



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:53 PM GMT

PDB ID : 1D0H
Title : THE HC FRAGMENT OF TETANUS TOXIN COMPLEXED WITH N-AC
ETYL-GALACTOSAMINE
Authors : Emsley, P.; Fotinou, C.; Black, I.; Fairweather, N.F.; Charles, I.G.; Watts, C.;
Hewitt, E.; Isaacs, N.W.
Deposited on : 1999-09-10
Resolution : 2.10 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

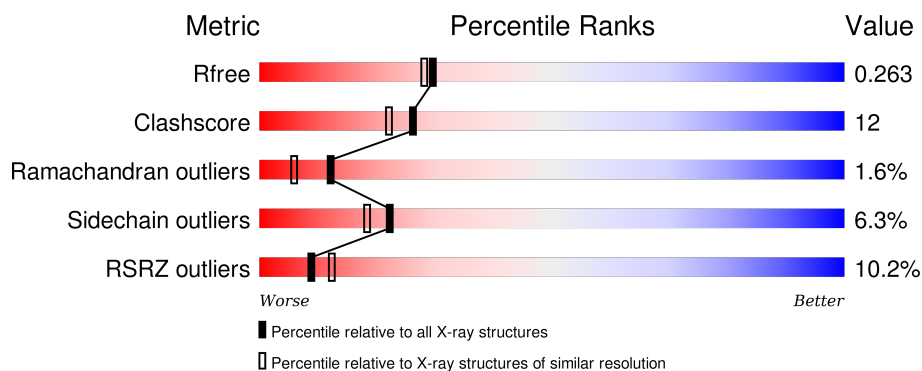
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	469	<div> <div>10%</div> <div>67%</div> <div>23%</div> <div>• 6%</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
2	A2G	A	601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A2G	A	602	-	-	-	X

2 Entry composition [i](#)

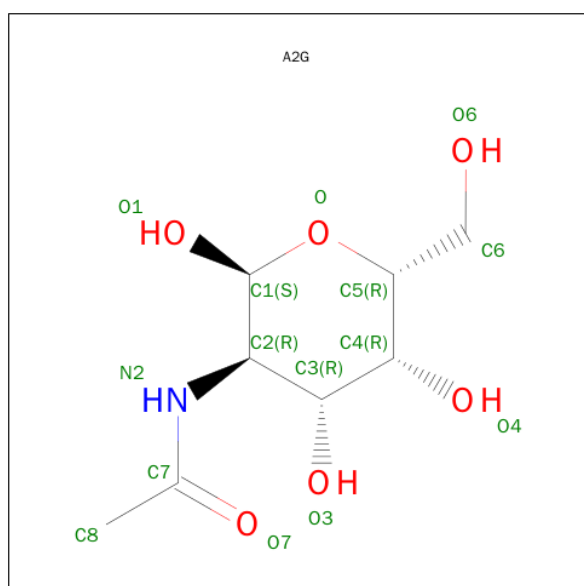
There are 4 unique types of molecules in this entry. The entry contains 4099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (TETANUS TOXIN HC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3563	2282	597	675	9			

- Molecule 2 is N-ACETYL-D-GALACTOSAMINE (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	501	Total	O	0	0
			501	501		

- Molecule 1: PROTEIN (TETANUS TOXIN HC)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.08 Å 70.88 Å 122.24 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 38.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.10) 99.6 (38.10-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.10 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.270 0.200 , 0.263	Depositor DCC
R_{free} test set	1764 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.3	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 34614 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4099	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: SO4, 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	0.53	0/3644	1.27	13/4945 (0.3%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1168	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	A	1168	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	957	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	1222	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	1123	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	1170	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	A	1128	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	1006	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	1187	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	1170	TYR	CB-CG-CD1	5.54	124.32	121.00
1	A	1226	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	890	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	957	ARG	CD-NE-CZ	5.11	130.75	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1065	ARG	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	3563	0	3516	87	0
2	A	30	0	29	3	0
3	A	5	0	0	0	0
4	A	501	0	0	13	0
All	All	4099	0	3545	88	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 12.

All (88) 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:1141:GLN:HE21	1:A:1142:LEU:H	1.05	0.98
1:A:1199:TYR:HE2	2:A:602:A2G:H1	1.41	0.83
1:A:972:ASN:HD21	1:A:1078:ASN:H	1.31	0.78
1:A:1270:THR:HG22	1:A:1284:LEU:CD2	2.14	0.76
1:A:929:GLU:H	1:A:929:GLU:CD	1.89	0.74
1:A:1093:CYS:HB3	4:A:207:HOH:O	1.89	0.71
1:A:1297:LYS:NZ	1:A:1298:ILE:HD11	2.04	0.71
1:A:1270:THR:HG22	1:A:1284:LEU:HD23	1.72	0.71
1:A:1141:GLN:NE2	1:A:1142:LEU:H	1.84	0.70
1:A:1223:ARG:HG2	1:A:1223:ARG:HH11	1.58	0.69
1:A:1182:PRO:O	1:A:1183:ASN:HB2	1.92	0.67
2:A:602:A2G:H8	4:A:252:HOH:O	1.94	0.67
1:A:1181:THR:HB	1:A:1182:PRO:HD2	1.76	0.67
1:A:1053:MET:SD	4:A:128:HOH:O	2.53	0.67
1:A:1199:TYR:CE2	2:A:602:A2G:H1	2.29	0.63
1:A:949:ASN:ND2	1:A:1040:ARG:H	1.98	0.62
1:A:1297:LYS:HZ1	1:A:1298:ILE:HD11	1.64	0.62
1:A:1017:ARG:HB2	4:A:301:HOH:O	2.00	0.61
1:A:944:ASN:O	1:A:948:ASN:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:THR:HB	1:A:1013:GLN:HG2	1.84	0.60
1:A:945:ASP:HB3	4:A:77:HOH:O	2.02	0.60
1:A:1097:ASN:ND2	1:A:1100:GLU:H	2.01	0.59
1:A:1083:TYR:OH	1:A:1310:GLU:HG3	2.05	0.56
1:A:1145:ILE:HD11	4:A:195:HOH:O	2.05	0.56
1:A:1180:TYR:HA	1:A:1197:LYS:NZ	2.20	0.56
1:A:907:ILE:HD12	1:A:936:HIS:CE1	2.41	0.56
1:A:1205:ASN:HB2	4:A:504:HOH:O	2.07	0.55
1:A:946:MET:HA	1:A:1064:ILE:O	2.07	0.55
1:A:876:ASP:HB2	1:A:879:VAL:HG23	1.88	0.54
1:A:1180:TYR:HA	1:A:1197:LYS:HZ2	1.72	0.54
1:A:891:ILE:HG12	1:A:896:ILE:HG12	1.89	0.54
1:A:1261:LYS:O	1:A:1262:ASN:HB2	2.08	0.53
1:A:924:HIS:HD2	1:A:1085:SER:OG	1.92	0.53
1:A:1270:THR:HG22	1:A:1284:LEU:HD22	1.90	0.52
1:A:1130:LEU:HD22	1:A:1303:TRP:HB3	1.91	0.52
1:A:987:ILE:HB	1:A:1005:LYS:NZ	2.25	0.51
1:A:1256:LYS:HE2	1:A:1258:TYR:CZ	2.46	0.51
1:A:948:ASN:ND2	1:A:949:ASN:H	2.07	0.51
1:A:932:GLU:OE1	1:A:1073:LYS:HD3	2.11	0.51
1:A:983:HIS:CD2	1:A:983:HIS:O	2.65	0.50
1:A:1067:ASP:OD1	1:A:1068:ASN:N	2.45	0.50
1:A:1097:ASN:HB2	1:A:1098:PRO:HD2	1.94	0.49
1:A:1130:LEU:CD2	1:A:1303:TRP:HB3	2.42	0.49
1:A:1033:PHE:HZ	1:A:1104:LEU:HD13	1.76	0.49
1:A:1223:ARG:CG	1:A:1223:ARG:NH1	2.73	0.49
1:A:1170:TYR:CE1	1:A:1308:THR:HA	2.48	0.49
1:A:999:ASN:OD1	1:A:1017:ARG:HD2	2.13	0.47
1:A:1033:PHE:CZ	1:A:1104:LEU:HD13	2.48	0.47
1:A:1005:LYS:HG3	1:A:1011:VAL:HG23	1.97	0.47
1:A:1003:THR:HG23	4:A:2:HOH:O	2.15	0.47
1:A:1075:ASP:O	1:A:1076:ARG:HB2	2.14	0.46
1:A:1137:SER:HA	4:A:69:HOH:O	2.14	0.46
1:A:1097:ASN:HB2	1:A:1098:PRO:CD	2.46	0.46
1:A:1053:MET:HE1	4:A:474:HOH:O	2.16	0.46
1:A:1146:THR:N	1:A:1227:VAL:O	2.46	0.45
1:A:1212:PRO:HB3	1:A:1229:TYR:CE2	2.51	0.45
1:A:1208:ILE:HD13	1:A:1238:LYS:HG2	1.97	0.45
1:A:1221:LEU:O	1:A:1223:ARG:NH1	2.49	0.45
1:A:1145:ILE:HG12	1:A:1146:THR:N	2.32	0.45
1:A:1145:ILE:HD12	4:A:423:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:ILE:HB	1:A:1005:LYS:HZ3	1.81	0.45
1:A:942:GLU:HG3	1:A:943:TYR:CD2	2.52	0.44
1:A:1223:ARG:HG2	1:A:1223:ARG:NH1	2.28	0.44
1:A:1017:ARG:HH11	1:A:1017:ARG:HD2	1.55	0.44
1:A:1029:ASN:HB3	1:A:1118:TRP:CZ3	2.53	0.44
1:A:947:PHE:CE1	1:A:1063:ALA:HB2	2.53	0.43
1:A:909:TYR:HB3	1:A:910:PRO:HD2	2.00	0.43
1:A:1181:THR:HB	1:A:1182:PRO:CD	2.46	0.43
1:A:963:ALA:O	1:A:967:GLU:HG3	2.19	0.43
1:A:981:LYS:HG3	1:A:1067:ASP:HB2	2.01	0.43
1:A:998:ASN:HD22	1:A:998:ASN:HA	1.66	0.42
1:A:976:ILE:HG13	1:A:977:ILE:HG13	2.01	0.42
1:A:1037:THR:O	1:A:1044:ALA:HA	2.20	0.42
1:A:987:ILE:HD12	1:A:1005:LYS:HE2	2.00	0.42
1:A:1178:LYS:HD2	1:A:1199:TYR:CE1	2.54	0.42
1:A:1003:THR:HG21	4:A:303:HOH:O	2.20	0.42
1:A:915:VAL:HB	1:A:916:PRO:HD2	2.00	0.42
1:A:946:MET:HG3	1:A:1063:ALA:HB1	2.02	0.41
1:A:1110:SER:HB2	4:A:326:HOH:O	2.19	0.41
1:A:1205:ASN:HD22	1:A:1206:GLU:H	1.68	0.41
1:A:1075:ASP:O	1:A:1076:ARG:CB	2.68	0.41
1:A:1222:ASP:OD2	1:A:1271:HIS:HD2	2.04	0.41
1:A:1182:PRO:O	1:A:1183:ASN:CB	2.63	0.41
1:A:1240:MET:HA	1:A:1256:LYS:O	2.21	0.41
1:A:972:ASN:ND2	1:A:1078:ASN:H	2.07	0.41
1:A:876:ASP:HB2	1:A:879:VAL:CG2	2.50	0.41
1:A:1066:GLU:HG2	1:A:1067:ASP:O	2.21	0.41
1:A:886:ILE:HB	1:A:941:ILE:HG21	2.03	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	439/469 (94%)	411 (94%)	21 (5%)	7 (2%)	12 6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	986	SER
1	A	988	GLY
1	A	1183	ASN
1	A	982	LYS
1	A	984	SER
1	A	1221	LEU
1	A	987	ILE

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	397/421 (94%)	372 (94%)	25 (6%)	22 18

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	876	ASP
1	A	905	SER
1	A	929	GLU
1	A	943	TYR
1	A	1003	THR
1	A	1066	GLU
1	A	1076	ARG
1	A	1094	LYS
1	A	1097	ASN
1	A	1104	LEU
1	A	1111	ILE
1	A	1122	LEU
1	A	1145	ILE
1	A	1161	LYS

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Mol	Chain	Res	Type
1	A	1167	ARG
1	A	1179	ARG
1	A	1185	GLU
1	A	1203	ASN
1	A	1205	ASN
1	A	1216	ASN
1	A	1219	ASN
1	A	1234	ILE
1	A	1238	LYS
1	A	1245	LEU
1	A	1284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	919	ASN
1	A	924	HIS
1	A	936	HIS
1	A	949	ASN
1	A	972	ASN
1	A	983	HIS
1	A	998	ASN
1	A	1013	GLN
1	A	1082	GLN
1	A	1097	ASN
1	A	1141	GLN
1	A	1203	ASN
1	A	1205	ASN
1	A	1207	HIS
1	A	1216	ASN
1	A	1271	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
2	A2G	A	601	-	15,15,15	0.34	0	17,21,21	1.04	2 (11%)
2	A2G	A	602	-	15,15,15	0.53	0	17,21,21	2.14	6 (35%)
3	SO4	A	701	-	4,4,4	0.97	0	6,6,6	0.22	0

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	A2G	A	601	-	-	0/6/26/26	0/1/1/1
2	A2G	A	602	-	-	0/6/26/26	0/1/1/1
3	SO4	A	701	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	A2G	C8-C7-N2	-2.64	111.05	116.11
2	A	602	A2G	C4-C3-C2	2.01	113.21	110.43
2	A	601	A2G	O3-C3-C2	2.02	113.78	109.66
2	A	602	A2G	O-C5-C4	2.12	113.66	109.68
2	A	601	A2G	O4-C4-C5	2.51	115.90	109.24
2	A	602	A2G	O7-C7-N2	3.01	128.00	121.86
2	A	602	A2G	C2-N2-C7	4.46	134.54	123.10
2	A	602	A2G	C1-O-C5	4.51	121.81	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	A2G	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	441/469 (94%)	0.51	45 (10%) 9 12	17, 30, 69, 100	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	ILE	10.6
1	A	985	LEU	10.1
1	A	983	HIS	9.9
1	A	1183	ASN	7.9
1	A	943	TYR	7.8
1	A	986	SER	7.3
1	A	984	SER	6.2
1	A	944	ASN	5.5
1	A	941	ILE	5.2
1	A	875	GLU	5.1
1	A	936	HIS	4.9
1	A	939	MET	4.9
1	A	938	ALA	4.7
1	A	940	ASP	4.7
1	A	1184	ASN	4.7
1	A	982	LYS	4.2
1	A	1076	ARG	4.0
1	A	1112	THR	3.7
1	A	948	ASN	3.7
1	A	1111	ILE	3.6
1	A	1182	PRO	3.5
1	A	876	ASP	3.5
1	A	1113	PHE	3.5
1	A	902	PHE	3.3
1	A	1181	THR	2.9
1	A	956	LEU	2.9
1	A	1065	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1032	VAL	2.8
1	A	1017	ARG	2.5
1	A	877	ILE	2.5
1	A	1068	ASN	2.5
1	A	879	VAL	2.4
1	A	903	ASN	2.3
1	A	1086	ILE	2.3
1	A	988	GLY	2.3
1	A	942	GLU	2.3
1	A	880	ILE	2.3
1	A	945	ASP	2.2
1	A	1078	ASN	2.2
1	A	1077	CYS	2.2
1	A	1220	ASN	2.1
1	A	946	MET	2.1
1	A	1233	GLY	2.1
1	A	1034	ILE	2.0
1	A	1048	ILE	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 carbohydrates 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. 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
2	A2G	A	601	15/15	0.84	0.30	7.25	52,55,58,59	0
2	A2G	A	602	15/15	0.80	0.26	4.99	68,70,71,71	0
3	SO4	A	701	5/5	0.93	0.21	-	56,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.