



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:43 PM UTC

PDB ID : 2QLI / pdb_00002qli
Title : mPlum E16Q mutant
Authors : Shu, X.; Remington, S.J.
Deposited on : 2007-07-12
Resolution : 1.34 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
Mogul : 2022.3.0, CSD as543be (2022)
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

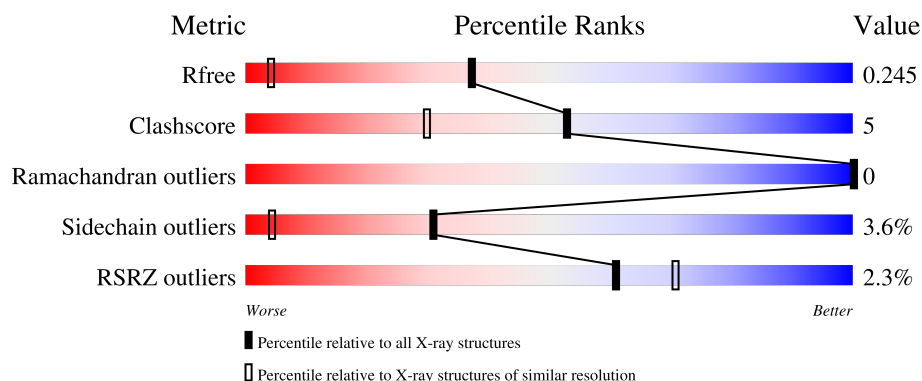
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	224	% 83% 11% • •
1	B	224	3% 76% 18% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3951 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 Fluorescent protein plum.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	2	0
			1730	1101	291	328	10			
1	B	216	Total	C	N	O	S	0	2	0
			1741	1107	291	333	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLN	GLU	engineered mutation	UNP Q5S3G7
B	16	GLN	GLU	engineered mutation	UNP Q5S3G7

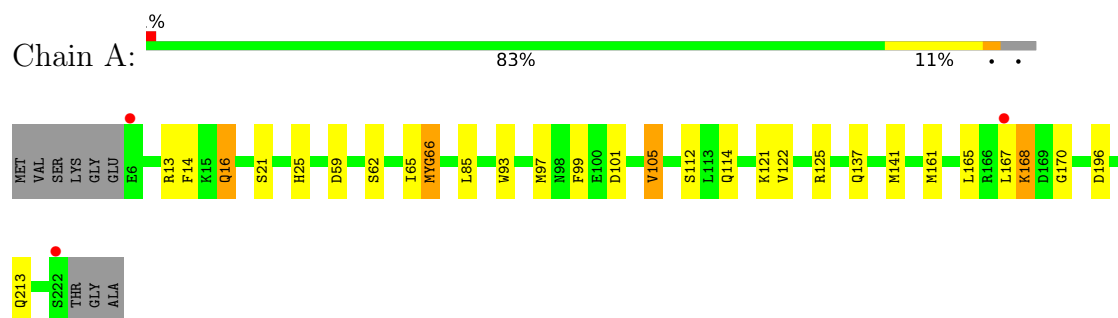
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	251	Total	O	0	0
			251	251		
2	B	229	Total	O	0	0
			229	229		

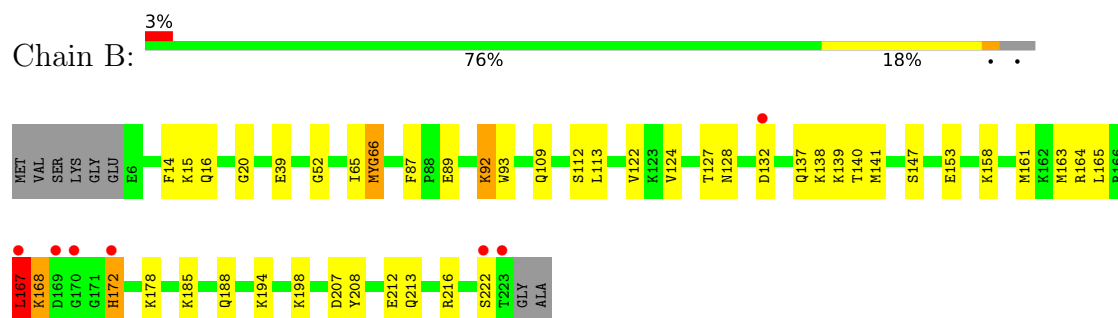
3 Residue-property plots [i](#)

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: Fluorescent protein plum



• Molecule 1: Fluorescent protein plum



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.16Å 77.90Å 96.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.34 10.00 – 1.34	Depositor EDS
% Data completeness (in resolution range)	87.8 (10.00-1.34) 85.7 (10.00-1.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.34Å)	Xtriage
Refinement program	SHELXL-97, TNT	Depositor
R, R_{free}	0.183 , 0.265 0.178 , 0.245	Depositor DCC
R_{free} test set	4791 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3951	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4429e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: NRQ

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	0.72	0/1753	1.55	17/2359 (0.7%)
1	B	0.67	0/1764	1.59	15/2373 (0.6%)
All	All	0.69	0/3517	1.57	32/4732 (0.7%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	SER	CA-C-N	13.47	145.95	121.70
1	B	222	SER	C-N-CA	13.47	145.95	121.70
1	A	125	ARG	CA-C-N	-10.87	114.68	122.18
1	A	125	ARG	C-N-CA	-10.87	114.68	122.18
1	A	16	GLN	OE1-CD-NE2	9.68	132.28	122.60
1	A	170	GLY	CA-C-N	-9.20	112.43	122.55
1	A	170	GLY	C-N-CA	-9.20	112.43	122.55
1	A	14	PHE	CA-CB-CG	9.15	122.95	113.80
1	B	132	ASP	CA-CB-CG	-9.06	103.54	112.60
1	B	172	HIS	CA-CB-CG	7.74	121.54	113.80
1	A	13	ARG	NE-CZ-NH2	-7.41	112.53	119.20
1	A	85	LEU	CA-C-O	7.39	128.43	119.49
1	B	167	LEU	CA-C-N	7.08	130.64	120.79
1	B	167	LEU	C-N-CA	7.08	130.64	120.79
1	B	112	SER	CA-C-O	-6.55	114.42	121.36
1	A	101	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	212	GLU	O-C-N	-6.37	114.91	123.19
1	B	93	TRP	CA-CB-CG	6.27	125.52	113.60
1	B	14	PHE	CA-CB-CG	6.21	120.01	113.80
1	B	168	LYS	O-C-N	6.12	128.63	122.08
1	B	87	PHE	CA-CB-CG	-5.84	107.96	113.80
1	B	15	LYS	CA-C-N	-5.51	113.19	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	LYS	C-N-CA	-5.51	113.19	122.29
1	B	188	GLN	N-CA-C	5.34	117.91	109.96
1	A	112	SER	CA-C-O	-5.31	115.56	121.51
1	A	137	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	114	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	16	GLN	CB-CG-CD	-5.20	103.76	112.60
1	A	93	TRP	CA-CB-CG	5.18	123.44	113.60
1	A	170	GLY	O-C-N	-5.13	116.85	122.65
1	A	121	LYS	CA-C-O	-5.04	114.91	120.30
1	A	196	ASP	CA-CB-CG	-5.01	107.59	112.60

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	1730	0	1666	9	0
1	B	1741	0	1679	25	0
2	A	251	0	0	0	0
2	B	229	0	0	6	0
All	All	3951	0	3345	34	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 (34) 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:97:MET:HB2	1:A:105[A]:VAL:HG13	1.59	0.84
1:A:141:MET:SD	1:A:168:LYS:HA	2.23	0.77
1:B:141:MET:SD	1:B:168:LYS:HA	2.29	0.72
1:A:62:SER:HA	1:A:65[B]:ILE:HD12	1.73	0.70
1:B:52:GLY:HA3	2:B:648:HOH:O	1.98	0.64
1:B:89:GLU:OE2	1:B:185:LYS:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:O	1:B:168:LYS:HG2	2.02	0.59
1:B:138:LYS:HE2	2:B:604:HOH:O	2.02	0.59
1:B:198:LYS:HE3	2:B:562:HOH:O	2.04	0.57
1:B:66:NRQ:HD2	1:B:161:MET:HE1	1.87	0.57
1:B:147:SER:OG	1:B:194:LYS:HE3	2.04	0.57
1:B:137:GLN:HB3	1:B:139:LYS:HE2	1.87	0.57
1:B:16:GLN:OE1	1:B:65[A]:ILE:HD12	2.05	0.56
1:B:65[B]:ILE:HB	1:B:66:NRQ:HB11	1.87	0.56
1:A:66:NRQ:HD2	1:A:161:MET:HE1	1.88	0.56
1:B:92:LYS:HG2	1:B:109:GLN:O	2.05	0.56
1:B:137:GLN:CB	1:B:139:LYS:HE2	2.36	0.56
1:B:207:ASP:O	1:B:208:TYR:HB2	2.10	0.52
1:B:140:THR:HG21	1:B:165:LEU:HD13	1.93	0.51
1:B:127[A]:THR:HG22	1:B:128:ASN:H	1.77	0.49
1:A:99:PHE:HE1	1:A:105[A]:VAL:HG12	1.79	0.47
1:B:153:GLU:OE1	1:B:158:LYS:HE2	2.14	0.47
1:B:16:GLN:OE1	1:B:65[A]:ILE:HG23	2.16	0.46
1:A:59:ASP:HB3	1:A:165:LEU:HD21	1.98	0.45
1:A:16:GLN:OE1	1:A:65[B]:ILE:HG23	2.17	0.45
1:B:20:GLY:HA3	1:B:124:VAL:O	2.16	0.44
1:A:21:SER:HA	1:A:25:HIS:O	2.17	0.44
1:B:216:ARG:NE	2:B:672:HOH:O	2.50	0.44
1:B:127[A]:THR:HG22	1:B:128:ASN:N	2.32	0.44
1:B:198:LYS:NZ	2:B:621:HOH:O	2.50	0.43
1:B:66:NRQ:CZ	1:B:163:MET:HE3	2.50	0.42
1:B:178:LYS:HD2	2:B:575:HOH:O	2.20	0.41
1:A:97:MET:HB2	1:A:105[A]:VAL:CG1	2.39	0.41
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.66	0.41

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	211/224 (94%)	207 (98%)	4 (2%)	0	100	100
1	B	212/224 (95%)	208 (98%)	4 (2%)	0	100	100
All	All	423/448 (94%)	415 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/189 (95%)	174 (97%)	6 (3%)	33	5
1	B	182/189 (96%)	174 (96%)	8 (4%)	25	2
All	All	362/378 (96%)	348 (96%)	14 (4%)	31	3

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105[A]	VAL
1	A	105[B]	VAL
1	A	122	VAL
1	A	167	LEU
1	A	168	LYS
1	A	213	GLN
1	B	39	GLU
1	B	92	LYS
1	B	113	LEU
1	B	122	VAL
1	B	164	ARG
1	B	167	LEU
1	B	172	HIS
1	B	213	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	NRQ	A	66	1	24,24,25	2.51	7 (29%)	24,32,34	2.70	11 (45%)
1	NRQ	B	66	1	24,24,25	2.42	8 (33%)	24,32,34	2.99	11 (45%)

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
1	NRQ	A	66	1	-	1/9/31/32	0/2/2/2
1	NRQ	B	66	1	-	3/9/31/32	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	NRQ	CA1-N1	5.81	1.40	1.27
1	A	66	NRQ	OH-CZ	-5.48	1.24	1.37
1	B	66	NRQ	C1-CA1	-4.72	1.41	1.48
1	B	66	NRQ	OH-CZ	-4.65	1.26	1.37
1	B	66	NRQ	CA1-N1	4.28	1.37	1.27
1	B	66	NRQ	CE2-CZ	4.08	1.46	1.39
1	A	66	NRQ	C1-N3	3.99	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	NRQ	CG2-CB2	-3.91	1.39	1.46
1	A	66	NRQ	CE1-CZ	3.91	1.46	1.39
1	A	66	NRQ	CE2-CZ	3.74	1.46	1.39
1	B	66	NRQ	C1-N3	3.51	1.43	1.38
1	A	66	NRQ	CG2-CB2	-3.47	1.40	1.46
1	B	66	NRQ	CE1-CZ	3.09	1.44	1.39
1	A	66	NRQ	CB2-CA2	2.32	1.37	1.35
1	B	66	NRQ	CB2-CA2	2.07	1.37	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	NRQ	O2-C2-CA2	8.35	136.35	131.02
1	B	66	NRQ	CD1-CE1-CZ	6.14	126.37	119.88
1	A	66	NRQ	CA2-C2-N3	6.07	108.60	103.50
1	A	66	NRQ	CB2-CA2-N2	5.51	136.24	128.76
1	A	66	NRQ	CB2-CA2-C2	-5.04	116.25	122.36
1	B	66	NRQ	CE1-CZ-CE2	-4.20	113.08	119.77
1	A	66	NRQ	C3-CA3-N3	3.81	121.10	112.43
1	B	66	NRQ	CG2-CB2-CA2	3.59	134.13	129.87
1	B	66	NRQ	CA2-C2-N3	3.52	106.46	103.50
1	B	66	NRQ	O2-C2-N3	-3.45	117.12	124.31
1	B	66	NRQ	CB2-CA2-N2	3.30	133.24	128.76
1	A	66	NRQ	CG2-CB2-CA2	-3.21	126.05	129.87
1	A	66	NRQ	O2-C2-CA2	3.16	133.04	131.02
1	A	66	NRQ	O3-C3-CA3	-2.93	112.29	125.47
1	A	66	NRQ	O2-C2-N3	-2.86	118.35	124.31
1	B	66	NRQ	CA2-N2-C1	2.83	109.30	104.09
1	B	66	NRQ	CB2-CA2-C2	-2.59	119.22	122.36
1	B	66	NRQ	CE2-CD2-CG2	2.49	124.44	121.22
1	B	66	NRQ	C2-CA2-N2	-2.41	107.22	108.95
1	A	66	NRQ	CE1-CZ-CE2	-2.34	116.04	119.77
1	A	66	NRQ	CD2-CE2-CZ	2.16	122.16	119.88
1	A	66	NRQ	C2-CA2-N2	-2.03	107.49	108.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	66	NRQ	C2-CA2-CB2-CG2
1	A	66	NRQ	CB1-CG1-SD-CE
1	B	66	NRQ	CB1-CG1-SD-CE

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Mol	Chain	Res	Type	Atoms
1	B	66	NRQ	N2-CA2-CB2-CG2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	NRQ	1	0
1	B	66	NRQ	3	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	66:NRQ	C3	69:SER	N	1.18

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	214/224 (95%)	-0.10	3 (1%) 73 82	14, 24, 36, 54	2 (0%)
1	B	215/224 (95%)	0.14	7 (3%) 49 60	15, 27, 48, 72	2 (0%)
All	All	429/448 (95%)	0.02	10 (2%) 61 71	14, 25, 43, 72	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	THR	6.4
1	B	172	HIS	3.7
1	A	222	SER	3.0
1	B	132	ASP	2.9
1	B	167	LEU	2.8
1	A	6	GLU	2.8
1	B	169	ASP	2.8
1	A	167	LEU	2.5
1	B	170	GLY	2.5
1	B	222	SER	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
1	NRQ	B	66	23/24	0.96	0.07	18,22,27,29	0
1	NRQ	A	66	23/24	0.97	0.06	17,21,24,25	0

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.