



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 04:02 PM JST

PDB ID : 7CTN
Title : Structure of the 328-692 fragment of FlhA (E351A/D356A)
Authors : Kida, M.; Takekawa, N.; Kinoshita, M.; Inoue, Y.; Minamino, T.; Imada, K.
Deposited on : 2020-08-19
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

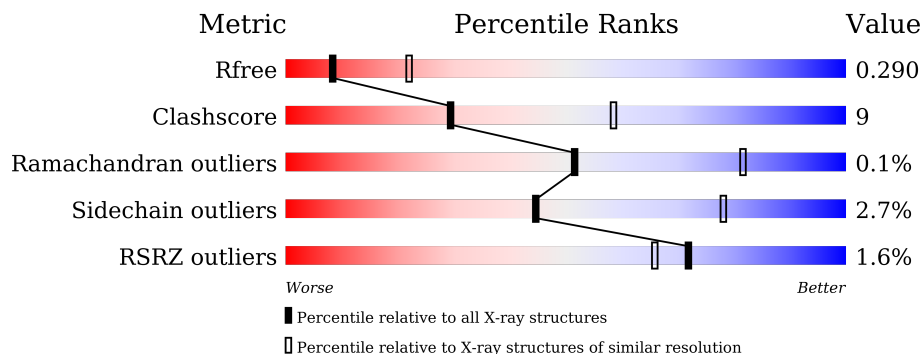
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	369	 2% 66% 26% • 7%
1	B	369	 % 73% 17% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5252 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 Flagellar biosynthesis protein FlhA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	345	Total	C	N	O	S	0	0	0
			2666	1688	476	493	9			
1	B	334	Total	C	N	O	S	0	0	0
			2586	1637	462	478	9			

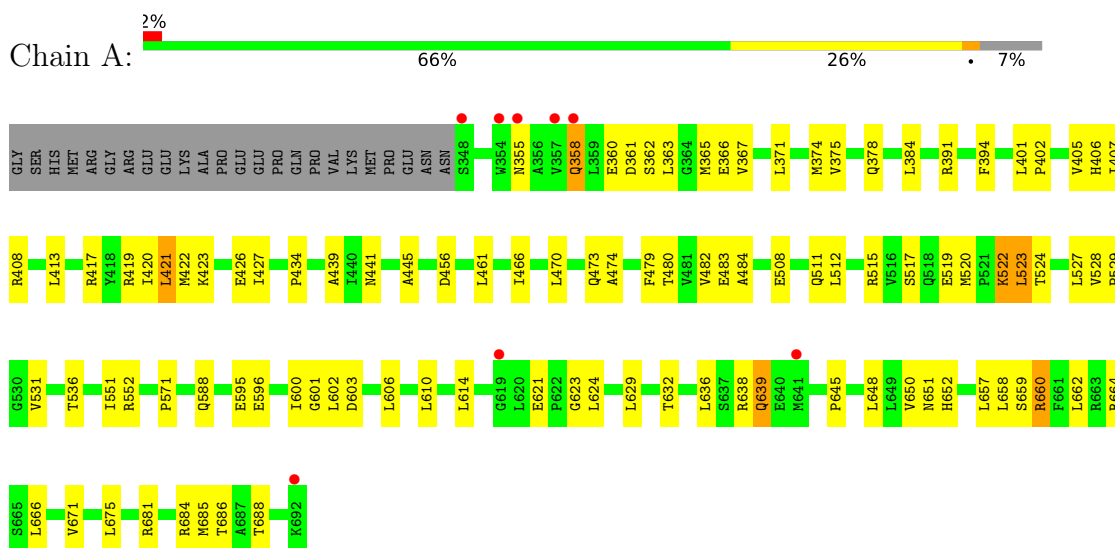
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	GLY	-	expression tag	UNP P40729
A	325	SER	-	expression tag	UNP P40729
A	326	HIS	-	expression tag	UNP P40729
A	327	MET	-	expression tag	UNP P40729
A	351	ALA	GLU	engineered mutation	UNP P40729
A	356	ALA	ASP	engineered mutation	UNP P40729
B	324	GLY	-	expression tag	UNP P40729
B	325	SER	-	expression tag	UNP P40729
B	326	HIS	-	expression tag	UNP P40729
B	327	MET	-	expression tag	UNP P40729
B	351	ALA	GLU	engineered mutation	UNP P40729
B	356	ALA	ASP	engineered mutation	UNP P40729

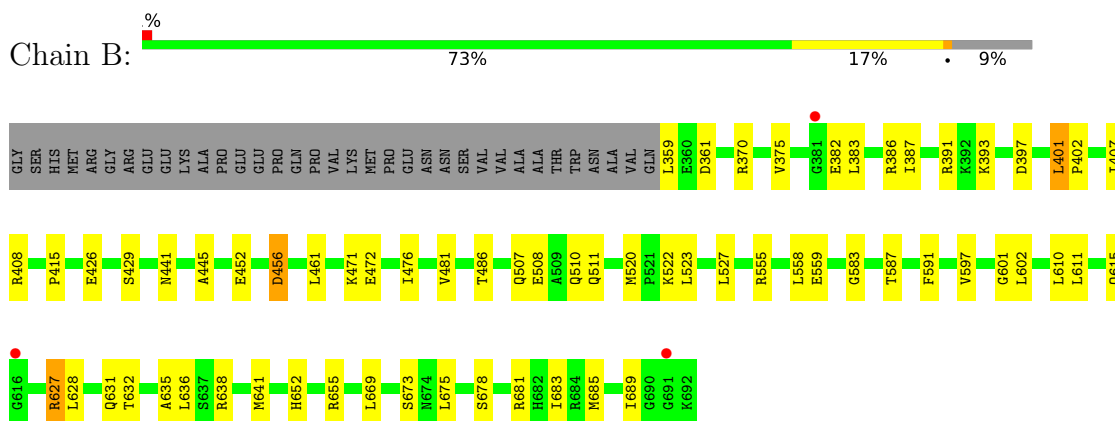
3 Residue-property plots [i](#)

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: Flagellar biosynthesis protein FlhA



- Molecule 1: Flagellar biosynthesis protein FlhA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.71Å 96.15Å 114.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.52 – 2.80 73.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (73.52-2.80) 96.3 (73.52-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.82Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.232 , 0.290 0.232 , 0.290	Depositor DCC
R_{free} test set	1903 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtrriage
Anisotropy	0.550	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5252	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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 [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	0.26	0/2712	0.48	2/3683 (0.1%)
1	B	0.26	0/2630	0.46	1/3568 (0.0%)
All	All	0.26	0/5342	0.47	3/7251 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	LEU	CA-CB-CG	7.11	131.64	115.30
1	A	523	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	359	LEU	CA-CB-CG	5.56	128.09	115.30

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	2666	0	2734	65	0
1	B	2586	0	2656	36	0
All	All	5252	0	5390	101	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 9.

All (101) 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:627:ARG:NH1	1:B:631:GLN:OE1	2.11	0.84
1:A:362:SER:HA	1:A:423:LYS:HG3	1.63	0.79
1:B:375:VAL:HG11	1:B:407:ILE:HG21	1.65	0.78
1:A:522:LYS:HG2	1:A:523:LEU:HD23	1.67	0.77
1:B:386:ARG:NH1	1:B:486:THR:OG1	2.22	0.73
1:A:522:LYS:HD3	1:A:522:LYS:H	1.52	0.72
1:A:639:GLN:OE1	1:A:686:THR:OG1	2.09	0.69
1:A:629:LEU:HD23	1:A:662:LEU:HD23	1.75	0.68
1:A:355:ASN:O	1:A:358:GLN:NE2	2.27	0.68
1:A:621:GLU:HG3	1:A:623:GLY:H	1.57	0.68
1:B:597:VAL:HB	1:B:683:ILE:HG22	1.75	0.68
1:B:610:LEU:HD21	1:B:628:LEU:HD11	1.77	0.67
1:A:474:ALA:HB1	1:A:479:PHE:HB2	1.77	0.66
1:A:365:MET:HB3	1:A:407:ILE:HG22	1.79	0.64
1:B:523:LEU:HD21	1:B:559:GLU:HG3	1.80	0.63
1:A:508:GLU:HA	1:A:511:GLN:HE21	1.62	0.63
1:A:527:LEU:HD12	1:A:531:VAL:HB	1.81	0.63
1:B:601:GLY:HA3	1:B:685:MET:HE3	1.80	0.62
1:A:614:LEU:HD11	1:A:657:LEU:HD22	1.80	0.62
1:A:512:LEU:HG	1:A:515:ARG:HH21	1.65	0.61
1:A:470:LEU:HD12	1:A:473:GLN:HG3	1.82	0.61
1:B:587:THR:HG21	1:B:678:SER:H	1.67	0.59
1:B:391:ARG:NH1	1:B:402:PRO:O	2.36	0.58
1:B:426:GLU:OE2	1:B:429:SER:OG	2.21	0.58
1:B:635:ALA:HA	1:B:638:ARG:HE	1.68	0.58
1:A:367:VAL:HG22	1:A:371:LEU:HB2	1.84	0.58
1:A:391:ARG:NH1	1:A:402:PRO:O	2.38	0.57
1:A:361:ASP:OD1	1:A:406:HIS:HB2	2.05	0.57
1:B:382:GLU:O	1:B:386:ARG:HG3	2.06	0.56
1:A:363:LEU:HD23	1:A:405:VAL:HG22	1.87	0.56
1:A:517:SER:HA	1:A:524:THR:HG21	1.87	0.56
1:B:361:ASP:OD2	1:B:408:ARG:NH2	2.38	0.56
1:B:632:THR:HG22	1:B:689:ILE:HD13	1.89	0.55
1:B:602:LEU:HD21	1:B:610:LEU:HD22	1.89	0.55
1:A:588:GLN:OE1	1:A:681:ARG:NH1	2.41	0.54
1:A:371:LEU:HD23	1:A:434:PRO:HG3	1.88	0.54
1:A:456:ASP:OD1	1:A:461:LEU:N	2.37	0.54
1:A:603:ASP:HB3	1:A:606:LEU:HB2	1.91	0.53
1:A:413:LEU:HD11	1:A:419:ARG:HG3	1.89	0.53
1:A:610:LEU:HD21	1:A:658:LEU:HD21	1.91	0.53
1:A:375:VAL:O	1:A:384:LEU:HD21	2.09	0.52
1:A:439:ALA:HB2	1:A:466:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:LEU:HG	1:A:650:VAL:HG23	1.92	0.51
1:B:591:PHE:O	1:B:681:ARG:NH1	2.41	0.51
1:A:638:ARG:NH2	1:A:688:THR:H	2.09	0.50
1:A:519:GLU:HG3	1:A:520:MET:HG3	1.93	0.50
1:A:639:GLN:NE2	1:A:645:PRO:O	2.45	0.50
1:A:601:GLY:HA3	1:A:685:MET:SD	2.52	0.50
1:A:358:GLN:HG2	1:A:358:GLN:O	2.11	0.49
1:B:652:HIS:CG	1:B:675:LEU:HD22	2.47	0.49
1:A:595:GLU:HG3	1:A:596:GLU:H	1.78	0.49
1:A:596:GLU:OE1	1:A:684:ARG:HD3	2.12	0.49
1:B:628:LEU:O	1:B:632:THR:HG23	2.12	0.49
1:B:456:ASP:OD2	1:B:461:LEU:HB2	2.13	0.49
1:A:441:ASN:OD1	1:A:445:ALA:HB3	2.14	0.48
1:A:536:THR:HG22	1:A:571:PRO:HG3	1.96	0.47
1:B:472:GLU:O	1:B:476:ILE:HG13	2.15	0.47
1:B:636:LEU:HD11	1:B:669:LEU:HB2	1.97	0.47
1:A:421:LEU:CB	1:A:426:GLU:HA	2.44	0.47
1:B:632:THR:HA	1:B:689:ILE:HG12	1.95	0.47
1:A:421:LEU:HB3	1:A:426:GLU:HA	1.97	0.47
1:A:361:ASP:O	1:A:423:LYS:HA	2.14	0.46
1:A:552:ARG:HA	1:A:552:ARG:HD2	1.72	0.46
1:A:365:MET:HE3	1:A:407:ILE:HG21	1.97	0.46
1:A:394:PHE:CD2	1:A:402:PRO:HG3	2.51	0.46
1:B:471:LYS:HG3	1:B:481:VAL:HG11	1.97	0.46
1:A:422:MET:HB2	1:A:422:MET:HE2	1.50	0.46
1:B:383:LEU:O	1:B:387:ILE:HG13	2.15	0.46
1:B:587:THR:HG21	1:B:678:SER:N	2.31	0.45
1:A:660:ARG:O	1:A:664:ARG:NH1	2.50	0.45
1:B:583:GLY:O	1:B:587:THR:HG23	2.17	0.45
1:A:366:GLU:HG3	1:A:419:ARG:HB2	1.99	0.45
1:B:393:LYS:NZ	1:B:397:ASP:OD2	2.42	0.45
1:A:407:ILE:O	1:A:408:ARG:HG3	2.18	0.44
1:A:483:GLU:HG2	1:A:484:ALA:H	1.83	0.44
1:A:600:ILE:HG12	1:A:639:GLN:HG3	1.99	0.43
1:B:611:LEU:O	1:B:615:GLN:HG3	2.17	0.43
1:B:370:ARG:HG3	1:B:415:PRO:HB3	2.00	0.43
1:A:421:LEU:HA	1:A:427:ILE:HG12	2.00	0.43
1:B:527:LEU:HD23	1:B:558:LEU:HD22	2.00	0.43
1:B:401:LEU:HD23	1:B:402:PRO:HD2	2.00	0.43
1:A:621:GLU:HB3	1:A:624:LEU:HD12	2.01	0.43
1:A:650:VAL:HG12	1:A:651:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ARG:O	1:B:631:GLN:HG3	2.19	0.42
1:A:480:THR:HG22	1:A:482:VAL:HG23	2.01	0.42
1:A:652:HIS:CG	1:A:675:LEU:HD22	2.54	0.42
1:A:602:LEU:HD12	1:A:602:LEU:HA	1.93	0.42
1:B:655:ARG:HD3	1:B:673:SER:HB2	2.01	0.42
1:A:401:LEU:HA	1:A:402:PRO:HD3	1.95	0.41
1:A:636:LEU:HD12	1:A:666:LEU:HD13	2.02	0.41
1:A:365:MET:HG3	1:A:420:ILE:HG12	2.02	0.41
1:B:508:GLU:HA	1:B:511:GLN:HB2	2.01	0.41
1:B:522:LYS:HD2	1:B:522:LYS:HA	1.86	0.41
1:A:659:SER:HA	1:A:671:VAL:HG21	2.03	0.41
1:A:551:ILE:HG22	1:A:551:ILE:O	2.19	0.41
1:A:528:VAL:HA	1:A:529:PRO:HA	1.93	0.41
1:A:522:LYS:HD3	1:A:522:LYS:N	2.28	0.40
1:A:371:LEU:HD22	1:A:374:MET:HE1	2.03	0.40
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.77	0.40
1:A:632:THR:HG21	1:A:662:LEU:HD22	2.03	0.40
1:B:441:ASN:CG	1:B:445:ALA:HB3	2.42	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	343/369 (93%)	329 (96%)	13 (4%)	1 (0%)	41	72
1	B	332/369 (90%)	319 (96%)	13 (4%)	0	100	100
All	All	675/738 (92%)	648 (96%)	26 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLU

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	286/307 (93%)	280 (98%)	6 (2%)	53 84
1	B	278/307 (91%)	269 (97%)	9 (3%)	39 73
All	All	564/614 (92%)	549 (97%)	15 (3%)	44 78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	A	378	GLN
1	A	417	ARG
1	A	522	LYS
1	A	639	GLN
1	A	660	ARG
1	B	401	LEU
1	B	452	GLU
1	B	456	ASP
1	B	507	GLN
1	B	510	GLN
1	B	520	MET
1	B	555	ARG
1	B	627	ARG
1	B	641	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	A	511	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 monosaccharides 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	345/369 (93%)	0.00	8 (2%) 60 51	35, 70, 119, 177	0
1	B	334/369 (90%)	-0.10	3 (0%) 84 80	25, 65, 102, 164	0
All	All	679/738 (92%)	-0.05	11 (1%) 72 66	25, 67, 111, 177	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	LYS	5.2
1	B	381	GLY	4.0
1	A	354	TRP	3.2
1	A	355	ASN	3.1
1	A	358	GLN	3.0
1	B	616	GLY	2.9
1	A	357	VAL	2.7
1	A	641	MET	2.2
1	A	619	GLY	2.1
1	A	348	SER	2.1
1	B	691	GLY	2.1

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 monosaccharides 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.