



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2020 – 02:41 PM BST

PDB ID : 6Y65
Title : Structure of apo Goose Hemorrhagic Polyomavirus VP1
Authors : Stroh, L.J.; Rustmeier, N.H.; Stehle, T.
Deposited on : 2020-02-26
Resolution : 1.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.14.3.dev2
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) : 2.14.3.dev2

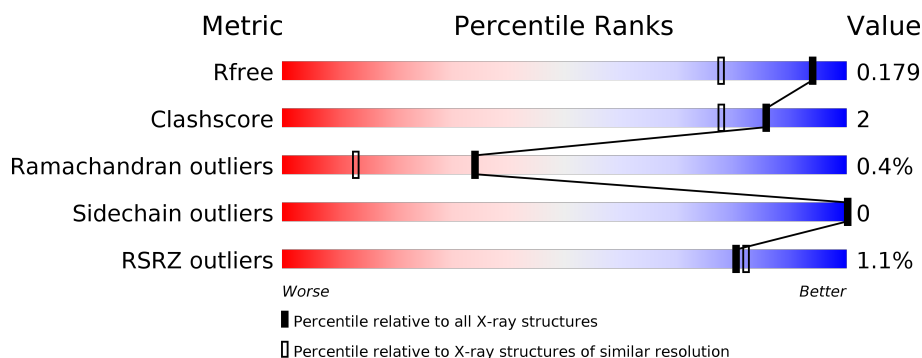
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	287	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	BBB	287	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	CCC	287	<div> <div></div> <div> <div></div> <div>88%</div> <div>5%</div> <div>8%</div> </div> </div>
1	DDD	287	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
1	EEE	287	<div> <div></div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
1	FFF	287	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>•</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	GGG	287	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>87%</div><div>6%7%</div></div>
1	HHH	287	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>%</div><div>87%</div><div>7%7%</div></div>
1	III	287	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>%</div><div>88%</div><div>5%7%</div></div>
1	JJJ	287	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>89%</div><div>•8%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24379 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	265	Total	C	N	O	S	0	10	1
			2061	1297	352	393	19			
1	BBB	265	Total	C	N	O	S	0	8	0
			2048	1291	348	390	19			
1	CCC	265	Total	C	N	O	S	0	11	0
			2065	1300	348	398	19			
1	DDD	265	Total	C	N	O	S	0	9	0
			2050	1290	349	392	19			
1	EEE	264	Total	C	N	O	S	0	8	0
			2047	1288	348	392	19			
1	FFF	268	Total	C	N	O	S	0	10	0
			2080	1308	353	399	20			
1	GGG	267	Total	C	N	O	S	0	10	0
			2076	1305	352	399	20			
1	HHH	268	Total	C	N	O	S	0	9	0
			2079	1306	355	398	20			
1	III	267	Total	C	N	O	S	0	10	0
			2073	1306	353	394	20			
1	JJJ	264	Total	C	N	O	S	0	8	0
			2042	1286	348	389	19			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP Q80FI3
AAA	1	GLY	-	expression tag	UNP Q80FI3
AAA	2	SER	-	expression tag	UNP Q80FI3
AAA	3	SER	-	expression tag	UNP Q80FI3
AAA	4	HIS	-	expression tag	UNP Q80FI3
AAA	5	HIS	-	expression tag	UNP Q80FI3
AAA	6	HIS	-	expression tag	UNP Q80FI3
AAA	7	HIS	-	expression tag	UNP Q80FI3
AAA	8	HIS	-	expression tag	UNP Q80FI3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	9	HIS	-	expression tag	UNP Q80FI3
AAA	10	SER	-	expression tag	UNP Q80FI3
AAA	11	SER	-	expression tag	UNP Q80FI3
AAA	12	GLY	-	expression tag	UNP Q80FI3
AAA	13	LEU	-	expression tag	UNP Q80FI3
AAA	14	VAL	-	expression tag	UNP Q80FI3
AAA	15	PRO	-	expression tag	UNP Q80FI3
AAA	16	ARG	-	expression tag	UNP Q80FI3
AAA	17	GLY	-	expression tag	UNP Q80FI3
AAA	18	SER	-	expression tag	UNP Q80FI3
AAA	19	HIS	-	expression tag	UNP Q80FI3
AAA	20	MET	-	expression tag	UNP Q80FI3
BBB	0	MET	-	initiating methionine	UNP Q80FI3
BBB	1	GLY	-	expression tag	UNP Q80FI3
BBB	2	SER	-	expression tag	UNP Q80FI3
BBB	3	SER	-	expression tag	UNP Q80FI3
BBB	4	HIS	-	expression tag	UNP Q80FI3
BBB	5	HIS	-	expression tag	UNP Q80FI3
BBB	6	HIS	-	expression tag	UNP Q80FI3
BBB	7	HIS	-	expression tag	UNP Q80FI3
BBB	8	HIS	-	expression tag	UNP Q80FI3
BBB	9	HIS	-	expression tag	UNP Q80FI3
BBB	10	SER	-	expression tag	UNP Q80FI3
BBB	11	SER	-	expression tag	UNP Q80FI3
BBB	12	GLY	-	expression tag	UNP Q80FI3
BBB	13	LEU	-	expression tag	UNP Q80FI3
BBB	14	VAL	-	expression tag	UNP Q80FI3
BBB	15	PRO	-	expression tag	UNP Q80FI3
BBB	16	ARG	-	expression tag	UNP Q80FI3
BBB	17	GLY	-	expression tag	UNP Q80FI3
BBB	18	SER	-	expression tag	UNP Q80FI3
BBB	19	HIS	-	expression tag	UNP Q80FI3
BBB	20	MET	-	expression tag	UNP Q80FI3
CCC	0	MET	-	initiating methionine	UNP Q80FI3
CCC	1	GLY	-	expression tag	UNP Q80FI3
CCC	2	SER	-	expression tag	UNP Q80FI3
CCC	3	SER	-	expression tag	UNP Q80FI3
CCC	4	HIS	-	expression tag	UNP Q80FI3
CCC	5	HIS	-	expression tag	UNP Q80FI3
CCC	6	HIS	-	expression tag	UNP Q80FI3
CCC	7	HIS	-	expression tag	UNP Q80FI3
CCC	8	HIS	-	expression tag	UNP Q80FI3

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	9	HIS	-	expression tag	UNP Q80FI3
CCC	10	SER	-	expression tag	UNP Q80FI3
CCC	11	SER	-	expression tag	UNP Q80FI3
CCC	12	GLY	-	expression tag	UNP Q80FI3
CCC	13	LEU	-	expression tag	UNP Q80FI3
CCC	14	VAL	-	expression tag	UNP Q80FI3
CCC	15	PRO	-	expression tag	UNP Q80FI3
CCC	16	ARG	-	expression tag	UNP Q80FI3
CCC	17	GLY	-	expression tag	UNP Q80FI3
CCC	18	SER	-	expression tag	UNP Q80FI3
CCC	19	HIS	-	expression tag	UNP Q80FI3
CCC	20	MET	-	expression tag	UNP Q80FI3
DDD	0	MET	-	initiating methionine	UNP Q80FI3
DDD	1	GLY	-	expression tag	UNP Q80FI3
DDD	2	SER	-	expression tag	UNP Q80FI3
DDD	3	SER	-	expression tag	UNP Q80FI3
DDD	4	HIS	-	expression tag	UNP Q80FI3
DDD	5	HIS	-	expression tag	UNP Q80FI3
DDD	6	HIS	-	expression tag	UNP Q80FI3
DDD	7	HIS	-	expression tag	UNP Q80FI3
DDD	8	HIS	-	expression tag	UNP Q80FI3
DDD	9	HIS	-	expression tag	UNP Q80FI3
DDD	10	SER	-	expression tag	UNP Q80FI3
DDD	11	SER	-	expression tag	UNP Q80FI3
DDD	12	GLY	-	expression tag	UNP Q80FI3
DDD	13	LEU	-	expression tag	UNP Q80FI3
DDD	14	VAL	-	expression tag	UNP Q80FI3
DDD	15	PRO	-	expression tag	UNP Q80FI3
DDD	16	ARG	-	expression tag	UNP Q80FI3
DDD	17	GLY	-	expression tag	UNP Q80FI3
DDD	18	SER	-	expression tag	UNP Q80FI3
DDD	19	HIS	-	expression tag	UNP Q80FI3
DDD	20	MET	-	expression tag	UNP Q80FI3
EEE	0	MET	-	initiating methionine	UNP Q80FI3
EEE	1	GLY	-	expression tag	UNP Q80FI3
EEE	2	SER	-	expression tag	UNP Q80FI3
EEE	3	SER	-	expression tag	UNP Q80FI3
EEE	4	HIS	-	expression tag	UNP Q80FI3
EEE	5	HIS	-	expression tag	UNP Q80FI3
EEE	6	HIS	-	expression tag	UNP Q80FI3
EEE	7	HIS	-	expression tag	UNP Q80FI3
EEE	8	HIS	-	expression tag	UNP Q80FI3

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	9	HIS	-	expression tag	UNP Q80FI3
EEE	10	SER	-	expression tag	UNP Q80FI3
EEE	11	SER	-	expression tag	UNP Q80FI3
EEE	12	GLY	-	expression tag	UNP Q80FI3
EEE	13	LEU	-	expression tag	UNP Q80FI3
EEE	14	VAL	-	expression tag	UNP Q80FI3
EEE	15	PRO	-	expression tag	UNP Q80FI3
EEE	16	ARG	-	expression tag	UNP Q80FI3
EEE	17	GLY	-	expression tag	UNP Q80FI3
EEE	18	SER	-	expression tag	UNP Q80FI3
EEE	19	HIS	-	expression tag	UNP Q80FI3
EEE	20	MET	-	expression tag	UNP Q80FI3
FFF	0	MET	-	initiating methionine	UNP Q80FI3
FFF	1	GLY	-	expression tag	UNP Q80FI3
FFF	2	SER	-	expression tag	UNP Q80FI3
FFF	3	SER	-	expression tag	UNP Q80FI3
FFF	4	HIS	-	expression tag	UNP Q80FI3
FFF	5	HIS	-	expression tag	UNP Q80FI3
FFF	6	HIS	-	expression tag	UNP Q80FI3
FFF	7	HIS	-	expression tag	UNP Q80FI3
FFF	8	HIS	-	expression tag	UNP Q80FI3
FFF	9	HIS	-	expression tag	UNP Q80FI3
FFF	10	SER	-	expression tag	UNP Q80FI3
FFF	11	SER	-	expression tag	UNP Q80FI3
FFF	12	GLY	-	expression tag	UNP Q80FI3
FFF	13	LEU	-	expression tag	UNP Q80FI3
FFF	14	VAL	-	expression tag	UNP Q80FI3
FFF	15	PRO	-	expression tag	UNP Q80FI3
FFF	16	ARG	-	expression tag	UNP Q80FI3
FFF	17	GLY	-	expression tag	UNP Q80FI3
FFF	18	SER	-	expression tag	UNP Q80FI3
FFF	19	HIS	-	expression tag	UNP Q80FI3
FFF	20	MET	-	expression tag	UNP Q80FI3
GGG	0	MET	-	initiating methionine	UNP Q80FI3
GGG	1	GLY	-	expression tag	UNP Q80FI3
GGG	2	SER	-	expression tag	UNP Q80FI3
GGG	3	SER	-	expression tag	UNP Q80FI3
GGG	4	HIS	-	expression tag	UNP Q80FI3
GGG	5	HIS	-	expression tag	UNP Q80FI3
GGG	6	HIS	-	expression tag	UNP Q80FI3
GGG	7	HIS	-	expression tag	UNP Q80FI3
GGG	8	HIS	-	expression tag	UNP Q80FI3

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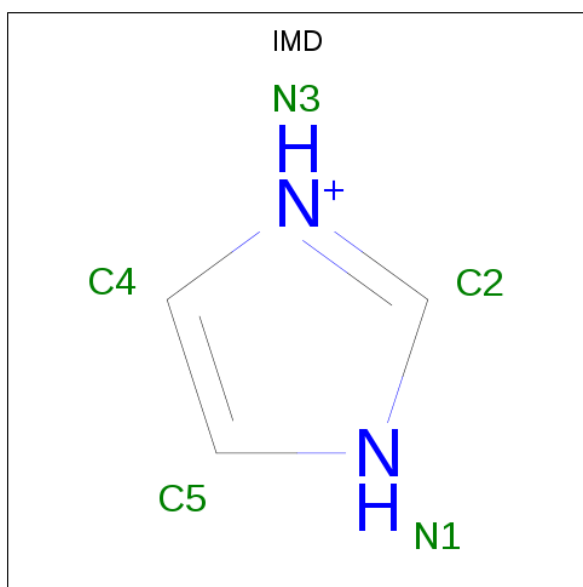
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	9	HIS	-	expression tag	UNP Q80FI3
GGG	10	SER	-	expression tag	UNP Q80FI3
GGG	11	SER	-	expression tag	UNP Q80FI3
GGG	12	GLY	-	expression tag	UNP Q80FI3
GGG	13	LEU	-	expression tag	UNP Q80FI3
GGG	14	VAL	-	expression tag	UNP Q80FI3
GGG	15	PRO	-	expression tag	UNP Q80FI3
GGG	16	ARG	-	expression tag	UNP Q80FI3
GGG	17	GLY	-	expression tag	UNP Q80FI3
GGG	18	SER	-	expression tag	UNP Q80FI3
GGG	19	HIS	-	expression tag	UNP Q80FI3
GGG	20	MET	-	expression tag	UNP Q80FI3
HHH	0	MET	-	initiating methionine	UNP Q80FI3
HHH	1	GLY	-	expression tag	UNP Q80FI3
HHH	2	SER	-	expression tag	UNP Q80FI3
HHH	3	SER	-	expression tag	UNP Q80FI3
HHH	4	HIS	-	expression tag	UNP Q80FI3
HHH	5	HIS	-	expression tag	UNP Q80FI3
HHH	6	HIS	-	expression tag	UNP Q80FI3
HHH	7	HIS	-	expression tag	UNP Q80FI3
HHH	8	HIS	-	expression tag	UNP Q80FI3
HHH	9	HIS	-	expression tag	UNP Q80FI3
HHH	10	SER	-	expression tag	UNP Q80FI3
HHH	11	SER	-	expression tag	UNP Q80FI3
HHH	12	GLY	-	expression tag	UNP Q80FI3
HHH	13	LEU	-	expression tag	UNP Q80FI3
HHH	14	VAL	-	expression tag	UNP Q80FI3
HHH	15	PRO	-	expression tag	UNP Q80FI3
HHH	16	ARG	-	expression tag	UNP Q80FI3
HHH	17	GLY	-	expression tag	UNP Q80FI3
HHH	18	SER	-	expression tag	UNP Q80FI3
HHH	19	HIS	-	expression tag	UNP Q80FI3
HHH	20	MET	-	expression tag	UNP Q80FI3
III	0	MET	-	initiating methionine	UNP Q80FI3
III	1	GLY	-	expression tag	UNP Q80FI3
III	2	SER	-	expression tag	UNP Q80FI3
III	3	SER	-	expression tag	UNP Q80FI3
III	4	HIS	-	expression tag	UNP Q80FI3
III	5	HIS	-	expression tag	UNP Q80FI3
III	6	HIS	-	expression tag	UNP Q80FI3
III	7	HIS	-	expression tag	UNP Q80FI3
III	8	HIS	-	expression tag	UNP Q80FI3

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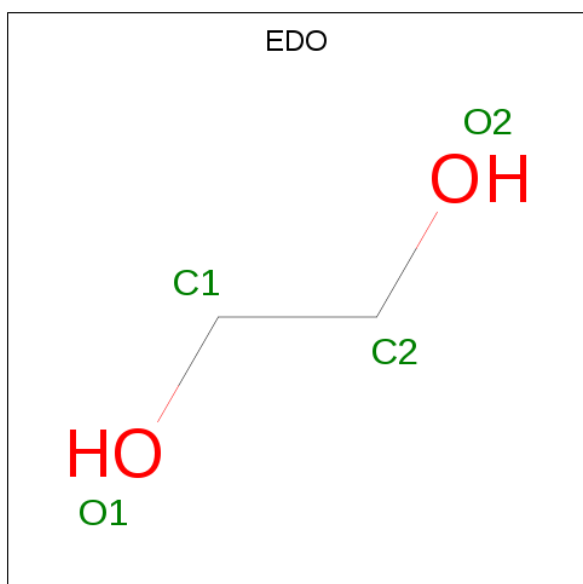
Chain	Residue	Modelled	Actual	Comment	Reference
III	9	HIS	-	expression tag	UNP Q80FI3
III	10	SER	-	expression tag	UNP Q80FI3
III	11	SER	-	expression tag	UNP Q80FI3
III	12	GLY	-	expression tag	UNP Q80FI3
III	13	LEU	-	expression tag	UNP Q80FI3
III	14	VAL	-	expression tag	UNP Q80FI3
III	15	PRO	-	expression tag	UNP Q80FI3
III	16	ARG	-	expression tag	UNP Q80FI3
III	17	GLY	-	expression tag	UNP Q80FI3
III	18	SER	-	expression tag	UNP Q80FI3
III	19	HIS	-	expression tag	UNP Q80FI3
III	20	MET	-	expression tag	UNP Q80FI3
JJJ	0	MET	-	initiating methionine	UNP Q80FI3
JJJ	1	GLY	-	expression tag	UNP Q80FI3
JJJ	2	SER	-	expression tag	UNP Q80FI3
JJJ	3	SER	-	expression tag	UNP Q80FI3
JJJ	4	HIS	-	expression tag	UNP Q80FI3
JJJ	5	HIS	-	expression tag	UNP Q80FI3
JJJ	6	HIS	-	expression tag	UNP Q80FI3
JJJ	7	HIS	-	expression tag	UNP Q80FI3
JJJ	8	HIS	-	expression tag	UNP Q80FI3
JJJ	9	HIS	-	expression tag	UNP Q80FI3
JJJ	10	SER	-	expression tag	UNP Q80FI3
JJJ	11	SER	-	expression tag	UNP Q80FI3
JJJ	12	GLY	-	expression tag	UNP Q80FI3
JJJ	13	LEU	-	expression tag	UNP Q80FI3
JJJ	14	VAL	-	expression tag	UNP Q80FI3
JJJ	15	PRO	-	expression tag	UNP Q80FI3
JJJ	16	ARG	-	expression tag	UNP Q80FI3
JJJ	17	GLY	-	expression tag	UNP Q80FI3
JJJ	18	SER	-	expression tag	UNP Q80FI3
JJJ	19	HIS	-	expression tag	UNP Q80FI3
JJJ	20	MET	-	expression tag	UNP Q80FI3

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	N	0	0
			5	3	2		
2	BBB	1	Total	C	N	0	0
			5	3	2		
2	DDD	1	Total	C	N	0	0
			5	3	2		
2	III	1	Total	C	N	0	0
			5	3	2		
2	JJJ	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	AAA	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0
3	BBB	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	CCC	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0
3	DDD	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	EEE	1	Total	C	O	0	0
			4	2	2		
3	EEE	1	Total	C	O	0	0
			4	2	2		
3	EEE	1	Total	C	O	0	0
			4	2	2		
3	EEE	1	Total	C	O	0	0
			4	2	2		
3	EEE	1	Total	C	O	0	0
			4	2	2		
3	EEE	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	FFF	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	GGG	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	HHH	1	Total	C	O	0	0
			4	2	2		
3	III	1	Total	C	O	0	0
			4	2	2		
3	III	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	III	1	Total 4	C 2	O 2	0	0
3	III	1	Total 4	C 2	O 2	0	0
3	III	1	Total 4	C 2	O 2	0	0
3	III	1	Total 4	C 2	O 2	0	0
3	III	1	Total 4	C 2	O 2	0	0
3	III	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0
3	JJJ	1	Total 4	C 2	O 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	DDD	2	Total 2	Cl 2	0	0
4	AAA	1	Total 1	Cl 1	0	0
4	CCC	2	Total 2	Cl 2	0	0
4	III	2	Total 2	Cl 2	0	0
4	HHH	2	Total 2	Cl 2	0	0
4	JJJ	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	FFF	2	Total 2	Cl 2	0	0
4	EEE	1	Total 1	Cl 1	0	0
4	BBB	2	Total 2	Cl 2	0	0
4	GGG	2	Total 2	Cl 2	0	0

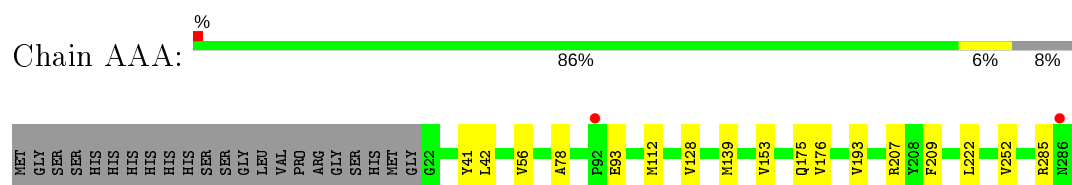
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	339	Total 343	O 343	0	4
5	BBB	321	Total 324	O 324	0	3
5	CCC	332	Total 335	O 335	0	3
5	DDD	310	Total 313	O 313	0	3
5	EEE	337	Total 342	O 342	0	5
5	FFF	316	Total 318	O 318	0	2
5	GGG	334	Total 336	O 336	0	2
5	HHH	346	Total 351	O 351	0	5
5	III	330	Total 332	O 332	0	2
5	JJJ	324	Total 330	O 330	0	6

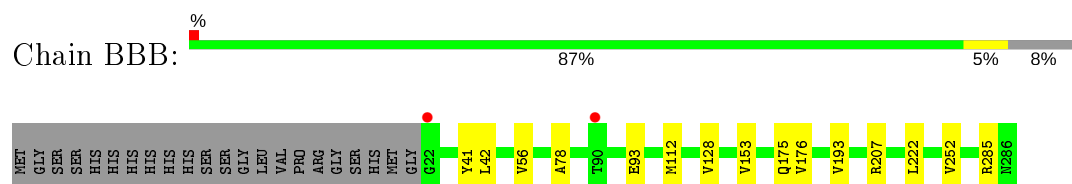
3 Residue-property plots [i](#)

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.

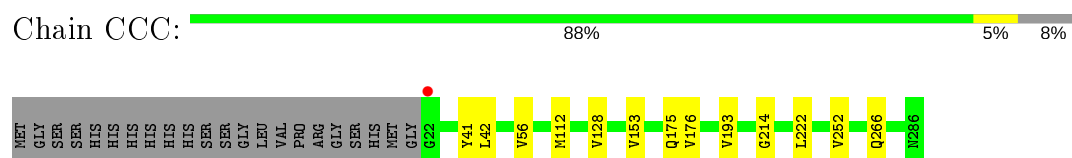
- Molecule 1: Capsid protein VP1



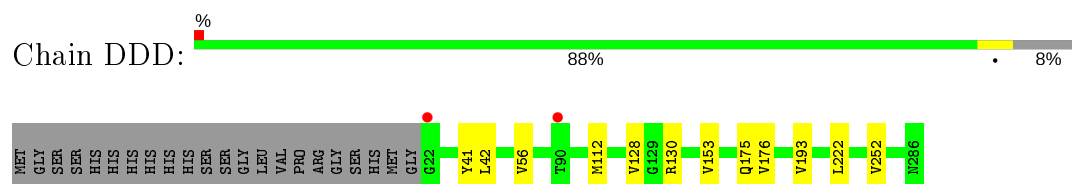
- Molecule 1: Capsid protein VP1



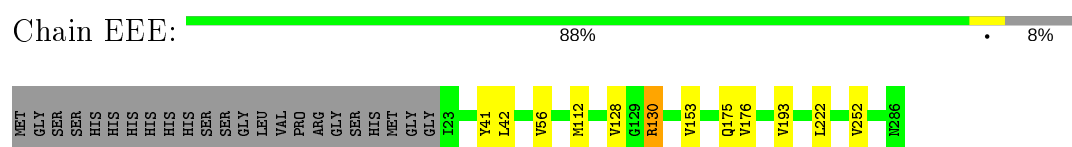
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

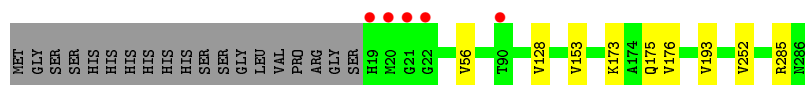


- Molecule 1: Capsid protein VP1

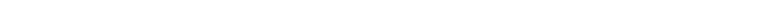


- Molecule 1: Capsid protein VP1

Chain FFF:  2% 90% 7%

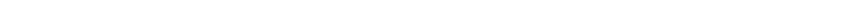


- Molecule 1: Capsid protein VP1

Chain GGG:  2% 87% 6% 7%

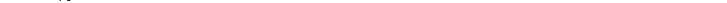


- Molecule 1: Capsid protein VP1

Chain HHH:  %

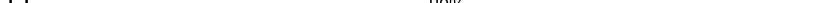


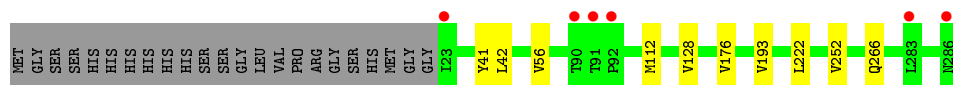
- Molecule 1: Capsid protein VP1

Chain III:  %



- Molecule 1: Capsid protein VP1

Chain JJJ: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.29 Å 90.41 Å 100.84 Å 94.05° 97.90° 108.06°	Depositor
Resolution (Å)	45.97 – 1.45 45.96 – 1.45	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.97-1.45) 95.4 (45.96-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.45 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.148 , 0.170 0.158 , 0.179	Depositor DCC
R_{free} test set	4875 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24379	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: CL, EDO, IMD

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	0.61	0/2115	0.79	1/2886 (0.0%)
1	BBB	0.61	0/2102	0.78	2/2869 (0.1%)
1	CCC	0.61	0/2119	0.76	0/2891
1	DDD	0.61	0/2101	0.76	0/2867
1	EEE	0.60	0/2098	0.77	1/2863 (0.0%)
1	FFF	0.61	0/2134	0.78	0/2911
1	GGG	0.61	0/2130	0.77	0/2904
1	HHH	0.61	0/2131	0.77	2/2906 (0.1%)
1	III	0.61	0/2124	0.78	1/2896 (0.0%)
1	JJJ	0.61	0/2093	0.77	0/2858
All	All	0.61	0/21147	0.77	7/28851 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	207	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	HHH	79	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	III	207	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	BBB	207	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	HHH	130	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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	AAA	2061	0	2017	12	0
1	BBB	2048	0	2004	12	0
1	CCC	2065	0	2008	8	0
1	DDD	2050	0	1998	9	0
1	EEE	2047	0	1999	8	0
1	FFF	2080	0	2028	7	0
1	GGG	2076	0	2026	18	0
1	HHH	2079	0	2025	10	0
1	III	2073	0	2028	9	0
1	JJJ	2042	0	1995	12	0
2	AAA	5	0	5	0	0
2	BBB	5	0	5	0	0
2	DDD	5	0	5	0	0
2	III	5	0	5	0	0
2	JJJ	5	0	5	0	0
3	AAA	44	0	66	0	0
3	BBB	48	0	72	0	0
3	CCC	40	0	60	0	0
3	DDD	40	0	60	0	0
3	EEE	32	0	48	0	0
3	FFF	40	0	60	0	0
3	GGG	48	0	72	1	0
3	HHH	40	0	60	1	0
3	III	32	0	48	0	0
3	JJJ	28	0	42	0	0
4	AAA	1	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
4	DDD	2	0	0	0	0
4	EEE	1	0	0	0	0
4	FFF	2	0	0	0	0
4	GGG	2	0	0	0	0
4	HHH	2	0	0	0	0
4	III	2	0	0	0	0
4	JJJ	1	0	0	0	0
5	AAA	343	0	0	1	0
5	BBB	324	0	0	1	0
5	CCC	335	0	0	0	0
5	DDD	313	0	0	0	0
5	EEE	342	0	0	1	0
5	FFF	318	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	GGG	336	0	0	1	0
5	HHH	351	0	0	1	0
5	III	332	0	0	0	0
5	JJJ	330	0	0	0	0
All	All	24379	0	20741	93	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.

The worst 5 of 93 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:GGG:86:ASN:HB2	1:GGG:89:MET:HE3	1.46	0.97
1:GGG:86:ASN:CB	1:GGG:89:MET:HE3	2.12	0.79
1:III:112[B]:MET:HE1	1:III:222:LEU:CD1	2.22	0.69
1:HHH:19:HIS:N	5:HHH:401:HOH:O	2.27	0.68
1:III:193:VAL:HG21	1:III:252:VAL:HG21	1.79	0.65

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	AAA	273/287 (95%)	265 (97%)	7 (3%)	1 (0%)	34	13
1	BBB	271/287 (94%)	262 (97%)	8 (3%)	1 (0%)	34	13
1	CCC	274/287 (96%)	265 (97%)	8 (3%)	1 (0%)	34	13
1	DDD	272/287 (95%)	264 (97%)	7 (3%)	1 (0%)	34	13
1	EEE	270/287 (94%)	261 (97%)	8 (3%)	1 (0%)	34	13
1	FFF	276/287 (96%)	268 (97%)	7 (2%)	1 (0%)	34	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GGG	275/287 (96%)	266 (97%)	8 (3%)	1 (0%)	34	13
1	HHH	275/287 (96%)	266 (97%)	8 (3%)	1 (0%)	34	13
1	III	275/287 (96%)	266 (97%)	8 (3%)	1 (0%)	34	13
1	JJJ	270/287 (94%)	261 (97%)	8 (3%)	1 (0%)	34	13
All	All	2731/2870 (95%)	2644 (97%)	77 (3%)	10 (0%)	34	13

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	176	VAL
1	JJJ	176	VAL
1	BBB	176	VAL
1	CCC	176	VAL
1	DDD	176	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	230/243 (95%)	230 (100%)	0	100	100
1	BBB	227/243 (93%)	227 (100%)	0	100	100
1	CCC	229/243 (94%)	229 (100%)	0	100	100
1	DDD	227/243 (93%)	227 (100%)	0	100	100
1	EEE	228/243 (94%)	228 (100%)	0	100	100
1	FFF	231/243 (95%)	231 (100%)	0	100	100
1	GGG	231/243 (95%)	231 (100%)	0	100	100
1	HHH	231/243 (95%)	231 (100%)	0	100	100
1	III	229/243 (94%)	229 (100%)	0	100	100
1	JJJ	227/243 (93%)	227 (100%)	0	100	100
All	All	2290/2430 (94%)	2290 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 120 ligands modelled in this entry, 17 are monoatomic - leaving 103 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	$\# Z > 2$
3	EDO	FFF	303	-	3,3,3	0.13	0	2,2,2	0.12	0
3	EDO	CCC	305	-	3,3,3	0.05	0	2,2,2	0.43	0
3	EDO	DDD	303	-	3,3,3	0.04	0	2,2,2	0.08	0
3	EDO	JJJ	304	-	3,3,3	0.20	0	2,2,2	0.41	0
3	EDO	CCC	303	-	3,3,3	0.08	0	2,2,2	0.09	0
2	IMD	DDD	301	-	3,5,5	0.24	0	4,5,5	0.88	0
3	EDO	BBB	307	-	3,3,3	0.08	0	2,2,2	0.21	0
3	EDO	HHH	304	-	3,3,3	0.17	0	2,2,2	0.40	0
3	EDO	AAA	311	-	3,3,3	0.07	0	2,2,2	0.08	0
3	EDO	III	303	-	3,3,3	0.07	0	2,2,2	0.08	0
3	EDO	AAA	309	-	3,3,3	0.09	0	2,2,2	0.27	0
3	EDO	GGG	309	-	3,3,3	0.07	0	2,2,2	0.29	0
3	EDO	III	306	-	3,3,3	0.17	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IMD	JJJ	301	-	3,5,5	0.30	0	4,5,5	0.94	0
3	EDO	AAA	305	-	3,3,3	0.09	0	2,2,2	0.12	0
3	EDO	AAA	303	-	3,3,3	0.26	0	2,2,2	0.15	0
3	EDO	DDD	311	-	3,3,3	0.08	0	2,2,2	0.25	0
3	EDO	BBB	309	-	3,3,3	0.07	0	2,2,2	0.14	0
3	EDO	DDD	307	-	3,3,3	0.09	0	2,2,2	0.18	0
3	EDO	GGG	301	-	3,3,3	0.20	0	2,2,2	0.25	0
3	EDO	CCC	309	-	3,3,3	0.12	0	2,2,2	0.13	0
3	EDO	CCC	307	-	3,3,3	0.07	0	2,2,2	0.17	0
3	EDO	HHH	307	-	3,3,3	0.10	0	2,2,2	0.22	0
3	EDO	III	307	-	3,3,3	0.07	0	2,2,2	0.21	0
3	EDO	EEE	307	-	3,3,3	0.07	0	2,2,2	0.25	0
3	EDO	JJJ	305	-	3,3,3	0.13	0	2,2,2	0.26	0
3	EDO	FFF	306	-	3,3,3	0.10	0	2,2,2	0.30	0
3	EDO	FFF	308	-	3,3,3	0.16	0	2,2,2	0.32	0
3	EDO	JJJ	307	-	3,3,3	0.08	0	2,2,2	0.21	0
3	EDO	GGG	306	-	3,3,3	0.19	0	2,2,2	0.22	0
3	EDO	EEE	302	-	3,3,3	0.09	0	2,2,2	0.15	0
3	EDO	HHH	303	-	3,3,3	0.09	0	2,2,2	0.19	0
3	EDO	DDD	302	-	3,3,3	0.17	0	2,2,2	0.18	0
3	EDO	CCC	302	-	3,3,3	0.09	0	2,2,2	0.07	0
3	EDO	HHH	309	-	3,3,3	0.40	0	2,2,2	0.28	0
3	EDO	JJJ	302	-	3,3,3	0.16	0	2,2,2	0.08	0
3	EDO	GGG	305	-	3,3,3	0.21	0	2,2,2	0.49	0
3	EDO	BBB	310	-	3,3,3	0.09	0	2,2,2	0.08	0
3	EDO	EEE	303	-	3,3,3	0.18	0	2,2,2	0.37	0
3	EDO	FFF	310	-	3,3,3	0.13	0	2,2,2	0.14	0
3	EDO	AAA	307	-	3,3,3	0.04	0	2,2,2	0.17	0
3	EDO	EEE	305	-	3,3,3	0.06	0	2,2,2	0.08	0
3	EDO	BBB	312	-	3,3,3	0.29	0	2,2,2	0.07	0
3	EDO	III	304	-	3,3,3	0.14	0	2,2,2	0.48	0
3	EDO	EEE	308	-	3,3,3	0.22	0	2,2,2	0.14	0
3	EDO	FFF	305	-	3,3,3	0.12	0	2,2,2	0.42	0
3	EDO	DDD	306	-	3,3,3	0.10	0	2,2,2	0.16	0
3	EDO	AAA	310	-	3,3,3	0.10	0	2,2,2	0.22	0
3	EDO	AAA	312	-	3,3,3	0.19	0	2,2,2	0.14	0
3	EDO	III	305	-	3,3,3	0.04	0	2,2,2	0.24	0
3	EDO	AAA	304	-	3,3,3	0.21	0	2,2,2	0.16	0
3	EDO	CCC	304	-	3,3,3	0.16	0	2,2,2	0.25	0
3	EDO	BBB	306	-	3,3,3	0.26	0	2,2,2	0.20	0
3	EDO	FFF	304	-	3,3,3	0.13	0	2,2,2	0.16	0
3	EDO	AAA	302	-	3,3,3	0.14	0	2,2,2	0.06	0
3	EDO	BBB	311	-	3,3,3	0.26	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	HHH	305	-	3,3,3	0.14	0	2,2,2	0.32	0
3	EDO	JJJ	308	-	3,3,3	0.16	0	2,2,2	0.12	0
2	IMD	BBB	301	-	3,5,5	0.25	0	4,5,5	0.94	0
3	EDO	CCC	301	-	3,3,3	0.20	0	2,2,2	0.10	0
3	EDO	GGG	310	-	3,3,3	0.18	0	2,2,2	0.29	0
3	EDO	GGG	307	-	3,3,3	0.18	0	2,2,2	0.22	0
3	EDO	EEE	301	-	3,3,3	0.13	0	2,2,2	0.16	0
3	EDO	HHH	310	-	3,3,3	0.22	0	2,2,2	0.15	0
3	EDO	GGG	308	-	3,3,3	0.12	0	2,2,2	0.33	0
3	EDO	GGG	312	-	3,3,3	0.10	0	2,2,2	0.21	0
3	EDO	HHH	301	-	3,3,3	0.07	0	2,2,2	0.09	0
3	EDO	BBB	302	-	3,3,3	0.07	0	2,2,2	0.29	0
3	EDO	FFF	301	-	3,3,3	0.12	0	2,2,2	0.22	0
3	EDO	III	302	-	3,3,3	0.09	0	2,2,2	0.15	0
3	EDO	III	309	-	3,3,3	0.10	0	2,2,2	0.15	0
3	EDO	CCC	310	-	3,3,3	0.12	0	2,2,2	0.11	0
3	EDO	DDD	305	-	3,3,3	0.23	0	2,2,2	0.43	0
3	EDO	HHH	302	-	3,3,3	0.05	0	2,2,2	0.18	0
3	EDO	GGG	303	-	3,3,3	0.08	0	2,2,2	0.10	0
3	EDO	CCC	306	-	3,3,3	0.20	0	2,2,2	0.39	0
3	EDO	BBB	313	-	3,3,3	0.17	0	2,2,2	0.02	0
3	EDO	BBB	305	-	3,3,3	0.15	0	2,2,2	0.12	0
3	EDO	CCC	308	-	3,3,3	0.09	0	2,2,2	0.24	0
3	EDO	GGG	304	-	3,3,3	0.10	0	2,2,2	0.10	0
3	EDO	EEE	306	-	3,3,3	0.12	0	2,2,2	0.36	0
3	EDO	FFF	302	-	3,3,3	0.16	0	2,2,2	0.13	0
3	EDO	FFF	307	-	3,3,3	0.14	0	2,2,2	0.14	0
3	EDO	DDD	309	-	3,3,3	0.07	0	2,2,2	0.31	0
3	EDO	EEE	304	-	3,3,3	0.11	0	2,2,2	0.26	0
3	EDO	GGG	302	-	3,3,3	0.19	0	2,2,2	0.21	0
3	EDO	JJJ	306	-	3,3,3	0.13	0	2,2,2	0.19	0
3	EDO	GGG	311	-	3,3,3	0.23	0	2,2,2	0.17	0
3	EDO	AAA	306	-	3,3,3	0.13	0	2,2,2	0.45	0
2	IMD	AAA	301	-	3,5,5	0.22	0	4,5,5	0.79	0
3	EDO	III	308	-	3,3,3	0.10	0	2,2,2	0.15	0
3	EDO	HHH	308	-	3,3,3	0.10	0	2,2,2	0.27	0
3	EDO	DDD	308	-	3,3,3	0.15	0	2,2,2	0.29	0
3	EDO	DDD	310	-	3,3,3	0.06	0	2,2,2	0.15	0
2	IMD	III	301	-	3,5,5	0.44	0	4,5,5	0.94	0
3	EDO	BBB	308	-	3,3,3	0.11	0	2,2,2	0.32	0
3	EDO	BBB	304	-	3,3,3	0.08	0	2,2,2	0.45	0
3	EDO	AAA	308	-	3,3,3	0.09	0	2,2,2	0.16	0
3	EDO	JJJ	303	-	3,3,3	0.20	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	DDD	304	-	3,3,3	0.19	0	2,2,2	0.05	0
3	EDO	FFF	309	-	3,3,3	0.08	0	2,2,2	0.22	0
3	EDO	HHH	306	-	3,3,3	0.11	0	2,2,2	0.18	0
3	EDO	BBB	303	-	3,3,3	0.06	0	2,2,2	0.07	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
3	EDO	FFF	303	-	-	0/1/1/1	-
3	EDO	CCC	305	-	-	0/1/1/1	-
3	EDO	HHH	307	-	-	1/1/1/1	-
3	EDO	JJJ	304	-	-	1/1/1/1	-
3	EDO	CCC	303	-	-	1/1/1/1	-
2	IMD	DDD	301	-	-	-	0/1/1/1
3	EDO	BBB	307	-	-	0/1/1/1	-
3	EDO	HHH	304	-	-	1/1/1/1	-
3	EDO	AAA	311	-	-	1/1/1/1	-
3	EDO	III	303	-	-	1/1/1/1	-
3	EDO	AAA	309	-	-	0/1/1/1	-
3	EDO	GGG	309	-	-	1/1/1/1	-
3	EDO	III	306	-	-	0/1/1/1	-
2	IMD	JJJ	301	-	-	-	0/1/1/1
3	EDO	AAA	305	-	-	1/1/1/1	-
3	EDO	AAA	303	-	-	0/1/1/1	-
3	EDO	DDD	311	-	-	1/1/1/1	-
3	EDO	BBB	309	-	-	0/1/1/1	-
3	EDO	DDD	307	-	-	1/1/1/1	-
3	EDO	GGG	301	-	-	0/1/1/1	-
3	EDO	CCC	309	-	-	1/1/1/1	-
3	EDO	CCC	307	-	-	1/1/1/1	-
3	EDO	DDD	303	-	-	0/1/1/1	-
3	EDO	III	307	-	-	1/1/1/1	-
3	EDO	EEE	307	-	-	0/1/1/1	-
3	EDO	JJJ	305	-	-	1/1/1/1	-
3	EDO	FFF	306	-	-	0/1/1/1	-
3	EDO	FFF	308	-	-	0/1/1/1	-
3	EDO	JJJ	307	-	-	1/1/1/1	-
3	EDO	GGG	306	-	-	0/1/1/1	-
3	EDO	EEE	302	-	-	1/1/1/1	-
3	EDO	HHH	303	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	DDD	302	-	-	0/1/1/1	-
3	EDO	CCC	302	-	-	0/1/1/1	-
3	EDO	HHH	309	-	-	0/1/1/1	-
3	EDO	JJJ	302	-	-	0/1/1/1	-
3	EDO	GGG	305	-	-	0/1/1/1	-
3	EDO	BBB	310	-	-	0/1/1/1	-
3	EDO	EEE	303	-	-	1/1/1/1	-
3	EDO	FFF	310	-	-	1/1/1/1	-
3	EDO	AAA	307	-	-	0/1/1/1	-
3	EDO	EEE	305	-	-	0/1/1/1	-
3	EDO	BBB	312	-	-	0/1/1/1	-
3	EDO	III	304	-	-	0/1/1/1	-
3	EDO	EEE	308	-	-	0/1/1/1	-
3	EDO	FFF	305	-	-	1/1/1/1	-
3	EDO	DDD	306	-	-	0/1/1/1	-
3	EDO	AAA	310	-	-	1/1/1/1	-
3	EDO	AAA	312	-	-	0/1/1/1	-
3	EDO	III	305	-	-	1/1/1/1	-
3	EDO	AAA	304	-	-	0/1/1/1	-
3	EDO	CCC	304	-	-	0/1/1/1	-
3	EDO	BBB	306	-	-	1/1/1/1	-
3	EDO	FFF	304	-	-	0/1/1/1	-
3	EDO	AAA	302	-	-	0/1/1/1	-
3	EDO	BBB	311	-	-	1/1/1/1	-
3	EDO	HHH	305	-	-	0/1/1/1	-
3	EDO	JJJ	308	-	-	0/1/1/1	-
2	IMD	BBB	301	-	-	-	0/1/1/1
3	EDO	CCC	301	-	-	0/1/1/1	-
3	EDO	GGG	310	-	-	0/1/1/1	-
3	EDO	GGG	307	-	-	1/1/1/1	-
3	EDO	EEE	301	-	-	0/1/1/1	-
3	EDO	HHH	310	-	-	0/1/1/1	-
3	EDO	GGG	308	-	-	0/1/1/1	-
3	EDO	GGG	312	-	-	1/1/1/1	-
3	EDO	HHH	301	-	-	0/1/1/1	-
3	EDO	BBB	302	-	-	0/1/1/1	-
3	EDO	FFF	301	-	-	0/1/1/1	-
3	EDO	III	302	-	-	0/1/1/1	-
3	EDO	III	309	-	-	0/1/1/1	-
3	EDO	CCC	310	-	-	0/1/1/1	-
3	EDO	DDD	305	-	-	1/1/1/1	-
3	EDO	HHH	302	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	GGG	303	-	-	1/1/1/1	-
3	EDO	CCC	306	-	-	1/1/1/1	-
3	EDO	BBB	313	-	-	0/1/1/1	-
3	EDO	BBB	305	-	-	0/1/1/1	-
3	EDO	CCC	308	-	-	0/1/1/1	-
3	EDO	GGG	304	-	-	0/1/1/1	-
3	EDO	EEE	306	-	-	0/1/1/1	-
3	EDO	FFF	302	-	-	0/1/1/1	-
3	EDO	FFF	307	-	-	0/1/1/1	-
3	EDO	DDD	309	-	-	1/1/1/1	-
3	EDO	EEE	304	-	-	0/1/1/1	-
3	EDO	GGG	302	-	-	0/1/1/1	-
3	EDO	JJJ	306	-	-	0/1/1/1	-
3	EDO	GGG	311	-	-	0/1/1/1	-
3	EDO	AAA	306	-	-	0/1/1/1	-
2	IMD	AAA	301	-	-	-	0/1/1/1
3	EDO	III	308	-	-	0/1/1/1	-
3	EDO	HHH	308	-	-	1/1/1/1	-
3	EDO	DDD	308	-	-	0/1/1/1	-
3	EDO	DDD	310	-	-	1/1/1/1	-
2	IMD	III	301	-	-	-	0/1/1/1
3	EDO	BBB	308	-	-	0/1/1/1	-
3	EDO	BBB	304	-	-	0/1/1/1	-
3	EDO	AAA	308	-	-	0/1/1/1	-
3	EDO	JJJ	303	-	-	1/1/1/1	-
3	EDO	DDD	304	-	-	1/1/1/1	-
3	EDO	FFF	309	-	-	1/1/1/1	-
3	EDO	HHH	306	-	-	1/1/1/1	-
3	EDO	BBB	303	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	306	EDO	O1-C1-C2-O2
3	JJJ	304	EDO	O1-C1-C2-O2
3	GGG	309	EDO	O1-C1-C2-O2
3	HHH	307	EDO	O1-C1-C2-O2
3	JJJ	307	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	GGG	306	EDO	1	0
3	HHH	309	EDO	1	0
3	GGG	307	EDO	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	AAA	265/287 (92%)	-0.28	2 (0%) 86 87	7, 11, 23, 32	0
1	BBB	265/287 (92%)	-0.34	2 (0%) 86 87	7, 11, 21, 35	0
1	CCC	265/287 (92%)	-0.36	1 (0%) 92 94	8, 12, 20, 38	0
1	DDD	265/287 (92%)	-0.28	2 (0%) 86 87	8, 12, 23, 36	0
1	EEE	264/287 (91%)	-0.35	0 100 100	7, 11, 22, 33	0
1	FFF	268/287 (93%)	-0.22	5 (1%) 66 68	8, 12, 29, 49	0
1	GGG	267/287 (93%)	-0.23	7 (2%) 56 58	7, 10, 24, 45	0
1	HHH	268/287 (93%)	-0.33	2 (0%) 87 89	8, 11, 20, 41	0
1	III	267/287 (93%)	-0.29	3 (1%) 80 82	8, 12, 22, 42	0
1	JJJ	264/287 (91%)	-0.19	6 (2%) 60 63	7, 11, 28, 45	0
All	All	2658/2870 (92%)	-0.29	30 (1%) 80 82	7, 11, 23, 49	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	GGG	21	GLY	7.1
1	III	21	GLY	6.4
1	FFF	21	GLY	6.0
1	JJJ	90	THR	5.2
1	GGG	22	GLY	4.5

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 ⓘ

There are no monosaccharides in this entry.

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	EDO	DDD	310	4/4	0.63	0.28	50,50,50,53	0
3	EDO	FFF	310	4/4	0.66	0.19	34,36,38,41	0
3	EDO	CCC	308	4/4	0.67	0.21	42,42,42,44	0
3	EDO	AAA	310	4/4	0.72	0.18	49,50,51,51	0
3	EDO	GGG	312	4/4	0.73	0.37	42,47,47,50	0
3	EDO	DDD	308	4/4	0.75	0.18	33,33,34,34	0
3	EDO	FFF	309	4/4	0.75	0.20	50,50,52,52	0
3	EDO	EEE	302	4/4	0.76	0.15	35,36,36,37	0
3	EDO	JJJ	307	4/4	0.76	0.12	46,50,50,51	0
3	EDO	GGG	304	4/4	0.77	0.17	33,33,34,36	0
3	EDO	BBB	312	4/4	0.78	0.35	32,34,35,37	0
3	EDO	BBB	310	4/4	0.78	0.21	51,52,52,52	0
3	EDO	AAA	311	4/4	0.79	0.21	34,34,36,36	0
3	EDO	CCC	310	4/4	0.80	0.17	36,38,40,45	0
3	EDO	HHH	309	4/4	0.80	0.29	30,31,32,33	0
3	EDO	JJJ	303	4/4	0.80	0.15	28,28,29,33	0
3	EDO	DDD	304	4/4	0.80	0.14	29,30,30,31	0
3	EDO	AAA	305	4/4	0.80	0.15	33,33,34,34	0
3	EDO	AAA	308	4/4	0.81	0.14	42,43,43,45	0
3	EDO	III	308	4/4	0.81	0.12	38,38,40,41	0
3	EDO	III	306	4/4	0.82	0.14	32,36,37,39	0
3	EDO	JJJ	304	4/4	0.82	0.15	27,29,31,33	0
3	EDO	DDD	309	4/4	0.83	0.19	42,44,44,45	0
3	EDO	GGG	305	4/4	0.83	0.17	25,26,27,31	0
3	EDO	CCC	304	4/4	0.83	0.17	26,29,31,34	0
3	EDO	HHH	307	4/4	0.83	0.24	44,45,45,47	0
3	EDO	GGG	307	4/4	0.84	0.12	25,27,27,30	0
3	EDO	BBB	305	4/4	0.84	0.14	27,28,28,29	0
3	EDO	GGG	308	4/4	0.84	0.19	26,28,29,29	0
3	EDO	HHH	305	4/4	0.84	0.16	26,30,31,33	0
3	EDO	III	305	4/4	0.85	0.14	33,37,37,40	0
3	EDO	CCC	303	4/4	0.85	0.12	29,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	EEE	303	4/4	0.85	0.16	28,29,31,34	0
3	EDO	HHH	303	4/4	0.85	0.14	28,28,30,32	0
3	EDO	III	303	4/4	0.85	0.15	34,34,34,37	0
3	EDO	HHH	304	4/4	0.85	0.15	24,26,28,31	0
3	EDO	BBB	307	4/4	0.86	0.18	28,29,29,30	0
3	EDO	DDD	311	4/4	0.86	0.18	43,44,44,45	0
3	EDO	FFF	305	4/4	0.86	0.14	25,26,27,31	0
3	EDO	BBB	306	4/4	0.86	0.12	21,23,25,29	0
3	EDO	FFF	304	4/4	0.87	0.13	30,31,32,34	0
3	EDO	EEE	306	4/4	0.87	0.14	27,31,32,32	0
3	EDO	HHH	306	4/4	0.87	0.16	37,38,39,41	0
3	EDO	BBB	308	4/4	0.88	0.11	28,30,32,32	0
3	EDO	CCC	307	4/4	0.88	0.09	42,42,43,44	0
4	CL	HHH	312	1/1	0.88	0.09	45,45,45,45	0
3	EDO	CCC	302	4/4	0.88	0.12	25,27,27,32	0
3	EDO	FFF	308	4/4	0.88	0.11	32,34,34,35	0
3	EDO	JJJ	308	4/4	0.88	0.13	33,36,37,39	0
3	EDO	AAA	312	4/4	0.89	0.13	31,32,33,37	0
3	EDO	III	309	4/4	0.89	0.22	47,48,48,49	0
3	EDO	BBB	311	4/4	0.89	0.25	33,33,33,36	0
3	EDO	GGG	303	4/4	0.89	0.11	25,25,27,27	0
3	EDO	JJJ	306	4/4	0.89	0.14	31,31,33,35	0
3	EDO	BBB	313	4/4	0.89	0.15	36,38,38,41	0
3	EDO	AAA	306	4/4	0.89	0.14	25,25,26,29	0
3	EDO	AAA	307	4/4	0.89	0.10	34,35,36,37	0
3	EDO	HHH	308	4/4	0.90	0.19	31,31,31,32	0
3	EDO	CCC	309	4/4	0.90	0.13	47,49,50,50	0
3	EDO	GGG	310	4/4	0.90	0.19	23,28,30,36	0
3	EDO	FFF	307	4/4	0.90	0.22	30,30,31,31	0
3	EDO	III	307	4/4	0.90	0.20	48,48,48,50	0
3	EDO	CCC	306	4/4	0.90	0.14	30,30,30,32	0
3	EDO	HHH	310	4/4	0.90	0.12	34,36,37,40	0
3	EDO	EEE	308	4/4	0.90	0.17	33,37,38,41	0
3	EDO	GGG	309	4/4	0.90	0.14	40,41,42,43	0
3	EDO	BBB	309	4/4	0.91	0.13	34,35,35,36	0
3	EDO	AAA	304	4/4	0.91	0.11	23,23,23,26	0
3	EDO	III	302	4/4	0.91	0.11	24,25,26,27	0
3	EDO	GGG	311	4/4	0.91	0.16	31,35,36,41	0
3	EDO	DDD	307	4/4	0.91	0.10	31,32,32,34	0
3	EDO	EEE	307	4/4	0.91	0.12	40,40,41,42	0
3	EDO	EEE	305	4/4	0.91	0.19	26,27,28,29	0
3	EDO	JJJ	305	4/4	0.91	0.12	27,29,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	DDD	306	4/4	0.92	0.12	24,26,26,27	0
3	EDO	DDD	303	4/4	0.92	0.10	24,24,25,27	0
3	EDO	EEE	301	4/4	0.92	0.10	22,22,22,26	0
3	EDO	DDD	305	4/4	0.92	0.12	23,27,29,32	0
3	EDO	BBB	303	4/4	0.92	0.10	29,29,30,33	0
4	CL	HHH	311	1/1	0.93	0.04	43,43,43,43	0
4	CL	AAA	313	1/1	0.93	0.05	48,48,48,48	0
3	EDO	FFF	303	4/4	0.93	0.09	24,24,25,28	0
4	CL	III	310	1/1	0.93	0.13	43,43,43,43	0
4	CL	GGG	313	1/1	0.93	0.09	42,42,42,42	0
3	EDO	HHH	302	4/4	0.93	0.08	25,26,26,29	0
3	EDO	III	304	4/4	0.94	0.11	23,25,26,29	0
4	CL	III	311	1/1	0.94	0.06	37,37,37,37	0
4	CL	EEE	309	1/1	0.95	0.06	41,41,41,41	0
4	CL	BBB	314	1/1	0.95	0.07	42,42,42,42	0
3	EDO	BBB	304	4/4	0.95	0.11	24,25,26,30	0
3	EDO	AAA	309	4/4	0.95	0.12	19,24,27,29	0
3	EDO	GGG	301	4/4	0.95	0.10	13,13,14,17	0
3	EDO	FFF	306	4/4	0.95	0.12	24,26,29,30	0
3	EDO	JJJ	302	4/4	0.95	0.08	23,23,24,24	0
3	EDO	FFF	302	4/4	0.95	0.09	13,15,15,17	0
3	EDO	CCC	301	4/4	0.95	0.08	16,17,18,19	0
4	CL	CCC	311	1/1	0.95	0.05	46,46,46,46	0
3	EDO	BBB	302	4/4	0.96	0.08	15,16,16,19	0
2	IMD	JJJ	301	5/5	0.96	0.07	10,10,11,11	0
4	CL	CCC	312	1/1	0.96	0.07	34,34,34,34	0
2	IMD	BBB	301	5/5	0.96	0.07	11,11,12,12	0
4	CL	BBB	315	1/1	0.96	0.07	35,35,35,35	0
3	EDO	AAA	302	4/4	0.96	0.07	13,13,13,16	0
3	EDO	GGG	306	4/4	0.96	0.09	18,20,22,23	0
3	EDO	DDD	302	4/4	0.96	0.07	15,15,16,16	0
4	CL	DDD	313	1/1	0.97	0.05	40,40,40,40	0
3	EDO	GGG	302	4/4	0.97	0.06	12,14,14,17	0
4	CL	FFF	311	1/1	0.97	0.05	40,40,40,40	0
4	CL	GGG	314	1/1	0.97	0.07	36,36,36,36	0
3	EDO	EEE	304	4/4	0.97	0.08	19,22,25,26	0
3	EDO	AAA	303	4/4	0.97	0.06	14,16,17,21	0
2	IMD	DDD	301	5/5	0.97	0.06	10,11,11,11	0
3	EDO	HHH	301	4/4	0.97	0.07	15,15,15,17	0
2	IMD	III	301	5/5	0.97	0.07	10,10,10,10	0
4	CL	FFF	312	1/1	0.98	0.07	36,36,36,36	0
3	EDO	FFF	301	4/4	0.98	0.06	16,17,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	CCC	305	4/4	0.98	0.06	16,20,22,24	0
2	IMD	AAA	301	5/5	0.98	0.06	11,11,12,12	0
4	CL	DDD	312	1/1	0.98	0.08	44,44,44,44	0
4	CL	JJJ	309	1/1	0.98	0.05	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.