



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:21 AM GMT

PDB ID : 2GTH
Title : crystal structure of the wildtype MHV coronavirus non-structural protein nsp15
Authors : Xu, X.; Zhai, Y.; Sun, F.; Lou, Z.; Su, D.; Rao, Z.
Deposited on : 2006-04-28
Resolution : 2.70 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 ⓘ](#)) 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

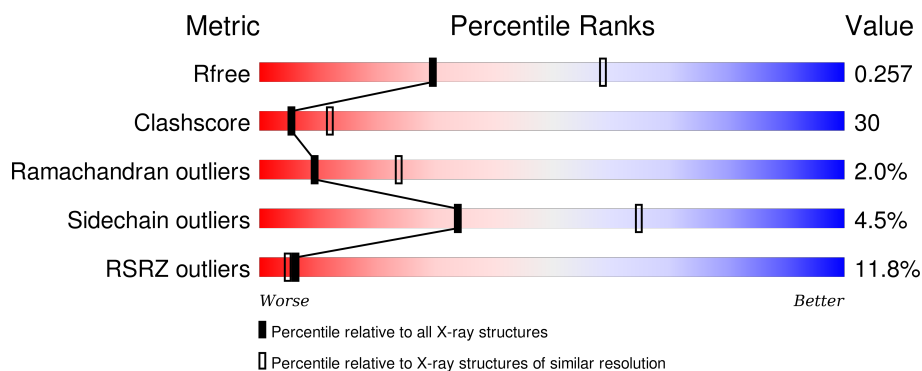
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	370	<div> <div>11%</div> <div>54%</div> <div>37%</div> <div>• 6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3014 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 Replicase polypeptide 1ab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	348	2764	1762	462	526	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	UNP P16342

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	250	Total	O	0	0
			250	250		

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.44Å 86.44Å 219.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 43.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 96.0 (43.22-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.256 0.196 , 0.257	Depositor DCC
R_{free} test set	517 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 76.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 10397 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3014	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	0/2817	0.72	0/3807

There are no bond length outliers.

There are no bond angle outliers.

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	2764	0	2732	164	0
2	A	250	0	0	42	0
All	All	3014	0	2732	164	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 30.

All (164) 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:254:SER:HA	1:A:256:GLN:HE21	1.13	1.12
1:A:147:MET:HE3	2:A:594:HOH:O	1.62	0.97
1:A:303:ILE:HG12	1:A:366:VAL:HG21	1.48	0.94
1:A:339:LEU:HD11	1:A:361:CYS:HA	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:O	1:A:331:VAL:HG12	1.69	0.91
1:A:333:ILE:HG22	2:A:492:HOH:O	1.76	0.83
1:A:339:LEU:HD21	1:A:361:CYS:HA	1.64	0.78
1:A:231:PHE:CE2	1:A:280:ILE:HG13	2.18	0.78
1:A:337:LEU:HD13	1:A:359:LEU:HD22	1.67	0.77
1:A:168:ASP:HB3	2:A:559:HOH:O	1.83	0.76
1:A:317:LYS:HD2	1:A:320:CYS:HB2	1.67	0.76
1:A:320:CYS:HB3	2:A:471:HOH:O	1.85	0.76
1:A:300:ASP:HA	2:A:385:HOH:O	1.85	0.74
1:A:329:ASP:O	1:A:333:ILE:HG12	1.87	0.74
1:A:87:ASP:HB2	2:A:510:HOH:O	1.88	0.73
1:A:331:VAL:O	1:A:334:VAL:HG22	1.90	0.71
1:A:251:ALA:HA	1:A:256:GLN:HE22	1.56	0.71
1:A:128:PHE:CZ	1:A:176:ARG:HG3	2.25	0.71
1:A:293:ILE:HG23	1:A:306:TYR:HB3	1.75	0.67
1:A:252:LYS:HD3	1:A:253:TYR:CZ	2.30	0.67
1:A:339:LEU:CD1	1:A:361:CYS:HA	2.24	0.67
1:A:295:GLU:HG2	1:A:298:THR:HG23	1.77	0.67
1:A:298:THR:HB	2:A:449:HOH:O	1.95	0.66
1:A:110:ILE:HG22	1:A:113:LEU:HD12	1.77	0.66
1:A:340:LYS:HE3	1:A:340:LYS:HA	1.78	0.65
1:A:135:VAL:HB	2:A:612:HOH:O	1.97	0.65
1:A:228:LEU:CD1	1:A:286:GLN:HE21	2.10	0.65
1:A:87:ASP:HB3	1:A:90:LYS:HB3	1.77	0.65
1:A:252:LYS:HD3	1:A:253:TYR:CE1	2.33	0.64
1:A:300:ASP:HB2	2:A:403:HOH:O	1.97	0.64
1:A:295:GLU:HG2	1:A:298:THR:CG2	2.29	0.62
1:A:339:LEU:HD11	1:A:361:CYS:CA	2.27	0.62
1:A:242:MET:CE	1:A:280:ILE:HG12	2.29	0.62
1:A:303:ILE:HG12	1:A:366:VAL:CG2	2.26	0.62
1:A:132:ARG:HD3	2:A:401:HOH:O	1.99	0.62
1:A:97:SER:HA	2:A:406:HOH:O	1.99	0.61
1:A:0:SER:N	2:A:407:HOH:O	2.28	0.61
1:A:26:VAL:C	1:A:27:ILE:HD12	2.21	0.61
1:A:261:GLU:HB2	2:A:560:HOH:O	1.99	0.60
1:A:241:PHE:HD2	1:A:242:MET:CE	2.14	0.60
1:A:273:ILE:O	1:A:317:LYS:HE2	2.02	0.60
1:A:228:LEU:HD12	1:A:286:GLN:HE21	1.66	0.59
1:A:77:ILE:HG13	2:A:612:HOH:O	2.02	0.59
1:A:339:LEU:HD21	1:A:361:CYS:CA	2.31	0.58
1:A:272:ILE:N	1:A:272:ILE:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HD3	1:A:166:ASP:HA	1.86	0.57
1:A:27:ILE:N	1:A:27:ILE:HD12	2.19	0.56
1:A:246:ASP:O	1:A:250:ILE:HG13	2.05	0.56
1:A:185:SER:HB2	2:A:494:HOH:O	2.05	0.56
1:A:94:PHE:HA	2:A:510:HOH:O	2.04	0.56
1:A:6:VAL:HG21	1:A:24:CYS:SG	2.46	0.56
1:A:303:ILE:CG1	1:A:366:VAL:HG21	2.31	0.56
1:A:242:MET:HE1	1:A:280:ILE:HG12	1.86	0.56
1:A:339:LEU:CD2	1:A:361:CYS:HA	2.34	0.56
1:A:219:GLY:HA2	1:A:349:ASN:OD1	2.06	0.56
1:A:339:LEU:HA	2:A:457:HOH:O	2.06	0.55
1:A:262:HIS:NE2	1:A:363:GLU:OE1	2.34	0.55
1:A:234:ARG:NH2	2:A:419:HOH:O	2.37	0.54
1:A:237:MET:HE1	1:A:327:LEU:C	2.29	0.53
1:A:128:PHE:CD1	1:A:136:TYR:HB2	2.44	0.53
1:A:307:PHE:CE1	1:A:318:SER:HA	2.43	0.53
1:A:147:MET:CE	2:A:594:HOH:O	2.37	0.53
1:A:141:LYS:HD2	1:A:172:TRP:CZ2	2.44	0.53
1:A:0:SER:HA	2:A:551:HOH:O	2.09	0.52
1:A:90:LYS:HE2	2:A:510:HOH:O	2.10	0.52
1:A:47:THR:HG22	1:A:92:SER:OG	2.10	0.52
1:A:170:GLU:HB2	2:A:485:HOH:O	2.08	0.52
1:A:337:LEU:HA	2:A:554:HOH:O	2.10	0.52
1:A:98:THR:HA	2:A:372:HOH:O	2.08	0.52
1:A:339:LEU:HD13	1:A:359:LEU:HD11	1.92	0.51
1:A:359:LEU:HG	1:A:359:LEU:O	2.10	0.51
1:A:241:PHE:HD2	1:A:242:MET:HE2	1.75	0.51
1:A:128:PHE:CG	1:A:136:TYR:HB2	2.45	0.51
1:A:346:VAL:HG13	1:A:357:PHE:HB2	1.92	0.51
1:A:339:LEU:O	1:A:340:LYS:HE3	2.09	0.51
1:A:338:ASN:ND2	2:A:585:HOH:O	2.43	0.51
1:A:343:SER:HB2	1:A:360:TRP:CZ3	2.45	0.51
1:A:71:LEU:HD23	1:A:351:ASP:HB3	1.92	0.51
1:A:66:HIS:CE1	1:A:155:ASP:HB3	2.46	0.51
1:A:87:ASP:O	1:A:91:ASP:N	2.45	0.50
1:A:293:ILE:N	1:A:293:ILE:HD12	2.26	0.50
1:A:237:MET:HE3	1:A:327:LEU:HB3	1.94	0.50
1:A:98:THR:O	1:A:106:ASP:HA	2.12	0.50
1:A:291:LEU:HD22	1:A:308:ILE:HG23	1.93	0.50
1:A:159:VAL:HA	2:A:609:HOH:O	2.12	0.50
1:A:65:PRO:HG3	1:A:156:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:O	1:A:6:VAL:HG23	2.12	0.49
1:A:360:TRP:C	1:A:362:ASN:H	2.15	0.49
1:A:345:VAL:HG22	2:A:433:HOH:O	2.12	0.49
1:A:233:PRO:HG3	1:A:242:MET:HG3	1.94	0.49
1:A:254:SER:HA	1:A:256:GLN:NE2	1.99	0.49
1:A:294:GLN:HB2	1:A:307:PHE:HB3	1.94	0.49
1:A:140:THR:HA	2:A:587:HOH:O	2.13	0.49
1:A:80:CYS:HB3	1:A:83:HIS:CE1	2.47	0.49
1:A:242:MET:HE2	1:A:284:ARG:HB2	1.94	0.48
1:A:79:VAL:HG22	1:A:80:CYS:N	2.28	0.48
1:A:3:GLU:HG3	1:A:22:LEU:O	2.13	0.48
1:A:340:LYS:CE	1:A:340:LYS:HA	2.43	0.48
1:A:325:LEU:HD13	2:A:436:HOH:O	2.14	0.47
1:A:237:MET:CE	1:A:327:LEU:HB3	2.45	0.47
1:A:87:ASP:CB	2:A:510:HOH:O	2.54	0.47
1:A:141:LYS:HD2	1:A:172:TRP:CH2	2.50	0.47
1:A:237:MET:CE	1:A:328:ASP:N	2.78	0.47
1:A:241:PHE:CD2	1:A:242:MET:HE2	2.50	0.47
1:A:93:VAL:C	2:A:510:HOH:O	2.53	0.47
1:A:242:MET:HE1	1:A:280:ILE:O	2.15	0.46
1:A:18:ARG:HB3	2:A:599:HOH:O	2.13	0.46
1:A:253:TYR:O	1:A:254:SER:C	2.53	0.46
1:A:360:TRP:O	1:A:362:ASN:N	2.49	0.46
1:A:152:GLN:HB3	2:A:395:HOH:O	2.15	0.46
1:A:237:MET:HE2	1:A:328:ASP:N	2.30	0.46
1:A:337:LEU:HD13	1:A:359:LEU:CD2	2.44	0.45
1:A:217:ALA:C	1:A:219:GLY:H	2.20	0.45
1:A:8:ASN:HB3	1:A:14:HIS:O	2.17	0.45
1:A:255:LEU:HD13	1:A:260:PHE:CE2	2.52	0.45
1:A:272:ILE:HA	1:A:316:SER:O	2.17	0.45
1:A:25:ALA:HB1	1:A:27:ILE:HD11	1.98	0.45
1:A:360:TRP:C	1:A:362:ASN:N	2.70	0.45
1:A:242:MET:HE3	1:A:280:ILE:HG12	1.96	0.44
1:A:226:ARG:CZ	1:A:231:PHE:CZ	3.01	0.44
1:A:284:ARG:O	1:A:287:GLN:HB2	2.17	0.44
1:A:285:ARG:O	1:A:287:GLN:N	2.51	0.44
1:A:16:ASP:OD1	1:A:18:ARG:NH2	2.39	0.44
1:A:338:ASN:HB3	2:A:513:HOH:O	2.17	0.44
1:A:307:PHE:CZ	1:A:318:SER:HA	2.52	0.44
1:A:308:ILE:HG13	2:A:471:HOH:O	2.18	0.44
1:A:128:PHE:CE1	1:A:176:ARG:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:HD21	1:A:361:CYS:C	2.38	0.43
1:A:329:ASP:HB3	2:A:436:HOH:O	2.18	0.43
1:A:52:ASN:O	1:A:55:VAL:HG12	2.19	0.43
1:A:9:LEU:HD12	1:A:9:LEU:HA	1.83	0.43
1:A:339:LEU:HD21	1:A:361:CYS:O	2.18	0.43
1:A:27:ILE:CD1	1:A:27:ILE:N	2.82	0.43
1:A:320:CYS:HA	2:A:453:HOH:O	2.19	0.42
1:A:95:CYS:HB2	2:A:384:HOH:O	2.20	0.42
1:A:255:LEU:HD13	1:A:260:PHE:CD2	2.53	0.42
1:A:47:THR:HB	1:A:48:PRO:HD2	2.01	0.42
1:A:291:LEU:HD22	1:A:308:ILE:CG2	2.48	0.42
1:A:131:CYS:O	1:A:176:ARG:NH1	2.52	0.42
1:A:257:ASP:O	1:A:258:TYR:CD2	2.73	0.42
1:A:356:GLN:HB3	1:A:356:GLN:HE21	1.66	0.42
1:A:255:LEU:O	1:A:256:GLN:C	2.57	0.42
1:A:231:PHE:CZ	1:A:280:ILE:HG13	2.53	0.42
1:A:261:GLU:O	1:A:265:TYR:HB2	2.19	0.42
1:A:36:GLN:HA	1:A:36:GLN:OE1	2.19	0.42
1:A:303:ILE:HD11	1:A:323:ILE:HD12	2.02	0.42
1:A:285:ARG:C	1:A:287:GLN:N	2.73	0.42
1:A:99:TYR:O	1:A:100:LYS:HB2	2.20	0.42
1:A:339:LEU:CG	1:A:361:CYS:HA	2.49	0.41
1:A:87:ASP:OD1	1:A:89:ALA:HB3	2.20	0.41
1:A:345:VAL:HG13	1:A:345:VAL:O	2.20	0.41
1:A:32:ILE:HD12	1:A:32:ILE:N	2.35	0.41
1:A:3:GLU:HB3	1:A:21:GLU:HB3	2.03	0.41
1:A:334:VAL:O	1:A:337:LEU:HB2	2.20	0.41
1:A:235:SER:OG	1:A:238:GLU:HG3	2.20	0.41
1:A:57:LEU:HD13	1:A:93:VAL:HG21	2.03	0.41
1:A:258:TYR:HA	2:A:588:HOH:O	2.21	0.40
1:A:46:ASN:ND2	2:A:467:HOH:O	2.47	0.40
1:A:147:MET:CE	1:A:172:TRP:HB3	2.51	0.40
1:A:231:PHE:HE2	1:A:280:ILE:HG13	1.76	0.40
1:A:349:ASN:HA	1:A:353:LYS:O	2.21	0.40
1:A:250:ILE:O	1:A:250:ILE:HG22	2.22	0.40
1:A:344:LYS:HG2	2:A:456:HOH:O	2.21	0.40
1:A:288:LYS:HA	2:A:511:HOH:O	2.22	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	344/370 (93%)	317 (92%)	20 (6%)	7 (2%)	9 24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	LEU
1	A	342	VAL
1	A	256	GLN
1	A	218	ARG
1	A	286	GLN
1	A	361	CYS
1	A	101	VAL

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	313/331 (95%)	299 (96%)	14 (4%)	34 65

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	16	ASP
1	A	37	ASN
1	A	109	CYS

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Mol	Chain	Res	Type
1	A	131	CYS
1	A	228	LEU
1	A	270	GLN
1	A	278	LEU
1	A	299	TYR
1	A	318	SER
1	A	338	ASN
1	A	340	LYS
1	A	354	ASP
1	A	365	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	269	ASN
1	A	286	GLN
1	A	287	GLN
1	A	338	ASN
1	A	356	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 [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

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	348/370 (94%)	0.33	41 (11%) 6 5	10, 26, 63, 76	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	VAL	4.9
1	A	258	TYR	4.7
1	A	362	ASN	4.4
1	A	368	THR	4.2
1	A	343	SER	4.0
1	A	338	ASN	3.7
1	A	361	CYS	3.7
1	A	253	TYR	3.5
1	A	360	TRP	3.5
1	A	166	ASP	3.4
1	A	260	PHE	3.3
1	A	236	GLU	3.3
1	A	235	SER	3.2
1	A	339	LEU	3.2
1	A	239	LYS	3.1
1	A	247	ASP	3.1
1	A	327	LEU	3.0
1	A	335	LYS	3.0
1	A	244	LEU	2.9
1	A	340	LYS	2.9
1	A	336	SER	2.7
1	A	326	LEU	2.6
1	A	257	ASP	2.6
1	A	249	PHE	2.5
1	A	359	LEU	2.5
1	A	240	ASP	2.4
1	A	234	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	237	MET	2.4
1	A	193	SER	2.3
1	A	369	PHE	2.3
1	A	256	GLN	2.3
1	A	261	GLU	2.2
1	A	242	MET	2.2
1	A	250	ILE	2.2
1	A	269	ASN	2.2
1	A	358	MET	2.2
1	A	344	LYS	2.1
1	A	255	LEU	2.1
1	A	289	SER	2.1
1	A	243	ASP	2.0
1	A	331	VAL	2.0

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.