



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:41 PM UTC

PDB ID : 3RA4 / pdb_00003ra4
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 : 2011-03-27
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

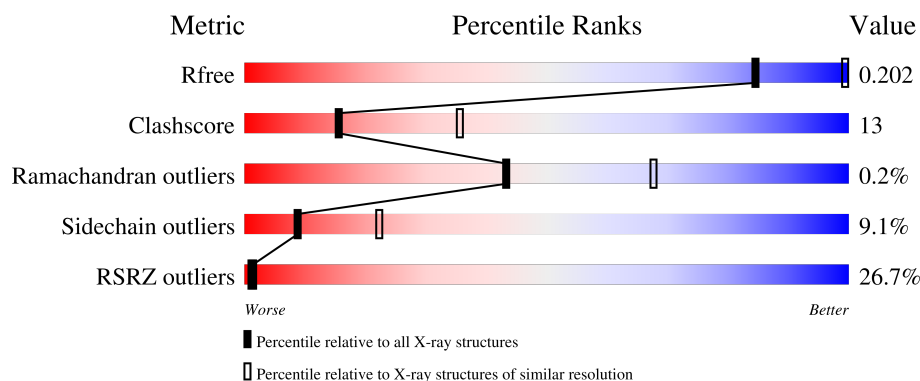
1 Overall quality at a glance

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	26% 75% 20% 5%
2	D	2	100% 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4249 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 a DNA chain called DNA (5'-D(*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	P	0	0	0
			37	19	8	9	1			

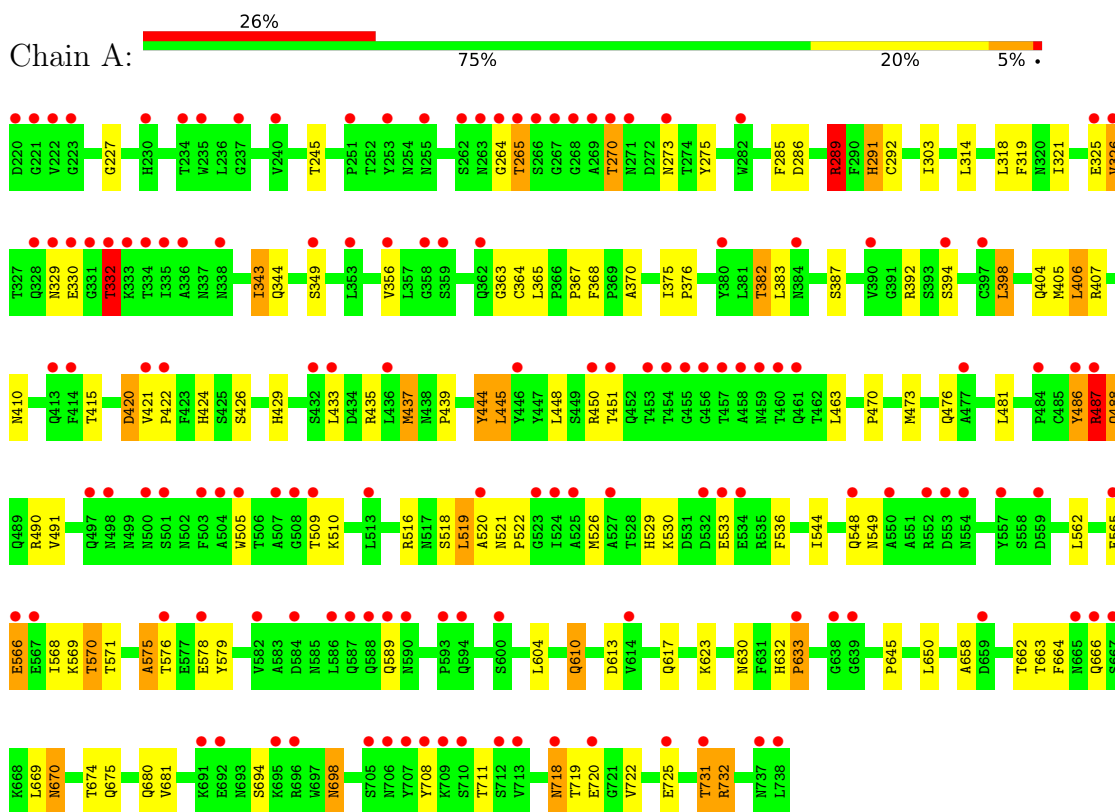
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	D	1	Total	O	0	0
			1	1		

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: Capsid protein



• Molecule 2: DNA (5'-D(*CP*A)-3')



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)	(Not available) (40.00-2.70) 92.9 (40.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.213 0.203 , 0.202	Depositor DCC
R_{free} test set	12162 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.3	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	0.38	EDS
Total number of atoms	4249	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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	0.53	2/4259 (0.0%)	1.05	28/5811 (0.5%)
2	D	0.43	0/41	0.90	0/61
All	All	0.53	2/4300 (0.0%)	1.05	28/5872 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	THR	CA-CB	5.93	1.60	1.53
1	A	289	ARG	C-N	5.31	1.40	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	THR	N-CA-C	-11.61	99.12	113.28
1	A	488	GLN	OE1-CD-NE2	-10.28	112.32	122.60
1	A	725	GLU	CA-C-N	7.64	128.03	119.32
1	A	725	GLU	C-N-CA	7.64	128.03	119.32
1	A	658	ALA	N-CA-C	-7.42	100.10	110.35
1	A	732	ARG	N-CA-C	6.58	120.14	108.24
1	A	486	TYR	N-CA-C	-6.56	97.67	108.76
1	A	488	GLN	CG-CD-NE2	6.55	126.22	116.40
1	A	303	ILE	N-CA-C	6.40	119.09	111.09
1	A	487	ARG	CA-C-N	-6.18	112.98	122.62
1	A	487	ARG	C-N-CA	-6.18	112.98	122.62
1	A	664	PHE	N-CA-C	6.10	118.84	110.24
1	A	694	SER	N-CA-C	5.81	118.88	110.28
1	A	487	ARG	N-CA-C	5.78	119.37	110.42
1	A	375	ILE	CA-C-N	5.46	125.41	119.78
1	A	375	ILE	C-N-CA	5.46	125.41	119.78
1	A	579	TYR	N-CA-C	-5.45	104.99	111.69
1	A	444	TYR	N-CA-C	-5.43	106.70	113.38
1	A	292	CYS	N-CA-C	-5.39	106.20	112.89
1	A	407	ARG	N-CA-C	-5.32	102.59	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	ALA	N-CA-C	-5.31	99.32	108.56
1	A	675	GLN	N-CA-C	5.29	116.88	108.79
1	A	575	ALA	N-CA-C	5.27	118.49	111.75
1	A	365	LEU	CA-C-N	5.26	123.50	119.66
1	A	365	LEU	C-N-CA	5.26	123.50	119.66
1	A	343	ILE	N-CA-C	-5.20	100.88	108.99
1	A	708	TYR	N-CA-C	5.13	117.47	110.55
1	A	666	GLN	N-CA-C	5.03	117.49	111.71

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	108	0
2	D	37	0	24	9	0
3	A	75	0	0	0	0
3	D	1	0	0	0	0
All	All	4249	0	3917	108	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 13.

All (108) 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	0.95	1.07
1:A:382:THR:HG21	1:A:394:SER:H	1.25	1.01
1:A:289:ARG:HG2	1:A:289:ARG:NH1	1.71	1.00
1:A:487:ARG:HG3	1:A:488:GLN:N	1.77	0.98
1:A:486:TYR:O	1:A:526:MET:HE1	1.67	0.94
1:A:718:ASN:HB3	1:A:720:GLU:H	1.32	0.91
1:A:289:ARG:HH11	1:A:289:ARG:CG	1.82	0.91
1:A:698:ASN:HD22	1:A:698:ASN:H	1.22	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASP:HB3	2:D:1:DC:N4	1.91	0.85
1:A:632:HIS:N	1:A:633:PRO:HD3	1.96	0.81
1:A:426:SER:HA	1:A:731:THR:HG23	1.67	0.75
1:A:529:HIS:CG	1:A:533:GLU:O	2.39	0.75
1:A:633:PRO:HD2	2:D:2:DA:H2''	1.71	0.73
1:A:529:HIS:CD2	1:A:533:GLU:O	2.43	0.72
1:A:566:GLU:O	1:A:569:LYS:HG3	1.92	0.68
1:A:429:HIS:HB2	1:A:570:THR:HG21	1.75	0.68
1:A:630:ASN:OD1	1:A:633:PRO:HG3	1.95	0.67
1:A:487:ARG:CG	1:A:488:GLN:N	2.55	0.66
1:A:698:ASN:H	1:A:698:ASN:ND2	1.89	0.66
1:A:486:TYR:O	1:A:526:MET:CE	2.44	0.65
1:A:329:ASN:O	1:A:332:THR:HG23	1.98	0.63
1:A:632:HIS:N	1:A:633:PRO:CD	2.61	0.63
1:A:363:GLY:HA3	1:A:376:PRO:HG3	1.82	0.62
1:A:718:ASN:HB2	1:A:722:VAL:H	1.65	0.61
1:A:420:ASP:HB3	2:D:1:DC:H41	1.63	0.61
1:A:420:ASP:C	2:D:1:DC:N4	2.59	0.60
1:A:321:ILE:CD1	1:A:406:LEU:HD12	2.31	0.60
1:A:314:LEU:C	1:A:314:LEU:HD12	2.27	0.60
1:A:383:LEU:HD12	1:A:392:ARG:HB2	1.84	0.60
1:A:421:VAL:HG22	1:A:422:PRO:HD2	1.83	0.60
1:A:321:ILE:HD13	1:A:343:ILE:HD11	1.83	0.59
1:A:422:PRO:HG3	2:D:1:DC:H2'	1.85	0.58
1:A:420:ASP:CB	2:D:1:DC:H41	2.17	0.56
1:A:285:PHE:CZ	1:A:318:LEU:HD21	2.43	0.54
1:A:450:ARG:HH11	1:A:450:ARG:HG3	1.71	0.54
1:A:326:VAL:HG13	1:A:674:THR:HG22	1.89	0.54
1:A:439:PRO:O	1:A:470:PRO:HB3	2.09	0.53
1:A:610:GLN:HE21	1:A:610:GLN:CA	2.20	0.53
1:A:435:ARG:CZ	1:A:473:MET:HE3	2.38	0.53
1:A:623:LYS:HB2	1:A:645:PRO:HG3	1.90	0.52
1:A:570:THR:HG23	1:A:571:THR:HG23	1.91	0.52
1:A:321:ILE:HD12	1:A:406:LEU:HD12	1.92	0.52
1:A:510:LYS:HB3	1:A:518:SER:O	2.08	0.52
1:A:264:GLY:CA	1:A:387:SER:HB3	2.40	0.52
1:A:613:ASP:OD1	1:A:731:THR:HG22	2.11	0.51
1:A:329:ASN:O	1:A:332:THR:CG2	2.58	0.51
1:A:568:ILE:C	1:A:570:THR:N	2.69	0.51
1:A:289:ARG:NH1	1:A:617:GLN:O	2.41	0.51
1:A:487:ARG:NH1	1:A:576:THR:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:C	1:A:332:THR:H	2.18	0.50
1:A:435:ARG:NE	1:A:473:MET:HE3	2.26	0.50
1:A:405:MET:C	1:A:406:LEU:HD23	2.37	0.50
1:A:421:VAL:HG22	1:A:422:PRO:CD	2.41	0.50
1:A:565:GLU:O	1:A:568:ILE:HG12	2.12	0.50
1:A:424:HIS:CD2	1:A:731:THR:HG21	2.47	0.49
1:A:670:ASN:H	1:A:670:ASN:HD22	1.61	0.49
1:A:398:LEU:N	1:A:398:LEU:HD23	2.28	0.49
1:A:289:ARG:NH1	1:A:289:ARG:CG	2.53	0.49
1:A:731:THR:HG22	1:A:732:ARG:HG3	1.94	0.48
1:A:326:VAL:HG13	1:A:674:THR:CG2	2.43	0.48
1:A:264:GLY:HA3	1:A:387:SER:HB3	1.96	0.47
1:A:670:ASN:HD22	1:A:670:ASN:C	2.22	0.47
1:A:289:ARG:HD2	1:A:364:CYS:SG	2.53	0.47
1:A:426:SER:HA	1:A:731:THR:CG2	2.39	0.47
1:A:368:PHE:CE2	1:A:370:ALA:HB3	2.51	0.46
1:A:406:LEU:HB3	1:A:410:ASN:HB2	1.97	0.46
1:A:422:PRO:CG	2:D:1:DC:H2'	2.46	0.46
1:A:529:HIS:HD2	1:A:530:LYS:O	1.99	0.46
1:A:533:GLU:HB3	1:A:536:PHE:HD1	1.81	0.46
1:A:404:GLN:HE21	1:A:406:LEU:HD22	1.81	0.45
1:A:451:THR:HG22	1:A:451:THR:O	2.14	0.45
1:A:437:MET:HG2	1:A:476:GLN:OE1	2.16	0.45
1:A:286:ASP:O	1:A:364:CYS:HA	2.17	0.45
1:A:444:TYR:CE2	1:A:445:LEU:HD13	2.52	0.45
1:A:610:GLN:NE2	1:A:610:GLN:HA	2.32	0.44
1:A:344:GLN:HG2	1:A:405:MET:HG2	2.00	0.44
1:A:406:LEU:HD23	1:A:406:LEU:N	2.32	0.44
1:A:321:ILE:HD13	1:A:343:ILE:CD1	2.46	0.44
1:A:450:ARG:HG3	1:A:450:ARG:NH1	2.32	0.44
1:A:382:THR:HG21	1:A:394:SER:N	2.10	0.44
1:A:424:HIS:NE2	1:A:731:THR:HG21	2.33	0.43
1:A:291:HIS:CD2	1:A:367:PRO:HG3	2.53	0.43
1:A:398:LEU:CD1	1:A:650:LEU:HD22	2.49	0.43
1:A:670:ASN:C	1:A:670:ASN:ND2	2.74	0.43
1:A:568:ILE:C	1:A:570:THR:H	2.26	0.43
1:A:227:GLY:HA3	1:A:319:PHE:CD1	2.53	0.43
1:A:270:THR:HG23	1:A:273:ASN:HD22	1.82	0.43
1:A:330:GLU:O	1:A:332:THR:N	2.51	0.43
1:A:505:TRP:CZ3	1:A:519:LEU:HD13	2.53	0.43
1:A:291:HIS:CE1	1:A:367:PRO:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLN:HE21	1:A:610:GLN:HA	1.84	0.43
1:A:275:TYR:CD1	1:A:275:TYR:C	2.97	0.43
1:A:245:THR:HA	1:A:681:VAL:O	2.19	0.42
1:A:406:LEU:HB3	1:A:410:ASN:CB	2.49	0.42
1:A:526:MET:HB2	1:A:575:ALA:HB2	2.01	0.42
1:A:426:SER:CA	1:A:731:THR:HG23	2.42	0.42
1:A:670:ASN:HD22	1:A:670:ASN:N	2.17	0.42
1:A:544:ILE:HG23	1:A:562:LEU:HD23	2.03	0.41
1:A:610:GLN:CA	1:A:610:GLN:NE2	2.83	0.41
1:A:718:ASN:HB3	1:A:720:GLU:N	2.16	0.41
1:A:490:ARG:HD2	1:A:536:PHE:CG	2.55	0.41
1:A:420:ASP:C	2:D:1:DC:H41	2.29	0.41
1:A:488:GLN:HA	1:A:509:THR:OG1	2.21	0.41
1:A:291:HIS:NE2	1:A:367:PRO:HG3	2.36	0.41
1:A:451:THR:O	1:A:451:THR:CG2	2.70	0.40
1:A:420:ASP:HB3	2:D:1:DC:H42	1.78	0.40
1:A:265:THR:O	1:A:265:THR:HG23	2.21	0.40
1:A:521:ASN:HA	1:A:522:PRO:HA	1.86	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	517/519 (100%)	499 (96%)	17 (3%)	1 (0%)	43 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	633	PRO

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	453/453 (100%)	412 (91%)	41 (9%)	9 22

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	THR
1	A	270	THR
1	A	289	ARG
1	A	291	HIS
1	A	325	GLU
1	A	326	VAL
1	A	332	THR
1	A	349	SER
1	A	356	VAL
1	A	382	THR
1	A	398	LEU
1	A	406	LEU
1	A	415	THR
1	A	420	ASP
1	A	433	LEU
1	A	437	MET
1	A	445	LEU
1	A	448	LEU
1	A	463	LEU
1	A	481	LEU
1	A	487	ARG
1	A	491	VAL
1	A	516	ARG
1	A	519	LEU
1	A	548	GLN
1	A	549	ASN
1	A	566	GLU
1	A	570	THR
1	A	578	GLU
1	A	589	GLN

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Mol	Chain	Res	Type
1	A	604	LEU
1	A	610	GLN
1	A	662	THR
1	A	663	THR
1	A	669	LEU
1	A	670	ASN
1	A	680	GLN
1	A	698	ASN
1	A	711	THR
1	A	718	ASN
1	A	731	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	A	260	GLN
1	A	263	ASN
1	A	273	ASN
1	A	361	HIS
1	A	429	HIS
1	A	467	GLN
1	A	521	ASN
1	A	529	HIS
1	A	549	ASN
1	A	599	ASN
1	A	601	GLN
1	A	610	GLN
1	A	653	ASN
1	A	665	ASN
1	A	666	GLN
1	A	670	ASN
1	A	698	ASN
1	A	718	ASN

5.3.3 RNA ⓘ

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%)	1.60	137 (26%)  	33, 42, 63, 101	0
2	D	2/2 (100%)	7.05	2 (100%)  	40, 40, 40, 57	2 (100%)
All	All	521/521 (100%)	1.62	139 (26%)  	33, 42, 63, 101	2 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	DC	10.0
1	A	268	GLY	7.0
1	A	330	GLU	6.9
1	A	220	ASP	6.6
1	A	267	GLY	6.3
1	A	456	GLY	6.2
1	A	589	GLN	6.0
1	A	457	THR	5.7
1	A	331	GLY	5.5
1	A	329	ASN	5.3
1	A	328	GLN	5.2
1	A	553	ASP	5.1
1	A	455	GLY	4.6
1	A	460	THR	4.5
1	A	266	SER	4.4
1	A	336	ALA	4.4
1	A	269	ALA	4.3
1	A	738	LEU	4.1
2	D	2	DA	4.1
1	A	332	THR	4.0
1	A	333	LYS	3.9
1	A	578	GLU	3.8
1	A	454	THR	3.8
1	A	691	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	707	TYR	3.7
1	A	534	GLU	3.6
1	A	459	ASN	3.6
1	A	532	ASP	3.6
1	A	436	LEU	3.6
1	A	706	ASN	3.5
1	A	234	THR	3.4
1	A	237	GLY	3.4
1	A	461	GLN	3.3
1	A	338	ASN	3.3
1	A	326	VAL	3.3
1	A	221	GLY	3.3
1	A	265	THR	3.3
1	A	508	GLY	3.3
1	A	659	ASP	3.3
1	A	458	ALA	3.2
1	A	359	SER	3.1
1	A	253	TYR	3.1
1	A	586	LEU	3.0
1	A	638	GLY	3.0
1	A	477	ALA	3.0
1	A	708	TYR	3.0
1	A	362	GLN	3.0
1	A	270	THR	3.0
1	A	557	TYR	3.0
1	A	325	GLU	2.9
1	A	271	ASN	2.9
1	A	223	GLY	2.9
1	A	264	GLY	2.9
1	A	222	VAL	2.9
1	A	501	SER	2.8
1	A	576	THR	2.8
1	A	567	GLU	2.8
1	A	695	LYS	2.7
1	A	552	ARG	2.7
1	A	486	TYR	2.7
1	A	453	THR	2.7
1	A	255	ASN	2.7
1	A	500	ASN	2.6
1	A	513	LEU	2.6
1	A	262	SER	2.6
1	A	593	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	548	GLN	2.6
1	A	230	HIS	2.6
1	A	380	TYR	2.6
1	A	356	VAL	2.5
1	A	421	VAL	2.5
1	A	523	GLY	2.5
1	A	507	ALA	2.5
1	A	666	GLN	2.5
1	A	384	ASN	2.5
1	A	450	ARG	2.4
1	A	588	GLN	2.4
1	A	282	TRP	2.4
1	A	240	VAL	2.4
1	A	696	ARG	2.4
1	A	665	ASN	2.4
1	A	705	SER	2.4
1	A	497	GLN	2.4
1	A	334	THR	2.3
1	A	590	ASN	2.3
1	A	737	ASN	2.3
1	A	692	GLU	2.3
1	A	720	GLU	2.3
1	A	584	ASP	2.3
1	A	600	SER	2.3
1	A	639	GLY	2.3
1	A	504	ALA	2.3
1	A	520	ALA	2.3
1	A	527	ALA	2.3
1	A	335	ILE	2.3
1	A	713	VAL	2.3
1	A	503	PHE	2.3
1	A	587	GLN	2.3
1	A	414	PHE	2.3
1	A	446	TYR	2.3
1	A	554	ASN	2.3
1	A	422	PRO	2.3
1	A	487	ARG	2.3
1	A	667	SER	2.3
1	A	273	ASN	2.2
1	A	349	SER	2.2
1	A	390	VAL	2.2
1	A	525	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	709	LYS	2.2
1	A	509	THR	2.2
1	A	550	ALA	2.2
1	A	397	CYS	2.2
1	A	565	GLU	2.2
1	A	263	ASN	2.2
1	A	594	GLN	2.2
1	A	559	ASP	2.2
1	A	712	SER	2.2
1	A	533	GLU	2.2
1	A	731	THR	2.2
1	A	484	PRO	2.2
1	A	394	SER	2.2
1	A	413	GLN	2.1
1	A	718	ASN	2.1
1	A	353	LEU	2.1
1	A	235	TRP	2.1
1	A	251	PRO	2.1
1	A	433	LEU	2.1
1	A	498	ASN	2.1
1	A	614	VAL	2.1
1	A	725	GLU	2.1
1	A	432	SER	2.1
1	A	566	GLU	2.1
1	A	451	THR	2.1
1	A	710	SER	2.0
1	A	582	VAL	2.0
1	A	505	TRP	2.0
1	A	633	PRO	2.0
1	A	358	GLY	2.0
1	A	524	ILE	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.