



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 03:53 AM EST

PDB ID : 6EGU  
Title : Structure of RVFV envelope protein Gc in postfusion conformation in complex with 1,2-dipropionyl-sn-glycero-3-phosphocholine  
Authors : GUARDADO-CALVO, P.; REY, F.A.  
Deposited on : unknown  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

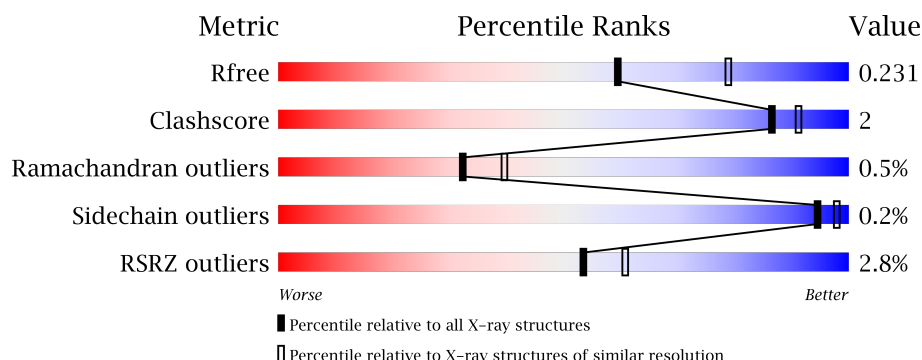
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	531	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>5%</div> <div>17%</div> </div> </div>
1	B	531	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>17%</div> </div> </div>
1	C	531	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>5%</div> <div>16%</div> </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	NAG	A	1303	-	-	-	X
2	NAG	B	1303	-	-	-	X
4	43Y	A	1305	X	-	-	X
4	43Y	B	1305	X	-	-	X
4	43Y	C	1303	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11294 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 RVFV ENVELOPE PROTEIN GC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3368	2087	581	671	29			
1	B	440	Total	C	N	O	S	0	2	0
			3354	2078	580	667	29			
1	C	444	Total	C	N	O	S	0	1	0
			3381	2095	583	674	29			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	821	HIS	TRP	engineered mutation	UNP A2T087
A	1159	ASP	-	expression tag	UNP A2T087
A	1160	PRO	-	expression tag	UNP A2T087
A	1161	THR	-	expression tag	UNP A2T087
A	1162	GLY	-	expression tag	UNP A2T087
A	1163	ASP	-	expression tag	UNP A2T087
A	1164	TYR	-	expression tag	UNP A2T087
A	1165	LYS	-	expression tag	UNP A2T087
A	1166	ASP	-	expression tag	UNP A2T087
A	1167	ASP	-	expression tag	UNP A2T087
A	1168	ASP	-	expression tag	UNP A2T087
A	1169	ASP	-	expression tag	UNP A2T087
A	1170	ALA	-	expression tag	UNP A2T087
A	1171	GLY	-	expression tag	UNP A2T087
A	1172	PRO	-	expression tag	UNP A2T087
A	1173	GLY	-	expression tag	UNP A2T087
A	1174	TRP	-	expression tag	UNP A2T087
A	1175	SER	-	expression tag	UNP A2T087
A	1176	HIS	-	expression tag	UNP A2T087
A	1177	PRO	-	expression tag	UNP A2T087
A	1178	GLN	-	expression tag	UNP A2T087
A	1179	PHE	-	expression tag	UNP A2T087
A	1180	GLU	-	expression tag	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1181	LYS	-	expression tag	UNP A2T087
A	1182	GLY	-	expression tag	UNP A2T087
A	1183	GLY	-	expression tag	UNP A2T087
A	1184	GLY	-	expression tag	UNP A2T087
A	1185	SER	-	expression tag	UNP A2T087
A	1186	GLY	-	expression tag	UNP A2T087
A	1187	GLY	-	expression tag	UNP A2T087
A	1188	GLY	-	expression tag	UNP A2T087
A	1189	SER	-	expression tag	UNP A2T087
A	1190	GLY	-	expression tag	UNP A2T087
A	1191	GLY	-	expression tag	UNP A2T087
A	1192	GLY	-	expression tag	UNP A2T087
A	1193	SER	-	expression tag	UNP A2T087
A	1194	TRP	-	expression tag	UNP A2T087
A	1195	SER	-	expression tag	UNP A2T087
A	1196	HIS	-	expression tag	UNP A2T087
A	1197	PRO	-	expression tag	UNP A2T087
A	1198	GLN	-	expression tag	UNP A2T087
A	1199	PHE	-	expression tag	UNP A2T087
A	1200	GLU	-	expression tag	UNP A2T087
A	1201	LYS	-	expression tag	UNP A2T087
A	1202	GLY	-	expression tag	UNP A2T087
A	1203	GLY	-	expression tag	UNP A2T087
A	1204	GLY	-	expression tag	UNP A2T087
A	1205	SER	-	expression tag	UNP A2T087
A	1206	GLY	-	expression tag	UNP A2T087
A	1207	GLY	-	expression tag	UNP A2T087
A	1208	GLY	-	expression tag	UNP A2T087
A	1209	SER	-	expression tag	UNP A2T087
A	1210	GLY	-	expression tag	UNP A2T087
A	1211	GLY	-	expression tag	UNP A2T087
A	1212	GLY	-	expression tag	UNP A2T087
A	1213	SER	-	expression tag	UNP A2T087
A	1214	TRP	-	expression tag	UNP A2T087
A	1215	SER	-	expression tag	UNP A2T087
A	1216	HIS	-	expression tag	UNP A2T087
A	1217	PRO	-	expression tag	UNP A2T087
A	1218	GLN	-	expression tag	UNP A2T087
A	1219	PHE	-	expression tag	UNP A2T087
A	1220	GLU	-	expression tag	UNP A2T087
A	1221	LYS	-	expression tag	UNP A2T087
B	821	HIS	TRP	engineered mutation	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1159	ASP	-	expression tag	UNP A2T087
B	1160	PRO	-	expression tag	UNP A2T087
B	1161	THR	-	expression tag	UNP A2T087
B	1162	GLY	-	expression tag	UNP A2T087
B	1163	ASP	-	expression tag	UNP A2T087
B	1164	TYR	-	expression tag	UNP A2T087
B	1165	LYS	-	expression tag	UNP A2T087
B	1166	ASP	-	expression tag	UNP A2T087
B	1167	ASP	-	expression tag	UNP A2T087
B	1168	ASP	-	expression tag	UNP A2T087
B	1169	ASP	-	expression tag	UNP A2T087
B	1170	ALA	-	expression tag	UNP A2T087
B	1171	GLY	-	expression tag	UNP A2T087
B	1172	PRO	-	expression tag	UNP A2T087
B	1173	GLY	-	expression tag	UNP A2T087
B	1174	TRP	-	expression tag	UNP A2T087
B	1175	SER	-	expression tag	UNP A2T087
B	1176	HIS	-	expression tag	UNP A2T087
B	1177	PRO	-	expression tag	UNP A2T087
B	1178	GLN	-	expression tag	UNP A2T087
B	1179	PHE	-	expression tag	UNP A2T087
B	1180	GLU	-	expression tag	UNP A2T087
B	1181	LYS	-	expression tag	UNP A2T087
B	1182	GLY	-	expression tag	UNP A2T087
B	1183	GLY	-	expression tag	UNP A2T087
B	1184	GLY	-	expression tag	UNP A2T087
B	1185	SER	-	expression tag	UNP A2T087
B	1186	GLY	-	expression tag	UNP A2T087
B	1187	GLY	-	expression tag	UNP A2T087
B	1188	GLY	-	expression tag	UNP A2T087
B	1189	SER	-	expression tag	UNP A2T087
B	1190	GLY	-	expression tag	UNP A2T087
B	1191	GLY	-	expression tag	UNP A2T087
B	1192	GLY	-	expression tag	UNP A2T087
B	1193	SER	-	expression tag	UNP A2T087
B	1194	TRP	-	expression tag	UNP A2T087
B	1195	SER	-	expression tag	UNP A2T087
B	1196	HIS	-	expression tag	UNP A2T087
B	1197	PRO	-	expression tag	UNP A2T087
B	1198	GLN	-	expression tag	UNP A2T087
B	1199	PHE	-	expression tag	UNP A2T087
B	1200	GLU	-	expression tag	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1201	LYS	-	expression tag	UNP A2T087
B	1202	GLY	-	expression tag	UNP A2T087
B	1203	GLY	-	expression tag	UNP A2T087
B	1204	GLY	-	expression tag	UNP A2T087
B	1205	SER	-	expression tag	UNP A2T087
B	1206	GLY	-	expression tag	UNP A2T087
B	1207	GLY	-	expression tag	UNP A2T087
B	1208	GLY	-	expression tag	UNP A2T087
B	1209	SER	-	expression tag	UNP A2T087
B	1210	GLY	-	expression tag	UNP A2T087
B	1211	GLY	-	expression tag	UNP A2T087
B	1212	GLY	-	expression tag	UNP A2T087
B	1213	SER	-	expression tag	UNP A2T087
B	1214	TRP	-	expression tag	UNP A2T087
B	1215	SER	-	expression tag	UNP A2T087
B	1216	HIS	-	expression tag	UNP A2T087
B	1217	PRO	-	expression tag	UNP A2T087
B	1218	GLN	-	expression tag	UNP A2T087
B	1219	PHE	-	expression tag	UNP A2T087
B	1220	GLU	-	expression tag	UNP A2T087
B	1221	LYS	-	expression tag	UNP A2T087
C	821	HIS	TRP	engineered mutation	UNP A2T087
C	1159	ASP	-	expression tag	UNP A2T087
C	1160	PRO	-	expression tag	UNP A2T087
C	1161	THR	-	expression tag	UNP A2T087
C	1162	GLY	-	expression tag	UNP A2T087
C	1163	ASP	-	expression tag	UNP A2T087
C	1164	TYR	-	expression tag	UNP A2T087
C	1165	LYS	-	expression tag	UNP A2T087
C	1166	ASP	-	expression tag	UNP A2T087
C	1167	ASP	-	expression tag	UNP A2T087
C	1168	ASP	-	expression tag	UNP A2T087
C	1169	ASP	-	expression tag	UNP A2T087
C	1170	ALA	-	expression tag	UNP A2T087
C	1171	GLY	-	expression tag	UNP A2T087
C	1172	PRO	-	expression tag	UNP A2T087
C	1173	GLY	-	expression tag	UNP A2T087
C	1174	TRP	-	expression tag	UNP A2T087
C	1175	SER	-	expression tag	UNP A2T087
C	1176	HIS	-	expression tag	UNP A2T087
C	1177	PRO	-	expression tag	UNP A2T087
C	1178	GLN	-	expression tag	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	PHE	-	expression tag	UNP A2T087
C	1180	GLU	-	expression tag	UNP A2T087
C	1181	LYS	-	expression tag	UNP A2T087
C	1182	GLY	-	expression tag	UNP A2T087
C	1183	GLY	-	expression tag	UNP A2T087
C	1184	GLY	-	expression tag	UNP A2T087
C	1185	SER	-	expression tag	UNP A2T087
C	1186	GLY	-	expression tag	UNP A2T087
C	1187	GLY	-	expression tag	UNP A2T087
C	1188	GLY	-	expression tag	UNP A2T087
C	1189	SER	-	expression tag	UNP A2T087
C	1190	GLY	-	expression tag	UNP A2T087
C	1191	GLY	-	expression tag	UNP A2T087
C	1192	GLY	-	expression tag	UNP A2T087
C	1193	SER	-	expression tag	UNP A2T087
C	1194	TRP	-	expression tag	UNP A2T087
C	1195	SER	-	expression tag	UNP A2T087
C	1196	HIS	-	expression tag	UNP A2T087
C	1197	PRO	-	expression tag	UNP A2T087
C	1198	GLN	-	expression tag	UNP A2T087
C	1199	PHE	-	expression tag	UNP A2T087
C	1200	GLU	-	expression tag	UNP A2T087
C	1201	LYS	-	expression tag	UNP A2T087
C	1202	GLY	-	expression tag	UNP A2T087
C	1203	GLY	-	expression tag	UNP A2T087
C	1204	GLY	-	expression tag	UNP A2T087
C	1205	SER	-	expression tag	UNP A2T087
C	1206	GLY	-	expression tag	UNP A2T087
C	1207	GLY	-	expression tag	UNP A2T087
C	1208	GLY	-	expression tag	UNP A2T087
C	1209	SER	-	expression tag	UNP A2T087
C	1210	GLY	-	expression tag	UNP A2T087
C	1211	GLY	-	expression tag	UNP A2T087
C	1212	GLY	-	expression tag	UNP A2T087
C	1213	SER	-	expression tag	UNP A2T087
C	1214	TRP	-	expression tag	UNP A2T087
C	1215	SER	-	expression tag	UNP A2T087
C	1216	HIS	-	expression tag	UNP A2T087
C	1217	PRO	-	expression tag	UNP A2T087
C	1218	GLN	-	expression tag	UNP A2T087
C	1219	PHE	-	expression tag	UNP A2T087
C	1220	GLU	-	expression tag	UNP A2T087

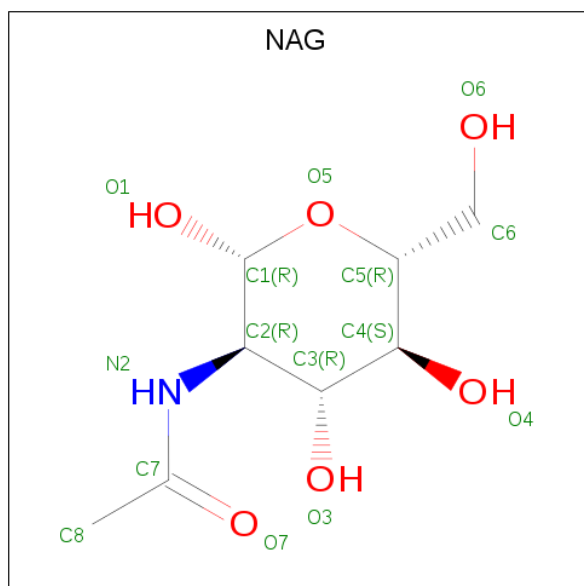
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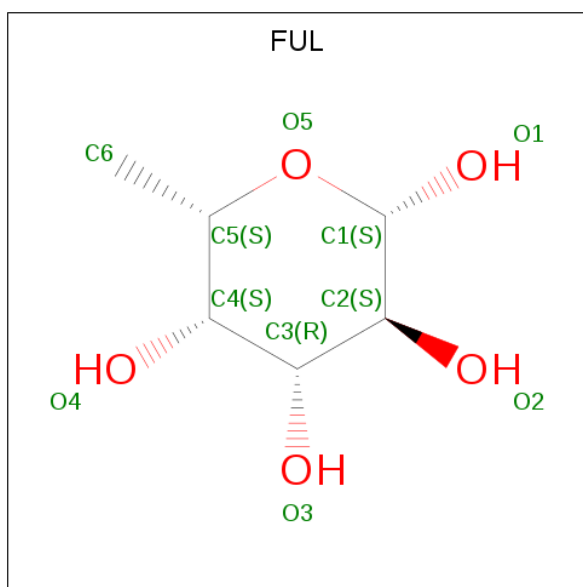
Chain	Residue	Modelled	Actual	Comment	Reference
C	1221	LYS	-	expression tag	UNP A2T087

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



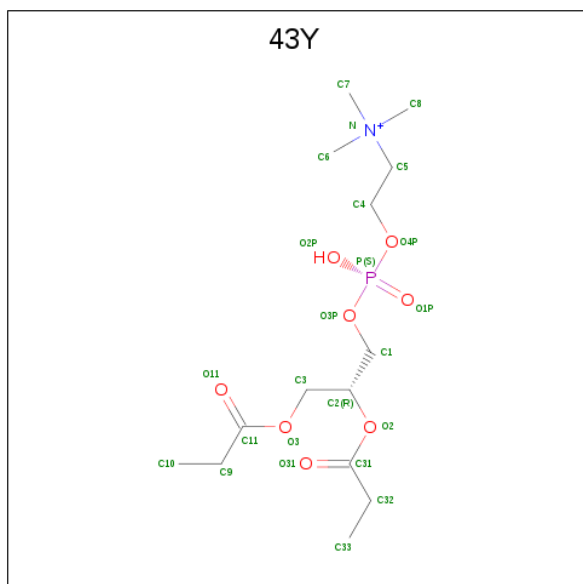
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

- Molecule 3 is BETA-L-FUCOSE (three-letter code: FUL) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is [(2R)-3-[oxidanyl-[2-(trimethyl- $\text{N}^{\{4\}}$ -azanyl)ethoxy]phosphoryl]oxy-2-propa noyloxy-propyl] propanoate (three-letter code: 43Y) (formula:  $\text{C}_{14}\text{H}_{29}\text{NO}_8\text{P}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			24	14	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			19	11	1	6	1		
4	C	1	Total	C	N	O	P	0	0
			24	14	1	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	356	Total	O	0	0
			356	356		
5	B	330	Total	O	0	0
			330	330		
5	C	306	Total	O	0	0
			306	306		



HIS PRO GLN PHE GLU LYS GLY GLY GLY SER SER GLY GLY GLY GLY SER TRP TRP HIS HIS PRO PRO GLN PHE GLU LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.57Å 195.73Å 65.50Å 90.00° 113.96° 90.00°	Depositor
Resolution (Å)	37.88 – 2.30 37.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.88-2.30) 99.9 (37.88-2.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.180 , 0.232 0.178 , 0.231	Depositor DCC
$R_{free}$ test set	3305 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: FUL, NAG, 43Y

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	0.27	0/3428	0.43	0/4631
1	B	0.27	0/3419	0.43	0/4618
1	C	0.26	0/3441	0.42	0/4649
All	All	0.27	0/10288	0.43	0/13898

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	3368	0	3235	14	0
1	B	3354	0	3227	20	0
1	C	3381	0	3249	14	0
2	A	42	0	38	0	0
2	B	42	0	38	1	0
2	C	28	0	26	0	0
3	A	10	0	10	0	0
3	B	10	0	10	1	0
4	A	24	0	29	3	0
4	B	19	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	24	0	29	3	0
5	A	356	0	0	1	0
5	B	330	0	0	0	0
5	C	306	0	0	1	0
All	All	11294	0	9913	50	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 2.

All (50) 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:B:1030:ASP:OD1	1:B:1106:ARG:NH2	2.25	0.68
1:A:785:VAL:HG13	1:A:786:ASN:H	1.57	0.67
1:C:861:LEU:HD12	1:C:873:ILE:HD11	1.76	0.67
1:B:735:LYS:HE3	1:B:1021:ASP:HA	1.79	0.65
1:C:1029:CYS:O	1:C:1106:ARG:NH2	2.31	0.63
1:A:757:ARG:HB2	1:A:854:ASP:HB2	1.82	0.61
1:B:693:GLU:O	1:B:722[A]:ARG:NH1	2.35	0.60
1:B:785:VAL:HG13	1:B:786:ASN:H	1.68	0.59
1:B:700:ARG:HH21	1:B:737:VAL:HG13	1.69	0.57
1:B:776:ARG:HD2	1:B:799:GLU:OE1	2.07	0.54
1:A:962:GLN:NE2	1:A:1129:GLU:OE2	2.38	0.54
1:C:780:VAL:HG21	4:C:1303:43Y:H5	1.90	0.54
1:C:721:ILE:HD13	1:C:1013:LEU:HD11	1.90	0.54
1:C:1073:LEU:HD21	1:C:1084:GLN:HB3	1.91	0.53
1:B:774:SER:HB2	1:B:1133:VAL:HB	1.89	0.53
1:A:780:VAL:HG21	4:A:1305:43Y:H5	1.92	0.51
1:B:746:LYS:HB2	1:B:864:THR:HB	1.92	0.51
1:B:847:LEU:HD12	1:B:972:PRO:HB2	1.93	0.50
1:B:752:SER:OG	1:B:857:HIS:NE2	2.46	0.49
1:B:993:SER:HB3	1:B:1000:GLN:HG3	1.94	0.49
1:B:1063:HIS:NE2	1:B:1105:GLU:OE2	2.42	0.48
1:A:715:LEU:HD23	1:A:737:VAL:HG11	1.96	0.48
1:A:1017:ASN:ND2	5:A:1404:HOH:O	2.37	0.48
1:A:949:ARG:HB2	1:A:953:LEU:HD12	1.95	0.47
1:A:729:GLU:HG3	1:A:748:LYS:HB2	1.96	0.47
1:B:785:VAL:HG23	5:C:1688:HOH:O	2.14	0.47
4:C:1303:43Y:H8	4:C:1303:43Y:H20	1.59	0.46
2:B:1303:NAG:H61	3:B:1304:FUL:H2	1.68	0.46
1:C:731:CYS:HB3	1:C:744:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ILE:HD11	1:A:861:LEU:HD13	1.99	0.45
1:B:892:LEU:HB3	1:B:1010:ASP:HB2	1.98	0.44
1:B:1073:LEU:HD21	1:B:1084:GLN:HB3	2.00	0.44
1:C:757:ARG:HB2	1:C:854:ASP:HB2	2.00	0.44
1:A:847:LEU:HD12	1:A:972:PRO:HB2	1.99	0.44
1:C:777:CYS:HB2	4:C:1303:43Y:H6	1.99	0.43
1:C:844:LYS:HE3	1:C:844:LYS:HB2	1.83	0.42
1:A:844:LYS:HD3	1:A:844:LYS:HA	1.91	0.42
1:A:957:LYS:HE3	1:A:959:MET:HE2	2.01	0.42
4:A:1305:43Y:H8	4:A:1305:43Y:H19	1.73	0.42
1:C:847:LEU:HD12	1:C:972:PRO:HB2	2.02	0.42
1:B:826:PHE:N	4:B:1305:43Y:O31	2.47	0.41
1:B:701:ILE:HG21	1:C:695:ILE:HG21	2.02	0.41
1:B:1062:ALA:HB3	1:B:1071:ILE:HB	2.01	0.41
1:C:772:LEU:HD23	1:C:1131:THR:HB	2.02	0.41
1:A:1080:LYS:HB3	1:A:1080:LYS:HE2	1.84	0.41
1:C:931:GLU:OE1	1:C:970:ILE:N	2.51	0.41
1:B:1094:GLU:HG3	1:B:1109:LEU:HD11	2.03	0.41
1:B:738:LYS:HE3	1:B:738:LYS:HB2	1.89	0.40
1:A:777:CYS:SG	4:A:1305:43Y:H6	2.62	0.40
1:C:843:ARG:HG2	1:C:843:ARG:H	1.59	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	439/531 (83%)	427 (97%)	10 (2%)	2 (0%)	32	39
1	B	438/531 (82%)	423 (97%)	13 (3%)	2 (0%)	32	39
1	C	441/531 (83%)	427 (97%)	12 (3%)	2 (0%)	32	39
All	All	1318/1593 (83%)	1277 (97%)	35 (3%)	6 (0%)	32	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	785	VAL
1	B	785	VAL
1	A	960	ILE
1	B	960	ILE
1	C	785	VAL
1	C	960	ILE

### 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	382/443 (86%)	380 (100%)	2 (0%)	91	96
1	B	381/443 (86%)	381 (100%)	0	100	100
1	C	384/443 (87%)	384 (100%)	0	100	100
All	All	1147/1329 (86%)	1145 (100%)	2 (0%)	94	98

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

Mol	Chain	Res	Type
1	A	699	SER
1	A	722	ARG

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

### 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](#)

13 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	NAG	A	1301	1	14,14,15	0.26	0	15,19,21	0.49	0
2	NAG	A	1302	1	14,14,15	0.36	0	15,19,21	0.43	0
2	NAG	A	1303	1,3	14,14,15	0.46	0	15,19,21	0.45	0
3	FUL	A	1304	2	9,10,11	0.87	0	13,14,16	1.22	1 (7%)
4	43Y	A	1305	-	23,23,23	1.00	1 (4%)	28,31,31	0.86	1 (3%)
2	NAG	B	1301	1	14,14,15	0.22	0	15,19,21	0.54	0
2	NAG	B	1302	1	14,14,15	0.31	0	15,19,21	0.44	0
2	NAG	B	1303	1,3	14,14,15	0.26	0	15,19,21	0.44	0
3	FUL	B	1304	2	9,10,11	1.06	1 (11%)	13,14,16	1.42	2 (15%)
4	43Y	B	1305	-	18,18,23	0.85	0	22,25,31	0.93	1 (4%)
2	NAG	C	1301	1	14,14,15	0.35	0	15,19,21	0.46	0
2	NAG	C	1302	1	14,14,15	0.26	0	15,19,21	0.45	0
4	43Y	C	1303	-	23,23,23	1.00	1 (4%)	28,31,31	0.83	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	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1,3	-	0/6/23/26	0/1/1/1
3	FUL	A	1304	2	-	0/0/17/20	0/1/1/1
4	43Y	A	1305	-	1/1/5/5	0/27/27/27	0/0/0/0
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1303	1,3	-	0/6/23/26	0/1/1/1
3	FUL	B	1304	2	-	0/0/17/20	0/1/1/1
4	43Y	B	1305	-	1/1/4/5	0/20/20/27	0/0/0/0
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	43Y	C	1303	-	1/1/5/5	0/27/27/27	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1304	FUL	C2-C3	2.53	1.55	1.52
4	A	1305	43Y	P-O1P	3.07	1.62	1.50
4	C	1303	43Y	P-O1P	3.17	1.62	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1305	43Y	C3-O3-C11	-2.17	110.59	117.13
4	B	1305	43Y	O2-C2-C1	2.24	110.85	105.88
3	A	1304	FUL	C1-O5-C5	2.49	117.90	112.39
3	B	1304	FUL	C1-O5-C5	2.56	118.06	112.39
3	B	1304	FUL	C1-C2-C3	2.81	113.22	109.65

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1305	43Y	C2
4	C	1303	43Y	C2
4	A	1305	43Y	C2

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1305	43Y	3	0
2	B	1303	NAG	1	0
3	B	1304	FUL	1	0
4	B	1305	43Y	1	0
4	C	1303	43Y	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, 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	443/531 (83%)	-0.25	10 (2%) 61 67	14, 23, 47, 92	0
1	B	440/531 (82%)	-0.19	9 (2%) 65 72	15, 25, 54, 87	0
1	C	444/531 (83%)	-0.03	18 (4%) 38 45	14, 26, 61, 128	0
All	All	1327/1593 (83%)	-0.16	37 (2%) 53 61	14, 25, 57, 128	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	710	ASN	4.5
1	A	706	THR	4.4
1	C	802	PHE	3.8
1	C	1136	LYS	3.8
1	A	804	GLY	3.5
1	C	1032	ALA	3.4
1	A	1136	LYS	3.4
1	B	737	VAL	3.3
1	C	804	GLY	3.2
1	A	996	ASN	3.1
1	C	826	PHE	3.1
1	C	994	LYS	3.1
1	A	995	GLY	3.0
1	A	707	GLU	3.0
1	C	1054	SER	2.9
1	C	801	SER	2.9
1	B	740	ASP	2.6
1	B	1079	THR	2.6
1	C	1033	PHE	2.6
1	C	844	LYS	2.5
1	C	709	VAL	2.5
1	C	884	ASN	2.5
1	A	997	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	805	GLU	2.4
1	A	802	PHE	2.4
1	B	1134	ASN	2.2
1	B	711	THR	2.2
1	B	866	PHE	2.1
1	B	742	THR	2.1
1	B	996	ASN	2.1
1	C	1077	ASN	2.1
1	C	1078	GLY	2.1
1	A	1135	PRO	2.0
1	C	842	VAL	2.0
1	C	1079	THR	2.0
1	B	842	VAL	2.0
1	C	1134	ASN	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	43Y	B	1305	19/24	0.74	0.37	3.69	68,87,114,114	0
2	NAG	B	1303	14/15	0.89	0.25	3.13	40,44,56,63	0
2	NAG	A	1303	14/15	0.88	0.27	3.06	45,50,59,61	0
4	43Y	A	1305	24/24	0.91	0.21	2.49	32,55,61,62	0
2	NAG	C	1302	14/15	0.84	0.29	1.78	38,48,50,51	0
2	NAG	B	1302	14/15	0.85	0.18	1.11	34,41,45,48	0
2	NAG	A	1302	14/15	0.93	0.19	0.95	31,38,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	43Y	C	1303	24/24	0.94	0.20	0.94	24,43,49,49	0
2	NAG	A	1301	14/15	0.70	0.28	-	56,63,65,67	0
2	NAG	B	1301	14/15	0.74	0.39	-	47,58,60,60	0
2	NAG	C	1301	14/15	0.77	0.32	-	55,61,66,68	0
3	FUL	B	1304	10/11	0.79	0.40	-	69,80,91,92	0
3	FUL	A	1304	10/11	0.73	0.39	-	65,74,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.