



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:59 AM BST

PDB ID : 4CJB  
Title : orthorhombic crystal form of Bogt6a E192Q in complex with GalNAc  
Authors : Pham, T.; Stinson, B.; Thiyagarajan, N.; Lizotte-Waniewski, M.; Brew, K.;  
Acharya, K.R.  
Deposited on : 2013-12-19  
Resolution : 2.78 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

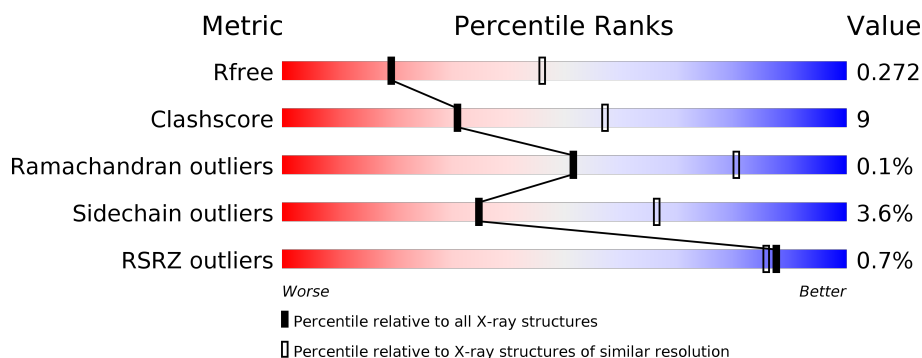
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	246	
1	B	246	
1	C	246	
1	D	246	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8060 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.

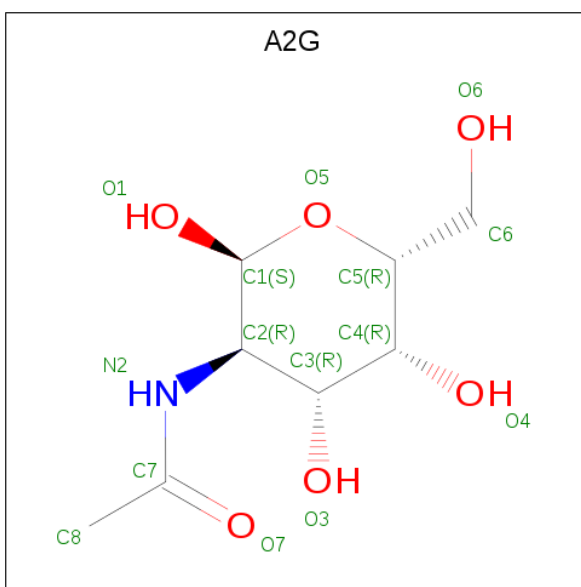
- Molecule 1 is a protein called GLYCOSYLTRANSFERASE FAMILY 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total 1973	C 1291	N 320	O 355	S 7	10	0	0
1	B	236	Total 1973	C 1291	N 320	O 355	S 7	7	0	0
1	C	237	Total 1977	C 1293	N 321	O 356	S 7	10	0	0
1	D	235	Total 1961	C 1282	N 319	O 353	S 7	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLN	GLU	engineered mutation	UNP A7LVT2
B	192	GLN	GLU	engineered mutation	UNP A7LVT2
C	192	GLN	GLU	engineered mutation	UNP A7LVT2
D	192	GLN	GLU	engineered mutation	UNP A7LVT2

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

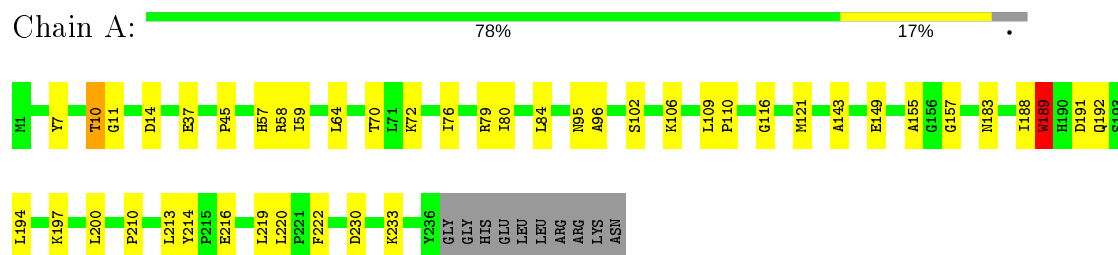
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	32	Total	O	0	0
			32	32		
3	C	20	Total	O	0	0
			20	20		
3	D	17	Total	O	0	0
			17	17		

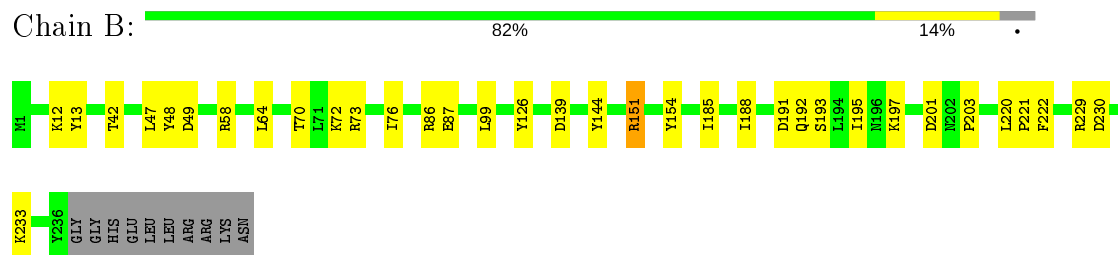
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

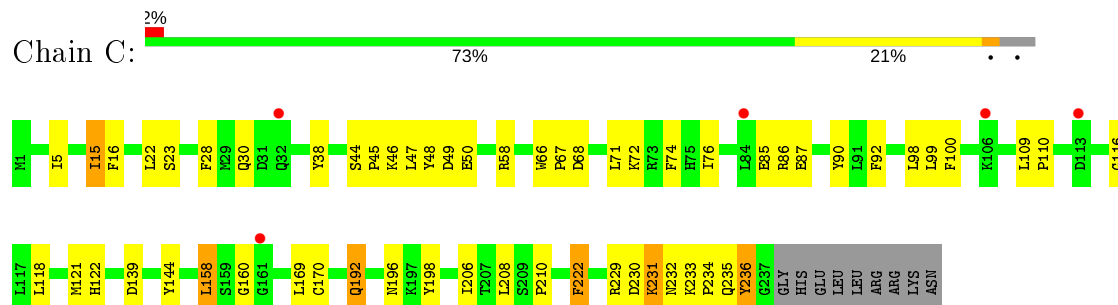
#### • Molecule 1: GLYCOSYLTRANSFERASE FAMILY 6



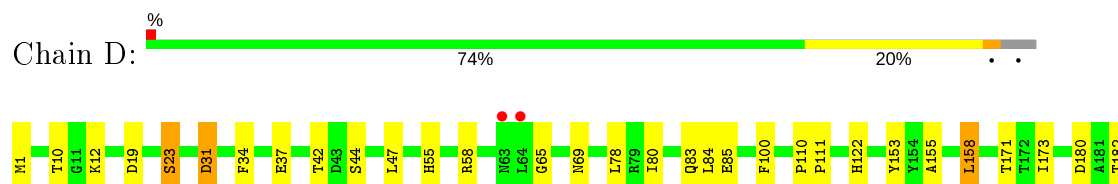
#### • Molecule 1: GLYCOSYLTRANSFERASE FAMILY 6



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W183	H184	I185	I188	W189	H190	D191	Q192	S193	L194	I195	W196	K197	Y198	D201	L213	Y214	P215	W218	L219	L220	F221	F222	I228	R229	D230	K231	R232	K233	P234	Q235	TYR	GLY	GLY	HIS	GLU	LEU	LEU	ARG	ARG	LYS	ASN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.12Å 115.60Å 126.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.63 – 2.78 67.63 – 2.78	Depositor EDS
% Data completeness (in resolution range)	97.6 (67.63-2.78) 91.4 (67.63-2.78)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.231 , 0.274 0.231 , 0.272	Depositor DCC
$R_{free}$ test set	1495 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/2038	0.50	1/2768 (0.0%)
1	B	0.39	0/2038	0.51	0/2768
1	C	0.46	0/2042	0.55	1/2773 (0.0%)
1	D	0.39	0/2025	0.53	1/2750 (0.0%)
All	All	0.41	0/8143	0.52	3/11059 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	TRP	N-CA-C	-5.45	96.29	111.00
1	C	158	LEU	CA-CB-CG	5.15	127.15	115.30
1	D	158	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1973	0	1914	32	0
1	B	1973	0	1914	21	0
1	C	1977	0	1917	48	0
1	D	1961	0	1905	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	12	5	0
2	B	15	0	12	0	0
2	C	15	0	12	1	0
2	D	15	0	12	2	0
3	A	47	0	0	1	0
3	B	32	0	0	1	0
3	C	20	0	0	0	0
3	D	17	0	0	0	0
All	All	8060	0	7698	141	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 9.

All (141) 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:C:233:LYS:HG3	1:C:234:PRO:CD	1.36	1.51
1:A:188:ILE:HD12	1:A:188:ILE:O	1.42	1.14
1:D:153:TYR:OH	1:D:192:GLN:OE1	1.65	1.13
1:C:233:LYS:HG3	1:C:234:PRO:HD3	1.29	1.09
1:D:191:ASP:O	1:D:195:ILE:HD12	1.53	1.08
1:C:233:LYS:CG	1:C:234:PRO:CD	2.32	1.08
1:C:231:LYS:O	1:C:232:ASN:HB2	1.55	1.05
1:C:233:LYS:HG3	1:C:234:PRO:HD2	1.02	0.99
1:C:233:LYS:CG	1:C:234:PRO:HD2	1.89	0.99
1:A:191:ASP:OD2	2:A:1237:A2G:O3	1.83	0.95
1:D:188:ILE:HG23	1:D:188:ILE:O	1.70	0.91
1:B:73:ARG:NH1	1:B:191:ASP:OD2	2.06	0.88
1:D:153:TYR:CZ	1:D:192:GLN:OE1	2.29	0.86
1:C:44:SER:O	1:C:58:ARG:NH2	2.12	0.82
1:C:233:LYS:CG	1:C:234:PRO:HD3	2.06	0.81
1:D:191:ASP:O	1:D:195:ILE:CD1	2.30	0.79
1:B:151:ARG:HH12	1:B:203:PRO:HB3	1.49	0.77
1:D:153:TYR:CE2	1:D:192:GLN:OE1	2.38	0.77
1:A:189:TRP:CD1	1:A:189:TRP:N	2.53	0.76
1:D:230:ASP:HB3	1:D:233:LYS:HG2	1.67	0.76
1:A:188:ILE:O	1:A:188:ILE:CD1	2.30	0.75
1:C:231:LYS:O	1:C:232:ASN:CB	2.30	0.74
1:D:31:ASP:N	1:D:31:ASP:OD1	2.20	0.72
1:C:230:ASP:O	1:C:233:LYS:HB2	1.88	0.72
1:D:188:ILE:CG2	1:D:188:ILE:O	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD13	2:A:1237:A2G:H8	1.72	0.70
1:A:230:ASP:HB3	1:A:233:LYS:HD3	1.74	0.69
1:C:15:ILE:HG13	1:C:236:TYR:HB3	1.76	0.68
1:A:157:GLY:HA3	2:A:1237:A2G:H8B	1.78	0.66
1:C:234:PRO:O	1:C:235:GLN:C	2.30	0.65
1:C:99:LEU:HB2	1:C:229:ARG:HH11	1.62	0.65
1:C:192:GLN:O	1:C:196:ASN:ND2	2.19	0.64
1:C:230:ASP:C	1:C:230:ASP:OD1	2.30	0.64
1:D:44:SER:O	1:D:58:ARG:NH2	2.31	0.64
1:A:121:MET:HB2	1:A:210:PRO:HD3	1.78	0.64
1:C:231:LYS:C	1:C:233:LYS:H	2.00	0.63
1:C:46:LYS:NZ	1:C:47:LEU:O	2.32	0.62
1:C:118:LEU:HD11	1:C:208:LEU:HG	1.81	0.62
1:C:210:PRO:HG2	1:C:222:PHE:CZ	2.35	0.61
1:B:58:ARG:NH1	3:B:2006:HOH:O	2.34	0.61
1:B:230:ASP:HB3	1:B:233:LYS:HG3	1.83	0.60
1:D:122:HIS:HE2	2:D:1236:A2G:H3	1.67	0.60
1:D:78:LEU:HD11	1:D:171:THR:HA	1.83	0.60
1:B:192:GLN:HA	1:B:195:ILE:HG22	1.82	0.60
1:A:95:ASN:HD21	2:A:1237:A2G:H3	1.65	0.60
1:B:197:LYS:NZ	1:B:201:ASP:OD2	2.35	0.60
1:D:1:MET:HB2	1:D:34:PHE:CE1	2.37	0.59
1:C:230:ASP:O	1:C:233:LYS:CB	2.50	0.59
1:D:42:THR:HG21	1:D:47:LEU:HD21	1.84	0.58
1:A:143:ALA:HA	1:A:197:LYS:HG3	1.85	0.57
1:C:16:PHE:HB3	1:C:229:ARG:HH21	1.70	0.57
1:C:121:MET:HB2	1:C:210:PRO:HD3	1.87	0.56
1:B:99:LEU:HB2	1:B:229:ARG:HH11	1.70	0.56
1:A:72:LYS:NZ	3:A:2018:HOH:O	2.39	0.55
1:D:189:TRP:HA	1:D:189:TRP:CE3	2.41	0.55
1:D:188:ILE:O	1:D:189:TRP:HB2	2.05	0.55
1:A:45:PRO:O	1:A:58:ARG:NH1	2.39	0.55
1:A:76:ILE:O	1:A:79:ARG:HG2	2.05	0.55
1:A:210:PRO:HG2	1:A:222:PHE:CE2	2.43	0.54
1:C:110:PRO:HB2	1:C:116:GLY:HA2	1.88	0.54
1:A:191:ASP:OD1	1:A:191:ASP:N	2.32	0.54
1:A:37:GLU:OE1	1:A:57:HIS:NE2	2.34	0.53
1:C:86:ARG:HG3	1:C:87:GLU:HG3	1.90	0.52
1:C:233:LYS:HB3	1:C:236:TYR:HE1	1.75	0.52
1:C:92:PHE:HD1	1:C:160:GLY:HA3	1.75	0.52
1:C:118:LEU:HD13	1:C:206:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LYS:HD2	1:D:234:PRO:HD2	1.91	0.51
1:B:151:ARG:HE	1:B:154:TYR:HE1	1.59	0.51
1:C:230:ASP:OD1	1:C:231:LYS:O	2.29	0.50
1:D:191:ASP:OD1	1:D:191:ASP:N	2.45	0.50
1:D:188:ILE:O	1:D:193:SER:OG	2.29	0.50
1:C:50:GLU:OE2	1:C:58:ARG:HD2	2.11	0.50
1:C:230:ASP:O	1:C:230:ASP:OD1	2.30	0.49
1:C:139:ASP:HA	1:C:144:TYR:CG	2.48	0.49
1:C:48:TYR:CD1	1:C:49:ASP:HB2	2.47	0.49
1:A:189:TRP:HD1	1:A:189:TRP:H	1.61	0.48
1:A:214:TYR:CE1	1:B:221:PRO:HB3	2.49	0.48
1:B:86:ARG:HG3	1:B:87:GLU:HG3	1.96	0.48
1:A:110:PRO:HB2	1:A:116:GLY:HA2	1.97	0.47
1:D:80:ILE:HG13	1:D:83:GLN:HB3	1.96	0.47
1:A:188:ILE:HD12	1:A:188:ILE:C	2.24	0.47
1:C:98:LEU:O	1:C:229:ARG:NH1	2.48	0.47
1:C:74:PHE:HD2	1:C:170:CYS:HA	1.81	0.46
1:D:197:LYS:NZ	1:D:201:ASP:OD2	2.48	0.46
1:D:19:ASP:O	1:D:23:SER:HB2	2.15	0.46
1:D:65:GLY:N	1:D:69:ASN:OD1	2.48	0.46
1:A:143:ALA:HB2	1:A:194:LEU:HD13	1.97	0.46
1:C:72:LYS:O	1:C:76:ILE:HG12	2.16	0.46
1:B:48:TYR:CD2	1:B:49:ASP:HB2	2.51	0.45
1:D:188:ILE:O	1:D:189:TRP:CB	2.65	0.45
1:D:1:MET:HB2	1:D:34:PHE:HE1	1.78	0.45
1:A:7:TYR:CE1	1:A:96:ALA:HA	2.52	0.45
1:D:215:PRO:HB2	1:D:218:TRP:CD1	2.52	0.45
1:C:68:ASP:HA	1:C:71:LEU:HB3	1.99	0.45
1:D:220:LEU:HB3	1:D:222:PHE:CE1	2.52	0.45
1:A:149:GLU:HG3	1:A:200:LEU:HD11	1.98	0.45
1:D:1:MET:HB2	1:D:34:PHE:CD1	2.52	0.45
1:B:70:THR:O	1:B:191:ASP:HB3	2.17	0.44
1:C:122:HIS:CE1	2:C:1238:A2G:H8A	2.52	0.44
1:C:231:LYS:C	1:C:233:LYS:N	2.63	0.44
1:C:233:LYS:HB3	1:C:236:TYR:CE1	2.52	0.44
1:C:45:PRO:O	1:C:58:ARG:NH1	2.38	0.44
1:C:5:ILE:HD12	1:C:38:TYR:HE1	1.82	0.44
1:B:151:ARG:NH1	1:B:203:PRO:HB3	2.26	0.44
1:D:173:ILE:HD11	1:D:198:TYR:HB2	1.99	0.44
1:D:215:PRO:HA	1:D:228:ILE:HB	2.00	0.44
1:C:23:SER:HB2	1:C:100:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:TRP:HA	1:D:189:TRP:HE3	1.83	0.44
1:A:155:ALA:HB1	2:A:1237:A2G:O7	2.18	0.44
1:D:180:ASP:HB3	1:D:185:ILE:O	2.18	0.44
1:D:155:ALA:HB1	2:D:1236:A2G:H6	2.00	0.44
1:B:42:THR:HG21	1:B:47:LEU:HD21	1.99	0.44
1:D:182:THR:C	1:D:184:HIS:H	2.21	0.44
1:A:106:LYS:HA	1:A:109:LEU:HD13	2.00	0.43
1:A:59:ILE:HD13	1:A:80:ILE:HD13	2.00	0.43
1:C:99:LEU:HB2	1:C:229:ARG:NH1	2.32	0.43
1:D:189:TRP:O	1:D:192:GLN:HB3	2.18	0.43
1:A:219:LEU:HD21	1:B:126:TYR:CE2	2.54	0.43
1:B:139:ASP:HA	1:B:144:TYR:CG	2.52	0.43
1:C:66:TRP:CE2	1:C:67:PRO:HB3	2.53	0.43
1:B:151:ARG:H	1:B:151:ARG:HG3	1.55	0.43
1:D:37:GLU:CD	1:D:55:HIS:HD1	2.22	0.43
1:A:7:TYR:CZ	1:A:96:ALA:HA	2.54	0.43
1:D:233:LYS:HD3	1:D:233:LYS:HA	1.85	0.43
1:C:5:ILE:HD12	1:C:38:TYR:CE1	2.53	0.42
1:B:72:LYS:O	1:B:76:ILE:HG13	2.18	0.42
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.92	0.42
1:D:110:PRO:HA	1:D:111:PRO:HD3	1.86	0.42
1:D:231:LYS:HG3	1:D:231:LYS:HZ3	1.69	0.42
1:B:12:LYS:HZ1	1:B:13:TYR:HE1	1.65	0.42
1:A:216:GLU:HG3	1:B:222:PHE:HA	2.01	0.42
1:C:169:LEU:HD12	1:C:198:TYR:CE1	2.55	0.42
1:C:5:ILE:HD11	1:C:28:PHE:CE2	2.55	0.42
1:C:90:TYR:CE2	1:C:109:LEU:HD13	2.56	0.41
1:D:234:PRO:HG2	1:D:235:GLN:OE1	2.21	0.41
1:A:10:THR:OG1	1:A:11:GLY:N	2.54	0.40
1:B:188:ILE:HG12	1:B:188:ILE:H	1.65	0.40
1:D:23:SER:OG	1:D:100:PHE:O	2.40	0.40
1:D:37:GLU:OE2	1:D:55:HIS:ND1	2.54	0.40
1:A:14:ASP:N	1:A:14:ASP:OD1	2.54	0.40
1:A:214:TYR:CE2	1:A:220:LEU:HB2	2.56	0.40

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	234/246 (95%)	226 (97%)	7 (3%)	1 (0%)	34	64
1	B	234/246 (95%)	226 (97%)	8 (3%)	0	100	100
1	C	235/246 (96%)	225 (96%)	10 (4%)	0	100	100
1	D	233/246 (95%)	223 (96%)	10 (4%)	0	100	100
All	All	936/984 (95%)	900 (96%)	35 (4%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASN

### 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	213/221 (96%)	206 (97%)	7 (3%)	38	69
1	B	213/221 (96%)	208 (98%)	5 (2%)	50	79
1	C	213/221 (96%)	204 (96%)	9 (4%)	30	60
1	D	212/221 (96%)	202 (95%)	10 (5%)	26	56
All	All	851/884 (96%)	820 (96%)	31 (4%)	35	66

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	64	LEU
1	A	70	THR
1	A	84	LEU
1	A	102	SER
1	A	189	TRP
1	A	192	GLN
1	B	64	LEU
1	B	151	ARG
1	B	185	ILE
1	B	193	SER
1	B	220	LEU
1	C	15	ILE
1	C	22	LEU
1	C	30	GLN
1	C	85	GLU
1	C	158	LEU
1	C	192	GLN
1	C	222	PHE
1	C	231	LYS
1	C	236	TYR
1	D	10	THR
1	D	12	LYS
1	D	23	SER
1	D	31	ASP
1	D	84	LEU
1	D	85	GLU
1	D	158	LEU
1	D	188	ILE
1	D	194	LEU
1	D	222	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	B	192	GLN
1	C	130	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	D	1236	-	15,15,15	0.41	0	21,21,21	0.71	0
2	A2G	C	1238	-	15,15,15	0.45	0	21,21,21	1.86	3 (14%)
2	A2G	B	1237	-	15,15,15	0.53	0	21,21,21	1.53	3 (14%)
2	A2G	A	1237	-	15,15,15	0.56	0	21,21,21	1.74	4 (19%)

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	D	1236	-	-	4/6/26/26	0/1/1/1
2	A2G	C	1238	-	-	4/6/26/26	0/1/1/1
2	A2G	B	1237	-	-	2/6/26/26	0/1/1/1
2	A2G	A	1237	-	-	3/6/26/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	1238	A2G	C1-O5-C5	4.88	122.88	113.66
2	C	1238	A2G	O5-C1-C2	4.62	114.16	109.52
2	B	1237	A2G	O5-C1-C2	4.55	114.09	109.52
2	C	1238	A2G	O5-C5-C4	4.48	117.83	109.69
2	A	1237	A2G	O5-C1-C2	4.26	113.80	109.52
2	A	1237	A2G	C1-C2-C3	4.20	116.27	110.54
2	A	1237	A2G	C4-C3-C2	3.32	115.21	110.34
2	B	1237	A2G	C1-C2-C3	3.24	114.97	110.54
2	A	1237	A2G	C3-C4-C5	2.31	114.36	110.24
2	B	1237	A2G	O5-C5-C6	2.24	112.00	106.44

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1238	A2G	O7-C7-N2-C2
2	C	1238	A2G	C8-C7-N2-C2
2	D	1236	A2G	O7-C7-N2-C2
2	D	1236	A2G	C8-C7-N2-C2
2	D	1236	A2G	C4-C5-C6-O6
2	D	1236	A2G	O5-C5-C6-O6
2	B	1237	A2G	O7-C7-N2-C2
2	B	1237	A2G	C8-C7-N2-C2
2	A	1237	A2G	C8-C7-N2-C2
2	A	1237	A2G	O7-C7-N2-C2
2	C	1238	A2G	C3-C2-N2-C7
2	A	1237	A2G	O5-C5-C6-O6
2	C	1238	A2G	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1236	A2G	2	0
2	C	1238	A2G	1	0
2	A	1237	A2G	5	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	236/246 (95%)	-0.17	0	100 100	15, 28, 46, 65	3 (1%)
1	B	236/246 (95%)	-0.03	0	100 100	16, 34, 58, 80	2 (0%)
1	C	237/246 (96%)	0.27	5 (2%)	63 59	20, 49, 75, 89	3 (1%)
1	D	235/246 (95%)	0.16	2 (0%)	84 82	24, 51, 72, 82	3 (1%)
All	All	944/984 (95%)	0.06	7 (0%)	87 86	15, 39, 68, 89	11 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	ASP	3.1
1	C	32	GLN	2.8
1	D	63	ASN	2.7
1	C	161	GLY	2.5
1	D	64	LEU	2.4
1	C	84	LEU	2.3
1	C	106	LYS	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A2G	D	1236	15/15	0.70	0.33	33,46,61,63	15
2	A2G	C	1238	15/15	0.70	0.39	27,36,43,51	15
2	A2G	A	1237	15/15	0.75	0.37	30,40,46,48	15
2	A2G	B	1237	15/15	0.76	0.33	35,41,52,55	15

## 6.5 Other polymers [i](#)

There are no such residues in this entry.