



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 05:10 pm GMT

PDB ID : 1VPS
Title : POLYOMAVIRUS VP1 PENTAMER COMPLEXED WITH A DISIALYLATED HEXASACCHARIDE
Authors : Stehle, T.; Harrison, S.C.
Deposited on : 1997-03-07
Resolution : 1.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

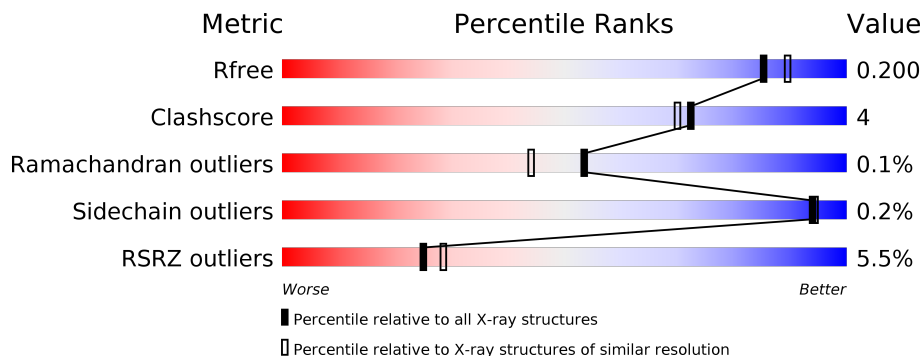
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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 ≥ 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	289	 7% 90% 8%
1	B	289	 4% 90% 10%
1	C	289	 6% 91% 8%
1	D	289	 6% 90% 8%
1	E	289	 6% 91% 8%

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	A	4	-	-	-	X
2	SIA	B	4	-	-	-	X
2	SIA	C	4	-	-	-	X
2	SIA	E	4	-	-	-	X
4	NAG	C	3	-	-	-	X
4	NAG	E	3	-	-	-	X

2 Entry composition [i](#)

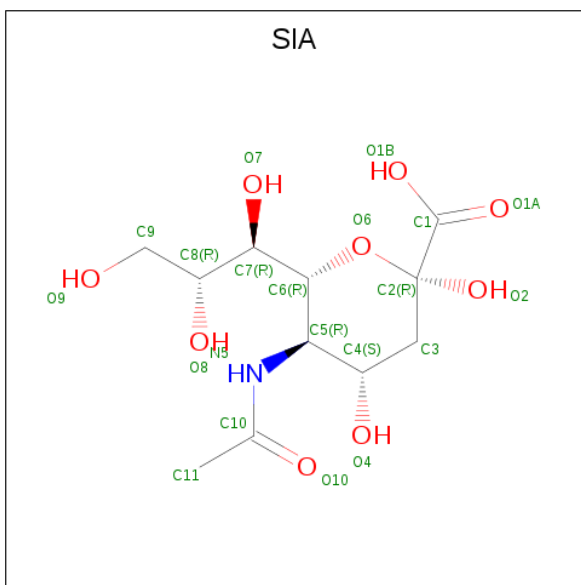
There are 5 unique types of molecules in this entry. The entry contains 13591 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 POLYOMAVIRUS VP1 PENTAMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	Total 2220	C 1404	N 373	O 432	S 11	0	0	0
1	B	289	Total 2254	C 1427	N 378	O 438	S 11	0	0	0
1	C	285	Total 2220	C 1404	N 373	O 432	S 11	0	0	0
1	D	285	Total 2220	C 1404	N 373	O 432	S 11	0	0	0
1	E	285	Total 2220	C 1404	N 373	O 432	S 11	0	0	0

- Molecule 2 is O-SIALIC ACID (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



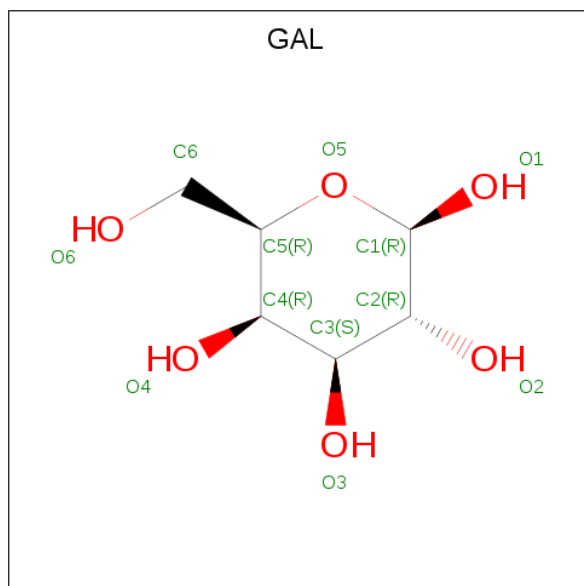
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 20	C 11	N 1	O 8	0	0

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

- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



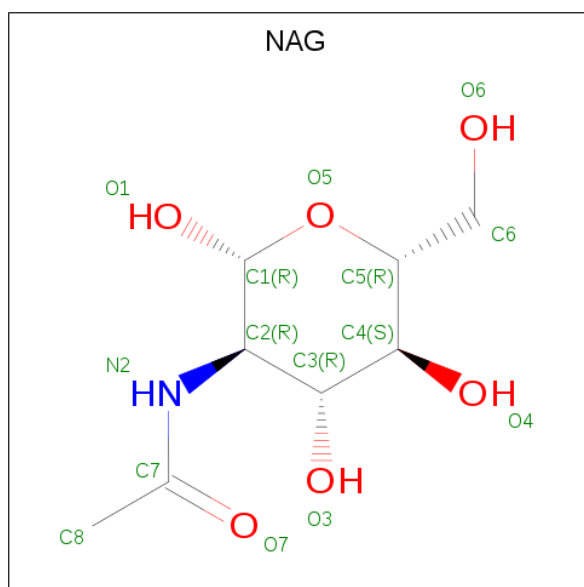
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	Total 11	C 6	O 5	0	0
3	B	1	Total 11	C 6	O 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total	O	0	0
			391	391		

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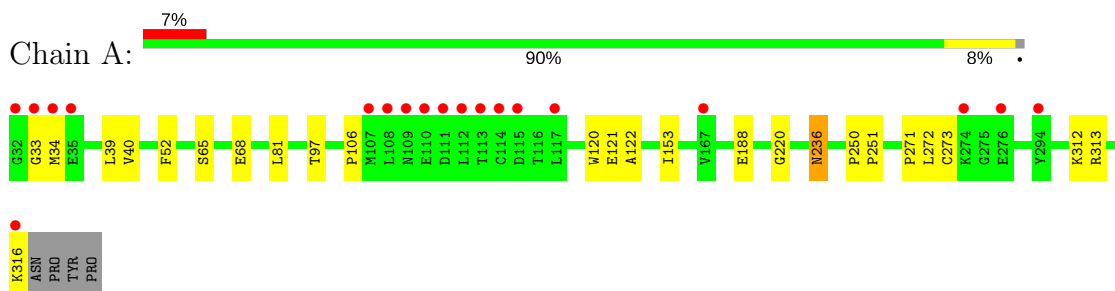
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	444	Total 444	O 444	0	0
5	C	452	Total 452	O 452	0	0
5	D	436	Total 436	O 436	0	0
5	E	404	Total 404	O 404	0	0

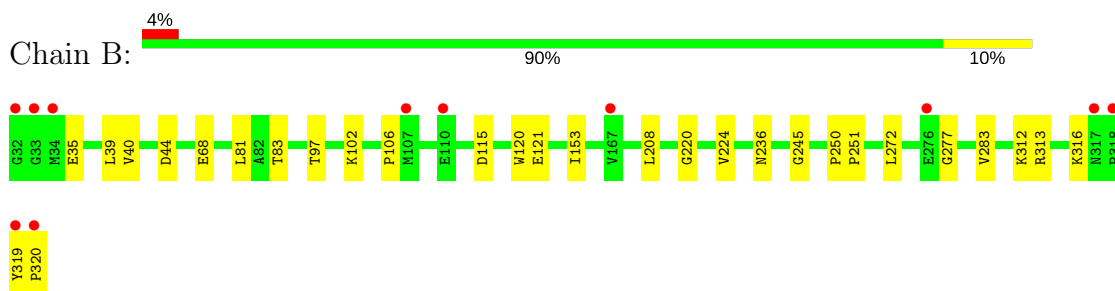
3 Residue-property plots

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

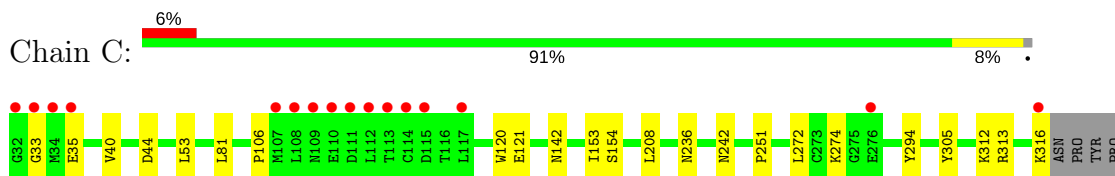
- Molecule 1: POLYOMAVIRUS VP1 PENTAMER



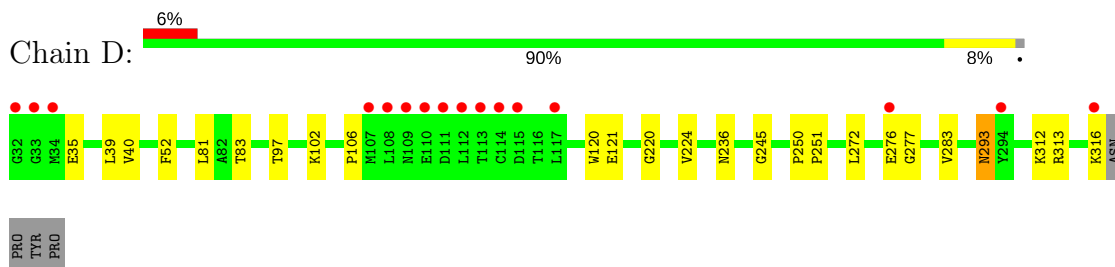
- Molecule 1: POLYOMAVIRUS VP1 PENTAMER



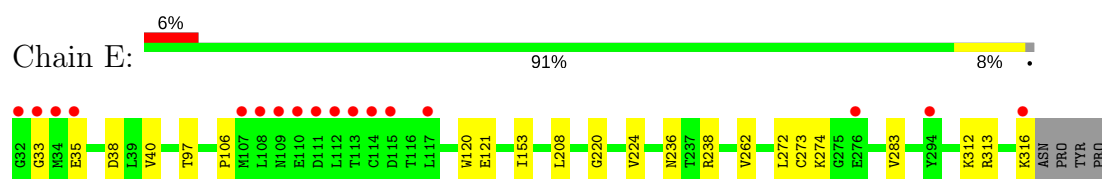
- Molecule 1: POLYOMAVIRUS VP1 PENTAMER



- Molecule 1: POLYOMAVIRUS VP1 PENTAMER



- Molecule 1: POLYOMAVIRUS VP1 PENTAMER



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.50Å 221.50Å 99.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90 24.74 – 1.92	Depositor EDS
% Data completeness (in resolution range)	85.6 (20.00-1.90) 88.7 (24.74-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.92Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.205 0.174 , 0.200	Depositor DCC
R_{free} test set	7533 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13591	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SIA, GAL, NAG

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	0.38	0/2273	0.63	0/3098
1	B	0.39	0/2310	0.65	0/3151
1	C	0.40	0/2273	0.65	0/3098
1	D	0.42	1/2273 (0.0%)	0.64	0/3098
1	E	0.38	0/2273	0.63	0/3098
All	All	0.39	1/11402 (0.0%)	0.64	0/15543

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	293	ASN	C-N	-5.84	1.20	1.34

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	2220	0	2187	15	0
1	B	2254	0	2216	20	0
1	C	2220	0	2187	20	0
1	D	2220	0	2187	18	0
1	E	2220	0	2187	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	0	34	0	0
2	B	40	0	34	1	0
2	C	40	0	34	0	0
2	D	40	0	34	1	0
2	E	40	0	34	0	0
3	A	11	0	9	0	0
3	B	11	0	9	0	0
3	C	11	0	9	0	0
3	D	11	0	9	0	0
3	E	11	0	9	0	0
4	A	15	0	13	0	0
4	B	15	0	13	0	0
4	C	15	0	13	0	0
4	D	15	0	13	0	0
4	E	15	0	13	0	0
5	A	391	0	0	3	0
5	B	444	0	0	6	0
5	C	452	0	0	3	0
5	D	436	0	0	2	0
5	E	404	0	0	6	0
All	All	13591	0	11244	83	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 4.

All (83) 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:273:CYS:SG	5:A:651:HOH:O	2.50	0.69
1:C:35:GLU:HB3	1:C:316:LYS:HB2	1.75	0.68
1:D:35:GLU:HB3	1:D:316:LYS:HB2	1.75	0.66
1:E:273:CYS:SG	5:E:705:HOH:O	2.50	0.66
1:B:35:GLU:HB3	1:B:316:LYS:HB2	1.85	0.57
1:A:33:GLY:O	1:A:316:LYS:HB3	2.04	0.57
1:E:35:GLU:HB3	1:E:316:LYS:HB2	1.87	0.57
1:C:106:PRO:HG2	1:C:120:TRP:CZ2	2.41	0.56
1:D:102:LYS:NZ	1:D:277:GLY:HA3	2.20	0.56
1:E:262:VAL:HG13	5:E:692:HOH:O	2.06	0.56
1:B:153:ILE:HA	1:C:81:LEU:HD21	1.87	0.56
1:C:305:TYR:HE1	5:C:502:HOH:O	1.88	0.56
1:D:39:LEU:HD23	1:D:313:ARG:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:TYR:HD2	5:C:717:HOH:O	1.90	0.55
1:B:224:VAL:HG11	1:B:283:VAL:HG21	1.90	0.54
5:B:626:HOH:O	1:C:294:TYR:HA	2.07	0.54
1:D:102:LYS:HZ1	1:D:277:GLY:HA3	1.73	0.54
1:A:81:LEU:HD21	1:E:153:ILE:HA	1.90	0.53
1:D:121:GLU:OE1	1:D:313:ARG:HD3	2.09	0.53
1:B:115:ASP:HB2	5:B:651:HOH:O	2.08	0.52
1:C:153:ILE:HA	1:D:81:LEU:HD21	1.91	0.52
1:B:106:PRO:HG2	1:B:120:TRP:CZ2	2.44	0.52
1:A:121:GLU:OE1	1:A:313:ARG:HD3	2.10	0.51
5:B:749:HOH:O	1:C:242:ASN:HB2	2.09	0.51
1:C:236:ASN:ND2	1:C:272:LEU:O	2.44	0.51
1:C:121:GLU:OE1	1:C:313:ARG:HD3	2.10	0.51
1:B:102:LYS:NZ	1:B:277:GLY:HA3	2.27	0.49
1:E:208:LEU:HD13	5:E:694:HOH:O	2.12	0.49
1:E:121:GLU:OE1	1:E:313:ARG:HD3	2.13	0.49
1:E:40:VAL:HB	1:E:312:LYS:HB2	1.94	0.49
1:E:238:ARG:HD3	5:E:637:HOH:O	2.13	0.48
1:A:65:SER:HB3	1:A:68:GLU:HB2	1.95	0.48
1:B:236:ASN:ND2	1:B:272:LEU:O	2.46	0.48
1:C:53:LEU:HG	5:C:759:HOH:O	2.13	0.48
1:D:293:ASN:HB3	5:D:733:HOH:O	2.13	0.48
1:D:106:PRO:HG2	1:D:120:TRP:CZ2	2.49	0.48
1:A:39:LEU:HD23	1:A:313:ARG:HD2	1.96	0.47
1:A:106:PRO:HG2	1:A:120:TRP:CZ2	2.49	0.47
1:C:236:ASN:ND2	1:C:274:LYS:HE3	2.29	0.47
1:C:236:ASN:HD22	1:C:274:LYS:HE3	1.79	0.47
1:C:33:GLY:O	1:C:316:LYS:HB3	2.14	0.47
1:E:236:ASN:ND2	1:E:272:LEU:O	2.48	0.47
1:E:106:PRO:HG2	1:E:120:TRP:CZ2	2.50	0.47
1:E:97:THR:OG1	1:E:220:GLY:HA2	2.15	0.46
1:E:224:VAL:HG11	1:E:283:VAL:HG21	1.97	0.46
1:E:33:GLY:O	1:E:316:LYS:HB3	2.16	0.46
1:D:40:VAL:HB	1:D:312:LYS:HB2	1.97	0.46
1:B:121:GLU:OE1	1:B:313:ARG:HD3	2.16	0.45
1:B:44:ASP:O	1:B:312:LYS:HE3	2.17	0.45
1:A:40:VAL:HB	1:A:312:LYS:HB2	1.99	0.45
5:A:679:HOH:O	1:B:208:LEU:HD13	2.17	0.45
1:B:319:TYR:HA	1:B:320:PRO:HD3	1.80	0.44
5:B:751:HOH:O	1:C:208:LEU:HD13	2.17	0.44
1:E:38:ASP:HB2	5:E:573:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:THR:HG23	2:B:4:SIA:H91	2.00	0.44
1:D:224:VAL:HG11	1:D:283:VAL:HG21	2.00	0.44
1:B:68:GLU:HG2	5:B:752:HOH:O	2.18	0.43
1:D:97:THR:OG1	1:D:220:GLY:HA2	2.18	0.43
1:A:153:ILE:HA	1:B:81:LEU:HD21	2.00	0.43
1:D:52:PHE:HB2	5:E:694:HOH:O	2.18	0.43
1:B:39:LEU:HD23	1:B:313:ARG:HD2	2.01	0.43
1:B:40:VAL:HB	1:B:312:LYS:HB2	2.01	0.43
1:B:251:PRO:HG3	5:B:727:HOH:O	2.19	0.42
1:C:40:VAL:HB	1:C:312:LYS:HB2	1.99	0.42
1:D:236:ASN:ND2	1:D:272:LEU:O	2.50	0.42
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.95	0.42
1:A:122:ALA:HB3	1:A:271:PRO:HD2	2.02	0.42
1:D:83:THR:HG23	2:D:4:SIA:H91	2.02	0.42
1:E:106:PRO:HG2	1:E:120:TRP:HZ2	1.83	0.42
1:D:276:GLU:HB3	5:D:722:HOH:O	2.20	0.41
1:C:274:LYS:HE2	1:C:274:LYS:HB3	1.92	0.41
1:A:251:PRO:HD2	1:B:245:GLY:HA3	2.02	0.41
1:A:97:THR:OG1	1:A:220:GLY:HA2	2.19	0.41
1:C:142:ASN:HB2	1:C:154:SER:OG	2.20	0.41
1:D:106:PRO:HG2	1:D:120:TRP:HZ2	1.84	0.41
1:E:274:LYS:HE2	1:E:274:LYS:HB3	1.89	0.41
1:C:251:PRO:HD2	1:D:245:GLY:HA3	2.03	0.40
1:D:250:PRO:HA	1:D:251:PRO:HD3	1.96	0.40
1:A:236:ASN:ND2	1:A:272:LEU:O	2.55	0.40
1:C:44:ASP:O	1:C:312:LYS:HE3	2.21	0.40
1:A:52:PHE:HB3	5:A:656:HOH:O	2.21	0.40
1:B:97:THR:OG1	1:B:220:GLY:HA2	2.21	0.40
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.89	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	283/289 (98%)	273 (96%)	9 (3%)	1 (0%)	36	25
1	B	287/289 (99%)	273 (95%)	14 (5%)	0	100	100
1	C	283/289 (98%)	268 (95%)	15 (5%)	0	100	100
1	D	283/289 (98%)	272 (96%)	11 (4%)	0	100	100
1	E	283/289 (98%)	271 (96%)	12 (4%)	0	100	100
All	All	1419/1445 (98%)	1357 (96%)	61 (4%)	1 (0%)	53	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	MET

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	249/253 (98%)	247 (99%)	2 (1%)	83	83
1	B	253/253 (100%)	253 (100%)	0	100	100
1	C	249/253 (98%)	249 (100%)	0	100	100
1	D	249/253 (98%)	249 (100%)	0	100	100
1	E	249/253 (98%)	249 (100%)	0	100	100
All	All	1249/1265 (99%)	1247 (100%)	2 (0%)	94	94

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

Mol	Chain	Res	Type
1	A	188	GLU
1	A	236	ASN

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](#)

20 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	3	17,20,21	0.50	0	19,28,31	0.79	1 (5%)
3	GAL	A	2	2,4	11,11,12	0.47	0	15,15,17	0.52	0
4	NAG	A	3	3,2	15,15,15	0.85	1 (6%)	21,21,21	1.32	5 (23%)
2	SIA	A	4	4	17,20,21	1.39	2 (11%)	19,28,31	0.80	1 (5%)
2	SIA	B	1	3	17,20,21	0.51	0	19,28,31	0.68	0
3	GAL	B	2	2,4	11,11,12	0.40	0	15,15,17	0.63	0
4	NAG	B	3	3,2	15,15,15	0.47	0	21,21,21	0.54	0
2	SIA	B	4	4	17,20,21	0.74	0	19,28,31	0.82	1 (5%)
2	SIA	C	1	3	17,20,21	0.52	0	19,28,31	0.71	0
3	GAL	C	2	2,4	11,11,12	0.72	0	15,15,17	0.66	0
4	NAG	C	3	3,2	15,15,15	0.92	1 (6%)	21,21,21	1.13	1 (4%)
2	SIA	C	4	4	17,20,21	1.06	1 (5%)	19,28,31	0.82	1 (5%)
2	SIA	D	1	3	17,20,21	0.43	0	19,28,31	0.68	0
3	GAL	D	2	2,4	11,11,12	0.41	0	15,15,17	0.58	0
4	NAG	D	3	3,2	15,15,15	0.52	0	21,21,21	0.83	0
2	SIA	D	4	4	17,20,21	0.87	0	19,28,31	1.14	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	E	1	3	17,20,21	0.53	0	19,28,31	0.70	0
3	GAL	E	2	2,4	11,11,12	0.61	0	15,15,17	0.51	0
4	NAG	E	3	3,2	15,15,15	0.74	0	21,21,21	0.93	1 (4%)
2	SIA	E	4	4	17,20,21	0.87	1 (5%)	19,28,31	0.87	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	3	-	0/14/34/38	0/1/1/1
3	GAL	A	2	2,4	-	0/2/19/22	0/1/1/1
4	NAG	A	3	3,2	-	0/6/26/26	0/1/1/1
2	SIA	A	4	4	-	0/14/34/38	0/1/1/1
2	SIA	B	1	3	-	0/14/34/38	0/1/1/1
3	GAL	B	2	2,4	-	0/2/19/22	0/1/1/1
4	NAG	B	3	3,2	-	0/6/26/26	0/1/1/1
2	SIA	B	4	4	-	0/14/34/38	0/1/1/1
2	SIA	C	1	3	-	0/14/34/38	0/1/1/1
3	GAL	C	2	2,4	-	0/2/19/22	0/1/1/1
4	NAG	C	3	3,2	-	0/6/26/26	0/1/1/1
2	SIA	C	4	4	-	0/14/34/38	0/1/1/1
2	SIA	D	1	3	-	0/14/34/38	0/1/1/1
3	GAL	D	2	2,4	-	0/2/19/22	0/1/1/1
4	NAG	D	3	3,2	-	0/6/26/26	0/1/1/1
2	SIA	D	4	4	-	0/14/34/38	0/1/1/1
2	SIA	E	1	3	-	0/14/34/38	0/1/1/1
3	GAL	E	2	2,4	-	0/2/19/22	0/1/1/1
4	NAG	E	3	3,2	-	0/6/26/26	0/1/1/1
2	SIA	E	4	4	-	0/14/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	NAG	C1-C2	2.11	1.55	1.52
4	A	3	NAG	C1-C2	2.24	1.55	1.52
2	E	4	SIA	C4-C5	2.39	1.55	1.53
2	C	4	SIA	C4-C5	2.91	1.55	1.53
2	A	4	SIA	C4-C5	3.19	1.56	1.53
2	A	4	SIA	C3-C4	3.22	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	SIA	C3-C4-C5	-4.05	106.57	111.46
2	E	4	SIA	C8-C7-C6	-2.97	107.33	113.03
2	A	4	SIA	C8-C7-C6	-2.83	107.59	113.03
4	C	3	NAG	C1-C2-N2	-2.76	107.53	110.73
2	B	4	SIA	C8-C7-C6	-2.63	107.99	113.03
2	C	4	SIA	C8-C7-C6	-2.26	108.70	113.03
4	A	3	NAG	C3-C4-C5	-2.23	106.24	110.24
2	A	1	SIA	C8-C7-C6	-2.12	108.96	113.03
4	A	3	NAG	C1-C2-N2	-2.06	108.34	110.73
4	E	3	NAG	C6-C5-C4	2.18	118.14	112.99
4	A	3	NAG	C6-C5-C4	2.24	118.28	112.99
4	A	3	NAG	C1-C2-C3	2.33	113.72	110.54
4	A	3	NAG	O5-C1-C2	2.88	112.41	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	SIA	1	0
2	D	4	SIA	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, 95th 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 ²)	Q<0.9
1	A	285/289 (98%)	0.14	19 (6%) 18 20	16, 25, 59, 95	0
1	B	289/289 (100%)	-0.07	11 (3%) 40 44	14, 22, 53, 82	0
1	C	285/289 (98%)	0.03	16 (5%) 24 28	14, 20, 54, 92	0
1	D	285/289 (98%)	0.06	16 (5%) 24 28	13, 20, 57, 92	0
1	E	285/289 (98%)	0.13	17 (5%) 22 25	17, 25, 59, 94	0
All	All	1429/1445 (98%)	0.06	79 (5%) 25 28	13, 22, 58, 95	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	LEU	14.2
1	A	112	LEU	13.4
1	D	112	LEU	12.6
1	E	113	THR	11.3
1	A	113	THR	11.2
1	E	112	LEU	10.6
1	D	33	GLY	10.6
1	C	113	THR	10.4
1	E	114	CYS	10.0
1	D	113	THR	9.9
1	C	33	GLY	9.9
1	B	32	GLY	9.3
1	A	114	CYS	9.2
1	D	114	CYS	9.0
1	A	111	ASP	8.7
1	D	32	GLY	8.6
1	E	32	GLY	8.5
1	E	33	GLY	8.4
1	C	114	CYS	8.1
1	A	33	GLY	7.9

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Mol	Chain	Res	Type	RSRZ
1	D	111	ASP	7.8
1	B	33	GLY	7.8
1	E	111	ASP	7.7
1	E	110	GLU	7.4
1	C	111	ASP	7.4
1	D	34	MET	7.0
1	A	34	MET	6.5
1	C	32	GLY	6.4
1	D	110	GLU	6.3
1	A	110	GLU	6.2
1	E	34	MET	6.2
1	A	32	GLY	6.1
1	C	107	MET	6.0
1	E	107	MET	5.7
1	B	320	PRO	5.4
1	C	34	MET	5.3
1	C	110	GLU	5.3
1	E	316	LYS	5.1
1	D	276	GLU	5.0
1	A	115	ASP	5.0
1	E	115	ASP	4.9
1	A	109	ASN	4.7
1	D	109	ASN	4.7
1	C	115	ASP	4.7
1	C	276	GLU	4.6
1	E	109	ASN	4.5
1	D	107	MET	4.4
1	B	107	MET	4.4
1	D	115	ASP	4.3
1	A	107	MET	4.3
1	B	276	GLU	4.0
1	B	317	ASN	4.0
1	C	316	LYS	4.0
1	E	276	GLU	3.9
1	A	316	LYS	3.8
1	A	294	TYR	3.8
1	A	117	LEU	3.8
1	B	110	GLU	3.6
1	A	276	GLU	3.5
1	D	316	LYS	3.5
1	B	34	MET	3.3
1	E	117	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	109	ASN	3.2
1	A	108	LEU	3.1
1	C	35	GLU	3.0
1	E	294	TYR	3.0
1	D	108	LEU	2.9
1	E	108	LEU	2.9
1	B	318	PRO	2.8
1	C	108	LEU	2.8
1	B	319	TYR	2.7
1	C	117	LEU	2.5
1	A	35	GLU	2.5
1	E	35	GLU	2.5
1	D	117	LEU	2.4
1	B	167	VAL	2.3
1	D	294	TYR	2.2
1	A	274	LYS	2.2
1	A	167	VAL	2.1

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SIA	B	4	20/21	0.50	0.51	80,82,83,84	0
2	SIA	C	4	20/21	0.51	0.55	67,71,77,77	0
2	SIA	E	4	20/21	0.54	0.50	78,81,82,82	0
4	NAG	E	3	15/15	0.55	0.41	59,69,74,78	0
2	SIA	A	4	20/21	0.58	0.45	66,71,73,73	0
4	NAG	B	3	15/15	0.62	0.40	53,66,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	3	15/15	0.63	0.37	54,62,66,69	0
4	NAG	C	3	15/15	0.63	0.43	46,58,63,67	0
2	SIA	D	4	20/21	0.71	0.23	46,56,62,63	0
4	NAG	D	3	15/15	0.75	0.27	41,51,53,54	0
3	GAL	E	2	11/12	0.83	0.15	40,46,51,53	0
2	SIA	E	1	20/21	0.90	0.11	31,34,37,38	0
2	SIA	A	1	20/21	0.90	0.11	28,32,36,40	0
2	SIA	D	1	20/21	0.92	0.12	23,25,29,33	0
3	GAL	C	2	11/12	0.92	0.09	28,32,35,38	0
3	GAL	A	2	11/12	0.92	0.13	37,44,46,48	0
2	SIA	B	1	20/21	0.92	0.11	24,27,31,35	0
2	SIA	C	1	20/21	0.93	0.10	22,24,29,34	0
3	GAL	B	2	11/12	0.93	0.10	32,37,41,44	0
3	GAL	D	2	11/12	0.93	0.09	28,31,33,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.