Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 07:47 AM EDT

PDB ID	:	2QQK
Title	:	Neuropilin-2 a1a2b1b2 Domains in Complex with a Semaphorin-Blocking Fab
Authors	:	Appleton, B.A.; Wiesmann, C.
Deposited on	:	2007-07-26
Resolution	:	2.75 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 (i)) were used in the production of this report:

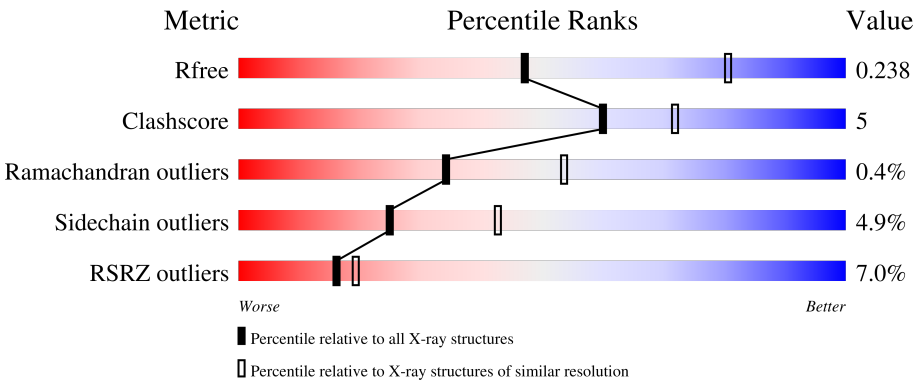
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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
1	A	579	7%, 82%, 11%, • 7%
2	H	231	5%, 82%, 12%, • 5%
3	L	214	7%, 81%, 16%, ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1	X	-	-	-
4	NAG	A	602	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7621 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 Neuropilin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	541	4304	2733	741	809	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	HIS	-	expression tag	UNP O60462
A	597	HIS	-	expression tag	UNP O60462
A	598	HIS	-	expression tag	UNP O60462
A	599	HIS	-	expression tag	UNP O60462
A	600	HIS	-	expression tag	UNP O60462
A	601	HIS	-	expression tag	UNP O60462

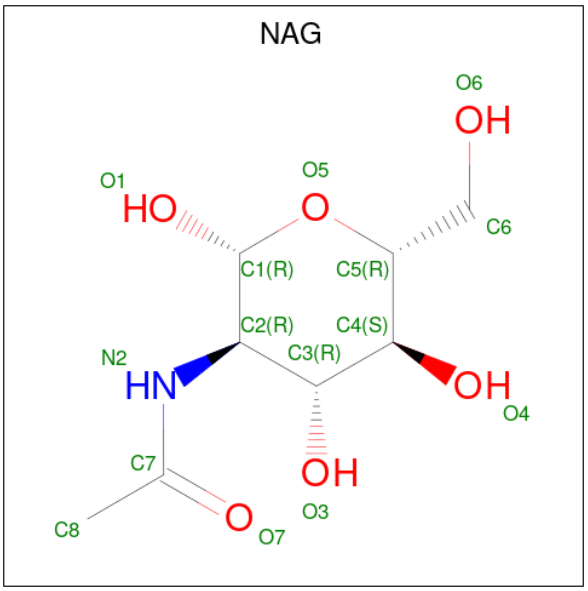
- Molecule 2 is a protein called Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1667	1056	282	323	6	0	0	0

- Molecule 3 is a protein called Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	211	1622	1021	269	327	5	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



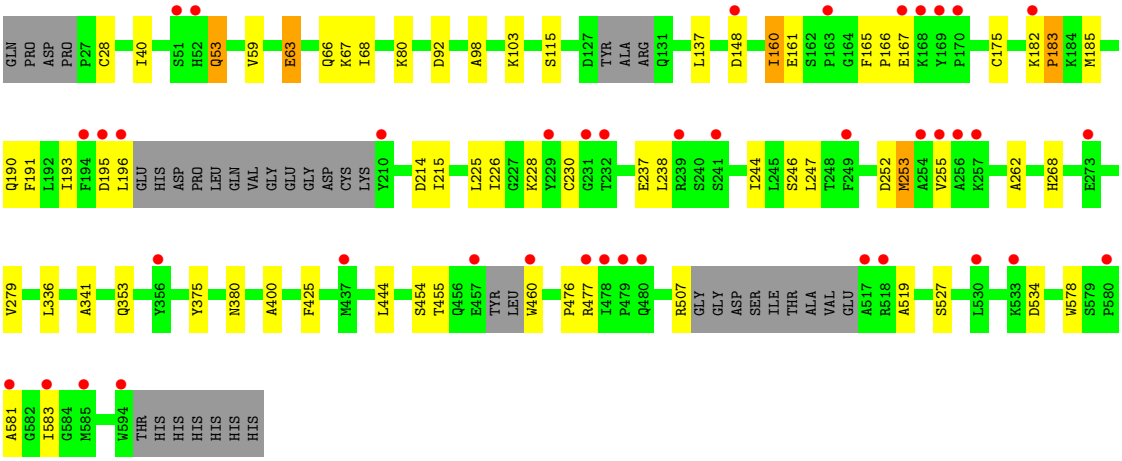
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

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.

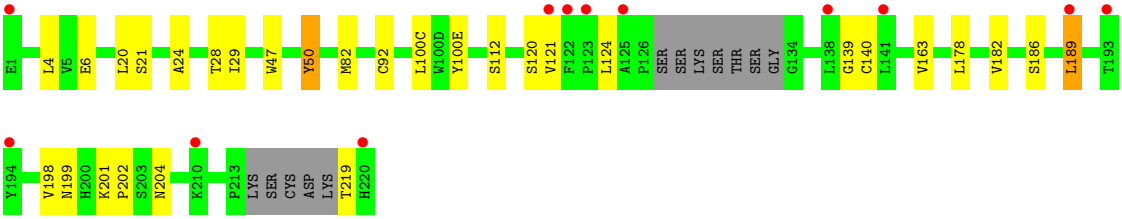
- Molecule 1: Neuropilin-2

Chain A:



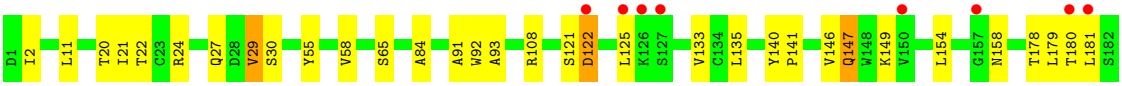
- Molecule 2: Antibody Heavy Chain

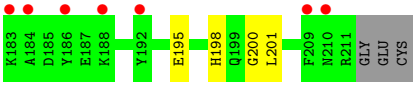
Chain H:



- Molecule 3: Antibody Light Chain

Chain L:




K183
A184
D185
Y186
E187
K188
Y192
E195
H198
Q199
G200
L201
F209
N210
R211
GLY
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.28Å 105.87Å 92.40Å 90.00° 98.83° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 42.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.75) 98.9 (42.91-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.54 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.243 0.189 , 0.238	Depositor DCC
R_{free} test set	1830 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 72.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7621	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.48	0/4421	0.62	0/6000
2	H	0.56	0/1709	0.64	0/2328
3	L	0.63	0/1659	0.66	0/2256
All	All	0.53	0/7789	0.63	0/10584

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	4304	0	4146	36	0
2	H	1667	0	1616	18	0
3	L	1622	0	1578	16	0
4	A	28	0	26	0	0
All	All	7621	0	7366	69	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 (69) 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:244:ILE:HD11	1:A:444:LEU:HD13	1.56	0.87
1:A:519:ALA:HB2	1:A:581:ALA:HB3	1.69	0.75
1:A:215:ILE:HG12	1:A:247:LEU:HD22	1.76	0.67
1:A:191:PHE:CD2	1:A:262:ALA:HB2	2.31	0.65
2:H:178:LEU:C	2:H:178:LEU:HD12	2.19	0.62
1:A:59:VAL:HG12	1:A:68:ILE:HD13	1.82	0.61
1:A:63:GLU:OE1	1:A:66:GLN:NE2	2.34	0.59
1:A:165:PHE:HZ	1:A:193:ILE:HD11	1.67	0.59
1:A:455:THR:HG21	1:A:460:TRP:CD2	2.39	0.58
3:L:2:ILE:HD12	3:L:93:ALA:HB2	1.86	0.57
2:H:4:LEU:HD23	2:H:92:CYS:SG	2.46	0.56
1:A:185:MET:HE3	1:A:268:HIS:CA	2.36	0.56
3:L:147:GLN:HE22	3:L:154:LEU:HD23	1.72	0.55
3:L:180:THR:O	3:L:181:LEU:HD12	2.07	0.54
1:A:214:ASP:HB2	1:A:225:LEU:HD11	1.88	0.54
3:L:198:HIS:CD2	3:L:200:GLY:H	2.25	0.54
3:L:122:ASP:HA	3:L:125:LEU:HD13	1.90	0.54
1:A:244:ILE:CD1	1:A:444:LEU:HD13	2.36	0.53
2:H:20:LEU:HG	2:H:82:MET:HE2	1.91	0.53
1:A:53:GLN:HE21	1:A:53:GLN:C	2.12	0.52
1:A:237:GLU:O	1:A:238:LEU:HD23	2.10	0.51
2:H:24:ALA:CB	2:H:29:ILE:HG23	2.42	0.50
2:H:47:TRP:HZ2	2:H:50:TYR:CD2	2.28	0.50
1:A:160:ILE:HD12	1:A:161:GLU:N	2.27	0.49
1:A:215:ILE:HG22	1:A:226:ILE:HD11	1.93	0.49
1:A:185:MET:HE3	1:A:268:HIS:HA	1.95	0.48
1:A:246:SER:C	1:A:247:LEU:HD23	2.34	0.48
1:A:92:ASP:O	1:A:98:ALA:HB1	2.13	0.48
1:A:40:ILE:HD12	1:A:137:LEU:HD11	1.96	0.47
3:L:133:VAL:HG22	3:L:178:THR:HG23	1.95	0.47
1:A:196:LEU:HD12	1:A:230:CYS:HA	1.97	0.47
1:A:578:TRP:CE3	1:A:583:ILE:HD11	2.50	0.47
3:L:147:GLN:NE2	3:L:154:LEU:HD23	2.30	0.46
3:L:11:LEU:C	3:L:11:LEU:HD12	2.36	0.46
1:A:185:MET:HE3	1:A:268:HIS:N	2.30	0.46
1:A:59:VAL:HG12	1:A:68:ILE:CD1	2.45	0.46
2:H:121:VAL:HG11	2:H:198:VAL:HG21	1.98	0.45
2:H:47:TRP:CZ2	2:H:50:TYR:CD2	3.04	0.45
1:A:252:ASP:OD1	1:A:253:MET:N	2.47	0.45
2:H:100(E):TYR:HB2	3:L:91:ALA:HB1	1.99	0.45
2:H:163:VAL:HG22	2:H:182:VAL:HB	1.98	0.44
2:H:199:ASN:HD21	2:H:201:LYS:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:55:TYR:O	3:L:58:VAL:HG23	2.18	0.44
1:A:68:ILE:H	1:A:115:SER:HB3	1.83	0.44
2:H:201:LYS:N	2:H:202:PRO:CD	2.80	0.44
1:A:215:ILE:O	1:A:225:LEU:HD12	2.18	0.43
1:A:341:ALA:HB3	1:A:425:PHE:HB2	2.01	0.43
3:L:158:ASN:O	3:L:179:LEU:HD12	2.19	0.43
1:A:253:MET:HA	1:A:253:MET:HE2	2.01	0.43
3:L:121:SER:O	3:L:122:ASP:C	2.56	0.42
1:A:165:PHE:CZ	1:A:193:ILE:HD11	2.50	0.42
1:A:375:TYR:OH	1:A:400:ALA:HB3	2.20	0.42
1:A:214:ASP:HB3	1:A:228:LYS:HA	2.01	0.42
1:A:247:LEU:HD23	1:A:247:LEU:N	2.35	0.42
2:H:186:SER:HA	2:H:189:LEU:HD23	2.02	0.42
1:A:215:ILE:CG2	1:A:226:ILE:HD11	2.49	0.42
2:H:178:LEU:C	2:H:178:LEU:CD1	2.86	0.42
3:L:140:TYR:CG	3:L:141:PRO:HA	2.55	0.41
1:A:454:SER:O	1:A:476:PRO:HA	2.20	0.41
3:L:146:VAL:O	3:L:146:VAL:HG12	2.20	0.41
1:A:165:PHE:CG	1:A:166:PRO:HA	2.56	0.41
3:L:149:LYS:NZ	3:L:195:GLU:OE1	2.52	0.41
2:H:6:GLU:HA	2:H:21:SER:O	2.21	0.41
2:H:24:ALA:CB	2:H:29:ILE:CG2	2.99	0.41
2:H:124:LEU:HD12	2:H:140:CYS:N	2.36	0.41
2:H:24:ALA:HB2	2:H:29:ILE:CG2	2.51	0.40
1:A:182:LYS:CG	1:A:183:PRO:HD2	2.51	0.40
3:L:29:VAL:HG22	3:L:92:TRP:HB2	2.04	0.40
2:H:124:LEU:HD12	2:H:139:GLY:C	2.41	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	531/579 (92%)	483 (91%)	45 (8%)	3 (1%)	25	42
2	H	213/231 (92%)	203 (95%)	10 (5%)	0	100	100
3	L	209/214 (98%)	194 (93%)	14 (7%)	1 (0%)	29	47
All	All	953/1024 (93%)	880 (92%)	69 (7%)	4 (0%)	34	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	A	80	LYS
1	A	255	VAL
3	L	84	ALA

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	470/502 (94%)	450 (96%)	20 (4%)	29	48
2	H	182/193 (94%)	174 (96%)	8 (4%)	28	47
3	L	184/186 (99%)	171 (93%)	13 (7%)	14	26
All	All	836/881 (95%)	795 (95%)	41 (5%)	25	43

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

Mol	Chain	Res	Type
1	A	28	CYS
1	A	53	GLN
1	A	63	GLU
1	A	67	LYS
1	A	103	LYS
1	A	148	ASP
1	A	160	ILE
1	A	167	GLU
1	A	175	CYS

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Mol	Chain	Res	Type
1	A	190	GLN
1	A	195	ASP
1	A	253	MET
1	A	279	VAL
1	A	336	LEU
1	A	353	GLN
1	A	380	ASN
1	A	477	ARG
1	A	507	ARG
1	A	527	SER
1	A	534	ASP
2	H	28	THR
2	H	50	TYR
2	H	100(C)	LEU
2	H	112	SER
2	H	120	SER
2	H	189	LEU
2	H	204	ASN
2	H	219	THR
3	L	20	THR
3	L	21	ILE
3	L	22	THR
3	L	24	ARG
3	L	27	GLN
3	L	29	VAL
3	L	30	SER
3	L	65	SER
3	L	108	ARG
3	L	122	ASP
3	L	135	LEU
3	L	147	GLN
3	L	201	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	71	ASN
1	A	171	HIS
1	A	190	GLN
1	A	353	GLN
1	A	354	ASN

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Mol	Chain	Res	Type
1	A	456	GLN
1	A	569	GLN
2	H	199	ASN
3	L	124	GLN
3	L	198	HIS
3	L	210	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	602	1	14,14,15	0.53	0	17,19,21	1.49	2 (11%)
4	NAG	A	1	1	14,14,15	0.68	0	17,19,21	1.80	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	602	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	A	1	1	1/1/5/7	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	NAG	C1-O5-C5	4.75	118.63	112.19
4	A	1	NAG	C3-C4-C5	3.94	117.27	110.24
4	A	1	NAG	C1-O5-C5	3.83	117.39	112.19
4	A	1	NAG	O5-C5-C4	2.91	117.91	110.83
4	A	602	NAG	O5-C5-C6	2.90	111.76	107.20
4	A	1	NAG	O5-C1-C2	-2.60	107.18	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1	NAG	C1
4	A	602	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	602	NAG	C8-C7-N2-C2
4	A	602	NAG	O7-C7-N2-C2
4	A	1	NAG	C1-C2-N2-C7
4	A	1	NAG	C4-C5-C6-O6
4	A	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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			OWAB(Å^2)	Q<0.9
1	A	541/579 (93%)	0.44	41 (7%)	13	16	58, 92, 122, 137	0
2	H	219/231 (94%)	0.12	12 (5%)	25	30	53, 78, 111, 117	0
3	L	211/214 (98%)	0.23	15 (7%)	16	19	49, 67, 117, 125	0
All	All	971/1024 (94%)	0.32	68 (7%)	16	19	49, 85, 119, 137	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	184	ALA	6.3
1	A	168	LYS	4.8
3	L	188	LYS	4.8
3	L	192	TYR	4.6
1	A	517	ALA	4.4
3	L	157	GLY	4.3
1	A	170	PRO	4.2
2	H	194	TYR	4.1
1	A	457	GLU	4.1
3	L	186	TYR	3.9
1	A	232	THR	3.9
1	A	169	TYR	3.9
1	A	195	ASP	3.7
2	H	122	PHE	3.6
2	H	189	LEU	3.6
1	A	167	GLU	3.6
1	A	256	ALA	3.5
3	L	210	ASN	3.5
1	A	530	LEU	3.5
2	H	138	LEU	3.4
1	A	533	LYS	3.3
3	L	209	PHE	3.3
2	H	210	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	231	GLY	3.1
1	A	580	PRO	3.1
1	A	52	HIS	3.0
1	A	229	TYR	3.0
1	A	163	PRO	3.0
1	A	479	PRO	3.0
1	A	581	ALA	2.9
1	A	594	TRP	2.8
1	A	480	GLN	2.8
2	H	125	ALA	2.8
2	H	1	GLU	2.8
3	L	180	THR	2.7
3	L	127	SER	2.7
3	L	126	LYS	2.6
3	L	150	VAL	2.6
2	H	123	PRO	2.6
2	H	220	HIS	2.6
2	H	121	VAL	2.5
1	A	583	ILE	2.5
3	L	125	LEU	2.5
1	A	194	PHE	2.5
2	H	141	LEU	2.5
1	A	477	ARG	2.4
1	A	460	TRP	2.4
2	H	193	THR	2.3
3	L	122	ASP	2.3
1	A	51	SER	2.3
1	A	249	PHE	2.3
1	A	196	LEU	2.3
3	L	181	LEU	2.3
1	A	254	ALA	2.2
1	A	478	ILE	2.2
1	A	273	GLU	2.2
1	A	182	LYS	2.2
1	A	210	TYR	2.2
1	A	585	MET	2.1
1	A	239	ARG	2.1
1	A	518	ARG	2.1
1	A	257	LYS	2.1
1	A	241	SER	2.1
1	A	148	ASP	2.1
1	A	437	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	356	TYR	2.0
1	A	255	VAL	2.0
3	L	183	LYS	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	602	14/15	0.69	0.22	118,120,122,122	0
4	NAG	A	1	14/15	0.78	0.14	122,133,136,136	0

6.5 Other polymers (i)

There are no such residues in this entry.