



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2016 – 11:04 PM EDT

PDB ID : 5JLV  
Title : Receptor binding domain of Botulinum neurotoxin A in complex with human glycosylated SV2C  
Authors : Yao, G.; Zhang, S.; Mahrhold, S.; Lam, K.; Stern, D.; Bagramyan, K.; Perry, K.; Kalkum, M.; Rummel, A.; Dong, M.; Jin, R.  
Deposited on : 2016-04-27  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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-20027939

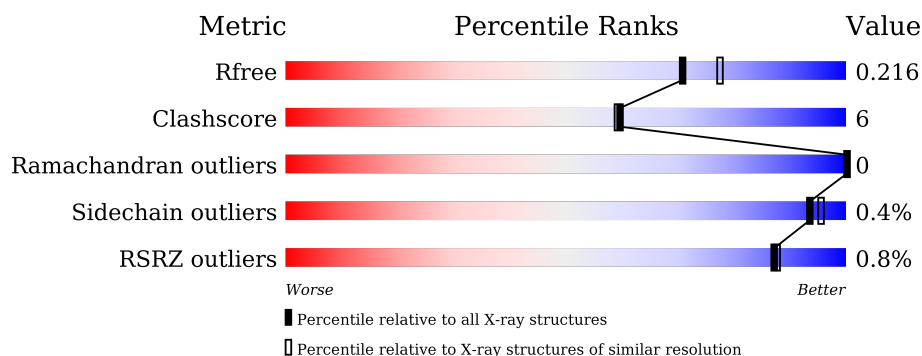
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	428	<div> <div>86%</div> <div>14%</div> <div>.</div> </div>
1	B	428	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	C	117	<div> <div>68%</div> <div>15%</div> <div>17%</div> </div>
2	D	117	<div> <div>69%</div> <div>9%</div> <div>22%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1301	-	-	-	X
4	PO4	A	1303	-	-	X	X
4	PO4	B	1303	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9428 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	3	5	0
			3538	2252	613	659	14			
1	B	425	Total	C	N	O	S	4	3	0
			3527	2246	610	657	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	869	GLY	-	expression tag	UNP P10845
A	870	PRO	-	expression tag	UNP P10845
A	871	MET	-	expression tag	UNP P10845
A	1158	ALA	THR	engineered mutation	UNP P10845
B	869	GLY	-	expression tag	UNP P10845
B	870	PRO	-	expression tag	UNP P10845
B	871	MET	-	expression tag	UNP P10845
B	1158	ALA	THR	engineered mutation	UNP P10845

- Molecule 2 is a protein called Synaptic vesicle glycoprotein 2C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	97	Total	C	N	O	S	0	0	0
			812	521	129	157	5			
2	D	91	Total	C	N	O	S	0	0	0
			764	493	118	148	5			

There are 44 discrepancies between the modelled and reference sequences:

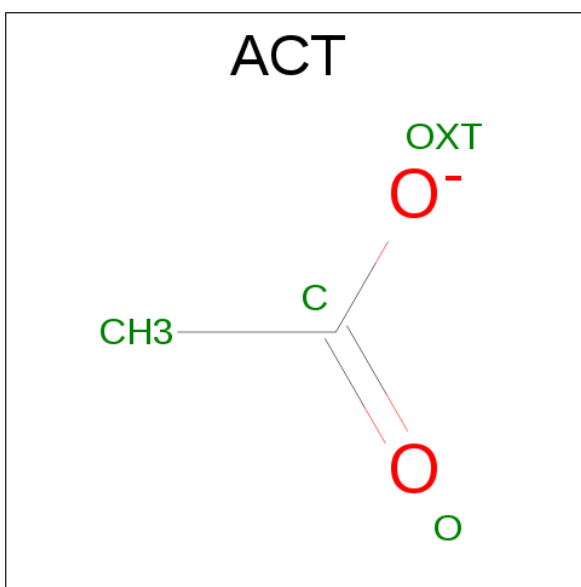
Chain	Residue	Modelled	Actual	Comment	Reference
C	451	SER	-	expression tag	UNP Q496J9
C	452	HIS	-	expression tag	UNP Q496J9
C	453	HIS	-	expression tag	UNP Q496J9
C	454	HIS	-	expression tag	UNP Q496J9

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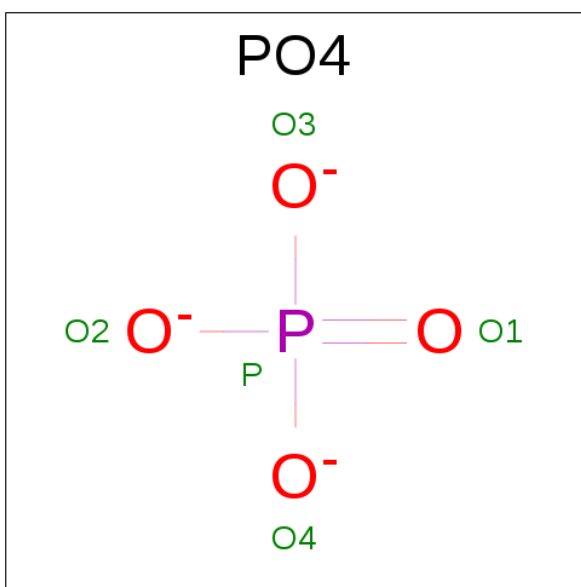
Chain	Residue	Modelled	Actual	Comment	Reference
C	455	HIS	-	expression tag	UNP Q496J9
C	456	HIS	-	expression tag	UNP Q496J9
C	457	HIS	-	expression tag	UNP Q496J9
C	458	HIS	-	expression tag	UNP Q496J9
C	459	HIS	-	expression tag	UNP Q496J9
C	460	HIS	-	expression tag	UNP Q496J9
C	461	SER	-	expression tag	UNP Q496J9
C	462	GLY	-	expression tag	UNP Q496J9
C	463	GLY	-	expression tag	UNP Q496J9
C	464	GLY	-	expression tag	UNP Q496J9
C	465	SER	-	expression tag	UNP Q496J9
C	466	GLY	-	expression tag	UNP Q496J9
C	467	GLY	-	expression tag	UNP Q496J9
C	468	GLY	-	expression tag	UNP Q496J9
C	469	ILE	-	expression tag	UNP Q496J9
C	470	GLU	-	expression tag	UNP Q496J9
C	471	GLY	-	expression tag	UNP Q496J9
C	472	ARG	-	expression tag	UNP Q496J9
D	451	SER	-	expression tag	UNP Q496J9
D	452	HIS	-	expression tag	UNP Q496J9
D	453	HIS	-	expression tag	UNP Q496J9
D	454	HIS	-	expression tag	UNP Q496J9
D	455	HIS	-	expression tag	UNP Q496J9
D	456	HIS	-	expression tag	UNP Q496J9
D	457	HIS	-	expression tag	UNP Q496J9
D	458	HIS	-	expression tag	UNP Q496J9
D	459	HIS	-	expression tag	UNP Q496J9
D	460	HIS	-	expression tag	UNP Q496J9
D	461	SER	-	expression tag	UNP Q496J9
D	462	GLY	-	expression tag	UNP Q496J9
D	463	GLY	-	expression tag	UNP Q496J9
D	464	GLY	-	expression tag	UNP Q496J9
D	465	SER	-	expression tag	UNP Q496J9
D	466	GLY	-	expression tag	UNP Q496J9
D	467	GLY	-	expression tag	UNP Q496J9
D	468	GLY	-	expression tag	UNP Q496J9
D	469	ILE	-	expression tag	UNP Q496J9
D	470	GLU	-	expression tag	UNP Q496J9
D	471	GLY	-	expression tag	UNP Q496J9
D	472	ARG	-	expression tag	UNP Q496J9

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



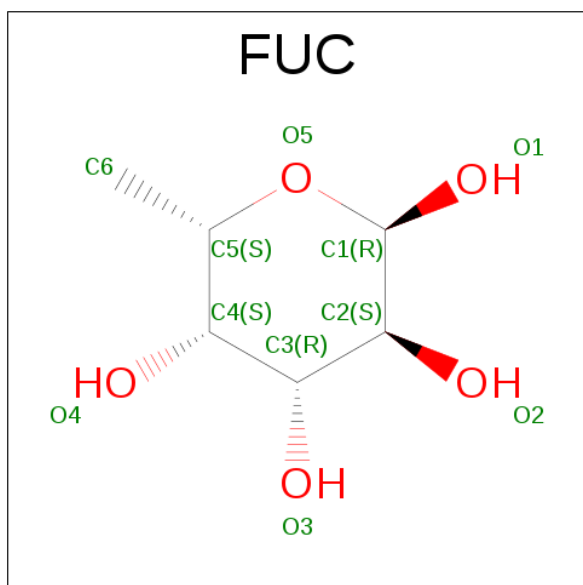
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

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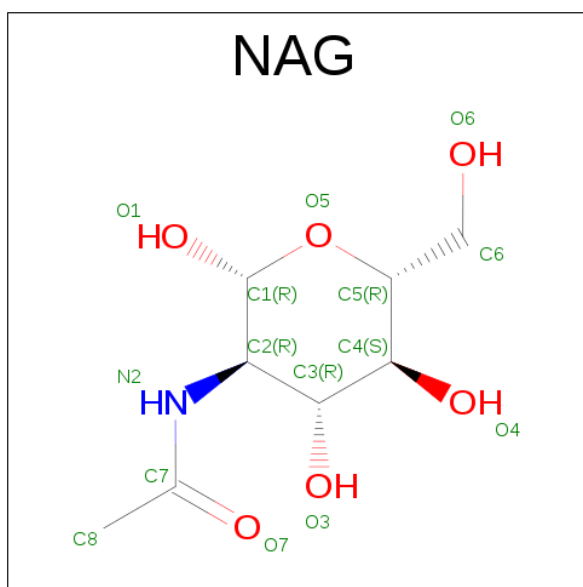
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



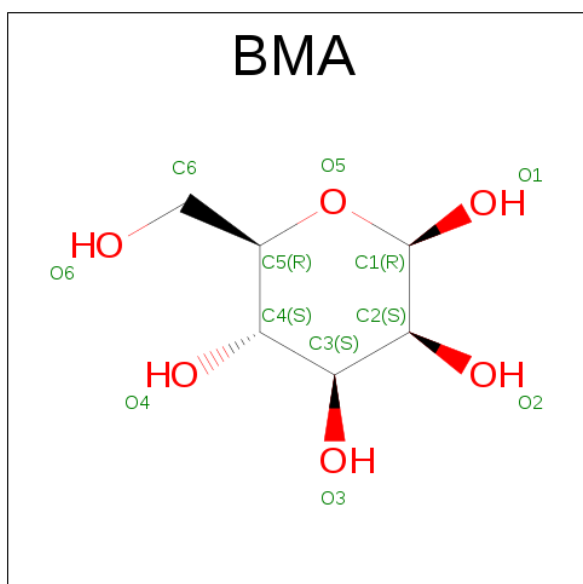
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).





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

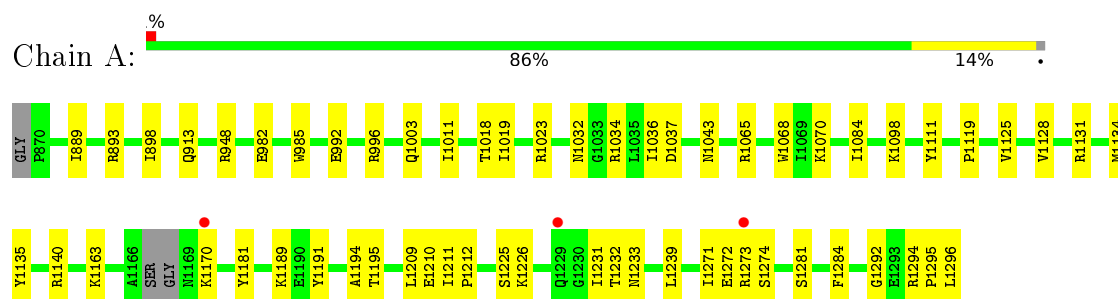
- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	276	Total	O		0	0
			276	276			
8	B	270	Total	O		0	0
			270	270			
8	C	81	Total	O		0	0
			81	81			
8	D	32	Total	O		0	0
			32	32			

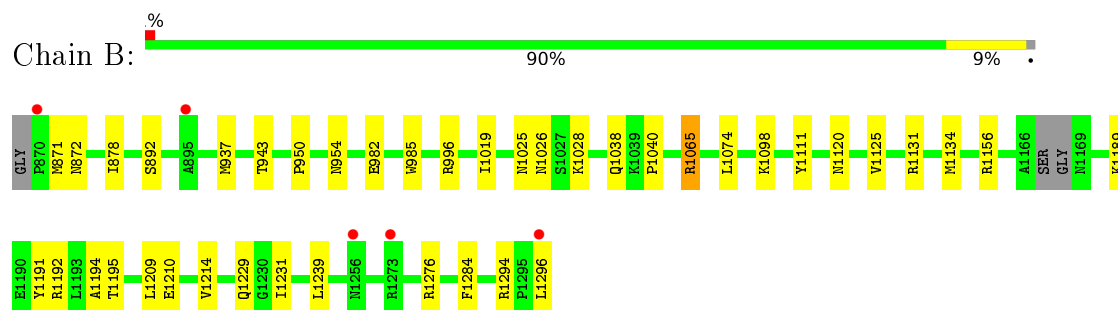
### 3 Residue-property plots [i](#)

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.

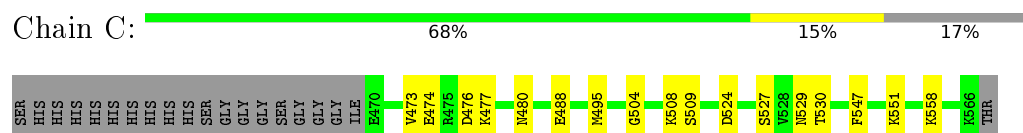
#### • Molecule 1: Botulinum neurotoxin type A



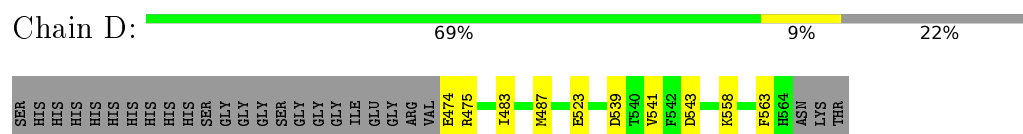
#### • Molecule 1: Botulinum neurotoxin type A



#### • Molecule 2: Synaptic vesicle glycoprotein 2C



#### • Molecule 2: Synaptic vesicle glycoprotein 2C



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.00Å 111.85Å 126.25Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	123.81 – 2.00 123.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (123.81-2.00) 93.8 (123.81-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.175 , 0.216 0.177 , 0.216	Depositor DCC
$R_{free}$ test set	4675 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.5	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	0.96	EDS
Total number of atoms	9428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: ACT, PO4, BMA, NAG, FUC

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	0.48	0/3614	0.54	0/4885
1	B	0.43	0/3600	0.53	0/4866
2	C	0.47	0/833	0.51	0/1119
2	D	0.39	0/785	0.44	0/1056
All	All	0.45	0/8832	0.53	0/11926

There are no bond length outliers.

There are no bond angle outliers.

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	3538	0	3498	49	0
1	B	3527	0	3486	30	0
2	C	812	0	749	11	0
2	D	764	0	700	10	0
3	A	4	0	3	1	0
3	B	8	0	6	1	0
4	A	10	0	0	5	0
4	B	5	0	0	4	0
5	C	10	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	10	0	0
6	C	42	0	36	1	0
6	D	28	0	24	4	0
7	C	11	0	10	0	0
8	A	276	0	0	16	0
8	B	270	0	0	9	0
8	C	81	0	0	3	0
8	D	32	0	0	0	0
All	All	9428	0	8532	99	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 (99) 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:1294:ARG:HG2	8:A:1430:HOH:O	1.72	0.89
1:A:996:ARG:HH22	4:A:1303:PO4:P	1.97	0.87
1:B:996:ARG:NH2	4:B:1303:PO4:O2	2.07	0.87
1:B:996:ARG:HH22	4:B:1303:PO4:P	2.07	0.76
2:C:476:ASP:HA	8:C:733:HOH:O	1.88	0.74
2:C:495:MET:SD	8:C:733:HOH:O	2.46	0.74
1:B:1156:ARG:NH1	8:B:1401:HOH:O	2.22	0.73
1:B:1276:ARG:HE	3:B:1301:ACT:H3	1.53	0.73
1:A:996:ARG:NH2	4:A:1303:PO4:O4	2.22	0.69
1:A:1037:ASP:HB2	8:A:1515:HOH:O	1.93	0.68
1:A:982:GLU:OE1	4:A:1303:PO4:O3	2.12	0.67
1:A:1119:PRO:O	1:A:1140:ARG:HD2	1.96	0.66
1:B:872:ASN:ND2	8:B:1405:HOH:O	2.28	0.66
3:A:1301:ACT:H3	8:A:1562:HOH:O	1.96	0.64
1:A:1135:TYR:OH	8:A:1401:HOH:O	2.14	0.62
1:A:996:ARG:NH2	4:A:1303:PO4:O1	2.33	0.61
1:A:1170:LYS:HB2	8:A:1664:HOH:O	1.99	0.61
1:A:1034:ARG:NH1	8:A:1404:HOH:O	2.34	0.61
2:D:483:ILE:HG21	2:D:487:MET:HE2	1.85	0.59
2:D:558:LYS:HD3	6:D:602:NAG:C8	2.33	0.58
1:B:950:PRO:O	1:B:1065:ARG:NH2	2.35	0.58
1:A:1098:LYS:NZ	8:A:1405:HOH:O	2.36	0.58
1:A:996:ARG:NH2	4:A:1303:PO4:P	2.75	0.58
1:A:1098:LYS:HB2	1:A:1233:ASN:HB3	1.87	0.57
1:A:1037:ASP:HB2	8:A:1639:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:LEU:HG	8:A:1430:HOH:O	2.04	0.57
1:B:1195:THR:HG22	1:B:1239:LEU:HD21	1.86	0.57
1:A:889:ILE:HA	1:A:898:ILE:HD13	1.87	0.56
1:A:1098:LYS:HG3	1:A:1231:ILE:HG23	1.86	0.56
1:B:871:MET:HA	8:B:1432:HOH:O	2.04	0.56
2:C:480:ASN:HB2	8:C:752:HOH:O	2.05	0.56
2:D:523:GLU:HA	2:D:543:ASP:O	2.05	0.56
1:B:1191:TYR:HE1	1:B:1210:GLU:OE2	1.89	0.56
2:D:558:LYS:HB3	6:D:602:NAG:H82	1.88	0.56
1:A:1272:GLU:O	1:A:1273:ARG:HB2	2.06	0.55
1:B:982:GLU:OE1	4:B:1303:PO4:O1	2.24	0.55
1:B:1229:GLN:HA	8:B:1402:HOH:O	2.08	0.54
1:A:1271:ILE:O	1:A:1274:SER:HB3	2.09	0.53
2:D:483:ILE:HG21	2:D:487:MET:CE	2.39	0.53
1:B:985:TRP:CD2	1:B:1019:ILE:HG21	2.44	0.52
1:A:992:GLU:HA	1:A:992:GLU:OE1	2.09	0.52
2:D:558:LYS:HD3	6:D:602:NAG:H82	1.92	0.51
1:B:954:ASN:HB2	8:B:1636:HOH:O	2.11	0.51
1:A:1043[A]:ASN:ND2	8:A:1411:HOH:O	2.43	0.49
1:A:1292:GLY:HA2	5:C:601:FUC:O5	2.13	0.49
1:B:1026:ASN:OD1	1:B:1040:PRO:HA	2.12	0.49
1:B:878:ILE:HG13	1:B:1074:LEU:HB3	1.95	0.49
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.47	0.48
1:A:1225:SER:CB	1:A:1232:THR:CG2	2.90	0.48
1:A:1189:LYS:NZ	1:A:1210:GLU:OE2	2.43	0.48
1:A:1163:LYS:HB2	1:A:1181:TYR:HB2	1.96	0.47
2:C:474:GLU:HB2	2:C:477:LYS:HG2	1.97	0.47
1:B:1120:ASN:HB3	8:B:1645:HOH:O	2.15	0.47
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.50	0.47
1:B:1189:LYS:NZ	8:B:1417:HOH:O	2.48	0.47
1:A:1131[A]:ARG:HA	1:A:1131[A]:ARG:HD3	1.55	0.46
1:B:1131:ARG:HD2	8:B:1505:HOH:O	2.13	0.46
2:C:488:GLU:HG3	2:C:508:LYS:HB2	1.98	0.46
1:A:1036:ILE:HG22	8:A:1515:HOH:O	2.16	0.46
2:C:547:PHE:HA	2:C:551:LYS:HG3	1.97	0.46
1:B:1028:LYS:HG2	1:B:1038:GLN:HB3	1.98	0.46
1:B:996:ARG:NH2	4:B:1303:PO4:P	2.82	0.45
1:A:1226:LYS:HD2	1:A:1281:SER:OG	2.16	0.45
1:B:1098:LYS:HD2	1:B:1231:ILE:HG23	1.98	0.45
1:B:1192:ARG:HG2	1:B:1214:VAL:HG11	1.98	0.45
1:B:1296:LEU:HD11	2:D:541:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:THR:HB	1:B:1074:LEU:HD12	1.97	0.45
1:B:1194:ALA:HB3	1:B:1209:LEU:HD12	1.99	0.45
2:C:473:VAL:HG13	2:C:474:GLU:HG3	1.98	0.45
1:A:1194:ALA:HB3	1:A:1209:LEU:HD23	1.99	0.45
1:B:1125:VAL:HG22	1:B:1134:MET:HG2	1.99	0.44
1:A:1070:LYS:HD2	8:A:1424:HOH:O	2.18	0.44
1:A:1128:VAL:HG11	1:A:1191:TYR:CE1	2.53	0.44
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.99	0.44
1:A:1032:ASN:HB2	1:A:1034:ARG:HH12	1.83	0.43
1:B:1294:ARG:HD3	2:D:539:ASP:O	2.18	0.43
1:B:1025:ASN:OD1	1:B:1026:ASN:ND2	2.52	0.43
2:D:474:GLU:HG2	2:D:475:ARG:H	1.84	0.43
1:A:985:TRP:CG	1:A:1019:ILE:HG21	2.54	0.43
1:A:893:ARG:NE	8:A:1420:HOH:O	2.51	0.43
1:A:1195:THR:HG22	1:A:1239:LEU:HD21	2.01	0.42
1:A:1125:VAL:HG22	1:A:1134:MET:HG2	2.01	0.42
1:B:1111:TYR:CG	1:B:1284:PHE:HB3	2.54	0.42
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	2.02	0.42
2:C:509:SER:HA	2:C:529:ASN:O	2.20	0.41
1:A:1211:ILE:N	1:A:1212:PRO:HD2	2.36	0.41
2:C:504:GLY:HA2	2:C:524:ASP:O	2.21	0.41
1:A:1070:LYS:CD	8:A:1424:HOH:O	2.69	0.41
2:C:558:LYS:HB3	6:C:602:NAG:H82	2.02	0.41
1:A:1018:THR:HG21	1:A:1084:ILE:HG12	2.03	0.41
2:D:558:LYS:CD	6:D:602:NAG:H82	2.51	0.41
1:A:1189:LYS:HE2	1:A:1210:GLU:OE2	2.20	0.40
1:B:892:SER:HA	8:B:1578:HOH:O	2.21	0.40
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	2.02	0.40
2:C:527:SER:HB2	2:C:530:THR:HB	2.03	0.40
1:A:1023:ARG:HB2	8:A:1494:HOH:O	2.22	0.40
1:A:1070:LYS:NZ	8:A:1424:HOH:O	2.53	0.40
1:A:1225:SER:HB2	1:A:1232:THR:CG2	2.51	0.40
1:A:1294:ARG:HA	1:A:1295:PRO:HD3	1.93	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	426/428 (100%)	408 (96%)	18 (4%)	0	100	100
1	B	424/428 (99%)	405 (96%)	19 (4%)	0	100	100
2	C	95/117 (81%)	94 (99%)	1 (1%)	0	100	100
2	D	89/117 (76%)	88 (99%)	1 (1%)	0	100	100
All	All	1034/1090 (95%)	995 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	397/393 (101%)	396 (100%)	1 (0%)	94	96
1	B	395/393 (100%)	393 (100%)	2 (0%)	92	94
2	C	92/106 (87%)	92 (100%)	0	100	100
2	D	87/106 (82%)	86 (99%)	1 (1%)	80	83
All	All	971/998 (97%)	967 (100%)	4 (0%)	93	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1065	ARG
1	B	937	MET

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Mol	Chain	Res	Type
1	B	1065	ARG
2	D	563	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1106	GLN
1	B	1172	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

14 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	$\# Z  > 2$
3	ACT	A	1301	-	0,3,3	0.00	-	0,3,3	0.00	-
4	PO4	A	1302	-	4,4,4	0.45	0	6,6,6	0.25	0
4	PO4	A	1303	-	4,4,4	2.25	3 (75%)	6,6,6	0.23	0
3	ACT	B	1301	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	B	1302	-	0,3,3	0.00	-	0,3,3	0.00	-
4	PO4	B	1303	-	4,4,4	2.25	3 (75%)	6,6,6	0.23	0
5	FUC	C	601	6	10,10,11	0.30	0	13,14,16	0.77	0
6	NAG	C	602	2,5,6	14,14,15	0.29	0	15,19,21	0.53	0
6	NAG	C	603	7,6	14,14,15	0.27	0	15,19,21	0.54	0
7	BMA	C	604	6	11,11,12	0.26	0	15,15,17	0.59	0
6	NAG	C	605	2	14,14,15	0.29	0	15,19,21	0.54	0
5	FUC	D	601	6	10,10,11	0.30	0	13,14,16	0.78	0
6	NAG	D	602	2,5,6	14,14,15	0.27	0	15,19,21	0.54	0
6	NAG	D	603	6	14,14,15	0.28	0	15,19,21	0.53	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
3	ACT	A	1301	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1302	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1303	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1301	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1302	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1303	-	-	0/0/0/0	0/0/0/0
5	FUC	C	601	6	-	0/0/17/20	0/1/1/1
6	NAG	C	602	2,5,6	-	0/6/23/26	0/1/1/1
6	NAG	C	603	7,6	-	0/6/23/26	0/1/1/1
7	BMA	C	604	6	-	0/2/19/22	0/1/1/1
6	NAG	C	605	2	-	0/6/23/26	0/1/1/1
5	FUC	D	601	6	-	0/0/17/20	0/1/1/1
6	NAG	D	602	2,5,6	-	0/6/23/26	0/1/1/1
6	NAG	D	603	6	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1303	PO4	P-O1	2.21	1.61	1.53
4	A	1303	PO4	P-O1	2.21	1.61	1.53
4	B	1303	PO4	P-O2	2.48	1.61	1.53
4	A	1303	PO4	P-O2	2.48	1.61	1.53
4	B	1303	PO4	P-O3	2.50	1.61	1.53
4	A	1303	PO4	P-O3	2.50	1.61	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	ACT	1	0
4	A	1303	PO4	5	0
3	B	1301	ACT	1	0
4	B	1303	PO4	4	0
5	C	601	FUC	1	0
6	C	602	NAG	1	0
6	D	602	NAG	4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	425/428 (99%)	-0.21	3 (0%) 89 89	19, 38, 68, 105	1 (0%)
1	B	425/428 (99%)	-0.20	5 (1%) 81 81	20, 42, 77, 104	1 (0%)
2	C	97/117 (82%)	-0.30	0 100 100	27, 42, 67, 83	0
2	D	91/117 (77%)	0.06	0 100 100	32, 58, 81, 115	0
All	All	1038/1090 (95%)	-0.19	8 (0%) 87 88	19, 41, 75, 115	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1273	ARG	4.6
1	B	1296	LEU	4.2
1	A	1229	GLN	3.2
1	A	1170	LYS	2.5
1	B	1256	ASN	2.2
1	B	870	PRO	2.1
1	B	895	ALA	2.0
1	B	1273	ARG	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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	A	1303	5/5	0.89	0.24	5.38	81,109,143,149	0
3	ACT	A	1301	4/4	0.82	0.21	3.71	53,59,66,68	0
3	ACT	B	1302	4/4	0.67	0.21	1.78	64,75,76,84	0
6	NAG	C	603	14/15	0.96	0.13	1.08	32,38,57,84	0
4	PO4	A	1302	5/5	0.94	0.11	0.56	43,51,56,76	0
6	NAG	D	602	14/15	0.92	0.12	0.53	36,41,46,49	0
5	FUC	D	601	10/11	0.96	0.10	0.11	41,52,57,62	0
3	ACT	B	1301	4/4	0.92	0.10	-0.53	45,49,53,57	0
5	FUC	C	601	10/11	0.96	0.09	-0.56	32,37,42,45	0
6	NAG	D	603	14/15	0.93	0.09	-0.70	37,43,60,70	0
6	NAG	C	602	14/15	0.95	0.09	-0.76	30,37,46,46	0
6	NAG	C	605	14/15	0.85	0.22	-	63,82,90,93	0
7	BMA	C	604	11/12	0.92	0.19	-	56,72,81,88	1
4	PO4	B	1303	5/5	0.84	0.22	-	105,112,130,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.