



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:56 PM GMT

PDB ID : 4X3R
Title : Avi-GCPII structure in complex with FITC-conjugated GCPII-specific inhibitor
Authors : Tykvart, J.; Konvalinka, J.
Deposited on : 2014-12-01
Resolution : 1.86 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

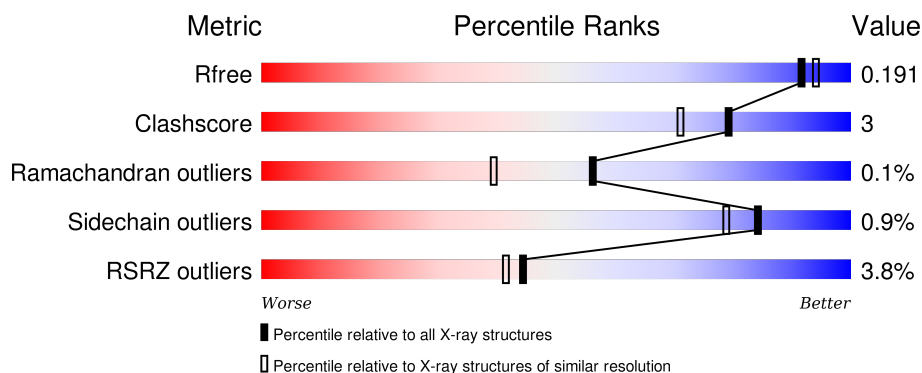
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	A	739	

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
5	NAG	A	1309	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	A	1319	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6517 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 Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	690	Total	C	N	O	S	0	8	0
			5540	3564	931	1026	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ARG	-	expression tag	UNP Q04609
A	13	SER	-	expression tag	UNP Q04609
A	14	GLY	-	expression tag	UNP Q04609
A	15	LEU	-	expression tag	UNP Q04609
A	16	ASN	-	expression tag	UNP Q04609
A	17	ASP	-	expression tag	UNP Q04609
A	18	ILE	-	expression tag	UNP Q04609
A	19	PHE	-	expression tag	UNP Q04609
A	20	GLU	-	expression tag	UNP Q04609
A	21	ALA	-	expression tag	UNP Q04609
A	22	GLN	-	expression tag	UNP Q04609
A	23	LYS	-	expression tag	UNP Q04609
A	24	ILE	-	expression tag	UNP Q04609
A	25	GLU	-	expression tag	UNP Q04609
A	26	TRP	-	expression tag	UNP Q04609
A	27	HIS	-	expression tag	UNP Q04609
A	28	GLU	-	expression tag	UNP Q04609
A	29	GLY	-	expression tag	UNP Q04609
A	30	SER	-	expression tag	UNP Q04609
A	31	GLY	-	expression tag	UNP Q04609
A	32	SER	-	expression tag	UNP Q04609
A	33	GLY	-	expression tag	UNP Q04609
A	34	SER	-	expression tag	UNP Q04609
A	35	GLU	-	expression tag	UNP Q04609
A	36	ASN	-	expression tag	UNP Q04609
A	37	LEU	-	expression tag	UNP Q04609
A	38	TYR	-	expression tag	UNP Q04609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	-	expression tag	UNP Q04609
A	40	GLN	-	expression tag	UNP Q04609
A	41	GLY	-	expression tag	UNP Q04609
A	42	ARG	-	expression tag	UNP Q04609
A	43	SER	-	expression tag	UNP Q04609

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0

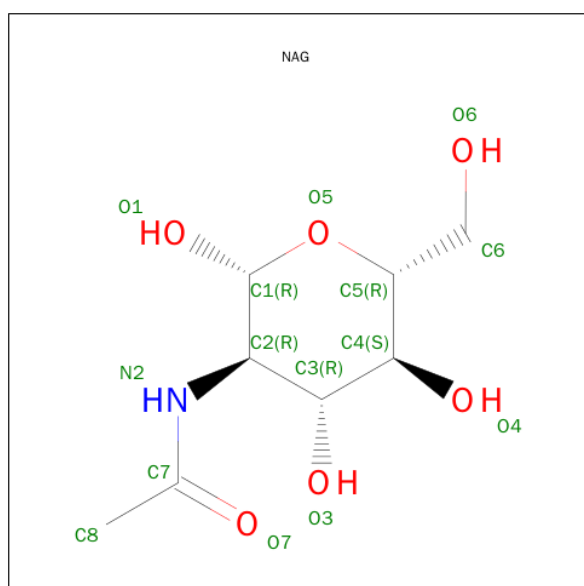
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

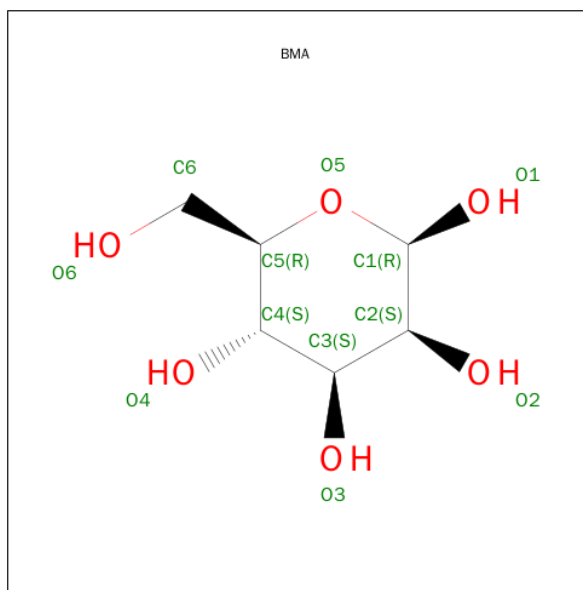
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



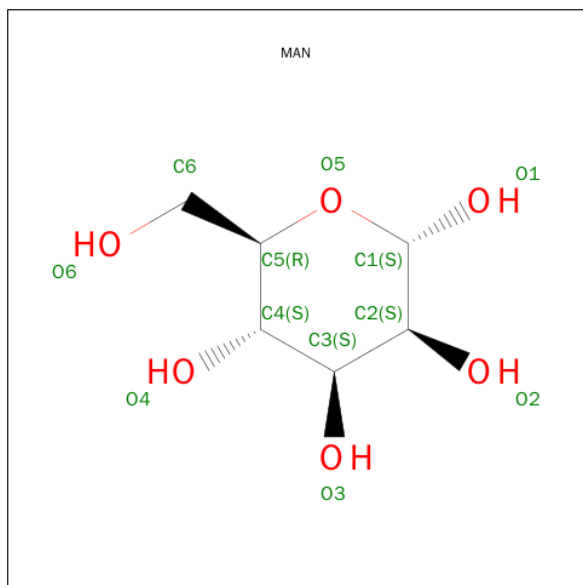
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



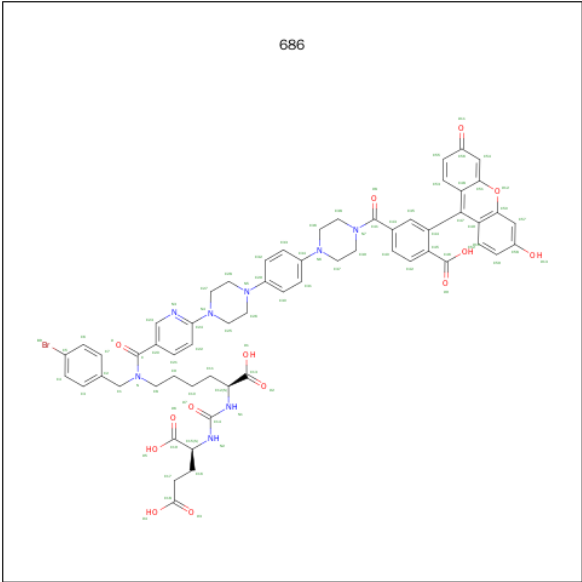
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is N-((1S)-5-[(4-bromobenzyl){6-[4-(4-{4-carboxy-3-(6-hydroxy-3-oxo-3H-xanthen-9-yl)benzoyl]piperazin-1-yl}phenyl)piperazin-1-yl]pyridin-3-yl}carbonyl)amino]-1-carboxypentyl}carbamoyl)-L-glutamic acid (three-letter code: 686) (formula: C₆₀H₅₉BrN₈O₁₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
8	A	1	138	3	95	16	24	0	1

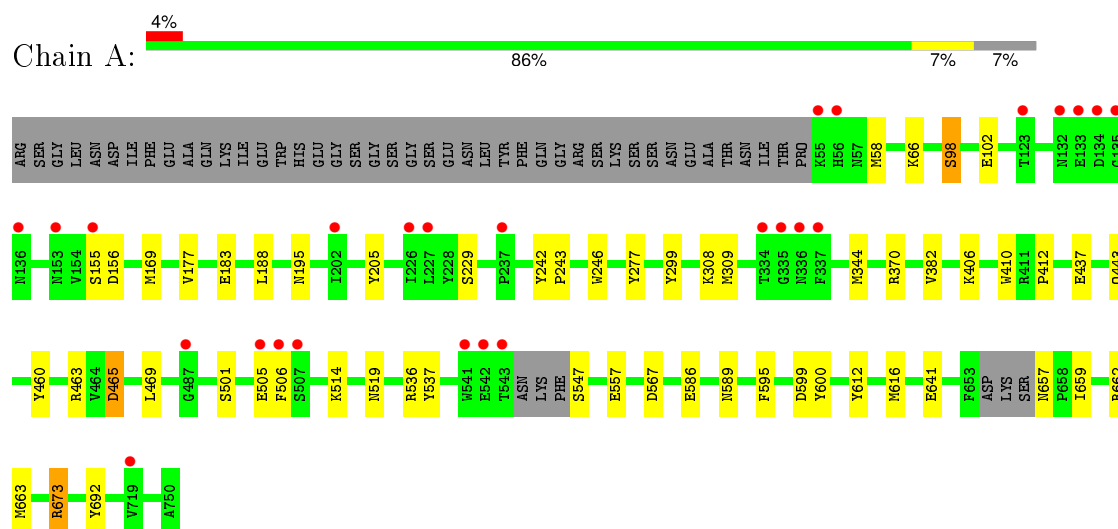
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	632	Total	O	0	5
			634	634		

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 errors 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: Glutamate carboxypeptidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.71Å 130.16Å 159.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.86 29.55 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.86) 99.5 (29.55-1.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.148 , 0.180 0.160 , 0.191	Depositor DCC
R_{free} test set	4426 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 88576 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6517	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, BMA, NAG, CL, CA, 686, 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	A	1.03	8/5715 (0.1%)	0.96	8/7743 (0.1%)

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
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	GLU	CD-OE2	-7.60	1.17	1.25
1	A	657	ASN	N-CA	7.50	1.61	1.46
1	A	557	GLU	CB-CG	-6.42	1.40	1.52
1	A	309	MET	CG-SD	-5.45	1.67	1.81
1	A	98	SER	CB-OG	-5.30	1.35	1.42
1	A	460	TYR	CG-CD1	5.21	1.46	1.39
1	A	501	SER	CB-OG	-5.19	1.35	1.42
1	A	277	TYR	CE1-CZ	5.12	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ASP	CB-CG-OD1	8.92	126.33	118.30
1	A	673	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	599	ASP	CB-CG-OD2	6.63	124.26	118.30
1	A	662	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	370	ARG	NE-CZ-NH1	6.21	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	673	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	465	ASP	CB-CG-OD2	-5.40	113.44	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain

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	5540	0	5400	31	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	168	0	149	2	0
6	A	22	0	19	0	0
7	A	11	0	10	0	0
8	A	138	0	99	17	0
9	A	634	0	0	5	0
All	All	6517	0	5677	40	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 3.

All (40) 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:659:ILE:O	1:A:663[B]:MET:HG3	1.85	0.77
8:A:1320[B]:686:O	8:A:1320[B]:686:H25	1.86	0.74
1:A:463[B]:ARG:HH22	8:A:1320[B]:686:H16	1.56	0.70
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463[B]:ARG:HH22	8:A:1320[B]:686:C23	2.13	0.62
1:A:465:ASP:OD2	8:A:1320[B]:686:H20	2.00	0.61
8:A:1320[B]:686:H19	9:A:1684:HOH:O	2.01	0.60
1:A:505:GLU:HB3	1:A:506:PHE:CD2	2.37	0.60
8:A:1320[B]:686:O	8:A:1320[B]:686:C9	2.50	0.58
1:A:463[B]:ARG:HG2	8:A:1320[B]:686:BR	2.61	0.55
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.43	0.54
1:A:505:GLU:HB3	1:A:506:PHE:CE2	2.43	0.53
1:A:169:MET:HA	1:A:344:MET:O	2.09	0.53
1:A:58:MET:CE	1:A:586:GLU:HG2	2.39	0.52
1:A:195:ASN:HD22	5:A:1311:NAG:H83	1.75	0.52
1:A:183:GLU:HG3	9:A:1956:HOH:O	2.11	0.51
1:A:463[B]:ARG:NH2	8:A:1320[B]:686:H16	2.24	0.50
1:A:66:LYS:HE2	9:A:1727:HOH:O	2.12	0.50
1:A:641:GLU:HG3	9:A:1805:HOH:O	2.13	0.49
1:A:155:SER:O	1:A:156:ASP:HB2	2.14	0.48
1:A:412:PRO:HA	1:A:589[B]:ASN:OD1	2.14	0.48
1:A:536:ARG:HG2	8:A:1320[B]:686:BR	2.70	0.47
8:A:1320[B]:686:C23	8:A:1320[B]:686:H18	2.45	0.46
8:A:1320[C]:686:H14	8:A:1320[C]:686:H8	1.76	0.46
1:A:469:LEU:O	1:A:595:PHE:HA	2.16	0.45
1:A:505:GLU:CB	1:A:506:PHE:CD2	3.00	0.45
8:A:1320[A]:686:H10	8:A:1320[A]:686:H5	1.83	0.45
1:A:246:TRP:CD1	5:A:1312:NAG:H83	2.53	0.44
8:A:1320[A]:686:C7	8:A:1320[A]:686:C20	2.95	0.44
1:A:514[A]:LYS:HD2	1:A:692:TYR:HE1	1.82	0.44
1:A:242:TYR:CG	1:A:243:PRO:HA	2.53	0.43
1:A:547:SER:N	8:A:1320[C]:686:C6	2.82	0.42
8:A:1320[C]:686:H5	8:A:1320[C]:686:H10	1.84	0.42
1:A:406:LYS:HA	1:A:410:TRP:O	2.19	0.42
1:A:465:ASP:OD2	8:A:1320[B]:686:C6	2.67	0.41
8:A:1320[B]:686:O7	8:A:1320[B]:686:C19	2.66	0.41
1:A:308:LYS:HB2	9:A:1537:HOH:O	2.20	0.41
1:A:98:SER:O	1:A:102:GLU:HG3	2.20	0.41
1:A:177:VAL:HG12	1:A:188:LEU:HD11	2.03	0.41
1:A:229:SER:O	1:A:299:TYR:HB3	2.21	0.41

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	692/739 (94%)	672 (97%)	19 (3%)	1 (0%)	56	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL

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	593/629 (94%)	587 (99%)	6 (1%)	82	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443[A]	GLN
1	A	443[B]	GLN
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	673	ARG

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

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 ⓘ

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 for Mogul analysis.

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$
5	NAG	A	1305	1,5	14,14,15	0.95	1 (7%)	15,19,21	1.99	6 (40%)
5	NAG	A	1306	5	14,14,15	0.86	0	15,19,21	1.79	5 (33%)
5	NAG	A	1307	1,5	14,14,15	1.26	1 (7%)	15,19,21	2.76	10 (66%)
5	NAG	A	1308	5	14,14,15	0.82	1 (7%)	15,19,21	1.43	1 (6%)
5	NAG	A	1309	1,5	14,14,15	1.12	2 (14%)	15,19,21	1.28	2 (13%)
5	NAG	A	1310	5	14,14,15	0.89	1 (7%)	15,19,21	1.99	5 (33%)
5	NAG	A	1311	1	14,14,15	0.90	1 (7%)	15,19,21	3.02	6 (40%)
5	NAG	A	1312	1	14,14,15	0.92	1 (7%)	15,19,21	2.40	8 (53%)
5	NAG	A	1313	1,5	14,14,15	1.13	0	15,19,21	1.73	5 (33%)
5	NAG	A	1314	5,6	14,14,15	0.77	0	15,19,21	1.25	0
6	BMA	A	1315	5	11,11,12	0.96	1 (9%)	15,15,17	1.59	5 (33%)
5	NAG	A	1316	1,5	14,14,15	1.20	0	15,19,21	1.11	2 (13%)
5	NAG	A	1317	5,6	14,14,15	1.03	1 (7%)	15,19,21	1.80	5 (33%)
6	BMA	A	1318	5,7	11,11,12	0.97	0	15,15,17	1.21	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	A	1319	6	11,11,12	0.92	1 (9%)	15,15,17	2.05	5 (33%)
8	686	A	1320[A]	2	44,53,91	0.94	1 (2%)	59,71,129	1.77	13 (22%)
8	686	A	1320[B]	-	30,39,91	0.81	2 (6%)	39,51,129	1.68	7 (17%)
8	686	A	1320[C]	2	44,53,91	0.90	2 (4%)	59,71,129	1.89	15 (25%)

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
5	NAG	A	1305	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1308	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1309	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1313	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1314	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1315	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1316	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1317	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1318	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	1319	6	-	0/2/19/22	0/1/1/1
8	686	A	1320[A]	2	-	0/38/58/92	0/4/4/9
8	686	A	1320[B]	-	-	0/30/40/92	0/2/2/9
8	686	A	1320[C]	2	-	0/38/58/92	0/4/4/9

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1317	NAG	O5-C1	-2.68	1.39	1.43
5	A	1305	NAG	C1-C2	-2.52	1.48	1.52
8	A	1320[B]	686	C15-N2	-2.19	1.43	1.46
5	A	1310	NAG	O3-C3	-2.19	1.37	1.43
7	A	1319	MAN	O2-C2	-2.14	1.38	1.43
8	A	1320[C]	686	C15-N2	-2.06	1.43	1.46
5	A	1309	NAG	C1-C2	2.03	1.55	1.52
5	A	1311	NAG	O5-C1	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1308	NAG	C4-C5	2.11	1.57	1.53
6	A	1315	BMA	C2-C3	2.12	1.55	1.52
8	A	1320[B]	686	C20-C	2.20	1.53	1.50
5	A	1307	NAG	C6-C5	2.28	1.60	1.51
8	A	1320[C]	686	C24-N4	2.34	1.42	1.37
5	A	1312	NAG	C3-C2	2.48	1.58	1.52
8	A	1320[A]	686	C24-N4	2.52	1.42	1.37
5	A	1309	NAG	C4-C5	2.81	1.59	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1312	NAG	O3-C3-C4	-4.82	99.48	110.36
7	A	1319	MAN	O2-C2-C1	-4.56	100.10	109.23
5	A	1311	NAG	O3-C3-C2	-4.47	99.81	109.37
5	A	1307	NAG	O4-C4-C3	-4.10	101.11	110.36
5	A	1310	NAG	C3-C4-C5	-3.64	103.74	110.23
5	A	1317	NAG	C3-C4-C5	-3.55	103.89	110.23
5	A	1313	NAG	O4-C4-C3	-3.54	102.37	110.36
8	A	1320[A]	686	O-C-N	-3.33	117.06	122.40
5	A	1312	NAG	O7-C7-C8	-3.31	115.98	122.07
8	A	1320[B]	686	BR-C5-C6	-3.18	114.47	119.29
8	A	1320[C]	686	C28-C27-N4	-3.17	104.67	110.59
8	A	1320[A]	686	C2-C1-N	-3.14	107.78	113.15
5	A	1305	NAG	O4-C4-C3	-2.96	103.69	110.36
6	A	1318	BMA	O3-C3-C2	-2.92	104.65	110.01
8	A	1320[B]	686	C19-C15-N2	-2.91	107.12	112.93
5	A	1307	NAG	O5-C5-C4	-2.91	105.31	110.13
5	A	1311	NAG	O7-C7-C8	-2.88	116.77	122.07
5	A	1306	NAG	C3-C4-C5	-2.87	105.11	110.23
5	A	1305	NAG	C2-N2-C7	-2.85	119.40	123.11
8	A	1320[A]	686	C22-C24-N3	-2.82	117.92	123.23
5	A	1317	NAG	O5-C5-C4	-2.81	105.47	110.13
8	A	1320[C]	686	C22-C24-N4	-2.76	117.24	121.66
5	A	1312	NAG	C3-C4-C5	-2.67	105.47	110.23
5	A	1310	NAG	O3-C3-C4	-2.64	104.41	110.36
5	A	1313	NAG	C3-C4-C5	-2.64	105.52	110.23
5	A	1313	NAG	O5-C5-C4	-2.54	105.92	110.13
8	A	1320[C]	686	C19-C15-N2	-2.50	107.94	112.93
7	A	1319	MAN	O5-C1-C2	-2.49	106.92	110.89
8	A	1320[A]	686	C19-C15-N2	-2.48	107.98	112.93
8	A	1320[A]	686	C28-C27-N4	-2.46	105.99	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1320[C]	686	C22-C24-N3	-2.46	118.58	123.23
5	A	1310	NAG	O7-C7-C8	-2.38	117.68	122.07
5	A	1307	NAG	C2-N2-C7	-2.36	120.03	123.11
5	A	1309	NAG	O3-C3-C2	-2.35	104.35	109.37
8	A	1320[C]	686	C11-C12-N1	-2.33	106.29	109.92
5	A	1313	NAG	O6-C6-C5	-2.29	103.64	111.30
8	A	1320[C]	686	C20-C23-N3	-2.29	120.04	123.64
8	A	1320[B]	686	C1-C2-C7	-2.28	116.50	120.78
5	A	1311	NAG	O7-C7-N2	-2.28	117.20	121.84
5	A	1307	NAG	O7-C7-C8	-2.28	117.88	122.07
5	A	1305	NAG	O7-C7-C8	-2.23	117.97	122.07
5	A	1317	NAG	O6-C6-C5	-2.21	103.91	111.30
6	A	1315	BMA	C1-O5-C5	-2.21	108.89	112.14
5	A	1313	NAG	C1-O5-C5	-2.19	108.92	112.14
8	A	1320[A]	686	C11-C12-N1	-2.14	106.58	109.92
8	A	1320[C]	686	O-C-N	-2.08	119.07	122.40
8	A	1320[A]	686	C22-C24-N4	-2.07	118.35	121.66
5	A	1316	NAG	C6-C5-C4	-2.06	107.83	112.99
8	A	1320[C]	686	O-C-C20	-2.04	116.28	120.16
5	A	1305	NAG	O7-C7-N2	2.01	125.94	121.84
5	A	1310	NAG	O7-C7-N2	2.02	125.97	121.84
5	A	1316	NAG	C1-O5-C5	2.03	115.13	112.14
8	A	1320[C]	686	BR-C5-C4	2.06	122.42	119.29
5	A	1307	NAG	C8-C7-N2	2.12	120.16	116.10
5	A	1306	NAG	O4-C4-C3	2.13	115.15	110.36
7	A	1319	MAN	C2-C3-C4	2.18	114.86	111.05
8	A	1320[A]	686	C20-C-N	2.19	121.67	118.77
5	A	1317	NAG	C6-C5-C4	2.20	118.49	112.99
5	A	1306	NAG	O4-C4-C5	2.20	115.03	109.23
6	A	1315	BMA	O2-C2-C3	2.25	114.72	110.19
6	A	1315	BMA	C3-C4-C5	2.27	114.28	110.23
8	A	1320[C]	686	C23-N3-C24	2.28	121.87	117.52
5	A	1307	NAG	O4-C4-C5	2.33	115.36	109.23
6	A	1315	BMA	O3-C3-C2	2.36	114.33	110.01
5	A	1312	NAG	O4-C4-C5	2.40	115.54	109.23
5	A	1312	NAG	O5-C5-C4	2.43	114.16	110.13
8	A	1320[A]	686	C23-N3-C24	2.43	122.17	117.52
8	A	1320[C]	686	C21-C22-C24	2.54	121.04	117.53
6	A	1315	BMA	O5-C5-C6	2.65	113.02	107.34
7	A	1319	MAN	O5-C5-C6	2.67	113.06	107.34
5	A	1312	NAG	C8-C7-N2	2.67	121.22	116.10
5	A	1309	NAG	C3-C4-C5	2.76	115.16	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1320[A]	686	C21-C22-C24	2.79	121.39	117.53
5	A	1307	NAG	C4-C3-C2	2.82	115.71	111.34
8	A	1320[B]	686	C16-C15-N2	2.90	114.46	109.92
7	A	1319	MAN	C1-O5-C5	3.09	116.68	112.14
5	A	1305	NAG	O5-C5-C6	3.14	114.07	107.34
5	A	1306	NAG	C2-N2-C7	3.23	127.30	123.11
5	A	1317	NAG	O3-C3-C4	3.30	117.81	110.36
5	A	1312	NAG	C1-O5-C5	3.30	117.00	112.14
8	A	1320[B]	686	C20-C-N	3.31	123.16	118.77
5	A	1306	NAG	C4-C3-C2	3.31	116.48	111.34
8	A	1320[B]	686	C24-N3-C23	3.34	122.95	116.82
5	A	1312	NAG	O3-C3-C2	3.35	116.55	109.37
5	A	1307	NAG	C6-C5-C4	3.69	122.25	112.99
5	A	1305	NAG	C1-O5-C5	3.71	117.60	112.14
5	A	1307	NAG	O5-C5-C6	3.99	115.88	107.34
8	A	1320[B]	686	BR-C5-C4	4.06	125.44	119.29
5	A	1310	NAG	O4-C4-C5	4.36	120.72	109.23
8	A	1320[C]	686	C16-C15-N2	4.41	116.82	109.92
8	A	1320[C]	686	C20-C-N	4.43	124.64	118.77
8	A	1320[A]	686	C16-C15-N2	4.46	116.89	109.92
5	A	1308	NAG	O4-C4-C5	4.47	121.02	109.23
5	A	1311	NAG	O5-C5-C6	4.71	117.42	107.34
5	A	1307	NAG	O6-C6-C5	5.03	128.11	111.30
8	A	1320[A]	686	N3-C24-N4	5.09	123.73	116.94
5	A	1311	NAG	C8-C7-N2	5.18	126.03	116.10
8	A	1320[C]	686	N3-C24-N4	5.43	124.17	116.94
8	A	1320[A]	686	C26-N5-C28	5.73	123.41	111.54
8	A	1320[C]	686	C26-N5-C28	5.90	123.75	111.54
5	A	1311	NAG	C1-O5-C5	6.48	121.66	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1311	NAG	1	0
5	A	1312	NAG	1	0
8	A	1320[A]	686	2	0
8	A	1320[B]	686	12	0
8	A	1320[C]	686	3	0

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	690/739 (93%)	-0.11	26 (3%) 44 41	16, 27, 49, 92	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	THR	6.3
1	A	541	TRP	3.9
1	A	135	GLY	3.5
1	A	155	SER	3.4
1	A	336	ASN	3.3
1	A	136	ASN	3.2
1	A	134	ASP	3.1
1	A	335	GLY	3.1
1	A	227	LEU	3.0
1	A	153	ASN	2.9
1	A	719	VAL	2.8
1	A	542	GLU	2.8
1	A	506	PHE	2.8
1	A	123	THR	2.7
1	A	55	LYS	2.6
1	A	507	SER	2.5
1	A	237	PRO	2.5
1	A	487	GLY	2.5
1	A	56	HIS	2.5
1	A	334	THR	2.4
1	A	337	PHE	2.4
1	A	133	GLU	2.3
1	A	132	ASN	2.3
1	A	202	ILE	2.2
1	A	226	ILE	2.0
1	A	505	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
7	MAN	A	1319	11/12	0.94	0.20	3.13	50,52,60,61	0
5	NAG	A	1309	14/15	0.87	0.18	2.25	39,43,49,57	0
5	NAG	A	1316	14/15	0.89	0.11	1.20	22,29,42,53	0
8	686	A	1320[A]	50/83	0.94	0.16	1.13	19,37,53,56	50
8	686	A	1320[C]	50/83	0.94	0.16	1.10	18,39,58,61	50
8	686	A	1320[B]	38/83	0.94	0.16	0.93	14,23,30,36	38
4	CA	A	1304	1/1	1.00	0.06	-0.34	17,17,17,17	0
3	CL	A	1303	1/1	1.00	0.11	-0.96	20,20,20,20	0
2	ZN	A	1301	1/1	1.00	0.08	-1.85	19,19,19,19	0
2	ZN	A	1302	1/1	1.00	0.07	-4.40	20,20,20,20	0
5	NAG	A	1317	14/15	0.90	0.27	-	40,48,57,61	0
5	NAG	A	1310	14/15	0.82	0.32	-	56,63,71,72	0
5	NAG	A	1313	14/15	0.94	0.14	-	28,30,35,44	0
5	NAG	A	1312	14/15	0.91	0.16	-	33,43,52,55	0
5	NAG	A	1311	14/15	0.74	0.20	-	60,71,80,86	0
5	NAG	A	1314	14/15	0.94	0.20	-	35,44,54,58	0
6	BMA	A	1315	11/12	0.73	0.35	-	60,67,72,80	0
5	NAG	A	1305	14/15	0.95	0.11	-	30,39,45,55	0
5	NAG	A	1308	14/15	0.78	0.43	-	69,75,82,91	0
6	BMA	A	1318	11/12	0.88	0.19	-	44,47,52,56	0
5	NAG	A	1306	14/15	0.67	0.30	-	41,58,68,70	0
5	NAG	A	1307	14/15	0.83	0.24	-	46,58,76,85	0

6.5 Other polymers

There are no such residues in this entry.