



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:27 PM UTC

PDB ID : 3RA2 / pdb_00003ra2
Title : Structural studies of AAV8 capsid transitions associated with endosomal trafficking
Authors : Nam, H.-J.; Gurda, B.; McKenna, R.; Porter, M.; Byrne, B.; Salganik, M.; Muzyczka, N.; Agbandje-McKenna, M.
Deposited on : 2011-03-26
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

<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

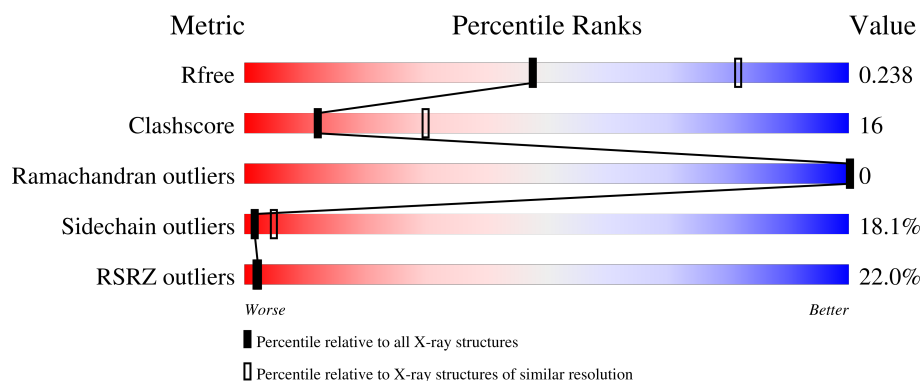
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	519	22% 66% 24% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4223 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4136	2609	716	798	13			

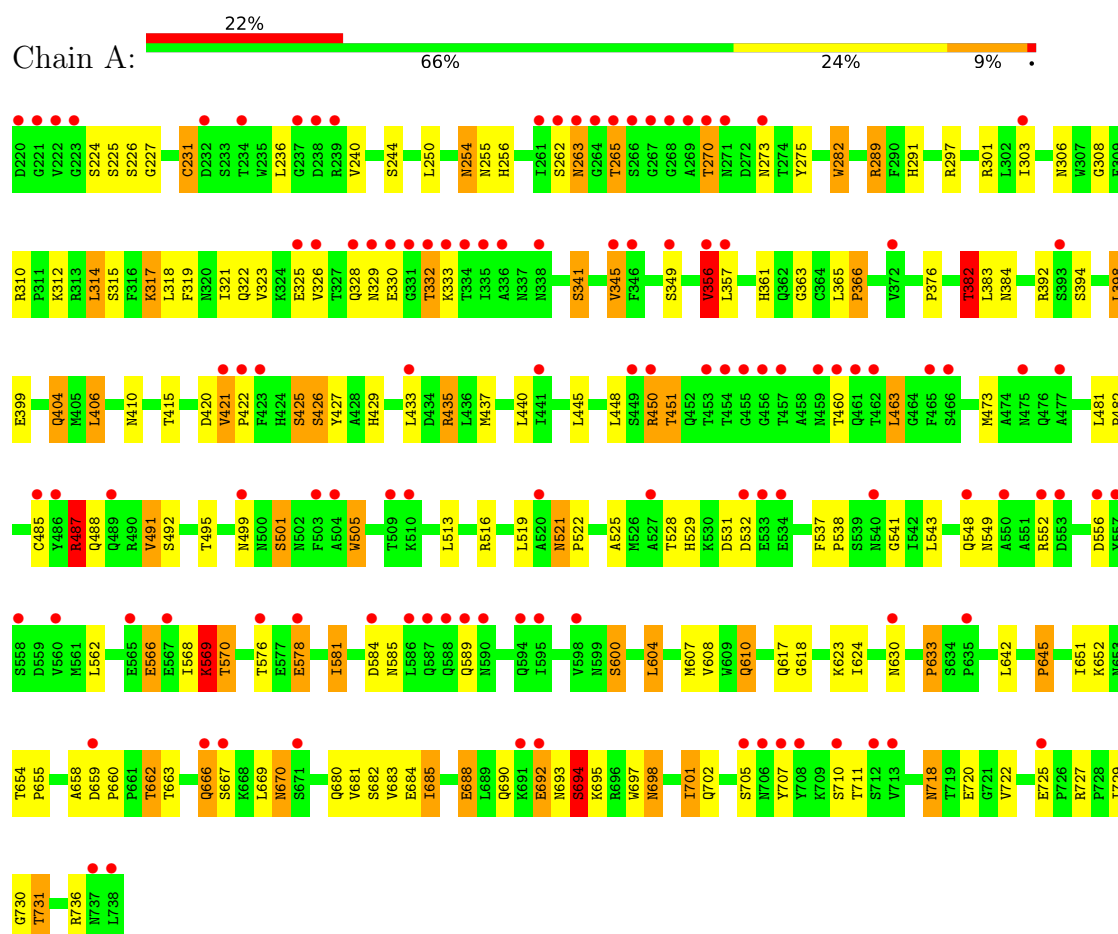
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total	O	0	0
			87	87		

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: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	257.94Å 257.94Å 448.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.8 (40.00-2.70) 86.7 (40.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.244 0.239 , 0.238	Depositor DCC
R_{free} test set	11064 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.34	EDS
Total number of atoms	4223	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 1.68% 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	2.01	25/4259 (0.6%)	1.08	17/5811 (0.3%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	GLY	C-O	-6.31	1.19	1.24
1	A	421	VAL	C-O	-6.20	1.20	1.24
1	A	608	VAL	C-O	-6.00	1.18	1.24
1	A	730	GLY	C-O	-5.96	1.18	1.23
1	A	240	VAL	C-O	-5.88	1.18	1.24
1	A	651	ILE	C-O	-5.80	1.18	1.24
1	A	521	ASN	C-O	-5.80	1.19	1.25
1	A	250	LEU	C-O	-5.69	1.18	1.24
1	A	729	ILE	C-O	-5.62	1.18	1.24
1	A	345	VAL	C-O	-5.60	1.18	1.24
1	A	525	ALA	CA-CB	-5.53	1.45	1.53
1	A	685	ILE	C-O	-5.46	1.18	1.24
1	A	366	PRO	C-O	-5.33	1.20	1.24
1	A	681	VAL	C-O	-5.31	1.18	1.24
1	A	658	ALA	CA-CB	-5.30	1.45	1.53
1	A	690	GLN	C-O	-5.28	1.18	1.24
1	A	308	GLY	C-O	-5.24	1.18	1.24
1	A	645	PRO	C-O	-5.22	1.18	1.24
1	A	624	ILE	CA-C	-5.20	1.49	1.53
1	A	688	GLU	C-O	-5.15	1.17	1.24
1	A	727	ARG	C-O	-5.15	1.19	1.24
1	A	633	PRO	CA-C	-5.14	1.48	1.53
1	A	306	ASN	C-O	-5.11	1.17	1.23
1	A	581	ILE	C-O	-5.09	1.19	1.24
1	A	356	VAL	C-O	-5.05	1.19	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ILE	N-CA-C	6.92	117.71	110.72
1	A	505	TRP	N-CA-C	-6.82	105.58	114.04
1	A	725	GLU	CA-C-N	6.80	126.26	118.85
1	A	725	GLU	C-N-CA	6.80	126.26	118.85
1	A	707	TYR	N-CA-C	6.75	118.72	111.36
1	A	697	TRP	N-CA-C	6.50	118.17	111.14
1	A	382	THR	CB-CA-C	-6.40	98.03	113.19
1	A	487	ARG	N-CA-C	6.13	119.35	110.28
1	A	357	LEU	N-CA-C	-6.03	103.00	110.41
1	A	569	LYS	N-CA-C	-5.78	106.07	113.01
1	A	658	ALA	N-CA-C	-5.74	102.43	110.35
1	A	694	SER	N-CA-C	5.49	118.40	110.28
1	A	421	VAL	N-CA-C	-5.46	104.71	109.19
1	A	618	GLY	N-CA-C	5.40	118.75	112.10
1	A	314	LEU	N-CA-C	5.06	116.89	109.24
1	A	282	TRP	N-CA-C	5.01	116.99	110.53
1	A	361	HIS	N-CA-C	5.01	117.31	110.55

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	4136	0	3893	125	0
2	A	87	0	0	1	0
All	All	4223	0	3893	125	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 16.

All (125) 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:289:ARG:HG2	1:A:289:ARG:HH11	1.05	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:SER:HB3	1:A:731:THR:HG23	1.31	1.08
1:A:289:ARG:HG2	1:A:289:ARG:NH1	1.69	0.96
1:A:666:GLN:O	1:A:666:GLN:HG3	1.62	0.96
1:A:289:ARG:HH11	1:A:289:ARG:CG	1.82	0.93
1:A:718:ASN:HB3	1:A:720:GLU:H	1.35	0.92
1:A:566:GLU:O	1:A:569:LYS:HG2	1.72	0.90
1:A:426:SER:HB3	1:A:731:THR:CG2	2.02	0.89
1:A:329:ASN:O	1:A:332:THR:HG23	1.74	0.87
1:A:426:SER:HA	1:A:731:THR:HG22	1.59	0.84
1:A:382:THR:HG21	1:A:394:SER:H	1.42	0.84
1:A:435:ARG:CD	1:A:473:MET:CE	2.58	0.82
1:A:698:ASN:HD22	1:A:698:ASN:H	1.23	0.81
1:A:255:ASN:O	1:A:256:HIS:HB2	1.79	0.79
1:A:731:THR:CG2	1:A:731:THR:O	2.30	0.78
1:A:329:ASN:HB3	1:A:330:GLU:OE1	1.83	0.77
1:A:566:GLU:HA	1:A:566:GLU:OE2	1.82	0.77
1:A:265:THR:O	1:A:265:THR:HG23	1.83	0.77
1:A:426:SER:HA	1:A:731:THR:CG2	2.15	0.76
1:A:718:ASN:HB2	1:A:722:VAL:H	1.49	0.75
1:A:566:GLU:OE2	1:A:566:GLU:CA	2.36	0.72
1:A:435:ARG:CD	1:A:473:MET:HE1	2.19	0.72
1:A:435:ARG:CD	1:A:473:MET:HE3	2.21	0.71
1:A:435:ARG:NE	1:A:473:MET:HE3	2.06	0.70
1:A:450:ARG:NH1	1:A:450:ARG:HG3	2.05	0.69
1:A:227:GLY:HA3	1:A:319:PHE:CD1	2.28	0.69
1:A:435:ARG:HD3	1:A:473:MET:CE	2.22	0.68
1:A:254:ASN:O	1:A:255:ASN:HB2	1.94	0.67
1:A:450:ARG:HG3	1:A:450:ARG:HH11	1.59	0.67
1:A:429:HIS:HB2	1:A:570:THR:HG21	1.76	0.67
1:A:566:GLU:O	1:A:569:LYS:CG	2.43	0.66
1:A:435:ARG:HD3	1:A:473:MET:HE3	1.78	0.65
1:A:610:GLN:HE21	1:A:610:GLN:CA	2.09	0.65
1:A:426:SER:CB	1:A:731:THR:CG2	2.75	0.65
1:A:330:GLU:OE1	1:A:330:GLU:N	2.30	0.65
1:A:662:THR:O	1:A:662:THR:CG2	2.46	0.64
1:A:435:ARG:NE	1:A:473:MET:CE	2.60	0.64
1:A:450:ARG:HH11	1:A:450:ARG:CG	2.11	0.64
1:A:398:LEU:N	1:A:398:LEU:HD23	2.13	0.63
1:A:531:ASP:O	1:A:532:ASP:HB2	1.97	0.63
1:A:698:ASN:H	1:A:698:ASN:ND2	1.92	0.62
1:A:297:ARG:HG3	1:A:301:ARG:CZ	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ASN:HB3	1:A:720:GLU:N	2.12	0.61
1:A:731:THR:HG23	1:A:731:THR:O	1.99	0.61
1:A:731:THR:HG22	1:A:731:THR:O	2.01	0.61
1:A:421:VAL:HG22	1:A:422:PRO:HD2	1.82	0.60
1:A:662:THR:O	1:A:662:THR:HG23	2.01	0.60
1:A:451:THR:O	1:A:451:THR:CG2	2.46	0.59
1:A:485:CYS:O	1:A:600:SER:HA	2.03	0.59
1:A:426:SER:CA	1:A:731:THR:CG2	2.82	0.58
1:A:670:ASN:H	1:A:670:ASN:HD22	1.50	0.58
1:A:321:ILE:CD1	1:A:406:LEU:HD12	2.34	0.58
1:A:312:LYS:HD3	1:A:688:GLU:OE2	2.04	0.58
1:A:255:ASN:O	1:A:256:HIS:CB	2.50	0.57
1:A:356:VAL:O	1:A:356:VAL:HG13	2.06	0.56
1:A:399:GLU:OE2	1:A:652:LYS:NZ	2.37	0.55
1:A:451:THR:O	1:A:451:THR:HG23	2.07	0.55
1:A:487:ARG:HG3	1:A:488:GLN:N	2.22	0.55
1:A:659:ASP:OD2	1:A:659:ASP:N	2.34	0.55
1:A:289:ARG:NH1	1:A:617:GLN:O	2.40	0.55
1:A:329:ASN:C	1:A:330:GLU:OE1	2.50	0.55
1:A:604:LEU:HB2	1:A:607:MET:HE3	1.90	0.54
1:A:231:CYS:SG	1:A:244:SER:HA	2.48	0.53
1:A:610:GLN:NE2	1:A:610:GLN:HA	2.23	0.53
1:A:382:THR:HG22	1:A:383:LEU:H	1.72	0.53
1:A:435:ARG:CZ	1:A:473:MET:CE	2.87	0.53
1:A:310:ARG:NH1	1:A:421:VAL:O	2.36	0.52
1:A:263:ASN:HB2	1:A:275:TYR:CE2	2.44	0.52
1:A:435:ARG:HD2	1:A:473:MET:HE1	1.90	0.52
1:A:323:VAL:HG11	1:A:341:SER:HB3	1.92	0.52
1:A:670:ASN:H	1:A:670:ASN:ND2	2.08	0.52
1:A:491:VAL:HG22	1:A:537:PHE:CE2	2.45	0.52
1:A:317:LYS:HD3	1:A:319:PHE:CD2	2.46	0.51
1:A:529:HIS:CD2	1:A:566:GLU:OE1	2.64	0.51
1:A:297:ARG:HG3	1:A:301:ARG:NH1	2.26	0.50
1:A:610:GLN:CA	1:A:610:GLN:NE2	2.71	0.50
1:A:314:LEU:C	1:A:314:LEU:HD12	2.37	0.50
1:A:404:GLN:NE2	1:A:406:LEU:CD2	2.75	0.50
1:A:692:GLU:HG2	1:A:693:ASN:N	2.25	0.49
1:A:421:VAL:HG22	1:A:422:PRO:CD	2.42	0.49
1:A:363:GLY:HA3	1:A:376:PRO:HG3	1.94	0.48
1:A:630:ASN:CG	1:A:633:PRO:HG3	2.38	0.48
1:A:482:PRO:O	1:A:607:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:THR:HG21	1:A:394:SER:N	2.21	0.47
1:A:425:SER:HB3	1:A:427:TYR:CE2	2.51	0.46
1:A:670:ASN:HD22	1:A:670:ASN:N	2.06	0.46
1:A:695:LYS:HA	1:A:695:LYS:HD2	1.61	0.46
1:A:384:ASN:OD1	1:A:516:ARG:NH2	2.49	0.46
1:A:578:GLU:H	1:A:578:GLU:HG3	1.45	0.45
1:A:328:GLN:OE1	1:A:333:LYS:HB2	2.15	0.45
1:A:435:ARG:HD3	1:A:473:MET:HE1	1.90	0.45
1:A:319:PHE:CD2	1:A:319:PHE:N	2.84	0.45
1:A:521:ASN:HA	1:A:522:PRO:HA	1.82	0.45
1:A:568:ILE:C	1:A:570:THR:H	2.24	0.45
1:A:670:ASN:HD22	1:A:670:ASN:C	2.25	0.44
1:A:435:ARG:CZ	1:A:473:MET:HE2	2.47	0.44
1:A:585:ASN:OD1	1:A:585:ASN:C	2.58	0.44
1:A:623:LYS:HB2	1:A:645:PRO:HG3	1.99	0.44
1:A:263:ASN:HD22	1:A:263:ASN:HA	1.49	0.44
1:A:568:ILE:C	1:A:570:THR:N	2.72	0.43
1:A:670:ASN:ND2	1:A:670:ASN:N	2.63	0.43
1:A:692:GLU:HG2	1:A:694:SER:H	1.83	0.43
1:A:491:VAL:HG23	1:A:492:SER:N	2.34	0.43
1:A:406:LEU:HB3	1:A:410:ASN:HB2	2.01	0.42
1:A:398:LEU:N	1:A:398:LEU:CD2	2.82	0.42
1:A:528:THR:HG23	1:A:538:PRO:HD3	2.02	0.42
1:A:718:ASN:HD22	1:A:718:ASN:HA	1.53	0.42
1:A:529:HIS:O	1:A:566:GLU:OE1	2.37	0.42
1:A:383:LEU:HD12	1:A:392:ARG:HB2	2.02	0.42
1:A:499:ASN:ND2	1:A:501:SER:OG	2.51	0.42
1:A:282:TRP:CE2	1:A:652:LYS:HD3	2.55	0.42
1:A:265:THR:O	1:A:265:THR:CG2	2.48	0.41
1:A:365:LEU:HA	1:A:366:PRO:HD3	1.92	0.41
1:A:654:THR:HA	1:A:655:PRO:HD3	1.93	0.41
1:A:610:GLN:HE21	1:A:610:GLN:HA	1.80	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.88	0.41
1:A:543:LEU:HA	2:A:13:HOH:O	2.20	0.41
1:A:659:ASP:HA	1:A:660:PRO:HD2	1.86	0.41
1:A:463:LEU:HD12	1:A:463:LEU:HA	1.84	0.41
1:A:329:ASN:CB	1:A:330:GLU:OE1	2.62	0.40
1:A:487:ARG:NH1	1:A:576:THR:O	2.52	0.40
1:A:270:THR:HG23	1:A:273:ASN:HD22	1.85	0.40
1:A:701:ILE:C	1:A:702:GLN:HG2	2.45	0.40
1:A:314:LEU:HA	1:A:684:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLN:O	1:A:549:ASN:HB3	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	517/519 (100%)	508 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	453/453 (100%)	371 (82%)	82 (18%)	2	5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	SER
1	A	225	SER
1	A	226	SER
1	A	231	CYS
1	A	236	LEU

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Mol	Chain	Res	Type
1	A	254	ASN
1	A	262	SER
1	A	263	ASN
1	A	265	THR
1	A	270	THR
1	A	289	ARG
1	A	291	HIS
1	A	315	SER
1	A	317	LYS
1	A	322	GLN
1	A	325	GLU
1	A	326	VAL
1	A	332	THR
1	A	341	SER
1	A	345	VAL
1	A	349	SER
1	A	356	VAL
1	A	382	THR
1	A	398	LEU
1	A	404	GLN
1	A	406	LEU
1	A	415	THR
1	A	420	ASP
1	A	425	SER
1	A	426	SER
1	A	433	LEU
1	A	435	ARG
1	A	437	MET
1	A	440	LEU
1	A	445	LEU
1	A	448	LEU
1	A	450	ARG
1	A	451	THR
1	A	460	THR
1	A	463	LEU
1	A	481	LEU
1	A	487	ARG
1	A	491	VAL
1	A	495	THR
1	A	501	SER
1	A	505	TRP
1	A	513	LEU

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Mol	Chain	Res	Type
1	A	519	LEU
1	A	552	ARG
1	A	556	ASP
1	A	562	LEU
1	A	566	GLU
1	A	569	LYS
1	A	570	THR
1	A	578	GLU
1	A	581	ILE
1	A	584	ASP
1	A	589	GLN
1	A	600	SER
1	A	604	LEU
1	A	610	GLN
1	A	642	LEU
1	A	662	THR
1	A	663	THR
1	A	666	GLN
1	A	667	SER
1	A	669	LEU
1	A	670	ASN
1	A	680	GLN
1	A	682	SER
1	A	683	VAL
1	A	685	ILE
1	A	692	GLU
1	A	694	SER
1	A	698	ASN
1	A	701	ILE
1	A	705	SER
1	A	710	SER
1	A	711	THR
1	A	718	ASN
1	A	731	THR
1	A	736	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	A	260	GLN
1	A	263	ASN

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Mol	Chain	Res	Type
1	A	273	ASN
1	A	322	GLN
1	A	404	GLN
1	A	467	GLN
1	A	479	ASN
1	A	499	ASN
1	A	529	HIS
1	A	549	ASN
1	A	601	GLN
1	A	610	GLN
1	A	665	ASN
1	A	670	ASN
1	A	698	ASN
1	A	718	ASN
1	A	737	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 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

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	519/519 (100%)	1.53	114 (21%) 2 2	25, 34, 59, 91	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	457	THR	7.5
1	A	267	GLY	7.0
1	A	456	GLY	7.0
1	A	329	ASN	6.0
1	A	460	THR	5.7
1	A	331	GLY	5.6
1	A	266	SER	5.6
1	A	268	GLY	5.2
1	A	330	GLU	5.1
1	A	265	THR	4.8
1	A	333	LYS	4.7
1	A	708	TYR	4.5
1	A	220	ASP	4.5
1	A	532	ASP	4.5
1	A	334	THR	4.3
1	A	461	GLN	4.2
1	A	707	TYR	4.2
1	A	328	GLN	4.1
1	A	504	ALA	4.0
1	A	691	LYS	4.0
1	A	325	GLU	3.9
1	A	589	GLN	3.7
1	A	269	ALA	3.7
1	A	356	VAL	3.6
1	A	738	LEU	3.6
1	A	453	THR	3.5
1	A	332	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	326	VAL	3.4
1	A	262	SER	3.4
1	A	237	GLY	3.4
1	A	578	GLU	3.4
1	A	588	GLN	3.3
1	A	459	ASN	3.3
1	A	264	GLY	3.3
1	A	455	GLY	3.3
1	A	586	LEU	3.2
1	A	336	ALA	3.2
1	A	534	GLU	3.2
1	A	553	ASP	3.2
1	A	393	SER	3.1
1	A	552	ARG	3.1
1	A	548	GLN	3.0
1	A	527	ALA	3.0
1	A	271	ASN	2.9
1	A	422	PRO	2.9
1	A	349	SER	2.9
1	A	421	VAL	2.9
1	A	556	ASP	2.8
1	A	222	VAL	2.8
1	A	273	ASN	2.8
1	A	223	GLY	2.8
1	A	450	ARG	2.8
1	A	263	ASN	2.7
1	A	261	ILE	2.7
1	A	540	ASN	2.7
1	A	433	LEU	2.7
1	A	533	GLU	2.7
1	A	520	ALA	2.6
1	A	485	CYS	2.6
1	A	706	ASN	2.6
1	A	710	SER	2.6
1	A	270	THR	2.6
1	A	594	GLN	2.6
1	A	630	ASN	2.6
1	A	462	THR	2.5
1	A	232	ASP	2.5
1	A	567	GLU	2.5
1	A	557	TYR	2.5
1	A	335	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	558	SER	2.5
1	A	221	GLY	2.5
1	A	560	VAL	2.5
1	A	595	ILE	2.4
1	A	584	ASP	2.4
1	A	692	GLU	2.4
1	A	338	ASN	2.4
1	A	345	VAL	2.4
1	A	466	SER	2.4
1	A	667	SER	2.4
1	A	477	ALA	2.4
1	A	550	ALA	2.4
1	A	705	SER	2.3
1	A	372	VAL	2.3
1	A	503	PHE	2.3
1	A	590	ASN	2.3
1	A	725	GLU	2.3
1	A	576	THR	2.3
1	A	238	ASP	2.3
1	A	465	PHE	2.3
1	A	666	GLN	2.2
1	A	441	ILE	2.2
1	A	486	TYR	2.2
1	A	449	SER	2.2
1	A	346	PHE	2.2
1	A	234	THR	2.2
1	A	737	ASN	2.2
1	A	475	ASN	2.2
1	A	635	PRO	2.2
1	A	712	SER	2.2
1	A	303	ILE	2.2
1	A	499	ASN	2.1
1	A	587	GLN	2.1
1	A	713	VAL	2.1
1	A	565	GLU	2.1
1	A	239	ARG	2.1
1	A	357	LEU	2.1
1	A	659	ASP	2.1
1	A	671	SER	2.1
1	A	423	PHE	2.1
1	A	454	THR	2.0
1	A	509	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	598	VAL	2.0
1	A	510	LYS	2.0
1	A	489	GLN	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.