



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:01 PM EDT

PDB ID : 4TQL / pdb_00004tql
Title : Computationally designed three helix bundle
Authors : Nannenga, B.L.; Oberdorfer, G.; DiMaio, F.; Baker, D.; Gonen, T.
Deposited on : 2014-06-11
Resolution : 2.80 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

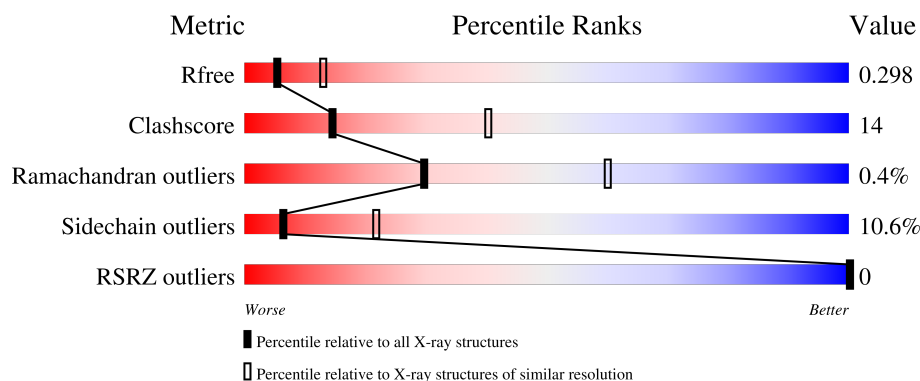
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	247	
1	B	247	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3888 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 Three helix bundle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1919	1221	328	353	17			
1	B	235	Total	C	N	O	S	0	0	0
			1962	1249	336	359	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	5	Total	O	0	0
			5	5		

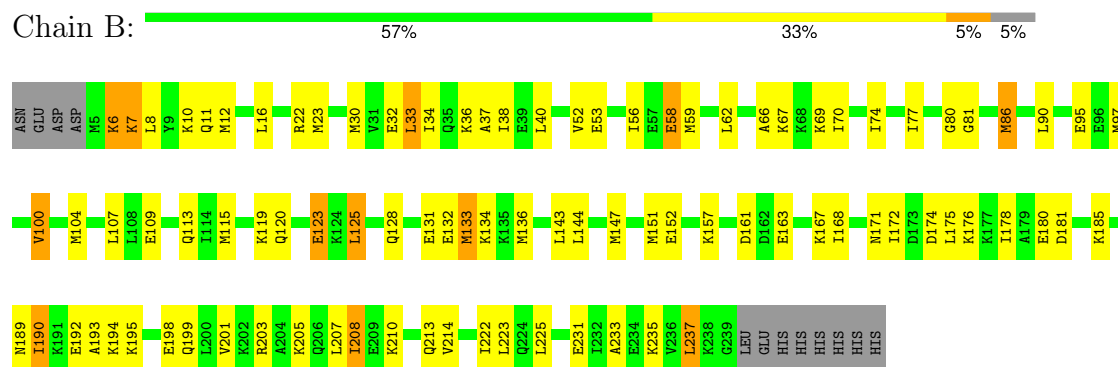
3 Residue-property plots [i](#)

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: Three helix bundle



• Molecule 1: Three helix bundle



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	24.88Å 41.55Å 133.20Å 98.94° 92.25° 90.06°	Depositor
Resolution (Å)	43.83 – 2.80 43.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (43.83-2.80) 93.9 (43.83-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.264 , 0.310 0.251 , 0.298	Depositor DCC
R_{free} test set	677 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l 0.400 for -h,k,-k-l 0.000 for -h,-k,k+l	Xtriage
Reported twinning fraction	0.500 for -h,k,-k-l	Depositor
Outliers	0 of 13451 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3888	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 26.19 % 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 2.7578e-03. 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 [i](#)

5.1 Standard geometry [i](#)

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	0.77	0/1921	1.02	1/2513 (0.0%)
1	B	0.77	0/1965	1.04	1/2571 (0.0%)
All	All	0.77	0/3886	1.03	2/5084 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	GLU	N-CA-C	-5.62	106.35	113.43
1	A	13	VAL	N-CA-C	-5.19	107.34	111.81

There are no chirality outliers.

There are no planarity outliers.

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	1919	0	2140	57	0
1	B	1962	0	2192	59	0
2	A	2	0	0	0	0
2	B	5	0	0	2	0
All	All	3888	0	4332	115	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 14.

All (115) 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:66:ALA:HB2	1:A:100:VAL:HG21	1.63	0.81
1:B:167:LYS:O	1:B:171:ASN:ND2	2.18	0.76
1:A:128:GLN:O	1:A:132:GLU:HG2	1.89	0.72
1:A:163:GLU:O	1:A:167:LYS:HG3	1.90	0.70
1:B:123:GLU:N	1:B:123:GLU:OE1	2.26	0.68
1:A:120:GLN:NE2	1:A:123:GLU:OE2	2.29	0.66
1:B:195:LYS:NZ	2:B:301:HOH:O	2.28	0.66
1:A:220:LYS:NZ	1:A:224:GLN:OE1	2.29	0.66
1:B:6:LYS:O	1:B:10:LYS:HG2	1.97	0.65
1:B:66:ALA:HB2	1:B:100:VAL:HG21	1.78	0.65
1:A:182:LEU:HD12	1:A:185:LYS:HE2	1.78	0.64
1:B:133:MET:HG3	1:B:190:ILE:HD12	1.80	0.64
1:A:67:LYS:HG3	1:A:225:LEU:HD11	1.78	0.64
1:B:12:MET:HE3	1:B:16:LEU:HD11	1.79	0.63
1:B:109:GLU:OE2	1:B:113:GLN:NE2	2.33	0.62
1:A:194:LYS:O	1:A:198:GLU:HG2	2.00	0.61
1:A:70:ILE:O	1:A:74:ILE:HG13	2.01	0.61
1:A:81:GLY:O	1:A:82:ASP:HB2	2.00	0.61
1:B:128:GLN:O	1:B:132:GLU:HG2	2.01	0.60
1:A:52:VAL:HG11	1:A:207:LEU:HB3	1.84	0.60
1:B:30:MET:HG2	1:B:136:MET:HE2	1.84	0.60
1:A:77:ILE:HG23	1:A:86:MET:HE3	1.83	0.59
1:B:12:MET:HG2	1:B:168:ILE:HD13	1.84	0.59
1:A:137:LYS:HG3	1:A:183:ILE:HD13	1.84	0.58
1:A:9:TYR:CE1	1:A:168:ILE:HG12	2.40	0.57
1:B:38:ILE:HD11	1:B:193:ALA:HB2	1.87	0.56
1:B:40:LEU:HD23	1:B:125:LEU:HD11	1.87	0.56
1:B:131:GLU:O	1:B:134:LYS:HB3	2.06	0.55
1:B:67:LYS:HG3	1:B:225:LEU:HD11	1.88	0.55
1:B:56:ILE:HA	1:B:59:MET:HE2	1.88	0.55
1:B:176:LYS:O	1:B:180:GLU:HG2	2.07	0.55
1:B:34:ILE:HD13	1:B:189:ASN:HB3	1.87	0.55
1:A:234:GLU:HA	1:A:237:LEU:HB2	1.89	0.54
1:B:22:ARG:HB3	1:B:143:LEU:HD11	1.88	0.54
1:B:131:GLU:OE1	1:B:134:LYS:HD2	2.07	0.54
1:A:176:LYS:O	1:A:180:GLU:HG2	2.08	0.54
1:A:27:TYR:CZ	1:A:185:LYS:HE3	2.42	0.54
1:A:34:ILE:HA	1:A:129:LEU:HD11	1.90	0.53
1:A:119:LYS:HE2	1:A:201:VAL:HG11	1.90	0.52
1:B:6:LYS:HB3	1:B:6:LYS:NZ	2.25	0.51
1:B:59:MET:HE1	1:B:214:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HZ1	1:B:205:LYS:HE3	1.75	0.50
1:B:77:ILE:HG23	1:B:86:MET:HE3	1.93	0.50
1:A:83:LYS:HD3	1:A:237:LEU:HD21	1.92	0.50
1:A:23:MET:HG2	1:A:140:MET:HG2	1.94	0.50
1:A:150:ARG:O	1:A:154:VAL:HG23	2.12	0.50
1:A:74:ILE:HG12	1:A:229:ALA:HB2	1.93	0.49
1:A:231:GLU:HB3	1:A:235:LYS:HZ2	1.77	0.49
1:A:202:LYS:HE3	1:A:206:GLN:NE2	2.28	0.49
1:B:7:LYS:HG3	1:B:8:LEU:N	2.28	0.49
1:B:185:LYS:NZ	2:B:302:HOH:O	2.42	0.49
1:A:202:LYS:HE3	1:A:206:GLN:HE22	1.77	0.49
1:B:174:ASP:O	1:B:178:ILE:HG12	2.13	0.49
1:A:137:LYS:HE2	1:A:141:GLU:OE2	2.13	0.48
1:B:11:GLN:HG2	1:B:11:GLN:O	2.12	0.48
1:B:77:ILE:C	1:B:80:GLY:H	2.21	0.48
1:A:231:GLU:O	1:A:235:LYS:HG3	2.13	0.48
1:B:199:GLN:O	1:B:203:ARG:HG2	2.14	0.48
1:A:76:GLN:OE1	1:A:89:LEU:HD21	2.13	0.48
1:B:194:LYS:O	1:B:198:GLU:HG2	2.14	0.47
1:A:231:GLU:HB3	1:A:235:LYS:NZ	2.28	0.47
1:B:52:VAL:HG11	1:B:207:LEU:HB3	1.95	0.47
1:A:43:LYS:NZ	1:B:120:GLN:OE1	2.48	0.47
1:A:69:LYS:HD3	1:A:96:GLU:CD	2.39	0.47
1:B:40:LEU:HB3	1:B:125:LEU:HD21	1.97	0.47
1:B:12:MET:HE3	1:B:16:LEU:CD1	2.45	0.46
1:B:163:GLU:O	1:B:167:LYS:HG3	2.16	0.46
1:A:9:TYR:OH	1:A:167:LYS:O	2.28	0.46
1:B:181:ASP:O	1:B:185:LYS:HG3	2.16	0.45
1:A:23:MET:HE3	1:A:179:ALA:HB2	1.98	0.45
1:B:37:ALA:O	1:B:40:LEU:HB2	2.16	0.45
1:A:9:TYR:CZ	1:A:167:LYS:HB3	2.52	0.45
1:B:36:LYS:O	1:B:40:LEU:HD13	2.17	0.45
1:A:12:MET:HG2	1:A:168:ILE:HD13	1.97	0.45
1:A:30:MET:HG2	1:A:136:MET:HE2	1.98	0.45
1:A:34:ILE:HD13	1:A:189:ASN:HB3	1.99	0.45
1:B:58:GLU:HB3	1:B:107:LEU:HD11	1.97	0.45
1:B:33:LEU:HD13	1:B:33:LEU:HA	1.83	0.45
1:A:23:MET:HE1	1:A:175:LEU:O	2.17	0.44
1:B:70:ILE:O	1:B:74:ILE:HG13	2.17	0.44
1:A:144:LEU:HD13	1:A:144:LEU:HA	1.83	0.44
1:B:237:LEU:HD22	1:B:237:LEU:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:O	1:A:218:LEU:HG	2.18	0.43
1:A:107:LEU:O	1:A:110:LYS:HB2	2.17	0.43
1:B:7:LYS:O	1:B:10:LYS:HB2	2.17	0.43
1:B:6:LYS:HG2	1:B:10:LYS:HE3	2.01	0.43
1:B:175:LEU:HA	1:B:178:ILE:HG12	1.98	0.43
1:B:151:MET:HE3	1:B:151:MET:HB3	1.85	0.43
1:A:108:LEU:HD11	1:A:212:LYS:HA	2.01	0.43
1:A:151:MET:HE3	1:A:151:MET:HB3	1.74	0.43
1:B:59:MET:HG2	1:B:104:MET:HG2	2.00	0.43
1:B:97:MET:HG3	1:B:222:ILE:HG21	2.00	0.42
1:A:99:LYS:O	1:A:103:LYS:HG3	2.20	0.42
1:A:179:ALA:O	1:A:183:ILE:HG13	2.20	0.42
1:A:30:MET:HB2	1:A:136:MET:HG3	2.02	0.42
1:B:119:LYS:HE2	1:B:201:VAL:HG13	2.01	0.42
1:B:144:LEU:HD13	1:B:147:MET:HE3	2.01	0.42
1:A:41:MET:SD	1:A:197:ALA:HB2	2.60	0.42
1:A:174:ASP:O	1:A:178:ILE:HG12	2.20	0.42
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.86	0.42
1:B:97:MET:HE2	1:B:97:MET:HB3	1.83	0.42
1:B:157:LYS:HA	1:B:157:LYS:HD2	1.60	0.42
1:B:231:GLU:HB3	1:B:235:LYS:NZ	2.34	0.41
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.74	0.41
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.82	0.41
1:A:201:VAL:HG12	1:A:205:LYS:HD2	2.01	0.41
1:B:32:GLU:O	1:B:36:LYS:HG3	2.21	0.41
1:B:115:MET:SD	1:B:208:ILE:HD13	2.61	0.41
1:A:10:LYS:HD3	1:A:10:LYS:HA	1.76	0.40
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.85	0.40
1:B:233:ALA:O	1:B:237:LEU:HB2	2.21	0.40
1:A:73:MET:O	1:A:76:GLN:HB2	2.21	0.40
1:A:180:GLU:O	1:A:184:LYS:HG2	2.21	0.40
1:A:86:MET:O	1:A:90:LEU:HD12	2.21	0.40
1:B:22:ARG:CB	1:B:143:LEU:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	225/247 (91%)	217 (96%)	7 (3%)	1 (0%)	30	60
1	B	233/247 (94%)	226 (97%)	6 (3%)	1 (0%)	30	60
All	All	458/494 (93%)	443 (97%)	13 (3%)	2 (0%)	30	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	B	81	GLY

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	211/228 (92%)	189 (90%)	22 (10%)	7	22
1	B	215/228 (94%)	192 (89%)	23 (11%)	6	21
All	All	426/456 (93%)	381 (89%)	45 (11%)	6	22

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	33	LEU
1	A	35	GLN
1	A	53	GLU

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Mol	Chain	Res	Type
1	A	58	GLU
1	A	69	LYS
1	A	86	MET
1	A	90	LEU
1	A	95	GLU
1	A	100	VAL
1	A	123	GLU
1	A	125	LEU
1	A	133	MET
1	A	147	MET
1	A	152	GLU
1	A	175	LEU
1	A	190	ILE
1	A	208	ILE
1	A	210	LYS
1	A	213	GLN
1	A	223	LEU
1	A	237	LEU
1	B	6	LYS
1	B	7	LYS
1	B	23	MET
1	B	33	LEU
1	B	53	GLU
1	B	58	GLU
1	B	69	LYS
1	B	86	MET
1	B	90	LEU
1	B	95	GLU
1	B	100	VAL
1	B	123	GLU
1	B	125	LEU
1	B	133	MET
1	B	152	GLU
1	B	161	ASP
1	B	172	ILE
1	B	190	ILE
1	B	208	ILE
1	B	210	LYS
1	B	213	GLN
1	B	223	LEU
1	B	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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	229/247 (92%)	-1.33	0 100 100	20, 33, 56, 66	0
1	B	235/247 (95%)	-1.23	0 100 100	17, 34, 58, 80	0
All	All	464/494 (93%)	-1.28	0 100 100	17, 34, 57, 80	0

There are no RSRZ outliers to report.

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.