



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID : 3S6X  
Title : Structure of reovirus attachment protein sigma1 in complex with alpha-2,3-sialyllactose  
Authors : Reiter, D.M.; Dermody, T.S.; Stehle, T.  
Deposited on : 2011-05-26  
Resolution : 2.25 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 (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

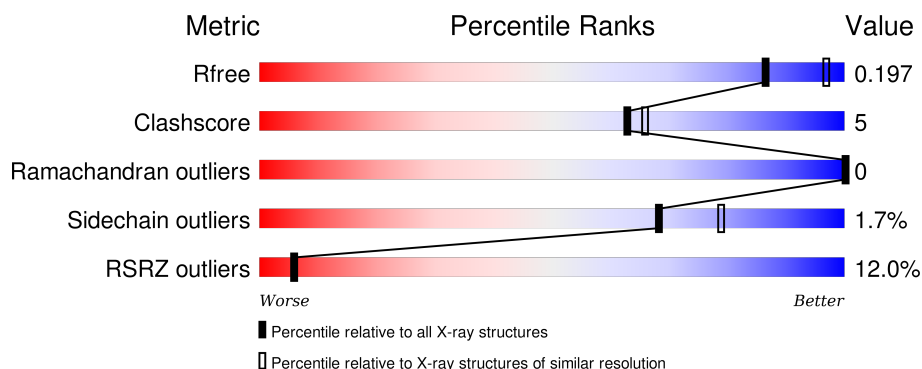
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	325	<div> <div>11%</div> <div>78% 11% 11%</div> </div>
1	B	325	<div> <div>11%</div> <div>79% 11% 9%</div> </div>
1	C	325	<div> <div>10%</div> <div>79% 10% 10%</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	GAL	C	2	-	-	-	X
2	BGC	C	3	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7624 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	1	0
			2210	1386	385	431	8			
1	B	295	Total	C	N	O	S	0	3	0
			2262	1417	396	441	8			
1	C	291	Total	C	N	O	S	1	0	0
			2211	1387	385	431	8			

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLN	-	EXPRESSION TAG	UNP P03528
A	132	ILE	-	EXPRESSION TAG	UNP P03528
A	133	GLU	-	EXPRESSION TAG	UNP P03528
A	134	ASP	-	EXPRESSION TAG	UNP P03528
A	135	LYS	-	EXPRESSION TAG	UNP P03528
A	136	ILE	-	EXPRESSION TAG	UNP P03528
A	137	GLU	-	EXPRESSION TAG	UNP P03528
A	138	GLU	-	EXPRESSION TAG	UNP P03528
A	139	ILE	-	EXPRESSION TAG	UNP P03528
A	140	LEU	-	EXPRESSION TAG	UNP P03528
A	141	SER	-	EXPRESSION TAG	UNP P03528
A	142	LYS	-	EXPRESSION TAG	UNP P03528
A	143	ILE	-	EXPRESSION TAG	UNP P03528
A	144	TYR	-	EXPRESSION TAG	UNP P03528
A	145	HIS	-	EXPRESSION TAG	UNP P03528
A	146	ILE	-	EXPRESSION TAG	UNP P03528
A	147	GLU	-	EXPRESSION TAG	UNP P03528
A	148	ASN	-	EXPRESSION TAG	UNP P03528
A	149	GLU	-	EXPRESSION TAG	UNP P03528
A	150	ILE	-	EXPRESSION TAG	UNP P03528
A	151	ALA	-	EXPRESSION TAG	UNP P03528
A	152	ARG	-	EXPRESSION TAG	UNP P03528
A	153	ILE	-	EXPRESSION TAG	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
A	154	LYS	-	EXPRESSION TAG	UNP P03528
A	155	LYS	-	EXPRESSION TAG	UNP P03528
A	156	LEU	-	EXPRESSION TAG	UNP P03528
A	157	ILE	-	EXPRESSION TAG	UNP P03528
A	158	GLY	-	EXPRESSION TAG	UNP P03528
A	159	GLU	-	EXPRESSION TAG	UNP P03528
A	160	GLY	-	EXPRESSION TAG	UNP P03528
A	161	SER	-	EXPRESSION TAG	UNP P03528
A	162	GLY	-	EXPRESSION TAG	UNP P03528
A	163	ARG	-	EXPRESSION TAG	UNP P03528
A	164	PRO	-	EXPRESSION TAG	UNP P03528
A	165	VAL	-	EXPRESSION TAG	UNP P03528
A	166	LEU	-	EXPRESSION TAG	UNP P03528
A	167	ASN	-	EXPRESSION TAG	UNP P03528
A	168	GLN	-	EXPRESSION TAG	UNP P03528
A	169	GLY	-	EXPRESSION TAG	UNP P03528
A	249	ILE	THR	ENGINEERED MUTATION	UNP P03528
A	408	THR	ALA	CONFLICT	UNP P03528
B	131	GLN	-	EXPRESSION TAG	UNP P03528
B	132	ILE	-	EXPRESSION TAG	UNP P03528
B	133	GLU	-	EXPRESSION TAG	UNP P03528
B	134	ASP	-	EXPRESSION TAG	UNP P03528
B	135	LYS	-	EXPRESSION TAG	UNP P03528
B	136	ILE	-	EXPRESSION TAG	UNP P03528
B	137	GLU	-	EXPRESSION TAG	UNP P03528
B	138	GLU	-	EXPRESSION TAG	UNP P03528
B	139	ILE	-	EXPRESSION TAG	UNP P03528
B	140	LEU	-	EXPRESSION TAG	UNP P03528
B	141	SER	-	EXPRESSION TAG	UNP P03528
B	142	LYS	-	EXPRESSION TAG	UNP P03528
B	143	ILE	-	EXPRESSION TAG	UNP P03528
B	144	TYR	-	EXPRESSION TAG	UNP P03528
B	145	HIS	-	EXPRESSION TAG	UNP P03528
B	146	ILE	-	EXPRESSION TAG	UNP P03528
B	147	GLU	-	EXPRESSION TAG	UNP P03528
B	148	ASN	-	EXPRESSION TAG	UNP P03528
B	149	GLU	-	EXPRESSION TAG	UNP P03528
B	150	ILE	-	EXPRESSION TAG	UNP P03528
B	151	ALA	-	EXPRESSION TAG	UNP P03528
B	152	ARG	-	EXPRESSION TAG	UNP P03528
B	153	ILE	-	EXPRESSION TAG	UNP P03528
B	154	LYS	-	EXPRESSION TAG	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	155	LYS	-	EXPRESSION TAG	UNP P03528
B	156	LEU	-	EXPRESSION TAG	UNP P03528
B	157	ILE	-	EXPRESSION TAG	UNP P03528
B	158	GLY	-	EXPRESSION TAG	UNP P03528
B	159	GLU	-	EXPRESSION TAG	UNP P03528
B	160	GLY	-	EXPRESSION TAG	UNP P03528
B	161	SER	-	EXPRESSION TAG	UNP P03528
B	162	GLY	-	EXPRESSION TAG	UNP P03528
B	163	ARG	-	EXPRESSION TAG	UNP P03528
B	164	PRO	-	EXPRESSION TAG	UNP P03528
B	165	VAL	-	EXPRESSION TAG	UNP P03528
B	166	LEU	-	EXPRESSION TAG	UNP P03528
B	167	ASN	-	EXPRESSION TAG	UNP P03528
B	168	GLN	-	EXPRESSION TAG	UNP P03528
B	169	GLY	-	EXPRESSION TAG	UNP P03528
B	249	ILE	THR	ENGINEERED MUTATION	UNP P03528
B	408	THR	ALA	CONFLICT	UNP P03528
C	131	GLN	-	EXPRESSION TAG	UNP P03528
C	132	ILE	-	EXPRESSION TAG	UNP P03528
C	133	GLU	-	EXPRESSION TAG	UNP P03528
C	134	ASP	-	EXPRESSION TAG	UNP P03528
C	135	LYS	-	EXPRESSION TAG	UNP P03528
C	136	ILE	-	EXPRESSION TAG	UNP P03528
C	137	GLU	-	EXPRESSION TAG	UNP P03528
C	138	GLU	-	EXPRESSION TAG	UNP P03528
C	139	ILE	-	EXPRESSION TAG	UNP P03528
C	140	LEU	-	EXPRESSION TAG	UNP P03528
C	141	SER	-	EXPRESSION TAG	UNP P03528
C	142	LYS	-	EXPRESSION TAG	UNP P03528
C	143	ILE	-	EXPRESSION TAG	UNP P03528
C	144	TYR	-	EXPRESSION TAG	UNP P03528
C	145	HIS	-	EXPRESSION TAG	UNP P03528
C	146	ILE	-	EXPRESSION TAG	UNP P03528
C	147	GLU	-	EXPRESSION TAG	UNP P03528
C	148	ASN	-	EXPRESSION TAG	UNP P03528
C	149	GLU	-	EXPRESSION TAG	UNP P03528
C	150	ILE	-	EXPRESSION TAG	UNP P03528
C	151	ALA	-	EXPRESSION TAG	UNP P03528
C	152	ARG	-	EXPRESSION TAG	UNP P03528
C	153	ILE	-	EXPRESSION TAG	UNP P03528
C	154	LYS	-	EXPRESSION TAG	UNP P03528
C	155	LYS	-	EXPRESSION TAG	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
C	156	LEU	-	EXPRESSION TAG	UNP P03528
C	157	ILE	-	EXPRESSION TAG	UNP P03528
C	158	GLY	-	EXPRESSION TAG	UNP P03528
C	159	GLU	-	EXPRESSION TAG	UNP P03528
C	160	GLY	-	EXPRESSION TAG	UNP P03528
C	161	SER	-	EXPRESSION TAG	UNP P03528
C	162	GLY	-	EXPRESSION TAG	UNP P03528
C	163	ARG	-	EXPRESSION TAG	UNP P03528
C	164	PRO	-	EXPRESSION TAG	UNP P03528
C	165	VAL	-	EXPRESSION TAG	UNP P03528
C	166	LEU	-	EXPRESSION TAG	UNP P03528
C	167	ASN	-	EXPRESSION TAG	UNP P03528
C	168	GLN	-	EXPRESSION TAG	UNP P03528
C	169	GLY	-	EXPRESSION TAG	UNP P03528
C	249	ILE	THR	ENGINEERED MUTATION	UNP P03528
C	408	THR	ALA	CONFLICT	UNP P03528

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			43	23	1	19		
2	B	3	Total	C	N	O	0	0
			43	23	1	19		
2	C	3	Total	C	N	O	0	0
			43	23	1	19		

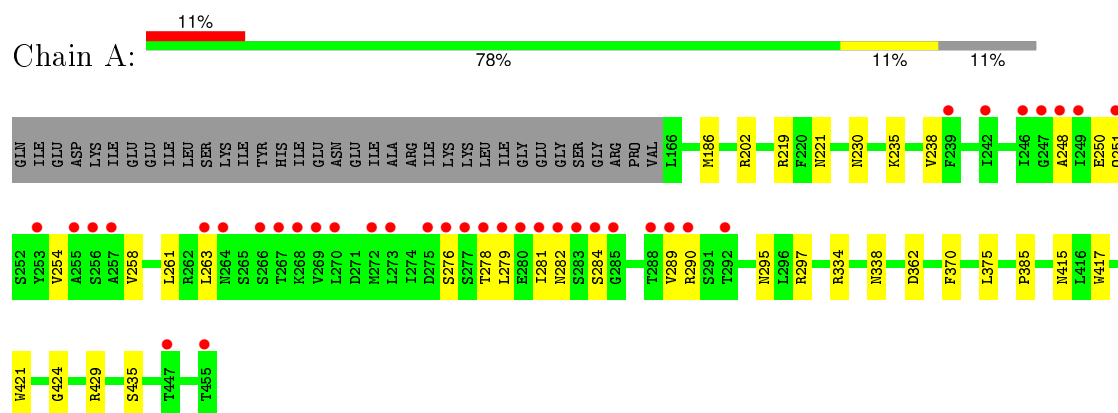
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	326	Total	O	0	0
			326	326		
3	B	253	Total	O	0	0
			253	253		
3	C	233	Total	O	0	0
			233	233		

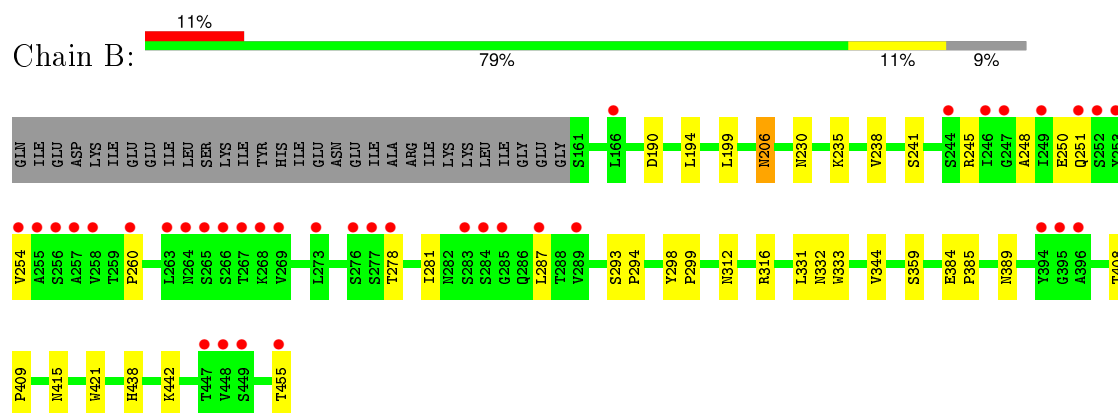
### 3 Residue-property plots [i](#)

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.

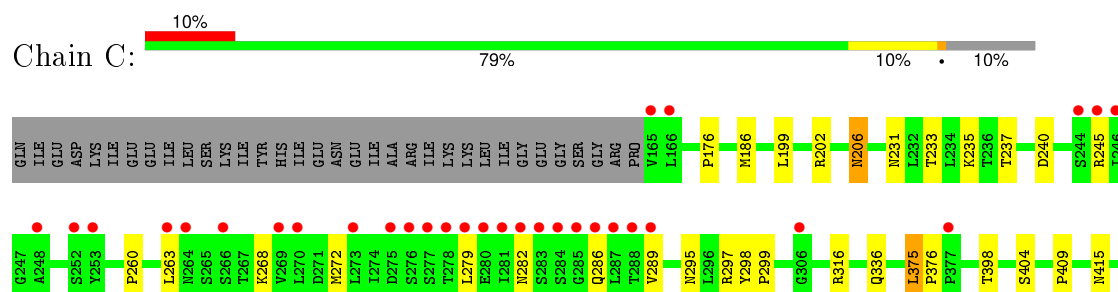
#### • Molecule 1: Outer capsid protein sigma-1



#### • Molecule 1: Outer capsid protein sigma-1



#### • Molecule 1: Outer capsid protein sigma-1





L428	
I440	
S441	
K442	
P451	
T455	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.15Å 333.18Å 58.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.61 – 2.25 38.61 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.4 (38.61-2.25) 95.4 (38.61-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.158 , 0.199 0.158 , 0.197	Depositor DCC
$R_{free}$ test set	3956 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 78323 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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, 0.375 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: SIA, BGC, GAL

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	0.32	0/2254	0.49	0/3069
1	B	0.33	0/2307	0.50	0/3141
1	C	0.32	0/2255	0.50	0/3070
All	All	0.32	0/6816	0.50	0/9280

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

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	2210	0	2170	25	0
1	B	2262	0	2225	31	0
1	C	2211	0	2173	32	0
2	A	43	0	37	1	0
2	B	43	0	37	0	0
2	C	43	0	37	3	0
3	A	326	0	0	2	5
3	B	253	0	0	9	6
3	C	233	0	0	6	2
All	All	7624	0	6679	72	8

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 5.

All (72) 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:332:ASN:HB3	3:B:693:HOH:O	1.83	0.77
1:B:250:GLU:OE2	1:C:245:ARG:HD2	1.87	0.74
1:A:221:ASN:HB2	1:C:233:THR:HG22	1.67	0.74
1:A:278:THR:HB	1:C:289:VAL:HG22	1.68	0.73
1:A:334:ARG:NE	3:A:707:HOH:O	2.22	0.72
1:C:440:ASN:ND2	3:C:818:HOH:O	2.24	0.70
1:B:389:ASN:HB3	3:B:814:HOH:O	1.94	0.67
2:C:1:SIA:C1	2:C:2:GAL:H4	2.24	0.66
1:B:190:ASP:OD1	3:B:530:HOH:O	2.14	0.65
1:B:316:ARG:NH1	3:B:890:HOH:O	1.98	0.65
1:C:336:GLN:NE2	3:C:498:HOH:O	2.30	0.63
1:A:289:VAL:HG22	1:B:278:THR:HB	1.80	0.62
1:A:186:MET:CE	1:C:199:LEU:HD22	2.30	0.62
1:C:375:LEU:HD13	1:C:376:PRO:HD2	1.81	0.62
1:A:282:ASN:OD1	1:A:284:SER:OG	2.09	0.61
1:A:254:VAL:HG22	1:C:263:LEU:HD13	1.83	0.60
1:A:276:SER:O	1:A:290:ARG:NH2	2.35	0.60
1:A:338:ASN:HB2	3:A:805:HOH:O	2.02	0.58
1:C:237:THR:HA	1:C:240:ASP:OD2	2.04	0.57
1:B:199:LEU:HD22	1:C:186:MET:CE	2.35	0.55
1:B:331:LEU:HD22	1:B:359[B]:SER:OG	2.07	0.54
1:C:282:ASN:HD21	1:C:286:GLN:HB2	1.72	0.54
1:B:235:LYS:O	1:B:238:VAL:HG12	2.09	0.53
1:B:442:LYS:HE2	3:B:527:HOH:O	2.08	0.52
1:A:295:ASN:HD21	1:A:297:ARG:HH22	1.57	0.52
1:B:281:ILE:HD12	1:C:260:PRO:HD3	1.92	0.51
1:C:282:ASN:ND2	1:C:286:GLN:HB2	2.26	0.51
1:C:398:THR:OG1	3:C:571:HOH:O	1.99	0.51
1:A:230:ASN:HB2	1:B:206:ASN:OD1	2.10	0.50
1:B:287:LEU:HB2	1:C:260:PRO:HG3	1.94	0.50
1:C:235:LYS:HG2	1:C:237:THR:HG23	1.94	0.49
1:C:442:LYS:HB2	1:C:442:LYS:NZ	2.28	0.48
1:B:230:ASN:HB2	1:C:206:ASN:OD1	2.14	0.48
1:B:194:LEU:HD21	1:C:176:PRO:HD3	1.95	0.47
1:C:316:ARG:HD3	3:C:515:HOH:O	2.14	0.47
1:A:279:LEU:HD23	1:A:289:VAL:HA	1.96	0.47
1:A:219:ARG:HB3	1:C:231:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:MET:HE2	1:C:199:LEU:HD22	1.96	0.47
1:A:261:LEU:HD21	1:C:272:MET:HB3	1.97	0.46
1:B:333:TRP:CA	3:B:803:HOH:O	2.63	0.46
1:B:248:ALA:O	1:B:251:GLN:HG2	2.17	0.45
1:A:258:VAL:O	1:A:261:LEU:HB2	2.16	0.45
2:C:2:GAL:O2	3:C:817:HOH:O	2.05	0.44
1:A:235:LYS:O	1:A:238:VAL:HG12	2.16	0.44
1:C:231:ASN:O	1:C:233:THR:HG23	2.16	0.44
1:A:421:TRP:CZ2	1:A:424:GLY:HA2	2.53	0.44
1:B:333:TRP:HA	3:B:803:HOH:O	2.16	0.44
1:B:199:LEU:HD22	1:C:186:MET:HE3	1.99	0.43
1:B:359[A]:SER:OG	1:B:438:HIS:O	2.35	0.43
1:B:333:TRP:N	3:B:803:HOH:O	2.51	0.43
1:B:293:SER:HA	1:B:294:PRO:HD3	1.87	0.43
1:B:298:TYR:CG	1:B:299:PRO:HA	2.54	0.43
1:C:295:ASN:HD21	1:C:297:ARG:HH22	1.67	0.42
2:C:3:BGC:H6C1	3:C:817:HOH:O	2.20	0.42
1:B:385:PRO:HD3	1:B:421:TRP:CG	2.54	0.42
1:A:250:GLU:O	1:C:268:LYS:NZ	2.37	0.42
1:A:263:LEU:HD13	1:B:254:VAL:HG22	2.02	0.42
1:A:385:PRO:HD3	1:A:421:TRP:CG	2.55	0.42
1:B:384:GLU:HA	1:B:385:PRO:HD3	1.92	0.42
1:B:344:VAL:HG21	1:C:451:PRO:HB3	2.01	0.42
1:C:298:TYR:CG	1:C:299:PRO:HA	2.55	0.41
1:C:298:TYR:CD1	1:C:299:PRO:HA	2.56	0.41
1:A:370:PHE:HB2	1:A:424:GLY:O	2.21	0.41
1:A:417:TRP:CZ2	1:A:429:ARG:HG2	2.56	0.41
1:C:279:LEU:HD23	1:C:289:VAL:HA	2.03	0.41
1:A:248:ALA:O	1:A:251:GLN:HG2	2.21	0.41
1:B:408:THR:HA	1:B:409:PRO:HD3	1.97	0.40
1:A:281:ILE:HD11	1:B:260:PRO:HD3	2.02	0.40
1:C:404:SER:HB3	1:C:409:PRO:HA	2.03	0.40
1:B:312[A]:ASN:ND2	3:B:551:HOH:O	2.55	0.40
1:B:241:SER:O	1:B:245:ARG:HG3	2.21	0.40
2:A:1:SIA:H32	2:A:2:GAL:H3	1.80	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:572:HOH:O	3:A:823:HOH:O[3_555]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:579:HOH:O	3:B:803:HOH:O[4_455]	1.97	0.23
3:B:631:HOH:O	3:B:834:HOH:O[3_555]	2.03	0.17
3:B:530:HOH:O	3:C:497:HOH:O[2_655]	2.03	0.17
3:A:557:HOH:O	3:B:752:HOH:O[4_455]	2.09	0.11
3:C:537:HOH:O	3:C:811:HOH:O[3_556]	2.11	0.09
3:A:778:HOH:O	3:B:533:HOH:O[4_455]	2.12	0.08
3:A:571:HOH:O	3:B:597:HOH:O[4_455]	2.18	0.02

## 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	289/325 (89%)	279 (96%)	10 (4%)	0	100	100
1	B	296/325 (91%)	288 (97%)	8 (3%)	0	100	100
1	C	289/325 (89%)	279 (96%)	10 (4%)	0	100	100
All	All	874/975 (90%)	846 (97%)	28 (3%)	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	247/278 (89%)	242 (98%)	5 (2%)	63	73
1	B	254/278 (91%)	251 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	247/278 (89%)	242 (98%)	5 (2%)	63	73
All	All	748/834 (90%)	735 (98%)	13 (2%)	68	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ARG
1	A	362	ASP
1	A	375	LEU
1	A	415	ASN
1	A	435	SER
1	B	206	ASN
1	B	415	ASN
1	B	455	THR
1	C	202	ARG
1	C	206	ASN
1	C	375	LEU
1	C	415	ASN
1	C	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	B	422	GLN
1	C	168	GLN
1	C	264	ASN
1	C	312	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 ⓘ

9 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	SIA	A	1	2	16,20,21	0.29	0	18,28,31	0.97	2 (11%)
2	GAL	A	2	2	11,11,12	0.58	0	14,15,17	1.04	1 (7%)
2	BGC	A	3	2	12,12,12	0.60	0	17,17,17	0.97	1 (5%)
2	SIA	B	1	2	16,20,21	0.24	0	18,28,31	0.56	0
2	GAL	B	2	2	11,11,12	0.68	0	14,15,17	1.38	1 (7%)
2	BGC	B	3	2	12,12,12	0.58	0	17,17,17	1.10	1 (5%)
2	SIA	C	1	2	16,20,21	0.37	0	18,28,31	0.79	0
2	GAL	C	2	2	11,11,12	0.58	0	14,15,17	0.78	0
2	BGC	C	3	2	12,12,12	0.57	0	17,17,17	0.96	1 (5%)

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	SIA	A	1	2	-	0/14/34/38	0/1/1/1
2	GAL	A	2	2	-	0/2/19/22	0/1/1/1
2	BGC	A	3	2	-	0/2/22/22	0/1/1/1
2	SIA	B	1	2	-	0/14/34/38	0/1/1/1
2	GAL	B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	B	3	2	-	0/2/22/22	0/1/1/1
2	SIA	C	1	2	-	0/14/34/38	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	GAL	O5-C1-C2	-2.36	107.03	110.86
2	A	1	SIA	C8-C7-C6	-2.30	108.39	113.01
2	A	1	SIA	O6-C6-C5	2.28	112.21	108.48
2	A	3	BGC	C3-C4-C5	2.28	114.17	110.20
2	C	3	BGC	C3-C4-C5	2.60	114.73	110.20
2	B	3	BGC	C3-C4-C5	2.74	114.97	110.20
2	B	2	GAL	C1-C2-C3	3.76	113.99	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SIA	1	0
2	A	2	GAL	1	0
2	C	1	SIA	1	0
2	C	2	GAL	2	0
2	C	3	BGC	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	290/325 (89%)	0.20	37 (12%) 5 5	21, 39, 119, 149	0
1	B	295/325 (90%)	0.31	37 (12%) 5 5	20, 39, 116, 137	2 (0%)
1	C	291/325 (89%)	0.17	31 (10%) 8 8	23, 44, 116, 144	3 (1%)
All	All	876/975 (89%)	0.23	105 (11%) 6 6	20, 41, 118, 149	5 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	SER	6.3
1	B	257	ALA	6.1
1	A	263	LEU	5.0
1	B	256	SER	4.9
1	C	166	LEU	4.7
1	B	252	SER	4.6
1	B	283	SER	4.5
1	A	257	ALA	4.5
1	B	263	LEU	4.4
1	B	269	VAL	4.2
1	B	455	THR	4.1
1	B	265	SER	3.9
1	A	289	VAL	3.7
1	A	267	THR	3.7
1	A	277	SER	3.7
1	C	266	SER	3.7
1	B	287	LEU	3.6
1	C	281	ILE	3.6
1	C	285	GLY	3.6
1	A	288	THR	3.5
1	A	248	ALA	3.5
1	A	269	VAL	3.5
1	A	270	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	3.4
1	A	246	ILE	3.4
1	B	166	LEU	3.4
1	C	273	LEU	3.3
1	A	242	ILE	3.3
1	C	277	SER	3.3
1	A	290	ARG	3.3
1	A	276	SER	3.3
1	B	284	SER	3.2
1	A	284	SER	3.1
1	B	249	ILE	3.0
1	A	273	LEU	3.0
1	C	269	VAL	2.9
1	A	256	SER	2.9
1	B	247	GLY	2.9
1	A	283	SER	2.9
1	A	251	GLN	2.9
1	C	253	TYR	2.8
1	B	251	GLN	2.8
1	A	292	THR	2.8
1	B	273	LEU	2.8
1	A	249	ILE	2.7
1	B	255	ALA	2.7
1	C	246	ILE	2.7
1	C	287	LEU	2.7
1	A	447	THR	2.7
1	C	284	SER	2.7
1	A	266	SER	2.6
1	C	282	ASN	2.6
1	B	276	SER	2.6
1	C	279	LEU	2.6
1	A	281	ILE	2.6
1	B	258	VAL	2.6
1	C	252	SER	2.6
1	A	272	MET	2.6
1	B	254	VAL	2.5
1	A	279	LEU	2.5
1	A	280	GLU	2.5
1	B	260	PRO	2.5
1	C	377	PRO	2.5
1	A	282	ASN	2.5
1	C	289	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	253	TYR	2.4
1	B	268	LYS	2.4
1	A	268	LYS	2.4
1	A	264	ASN	2.4
1	C	264	ASN	2.4
1	B	289	VAL	2.4
1	B	448	VAL	2.4
1	C	276	SER	2.4
1	B	267	THR	2.4
1	A	275	ASP	2.3
1	C	244	SER	2.3
1	C	278	THR	2.3
1	C	248	ALA	2.3
1	A	247	GLY	2.3
1	B	449	SER	2.3
1	B	246	ILE	2.3
1	A	278	THR	2.3
1	C	288	THR	2.3
1	B	266	SER	2.3
1	A	455	THR	2.2
1	B	253	TYR	2.2
1	C	280	GLU	2.2
1	A	255	ALA	2.2
1	B	277	SER	2.2
1	B	396	ALA	2.2
1	C	165	VAL	2.2
1	C	270	LEU	2.2
1	C	275	ASP	2.2
1	B	395	GLY	2.1
1	C	286	GLN	2.1
1	C	306	GLY	2.1
1	B	394	TYR	2.1
1	B	264	ASN	2.1
1	B	278	THR	2.1
1	B	285	GLY	2.1
1	B	447	THR	2.1
1	A	239	PHE	2.1
1	B	244	SER	2.1
1	C	263	LEU	2.0
1	C	245	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](#)

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
2	BGC	C	3	12/12	0.89	0.33	8.65	80,94,104,108	0
2	GAL	C	2	11/12	0.93	0.17	3.39	50,73,83,85	0
2	SIA	C	1	20/21	0.94	0.12	0.92	37,55,65,66	0
2	SIA	B	1	20/21	0.93	0.10	-0.26	39,51,68,74	0
2	SIA	A	1	20/21	0.95	0.09	-0.75	33,50,65,67	0
2	BGC	B	3	12/12	0.84	0.23	-	95,113,120,121	0
2	BGC	A	3	12/12	0.86	0.34	-	95,111,120,124	0
2	GAL	A	2	11/12	0.90	0.14	-	54,72,83,85	0
2	GAL	B	2	11/12	0.96	0.10	-	59,60,69,71	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.