



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2022 – 04:03 PM EDT

PDB ID : 7SJ5
Title : Bacteriophage lambda major capsid protein mutant - W308A
Authors : Davis, C.R.; Churchill, M.E.
Deposited on : 2021-10-15
Resolution : 2.69 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	:	2.29
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)	:	2.29

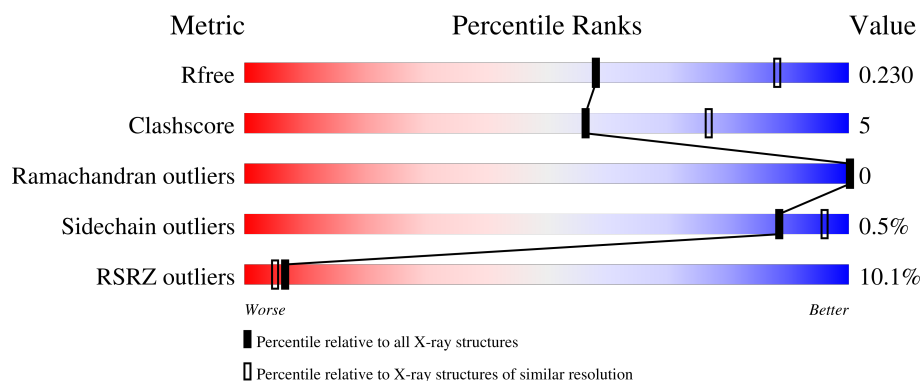
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	341	<div> <div>4%</div> <div>91%</div> <div>8%</div> </div>
1	B	341	<div> <div>3%</div> <div>89%</div> <div>11%</div> </div>
1	C	341	<div> <div>4%</div> <div>88%</div> <div>12%</div> </div>
1	D	341	<div> <div>29%</div> <div>78%</div> <div>21%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10801 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 Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2667	1677	457	520	13			
1	B	340	Total	C	N	O	S	0	0	0
			2667	1677	457	520	13			
1	C	340	Total	C	N	O	S	0	0	0
			2667	1677	457	520	13			
1	D	340	Total	C	N	O	S	0	0	0
			2637	1663	449	513	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ALA	TRP	engineered mutation	UNP P03713
B	308	ALA	TRP	engineered mutation	UNP P03713
C	308	ALA	TRP	engineered mutation	UNP P03713
D	308	ALA	TRP	engineered mutation	UNP P03713

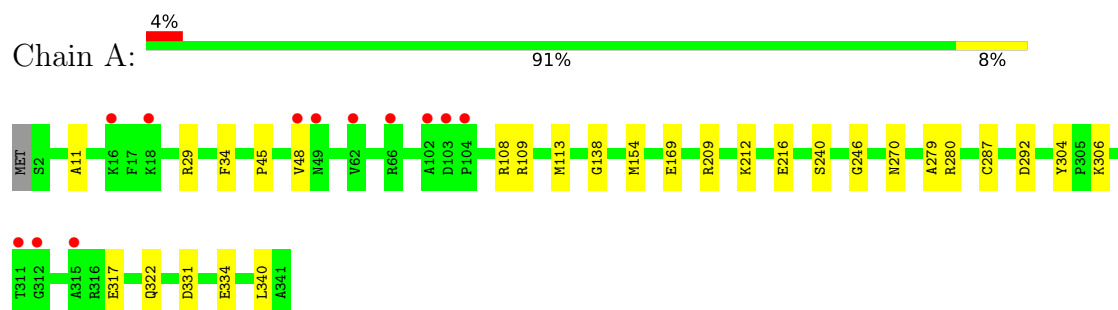
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total	O	0	0
			62	62		
2	B	65	Total	O	0	0
			65	65		
2	C	34	Total	O	0	0
			34	34		
2	D	2	Total	O	0	0
			2	2		

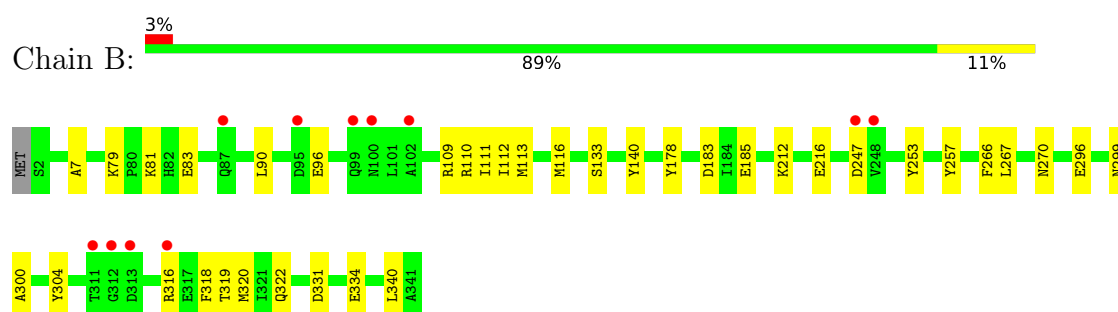
3 Residue-property plots [i](#)

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.

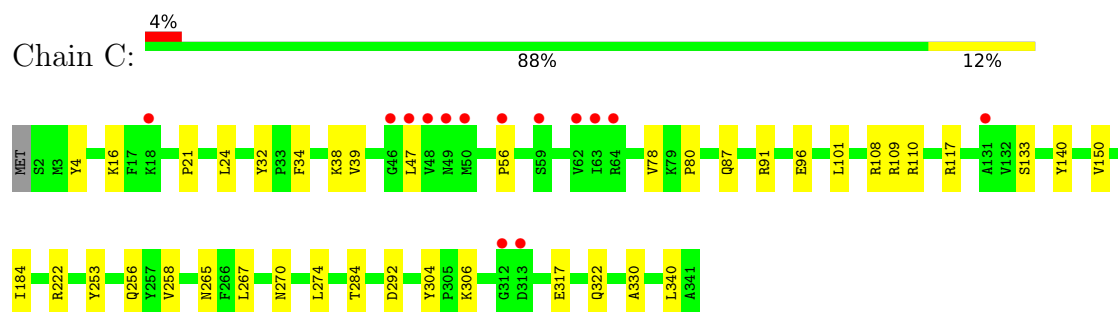
- Molecule 1: Major capsid protein



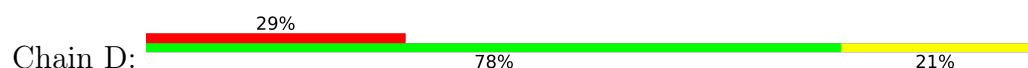
- Molecule 1: Major capsid protein

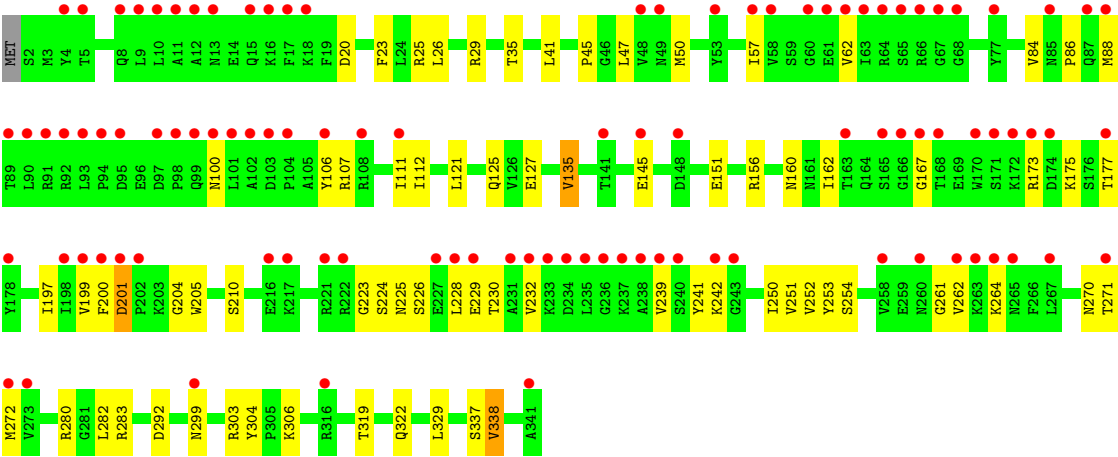


- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.15Å 95.30Å 113.12Å 90.00° 127.92° 90.00°	Depositor
Resolution (Å)	29.75 – 2.69 29.75 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.75-2.69) 99.6 (29.75-2.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.68Å)	Xtriage
Refinement program	PHENIX dev-3724	Depositor
R, R_{free}	0.207 , 0.230 0.207 , 0.230	Depositor DCC
R_{free} test set	2045 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10801	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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	0.25	0/2718	0.42	0/3677
1	B	0.25	0/2718	0.41	0/3677
1	C	0.25	0/2718	0.42	0/3677
1	D	0.25	0/2688	0.44	0/3642
All	All	0.25	0/10842	0.42	0/14673

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	2667	0	2633	17	0
1	B	2667	0	2633	20	0
1	C	2667	0	2633	23	0
1	D	2637	0	2588	51	0
2	A	62	0	0	0	0
2	B	65	0	0	0	0
2	C	34	0	0	1	0
2	D	2	0	0	0	0
All	All	10801	0	10487	105	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 (105) 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:D:304:TYR:HB2	1:D:322:GLN:HB2	1.70	0.72
1:D:239:VAL:HG22	1:D:254:SER:H	1.56	0.70
1:A:29:ARG:NH2	1:A:279:ALA:O	2.25	0.69
1:D:200:PHE:N	1:D:251:VAL:O	2.27	0.66
1:A:304:TYR:HB2	1:A:322:GLN:HB2	1.78	0.66
1:D:20:ASP:OD2	1:D:283:ARG:NH2	2.31	0.64
1:C:304:TYR:HB2	1:C:322:GLN:HB2	1.81	0.63
1:A:108:ARG:NH1	1:A:317:GLU:OE2	2.30	0.62
1:D:86:PRO:HD2	1:D:111:ILE:HD13	1.82	0.60
1:D:35:THR:OG1	1:D:299:ASN:ND2	2.34	0.60
1:C:78:VAL:HG12	1:C:80:PRO:HD3	1.84	0.59
1:A:209:ARG:HD3	1:B:185:GLU:HG3	1.83	0.59
1:D:57:ILE:HD11	1:D:151:GLU:HB2	1.83	0.59
1:B:96:GLU:OE2	1:B:110:ARG:NH1	2.36	0.58
1:A:212:LYS:NZ	1:A:216:GLU:OE2	2.36	0.58
1:C:256:GLN:HG2	1:C:265:ASN:HD22	1.69	0.57
1:D:41:LEU:HD13	1:D:50:MET:HG3	1.86	0.57
1:D:88:MET:O	1:D:107:ARG:NH2	2.38	0.57
1:C:109:ARG:NH2	1:D:145:GLU:O	2.39	0.55
1:C:108:ARG:NH1	1:C:317:GLU:OE2	2.40	0.55
1:D:224:SER:OG	1:D:241:TYR:OH	2.25	0.55
1:D:45:PRO:O	1:D:280:ARG:NH2	2.30	0.54
1:D:200:PHE:HA	1:D:270:ASN:ND2	2.22	0.54
1:C:270:ASN:HB3	1:C:340:LEU:HB2	1.90	0.54
1:B:304:TYR:HB2	1:B:322:GLN:HB2	1.90	0.53
1:D:201:ASP:HA	1:D:252:VAL:HG13	1.89	0.53
1:D:135:VAL:HG12	1:D:329:LEU:HD11	1.90	0.53
1:A:45:PRO:O	1:A:280:ARG:NH2	2.32	0.52
1:D:241:TYR:HB2	1:D:251:VAL:HA	1.91	0.52
1:D:84:VAL:HG21	1:D:319:THR:HG23	1.90	0.52
1:D:229:GLU:HG3	1:D:241:TYR:HE1	1.74	0.52
1:B:270:ASN:HB3	1:B:340:LEU:HB2	1.91	0.51
1:C:56:PRO:HA	1:C:150:VAL:HG12	1.92	0.51
1:B:212:LYS:NZ	1:B:216:GLU:OE2	2.44	0.51
1:D:239:VAL:HG11	1:D:253:TYR:HD1	1.75	0.50
1:D:205:TRP:CZ2	1:D:242:LYS:HD2	2.48	0.49
1:A:292:ASP:OD2	1:A:306:LYS:NZ	2.45	0.49
1:D:223:GLY:N	1:D:229:GLU:OE1	2.39	0.49
1:B:112:ILE:HG23	1:B:319:THR:HG21	1.95	0.49
1:C:253:TYR:HB3	1:C:267:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD21	1:B:111:ILE:HG13	1.93	0.49
1:C:16:LYS:HE2	1:C:117:ARG:HD3	1.94	0.48
1:C:292:ASP:OD2	1:C:306:LYS:NZ	2.46	0.48
1:D:272:MET:O	1:D:337:SER:HA	2.13	0.48
1:C:32:TYR:HB2	1:C:284:THR:HG22	1.95	0.48
1:D:200:PHE:CE1	1:D:250:ILE:HG23	2.48	0.48
1:B:7:ALA:HB2	1:B:296:GLU:HG2	1.95	0.48
1:D:26:LEU:O	1:D:29:ARG:NH1	2.42	0.48
1:D:167:GLY:O	1:D:173:ARG:NE	2.46	0.48
1:D:228:LEU:HD21	1:D:251:VAL:HG22	1.95	0.48
1:B:79:LYS:HG2	1:B:322:GLN:HG2	1.95	0.48
1:D:205:TRP:HZ2	1:D:242:LYS:HD2	1.79	0.48
1:C:91:ARG:O	1:C:110:ARG:NH2	2.47	0.47
1:D:162:ILE:HB	1:D:338:VAL:HB	1.97	0.47
1:B:83:GLU:HA	1:B:318:PHE:HA	1.97	0.47
1:B:116:MET:HE2	1:B:319:THR:HB	1.97	0.47
1:A:240:SER:OG	1:B:247:ASP:OD2	2.33	0.46
1:A:270:ASN:HB3	1:A:340:LEU:HB2	1.97	0.46
1:D:100:ASN:HB3	1:D:106:TYR:CD2	2.50	0.46
1:D:262:VAL:HG23	1:D:264:LYS:H	1.80	0.46
1:A:11:ALA:HA	1:D:261:GLY:O	2.16	0.46
1:A:246:GLY:O	1:C:222:ARG:HD3	2.16	0.46
1:D:20:ASP:O	1:D:25:ARG:NH2	2.50	0.45
1:C:96:GLU:HB3	1:C:101:LEU:HD11	1.99	0.45
1:D:292:ASP:OD2	1:D:306:LYS:NZ	2.39	0.45
1:C:133:SER:HB2	1:C:140:TYR:HB3	1.98	0.45
1:C:38:LYS:NZ	2:C:401:HOH:O	2.38	0.45
1:D:127:GLU:OE2	1:D:303:ARG:NH1	2.49	0.45
1:A:48:VAL:HG21	1:C:258:VAL:HG21	1.98	0.44
1:A:109:ARG:O	1:A:113:MET:HG2	2.17	0.44
1:D:197:ILE:HD11	1:D:251:VAL:HG21	1.99	0.44
1:B:257:TYR:HB3	1:B:266:PHE:CZ	2.53	0.44
1:D:239:VAL:HG13	1:D:253:TYR:HA	2.00	0.44
1:C:4:TYR:OH	1:C:109:ARG:HG3	2.18	0.44
1:A:331:ASP:HB3	1:A:334:GLU:HG3	2.00	0.43
1:C:21:PRO:HD2	1:C:24:LEU:HD12	2.01	0.43
1:D:226:SER:O	1:D:230:THR:OG1	2.32	0.43
1:C:34:PHE:HD2	1:C:39:VAL:HA	1.83	0.43
1:D:23:PHE:CE1	1:D:199:VAL:HG11	2.53	0.43
1:C:184:ILE:HG23	1:C:274:LEU:HD21	2.01	0.43
1:D:156:ARG:HD2	1:D:160:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:HG13	1:D:252:VAL:O	2.19	0.43
1:B:133:SER:HB2	1:B:140:TYR:HB3	2.00	0.43
1:D:229:GLU:O	1:D:232:VAL:HG22	2.19	0.43
1:D:121:LEU:O	1:D:125:GLN:HG2	2.19	0.42
1:D:204:GLY:HA3	1:D:270:ASN:CB	2.50	0.42
1:D:228:LEU:O	1:D:232:VAL:HG13	2.20	0.42
1:D:112:ILE:HG23	1:D:319:THR:HG21	2.01	0.42
1:C:47:LEU:HD11	1:C:330:ALA:HB1	2.02	0.42
1:B:253:TYR:HB3	1:B:267:LEU:HD22	2.02	0.41
1:D:241:TYR:HB2	1:D:250:ILE:O	2.20	0.41
1:C:222:ARG:HD2	1:C:222:ARG:N	2.35	0.41
1:A:169:GLU:OE1	1:A:169:GLU:N	2.49	0.41
1:A:34:PHE:O	1:A:287:CYS:HB2	2.21	0.41
1:B:299:ASN:OD1	1:B:300:ALA:N	2.44	0.41
1:B:109:ARG:O	1:B:113:MET:HG2	2.20	0.41
1:B:331:ASP:HB3	1:B:334:GLU:HG3	2.01	0.41
1:D:225:ASN:OD1	1:D:228:LEU:HB2	2.20	0.41
1:B:81:LYS:HB3	1:B:320:MET:HE2	2.03	0.40
1:D:47:LEU:HD21	1:D:282:LEU:HD11	2.03	0.40
1:D:57:ILE:HG12	1:D:62:VAL:HG22	2.03	0.40
1:B:178:TYR:OH	1:B:183:ASP:OD2	2.32	0.40
1:A:138:GLY:O	1:A:154:MET:HG2	2.22	0.40
1:D:175:LYS:NZ	1:D:210:SER:HB2	2.36	0.40
1:D:271:THR:HB	1:D:338:VAL:O	2.21	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	338/341 (99%)	327 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	338/341 (99%)	331 (98%)	7 (2%)	0	100	100
1	C	338/341 (99%)	332 (98%)	6 (2%)	0	100	100
1	D	338/341 (99%)	323 (96%)	15 (4%)	0	100	100
All	All	1352/1364 (99%)	1313 (97%)	39 (3%)	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	288/289 (100%)	288 (100%)	0	100	100
1	B	288/289 (100%)	287 (100%)	1 (0%)	92	98
1	C	288/289 (100%)	287 (100%)	1 (0%)	92	98
1	D	281/289 (97%)	277 (99%)	4 (1%)	67	86
All	All	1145/1156 (99%)	1139 (100%)	6 (0%)	88	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	316	ARG
1	C	87	GLN
1	D	135	VAL
1	D	177	THR
1	D	201	ASP
1	D	338	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	99	GLN
1	B	260	ASN

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Mol	Chain	Res	Type
1	C	265	ASN
1	D	114	GLN
1	D	115	ASN
1	D	260	ASN
1	D	289	GLN
1	D	299	ASN

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

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	340/341 (99%)	-0.02	12 (3%) 44 44	26, 49, 108, 157	0
1	B	340/341 (99%)	-0.00	11 (3%) 47 48	26, 51, 109, 167	0
1	C	340/341 (99%)	0.11	14 (4%) 37 36	35, 66, 114, 172	0
1	D	340/341 (99%)	1.51	100 (29%) 0 0	60, 108, 187, 229	0
All	All	1360/1364 (99%)	0.40	137 (10%) 7 5	26, 66, 155, 229	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91	ARG	10.3
1	D	341	ALA	9.8
1	D	237	LYS	8.7
1	D	242	LYS	8.1
1	D	9	LEU	8.0
1	D	11	ALA	8.0
1	D	236	GLY	8.0
1	D	238	ALA	7.5
1	D	102	ALA	7.1
1	D	17	PHE	6.3
1	D	92	ARG	6.3
1	A	312	GLY	6.1
1	B	312	GLY	6.0
1	D	64	ARG	6.0
1	D	106	TYR	5.9
1	D	62	VAL	5.5
1	D	104	PRO	5.4
1	D	67	GLY	5.4
1	D	53	TYR	5.4
1	D	262	VAL	5.2
1	D	94	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	63	ILE	5.2
1	D	178	TYR	5.2
1	D	216	GLU	5.2
1	D	12	ALA	5.2
1	D	98	PRO	5.1
1	D	172	LYS	5.0
1	D	66	ARG	4.9
1	D	239	VAL	4.9
1	D	222	ARG	4.8
1	D	272	MET	4.8
1	D	60	GLY	4.8
1	D	168	THR	4.7
1	D	89	THR	4.7
1	C	48	VAL	4.7
1	D	170	TRP	4.7
1	D	87	GLN	4.6
1	B	313	ASP	4.5
1	D	99	GLN	4.4
1	D	233	LYS	4.4
1	D	202	PRO	4.2
1	D	93	LEU	4.2
1	D	61	GLU	4.1
1	A	311	THR	4.0
1	D	90	LEU	4.0
1	D	5	THR	3.9
1	D	16	LYS	3.9
1	C	64	ARG	3.8
1	D	263	LYS	3.8
1	D	273	VAL	3.8
1	D	15	GLN	3.8
1	B	99	GLN	3.8
1	D	85	ASN	3.8
1	C	313	ASP	3.8
1	D	10	LEU	3.7
1	D	111	ILE	3.7
1	B	87	GLN	3.6
1	D	240	SER	3.6
1	D	18	LYS	3.6
1	D	100	ASN	3.5
1	D	171	SER	3.5
1	D	65	SER	3.5
1	D	173	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	243	GLY	3.5
1	C	47	LEU	3.5
1	D	258	VAL	3.4
1	D	177	THR	3.4
1	D	48	VAL	3.3
1	B	95	ASP	3.3
1	D	271	THR	3.3
1	B	102	ALA	3.2
1	D	8	GLN	3.2
1	A	104	PRO	3.2
1	D	265	ASN	3.2
1	C	18	LYS	3.1
1	D	264	LYS	3.1
1	D	13	ASN	3.1
1	D	165	SER	3.1
1	B	311	THR	3.0
1	D	231	ALA	3.0
1	D	4	TYR	3.0
1	A	62	VAL	3.0
1	C	312	GLY	3.0
1	D	57	ILE	3.0
1	D	49	ASN	3.0
1	D	234	ASP	3.0
1	A	18	LYS	3.0
1	D	235	LEU	2.9
1	C	46	GLY	2.9
1	D	166	GLY	2.9
1	D	167	GLY	2.9
1	C	50	MET	2.9
1	D	199	VAL	2.9
1	D	201	ASP	2.8
1	D	232	VAL	2.7
1	D	163	THR	2.7
1	B	100	ASN	2.7
1	D	221	ARG	2.7
1	C	63	ILE	2.7
1	D	260	ASN	2.7
1	C	62	VAL	2.7
1	C	49	ASN	2.6
1	D	217	LYS	2.6
1	D	141	THR	2.6
1	D	95	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	145	GLU	2.6
1	D	88	MET	2.6
1	D	229	GLU	2.6
1	D	227	GLU	2.6
1	D	108	ARG	2.6
1	D	101	LEU	2.5
1	D	97	ASP	2.4
1	D	174	ASP	2.4
1	D	58	VAL	2.4
1	A	66	ARG	2.3
1	D	103	ASP	2.3
1	D	267	LEU	2.3
1	D	200	PHE	2.2
1	A	48	VAL	2.2
1	A	49	ASN	2.2
1	A	102	ALA	2.2
1	B	247	ASP	2.2
1	D	316	ARG	2.2
1	C	59	SER	2.2
1	D	228	LEU	2.2
1	D	77	TYR	2.1
1	D	198	ILE	2.1
1	C	56	PRO	2.1
1	B	316	ARG	2.1
1	B	248	VAL	2.1
1	D	68	GLY	2.1
1	C	131	ALA	2.0
1	D	299	ASN	2.0
1	A	103	ASP	2.0
1	D	148	ASP	2.0
1	A	16	LYS	2.0
1	A	315	ALA	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 monosaccharides 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.