



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 08:19 PM BST

PDB ID : 6Y63
Title : Structure of Sheep Polyomavirus VP1 in complex with 3'-Sialyllactosamine
Authors : Stroh, L.J.; Rustmeier, N.H.; Stehle, T.
Deposited on : 2020-02-26
Resolution : 1.65 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:

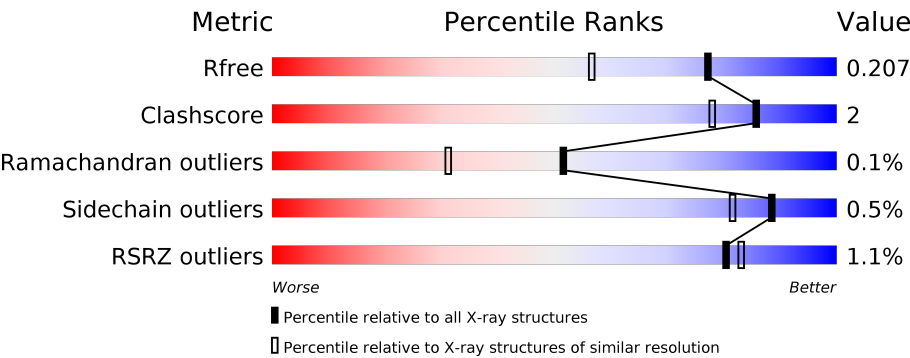
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 respectively. 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	AAA	293	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>83%5%12%</div></div>
1	BBB	293	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>81%15%</div></div>
1	CCC	293	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>85%12%</div></div>
1	DDD	293	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>83%5%12%</div></div>
1	EEE	293	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>82%15%</div></div>
1	FFF	293	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>83%14%</div></div>

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Mol	Chain	Length	Quality of chain
1	GGG	293	
1	HHH	293	
1	III	293	
1	JJJ	293	
2	A	2	
2	B	2	
2	C	2	
2	D	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22396 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	257	Total	C	N	O	S	0	2	0
			1998	1272	335	377	14			
1	BBB	249	Total	C	N	O	S	0	3	0
			1944	1246	324	361	13			
1	CCC	257	Total	C	N	O	S	0	2	0
			2002	1275	337	377	13			
1	DDD	257	Total	C	N	O	S	0	4	0
			2016	1283	335	384	14			
1	EEE	250	Total	C	N	O	S	0	2	0
			1954	1247	331	364	12			
1	FFF	253	Total	C	N	O	S	0	1	0
			1943	1241	325	364	13			
1	GGG	250	Total	C	N	O	S	0	3	0
			1955	1247	329	366	13			
1	HHH	256	Total	C	N	O	S	0	1	0
			1993	1270	335	375	13			
1	III	251	Total	C	N	O	S	0	1	0
			1933	1237	323	361	12			
1	JJJ	258	Total	C	N	O	S	0	0	0
			1973	1256	328	376	13			

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
AAA	0	GLY	-	expression tag	UNP A0A0E3ZCF3
AAA	1	SER	-	expression tag	UNP A0A0E3ZCF3
AAA	2	SER	-	expression tag	UNP A0A0E3ZCF3
AAA	3	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	4	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	5	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	6	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	7	HIS	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	8	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	9	SER	-	expression tag	UNP A0A0E3ZCF3
AAA	10	SER	-	expression tag	UNP A0A0E3ZCF3
AAA	11	GLY	-	expression tag	UNP A0A0E3ZCF3
AAA	12	LEU	-	expression tag	UNP A0A0E3ZCF3
AAA	13	VAL	-	expression tag	UNP A0A0E3ZCF3
AAA	14	PRO	-	expression tag	UNP A0A0E3ZCF3
AAA	15	ARG	-	expression tag	UNP A0A0E3ZCF3
AAA	16	GLY	-	expression tag	UNP A0A0E3ZCF3
AAA	17	SER	-	expression tag	UNP A0A0E3ZCF3
AAA	18	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	19	MET	-	expression tag	UNP A0A0E3ZCF3
AAA	95	SER	CYS	conflict	UNP A0A0E3ZCF3
BBB	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
BBB	0	GLY	-	expression tag	UNP A0A0E3ZCF3
BBB	1	SER	-	expression tag	UNP A0A0E3ZCF3
BBB	2	SER	-	expression tag	UNP A0A0E3ZCF3
BBB	3	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	4	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	5	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	6	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	7	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	8	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	9	SER	-	expression tag	UNP A0A0E3ZCF3
BBB	10	SER	-	expression tag	UNP A0A0E3ZCF3
BBB	11	GLY	-	expression tag	UNP A0A0E3ZCF3
BBB	12	LEU	-	expression tag	UNP A0A0E3ZCF3
BBB	13	VAL	-	expression tag	UNP A0A0E3ZCF3
BBB	14	PRO	-	expression tag	UNP A0A0E3ZCF3
BBB	15	ARG	-	expression tag	UNP A0A0E3ZCF3
BBB	16	GLY	-	expression tag	UNP A0A0E3ZCF3
BBB	17	SER	-	expression tag	UNP A0A0E3ZCF3
BBB	18	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	19	MET	-	expression tag	UNP A0A0E3ZCF3
BBB	95	SER	CYS	conflict	UNP A0A0E3ZCF3
CCC	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
CCC	0	GLY	-	expression tag	UNP A0A0E3ZCF3
CCC	1	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	2	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	3	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	4	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	5	HIS	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	6	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	7	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	8	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	9	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	10	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	11	GLY	-	expression tag	UNP A0A0E3ZCF3
CCC	12	LEU	-	expression tag	UNP A0A0E3ZCF3
CCC	13	VAL	-	expression tag	UNP A0A0E3ZCF3
CCC	14	PRO	-	expression tag	UNP A0A0E3ZCF3
CCC	15	ARG	-	expression tag	UNP A0A0E3ZCF3
CCC	16	GLY	-	expression tag	UNP A0A0E3ZCF3
CCC	17	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	18	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	19	MET	-	expression tag	UNP A0A0E3ZCF3
CCC	95	SER	CYS	conflict	UNP A0A0E3ZCF3
DDD	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
DDD	0	GLY	-	expression tag	UNP A0A0E3ZCF3
DDD	1	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	2	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	3	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	4	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	5	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	6	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	7	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	8	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	9	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	10	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	11	GLY	-	expression tag	UNP A0A0E3ZCF3
DDD	12	LEU	-	expression tag	UNP A0A0E3ZCF3
DDD	13	VAL	-	expression tag	UNP A0A0E3ZCF3
DDD	14	PRO	-	expression tag	UNP A0A0E3ZCF3
DDD	15	ARG	-	expression tag	UNP A0A0E3ZCF3
DDD	16	GLY	-	expression tag	UNP A0A0E3ZCF3
DDD	17	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	18	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	19	MET	-	expression tag	UNP A0A0E3ZCF3
DDD	95	SER	CYS	conflict	UNP A0A0E3ZCF3
EEE	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
EEE	0	GLY	-	expression tag	UNP A0A0E3ZCF3
EEE	1	SER	-	expression tag	UNP A0A0E3ZCF3
EEE	2	SER	-	expression tag	UNP A0A0E3ZCF3
EEE	3	HIS	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	4	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	5	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	6	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	7	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	8	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	9	SER	-	expression tag	UNP A0A0E3ZCF3
EEE	10	SER	-	expression tag	UNP A0A0E3ZCF3
EEE	11	GLY	-	expression tag	UNP A0A0E3ZCF3
EEE	12	LEU	-	expression tag	UNP A0A0E3ZCF3
EEE	13	VAL	-	expression tag	UNP A0A0E3ZCF3
EEE	14	PRO	-	expression tag	UNP A0A0E3ZCF3
EEE	15	ARG	-	expression tag	UNP A0A0E3ZCF3
EEE	16	GLY	-	expression tag	UNP A0A0E3ZCF3
EEE	17	SER	-	expression tag	UNP A0A0E3ZCF3
EEE	18	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	19	MET	-	expression tag	UNP A0A0E3ZCF3
EEE	95	SER	CYS	conflict	UNP A0A0E3ZCF3
FFF	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
FFF	0	GLY	-	expression tag	UNP A0A0E3ZCF3
FFF	1	SER	-	expression tag	UNP A0A0E3ZCF3
FFF	2	SER	-	expression tag	UNP A0A0E3ZCF3
FFF	3	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	4	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	5	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	6	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	7	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	8	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	9	SER	-	expression tag	UNP A0A0E3ZCF3
FFF	10	SER	-	expression tag	UNP A0A0E3ZCF3
FFF	11	GLY	-	expression tag	UNP A0A0E3ZCF3
FFF	12	LEU	-	expression tag	UNP A0A0E3ZCF3
FFF	13	VAL	-	expression tag	UNP A0A0E3ZCF3
FFF	14	PRO	-	expression tag	UNP A0A0E3ZCF3
FFF	15	ARG	-	expression tag	UNP A0A0E3ZCF3
FFF	16	GLY	-	expression tag	UNP A0A0E3ZCF3
FFF	17	SER	-	expression tag	UNP A0A0E3ZCF3
FFF	18	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	19	MET	-	expression tag	UNP A0A0E3ZCF3
FFF	95	SER	CYS	conflict	UNP A0A0E3ZCF3
GGG	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
GGG	0	GLY	-	expression tag	UNP A0A0E3ZCF3
GGG	1	SER	-	expression tag	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
GGG	2	SER	-	expression tag	UNP A0A0E3ZCF3
GGG	3	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	4	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	5	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	6	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	7	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	8	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	9	SER	-	expression tag	UNP A0A0E3ZCF3
GGG	10	SER	-	expression tag	UNP A0A0E3ZCF3
GGG	11	GLY	-	expression tag	UNP A0A0E3ZCF3
GGG	12	LEU	-	expression tag	UNP A0A0E3ZCF3
GGG	13	VAL	-	expression tag	UNP A0A0E3ZCF3
GGG	14	PRO	-	expression tag	UNP A0A0E3ZCF3
GGG	15	ARG	-	expression tag	UNP A0A0E3ZCF3
GGG	16	GLY	-	expression tag	UNP A0A0E3ZCF3
GGG	17	SER	-	expression tag	UNP A0A0E3ZCF3
GGG	18	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	19	MET	-	expression tag	UNP A0A0E3ZCF3
GGG	95	SER	CYS	conflict	UNP A0A0E3ZCF3
HHH	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
HHH	0	GLY	-	expression tag	UNP A0A0E3ZCF3
HHH	1	SER	-	expression tag	UNP A0A0E3ZCF3
HHH	2	SER	-	expression tag	UNP A0A0E3ZCF3
HHH	3	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	4	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	5	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	6	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	7	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	8	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	9	SER	-	expression tag	UNP A0A0E3ZCF3
HHH	10	SER	-	expression tag	UNP A0A0E3ZCF3
HHH	11	GLY	-	expression tag	UNP A0A0E3ZCF3
HHH	12	LEU	-	expression tag	UNP A0A0E3ZCF3
HHH	13	VAL	-	expression tag	UNP A0A0E3ZCF3
HHH	14	PRO	-	expression tag	UNP A0A0E3ZCF3
HHH	15	ARG	-	expression tag	UNP A0A0E3ZCF3
HHH	16	GLY	-	expression tag	UNP A0A0E3ZCF3
HHH	17	SER	-	expression tag	UNP A0A0E3ZCF3
HHH	18	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	19	MET	-	expression tag	UNP A0A0E3ZCF3
HHH	95	SER	CYS	conflict	UNP A0A0E3ZCF3
III	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3

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Chain	Residue	Modelled	Actual	Comment	Reference
III	0	GLY	-	expression tag	UNP A0A0E3ZCF3
III	1	SER	-	expression tag	UNP A0A0E3ZCF3
III	2	SER	-	expression tag	UNP A0A0E3ZCF3
III	3	HIS	-	expression tag	UNP A0A0E3ZCF3
III	4	HIS	-	expression tag	UNP A0A0E3ZCF3
III	5	HIS	-	expression tag	UNP A0A0E3ZCF3
III	6	HIS	-	expression tag	UNP A0A0E3ZCF3
III	7	HIS	-	expression tag	UNP A0A0E3ZCF3
III	8	HIS	-	expression tag	UNP A0A0E3ZCF3
III	9	SER	-	expression tag	UNP A0A0E3ZCF3
III	10	SER	-	expression tag	UNP A0A0E3ZCF3
III	11	GLY	-	expression tag	UNP A0A0E3ZCF3
III	12	LEU	-	expression tag	UNP A0A0E3ZCF3
III	13	VAL	-	expression tag	UNP A0A0E3ZCF3
III	14	PRO	-	expression tag	UNP A0A0E3ZCF3
III	15	ARG	-	expression tag	UNP A0A0E3ZCF3
III	16	GLY	-	expression tag	UNP A0A0E3ZCF3
III	17	SER	-	expression tag	UNP A0A0E3ZCF3
III	18	HIS	-	expression tag	UNP A0A0E3ZCF3
III	19	MET	-	expression tag	UNP A0A0E3ZCF3
III	95	SER	CYS	conflict	UNP A0A0E3ZCF3
JJJ	-1	MET	-	initiating methionine	UNP A0A0E3ZCF3
JJJ	0	GLY	-	expression tag	UNP A0A0E3ZCF3
JJJ	1	SER	-	expression tag	UNP A0A0E3ZCF3
JJJ	2	SER	-	expression tag	UNP A0A0E3ZCF3
JJJ	3	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	4	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	5	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	6	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	7	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	8	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	9	SER	-	expression tag	UNP A0A0E3ZCF3
JJJ	10	SER	-	expression tag	UNP A0A0E3ZCF3
JJJ	11	GLY	-	expression tag	UNP A0A0E3ZCF3
JJJ	12	LEU	-	expression tag	UNP A0A0E3ZCF3
JJJ	13	VAL	-	expression tag	UNP A0A0E3ZCF3
JJJ	14	PRO	-	expression tag	UNP A0A0E3ZCF3
JJJ	15	ARG	-	expression tag	UNP A0A0E3ZCF3
JJJ	16	GLY	-	expression tag	UNP A0A0E3ZCF3
JJJ	17	SER	-	expression tag	UNP A0A0E3ZCF3
JJJ	18	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	19	MET	-	expression tag	UNP A0A0E3ZCF3

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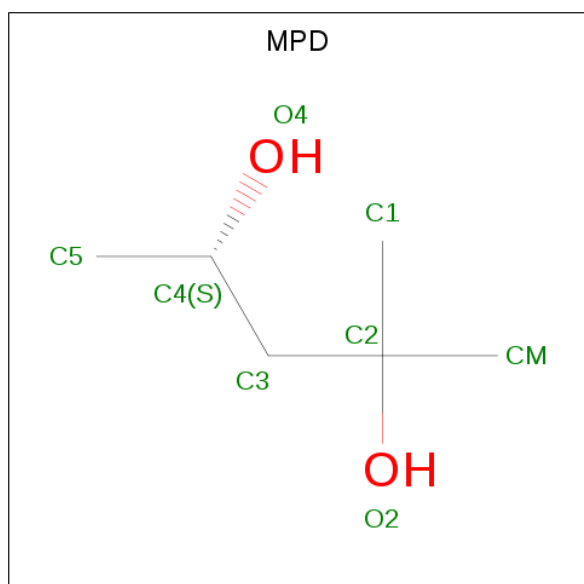
Chain	Residue	Modelled	Actual	Comment	Reference
JJJ	95	SER	CYS	conflict	UNP A0A0E3ZCF3

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	B	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	C	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	D	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			8	6	2		

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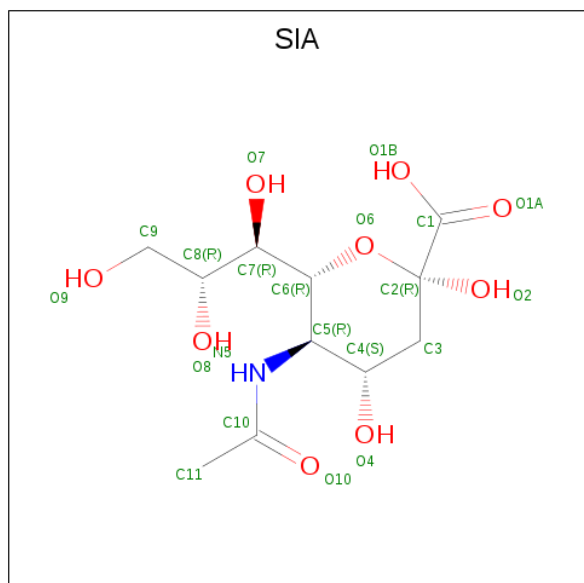
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			8	6	2		
3	BBB	1	Total	C	O	0	0
			8	6	2		
3	BBB	1	Total	C	O	0	0
			8	6	2		
3	BBB	1	Total	C	O	0	0
			8	6	2		
3	CCC	1	Total	C	O	0	0
			8	6	2		
3	DDD	1	Total	C	O	0	0
			8	6	2		
3	DDD	1	Total	C	O	0	0
			8	6	2		
3	EEE	1	Total	C	O	0	0
			8	6	2		
3	EEE	1	Total	C	O	0	0
			8	6	2		
3	FFF	1	Total	C	O	0	0
			8	6	2		
3	FFF	1	Total	C	O	0	0
			8	6	2		
3	FFF	1	Total	C	O	0	0
			8	6	2		
3	GGG	1	Total	C	O	0	0
			8	6	2		
3	GGG	1	Total	C	O	0	0
			8	6	2		
3	HHH	1	Total	C	O	0	0
			8	6	2		
3	HHH	1	Total	C	O	0	0
			8	6	2		
3	III	1	Total	C	O	0	0
			8	6	2		
3	III	1	Total	C	O	0	0
			8	6	2		
3	JJJ	1	Total	C	O	0	0
			8	6	2		
3	JJJ	1	Total	C	O	0	0
			8	6	2		
3	JJJ	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	DDD	2	Total	Mg	0	0
			2	2		
4	AAA	1	Total	Mg	0	0
			1	1		
4	CCC	1	Total	Mg	0	0
			1	1		
4	III	2	Total	Mg	0	0
			2	2		
4	HHH	1	Total	Mg	0	0
			1	1		
4	FFF	2	Total	Mg	0	0
			2	2		
4	BBB	1	Total	Mg	0	0
			1	1		
4	GGG	1	Total	Mg	0	0
			1	1		

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	EEE	1	Total	C	N	O	0	0
			21	11	1	9		
5	GGG	1	Total	C	N	O	0	0
			21	11	1	9		

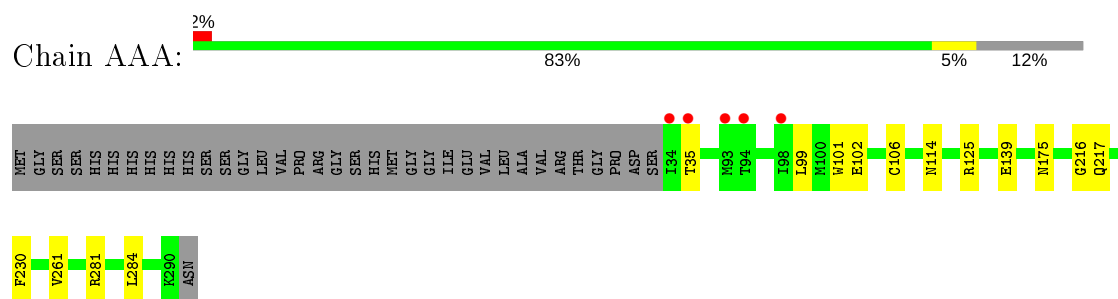
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	230	Total 232	O 232	0	2
6	BBB	230	Total 231	O 231	0	1
6	CCC	252	Total 256	O 256	0	4
6	DDD	296	Total 299	O 299	0	3
6	EEE	244	Total 247	O 247	0	3
6	FFF	175	Total 177	O 177	0	2
6	GGG	245	Total 247	O 247	0	2
6	HHH	237	Total 237	O 237	0	0
6	III	221	Total 223	O 223	0	2
6	JJJ	178	Total 179	O 179	0	1

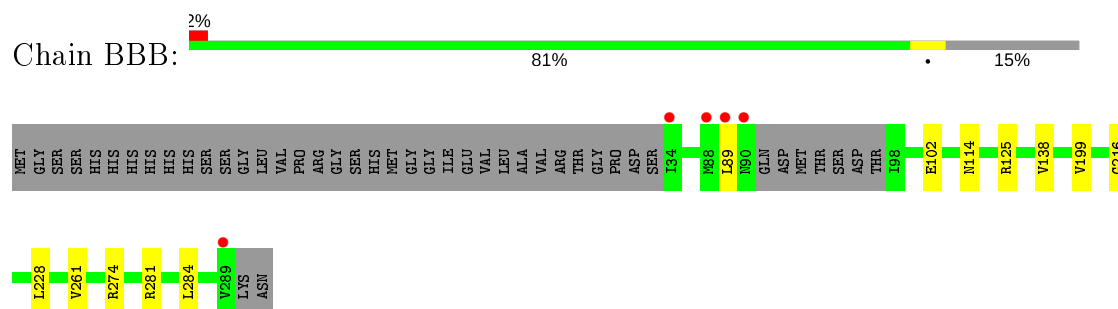
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

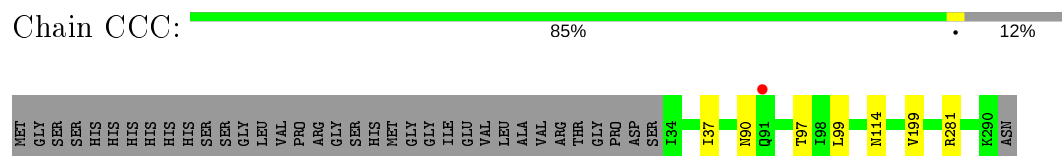
- Molecule 1: Capsid protein VP1



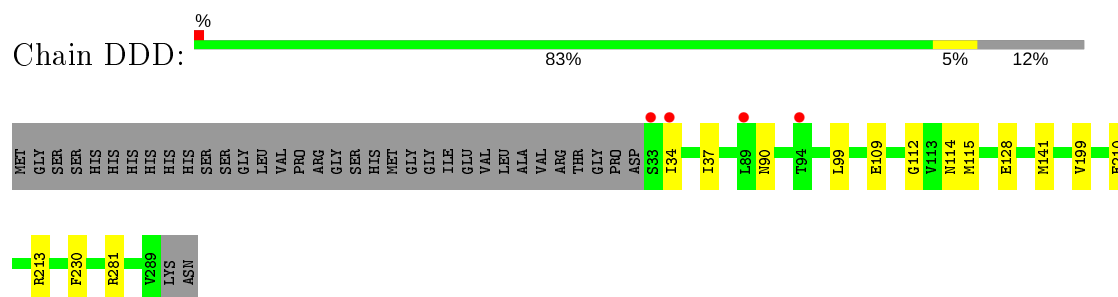
- Molecule 1: Capsid protein VP1




- Molecule 1: Capsid protein VP1

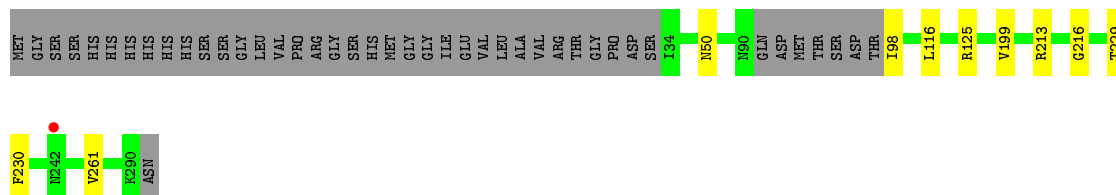


- Molecule 1: Capsid protein VP1




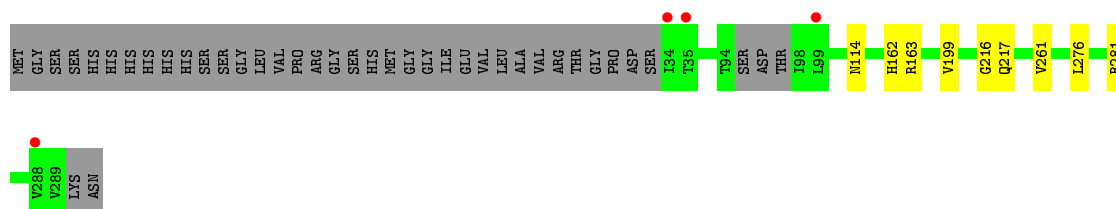
- Molecule 1: Capsid protein VP1

Chain EEE:  82% 15%




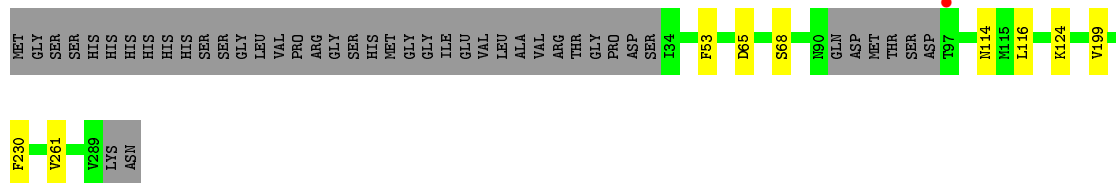
- Molecule 1: Capsid protein VP1

Chain FFF:  83% 14%




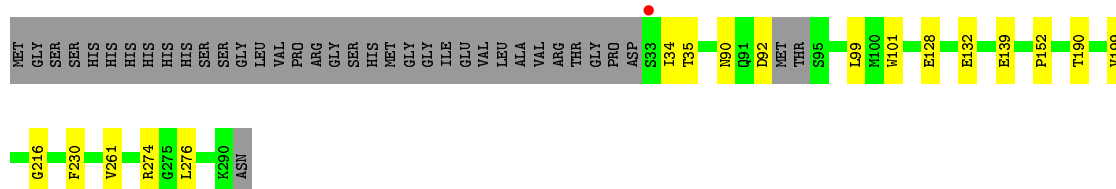
- Molecule 1: Capsid protein VP1

Chain GGG:  82% 15%




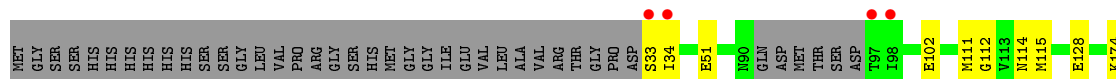
- Molecule 1: Capsid protein VP1

Chain HHH:  82% 13% 6%



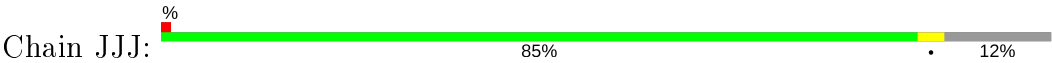
- Molecule 1: Capsid protein VP1

Chain III:  80% 14% 6%





• Molecule 1: Capsid protein VP1



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



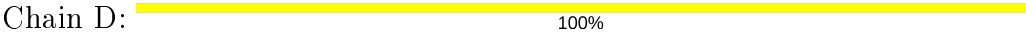
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.29 Å 79.93 Å 145.88 Å 90.00° 116.00° 90.00°	Depositor
Resolution (Å)	48.81 – 1.65 48.81 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.81-1.65) 99.8 (48.81-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.65 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.169 , 0.200 0.178 , 0.207	Depositor DCC
R_{free} test set	7413 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22396	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MPD, GAL, SIA

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	AAA	0.65	0/2053	0.79	0/2792
1	BBB	0.63	0/1998	0.80	0/2715
1	CCC	0.63	0/2057	0.80	0/2798
1	DDD	0.62	1/2071 (0.0%)	0.81	1/2817 (0.0%)
1	EEE	0.63	0/2008	0.79	1/2728 (0.0%)
1	FFF	0.64	0/1997	0.77	0/2716
1	GGG	0.62	0/2015	0.79	0/2737
1	HHH	0.63	0/2047	0.78	0/2781
1	III	0.62	0/1987	0.79	0/2703
1	JJJ	0.63	0/2025	0.79	0/2757
All	All	0.63	1/20258 (0.0%)	0.79	2/27544 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	109	GLU	CD-OE1	5.06	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	213	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	EEE	213	ARG	NE-CZ-NH2	-5.28	117.66	120.30

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	AAA	1998	0	1895	15	0
1	BBB	1944	0	1858	10	0
1	CCC	2002	0	1911	7	0
1	DDD	2016	0	1919	10	0
1	EEE	1954	0	1871	7	0
1	FFF	1943	0	1829	7	0
1	GGG	1955	0	1880	7	0
1	HHH	1993	0	1903	12	0
1	III	1933	0	1842	10	0
1	JJJ	1973	0	1855	10	0
2	A	32	0	28	0	0
2	B	32	0	28	0	0
2	C	32	0	28	0	0
2	D	32	0	28	1	0
3	AAA	16	0	28	1	0
3	BBB	24	0	42	1	0
3	CCC	8	0	14	0	0
3	DDD	16	0	28	3	0
3	EEE	16	0	28	2	0
3	FFF	24	0	42	2	0
3	GGG	16	0	28	2	0
3	HHH	16	0	28	0	0
3	III	16	0	28	1	0
3	JJJ	24	0	42	3	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	2	0	0	0	0
4	FFF	2	0	0	0	0
4	GGG	1	0	0	0	0
4	HHH	1	0	0	0	0
4	III	2	0	0	0	0
5	EEE	21	0	18	0	0
5	GGG	21	0	18	0	0
6	AAA	232	0	0	3	0
6	BBB	231	0	0	3	0
6	CCC	256	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	DDD	299	0	0	4	0
6	EEE	247	0	0	2	0
6	FFF	177	0	0	1	0
6	GGG	247	0	0	1	0
6	HHH	237	0	0	3	0
6	III	223	0	0	3	0
6	JJJ	179	0	0	2	0
All	All	22396	0	19219	86	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 (86) 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:CCC:97:THR:HG21	1:HHH:99:LEU:HD21	1.42	0.99
1:DDD:281:ARG:NH2	6:DDD:501:HOH:O	2.16	0.77
1:HHH:92:ASP:CB	6:HHH:619:HOH:O	2.35	0.74
1:BBB:281:ARG:NH1	6:BBB:401:HOH:O	2.21	0.72
3:FFF:403:MPD:H11	3:JJJ:401:MPD:HM1	1.72	0.71
1:AAA:281:ARG:NH2	6:AAA:401:HOH:O	2.25	0.69
1:III:33:SER:N	1:III:286:LYS:H	1.91	0.68
1:GGG:124:LYS:NZ	6:GGG:401:HOH:O	2.28	0.65
1:AAA:35:THR:CG2	1:AAA:101:TRP:CZ3	2.83	0.61
1:BBB:125[B]:ARG:NH1	6:BBB:403:HOH:O	2.33	0.61
1:AAA:99:LEU:HD13	1:JJJ:97:THR:HG21	1.82	0.60
3:III:304:MPD:O4	3:III:304:MPD:HM1	2.02	0.60
3:FFF:403:MPD:C1	3:JJJ:401:MPD:HM1	2.31	0.60
1:III:174:LYS:CG	6:III:591:HOH:O	2.48	0.60
1:CCC:97:THR:HG21	1:HHH:99:LEU:CD2	2.27	0.59
1:CCC:90:ASN:ND2	1:CCC:99:LEU:O	2.33	0.59
1:AAA:35:THR:HG21	1:AAA:101:TRP:CZ3	2.38	0.58
1:AAA:217:GLN:HG3	1:EEE:229:THR:HG22	1.86	0.58
1:HHH:35:THR:HG22	1:HHH:101:TRP:CZ3	2.39	0.58
1:AAA:125:ARG:HD2	6:AAA:582:HOH:O	2.06	0.55
1:CCC:281:ARG:NH1	6:CCC:503:HOH:O	2.39	0.55
1:AAA:35:THR:HG22	1:AAA:101:TRP:CZ3	2.42	0.55
1:DDD:128:GLU:HG2	6:DDD:695:HOH:O	2.07	0.54
1:DDD:90:ASN:HA	1:DDD:99:LEU:O	2.08	0.53
1:BBB:125[B]:ARG:HH21	1:BBB:125[B]:ARG:HG3	1.73	0.53
1:AAA:99:LEU:CD1	1:JJJ:97:THR:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:GGG:303:MPD:HM1	3:GGG:303:MPD:O4	2.10	0.51
1:III:128:GLU:OE2	1:III:269:LYS:NZ	2.34	0.51
1:AAA:175:ASN:ND2	6:AAA:402:HOH:O	2.38	0.51
1:BBB:125[B]:ARG:NH2	6:BBB:411:HOH:O	2.44	0.51
1:GGG:65:ASP:OD1	1:GGG:68:SER:OG	2.28	0.51
1:III:230:PHE:CZ	1:JJJ:216:GLY:HA3	2.47	0.50
1:AAA:102:GLU:O	1:AAA:284:LEU:HA	2.11	0.50
1:AAA:35:THR:HG21	1:AAA:101:TRP:CH2	2.47	0.50
6:III:424:HOH:O	2:D:2:SIA:C9	2.61	0.49
1:DDD:210:GLU:CG	6:DDD:747:HOH:O	2.61	0.49
1:CCC:37:ILE:HD12	1:CCC:37:ILE:C	2.33	0.48
3:DDD:402:MPD:HM1	3:DDD:402:MPD:O4	2.13	0.48
1:EEE:116:LEU:HD11	1:EEE:261[A]:VAL:HG11	1.95	0.48
3:JJJ:402:MPD:O4	3:JJJ:402:MPD:HM1	2.14	0.47
1:JJJ:141:MET:O	1:JJJ:141:MET:HG3	2.13	0.47
3:DDD:401:MPD:HM1	3:EEE:303:MPD:H31	1.96	0.47
3:BBB:305:MPD:HM1	3:BBB:305:MPD:O4	2.15	0.46
1:EEE:50:ASN:CB	6:EEE:612:HOH:O	2.64	0.46
1:GGG:116:LEU:HD11	1:GGG:261[B]:VAL:HG11	1.98	0.46
1:HHH:128:GLU:HG2	6:HHH:436:HOH:O	2.15	0.46
1:BBB:138:VAL:HG11	1:BBB:261[B]:VAL:HG23	1.97	0.46
1:FFF:114:ASN:HB2	1:GGG:199:VAL:O	2.16	0.46
1:FFF:281:ARG:NH2	6:FFF:501:HOH:O	2.49	0.45
3:AAA:304:MPD:HM1	3:AAA:304:MPD:O4	2.17	0.45
1:BBB:261[B]:VAL:HG22	1:BBB:274:ARG:O	2.17	0.45
1:JJJ:281:ARG:NH2	6:JJJ:506:HOH:O	2.49	0.45
1:GGG:114:ASN:HB2	1:HHH:199:VAL:O	2.17	0.45
1:BBB:114:ASN:HB2	1:CCC:199:VAL:O	2.17	0.44
1:DDD:210:GLU:CG	6:DDD:620:HOH:O	2.64	0.44
1:III:51:GLU:CB	6:III:620:HOH:O	2.65	0.44
1:III:114:ASN:HB2	1:JJJ:199:VAL:O	2.17	0.44
1:AAA:230:PHE:CZ	1:BBB:216:GLY:HA3	2.53	0.44
1:FFF:162:HIS:CE1	1:FFF:163:ARG:HG3	2.53	0.44
1:JJJ:125:ARG:HD2	6:JJJ:638:HOH:O	2.18	0.43
1:BBB:102:GLU:O	1:BBB:284:LEU:HA	2.19	0.43
1:HHH:261[A]:VAL:HG22	1:HHH:274:ARG:O	2.19	0.43
1:FFF:217:GLN:HG3	1:JJJ:229:THR:HG22	2.01	0.42
1:DDD:37:ILE:HD12	1:DDD:37:ILE:C	2.40	0.42
1:DDD:230:PHE:CZ	1:EEE:216:GLY:HA3	2.55	0.42
1:HHH:139:GLU:HG3	6:HHH:425:HOH:O	2.19	0.42
3:EEE:303:MPD:HM1	3:EEE:303:MPD:O4	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:216:GLY:HA3	1:EEE:230:PHE:CZ	2.55	0.42
1:GGG:53:PHE:CD1	3:GGG:302:MPD:H32	2.55	0.42
1:FFF:261[B]:VAL:HG11	1:FFF:276:LEU:HD12	2.02	0.41
1:HHH:261[A]:VAL:HG11	1:HHH:276:LEU:HD12	2.02	0.41
1:AAA:106:CYS:HA	1:AAA:281:ARG:O	2.20	0.41
6:CCC:673:HOH:O	3:DDD:402:MPD:H13	2.20	0.41
1:CCC:114:ASN:HB2	1:DDD:199:VAL:O	2.20	0.41
1:III:112:GLY:O	1:III:115:MET:HG2	2.20	0.41
1:EEE:125[B]:ARG:NH2	6:EEE:410:HOH:O	2.54	0.41
1:DDD:114:ASN:HB2	1:EEE:199:VAL:O	2.20	0.41
1:III:102:GLU:OE1	1:III:287:ARG:HD3	2.21	0.41
1:III:111:MET:HB2	1:III:277:PRO:HG2	2.02	0.41
1:AAA:114:ASN:HB2	1:BBB:199:VAL:O	2.20	0.41
1:FFF:216:GLY:HA3	1:JJJ:230:PHE:CZ	2.55	0.41
1:GGG:230:PHE:CZ	1:HHH:216:GLY:HA3	2.55	0.40
1:FFF:199:VAL:O	1:JJJ:114:ASN:HB2	2.21	0.40
1:DDD:112:GLY:O	1:DDD:115:MET:HG2	2.22	0.40
1:HHH:152:PRO:HB2	1:HHH:190:THR:CG2	2.51	0.40
1:HHH:230:PHE:CZ	1:III:216:GLY:HA3	2.56	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	AAA	257/293 (88%)	247 (96%)	10 (4%)	0	100	100
1	BBB	248/293 (85%)	238 (96%)	9 (4%)	1 (0%)	34	16
1	CCC	257/293 (88%)	246 (96%)	11 (4%)	0	100	100
1	DDD	259/293 (88%)	248 (96%)	11 (4%)	0	100	100
1	EEE	248/293 (85%)	239 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FFF	250/293 (85%)	241 (96%)	9 (4%)	0	100	100
1	GGG	249/293 (85%)	240 (96%)	9 (4%)	0	100	100
1	HHH	253/293 (86%)	243 (96%)	10 (4%)	0	100	100
1	III	248/293 (85%)	238 (96%)	8 (3%)	2 (1%)	19	5
1	JJJ	256/293 (87%)	246 (96%)	10 (4%)	0	100	100
All	All	2525/2930 (86%)	2426 (96%)	96 (4%)	3 (0%)	51	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	III	34	ILE
1	BBB	89	LEU
1	III	182	VAL

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	AAA	211/249 (85%)	208 (99%)	3 (1%)	67	46
1	BBB	204/249 (82%)	203 (100%)	1 (0%)	88	81
1	CCC	213/249 (86%)	213 (100%)	0	100	100
1	DDD	216/249 (87%)	214 (99%)	2 (1%)	78	66
1	EEE	207/249 (83%)	206 (100%)	1 (0%)	88	81
1	FFF	201/249 (81%)	201 (100%)	0	100	100
1	GGG	210/249 (84%)	210 (100%)	0	100	100
1	HHH	212/249 (85%)	209 (99%)	3 (1%)	67	46
1	III	203/249 (82%)	203 (100%)	0	100	100
1	JJJ	207/249 (83%)	206 (100%)	1 (0%)	88	81
All	All	2084/2490 (84%)	2073 (100%)	11 (0%)	88	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	139	GLU
1	AAA	261[A]	VAL
1	AAA	261[B]	VAL
1	BBB	228	LEU
1	DDD	34	ILE
1	DDD	141	MET
1	EEE	98	ILE
1	HHH	34	ILE
1	HHH	90	ASN
1	HHH	132	GLU
1	JJJ	223	GLN

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

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 ⓘ

8 monosaccharides 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	GAL	A	1	2	12,12,12	0.55	0	17,17,17	1.17	1 (5%)
2	SIA	A	2	2	17,20,21	0.46	0	21,28,31	1.09	2 (9%)
2	GAL	B	1	2	12,12,12	0.56	0	17,17,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	B	2	2	17,20,21	0.61	0	21,28,31	0.87	1 (4%)
2	GAL	C	1	2	12,12,12	0.66	0	17,17,17	1.56	2 (11%)
2	SIA	C	2	2	17,20,21	0.61	0	21,28,31	1.07	0
2	GAL	D	1	2	12,12,12	0.55	0	17,17,17	1.00	1 (5%)
2	SIA	D	2	2	17,20,21	0.56	0	21,28,31	0.86	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	GAL	A	1	2	-	0/2/22/22	0/1/1/1
2	SIA	A	2	2	-	0/14/34/38	0/1/1/1
2	GAL	B	1	2	-	0/2/22/22	0/1/1/1
2	SIA	B	2	2	-	2/14/34/38	0/1/1/1
2	GAL	C	1	2	-	1/2/22/22	0/1/1/1
2	SIA	C	2	2	-	0/14/34/38	0/1/1/1
2	GAL	D	1	2	-	0/2/22/22	0/1/1/1
2	SIA	D	2	2	-	2/14/34/38	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	C	1	GAL	O5-C5-C4	3.60	116.24	109.69
2	A	1	GAL	O5-C1-C2	-2.88	105.15	110.28
2	C	1	GAL	O3-C3-C2	-2.88	103.70	110.35
2	A	2	SIA	C4-C3-C2	2.47	114.24	109.81
2	B	2	SIA	C6-O6-C2	2.14	115.93	111.34
2	D	1	GAL	C6-C5-C4	-2.05	108.19	113.00
2	A	2	SIA	C8-C7-C6	-2.05	109.15	113.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	SIA	C7-C8-C9-O9
2	D	2	SIA	O8-C8-C9-O9
2	C	1	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	2	SIA	O8-C8-C9-O9
2	B	2	SIA	C7-C8-C9-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	SIA	1	0

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 11 are monoatomic - leaving 24 for Mogul analysis.

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	$\# Z > 2$
5	SIA	GGG	301	-	18,21,21	1.00	1 (5%)	21,31,31	1.50	3 (14%)
3	MPD	FFF	402	-	7,7,7	0.22	0	9,10,10	0.43	0
3	MPD	BBB	305	-	7,7,7	0.20	0	9,10,10	0.57	0
3	MPD	BBB	304	-	7,7,7	0.16	0	9,10,10	0.57	0
3	MPD	GGG	302	-	7,7,7	0.25	0	9,10,10	0.45	0
3	MPD	FFF	401	-	7,7,7	0.15	0	9,10,10	0.46	0
3	MPD	JJJ	402	-	7,7,7	0.19	0	9,10,10	0.72	0
3	MPD	FFF	403	-	7,7,7	0.19	0	9,10,10	0.55	0
3	MPD	AAA	303	-	7,7,7	0.19	0	9,10,10	0.42	0
3	MPD	AAA	304	-	7,7,7	0.27	0	9,10,10	0.69	0
3	MPD	III	304	-	7,7,7	0.21	0	9,10,10	0.62	0
3	MPD	HHH	304	-	7,7,7	0.29	0	9,10,10	0.70	0
3	MPD	HHH	303	-	7,7,7	0.24	0	9,10,10	0.45	0
5	SIA	EEE	301	-	18,21,21	1.08	1 (5%)	21,31,31	1.13	1 (4%)
3	MPD	BBB	303	-	7,7,7	0.21	0	9,10,10	0.38	0
3	MPD	CCC	401	-	7,7,7	0.19	0	9,10,10	0.47	0
3	MPD	EEE	302	-	7,7,7	0.15	0	9,10,10	0.43	0
3	MPD	JJJ	401	-	7,7,7	0.14	0	9,10,10	0.53	0
3	MPD	DDD	401	-	7,7,7	0.25	0	9,10,10	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	EEE	303	-	7,7,7	0.19	0	9,10,10	0.58	0
3	MPD	GGG	303	-	7,7,7	0.23	0	9,10,10	0.58	0
3	MPD	III	303	-	7,7,7	0.23	0	9,10,10	0.43	0
3	MPD	DDD	402	-	7,7,7	0.32	0	9,10,10	0.62	0
3	MPD	JJJ	403	-	7,7,7	0.16	0	9,10,10	0.69	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
5	SIA	GGG	301	-	-	2/14/38/38	0/1/1/1
3	MPD	FFF	402	-	-	0/5/5/5	-
3	MPD	BBB	305	-	-	2/5/5/5	-
3	MPD	BBB	304	-	-	0/5/5/5	-
3	MPD	GGG	302	-	-	0/5/5/5	-
3	MPD	FFF	401	-	-	1/5/5/5	-
3	MPD	JJJ	402	-	-	2/5/5/5	-
3	MPD	FFF	403	-	-	0/5/5/5	-
3	MPD	AAA	303	-	-	0/5/5/5	-
3	MPD	AAA	304	-	-	4/5/5/5	-
3	MPD	III	304	-	-	3/5/5/5	-
3	MPD	HHH	304	-	-	0/5/5/5	-
3	MPD	HHH	303	-	-	0/5/5/5	-
5	SIA	EEE	301	-	-	2/14/38/38	0/1/1/1
3	MPD	BBB	303	-	-	0/5/5/5	-
3	MPD	CCC	401	-	-	1/5/5/5	-
3	MPD	EEE	302	-	-	0/5/5/5	-
3	MPD	JJJ	401	-	-	1/5/5/5	-
3	MPD	DDD	401	-	-	0/5/5/5	-
3	MPD	EEE	303	-	-	2/5/5/5	-
3	MPD	GGG	303	-	-	3/5/5/5	-
3	MPD	III	303	-	-	0/5/5/5	-
3	MPD	DDD	402	-	-	3/5/5/5	-
3	MPD	JJJ	403	-	-	3/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	EEE	301	SIA	O2-C2	3.61	1.44	1.39
5	GGG	301	SIA	O2-C2	3.07	1.44	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	GGG	301	SIA	O8-C8-C9	-4.53	98.51	109.14
5	GGG	301	SIA	O7-C7-C6	-2.49	104.12	109.50
5	GGG	301	SIA	C9-C8-C7	2.40	117.62	112.41
5	EEE	301	SIA	O6-C6-C5	2.36	112.08	109.78

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	304	MPD	O2-C2-C3-C4
3	AAA	304	MPD	CM-C2-C3-C4
3	III	304	MPD	O2-C2-C3-C4
3	III	304	MPD	CM-C2-C3-C4
3	EEE	303	MPD	C2-C3-C4-C5
3	GGG	303	MPD	O2-C2-C3-C4
3	GGG	303	MPD	CM-C2-C3-C4
3	DDD	402	MPD	O2-C2-C3-C4
3	DDD	402	MPD	CM-C2-C3-C4
3	JJJ	403	MPD	O2-C2-C3-C4
3	JJJ	403	MPD	CM-C2-C3-C4
5	GGG	301	SIA	O7-C7-C8-C9
5	EEE	301	SIA	O8-C8-C9-O9
5	GGG	301	SIA	C6-C7-C8-C9
3	BBB	305	MPD	C2-C3-C4-C5
3	JJJ	402	MPD	C2-C3-C4-C5
3	JJJ	402	MPD	C2-C3-C4-O4
3	AAA	304	MPD	C1-C2-C3-C4
3	JJJ	401	MPD	C1-C2-C3-C4
3	GGG	303	MPD	C1-C2-C3-C4
3	DDD	402	MPD	C1-C2-C3-C4
3	JJJ	403	MPD	C1-C2-C3-C4
5	EEE	301	SIA	C7-C8-C9-O9
3	FFF	401	MPD	O2-C2-C3-C4
3	CCC	401	MPD	C2-C3-C4-C5
3	BBB	305	MPD	C2-C3-C4-O4
3	AAA	304	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	III	304	MPD	C2-C3-C4-O4
3	EEE	303	MPD	C2-C3-C4-O4

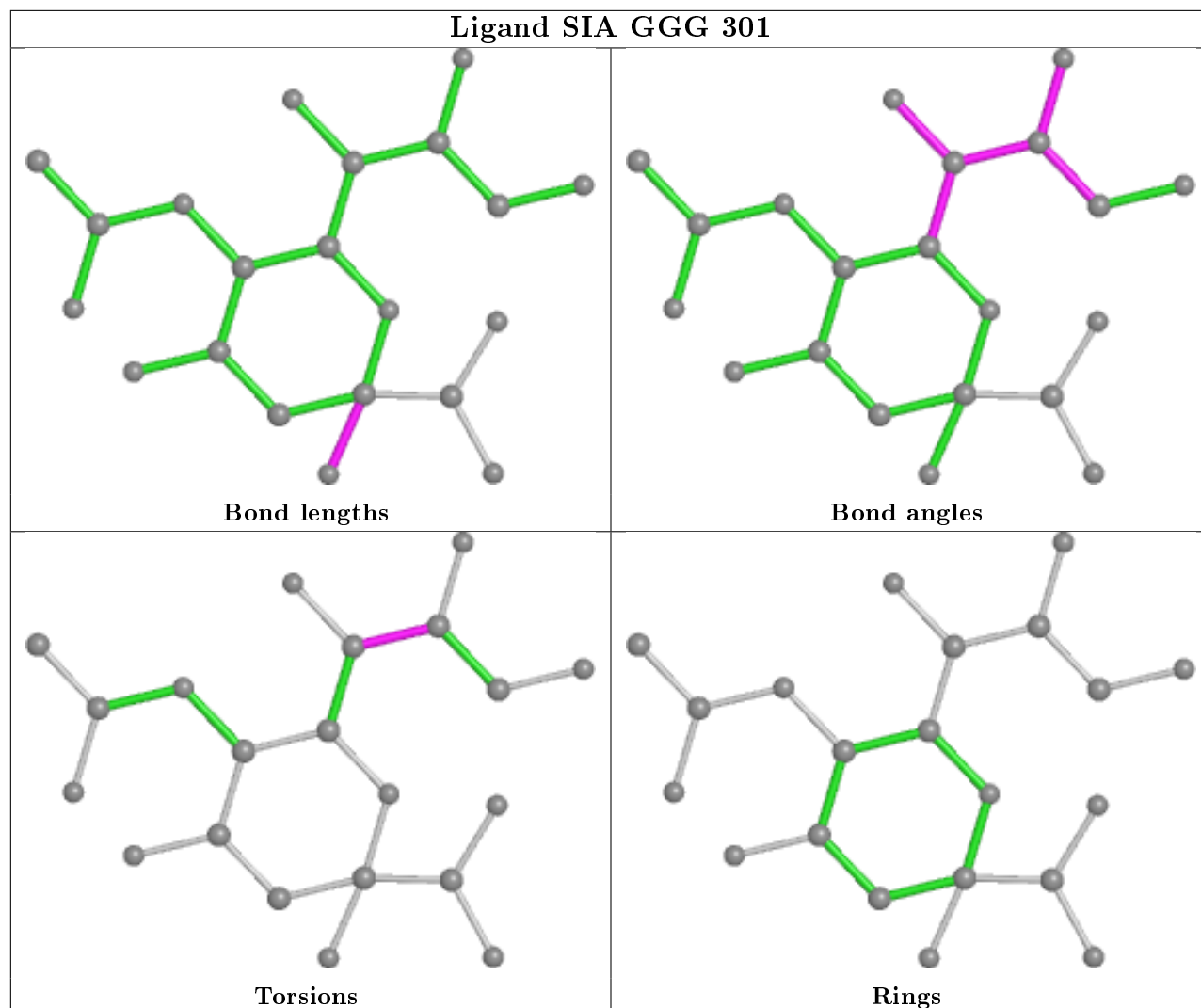
There are no ring outliers.

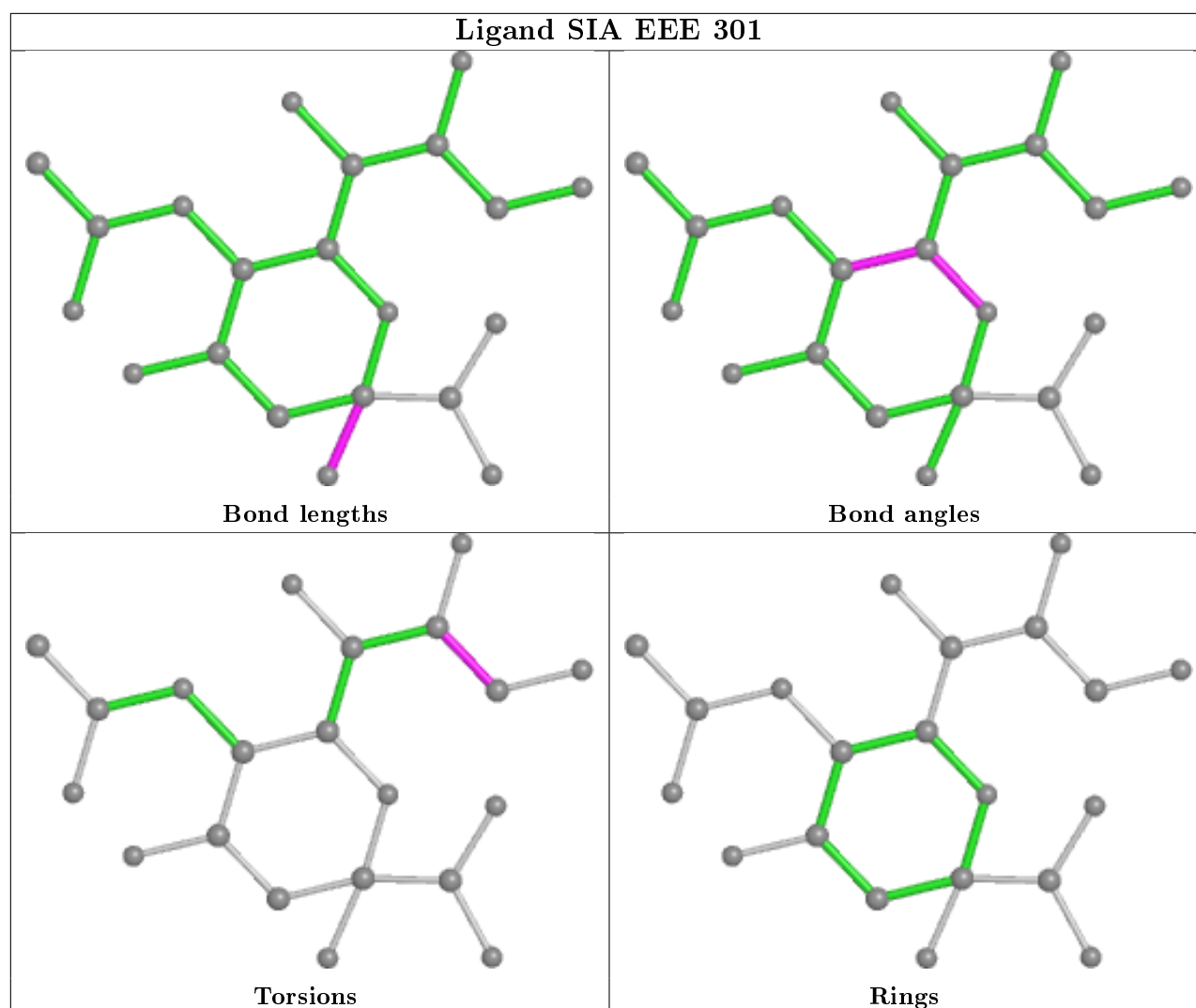
11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	305	MPD	1	0
3	GGG	302	MPD	1	0
3	JJJ	402	MPD	1	0
3	FFF	403	MPD	2	0
3	AAA	304	MPD	1	0
3	III	304	MPD	1	0
3	JJJ	401	MPD	2	0
3	DDD	401	MPD	1	0
3	EEE	303	MPD	2	0
3	GGG	303	MPD	1	0
3	DDD	402	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SIA GGG 301





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	AAA	257/293 (87%)	-0.32	5 (1%) 66 69	16, 22, 39, 64	0
1	BBB	249/293 (84%)	-0.42	5 (2%) 65 67	13, 21, 34, 60	0
1	CCC	257/293 (87%)	-0.47	1 (0%) 92 93	12, 19, 36, 50	0
1	DDD	257/293 (87%)	-0.47	4 (1%) 72 75	12, 17, 35, 42	0
1	EEE	250/293 (85%)	-0.37	1 (0%) 92 93	14, 19, 38, 50	0
1	FFF	253/293 (86%)	-0.20	4 (1%) 72 75	14, 26, 45, 57	0
1	GGG	250/293 (85%)	-0.39	1 (0%) 92 93	14, 21, 35, 47	0
1	HHH	256/293 (87%)	-0.46	1 (0%) 92 93	14, 19, 39, 56	0
1	III	251/293 (85%)	-0.37	5 (1%) 65 67	15, 21, 38, 54	0
1	JJJ	258/293 (88%)	-0.23	2 (0%) 86 88	16, 26, 41, 55	0
All	All	2538/2930 (86%)	-0.37	29 (1%) 80 83	12, 21, 38, 64	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	34	ILE	4.9
1	GGG	97	THR	3.5
1	AAA	93	MET	3.1
1	AAA	35	THR	2.9
1	AAA	34	ILE	2.8
1	FFF	35	THR	2.8
1	FFF	34	ILE	2.8
1	III	34	ILE	2.8
1	III	98	ILE	2.8
1	JJJ	50	ASN	2.5
1	EEE	242	ASN	2.4
1	DDD	94	THR	2.4
1	AAA	94	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	FFF	99	LEU	2.3
1	DDD	89	LEU	2.3
1	JJJ	34	ILE	2.3
1	DDD	33	SER	2.2
1	III	33	SER	2.2
1	DDD	34	ILE	2.2
1	BBB	289	VAL	2.2
1	III	289	VAL	2.1
1	AAA	98	ILE	2.1
1	BBB	88	MET	2.1
1	III	97	THR	2.0
1	BBB	90	ASN	2.0
1	FFF	288	VAL	2.0
1	BBB	89	LEU	2.0
1	HHH	33	SER	2.0
1	CCC	91	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	GAL	A	1	12/12	0.81	0.14	41,53,54,56	0
2	GAL	D	1	12/12	0.86	0.21	36,48,52,58	0
2	GAL	C	1	12/12	0.89	0.19	34,52,58,59	0
2	GAL	B	1	12/12	0.90	0.19	33,45,50,51	0
2	SIA	D	2	20/21	0.93	0.13	20,26,34,40	0
2	SIA	B	2	20/21	0.93	0.13	19,29,37,39	0
2	SIA	C	2	20/21	0.93	0.08	17,24,33,34	0
2	SIA	A	2	20/21	0.94	0.09	24,30,38,39	0

6.4 Ligands ⓘ

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.

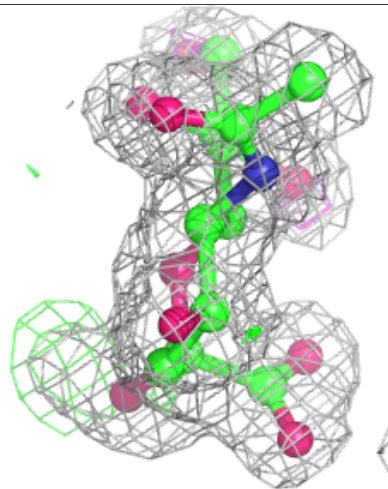
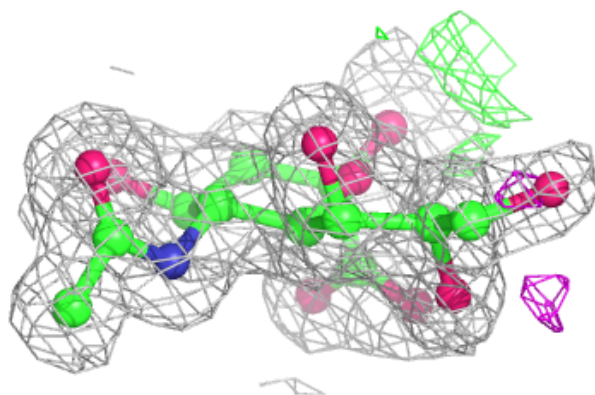
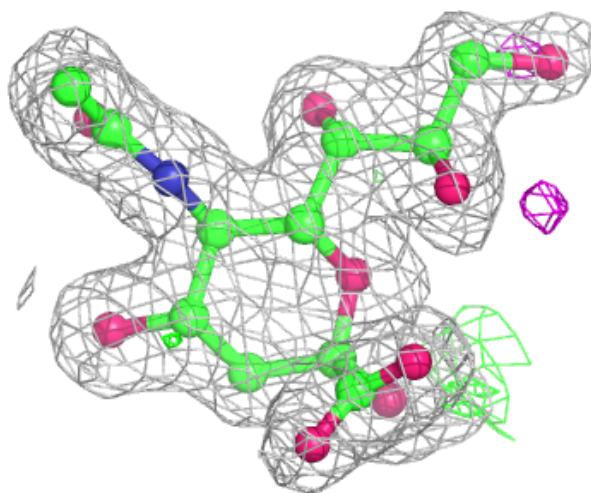
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	DDD	402	8/8	0.83	0.18	29,38,44,45	0
3	MPD	JJJ	402	8/8	0.84	0.18	35,42,49,52	0
3	MPD	BBB	305	8/8	0.84	0.22	25,35,47,47	0
3	MPD	EEE	302	8/8	0.85	0.12	31,36,40,41	0
3	MPD	EEE	303	8/8	0.85	0.19	35,44,50,53	0
3	MPD	III	304	8/8	0.85	0.17	32,42,50,51	0
3	MPD	BBB	304	8/8	0.86	0.13	36,48,54,54	0
3	MPD	FFF	403	8/8	0.86	0.13	37,46,56,56	0
3	MPD	JJJ	403	8/8	0.86	0.14	29,38,48,49	0
3	MPD	FFF	401	8/8	0.88	0.12	31,42,48,50	0
3	MPD	FFF	402	8/8	0.89	0.12	34,40,42,42	0
3	MPD	GGG	303	8/8	0.89	0.14	31,39,47,48	0
3	MPD	GGG	302	8/8	0.90	0.15	30,37,40,40	0
5	SIA	EEE	301	21/21	0.90	0.11	18,25,32,36	0
3	MPD	CCC	401	8/8	0.90	0.15	28,36,39,39	0
3	MPD	AAA	304	8/8	0.90	0.13	28,40,44,46	0
5	SIA	GGG	301	21/21	0.91	0.11	17,24,30,35	0
3	MPD	III	303	8/8	0.92	0.12	27,30,32,33	0
3	MPD	HHH	304	8/8	0.92	0.11	31,42,49,49	0
3	MPD	JJJ	401	8/8	0.92	0.14	35,40,42,43	0
3	MPD	AAA	303	8/8	0.93	0.09	31,34,37,37	0
4	MG	DDD	403	1/1	0.93	0.09	32,32,32,32	0
3	MPD	DDD	401	8/8	0.94	0.10	23,26,28,31	0
3	MPD	BBB	303	8/8	0.94	0.09	22,24,25,26	0
4	MG	FFF	405	1/1	0.94	0.11	40,40,40,40	0
3	MPD	HHH	303	8/8	0.95	0.07	24,28,29,30	0
4	MG	BBB	306	1/1	0.96	0.06	31,31,31,31	0
4	MG	FFF	404	1/1	0.96	0.06	34,34,34,34	0
4	MG	III	305	1/1	0.96	0.07	32,32,32,32	0
4	MG	CCC	402	1/1	0.97	0.04	28,28,28,28	0
4	MG	DDD	404	1/1	0.98	0.04	26,26,26,26	0
4	MG	GGG	304	1/1	0.98	0.07	27,27,27,27	0
4	MG	HHH	305	1/1	0.99	0.03	27,27,27,27	0
4	MG	AAA	305	1/1	0.99	0.05	22,22,22,22	0
4	MG	III	306	1/1	0.99	0.07	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

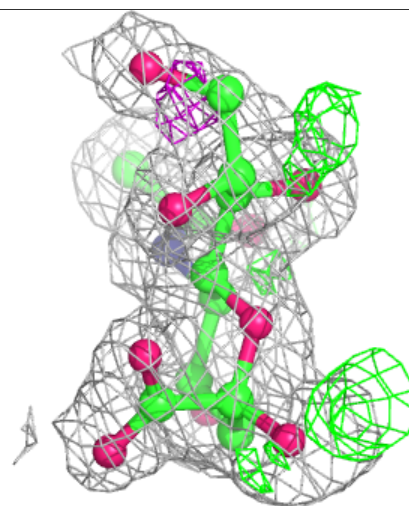
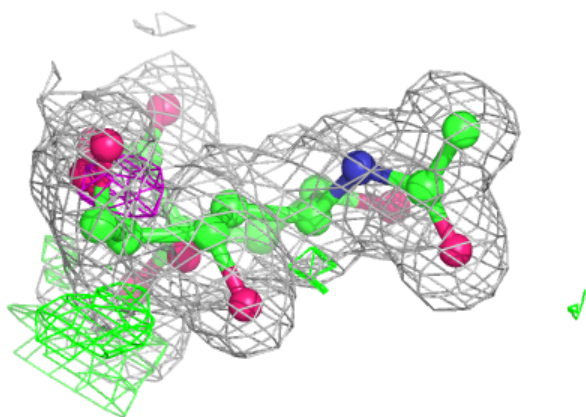
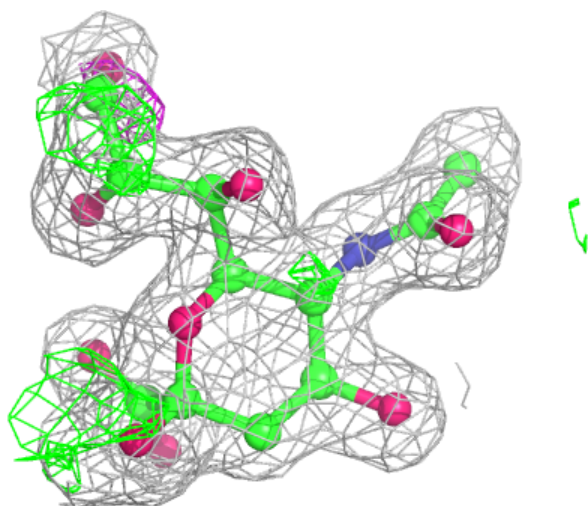
Electron density around SIA EEE 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SIA GGG 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.