

Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2024 – 01:22 pm BST

PDB ID	:	8QFT
Title	:	X-ray structure of non-toxic non-hemagglutinin (NTNH) protein from bo-
		tulinum neurotoxin serotype X
Authors	:	Skerlova, J.; Masuyer, G.; Stenmark, P.
Deposited on	:	2023-09-04
Resolution	:	3.30 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)	
Clashscore	141614	1205 (3.34-3.26)	
Ramachandran outliers	138981	1183 (3.34-3.26)	
Sidechain outliers	138945	1182 (3.34-3.26)	
RSRZ outliers	127900	1115 (3.34-3.26)	

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 <=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	
			15%	
1	А	1174	77%	23%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9710 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 non-toxic non-hemagglutinin protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	1174	Total 9710	C 6266	N 1530	O 1893	S 21	0	0	0



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: non-toxic non-hemagglutinin protein X





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	174.11Å 174.11Å 138.02Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	73.74 - 3.30	Depositor
Resolution (A)	73.63 - 3.30	EDS
% Data completeness	99.5 (73.74-3.30)	Depositor
(in resolution range)	99.5(73.63-3.30)	EDS
R _{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.50 (at 3.33 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
D D.	0.276 , 0.333	Depositor
Π, Π_{free}	0.286 , 0.338	DCC
R_{free} test set	1939 reflections (5.31%)	wwPDB-VP
Wilson B-factor $(Å^2)$	137.9	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.32, 168.4	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9710	wwPDB-VP
Average B, all atoms $(Å^2)$	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	А	0.29	0/9925	0.59	0/13473

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	А	9710	0	9491	184	0
All	All	9710	0	9491	184	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 10.

All (184) 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:102:LYS:HE3	1:A:434:LEU:HD21	1.61	0.81
1:A:123:LEU:HD22	1:A:162:LEU:HD13	1.60	0.81
1:A:852:HIS:O	1:A:853:THR:HG22	1.84	0.75
1:A:355:ASN:HB2	1:A:360:THR:HA	1.68	0.75
1:A:966:THR:O	1:A:966:THR:HG22	1.87	0.73



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:563:ILE:HD11	1:A:592:ILE:HD11	1.73	0.71
1:A:129:LEU:HB2	1:A:131:VAL:HG13	1.75	0.68
1:A:1160:LYS:HA	1:A:1165:PRO:HA	1.75	0.67
1:A:920:GLU:HB3	1:A:930:THR:HG23	1.76	0.67
1:A:607:MET:O	1:A:750:ASN:ND2	2.29	0.66
1:A:1080:LYS:NZ	1:A:1087:ASP:OD2	2.28	0.65
1:A:218:ILE:HG23	1:A:261:ASN:HD22	1.62	0.65
1:A:343:ASN:OD1	1:A:346:ASN:ND2	2.29	0.64
1:A:326:SER:OG	1:A:803:ASP:HB2	1.98	0.64
1:A:28:THR:HG21	1:A:55:PRO:HA	1.81	0.62
1:A:122:TYR:OH	1:A:163:ASN:ND2	2.34	0.61
1:A:186:LYS:O	1:A:187:PHE:HB3	2.00	0.61
1:A:985:SER:O	1:A:986:ASP:HB3	2.01	0.60
1:A:945:THR:HG23	1:A:958:PHE:HB2	1.84	0.60
1:A:875:PHE:N	1:A:976:GLU:OE1	2.33	0.59
1:A:852:HIS:O	1:A:853:THR:CG2	2.51	0.59
1:A:887:LEU:HD21	1:A:889:ILE:HD11	1.85	0.58
1:A:139:LYS:HD2	1:A:141:PHE:CE1	2.38	0.58
1:A:102:LYS:HB3	1:A:434:LEU:HD11	1.85	0.58
1:A:896:THR:OG1	1:A:985:SER:O	2.23	0.57
1:A:895:SER:O	1:A:987:ASN:ND2	2.32	0.57
1:A:489:MET:HA	1:A:682:LYS:NZ	2.20	0.56
1:A:163:ASN:HA	1:A:455:THR:HB	1.88	0.56
1:A:128:LEU:HG	1:A:130:TYR:H	1.70	0.55
1:A:247:ASN:ND2	1:A:799:ILE:O	2.40	0.55
1:A:1113:ASP:OD1	1:A:1115:ASN:N	2.39	0.55
1:A:409:TYR:O	1:A:603:ILE:HG21	2.07	0.55
1:A:1135:SER:HA	1:A:1140:ALA:HA	1.89	0.54
1:A:1033:ASN:HB2	1:A:1070:PHE:HB3	1.90	0.54
1:A:20:GLU:OE2	1:A:34:LYS:HD3	2.07	0.54
1:A:713:SER:HB3	1:A:809:THR:HG23	1.88	0.54
1:A:344:TYR:N	1:A:345:PRO:HD2	2.23	0.54
1:A:880:SER:HB3	1:A:950:ARG:H	1.73	0.54
1:A:1142:ARG:HH12	1:A:1144:SER:HA	1.73	0.53
1:A:621:TYR:O	1:A:621:TYR:CG	2.62	0.53
1:A:784:SER:HB2	1:A:787:GLU:HB3	1.90	0.53
1:A:228:LEU:H	1:A:379:GLN:HE22	1.56	0.53
1:A:1161:LEU:HD11	1:A:1166:LEU:HD23	1.90	0.53
1:A:482:SER:OG	1:A:512:TYR:HB3	2.09	0.53
1:A:496:THR:HB	1:A:510:LEU:HD11	1.91	0.52
1:A:457:LEU:N	1:A:458:PRO:HD3	2.25	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:97:VAL:HG23	1:A:100:GLY:H	1.75	0.52
1:A:687:PHE:HA	1:A:692:LEU:HD12	1.91	0.52
1:A:495:PHE:CD2	1:A:522:MET:HG3	2.44	0.52
1:A:54:GLU:OE2	1:A:158:GLN:NE2	2.42	0.52
1:A:764:LYS:HB3	1:A:768:LEU:HB3	1.90	0.52
1:A:228:LEU:N	1:A:379:GLN:HE22	2.07	0.52
1:A:837:ASN:ND2	1:A:869:PRO:O	2.41	0.52
1:A:292:LEU:HA	1:A:295:TYR:CD2	2.44	0.51
1:A:673:GLN:HE22	1:A:716:SER:CB	2.22	0.51
1:A:917:LEU:HB3	1:A:933:PHE:HD2	1.74	0.51
1:A:68:ILE:HB	1:A:154:ILE:HB	1.92	0.51
1:A:9:ILE:O	1:A:12:PRO:HD3	2.10	0.51
1:A:123:LEU:HD21	1:A:453:LYS:C	2.31	0.51
1:A:619:ARG:O	1:A:623:ASP:N	2.43	0.51
1:A:799:ILE:HG13	1:A:800:THR:HG23	1.93	0.51
1:A:894:GLU:O	1:A:914:ASN:N	2.44	0.50
1:A:139:LYS:HD3	1:A:140:PHE:N	2.26	0.50
1:A:764:LYS:HB3	1:A:768:LEU:CB	2.42	0.50
1:A:740:TYR:N	1:A:741:PRO:HD2	2.27	0.50
1:A:382:THR:HA	1:A:393:THR:HA	1.94	0.49
1:A:548:TYR:CZ	1:A:552:ILE:HD13	2.46	0.49
1:A:1054:LYS:HE2	1:A:1109:VAL:HG11	1.93	0.49
1:A:367:LYS:HE3	1:A:370:ASN:HB2	1.93	0.49
1:A:567:LEU:HD12	1:A:569:TRP:HE1	1.77	0.49
1:A:713:SER:HA	1:A:716:SER:HB3	1.94	0.49
1:A:129:LEU:HA	1:A:137:GLU:O	2.12	0.49
1:A:289:ASN:ND2	1:A:293:ASN:OD1	2.46	0.49
1:A:258:TRP:N	1:A:258:TRP:CD1	2.81	0.49
1:A:107:LEU:O	1:A:144:ASN:ND2	2.45	0.49
1:A:435:ASP:HB3	1:A:438:PHE:HB3	1.94	0.49
1:A:256:PRO:HD2	1:A:644:TYR:HE2	1.77	0.49
1:A:228:LEU:HD11	1:A:475:LEU:HD11	1.94	0.48
1:A:777:THR:O	1:A:781:THR:N	2.45	0.48
1:A:830:ILE:HD12	1:A:842:PHE:CG	2.48	0.48
1:A:113:PHE:HE1	1:A:282:LEU:HD11	1.78	0.48
1:A:632:TYR:HD1	1:A:782:PHE:CE1	2.32	0.48
1:A:883:ILE:HG12	1:A:997:ILE:HG12	1.94	0.48
1:A:252:PHE:CE1	1:A:253:THR:HG23	2.48	0.48
1:A:874:ASN:HA	1:A:976:GLU:OE1	2.14	0.48
1:A:762:ILE:HB	1:A:764:LYS:HE3	1.96	0.48
1:A:772:GLN:HA	1:A:775:GLU:OE1	2.14	0.48



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:434:LEU:N	1:A:434:LEU:HD23	2.28	0.48
1:A:1023:TYR:HA	1:A:1130:ASN:HB3	1.95	0.48
1:A:1096:ASP:HB3	1:A:1097:PRO:HD3	1.94	0.48
1:A:1142:ARG:NH1	1:A:1144:SER:HA	2.28	0.48
1:A:390:LEU:HD11	1:A:503:VAL:HG23	1.96	0.48
1:A:877:PHE:HD1	1:A:974:SER:HB2	1.79	0.47
1:A:223:LYS:NZ	1:A:398:GLU:OE2	2.47	0.47
1:A:870:THR:HG23	1:A:980:PRO:HA	1.96	0.47
1:A:231:ASP:HB2	1:A:599:TYR:HE1	1.80	0.47
1:A:843:ASP:HB3	1:A:865:TYR:CE1	2.49	0.47
1:A:592:ILE:HD12	1:A:733:PHE:CG	2.49	0.47
1:A:674:GLN:O	1:A:677:ILE:HG13	2.15	0.47
1:A:98:ILE:O	1:A:102:LYS:HG3	2.14	0.47
1:A:162:LEU:HD21	1:A:174:VAL:HG23	1.97	0.47
1:A:1048:LYS:H	1:A:1069:THR:HG21	1.79	0.47
1:A:1063:GLN:C	1:A:1065:THR:H	2.19	0.46
1:A:1099:ASN:OD1	1:A:1099:ASN:N	2.48	0.46
1:A:818:ILE:HB	1:A:833:GLU:HB3	1.96	0.46
1:A:83:TYR:O	1:A:87:ILE:HG12	2.16	0.46
1:A:877:PHE:HA	1:A:950:ARG:CZ	2.46	0.46
1:A:252:PHE:CD1	1:A:253:THR:HG23	2.50	0.46
1:A:563:ILE:HD11	1:A:592:ILE:CD1	2.44	0.46
1:A:1103:ILE:HG12	1:A:1118:THR:HG21	1.98	0.46
1:A:1091:ILE:HB	1:A:1101:ILE:HD12	1.98	0.46
1:A:278:TYR:O	1:A:283:LYS:N	2.48	0.46
1:A:122:TYR:OH	1:A:166:ASP:HB2	2.16	0.45
1:A:1059:ILE:O	1:A:1150:GLU:HA	2.15	0.45
1:A:714:ARG:HD3	1:A:814:ILE:HD12	1.97	0.45
1:A:773:ILE:O	1:A:777:THR:N	2.50	0.45
1:A:673:GLN:HE22	1:A:716:SER:HB2	1.80	0.45
1:A:933:PHE:CE1	1:A:957:CYS:SG	3.10	0.45
1:A:102:LYS:HG2	1:A:436:ASN:OD1	2.16	0.45
1:A:259:LEU:HG	1:A:261:ASN:OD1	2.17	0.45
1:A:2:ASP:HB2	1:A:440:ASP:OD2	2.17	0.45
1:A:479:TYR:O	1:A:483:GLN:HG2	2.17	0.45
1:A:484:THR:HG22	1:A:671:LYS:HE3	1.99	0.45
1:A:135:ASN:HB3	1:A:137:GLU:OE1	2.17	0.45
1:A:1076:LYS:HE2	1:A:1090:TYR:OH	2.16	0.44
1:A:637:PHE:O	1:A:641:LYS:HG3	2.18	0.44
1:A:1161:LEU:HD11	1:A:1166:LEU:CD2	2.47	0.44
1:A:249:TYR:HA	1:A:252:PHE:CE2	2.53	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:714:ARG:HH12	1:A:879:GLU:CD	2.21	0.44
1:A:824:ILE:HD12	1:A:825:ASN:H	1.82	0.44
1:A:130:TYR:HB2	1:A:135:ASN:HB2	2.00	0.44
1:A:1103:ILE:HA	1:A:1107:GLN:O	2.18	0.44
1:A:1019:TYR:HB3	1:A:1027:ILE:HG23	1.98	0.44
1:A:140:PHE:CD1	1:A:450:ALA:HB3	2.53	0.44
1:A:424:ILE:HG23	1:A:426:GLN:H	1.83	0.44
1:A:505:GLU:HB2	1:A:508:SER:HB2	2.00	0.44
1:A:1142:ARG:NH1	1:A:1143:LEU:O	2.51	0.43
1:A:517:HIS:HB2	1:A:551:ASP:OD2	2.17	0.43
1:A:383:TYR:HE2	1:A:390:LEU:HD23	1.84	0.43
1:A:260:SER:HB2	1:A:264:PHE:HB2	2.01	0.43
1:A:493:ILE:HD11	1:A:682:LYS:HE2	2.00	0.43
1:A:817:LEU:HA	1:A:832:ASP:OD2	2.17	0.43
1:A:121:LYS:H	1:A:450:ALA:HA	1.82	0.43
1:A:643:TYR:O	1:A:646:ILE:HG22	2.19	0.43
1:A:98:ILE:HG13	1:A:102:LYS:HD2	2.01	0.43
1:A:233:TYR:HB2	1:A:235:TYR:HE1	1.84	0.43
1:A:113:PHE:HD1	1:A:114:PRO:HD2	1.84	0.42
1:A:622:ASP:HB2	1:A:624:ILE:HG13	2.01	0.42
1:A:23:THR:O	1:A:32:GLN:NE2	2.52	0.42
1:A:807:ILE:HG22	1:A:808:LEU:HD22	2.01	0.42
1:A:852:HIS:C	1:A:853:THR:HG22	2.39	0.42
1:A:124:LEU:HD11	1:A:142:THR:HA	2.01	0.42
1:A:137:GLU:OE1	1:A:137:GLU:N	2.52	0.42
1:A:147:LEU:HD11	1:A:179:TYR:HB3	2.02	0.42
1:A:438:PHE:O	1:A:442:LEU:HG	2.20	0.42
1:A:500:TYR:HA	1:A:503:VAL:HG22	2.01	0.42
1:A:656:ILE:HA	1:A:659:ILE:HG22	2.02	0.41
1:A:50:ARG:NH2	1:A:151:GLY:O	2.48	0.41
1:A:882:SER:HB3	1:A:947:SER:HB2	2.01	0.41
1:A:1138:SER:O	1:A:1158:VAL:HG12	2.20	0.41
1:A:10:ASP:CG	1:A:11:SER:H	2.23	0.41
1:A:98:ILE:O	1:A:101:LYS:HG2	2.21	0.41
1:A:113:PHE:CE1	1:A:282:LEU:HD11	2.56	0.41
1:A:392:TYR:CG	1:A:503:VAL:HG12	2.56	0.41
1:A:673:GLN:NE2	1:A:716:SER:HB2	2.35	0.41
1:A:24:PHE:O	1:A:32:GLN:NE2	2.54	0.41
1:A:258:TRP:CZ2	1:A:644:TYR:HB3	2.55	0.41
1:A:270:THR:HA	1:A:273:GLU:OE2	2.21	0.41
1:A:592:ILE:HD12	1:A:733:PHE:CD1	2.56	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ASN:O	1:A:759:LEU:HG	2.20	0.41
1:A:121:LYS:HG3	1:A:122:TYR:N	2.36	0.41
1:A:1059:ILE:HD12	1:A:1143:LEU:HD21	2.01	0.41
1:A:9:ILE:HG12	1:A:81:GLN:HE22	1.86	0.41
1:A:123:LEU:HG	1:A:452:ASN:HA	2.03	0.41
1:A:123:LEU:HA	1:A:451:GLN:O	2.21	0.41
1:A:769:THR:OG1	1:A:772:GLN:HB3	2.21	0.41
1:A:489:MET:HA	1:A:682:LYS:HZ2	1.86	0.40
1:A:859:LEU:HD13	1:A:864:GLN:HB3	2.03	0.40
1:A:966:THR:O	1:A:966:THR:CG2	2.56	0.40
1:A:579:THR:HG22	1:A:580:ASN:OD1	2.21	0.40
1:A:174:VAL:HG23	1:A:174:VAL:O	2.21	0.40
1:A:1071:PHE:CD1	1:A:1071:PHE:N	2.88	0.40
1:A:714:ARG:HB2	1:A:811:ILE:HD11	2.03	0.40
1:A:1107:GLN:HG3	1:A:1108:ALA:N	2.36	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	А	1172/1174 (100%)	1073~(92%)	99~(8%)	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	Perce	ntiles
1	А	1107/1107~(100%)	1107 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	1174/1174~(100%)	0.78	179 (15%) 2 2	114, 214, 310, 415	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	125	LYS	10.5
1	А	427	TYR	8.2
1	А	37	ALA	7.8
1	А	289	ASN	7.6
1	А	19	ILE	7.6
1	А	143	SER	7.2
1	А	126	GLU	6.9
1	А	36	LYS	6.8
1	А	302	PHE	6.6
1	А	114	PRO	6.4
1	А	605	PRO	6.0
1	А	141	PHE	5.8
1	А	124	LEU	5.7
1	А	300	TYR	5.6
1	А	796	PHE	5.3
1	А	210	TYR	5.3
1	А	38	TYR	5.2
1	А	120	ASN	5.1
1	А	604	ILE	4.9
1	А	447	GLY	4.8
1	А	40	ILE	4.7
1	А	791	PHE	4.7
1	А	448	MET	4.7
1	А	566	VAL	4.5
1	А	308	TRP	4.5
1	А	115	PHE	4.5
1	А	221	PRO	4.5



8QFT

Mol	Chain	Res	Type	RSRZ
1	А	142	THR	4.5
1	А	463	GLY	4.5
1	А	654	TYR	4.4
1	А	21	PHE	4.3
1	А	961	GLY	4.3
1	А	134	GLU	4.3
1	А	614	LEU	4.2
1	А	249	TYR	4.2
1	А	445	ILE	4.2
1	А	140	PHE	4.0
1	А	758	VAL	4.0
1	А	500	TYR	4.0
1	A	136	PHE	4.0
1	А	132	ASN	4.0
1	А	106	LEU	3.9
1	А	613	PRO	3.9
1	А	113	PHE	3.9
1	А	24	PHE	3.8
1	А	446	GLN	3.8
1	А	449	ASN	3.8
1	А	569	TRP	3.8
1	А	61	GLU	3.8
1	А	592	ILE	3.8
1	А	43	HIS	3.8
1	А	315	PHE	3.8
1	А	119	THR	3.7
1	А	133	GLU	3.7
1	А	35	ILE	3.7
1	А	567	LEU	3.6
1	А	433	THR	3.6
1	А	636	LYS	3.4
1	A	187	PHE	3.3
1	A	782	PHE	3.3
1	A	1058	ALA	3.3
1	А	556	ARG	3.3
1	А	312	LEU	3.2
1	А	464	THR	3.2
1	A	290	ASN	3.2
1	А	368	ASP	3.2
1	А	46	VAL	3.2
1	A	837	ASN	3.2
1	А	461	SER	3.1



8QFT

Mol	Chain	Res	Type	RSRZ
1	А	531	ILE	3.1
1	А	298	GLN	3.1
1	А	282	LEU	3.1
1	А	1056	TYR	3.1
1	А	307	ILE	3.0
1	А	1105	ASN	3.0
1	А	617	MET	3.0
1	А	584	GLU	2.9
1	А	624	ILE	2.9
1	А	1137	ASN	2.9
1	А	595	LEU	2.9
1	А	640	LEU	2.8
1	А	304	ILE	2.8
1	A	371	PHE	2.8
1	A	548	TYR	2.8
1	А	465	ASP	2.8
1	A	944	ILE	2.8
1	A	1153	ILE	2.7
1	А	495	PHE	2.7
1	A	732	LEU	2.7
1	A	625	ASP	2.7
1	А	919	TRP	2.7
1	A	658	PHE	2.7
1	А	483	GLN	2.7
1	A	131	VAL	2.7
1	A	409	TYR	2.7
1	A	365	ILE	2.6
1	A	890	LEU	2.6
1	A	60	ASP	2.6
1	A	1059	ILE	2.6
1	A	22	ILE	2.6
1	A	306	LYS	2.6
1	A	224	LEU	2.6
1	A	244	PHE	2.5
1	A	353	PHE	2.5
1	A	218	ILE	2.5
1	A	413	MET	2.5
1	A	607	MET	2.5
1	А	34	LYS	2.5
1	A	296	LEU	2.5
1	A	602	PHE	2.4
1	А	428	LYS	2.4

Continued from previous page...



Mol	Chain	Res	Type	RSRZ
1	А	423	THR	2.4
1	А	203	LEU	2.4
1	А	1002	LEU	2.4
1	А	310	LEU	2.4
1	А	442	LEU	2.4
1	А	414	PHE	2.4
1	А	565	ALA	2.4
1	А	238	LEU	2.4
1	А	898	LEU	2.4
1	А	235	TYR	2.4
1	А	425	ASN	2.4
1	А	1110	LEU	2.4
1	А	107	LEU	2.4
1	А	264	PHE	2.4
1	А	373	ILE	2.4
1	А	983	ILE	2.4
1	А	935	PHE	2.4
1	А	20	GLU	2.4
1	А	552	ILE	2.4
1	А	826	ASP	2.4
1	А	726	PHE	2.4
1	А	866	ILE	2.3
1	А	91	PHE	2.3
1	А	426	GLN	2.3
1	А	623	ASP	2.3
1	А	444	PRO	2.3
1	А	744	LEU	2.3
1	А	583	PHE	2.3
1	А	183	PHE	2.3
1	А	223	LYS	2.3
1	А	665	CYS	2.3
1	А	44	ILE	2.3
1	А	917	LEU	2.2
1	А	647	VAL	2.2
1	А	137	GLU	2.2
1	А	121	LYS	2.2
1	А	879	GLU	2.2
1	А	359	ASN	2.2
1	А	1057	ILE	2.2
1	А	676	LEU	2.2
1	А	138	PHE	2.2
1	А	109	SER	2.2



Mol	Chain	Res	Type	RSRZ
1	А	233	TYR	2.2
1	А	887	LEU	2.2
1	А	400	ASN	2.2
1	А	323	ILE	2.2
1	А	643	TYR	2.2
1	А	331	ILE	2.2
1	А	443	PRO	2.1
1	А	1134	PHE	2.1
1	А	1091	ILE	2.1
1	А	740	TYR	2.1
1	А	657	GLN	2.1
1	А	271	PHE	2.1
1	А	570	ILE	2.1
1	А	838	LEU	2.1
1	А	105	SER	2.1
1	А	478	HIS	2.1
1	А	751	ILE	2.0
1	А	1122	LEU	2.0
1	А	1173	PHE	2.0
1	А	1115	ASN	2.0
1	A	631	ILE	2.0
1	A	1143	LEU	2.0
1	А	130	TYR	2.0
1	А	773	ILE	2.0
1	А	899	LEU	2.0
1	A	1132	LEU	2.0

Continued from previous page...

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.

