



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:07 PM UTC

PDB ID : 2AQL / pdb_00002aql
Title : Crystal Structure of the MRG15 MRG domain
Authors : Quioco, F.A.; Bowman, B.R.
Deposited on : 2005-08-18
Resolution : 2.30 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

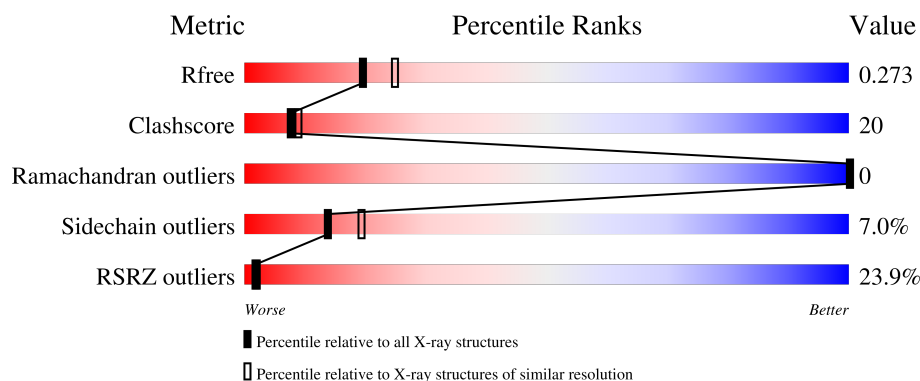
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	173	18% 57% 30% 5% 9%
1	B	173	25% 53% 28% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2648 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 Mortality factor 4-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1301	855	207	236	3			
1	B	152	Total	C	N	O	S	0	0	0
			1244	819	197	225	3			

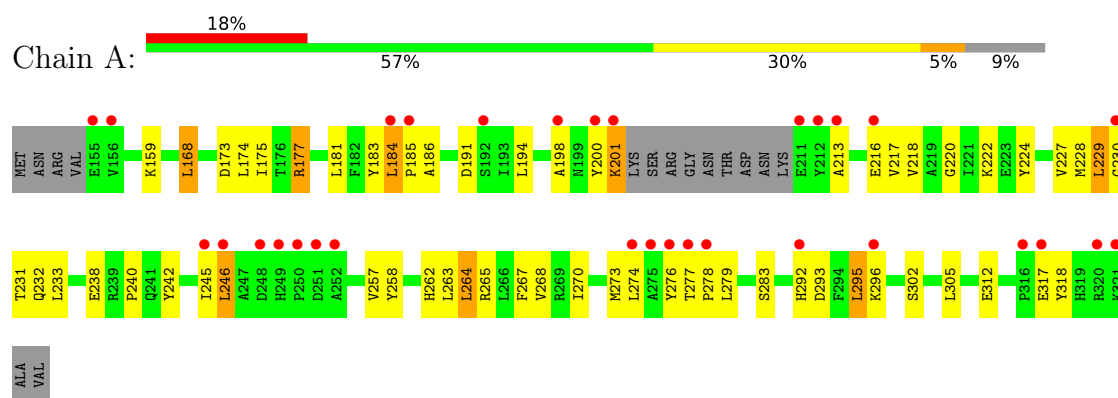
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	33	Total	O	0	0
			33	33		

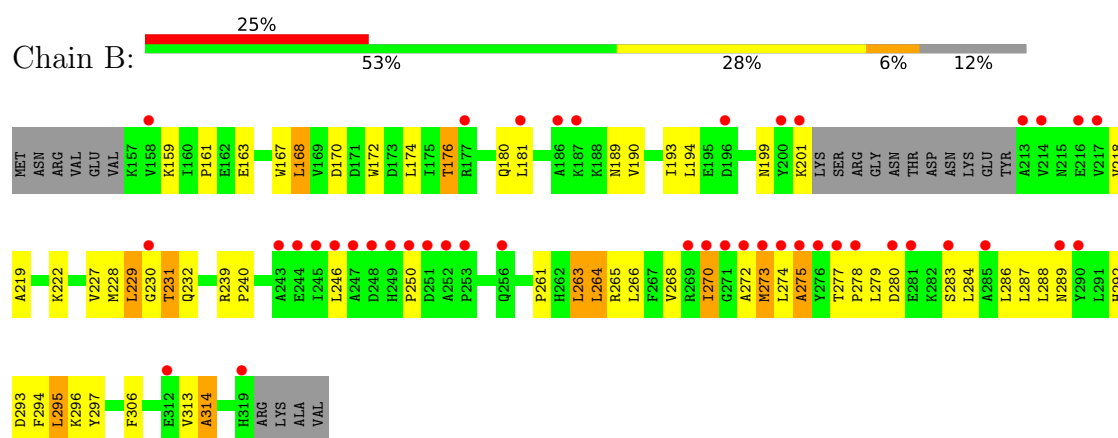
3 Residue-property plots

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: Mortality factor 4-like protein 1



• Molecule 1: Mortality factor 4-like protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	111.20Å 111.20Å 84.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.86 – 2.30 41.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (41.86-2.30) 97.0 (41.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.273 0.244 , 0.273	Depositor DCC
R_{free} test set	1666 reflections (7.25%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2648	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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	0.48	0/1336	1.09	8/1815 (0.4%)
1	B	0.46	1/1278 (0.1%)	1.04	5/1738 (0.3%)
All	All	0.47	1/2614 (0.0%)	1.06	13/3553 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	ALA	N-CA	5.27	1.53	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ALA	N-CA-C	16.99	133.11	112.38
1	A	184	LEU	CA-C-N	-12.83	103.80	119.84
1	A	184	LEU	C-N-CA	-12.83	103.80	119.84
1	A	184	LEU	N-CA-C	9.95	125.69	112.35
1	B	176	THR	N-CA-C	7.48	119.52	111.36
1	A	175	ILE	N-CA-C	7.47	117.54	110.74
1	A	233	LEU	N-CA-C	6.47	121.18	113.16
1	A	185	PRO	N-CA-C	-6.28	99.54	112.47
1	A	302	SER	N-CA-C	6.14	118.47	111.11
1	B	314	ALA	CA-C-N	5.25	123.49	119.66
1	B	314	ALA	C-N-CA	5.25	123.49	119.66
1	A	305	LEU	N-CA-C	5.08	117.93	111.69
1	B	229	LEU	N-CA-C	-5.06	102.21	110.20

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	1301	0	1299	56	0
1	B	1244	0	1243	61	0
2	A	70	0	0	2	0
2	B	33	0	0	1	0
All	All	2648	0	2542	102	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 20.

All (102) 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:B:159:LYS:H	1:B:292:HIS:HE1	1.20	0.89
1:A:227:VAL:HG21	1:B:273:MET:HG2	1.58	0.85
1:A:184:LEU:O	1:A:186:ALA:N	2.10	0.85
1:B:180:GLN:HG2	1:B:313:VAL:HA	1.59	0.83
1:B:168:LEU:HD13	1:B:264:LEU:HD13	1.61	0.82
1:A:231:THR:HG23	1:A:232:GLN:HG2	1.61	0.80
1:B:181:LEU:HD13	1:B:314:ALA:HB2	1.65	0.79
1:B:270:ILE:HD13	1:B:273:MET:HB3	1.67	0.77
1:A:227:VAL:HG13	1:B:228:MET:HG2	1.67	0.76
1:A:267:PHE:CD2	1:A:295:LEU:HD11	2.23	0.74
1:B:180:GLN:C	1:B:181:LEU:HD12	2.13	0.73
1:A:279:LEU:HD21	1:B:277:THR:HA	1.69	0.73
1:A:229:LEU:HD13	1:A:230:GLY:N	2.05	0.72
1:A:224:TYR:HE2	1:A:273:MET:HG2	1.54	0.71
1:A:159:LYS:H	1:A:292:HIS:HE1	1.38	0.71
1:A:277:THR:HG22	1:A:279:LEU:H	1.55	0.71
1:A:159:LYS:N	1:A:292:HIS:HE1	1.89	0.70
1:B:277:THR:HG22	1:B:284:LEU:HB2	1.74	0.70
1:B:181:LEU:CD1	1:B:314:ALA:HB2	2.21	0.69
1:A:168:LEU:HD13	1:A:264:LEU:HD13	1.76	0.67
1:A:227:VAL:HG21	1:B:273:MET:CG	2.23	0.67
1:A:240:PRO:HG2	1:A:318:TYR:CZ	2.31	0.66
1:B:194:LEU:HD12	1:B:222:LYS:HZ3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:HA	1:A:296:LYS:HE2	1.79	0.64
1:A:245:ILE:HG12	1:A:257:VAL:HG11	1.79	0.64
1:A:224:TYR:HE1	1:B:275:ALA:HB3	1.64	0.63
1:A:242:TYR:O	1:A:245:ILE:HG22	1.98	0.63
1:B:168:LEU:CD1	1:B:264:LEU:HD13	2.28	0.63
1:B:231:THR:CG2	1:B:232:GLN:HG2	2.29	0.62
1:B:231:THR:HG23	1:B:232:GLN:HG2	1.81	0.62
1:B:229:LEU:HD13	1:B:230:GLY:N	2.15	0.61
1:B:246:LEU:HD22	1:B:250:PRO:HA	1.82	0.61
1:B:194:LEU:HD12	1:B:222:LYS:NZ	2.16	0.60
1:A:220:GLY:HA2	1:B:275:ALA:HB1	1.84	0.60
1:B:265:ARG:O	1:B:268:VAL:HG22	2.01	0.60
1:A:276:TYR:HE2	1:B:219:ALA:HB1	1.67	0.59
1:A:227:VAL:O	1:B:231:THR:HG21	2.01	0.59
1:A:228:MET:SD	1:A:273:MET:HE2	2.42	0.59
1:B:199:ASN:O	1:B:201:LYS:HG3	2.03	0.59
1:A:277:THR:CG2	1:A:279:LEU:HG	2.33	0.59
1:A:159:LYS:H	1:A:292:HIS:CE1	2.18	0.58
1:B:170:ASP:O	1:B:174:LEU:HD23	2.04	0.57
1:A:265:ARG:O	1:A:268:VAL:HG22	2.04	0.57
1:B:194:LEU:HB3	1:B:218:VAL:HG13	1.87	0.56
1:A:227:VAL:CG1	1:B:228:MET:HG2	2.35	0.56
1:B:159:LYS:N	1:B:292:HIS:HE1	1.95	0.55
1:B:261:PRO:HD2	2:B:10:HOH:O	2.07	0.55
1:A:213:ALA:O	1:A:217:VAL:HG23	2.06	0.54
1:A:224:TYR:CE2	1:A:273:MET:HG2	2.40	0.54
1:B:239:ARG:HB2	1:B:240:PRO:HD3	1.91	0.53
1:A:279:LEU:HB3	1:A:283:SER:OG	2.08	0.53
1:B:273:MET:HA	1:B:273:MET:HE2	1.88	0.53
1:B:172:TRP:O	1:B:176:THR:HB	2.10	0.52
1:A:224:TYR:CD1	1:B:273:MET:HE1	2.45	0.51
1:A:277:THR:HG23	1:A:278:PRO:HD2	1.92	0.50
1:A:240:PRO:HG2	1:A:318:TYR:OH	2.11	0.50
1:B:294:PHE:O	1:B:297:TYR:HB3	2.12	0.50
1:A:200:TYR:O	1:A:201:LYS:HB2	2.12	0.50
1:B:161:PRO:HD3	1:B:295:LEU:HG	1.94	0.49
1:B:284:LEU:O	1:B:288:LEU:HB2	2.13	0.49
1:A:216:GLU:OE1	1:B:278:PRO:HB2	2.12	0.49
1:A:278:PRO:HG3	1:B:287:LEU:HD22	1.96	0.48
1:A:267:PHE:CG	1:A:295:LEU:HD11	2.48	0.48
1:B:228:MET:SD	1:B:273:MET:HG3	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLY:O	1:A:224:TYR:HD1	1.97	0.48
1:B:159:LYS:H	1:B:292:HIS:CE1	2.12	0.48
1:B:180:GLN:HG2	1:B:313:VAL:CA	2.38	0.48
1:A:168:LEU:CD1	1:A:264:LEU:HD13	2.43	0.47
1:A:231:THR:HG21	1:B:227:VAL:O	2.15	0.47
1:A:173:ASP:OD2	1:A:177:ARG:NH1	2.47	0.47
1:B:167:TRP:CD2	1:B:306:PHE:HB3	2.50	0.46
1:B:277:THR:N	1:B:278:PRO:CD	2.78	0.46
1:B:270:ILE:HD12	1:B:274:LEU:CD2	2.45	0.46
1:A:191:ASP:OD2	1:A:222:LYS:HD2	2.15	0.46
1:A:198:ALA:O	1:A:201:LYS:HD3	2.15	0.46
1:A:183:TYR:HD1	1:A:312:GLU:OE2	1.99	0.45
1:A:220:GLY:CA	1:B:275:ALA:HB1	2.46	0.45
1:A:238:GLU:OE1	1:A:262:HIS:HE1	1.99	0.45
1:B:170:ASP:O	1:B:174:LEU:CD2	2.64	0.45
1:B:266:LEU:O	1:B:270:ILE:HB	2.17	0.45
1:B:286:LEU:O	1:B:289:ASN:HB2	2.17	0.45
1:B:168:LEU:HD12	1:B:168:LEU:HA	1.88	0.44
1:A:168:LEU:HD13	1:A:264:LEU:CD1	2.46	0.44
1:A:262:HIS:HD2	2:A:1:HOH:O	2.01	0.44
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.32	0.43
1:B:229:LEU:HD13	1:B:229:LEU:C	2.42	0.43
1:B:167:TRP:CE2	1:B:306:PHE:HB3	2.54	0.43
1:A:184:LEU:HD11	1:A:258:TYR:CZ	2.53	0.43
1:B:280:ASP:OD2	1:B:283:SER:HB3	2.18	0.43
1:A:270:ILE:O	1:A:274:LEU:HG	2.20	0.42
1:B:272:ALA:C	1:B:274:LEU:H	2.27	0.41
1:B:189:ASN:O	1:B:193:ILE:HG13	2.20	0.41
1:A:246:LEU:HD22	1:B:239:ARG:CZ	2.51	0.41
1:A:274:LEU:C	1:A:276:TYR:N	2.76	0.41
1:B:293:ASP:HA	1:B:296:LYS:HD3	2.03	0.41
1:B:277:THR:C	1:B:279:LEU:N	2.78	0.41
1:B:168:LEU:HD13	1:B:264:LEU:CD1	2.42	0.40
1:A:201:LYS:HD3	1:A:201:LYS:N	2.36	0.40
1:A:292:HIS:HB3	2:A:70:HOH:O	2.20	0.40
1:A:194:LEU:HB3	1:A:218:VAL:HG13	2.04	0.40
1:A:277:THR:HG22	1:A:279:LEU:HG	2.01	0.40
1:B:190:VAL:HG22	1:B:263:LEU:HG	2.04	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	154/173 (89%)	148 (96%)	6 (4%)	0	100	100
1	B	148/173 (86%)	139 (94%)	9 (6%)	0	100	100
All	All	302/346 (87%)	287 (95%)	15 (5%)	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	139/152 (91%)	128 (92%)	11 (8%)	11	15
1	B	133/152 (88%)	125 (94%)	8 (6%)	17	25
All	All	272/304 (90%)	253 (93%)	19 (7%)	14	19

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	LEU
1	A	174	LEU
1	A	177	ARG
1	A	181	LEU
1	A	201	LYS
1	A	229	LEU
1	A	246	LEU
1	A	263	LEU

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Mol	Chain	Res	Type
1	A	264	LEU
1	A	295	LEU
1	A	317	GLU
1	B	163	GLU
1	B	168	LEU
1	B	231	THR
1	B	263	LEU
1	B	264	LEU
1	B	270	ILE
1	B	273	MET
1	B	295	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	215	ASN
1	A	232	GLN
1	A	241	GLN
1	A	262	HIS
1	A	292	HIS
1	B	180	GLN
1	B	232	GLN
1	B	262	HIS
1	B	289	ASN
1	B	292	HIS

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

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, 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	158/173 (91%)	1.04	31 (19%) 3 3	17, 30, 54, 64	0
1	B	152/173 (87%)	1.59	43 (28%) 1 1	22, 38, 60, 69	0
All	All	310/346 (89%)	1.31	74 (23%) 2 2	17, 35, 57, 69	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	LEU	8.7
1	B	247	ALA	7.6
1	B	213	ALA	6.4
1	A	320	ARG	6.3
1	B	249	HIS	6.1
1	B	248	ASP	5.5
1	B	271	GLY	5.2
1	B	275	ALA	4.2
1	B	283	SER	4.1
1	B	272	ALA	4.0
1	B	216	GLU	4.0
1	A	156	VAL	3.8
1	B	201	LYS	3.7
1	A	276	TYR	3.7
1	A	278	PRO	3.7
1	B	253	PRO	3.7
1	A	200	TYR	3.6
1	A	212	TYR	3.6
1	B	214	VAL	3.5
1	B	319	HIS	3.5
1	B	250	PRO	3.4
1	B	200	TYR	3.4
1	B	276	TYR	3.4
1	B	277	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	184	LEU	3.3
1	A	185	PRO	3.3
1	A	250	PRO	3.3
1	A	211	GLU	3.3
1	B	186	ALA	3.2
1	B	273	MET	3.2
1	A	249	HIS	3.2
1	B	269	ARG	3.1
1	B	280	ASP	3.1
1	B	270	ILE	3.1
1	A	248	ASP	3.0
1	B	251	ASP	3.0
1	A	230	GLY	3.0
1	B	196	ASP	3.0
1	B	246	LEU	2.9
1	A	275	ALA	2.9
1	A	213	ALA	2.8
1	A	252	ALA	2.8
1	B	244	GLU	2.7
1	B	158	VAL	2.6
1	B	278	PRO	2.6
1	B	230	GLY	2.6
1	A	246	LEU	2.5
1	A	292	HIS	2.5
1	B	245	ILE	2.5
1	A	155	GLU	2.5
1	A	316	PRO	2.5
1	A	321	LYS	2.5
1	B	243	ALA	2.5
1	B	217	VAL	2.5
1	B	289	ASN	2.5
1	B	252	ALA	2.5
1	A	245	ILE	2.4
1	A	192	SER	2.4
1	B	290	TYR	2.4
1	A	198	ALA	2.4
1	A	317	GLU	2.3
1	A	201	LYS	2.3
1	B	312	GLU	2.2
1	B	281	GLU	2.2
1	B	181	LEU	2.2
1	A	251	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	187	LYS	2.1
1	A	277	THR	2.1
1	A	296	LYS	2.1
1	B	256	GLN	2.1
1	B	285	ALA	2.1
1	B	177	ARG	2.1
1	A	216	GLU	2.0
1	A	274	LEU	2.0

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.