Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:58 am BST

PDB ID	:	3H71
Title	:	Crystal structure of Streptococcus pneumoniae D39 neuraminidase A precursor (NanA)
Authors	:	Hsiao, Y.-S.; Tong, L.
Deposited on	:	2009-04-24
Resolution	:	1.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

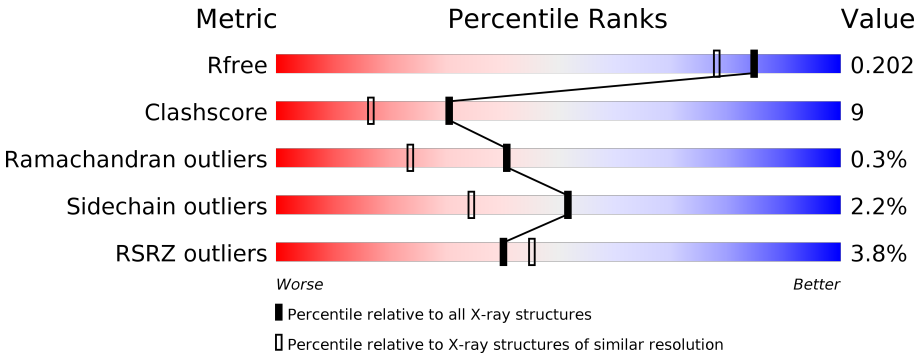
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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 <=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	477	5% 83% 14%
1	B	477	3% 83% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9263 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 Sialidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	Se	0	0	0
			3747	2347	661	727	12			
1	B	477	Total	C	N	O	Se	0	0	0
			3771	2363	664	732	12			

- Molecule 2 is water.

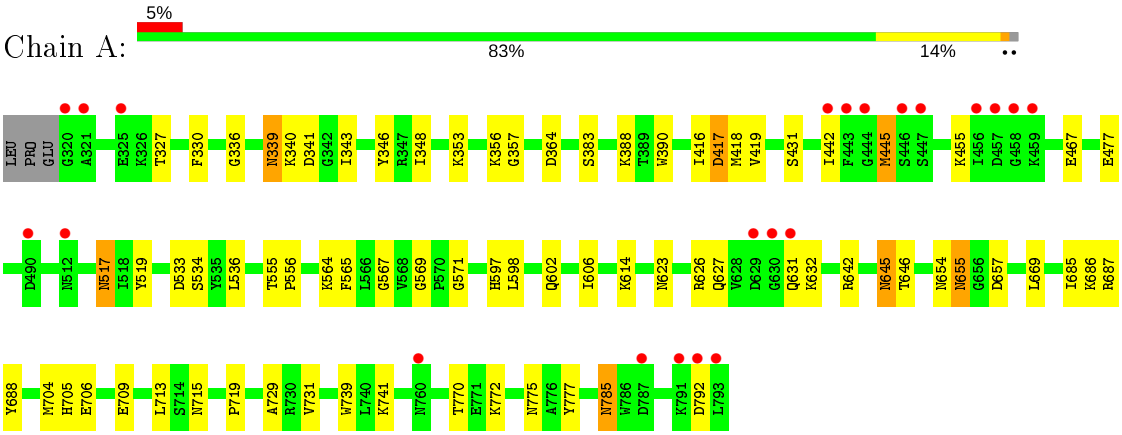
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	843	Total	O	0	0
			843	843		
2	B	902	Total	O	0	0
			902	902		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

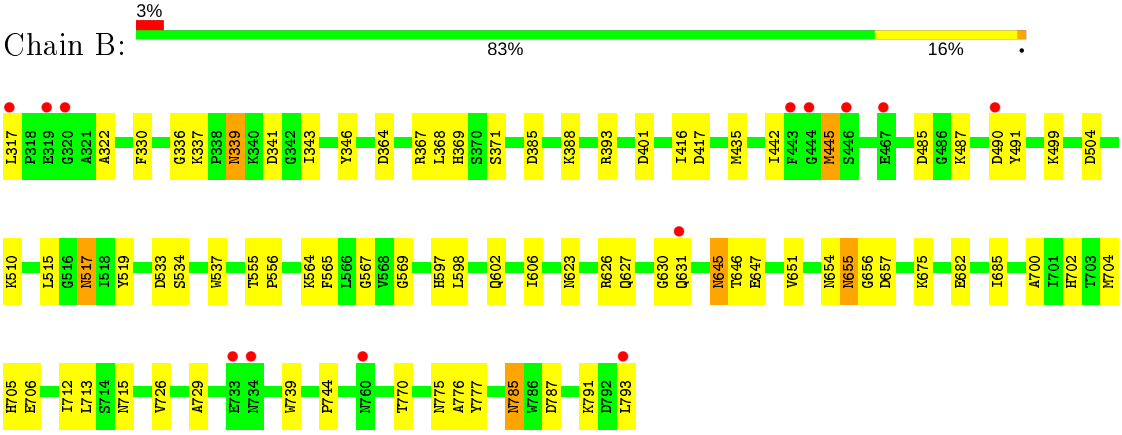
- Molecule 1: Sialidase A

Chain A:



- Molecule 1: Sialidase A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.04Å 47.67Å 137.27Å 90.00° 116.56° 90.00°	Depositor
Resolution (Å)	27.39 – 1.70 27.38 – 1.68	Depositor EDS
% Data completeness (in resolution range)	92.4 (27.39-1.70) 95.2 (27.38-1.68)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.11 (at 1.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.172 , 0.198 0.177 , 0.202	Depositor DCC
R_{free} test set	13261 reflections (7.17%)	wwPDB-VP
Wilson B-factor (Å^2)	10.5	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9263	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.30	0/3816	0.66	1/5133 (0.0%)
1	B	0.29	0/3841	0.65	1/5168 (0.0%)
All	All	0.30	0/7657	0.66	2/10301 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	569	GLY	N-CA-C	-6.98	95.65	113.10
1	A	569	GLY	N-CA-C	-6.88	95.89	113.10

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	3747	0	3664	61	0
1	B	3771	0	3688	75	0
2	A	843	0	0	11	0
2	B	902	0	0	10	0
All	All	9263	0	7352	136	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 (136) 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:517:ASN:HD22	1:A:519:TYR:H	1.14	0.94
1:B:517:ASN:HD22	1:B:519:TYR:H	1.13	0.92
1:A:336:GLY:H	1:A:775:ASN:HD21	1.26	0.80
1:B:445:MSE:HG2	1:B:564:LYS:HE2	1.64	0.80
1:B:336:GLY:H	1:B:775:ASN:HD21	1.31	0.78
1:B:510:LYS:HB2	1:B:515:LEU:HD11	1.66	0.77
1:A:418:MSE:CE	1:A:431:SER:HB2	2.14	0.77
1:A:517:ASN:ND2	1:A:519:TYR:H	1.84	0.75
1:B:401:ASP:HB3	2:B:1051:HOH:O	1.88	0.72
1:A:327:THR:HG21	2:A:1804:HOH:O	1.92	0.68
1:B:517:ASN:ND2	1:B:519:TYR:H	1.88	0.68
1:B:655:ASN:ND2	1:B:657:ASP:H	1.92	0.67
1:B:435:MSE:HE2	1:B:537:TRP:CZ2	2.30	0.66
1:A:339:ASN:ND2	1:A:341:ASP:H	1.94	0.66
1:A:418:MSE:HE1	1:A:431:SER:HB2	1.77	0.66
1:A:655:ASN:ND2	1:A:657:ASP:H	1.95	0.65
1:A:442:ILE:HD13	1:A:565:PHE:CD1	2.32	0.64
1:B:510:LYS:HB2	1:B:515:LEU:CD1	2.29	0.63
1:A:339:ASN:HD22	1:A:339:ASN:C	2.03	0.62
1:A:614:LYS:HE3	2:A:280:HOH:O	2.00	0.62
1:A:642:ARG:HH11	1:A:642:ARG:HG2	1.65	0.60
1:B:367:ARG:HH21	1:B:368:LEU:HD21	1.67	0.59
1:B:339:ASN:ND2	1:B:341:ASP:H	2.00	0.59
1:B:339:ASN:ND2	1:B:343:ILE:H	2.00	0.59
1:B:623:ASN:HD21	1:B:626:ARG:HH11	1.51	0.58
1:B:655:ASN:C	1:B:655:ASN:HD22	2.04	0.58
1:B:339:ASN:C	1:B:339:ASN:HD22	2.06	0.58
1:B:627:GLN:NE2	1:B:630:GLY:H	2.01	0.58
1:B:393:ARG:HD3	2:B:827:HOH:O	2.03	0.58
1:A:339:ASN:ND2	1:A:343:ILE:H	2.01	0.58
1:A:729:ALA:HB2	1:A:739:TRP:CE3	2.38	0.58
1:A:631:GLN:HG2	2:A:1123:HOH:O	2.04	0.58
1:B:364:ASP:OD2	1:B:416:ILE:HG13	2.05	0.57
1:A:533:ASP:CG	1:A:534:SER:H	2.07	0.57
1:A:709:GLU:HG2	1:A:731:VAL:HB	1.87	0.56
1:A:364:ASP:OD2	1:A:416:ILE:HG13	2.06	0.56
1:A:445:MSE:HG2	1:A:564:LYS:CE	2.36	0.56
1:B:787:ASP:HB3	1:B:791:LYS:HE3	1.87	0.56
1:B:499:LYS:HD2	1:B:504:ASP:HB3	1.86	0.56
1:B:655:ASN:HD22	1:B:656:GLY:N	2.04	0.56
1:A:602:GLN:HB3	1:A:646:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ASP:OD2	1:B:510:LYS:HD3	2.05	0.55
1:A:336:GLY:H	1:A:775:ASN:ND2	2.02	0.55
1:A:445:MSE:HG2	1:A:564:LYS:HE2	1.88	0.55
1:A:442:ILE:HG22	2:A:948:HOH:O	2.06	0.55
1:B:322:ALA:H	1:B:785:ASN:HD21	1.55	0.55
1:A:467:GLU:HG3	2:A:1160:HOH:O	2.06	0.54
1:A:555:THR:N	1:A:556:PRO:HD2	2.23	0.54
1:A:356:LYS:HE3	2:A:1298:HOH:O	2.07	0.54
1:B:627:GLN:HE21	1:B:630:GLY:H	1.56	0.53
1:B:369:HIS:CE1	1:B:371:SER:HB2	2.44	0.53
1:A:418:MSE:HE1	1:A:431:SER:CB	2.38	0.52
1:B:623:ASN:ND2	1:B:626:ARG:HH11	2.08	0.52
1:B:606:ILE:C	1:B:606:ILE:HD12	2.29	0.52
1:A:772:LYS:HG3	1:A:772:LYS:O	2.09	0.52
1:B:705:HIS:CE1	1:B:706:GLU:HG3	2.45	0.52
1:A:565:PHE:CZ	1:A:567:GLY:HA3	2.46	0.51
1:B:330:PHE:HB3	1:B:346:TYR:CG	2.45	0.51
1:A:339:ASN:ND2	1:A:339:ASN:C	2.63	0.51
1:A:627:GLN:OE1	1:A:632:LYS:HE2	2.11	0.51
1:B:744:PRO:HD2	1:B:793:LEU:HD12	1.93	0.51
1:B:367:ARG:HH21	1:B:368:LEU:HD11	1.74	0.51
1:B:533:ASP:CG	1:B:534:SER:H	2.13	0.51
1:B:343:ILE:HD13	1:B:367:ARG:HG3	1.91	0.51
1:B:445:MSE:CG	1:B:564:LYS:HE2	2.39	0.50
1:A:623:ASN:HD21	1:A:626:ARG:HH11	1.58	0.50
1:B:445:MSE:HE1	1:B:534:SER:HB2	1.93	0.50
1:A:455:LYS:HE3	2:A:1015:HOH:O	2.11	0.50
1:B:336:GLY:H	1:B:775:ASN:ND2	2.06	0.49
1:A:356:LYS:HE2	2:A:1782:HOH:O	2.12	0.49
1:A:353:LYS:HE3	1:A:357:GLY:HA2	1.95	0.49
1:B:442:ILE:HD11	1:B:598:LEU:HD21	1.95	0.49
1:A:340:LYS:HE3	2:A:1061:HOH:O	2.14	0.48
1:B:385:ASP:CG	1:B:388:LYS:HB3	2.34	0.48
1:A:330:PHE:HB3	1:A:346:TYR:CG	2.48	0.48
1:B:602:GLN:HB3	1:B:646:THR:HG22	1.95	0.48
1:B:726:VAL:O	1:B:726:VAL:HG23	2.14	0.48
1:A:785:ASN:HD22	1:A:785:ASN:C	2.17	0.48
1:A:741:LYS:HE3	1:A:792:ASP:OD1	2.14	0.48
1:B:445:MSE:HE1	1:B:534:SER:CB	2.44	0.48
1:A:623:ASN:HD21	1:A:645:ASN:HD21	1.62	0.47
1:B:337:LYS:HE3	2:B:1821:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ILE:HD12	1:A:685:ILE:N	2.30	0.47
1:B:646:THR:OG1	1:B:647:GLU:N	2.48	0.47
1:A:770:THR:HG23	1:A:777:TYR:CD1	2.49	0.47
1:A:623:ASN:ND2	1:A:626:ARG:HH11	2.13	0.47
1:B:555:THR:N	1:B:556:PRO:HD2	2.30	0.47
1:A:418:MSE:CE	1:A:431:SER:CB	2.89	0.46
1:A:642:ARG:NH1	1:A:642:ARG:HG2	2.29	0.46
1:B:682:GLU:HG3	2:B:1862:HOH:O	2.14	0.46
1:B:729:ALA:HB2	1:B:739:TRP:CE3	2.50	0.46
1:B:655:ASN:C	1:B:655:ASN:ND2	2.68	0.46
1:A:655:ASN:C	1:A:655:ASN:HD22	2.18	0.46
1:B:713:LEU:HD23	1:B:713:LEU:C	2.35	0.46
1:B:675:LYS:HE2	2:B:1862:HOH:O	2.15	0.45
1:A:388:LYS:HE3	2:A:1752:HOH:O	2.16	0.45
1:B:367:ARG:NH2	2:B:1064:HOH:O	2.48	0.45
1:A:602:GLN:CB	1:A:646:THR:HG22	2.46	0.45
1:A:418:MSE:HE3	1:A:431:SER:HB2	1.96	0.45
1:B:651:VAL:HG13	1:B:702:HIS:HB2	1.98	0.45
1:B:770:THR:HG23	1:B:777:TYR:CD1	2.52	0.45
1:B:322:ALA:H	1:B:785:ASN:ND2	2.15	0.45
1:B:435:MSE:HE2	1:B:537:TRP:HZ2	1.80	0.45
1:B:435:MSE:HG3	1:B:537:TRP:CE2	2.52	0.45
1:B:597:HIS:CG	1:B:598:LEU:H	2.35	0.45
1:A:705:HIS:CE1	1:A:706:GLU:HG3	2.52	0.44
1:B:367:ARG:NE	2:B:1003:HOH:O	2.51	0.44
1:A:606:ILE:HD12	1:A:606:ILE:C	2.37	0.44
1:B:675:LYS:HE3	2:B:1739:HOH:O	2.16	0.44
1:B:435:MSE:HG3	1:B:537:TRP:CZ2	2.52	0.44
1:A:348:ILE:HG21	1:A:417:ASP:HA	2.00	0.44
1:A:713:LEU:HD23	1:A:713:LEU:C	2.37	0.44
1:A:419:VAL:HA	1:A:571:GLY:O	2.18	0.44
1:A:655:ASN:C	1:A:655:ASN:ND2	2.71	0.43
1:B:339:ASN:C	1:B:339:ASN:ND2	2.71	0.43
1:A:597:HIS:CG	1:A:598:LEU:H	2.36	0.43
1:B:367:ARG:NH2	1:B:368:LEU:HD21	2.32	0.43
1:B:485:ASP:OD1	1:B:487:LYS:HG2	2.18	0.43
1:B:565:PHE:CZ	1:B:567:GLY:HA3	2.54	0.43
1:A:340:LYS:HG2	2:A:1136:HOH:O	2.17	0.43
1:B:606:ILE:O	1:B:606:ILE:HD12	2.19	0.43
1:B:700:ALA:HA	1:B:712:ILE:O	2.19	0.42
1:A:383:SER:HB2	1:A:390:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:ASP:CB	1:B:791:LYS:HE3	2.49	0.42
1:B:685:ILE:HD13	2:B:1089:HOH:O	2.19	0.42
1:B:654:ASN:HD21	1:B:704:MSE:SE	2.53	0.42
1:A:669:LEU:O	1:A:687:ARG:HA	2.20	0.42
1:B:623:ASN:HD21	1:B:645:ASN:HD21	1.68	0.42
1:A:686:LYS:HG2	1:A:688:TYR:CZ	2.55	0.42
1:B:776:ALA:HA	1:B:777:TYR:HA	1.79	0.41
1:B:491:TYR:CE2	1:B:510:LYS:HG2	2.56	0.41
1:B:510:LYS:CB	1:B:515:LEU:HD11	2.44	0.41
1:A:654:ASN:HD21	1:A:704:MSE:SE	2.53	0.41
1:B:785:ASN:HD22	1:B:785:ASN:H	1.69	0.40
1:B:401:ASP:HB3	2:B:1064:HOH:O	2.21	0.40
1:B:785:ASN:H	1:B:785:ASN:ND2	2.20	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	472/477 (99%)	448 (95%)	22 (5%)	2 (0%)	34 18
1	B	475/477 (100%)	450 (95%)	24 (5%)	1 (0%)	47 30
All	All	947/954 (99%)	898 (95%)	46 (5%)	3 (0%)	41 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	417	ASP
1	A	417	ASP
1	A	719	PRO

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	404/395 (102%)	395 (98%)	9 (2%)	52 34
1	B	407/395 (103%)	398 (98%)	9 (2%)	52 34
All	All	811/790 (103%)	793 (98%)	18 (2%)	52 34

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	ASN
1	A	445	MSE
1	A	477	GLU
1	A	517	ASN
1	A	536	LEU
1	A	645	ASN
1	A	655	ASN
1	A	715	ASN
1	A	785	ASN
1	B	317	LEU
1	B	339	ASN
1	B	445	MSE
1	B	517	ASN
1	B	631	GLN
1	B	645	ASN
1	B	655	ASN
1	B	715	ASN
1	B	785	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	ASN
1	A	517	ASN
1	A	523	ASN
1	A	623	ASN

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Mol	Chain	Res	Type
1	A	655	ASN
1	A	715	ASN
1	A	753	ASN
1	A	775	ASN
1	A	785	ASN
1	B	339	ASN
1	B	517	ASN
1	B	523	ASN
1	B	599	ASN
1	B	623	ASN
1	B	627	GLN
1	B	631	GLN
1	B	655	ASN
1	B	715	ASN
1	B	753	ASN
1	B	774	GLN
1	B	775	ASN
1	B	785	ASN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	462/477 (96%)	0.01	22 (4%) 30 34	3, 10, 25, 41	0
1	B	465/477 (97%)	-0.05	13 (2%) 53 57	4, 11, 24, 32	0
All	All	927/954 (97%)	-0.02	35 (3%) 40 45	3, 10, 24, 41	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	793	LEU	13.5
1	A	321	ALA	9.1
1	B	317	LEU	5.8
1	A	792	ASP	5.3
1	B	793	LEU	5.1
1	A	320	GLY	5.1
1	A	443	PHE	4.9
1	A	457	ASP	4.9
1	B	733	GLU	4.6
1	A	446	SER	4.6
1	A	442	ILE	4.3
1	A	631	GLN	4.2
1	A	629	ASP	3.8
1	B	443	PHE	3.7
1	A	630	GLY	3.5
1	A	760	ASN	3.5
1	B	734	ASN	3.3
1	A	447	SER	3.1
1	B	760	ASN	3.1
1	A	458	GLY	2.8
1	B	631	GLN	2.8
1	A	512	ASN	2.7
1	A	456	ILE	2.6
1	B	319	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	490	ASP	2.5
1	A	444	GLY	2.5
1	A	791	LYS	2.5
1	B	467	GLU	2.5
1	B	446	SER	2.4
1	A	787	ASP	2.4
1	A	325	GLU	2.3
1	B	320	GLY	2.3
1	A	459	LYS	2.3
1	B	444	GLY	2.2
1	A	490	ASP	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 carbohydrates 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.