



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:57 pm GMT

PDB ID : 2GH0
Title : Growth factor/receptor complex
Authors : Wang, X.Q.
Deposited on : 2006-03-24
Resolution : 1.92 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

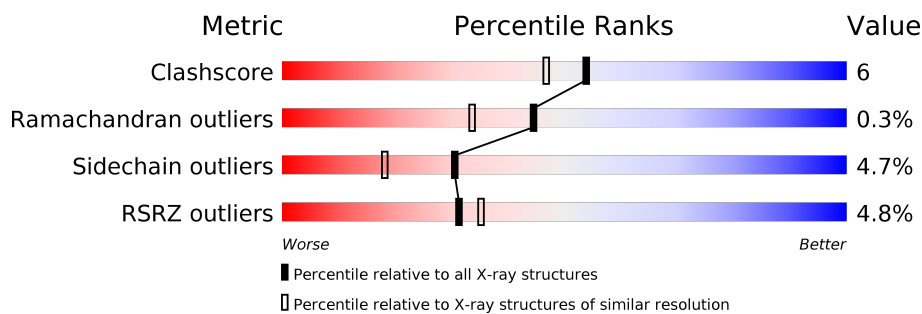
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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))
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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. 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	C	101	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	D	101	<div> <div>9%</div> <div>92%</div> <div>5%</div> <div>..</div> </div>
2	A	213	<div> <div>4%</div> <div>75%</div> <div>16%</div> <div>• 6%</div> </div>
2	B	213	<div> <div>5%</div> <div>77%</div> <div>13%</div> <div>• 7%</div> </div>

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
3	MAN	A	104	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4881 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 artemin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	100	Total	C	N	O	S	0	0	0
			758	463	153	134	8			
1	D	99	Total	C	N	O	S	0	0	0
			750	459	152	131	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	120	ASP	-	CLONING ARTIFACT	UNP Q5T4W7
C	121	PRO	-	CLONING ARTIFACT	UNP Q5T4W7
D	120	ASP	-	CLONING ARTIFACT	UNP Q5T4W7
D	121	PRO	-	CLONING ARTIFACT	UNP Q5T4W7

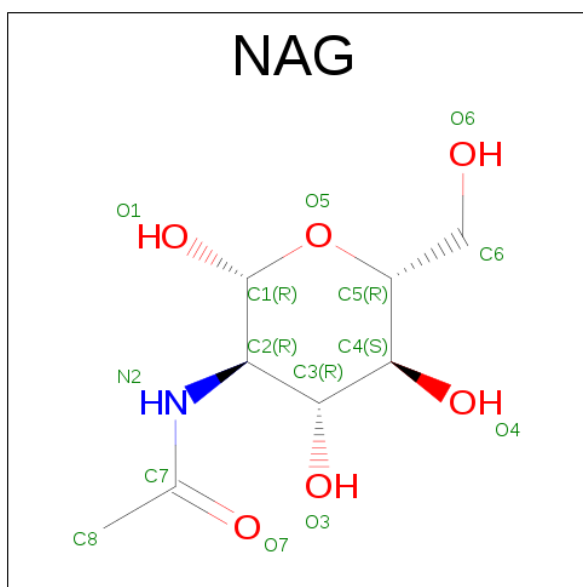
- Molecule 2 is a protein called GDNF family receptor alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	200	Total	C	N	O	S	0	0	0
			1535	946	284	280	25			
2	B	199	Total	C	N	O	S	0	0	0
			1527	942	283	277	25			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

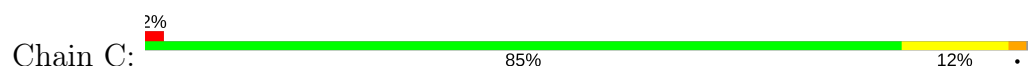
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	64	Total	O	0	0
			64	64		
5	C	35	Total	O	0	0
			35	35		
5	D	26	Total	O	0	0
			26	26		

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.

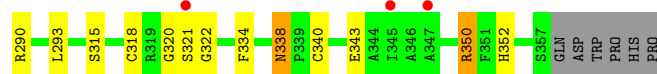
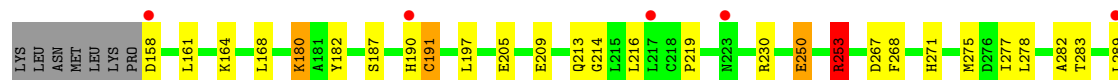
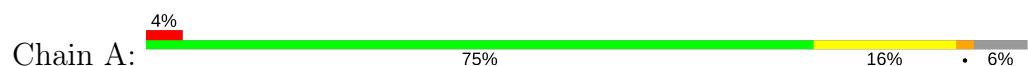
- Molecule 1: artemin



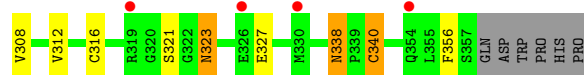
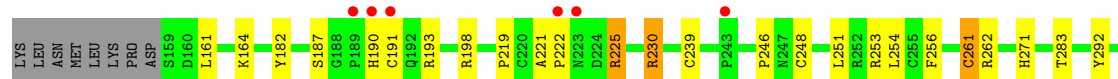
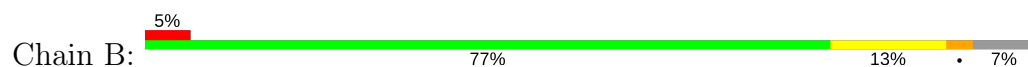
- Molecule 1: artemin



- Molecule 2: GDNF family receptor alpha-3



- Molecule 2: GDNF family receptor alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.68Å 41.46Å 119.86Å 90.00° 103.56° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 38.09 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.92) 93.4 (38.09-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.25 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.263 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4881	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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

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

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	C	0.86	0/774	0.85	0/1048
1	D	0.72	0/766	0.86	0/1036
2	A	1.14	9/1565 (0.6%)	0.97	7/2115 (0.3%)
2	B	0.86	1/1557 (0.1%)	0.85	3/2104 (0.1%)
All	All	0.94	10/4662 (0.2%)	0.89	10/6303 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	322	GLY	C-N	12.33	1.62	1.34
2	A	180	LYS	CE-NZ	7.95	1.69	1.49
2	A	350	ARG	CG-CD	7.10	1.69	1.51
2	A	250	GLU	CD-OE2	6.03	1.32	1.25
2	A	320	GLY	C-O	5.85	1.33	1.23
2	A	253	ARG	C-O	5.84	1.34	1.23
2	A	322	GLY	C-O	5.80	1.32	1.23
2	A	343	GLU	CG-CD	5.53	1.60	1.51
2	A	205	GLU	CB-CG	-5.22	1.42	1.52
2	B	261	CYS	CB-SG	5.11	1.91	1.82

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	ARG	NE-CZ-NH2	-12.06	114.27	120.30
2	A	230	ARG	NE-CZ-NH2	-9.55	115.53	120.30
2	B	230	ARG	NE-CZ-NH1	8.16	124.38	120.30
2	A	253	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	A	230	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	B	191	CYS	CA-CB-SG	-5.91	103.35	114.00
2	A	230	ARG	CG-CD-NE	-5.82	99.58	111.80
2	A	289	LEU	CB-CG-CD2	5.82	120.89	111.00
2	A	322	GLY	O-C-N	5.26	131.11	122.70
2	A	168	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	187	SER	Peptide

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	C	758	0	755	13	0
1	D	750	0	752	6	0
2	A	1535	0	1490	17	0
2	B	1527	0	1486	22	0
3	A	61	0	51	2	0
4	B	14	0	13	0	0
5	A	111	0	0	1	0
5	B	64	0	0	1	0
5	C	35	0	0	1	0
5	D	26	0	0	1	0
All	All	4881	0	4547	56	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 6.

All (56) 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)
2:A:180:LYS:CE	2:A:180:LYS:NZ	1.68	1.54
2:B:292:TYR:OH	2:B:312:VAL:HG21	1.43	1.14
2:B:323:ASN:H	2:B:323:ASN:HD22	1.23	0.84
1:C:154:CYS:H	1:C:185:GLN:NE2	1.88	0.71
2:B:292:TYR:OH	2:B:312:VAL:CG2	2.32	0.70
2:B:221:ALA:HB1	2:B:222:PRO:HD2	1.74	0.69
2:A:275:MET:HG2	2:A:282:ALA:HA	1.74	0.68
2:A:250:GLU:OE1	2:A:253:ARG:NH1	2.30	0.65
1:C:147:PHE:HE1	1:C:211:LEU:HD22	1.64	0.63
2:A:338:ASN:C	2:A:338:ASN:HD22	2.02	0.62
2:A:275:MET:CG	2:A:282:ALA:HA	2.31	0.60
1:C:154:CYS:H	1:C:185:GLN:HE21	1.48	0.60
2:B:323:ASN:H	2:B:323:ASN:ND2	1.96	0.59
2:B:338:ASN:C	2:B:338:ASN:HD22	2.08	0.57
2:A:180:LYS:CD	2:A:180:LYS:NZ	2.63	0.56
2:B:323:ASN:HD22	2:B:323:ASN:N	2.00	0.55
1:C:161:HIS:HE1	5:D:221:HOH:O	1.90	0.54
1:C:161:HIS:HD2	1:D:211:LEU:O	1.92	0.53
3:A:101:NAG:O3	3:A:102:BMA:C1	2.56	0.52
2:A:318:CYS:O	2:A:321:SER:OG	2.23	0.52
2:A:350:ARG:NH2	5:A:473:HOH:O	2.24	0.51
1:C:192:ARG:HG3	1:C:215:ALA:HB3	1.93	0.51
2:B:193:ARG:HG3	2:B:239:CYS:O	2.11	0.50
5:C:221:HOH:O	1:D:161:HIS:HE1	1.95	0.50
2:A:209:GLU:OE1	2:A:290:ARG:NH2	2.44	0.50
1:D:207:THR:HG22	2:B:187:SER:CB	2.43	0.49
2:B:251:LEU:HD22	2:B:316:CYS:HB3	1.95	0.49
2:B:323:ASN:ND2	2:B:323:ASN:N	2.60	0.49
2:A:216:LEU:HD23	2:A:293:LEU:HD22	1.94	0.48
2:B:256:PHE:O	2:B:262:ARG:HD3	2.14	0.48
2:B:338:ASN:HD21	2:B:340:CYS:HB3	1.78	0.48
2:B:225:ARG:NH1	2:B:308:VAL:HG13	2.30	0.47
2:B:198:ARG:HD2	2:B:198:ARG:HA	1.45	0.47
2:A:213:GLN:HG2	2:A:293:LEU:HD11	1.96	0.47
2:B:164:LYS:HD3	2:B:356:PHE:CE2	2.50	0.46
1:C:153:SER:OG	1:C:155:ARG:HG3	2.15	0.46
1:C:211:LEU:O	1:D:161:HIS:HD2	1.97	0.46
3:A:101:NAG:HO3	3:A:102:BMA:C1	2.29	0.45
1:D:202:ASN:O	1:D:203:SER:HB2	2.16	0.45
1:D:143:GLU:OE1	2:B:230:ARG:NH2	2.43	0.45
1:C:147:PHE:HE1	1:C:211:LEU:CD2	2.30	0.44
2:A:214:GLY:HA2	2:A:352:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:161:LEU:HD23	2:A:164:LYS:HD2	2.00	0.43
1:C:156:ARG:HE	1:C:156:ARG:HA	1.84	0.43
2:B:271:HIS:HD2	2:B:283:THR:OG1	2.01	0.43
2:B:161:LEU:HD12	2:B:219:PRO:HG2	2.01	0.42
2:A:315:SER:O	2:A:315:SER:OG	2.32	0.42
2:B:261:CYS:HB2	5:B:1121:HOH:O	2.20	0.41
1:C:202:ASN:O	1:C:203:SER:HB2	2.20	0.41
2:B:225:ARG:HH11	2:B:225:ARG:HG3	1.85	0.41
2:B:246:PRO:HG2	2:B:251:LEU:HD13	2.03	0.41
1:C:147:PHE:CE1	1:C:211:LEU:HD22	2.49	0.41
2:A:161:LEU:HD12	2:A:219:PRO:HG2	2.04	0.40
2:A:268:PHE:CE2	2:A:334:PHE:HD2	2.39	0.40
2:A:271:HIS:HD2	2:A:283:THR:OG1	2.05	0.40
1:C:140:ARG:O	1:C:200:ASP:HB2	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	C	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
1	D	97/101 (96%)	93 (96%)	4 (4%)	0	100	100
2	A	198/213 (93%)	190 (96%)	6 (3%)	2 (1%)	18	7
2	B	197/213 (92%)	189 (96%)	8 (4%)	0	100	100
All	All	590/628 (94%)	569 (96%)	19 (3%)	2 (0%)	44	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	190	HIS

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Mol	Chain	Res	Type
2	A	191	CYS

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	C	84/84 (100%)	82 (98%)	2 (2%)	54	46
1	D	83/84 (99%)	82 (99%)	1 (1%)	75	74
2	A	172/185 (93%)	162 (94%)	10 (6%)	23	12
2	B	171/185 (92%)	160 (94%)	11 (6%)	20	9
All	All	510/538 (95%)	486 (95%)	24 (5%)	30	18

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	156	ARG
1	C	211	LEU
1	D	211	LEU
2	A	158	ASP
2	A	182	TYR
2	A	191	CYS
2	A	197	LEU
2	A	253	ARG
2	A	267	ASP
2	A	277	ILE
2	A	278	LEU
2	A	338	ASN
2	A	340	CYS
2	B	182	TYR
2	B	190	HIS
2	B	225	ARG
2	B	248	CYS
2	B	253	ARG
2	B	254	LEU
2	B	321	SER

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Mol	Chain	Res	Type
2	B	323	ASN
2	B	327	GLU
2	B	338	ASN
2	B	340	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	161	HIS
1	C	185	GLN
1	D	161	HIS
2	A	271	HIS
2	A	323	ASN
2	A	338	ASN
2	B	192	GLN
2	B	271	HIS
2	B	323	ASN
2	B	338	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 ⓘ

5 carbohydrates 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
3	NAG	A	100	3,2	14,14,15	1.08	1 (7%)	15,19,21	2.37	6 (40%)
3	NAG	A	101	3	14,14,15	1.17	1 (7%)	15,19,21	1.87	3 (20%)
3	BMA	A	102	3	11,11,12	1.65	3 (27%)	13,15,17	3.21	6 (46%)
3	MAN	A	103	3	11,11,12	0.78	1 (9%)	13,15,17	2.19	5 (38%)
3	MAN	A	104	3	11,11,12	2.87	6 (54%)	13,15,17	2.23	6 (46%)

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
3	NAG	A	100	3,2	-	0/6/23/26	0/1/1/1
3	NAG	A	101	3	-	0/6/23/26	0/1/1/1
3	BMA	A	102	3	-	0/2/19/22	0/1/1/1
3	MAN	A	103	3	-	0/2/19/22	0/1/1/1
3	MAN	A	104	3	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	102	BMA	O3-C3	-3.08	1.35	1.43
3	A	101	NAG	O5-C5	-2.66	1.37	1.43
3	A	103	MAN	O3-C3	-2.20	1.37	1.43
3	A	104	MAN	C2-C3	-2.20	1.49	1.52
3	A	102	BMA	O2-C2	2.23	1.48	1.43
3	A	104	MAN	C4-C3	2.23	1.58	1.52
3	A	104	MAN	O5-C5	2.52	1.48	1.43
3	A	104	MAN	O5-C1	2.53	1.47	1.43
3	A	100	NAG	C1-C2	2.69	1.56	1.52
3	A	104	MAN	O3-C3	3.07	1.50	1.43
3	A	102	BMA	O5-C1	3.11	1.48	1.43
3	A	104	MAN	O4-C4	6.99	1.59	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	102	BMA	O3-C3-C4	-7.85	93.28	110.36
3	A	102	BMA	C1-O5-C5	-5.44	104.67	112.17
3	A	100	NAG	O5-C1-C2	-5.38	103.99	111.47
3	A	101	NAG	C4-C3-C2	-4.60	104.28	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	100	NAG	O4-C4-C3	-4.18	101.25	110.36
3	A	102	BMA	O5-C1-C2	-3.65	105.07	110.79
3	A	101	NAG	C2-N2-C7	-3.56	117.75	122.94
3	A	103	MAN	O3-C3-C4	-3.42	102.91	110.36
3	A	104	MAN	O4-C4-C3	-3.32	103.13	110.36
3	A	102	BMA	O6-C6-C5	-3.21	100.53	111.34
3	A	100	NAG	C3-C4-C5	-2.71	105.44	110.22
3	A	100	NAG	O6-C6-C5	-2.64	102.47	111.34
3	A	104	MAN	O2-C2-C1	-2.24	104.61	109.18
3	A	103	MAN	O2-C2-C1	-2.06	105.00	109.18
3	A	102	BMA	C3-C4-C5	-2.02	106.65	110.22
3	A	104	MAN	C1-C2-C3	2.05	112.25	109.65
3	A	103	MAN	C3-C4-C5	2.20	114.10	110.22
3	A	100	NAG	C4-C3-C2	2.24	114.30	111.02
3	A	103	MAN	O5-C1-C2	2.74	115.09	110.79
3	A	101	NAG	O3-C3-C2	2.79	115.37	109.39
3	A	100	NAG	C6-C5-C4	2.83	119.63	113.00
3	A	102	BMA	O4-C4-C5	2.87	116.51	109.28
3	A	104	MAN	O4-C4-C5	3.57	118.28	109.28
3	A	104	MAN	O5-C1-C2	3.72	116.62	110.79
3	A	104	MAN	C3-C4-C5	3.74	116.81	110.22
3	A	103	MAN	C1-O5-C5	4.35	118.16	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	101	NAG	2	0
3	A	102	BMA	2	0

5.6 Ligand geometry

1 ligand is 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	B	1100	2	14,14,15	0.65	0	15,19,21	1.22	1 (6%)

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	B	1100	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1100	NAG	C1-O5-C5	3.32	116.74	112.17

There are no chirality outliers.

There are no torsion outliers.

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

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	C	100/101 (99%)	0.16	2 (2%) 65 69	22, 33, 43, 47	0
1	D	99/101 (98%)	0.51	9 (9%) 10 11	29, 38, 54, 58	0
2	A	200/213 (93%)	0.53	8 (4%) 39 43	31, 36, 48, 56	0
2	B	199/213 (93%)	0.45	10 (5%) 30 33	27, 36, 48, 55	0
All	All	598/628 (95%)	0.44	29 (4%) 31 35	22, 36, 49, 58	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	175	ARG	5.1
2	B	190	HIS	4.9
2	B	222	PRO	4.9
2	B	243	PRO	4.5
1	D	171	ALA	4.1
1	D	138	GLY	3.9
2	B	319	ARG	3.7
1	D	157	ALA	3.5
2	B	326	GLU	3.4
1	D	133	ARG	3.4
1	D	156	ARG	3.4
2	B	354	GLN	3.2
2	A	190	HIS	3.1
1	C	156	ARG	2.9
1	D	181	ARG	2.8
1	D	155	ARG	2.8
2	A	345	ILE	2.8
1	C	210	ARG	2.6
2	A	158	ASP	2.6
2	A	321	SER	2.5
2	B	191	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	176	PRO	2.4
2	B	223	ASN	2.4
2	A	289	LEU	2.3
2	B	330	MET	2.3
2	A	347	ALA	2.3
2	B	189	PRO	2.2
2	A	223	ASN	2.1
2	A	217	LEU	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	MAN	A	104	11/12	0.88	0.24	2.58	37,49,55,58	0
3	NAG	A	100	14/15	0.95	0.20	1.19	30,32,37,41	0
3	NAG	A	101	14/15	0.95	0.16	0.14	24,31,38,39	0
3	BMA	A	102	11/12	0.87	0.14	-0.64	23,32,36,37	0
3	MAN	A	103	11/12	0.86	0.17	-	37,42,49,49	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	B	1100	14/15	0.91	0.15	-	39,47,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.