



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 06:41 AM EST

PDB ID : 3S6Z  
Title : Structure of reovirus attachment protein sigma1 in complex with alpha-2,8-dialylosactose  
Authors : Reiter, D.M.; Dermody, T.S.; Stehle, T.  
Deposited on : 2011-05-26  
Resolution : 2.28 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.

---

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-20030736  
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-20030736

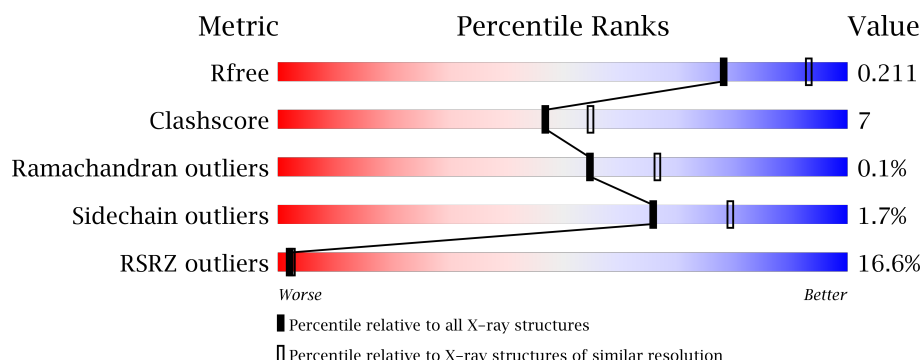
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (2.30-2.26)

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>14%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>11%</div> </div> </div>
1	B	325	<div> <div>16%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>9%</div> </div> </div>
1	C	325	<div> <div>15%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>10%</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	SIA	C	1	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7499 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	0	0
			2203	1381	384	430	8			
1	B	295	Total	C	N	O	S	0	1	0
			2243	1407	392	436	8			
1	C	292	Total	C	N	O	S	0	2	0
			2234	1402	389	435	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

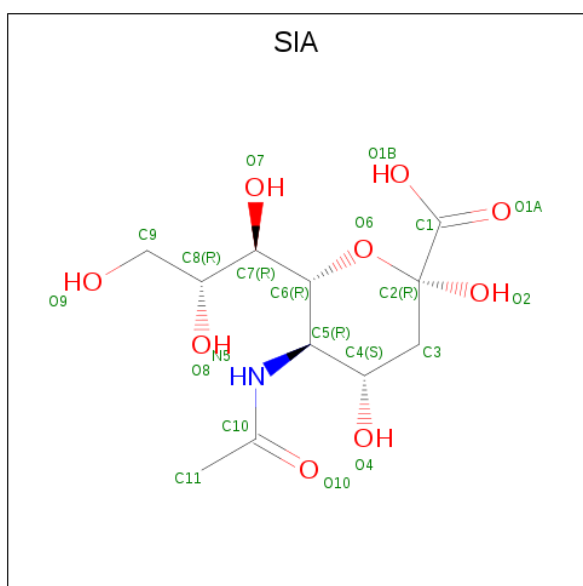
Chain	Residue	Modelled	Actual	Comment	Reference
B	155	LYS	-	EXPRESSION TAG	UNP P03528
B	156	LEU	-	EXPRESSION TAG	UNP P03528
B	157	ILE	-	EXPRESSION TAG	UNP P03528
B	158	GLY	-	EXPRESSION TAG	UNP P03528
B	159	GLU	-	EXPRESSION TAG	UNP P03528
B	160	GLY	-	EXPRESSION TAG	UNP P03528
B	161	SER	-	EXPRESSION TAG	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

*Continued on next page...*

Continued from previous page...

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 O-SIALIC ACID (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



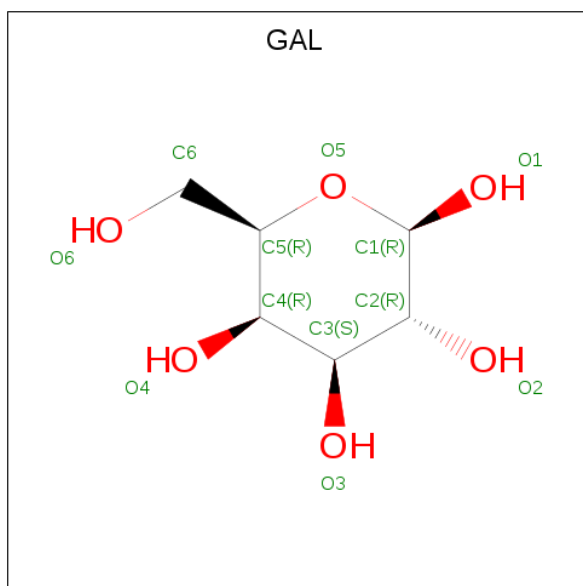
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	11	1	8		
2	A	1	Total	C	N	O	0	0
			20	11	1	8		
2	C	1	Total	C	N	O	0	0
			20	11	1	8		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

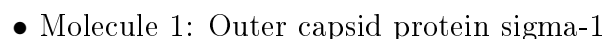
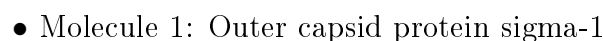
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	251	Total	O	0	0
			251	251		
4	B	240	Total	O	0	0
			240	240		
4	C	224	Total	O	0	0
			224	224		





- Molecule 1: Outer capsid protein sigma-1



## 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)	48.06 – 2.28 48.06 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.06-2.28) 96.0 (48.06-2.28)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, $R_{free}$	0.173 , 0.219 0.163 , 0.211	Depositor DCC
$R_{free}$ test set	3825 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7499	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, 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	0.34	0/2247	0.51	0/3059
1	B	0.36	0/2291	0.51	0/3119
1	C	0.33	0/2282	0.51	0/3107
All	All	0.34	0/6820	0.51	0/9285

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	2203	0	2162	30	0
1	B	2243	0	2210	30	0
1	C	2234	0	2201	48	1
2	A	40	0	33	6	0
2	C	40	0	33	1	0
3	A	12	0	11	5	0
3	C	12	0	11	1	0
4	A	251	0	0	4	3
4	B	240	0	0	6	2
4	C	224	0	0	10	6
All	All	7499	0	6661	95	9

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 7.

All (95) 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:180:ARG:NH1	4:C:515:HOH:O	2.07	0.88
1:A:221:ASN:HB2	1:C:233:THR:HG22	1.56	0.87
1:C:316:ARG:NH1	4:C:785:HOH:O	2.07	0.86
1:A:415:ASN:HD21	1:C:445:ALA:H	1.24	0.86
1:B:319:MET:HB2	1:B:375:LEU:HD22	1.64	0.80
1:A:278:THR:HB	1:C:289:VAL:HG22	1.64	0.79
1:A:245:ARG:NH1	1:C:250:GLU:OE1	2.17	0.78
1:B:389:ASN:HD22	1:B:422:GLN:HE22	1.33	0.76
2:A:2:SIA:H92	3:A:3:GAL:O3	1.89	0.73
1:A:415:ASN:HD21	1:C:445:ALA:N	1.91	0.67
1:B:168:GLN:OE1	4:B:506:HOH:O	2.14	0.65
1:A:289:VAL:HG22	1:B:278:THR:HB	1.78	0.65
1:C:323:ILE:HD13	1:C:336[A]:GLN:HE21	1.62	0.65
1:B:165:VAL:HA	1:C:165:VAL:O	1.98	0.64
1:A:415:ASN:ND2	1:C:445:ALA:H	1.94	0.63
1:A:262:ARG:NH2	1:A:271:ASP:OD2	2.30	0.63
1:A:276:SER:O	1:A:290:ARG:NH1	2.32	0.62
1:B:362:ASP:OD1	1:B:435:SER:HB3	1.99	0.62
1:B:282:ASN:HD21	1:B:286:GLN:HB2	1.64	0.62
1:C:398:THR:OG1	4:C:621:HOH:O	1.77	0.62
1:B:279:LEU:HD23	1:B:289:VAL:HA	1.82	0.60
1:B:332:ASN:O	1:B:333:TRP:HB3	2.03	0.59
1:A:272:MET:HE1	1:C:272:MET:SD	2.43	0.58
2:A:2:SIA:C1	3:A:3:GAL:C2	2.82	0.57
1:C:295:ASN:HD21	1:C:297:ARG:HH22	1.53	0.57
1:C:427:ARG:HD3	4:C:606:HOH:O	2.03	0.57
1:C:312[A]:ASN:HD21	1:C:316:ARG:HD3	1.70	0.56
1:C:323:ILE:HD13	1:C:336[A]:GLN:NE2	2.21	0.56
1:C:295:ASN:CG	1:C:297:ARG:HH12	2.08	0.55
1:C:166:LEU:HD13	1:C:166:LEU:H	1.70	0.55
1:A:277:SER:HA	1:A:290:ARG:HH11	1.72	0.55
1:B:282:ASN:ND2	1:B:286:GLN:HB2	2.21	0.55
1:C:378:LEU:HD12	4:C:617:HOH:O	2.05	0.55
1:C:167:ASN:O	1:C:168:GLN:HB3	2.07	0.55
1:B:442:LYS:HG3	4:B:776:HOH:O	2.07	0.55
1:B:262:ARG:HB3	1:B:271:ASP:OD1	2.08	0.54
1:C:316:ARG:HD3	4:C:512:HOH:O	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ALA:O	1:C:252:SER:OG	2.23	0.53
1:B:202:ARG:NH2	4:B:814:HOH:O	2.42	0.53
1:B:295:ASN:OD1	1:B:297:ARG:NH1	2.31	0.53
2:A:2:SIA:O1B	3:A:3:GAL:O2	2.24	0.52
1:A:263:LEU:HD13	1:B:254:VAL:HG22	1.91	0.52
1:A:245:ARG:HD2	1:C:250:GLU:OE2	2.09	0.52
1:A:427:ARG:HD2	4:A:601:HOH:O	2.11	0.51
1:B:332:ASN:O	1:B:333:TRP:CB	2.57	0.51
1:B:333:TRP:N	4:B:805:HOH:O	2.42	0.51
1:B:254:VAL:O	1:C:253:TYR:HA	2.09	0.51
1:A:422:GLN:HE21	1:A:422:GLN:HA	1.77	0.50
1:C:316:ARG:NH2	4:C:599:HOH:O	2.40	0.50
1:C:427:ARG:NH2	4:C:564:HOH:O	2.18	0.49
1:C:246:ILE:O	1:C:250:GLU:HG3	2.12	0.49
2:A:2:SIA:C1	3:A:3:GAL:H2	2.43	0.49
1:C:279:LEU:HD23	1:C:289:VAL:HA	1.95	0.48
1:C:224:GLN:HA	1:C:238:VAL:HG22	1.95	0.48
1:C:421:TRP:CZ2	1:C:424:GLY:HA2	2.48	0.48
1:B:181:ASN:ND2	4:B:823:HOH:O	2.47	0.48
1:C:282:ASN:HD21	1:C:286:GLN:HB2	1.78	0.48
1:B:237:THR:HA	1:B:240:ASP:OD2	2.14	0.47
1:C:237:THR:HA	1:C:240:ASP:OD2	2.14	0.47
1:C:295:ASN:ND2	1:C:297:ARG:HH12	2.13	0.46
1:B:268:LYS:NZ	1:C:250:GLU:O	2.48	0.46
1:A:453:SER:HB3	4:A:782:HOH:O	2.16	0.46
1:A:262:ARG:HD3	1:A:273:LEU:HD21	1.97	0.46
1:A:336:GLN:OE1	4:A:640:HOH:O	2.21	0.45
2:C:2:SIA:H32	3:C:3:GAL:H3	1.63	0.45
1:A:403:LEU:HD22	1:A:438:HIS:CD2	2.51	0.45
1:B:250:GLU:OE2	1:C:245:ARG:HD2	2.16	0.45
1:A:403:LEU:HD12	1:A:412:MET:HG3	1.99	0.45
1:C:404:SER:HB3	1:C:409:PRO:HA	1.98	0.45
1:B:199:LEU:HD22	1:C:186:MET:CE	2.46	0.45
1:B:318:SER:HB3	1:B:378:LEU:HD22	1.98	0.45
2:A:2:SIA:C1	3:A:3:GAL:HO2	2.28	0.44
1:A:335:VAL:HG23	4:A:94:HOH:O	2.18	0.44
1:C:385:PRO:HD3	1:C:421:TRP:CG	2.53	0.44
1:A:221:ASN:CB	1:C:233:THR:HG22	2.39	0.43
1:A:235:LYS:HB2	1:A:238:VAL:HG23	2.00	0.43
1:A:221:ASN:OD1	1:A:223:ASP:HB2	2.19	0.43
1:C:235:LYS:HB2	1:C:238:VAL:HG23	2.00	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ASN:OD1	1:C:224:GLN:HG3	2.19	0.43
1:A:222:THR:O	1:A:235:LYS:NZ	2.52	0.43
1:C:212:GLN:OE1	1:C:219:ARG:HD2	2.19	0.42
1:C:224:GLN:HA	1:C:238:VAL:CG2	2.49	0.42
1:A:221:ASN:HB2	1:C:233:THR:CG2	2.40	0.42
2:A:2:SIA:C2	2:A:2:SIA:H92	2.49	0.42
1:A:394:TYR:CZ	1:A:451:PRO:HD3	2.54	0.42
1:A:254:VAL:HG22	1:C:263:LEU:HD13	1.99	0.42
1:B:404:SER:HB3	1:B:409:PRO:HA	2.02	0.42
1:B:331:LEU:HD13	1:B:359[A]:SER:HB3	2.01	0.42
1:B:182:ASN:N	4:B:548:HOH:O	2.30	0.42
1:A:203:LEU:HD23	1:C:216:LEU:HB3	2.02	0.41
1:A:279:LEU:HD23	1:A:289:VAL:HA	2.02	0.41
1:B:331:LEU:HD22	1:B:359[B]:SER:OG	2.20	0.41
1:B:408:THR:HA	1:B:409:PRO:HD3	1.95	0.41
1:C:316:ARG:HD2	4:C:617:HOH:O	2.21	0.41
1:C:422:GLN:NE2	4:C:485:HOH:O	2.54	0.40

All (9) 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)
4:C:723:HOH:O	4:C:738:HOH:O[3_555]	1.81	0.39
1:C:336[B]:GLN:OE1	4:A:852:HOH:O[3_545]	1.82	0.38
4:A:460:HOH:O	4:B:653:HOH:O[2_665]	1.96	0.24
4:B:582:HOH:O	4:C:468:HOH:O[3_555]	2.00	0.20
4:C:724:HOH:O	4:C:738:HOH:O[3_555]	2.05	0.15
4:C:724:HOH:O	4:C:739:HOH:O[3_555]	2.08	0.12
4:C:529:HOH:O	4:C:637:HOH:O[2_665]	2.10	0.10
4:A:741:HOH:O	4:A:758:HOH:O[3_556]	2.10	0.10
4:C:739:HOH:O	4:C:740:HOH:O[3_545]	2.11	0.09

## 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	288/325 (89%)	278 (96%)	10 (4%)	0	100	100
1	B	294/325 (90%)	281 (96%)	12 (4%)	1 (0%)	44	54
1	C	292/325 (90%)	279 (96%)	13 (4%)	0	100	100
All	All	874/975 (90%)	838 (96%)	35 (4%)	1 (0%)	55	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	TRP

### 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	246/278 (88%)	244 (99%)	2 (1%)	85	92
1	B	251/278 (90%)	244 (97%)	7 (3%)	49	63
1	C	251/278 (90%)	247 (98%)	4 (2%)	68	81
All	All	748/834 (90%)	735 (98%)	13 (2%)	66	79

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

Mol	Chain	Res	Type
1	A	167	ASN
1	A	422	GLN
1	B	252	SER
1	B	295	ASN
1	B	316	ARG
1	B	375	LEU
1	B	415	ASN
1	B	422	GLN
1	B	448	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	166	LEU
1	C	202	ARG
1	C	415	ASN
1	C	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	251	GLN
1	A	397	GLN
1	A	415	ASN
1	A	422	GLN
1	B	182	ASN
1	B	422	GLN

### 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](#)

6 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	SIA	A	1	2	17,20,21	0.39	0	19,28,31	0.84	1 (5%)
2	SIA	A	2	3,2	17,20,21	0.31	0	19,28,31	0.95	1 (5%)
3	GAL	A	3	2	12,12,12	0.73	0	17,17,17	1.38	3 (17%)
2	SIA	C	1	2	17,20,21	0.41	0	19,28,31	0.77	0
2	SIA	C	2	3,2	17,20,21	0.39	0	19,28,31	0.91	1 (5%)
3	GAL	C	3	2	12,12,12	0.56	0	17,17,17	0.60	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	SIA	A	1	2	-	0/14/34/38	0/1/1/1
2	SIA	A	2	3,2	-	0/14/34/38	0/1/1/1
3	GAL	A	3	2	-	0/2/22/22	0/1/1/1
2	SIA	C	1	2	-	0/14/34/38	0/1/1/1
2	SIA	C	2	3,2	-	0/14/34/38	0/1/1/1
3	GAL	C	3	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	SIA	C6-C5-N5	-2.81	106.06	111.00
2	C	2	SIA	C3-C4-C5	-2.09	108.94	111.46
3	A	3	GAL	C4-C3-C2	2.01	114.39	110.84
2	A	1	SIA	C4-C3-C2	2.02	113.54	109.75
3	A	3	GAL	C3-C4-C5	2.97	115.45	110.22
3	A	3	GAL	C1-C2-C3	3.14	116.33	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	SIA	6	0
3	A	3	GAL	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	SIA	1	0
3	C	3	GAL	1	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	290/325 (89%)	0.40	44 (15%) <b>2</b> <b>3</b>	18, 37, 112, 141	0
1	B	295/325 (90%)	0.61	53 (17%) <b>2</b> <b>2</b>	15, 38, 109, 134	0
1	C	292/325 (89%)	0.45	49 (16%) <b>2</b> <b>2</b>	20, 42, 110, 141	1 (0%)
All	All	877/975 (89%)	0.49	146 (16%) <b>2</b> <b>2</b>	15, 39, 110, 141	1 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	LEU	8.9
1	A	257	ALA	7.1
1	B	257	ALA	7.1
1	A	273	LEU	7.0
1	A	263	LEU	6.9
1	C	273	LEU	6.1
1	C	283	SER	6.0
1	A	281	ILE	5.8
1	C	289	VAL	5.7
1	A	276	SER	5.7
1	A	272	MET	5.5
1	B	272	MET	5.5
1	C	281	ILE	5.5
1	B	256	SER	5.2
1	B	273	LEU	5.2
1	A	274	ILE	5.1
1	A	288	THR	5.0
1	C	285	GLY	4.9
1	A	277	SER	4.9
1	A	283	SER	4.8
1	B	260	PRO	4.8
1	B	166	LEU	4.8
1	B	258	VAL	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	291	SER	4.6
1	A	278	THR	4.6
1	C	279	LEU	4.5
1	C	287	LEU	4.5
1	A	290	ARG	4.5
1	A	289	VAL	4.5
1	B	263	LEU	4.4
1	B	252	SER	4.4
1	C	284	SER	4.4
1	A	258	VAL	4.3
1	C	272	MET	4.3
1	B	261	LEU	4.3
1	A	269	VAL	4.3
1	B	238	VAL	4.3
1	C	291	SER	4.2
1	A	256	SER	4.2
1	C	269	VAL	4.2
1	B	264	ASN	4.1
1	A	280	GLU	4.0
1	B	283	SER	4.0
1	C	166	LEU	4.0
1	C	276	SER	3.9
1	A	287	LEU	3.8
1	C	263	LEU	3.8
1	A	275	ASP	3.8
1	A	285	GLY	3.8
1	C	288	THR	3.7
1	B	274	ILE	3.7
1	C	290	ARG	3.6
1	B	266	SER	3.6
1	B	239	PHE	3.6
1	B	287	LEU	3.6
1	C	274	ILE	3.6
1	C	280	GLU	3.6
1	B	161	SER	3.6
1	B	247	GLY	3.6
1	A	292	THR	3.6
1	A	270	LEU	3.6
1	C	164	PRO	3.6
1	A	242	ILE	3.5
1	C	165	VAL	3.5
1	C	282	ASN	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	251	GLN	3.4
1	B	289	VAL	3.4
1	C	252	SER	3.4
1	A	252	SER	3.4
1	C	277	SER	3.4
1	B	265	SER	3.4
1	B	269	VAL	3.3
1	C	278	THR	3.3
1	B	285	GLY	3.2
1	B	277	SER	3.2
1	C	246	ILE	3.2
1	B	164	PRO	3.2
1	C	251	GLN	3.2
1	B	259	THR	3.1
1	B	248	ALA	3.1
1	B	276	SER	3.1
1	A	282	ASN	3.1
1	A	271	ASP	3.1
1	A	239	PHE	3.1
1	C	264	ASN	3.0
1	C	260	PRO	3.0
1	A	262	ARG	3.0
1	A	166	LEU	3.0
1	B	288	THR	3.0
1	C	168	GLN	3.0
1	B	268	LYS	2.9
1	B	165	VAL	2.9
1	A	293	SER	2.9
1	C	238	VAL	2.9
1	B	278	THR	2.8
1	C	286	GLN	2.8
1	A	284	SER	2.8
1	A	260	PRO	2.7
1	C	268	LYS	2.7
1	B	253	TYR	2.7
1	C	266	SER	2.7
1	B	226	GLN	2.7
1	A	259	THR	2.7
1	C	267	THR	2.7
1	C	270	LEU	2.7
1	B	279	LEU	2.6
1	C	240	ASP	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	267	THR	2.6
1	B	220	PHE	2.5
1	C	253	TYR	2.5
1	A	254	VAL	2.5
1	C	271	ASP	2.5
1	C	275	ASP	2.5
1	C	249	ILE	2.5
1	B	254	VAL	2.4
1	C	257	ALA	2.4
1	B	267	THR	2.4
1	B	255	ALA	2.4
1	A	286	GLN	2.4
1	A	266	SER	2.4
1	B	455	THR	2.4
1	C	261	LEU	2.3
1	A	253	TYR	2.3
1	B	284	SER	2.3
1	C	255	ALA	2.3
1	C	292	THR	2.3
1	B	270	LEU	2.2
1	C	237	THR	2.2
1	C	245	ARG	2.2
1	B	250	GLU	2.2
1	B	223	ASP	2.2
1	B	275	ASP	2.2
1	C	242	ILE	2.2
1	A	264	ASN	2.2
1	A	268	LYS	2.1
1	B	240	ASP	2.1
1	A	251	GLN	2.1
1	B	241	SER	2.1
1	B	281	ILE	2.1
1	B	236	THR	2.1
1	B	249	ILE	2.1
1	C	244	SER	2.1
1	A	245	ARG	2.0
1	B	286	GLN	2.0
1	C	236	THR	2.0
1	B	235	LYS	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
2	SIA	C	1	20/21	0.92	0.20	2.16	44,59,71,71	0
2	SIA	A	1	20/21	0.92	0.10	-0.52	36,46,67,68	0
3	GAL	A	3	12/12	0.68	0.30	-	87,110,117,121	0
3	GAL	C	3	12/12	0.70	0.51	-	115,136,141,143	0
2	SIA	C	2	20/21	0.88	0.23	-	35,71,101,104	0
2	SIA	A	2	20/21	0.78	0.21	-	47,73,110,111	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.