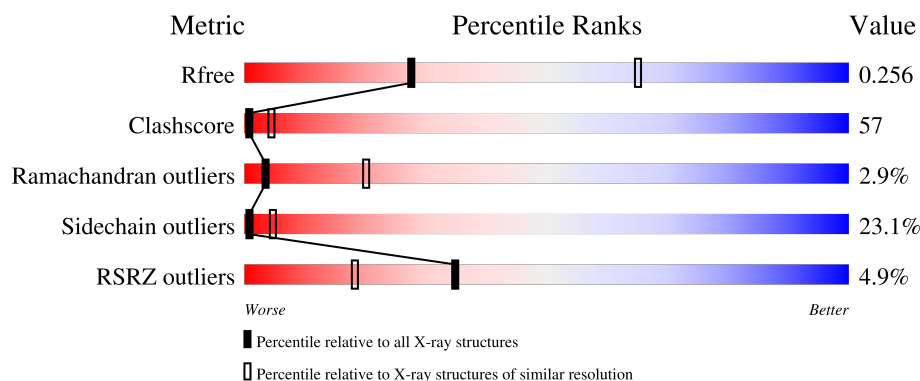
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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	196	

2 Entry composition

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			

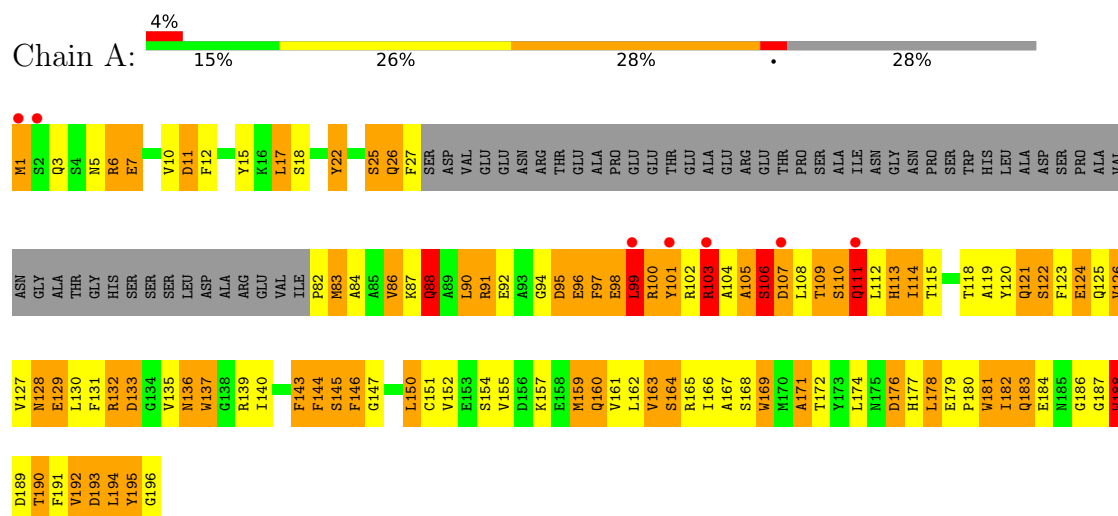
There is a discrepancy between the modelled and reference sequences:

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

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: Bcl-2-like protein 1



4 Data and refinement statistics

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 41.56 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (41.56-3.00) 91.5 (41.56-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.239 0.221 , 0.256	Depositor DCC
R_{free} test set	205 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	2.31	46/1176 (3.9%)	2.21	65/1589 (4.1%)

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	A	0	4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ASP	CA-C	-9.14	1.39	1.52
1	A	171	ALA	CA-CB	-8.85	1.39	1.53
1	A	11	ASP	N-CA	-8.71	1.35	1.46
1	A	189	ASP	CA-C	-8.67	1.41	1.53
1	A	18	SER	N-CA	-7.99	1.36	1.46
1	A	133	ASP	C-O	-7.92	1.16	1.24
1	A	195	TYR	CA-C	-7.77	1.42	1.52
1	A	109	THR	CA-C	7.56	1.62	1.52
1	A	126	VAL	N-CA	-7.32	1.37	1.46
1	A	137	TRP	N-CA	-7.25	1.37	1.46
1	A	188	TRP	CA-C	7.25	1.62	1.52
1	A	168	SER	CA-C	-7.20	1.43	1.52
1	A	135	VAL	CA-C	7.16	1.64	1.53
1	A	128	ASN	CA-C	-6.82	1.43	1.52
1	A	7	GLU	CA-C	-6.63	1.44	1.52
1	A	143	PHE	N-CA	-6.57	1.38	1.46
1	A	10	VAL	C-O	6.39	1.31	1.23
1	A	135	VAL	C-O	6.27	1.31	1.24
1	A	86	VAL	C-O	-6.16	1.17	1.24
1	A	124	GLU	N-CA	-6.15	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	SER	N-CA	-6.09	1.39	1.46
1	A	7	GLU	N-CA	-5.84	1.38	1.46
1	A	192	VAL	C-O	-5.82	1.17	1.24
1	A	90	LEU	N-CA	-5.74	1.38	1.46
1	A	118	THR	C-O	5.69	1.30	1.24
1	A	22	TYR	CA-C	-5.58	1.44	1.53
1	A	88	GLN	CA-CB	-5.58	1.44	1.53
1	A	107	ASP	C-O	5.57	1.32	1.24
1	A	109	THR	N-CA	5.56	1.53	1.46
1	A	160	GLN	CA-CB	-5.53	1.43	1.53
1	A	91	ARG	CA-C	5.45	1.60	1.52
1	A	7	GLU	CA-CB	-5.43	1.45	1.53
1	A	128	ASN	C-O	-5.41	1.17	1.24
1	A	122	SER	CA-C	-5.40	1.45	1.52
1	A	119	ALA	N-CA	5.38	1.52	1.45
1	A	188	TRP	CA-CB	-5.37	1.44	1.53
1	A	110	SER	CA-C	5.29	1.59	1.52
1	A	152	VAL	CA-C	-5.25	1.46	1.52
1	A	152	VAL	N-CA	-5.23	1.40	1.46
1	A	10	VAL	CA-C	-5.22	1.45	1.52
1	A	107	ASP	N-CA	5.21	1.53	1.46
1	A	187	GLY	N-CA	5.21	1.54	1.45
1	A	194	LEU	CA-C	-5.17	1.48	1.53
1	A	144	PHE	C-N	-5.03	1.27	1.33
1	A	183	GLN	CA-C	-5.02	1.45	1.52
1	A	115	THR	CA-C	-5.00	1.46	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	VAL	N-CA-C	12.10	122.82	110.23
1	A	106	SER	N-CA-CB	-11.57	90.83	110.50
1	A	105	ALA	CB-CA-C	11.10	127.15	110.50
1	A	176	ASP	N-CA-C	-10.94	98.13	112.68
1	A	3	GLN	N-CA-C	-10.57	100.12	113.23
1	A	110	SER	N-CA-C	9.84	122.00	111.28
1	A	95	ASP	N-CA-C	9.46	130.96	110.80
1	A	25	SER	N-CA-C	9.26	121.37	111.28
1	A	184	GLU	N-CA-C	-8.69	102.68	113.28
1	A	122	SER	N-CA-C	-8.31	101.76	112.23
1	A	181	TRP	N-CA-C	-8.06	101.25	112.45
1	A	88	GLN	CB-CG-CD	-7.60	99.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	SER	CB-CA-C	-7.57	98.07	110.79
1	A	109	THR	N-CA-C	7.52	120.43	111.33
1	A	133	ASP	CA-C-O	-7.27	113.14	119.97
1	A	106	SER	N-CA-C	-6.89	91.70	111.00
1	A	17	LEU	N-CA-C	6.73	118.27	111.07
1	A	135	VAL	CB-CA-C	-6.67	101.27	111.08
1	A	169	TRP	CA-C-N	-6.60	110.92	120.29
1	A	169	TRP	C-N-CA	-6.60	110.92	120.29
1	A	97	PHE	CA-C-N	-6.58	110.09	121.66
1	A	97	PHE	C-N-CA	-6.58	110.09	121.66
1	A	147	GLY	N-CA-C	-6.55	104.90	112.50
1	A	18	SER	N-CA-C	-6.44	104.26	111.28
1	A	95	ASP	CA-C-N	6.41	129.34	120.63
1	A	95	ASP	C-N-CA	6.41	129.34	120.63
1	A	177	HIS	N-CA-C	6.39	121.28	112.90
1	A	6	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	A	118	THR	CA-C-N	6.27	131.80	121.39
1	A	118	THR	C-N-CA	6.27	131.80	121.39
1	A	95	ASP	CB-CA-C	-6.20	98.08	110.42
1	A	192	VAL	CB-CA-C	-6.14	103.84	111.70
1	A	144	PHE	CA-C-O	6.12	127.03	120.24
1	A	192	VAL	CA-C-O	-6.09	115.08	121.41
1	A	96	GLU	N-CA-C	6.03	117.72	111.03
1	A	111	GLN	N-CA-C	-5.97	105.96	113.18
1	A	135	VAL	N-CA-C	5.89	119.09	109.78
1	A	176	ASP	CB-CA-C	5.82	119.96	110.24
1	A	160	GLN	CA-C-N	5.71	128.53	120.42
1	A	160	GLN	C-N-CA	5.71	128.53	120.42
1	A	165	ARG	N-CA-C	-5.69	104.71	111.03
1	A	17	LEU	CA-CB-CG	-5.69	96.38	116.30
1	A	160	GLN	N-CA-CB	-5.67	100.97	110.39
1	A	22	TYR	N-CA-C	-5.63	101.06	109.96
1	A	6	ARG	N-CA-C	-5.59	105.08	112.34
1	A	101	TYR	N-CA-C	5.58	122.69	110.80
1	A	195	TYR	CB-CA-C	-5.54	99.22	109.29
1	A	84	ALA	N-CA-C	-5.51	106.39	113.23
1	A	126	VAL	N-CA-CB	-5.50	103.53	110.57
1	A	90	LEU	CA-C-N	-5.47	113.15	120.54
1	A	90	LEU	C-N-CA	-5.47	113.15	120.54
1	A	195	TYR	N-CA-C	-5.45	106.80	113.50
1	A	194	LEU	O-C-N	5.43	128.24	122.38
1	A	143	PHE	N-CA-C	-5.40	104.63	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	LEU	N-CA-C	-5.32	106.62	113.01
1	A	103	ARG	N-CA-C	5.27	118.00	107.62
1	A	189	ASP	N-CA-C	-5.22	104.53	112.04
1	A	146	PHE	N-CA-C	5.21	116.96	111.28
1	A	190	THR	N-CA-C	-5.20	105.73	111.71
1	A	129	GLU	N-CA-C	5.18	117.59	111.33
1	A	152	VAL	CB-CA-C	-5.06	105.49	111.97
1	A	145	SER	N-CA-CB	-5.05	102.69	110.12
1	A	125	GLN	N-CA-C	5.05	117.68	111.82
1	A	6	ARG	CA-C-N	-5.03	112.87	122.53
1	A	6	ARG	C-N-CA	-5.03	112.87	122.53

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
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	127	0
All	All	1148	0	1093	127	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 57.

All (127) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.15
1:A:157:LYS:HD3	1:A:159:MET:HE2	1.29	1.08
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:HG3	1:A:83:MET:O	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:105:ALA:C	1:A:108:LEU:HB2	2.02	0.82
1:A:104:ALA:C	1:A:106:SER:CB	2.52	0.81
1:A:103:ARG:O	1:A:103:ARG:CG	2.30	0.79
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:CD	1:A:159:MET:HE2	2.12	0.76
1:A:107:ASP:O	1:A:111:GLN:CB	2.30	0.75
1:A:112:LEU:O	1:A:113:HIS:C	2.30	0.74
1:A:157:LYS:HD3	1:A:159:MET:CE	2.14	0.74
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:25:SER:C	1:A:27:PHE:H	2.01	0.68
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:136:ASN:HD22	1:A:136:ASN:C	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:5:ASN:C	1:A:7:GLU:H	2.07	0.62
1:A:136:ASN:HD22	1:A:139:ARG:H	1.45	0.62
1:A:105:ALA:HB1	1:A:146:PHE:HD1	1.66	0.61
1:A:5:ASN:C	1:A:7:GLU:N	2.59	0.59
1:A:15:TYR:CG	1:A:91:ARG:HG2	2.38	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:O	1:A:107:ASP:OD1	2.23	0.57
1:A:132:ARG:O	1:A:132:ARG:HG3	2.03	0.57
1:A:26:GLN:CD	1:A:26:GLN:H	2.13	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:107:ASP:C	1:A:111:GLN:HB2	2.30	0.55
1:A:101:TYR:HD1	1:A:103:ARG:CG	2.19	0.52
1:A:96:GLU:HG3	1:A:97:PHE:N	2.22	0.52
1:A:136:ASN:ND2	1:A:136:ASN:C	2.69	0.51
1:A:179:GLU:HA	1:A:179:GLU:OE1	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:NH2	1:A:132:ARG:HG2	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:106:SER:HA	1:A:109:THR:HG1	1.78	0.48
1:A:127:VAL:O	1:A:128:ASN:C	2.51	0.48
1:A:123:PHE:CE2	1:A:169:TRP:HB3	2.49	0.48
1:A:120:TYR:O	1:A:121:GLN:C	2.55	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:191:PHE:O	1:A:195:TYR:HB2	2.15	0.47
1:A:178:LEU:C	1:A:180:PRO:HD2	2.39	0.47
1:A:136:ASN:HA	1:A:181:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HA	1:A:17:LEU:HD23	1.70	0.47
1:A:99:LEU:N	1:A:99:LEU:HD23	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: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: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:83:MET:HE3	1:A:83:MET:HB2	1.44	0.45
1:A:88:GLN:HA	1:A:91:ARG:HD2	1.98	0.45
1:A:103:ARG:HG3	1:A:103:ARG:HH11	1.82	0.44
1:A:1:MET:C	1:A:1:MET:SD	2.99	0.44
1:A:17:LEU:HD22	1:A:22:TYR:HB2	1.99	0.44
1:A:123:PHE:HB2	1:A:169:TRP:CZ3	2.53	0.44
1:A:105:ALA:CA	1:A:106:SER:HB3	2.41	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:12:PHE:CD1	1:A:12:PHE:C	2.96	0.43
1:A:103:ARG:CG	1:A:103:ARG:HH11	2.30	0.43
1:A:171:ALA:O	1:A:172:THR:C	2.61	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:O	1:A:83:MET:CG	2.48	0.43
1:A:132:ARG:HG2	1:A:132:ARG:HH21	1.83	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:90:LEU:O	1:A:91:ARG:C	2.61	0.42
1:A:144:PHE:O	1:A:145:SER:C	2.59	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:CD2	1:A:22:TYR:N	2.87	0.42
1:A:127:VAL:HG12	1:A:131:PHE:HE2	1.85	0.42
1:A:123:PHE:O	1:A:124:GLU:C	2.64	0.41
1:A:123:PHE:CD1	1:A:169:TRP:HE3	2.38	0.41
1:A:166:ILE:O	1:A:167:ALA:C	2.63	0.41
1:A:181:TRP:O	1:A:182:ILE:C	2.62	0.40
1:A:101:TYR:CE1	1:A:103:ARG:NE	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:CG	1:A:103:ARG:NH1	2.84	0.40
1:A:140:ILE:O	1:A:143:PHE:HB3	2.21	0.40
1:A:5:ASN:HD22	1:A:5:ASN:HA	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%)	3	20

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%)	93 (77%)	28 (23%)	1	5

All (28) 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	86	VAL
1	A	87	LYS
1	A	88	GLN
1	A	98	GLU
1	A	99	LEU
1	A	100	ARG
1	A	103	ARG
1	A	111	GLN
1	A	114	ILE
1	A	121	GLN
1	A	122	SER
1	A	130	LEU
1	A	132	ARG
1	A	136	ASN
1	A	150	LEU
1	A	159	MET
1	A	163	VAL
1	A	164	SER
1	A	176	ASP
1	A	178	LEU
1	A	182	ILE
1	A	190	THR
1	A	193	ASP
1	A	194	LEU

Sometimes 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
1	A	19	GLN
1	A	88	GLN
1	A	113	HIS
1	A	125	GLN
1	A	136	ASN
1	A	175	ASN
1	A	183	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	0.03	7 (4%) 35 18	20, 43, 88, 113	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.0
1	A	101	TYR	3.2
1	A	107	ASP	3.1
1	A	111	GLN	2.8
1	A	99	LEU	2.6
1	A	2	SER	2.4
1	A	103	ARG	2.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.