



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:13 AM GMT

PDB ID : 2WNF
Title : CRYSTAL STRUCTURE OF A MAMMALIAN SIALYLTRANSFERASE IN
COMPLEX WITH GAL-BETA-1-3GALNAC-ORTHO-NITROPHENOL
Authors : Rao, F.V.; Rich, J.R.; Raikic, B.; Wakarchuk, W.W.; Withers, S.G.; Stry-
nadka, N.C.J.
Deposited on : 2009-07-09
Resolution : 1.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

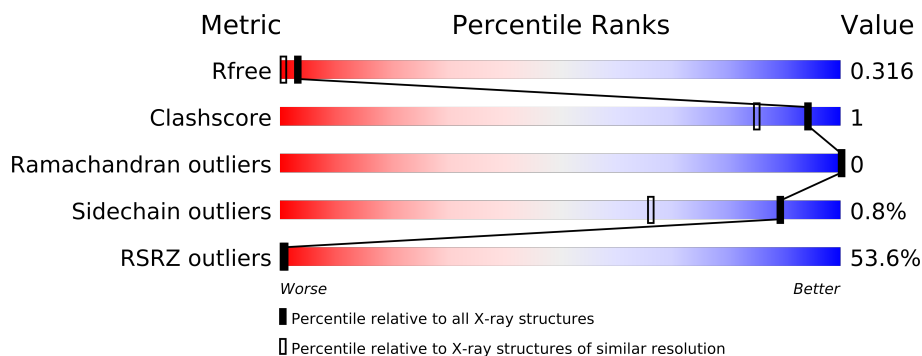
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.25 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}	66092	1021 (1.30-1.22)
Clashscore	79885	1125 (1.30-1.22)
Ramachandran outliers	78287	1075 (1.30-1.22)
Sidechain outliers	78261	1073 (1.30-1.22)
RSRZ outliers	66119	1021 (1.30-1.22)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	298	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CG3	A	1344	X	-

2 Entry composition i

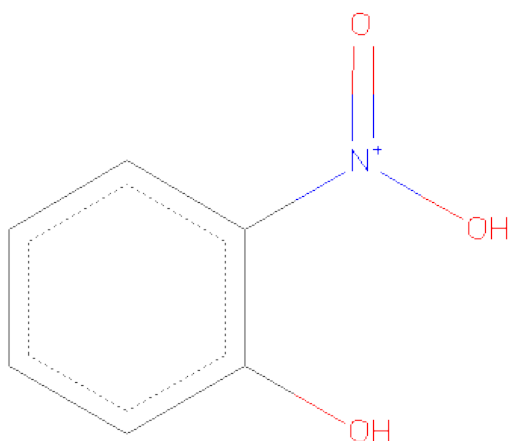
There are 4 unique types of molecules in this entry. The entry contains 2699 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CMP-N-ACETYLNEURAMINATE-BETA-GALACTOSAMIDE-ALPHA-2,3-SIALYLTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	Se	0	17	0
			2343	1493	415	424	8	3			

- Molecule 2 is HYDROXY(2-HYDROXYPHENYL)OXOAMMONIUM (three-letter code: CG3) (formula: C₆H₆NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			25	14	1	10		

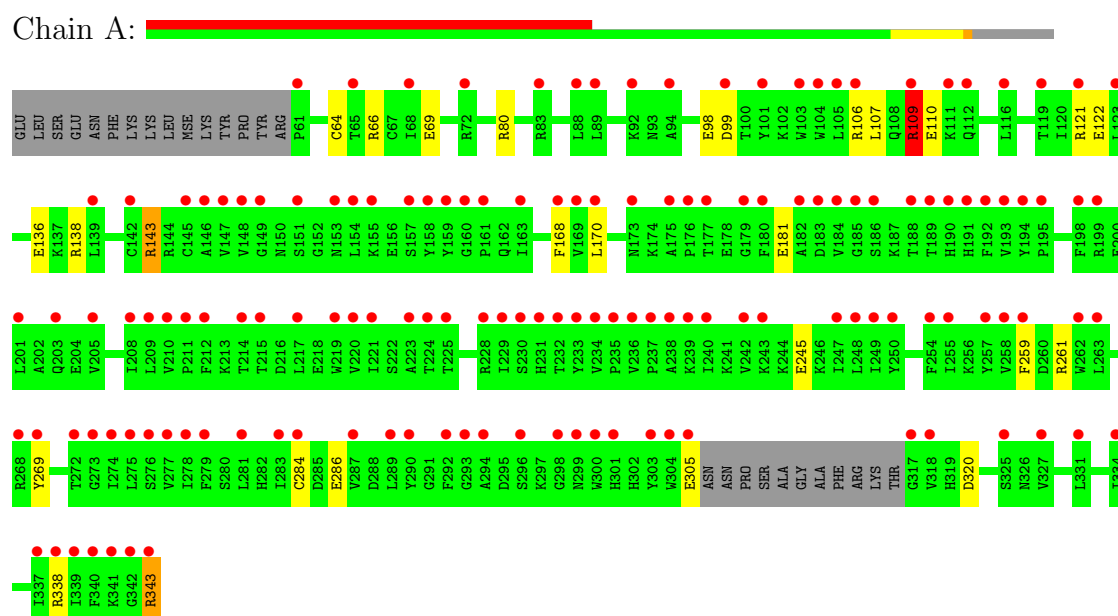
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	321	Total 321	O 321	0	0

3 Residue-property plots

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: CMP-N-ACETYLNEURAMINATE-BETA-GALACTOSAMIDE-ALPHA-2,3-SIALYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.99Å 78.35Å 99.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	1.29 – 1.25 32.93 – 1.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (1.29-1.25) 99.3 (32.93-1.24)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.180 , 0.195 0.308 , 0.316	Depositor DCC
R_{free} test set	4260 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	9.1	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.1	EDS
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 85219 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2699	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CG3, GAL, A2G

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	1.24	13/2423 (0.5%)	1.10	13/3271 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLU	CD-OE1	8.41	1.34	1.25
1	A	110	GLU	CB-CG	-6.79	1.39	1.52
1	A	69	GLU	CD-OE2	-6.43	1.18	1.25
1	A	98	GLU	CD-OE1	6.14	1.32	1.25
1	A	69	GLU	CB-CG	-6.13	1.40	1.52
1	A	245	GLU	CB-CG	-6.10	1.40	1.52
1	A	305	GLU	CG-CD	5.95	1.60	1.51
1	A	136	GLU	CD-OE2	5.42	1.31	1.25
1	A	259	PHE	CD2-CE2	5.35	1.50	1.39
1	A	245	GLU	CD-OE2	5.22	1.31	1.25
1	A	338	ARG	CB-CG	-5.19	1.38	1.52
1	A	286	GLU	CD-OE2	-5.10	1.20	1.25
1	A	109	ARG	CG-CD	-5.02	1.39	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	A	143	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	A	99	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	80	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	138	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	320	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	168	PHE	CB-CG-CD1	5.59	124.71	120.80
1	A	121[A]	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121[B]	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	170	LEU	CB-CG-CD2	5.28	119.97	111.00
1	A	343	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	261[A]	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	261[B]	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2343	0	2294	7	0
2	A	10	0	5	0	0
3	A	25	0	22	0	0
4	A	321	0	0	3	0
All	All	2699	0	2321	7	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122[A]:GLU:HG2	4:A:2093:HOH:O	1.60	1.02
1:A:106:ARG:O	1:A:109:ARG:HD2	2.01	0.61
1:A:122[A]:GLU:CG	4:A:2093:HOH:O	2.35	0.57
1:A:181:GLU:HB2	4:A:2167:HOH:O	2.08	0.54
1:A:143:ARG:HG2	1:A:284[B]:CYS:SG	2.59	0.42
1:A:107:LEU:HD22	1:A:269:TYR:HB3	2.02	0.41
1:A:64:CYS:HB2	1:A:66:ARG:O	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	285/298 (96%)	278 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	261/263 (99%)	259 (99%)	2 (1%)	89	66

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	343	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 chains 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

2 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	A2G	A	1345	3,2	12,14,15	0.88	0	15,19,21	1.33	1 (6%)
3	GAL	A	1346	3	10,11,12	1.32	2 (20%)	11,15,17	1.20	2 (18%)

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	A2G	A	1345	3,2	-	0/6/23/26	0/1/1/1
3	GAL	A	1346	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1346	GAL	O5-C5	2.20	1.49	1.45
3	A	1346	GAL	O2-C2	2.10	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1346	GAL	O5-C5-C4	-2.43	107.57	110.65
3	A	1346	GAL	C4-C3-C2	-2.41	107.27	110.50
3	A	1345	A2G	O-C5-C4	-2.30	107.74	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	$\# Z > 2$
2	CG3	A	1344	3	10,10,10	3.81	4 (40%)	13,13,13	4.23	9 (69%)

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
2	CG3	A	1344	3	-	0/3/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1344	CG3	OBI-NBG	9.08	1.42	1.23
2	A	1344	CG3	CBB-NBG	-6.45	1.34	1.46
2	A	1344	CG3	CAY-CAX	2.70	1.45	1.39
2	A	1344	CG3	OAO-CAW	2.65	1.42	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1344	CG3	OBH-NBG-OBI	-8.93	113.74	124.14
2	A	1344	CG3	OBH-NBG-CBB	-7.95	117.22	118.28
2	A	1344	CG3	CAY-CAZ-CBA	5.39	129.15	120.17
2	A	1344	CG3	CAX-CAW-CBB	4.83	125.28	118.68
2	A	1344	CG3	CAY-CAX-CAW	-3.26	115.72	120.05
2	A	1344	CG3	CAZ-CBA-CBB	-2.81	113.75	118.62
2	A	1344	CG3	OBI-NBG-CBB	2.29	125.42	119.20
2	A	1344	CG3	CAW-CBB-NBG	2.17	123.43	118.94
2	A	1344	CG3	CAZ-CAY-CAX	-2.13	116.61	120.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	272/298 (91%)	2.18	146 (53%) 0 1	10, 13, 18, 26	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	GLY	7.0
1	A	300	TRP	4.9
1	A	158	TYR	4.6
1	A	232	THR	4.6
1	A	147	VAL	4.5
1	A	192	PHE	4.4
1	A	208	ILE	4.4
1	A	279	PHE	4.3
1	A	275	LEU	4.3
1	A	111	LYS	4.2
1	A	201	LEU	4.2
1	A	193	VAL	4.2
1	A	274	ILE	4.2
1	A	154	LEU	4.1
1	A	182	ALA	4.0
1	A	250	TYR	3.9
1	A	255	ILE	3.8
1	A	290	TYR	3.8
1	A	301	HIS	3.8
1	A	304	TRP	3.8
1	A	277	VAL	3.8
1	A	209	LEU	3.7
1	A	210	VAL	3.7
1	A	180	PHE	3.7
1	A	106	ARG	3.7
1	A	170	LEU	3.7
1	A	254	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	318	VAL	3.6
1	A	148	VAL	3.6
1	A	159	TYR	3.6
1	A	194	TYR	3.6
1	A	299	ASN	3.6
1	A	303	TYR	3.5
1	A	236	VAL	3.5
1	A	240	ILE	3.5
1	A	212	PHE	3.4
1	A	198	PHE	3.4
1	A	168	PHE	3.3
1	A	284[A]	CYS	3.3
1	A	268	ARG	3.3
1	A	278	ILE	3.3
1	A	83	ARG	3.2
1	A	262	TRP	3.2
1	A	247	ILE	3.2
1	A	292	PHE	3.2
1	A	177	THR	3.2
1	A	234	VAL	3.2
1	A	289	LEU	3.2
1	A	276[A]	SER	3.1
1	A	145[A]	CYS	3.1
1	A	341[A]	LYS	3.1
1	A	281	LEU	3.1
1	A	229	ILE	3.0
1	A	105	LEU	3.0
1	A	179	GLY	3.0
1	A	163	ILE	3.0
1	A	188	THR	3.0
1	A	184	VAL	3.0
1	A	203	GLN	3.0
1	A	305	GLU	3.0
1	A	242	VAL	3.0
1	A	248	LEU	3.0
1	A	272	THR	3.0
1	A	283	ILE	2.9
1	A	169	VAL	2.9
1	A	221	ILE	2.9
1	A	175	ALA	2.9
1	A	219	TRP	2.9
1	A	339	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	2.8
1	A	104	TRP	2.8
1	A	176	PRO	2.8
1	A	185	GLY	2.8
1	A	223	ALA	2.8
1	A	340	PHE	2.8
1	A	146	ALA	2.7
1	A	249	ILE	2.7
1	A	205	VAL	2.7
1	A	287	VAL	2.7
1	A	230	SER	2.7
1	A	109	ARG	2.7
1	A	331	LEU	2.6
1	A	112	GLN	2.6
1	A	189	THR	2.6
1	A	228[A]	ARG	2.6
1	A	337	ILE	2.6
1	A	231[A]	HIS	2.6
1	A	103	TRP	2.6
1	A	233	TYR	2.6
1	A	149	GLY	2.5
1	A	342	GLY	2.5
1	A	257	TYR	2.5
1	A	142	CYS	2.5
1	A	116	LEU	2.4
1	A	238	ALA	2.4
1	A	220	VAL	2.4
1	A	296	SER	2.4
1	A	327	VAL	2.4
1	A	263	LEU	2.4
1	A	191	HIS	2.4
1	A	68	ILE	2.4
1	A	61	PRO	2.4
1	A	186[A]	SER	2.3
1	A	343	ARG	2.3
1	A	325[A]	SER	2.3
1	A	217	LEU	2.3
1	A	92[A]	LYS	2.3
1	A	157	SER	2.3
1	A	215	THR	2.3
1	A	155	LYS	2.3
1	A	239	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	225	THR	2.3
1	A	123	LEU	2.3
1	A	139	LEU	2.3
1	A	269	TYR	2.2
1	A	334	ILE	2.2
1	A	258	VAL	2.2
1	A	173	ASN	2.2
1	A	224	THR	2.2
1	A	121[A]	ARG	2.2
1	A	99	ASP	2.2
1	A	293	GLY	2.2
1	A	298	GLY	2.2
1	A	151	SER	2.2
1	A	88	LEU	2.2
1	A	101	TYR	2.2
1	A	338	ARG	2.2
1	A	65	THR	2.2
1	A	161	PRO	2.2
1	A	273	GLY	2.2
1	A	153	ASN	2.2
1	A	199	ARG	2.1
1	A	195	PRO	2.1
1	A	235	PRO	2.1
1	A	259	PHE	2.1
1	A	294	ALA	2.1
1	A	214	THR	2.1
1	A	89	LEU	2.1
1	A	211	PRO	2.1
1	A	237	PRO	2.1
1	A	190	HIS	2.1
1	A	119	THR	2.1
1	A	94	ALA	2.0
1	A	183	ASP	2.0
1	A	243	LYS	2.0
1	A	72	ARG	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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GAL	A	1346	11/12	0.19	1.21	13,14,16,18	0
3	A2G	A	1345	14/15	0.18	0.05	16,17,22,23	0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CG3	A	1344	10/10	0.22	0.95	20,23,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.