



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:42 AM UTC

PDB ID : 6Y65 / pdb_00006y65
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

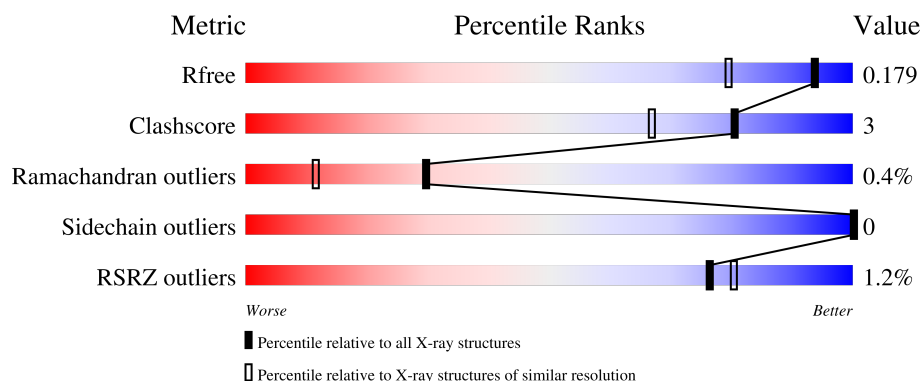
1 Overall quality at a glance

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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (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 of 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	86% 6% 8%
1	BBB	287	87% 5% 8%
1	CCC	287	86% 6% 8%
1	DDD	287	87% 5% 8%
1	EEE	287	88% • 8%

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Mol	Chain	Length	Quality of chain		
1	FFF	287	2%	89%	5% 7%
1	GGG	287	2%	86%	7% 7%
1	HHH	287	2%	87%	6% 7%
1	III	287	1%	87%	6% 7%
1	JJJ	287	2%	88%	• 8%

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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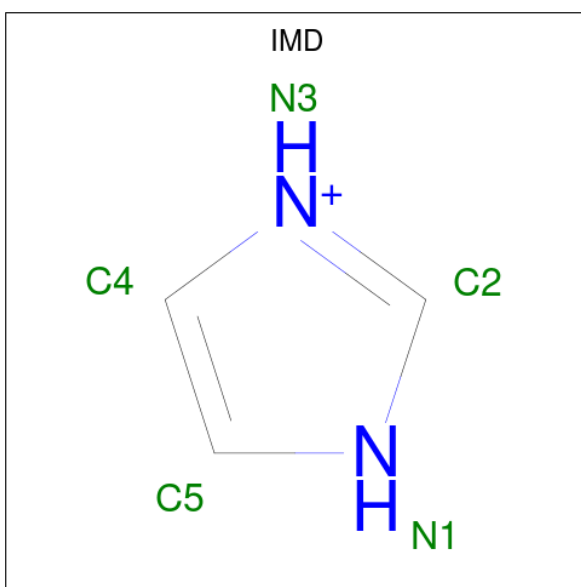
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	9	HIS	-	expression tag	UNP Q80FI3
GGG	10	SER	-	expression tag	UNP Q80FI3
GGG	11	SER	-	expression tag	UNP Q80FI3
GGG	12	GLY	-	expression tag	UNP Q80FI3
GGG	13	LEU	-	expression tag	UNP Q80FI3
GGG	14	VAL	-	expression tag	UNP Q80FI3
GGG	15	PRO	-	expression 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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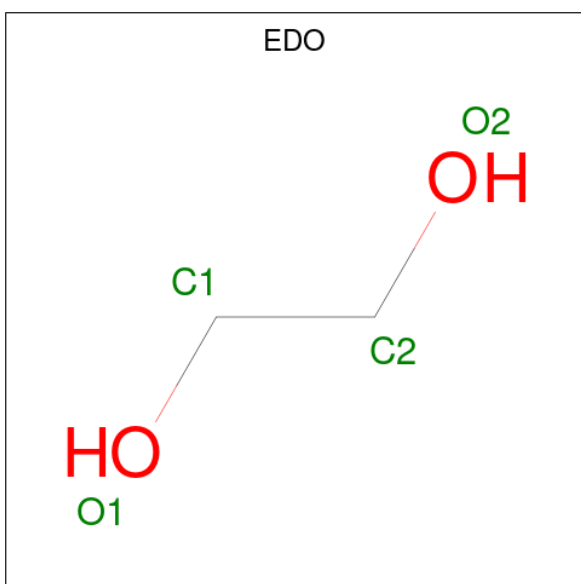
Chain	Residue	Modelled	Actual	Comment	Reference
III	9	HIS	-	expression tag	UNP Q80FI3
III	10	SER	-	expression tag	UNP Q80FI3
III	11	SER	-	expression tag	UNP Q80FI3
III	12	GLY	-	expression tag	UNP Q80FI3
III	13	LEU	-	expression tag	UNP Q80FI3
III	14	VAL	-	expression tag	UNP Q80FI3
III	15	PRO	-	expression 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 (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		
4	BBB	2	Total	Cl	0	0
			2	2		
4	CCC	2	Total	Cl	0	0
			2	2		
4	DDD	2	Total	Cl	0	0
			2	2		
4	EEE	1	Total	Cl	0	0
			1	1		
4	FFF	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	GGG	2	Total	Cl	0	0
			2	2		
4	HHH	2	Total	Cl	0	0
			2	2		
4	III	2	Total	Cl	0	0
			2	2		
4	JJJ	1	Total	Cl	0	0
			1	1		

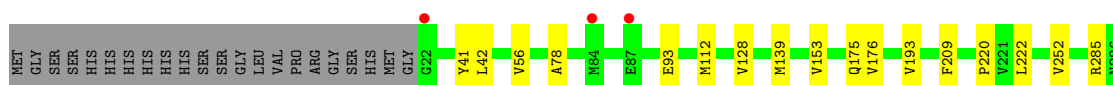
- Molecule 5 is water.

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

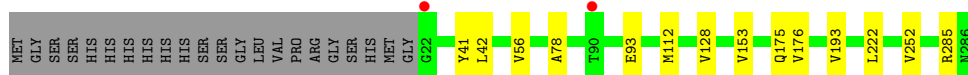
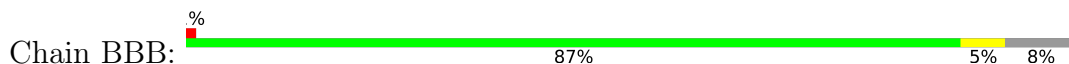
3 Residue-property plots [i](#)

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.

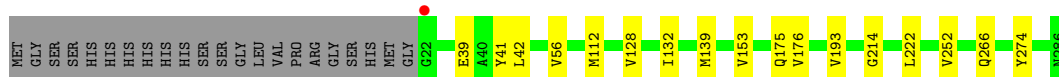
- Molecule 1: Capsid protein VP1



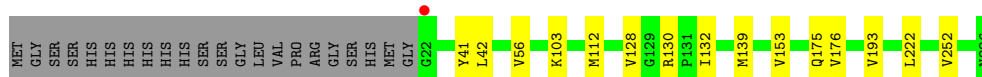
- Molecule 1: Capsid protein VP1



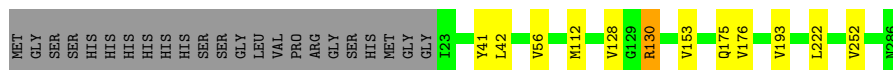
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

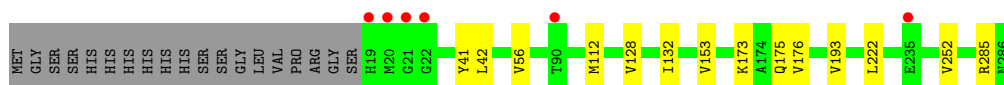


- Molecule 1: Capsid protein VP1



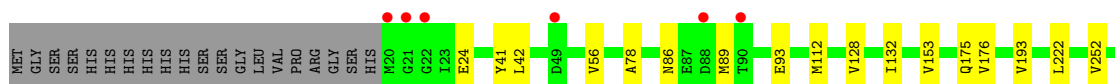
- Molecule 1: Capsid protein VP1

Chain FFF: 



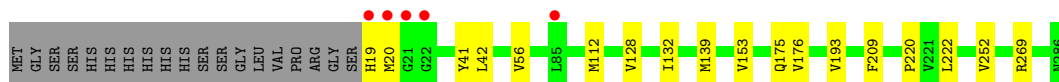
- Molecule 1: Capsid protein VP1

Chain GGG: 



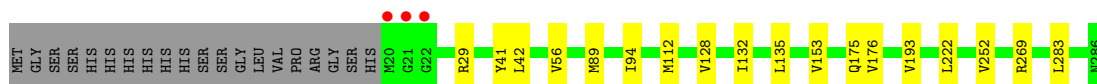
- Molecule 1: Capsid protein VP1

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	87.29Å 90.41Å 100.84Å 94.05° 97.90° 108.06°	Depositor
Resolution (Å)	45.97 – 1.45 45.97 – 1.45	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.97-1.45) 95.4 (45.97-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.45Å)	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 , 36.5	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

5.1 Standard geometry

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	0.89	0/2115	1.00	0/2886
1	BBB	0.90	0/2102	1.00	0/2869
1	CCC	0.89	0/2119	1.00	0/2891
1	DDD	0.90	0/2101	1.00	0/2867
1	EEE	0.88	0/2098	0.98	1/2863 (0.0%)
1	FFF	0.88	0/2134	1.03	0/2911
1	GGG	0.88	0/2130	0.98	0/2904
1	HHH	0.89	0/2131	0.99	0/2906
1	III	0.89	0/2124	1.00	0/2896
1	JJJ	0.90	0/2093	0.99	0/2858
All	All	0.89	0/21147	1.00	1/28851 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	130	ARG	CB-CA-C	-5.99	100.33	109.50

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	2061	0	2017	14	0
1	BBB	2048	0	2004	10	0
1	CCC	2065	0	2008	12	0
1	DDD	2050	0	1998	12	0
1	EEE	2047	0	1999	8	0
1	FFF	2080	0	2028	11	0
1	GGG	2076	0	2026	18	0
1	HHH	2079	0	2025	11	0
1	III	2073	0	2028	12	0
1	JJJ	2042	0	1995	11	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	1	0
5	EEE	342	0	0	1	0
5	FFF	318	0	0	2	0
5	GGG	336	0	0	1	0
5	HHH	351	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	III	332	0	0	0	0
5	JJJ	330	0	0	0	0
All	All	24379	0	20741	107	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 3.

The worst 5 of 107 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	0.96
1:BBB:112[B]:MET:HE1	1:BBB:222:LEU:CD1	2.01	0.91
1:III:112[B]:MET:HE1	1:III:222:LEU:CD1	2.03	0.88
1:GGG:112[B]:MET:HE1	1:GGG:222:LEU:CD1	2.06	0.85
1:JJJ:112[B]:MET:HE1	1:JJJ:222:LEU:CD1	2.05	0.85

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%)	30	11
1	BBB	271/287 (94%)	262 (97%)	8 (3%)	1 (0%)	30	11
1	CCC	274/287 (96%)	265 (97%)	8 (3%)	1 (0%)	30	11
1	DDD	272/287 (95%)	264 (97%)	7 (3%)	1 (0%)	30	11
1	EEE	270/287 (94%)	261 (97%)	8 (3%)	1 (0%)	30	11
1	FFF	276/287 (96%)	268 (97%)	7 (2%)	1 (0%)	30	11
1	GGG	275/287 (96%)	266 (97%)	8 (3%)	1 (0%)	30	11
1	HHH	275/287 (96%)	266 (97%)	8 (3%)	1 (0%)	30	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	III	275/287 (96%)	266 (97%)	8 (3%)	1 (0%)	30	11
1	JJJ	270/287 (94%)	261 (97%)	8 (3%)	1 (0%)	30	11
All	All	2731/2870 (95%)	2644 (97%)	77 (3%)	10 (0%)	30	11

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.

Sometimes 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 oligosaccharides 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	BBB	313	-	3,3,3	0.17	0	2,2,2	0.05	0
3	EDO	DDD	310	-	3,3,3	0.06	0	2,2,2	0.08	0
3	EDO	FFF	306	-	3,3,3	0.10	0	2,2,2	0.23	0
3	EDO	AAA	307	-	3,3,3	0.04	0	2,2,2	0.10	0
3	EDO	AAA	306	-	3,3,3	0.13	0	2,2,2	0.37	0
3	EDO	DDD	303	-	3,3,3	0.04	0	2,2,2	0.06	0
3	EDO	DDD	302	-	3,3,3	0.17	0	2,2,2	0.12	0
3	EDO	FFF	305	-	3,3,3	0.12	0	2,2,2	0.33	0
3	EDO	BBB	312	-	3,3,3	0.29	0	2,2,2	0.12	0
3	EDO	EEE	306	-	3,3,3	0.12	0	2,2,2	0.30	0
2	IMD	JJJ	301	-	5,5,5	0.25	0	5,5,5	0.78	0
3	EDO	AAA	302	-	3,3,3	0.12	0	2,2,2	0.11	0
3	EDO	GGG	311	-	3,3,3	0.23	0	2,2,2	0.14	0
3	EDO	CCC	307	-	3,3,3	0.07	0	2,2,2	0.11	0
3	EDO	GGG	312	-	3,3,3	0.10	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	III	302	-	3,3,3	0.08	0	2,2,2	0.17	0
3	EDO	GGG	310	-	3,3,3	0.17	0	2,2,2	0.22	0
3	EDO	GGG	306	-	3,3,3	0.19	0	2,2,2	0.14	0
3	EDO	HHH	310	-	3,3,3	0.23	0	2,2,2	0.14	0
3	EDO	EEE	304	-	3,3,3	0.11	0	2,2,2	0.21	0
3	EDO	DDD	309	-	3,3,3	0.07	0	2,2,2	0.24	0
3	EDO	III	304	-	3,3,3	0.13	0	2,2,2	0.40	0
3	EDO	HHH	301	-	3,3,3	0.07	0	2,2,2	0.04	0
3	EDO	CCC	310	-	3,3,3	0.12	0	2,2,2	0.09	0
3	EDO	DDD	311	-	3,3,3	0.08	0	2,2,2	0.17	0
3	EDO	DDD	306	-	3,3,3	0.09	0	2,2,2	0.09	0
3	EDO	GGG	301	-	3,3,3	0.21	0	2,2,2	0.18	0
3	EDO	BBB	305	-	3,3,3	0.14	0	2,2,2	0.11	0
3	EDO	III	305	-	3,3,3	0.04	0	2,2,2	0.16	0
3	EDO	EEE	308	-	3,3,3	0.22	0	2,2,2	0.17	0
3	EDO	JJJ	303	-	3,3,3	0.19	0	2,2,2	0.04	0
3	EDO	AAA	311	-	3,3,3	0.08	0	2,2,2	0.10	0
3	EDO	CCC	301	-	3,3,3	0.20	0	2,2,2	0.06	0
3	EDO	GGG	309	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	HHH	304	-	3,3,3	0.17	0	2,2,2	0.32	0
3	EDO	CCC	303	-	3,3,3	0.06	0	2,2,2	0.09	0
3	EDO	AAA	304	-	3,3,3	0.21	0	2,2,2	0.13	0
3	EDO	FFF	302	-	3,3,3	0.16	0	2,2,2	0.09	0
3	EDO	AAA	312	-	3,3,3	0.19	0	2,2,2	0.08	0
3	EDO	BBB	308	-	3,3,3	0.11	0	2,2,2	0.26	0
3	EDO	GGG	304	-	3,3,3	0.08	0	2,2,2	0.12	0
3	EDO	GGG	307	-	3,3,3	0.17	0	2,2,2	0.18	0
3	EDO	HHH	307	-	3,3,3	0.10	0	2,2,2	0.17	0
3	EDO	JJJ	307	-	3,3,3	0.08	0	2,2,2	0.14	0
3	EDO	CCC	306	-	3,3,3	0.20	0	2,2,2	0.31	0
3	EDO	HHH	309	-	3,3,3	0.41	0	2,2,2	0.32	0
3	EDO	EEE	301	-	3,3,3	0.13	0	2,2,2	0.13	0
3	EDO	AAA	310	-	3,3,3	0.10	0	2,2,2	0.16	0
3	EDO	III	306	-	3,3,3	0.16	0	2,2,2	0.21	0
3	EDO	FFF	303	-	3,3,3	0.13	0	2,2,2	0.10	0
3	EDO	III	303	-	3,3,3	0.06	0	2,2,2	0.03	0
3	EDO	CCC	305	-	3,3,3	0.04	0	2,2,2	0.35	0
3	EDO	DDD	305	-	3,3,3	0.23	0	2,2,2	0.35	0
3	EDO	DDD	307	-	3,3,3	0.09	0	2,2,2	0.11	0
3	EDO	DDD	304	-	3,3,3	0.18	0	2,2,2	0.06	0
3	EDO	FFF	310	-	3,3,3	0.12	0	2,2,2	0.08	0
3	EDO	HHH	306	-	3,3,3	0.12	0	2,2,2	0.11	0
2	IMD	AAA	301	-	5,5,5	0.24	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	III	308	-	3,3,3	0.10	0	2,2,2	0.11	0
3	EDO	HHH	303	-	3,3,3	0.09	0	2,2,2	0.12	0
3	EDO	CCC	308	-	3,3,3	0.09	0	2,2,2	0.17	0
3	EDO	JJJ	302	-	3,3,3	0.16	0	2,2,2	0.01	0
3	EDO	BBB	306	-	3,3,3	0.26	0	2,2,2	0.15	0
3	EDO	GGG	302	-	3,3,3	0.20	0	2,2,2	0.15	0
3	EDO	EEE	303	-	3,3,3	0.18	0	2,2,2	0.29	0
3	EDO	AAA	309	-	3,3,3	0.08	0	2,2,2	0.19	0
3	EDO	BBB	303	-	3,3,3	0.06	0	2,2,2	0.03	0
3	EDO	CCC	309	-	3,3,3	0.12	0	2,2,2	0.09	0
3	EDO	DDD	308	-	3,3,3	0.14	0	2,2,2	0.21	0
3	EDO	EEE	302	-	3,3,3	0.09	0	2,2,2	0.08	0
3	EDO	AAA	305	-	3,3,3	0.09	0	2,2,2	0.05	0
3	EDO	JJJ	308	-	3,3,3	0.16	0	2,2,2	0.08	0
3	EDO	FFF	301	-	3,3,3	0.12	0	2,2,2	0.15	0
3	EDO	JJJ	305	-	3,3,3	0.14	0	2,2,2	0.19	0
3	EDO	BBB	302	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	GGG	305	-	3,3,3	0.21	0	2,2,2	0.40	0
3	EDO	EEE	307	-	3,3,3	0.07	0	2,2,2	0.18	0
3	EDO	HHH	305	-	3,3,3	0.14	0	2,2,2	0.26	0
3	EDO	FFF	308	-	3,3,3	0.16	0	2,2,2	0.24	0
3	EDO	BBB	304	-	3,3,3	0.08	0	2,2,2	0.36	0
3	EDO	JJJ	304	-	3,3,3	0.19	0	2,2,2	0.32	0
3	EDO	III	307	-	3,3,3	0.07	0	2,2,2	0.13	0
3	EDO	FFF	304	-	3,3,3	0.13	0	2,2,2	0.09	0
3	EDO	CCC	304	-	3,3,3	0.16	0	2,2,2	0.18	0
2	IMD	DDD	301	-	5,5,5	0.30	0	5,5,5	0.70	0
3	EDO	BBB	311	-	3,3,3	0.26	0	2,2,2	0.15	0
2	IMD	BBB	301	-	5,5,5	0.26	0	5,5,5	0.77	0
3	EDO	EEE	305	-	3,3,3	0.06	0	2,2,2	0.02	0
3	EDO	AAA	308	-	3,3,3	0.09	0	2,2,2	0.09	0
3	EDO	HHH	302	-	3,3,3	0.04	0	2,2,2	0.13	0
3	EDO	FFF	309	-	3,3,3	0.08	0	2,2,2	0.15	0
3	EDO	III	309	-	3,3,3	0.10	0	2,2,2	0.09	0
3	EDO	AAA	303	-	3,3,3	0.26	0	2,2,2	0.11	0
3	EDO	HHH	308	-	3,3,3	0.10	0	2,2,2	0.20	0
2	IMD	III	301	-	5,5,5	0.48	0	5,5,5	0.77	0
3	EDO	GGG	303	-	3,3,3	0.09	0	2,2,2	0.04	0
3	EDO	GGG	308	-	3,3,3	0.11	0	2,2,2	0.26	0
3	EDO	BBB	307	-	3,3,3	0.08	0	2,2,2	0.14	0
3	EDO	FFF	307	-	3,3,3	0.14	0	2,2,2	0.18	0
3	EDO	BBB	310	-	3,3,3	0.09	0	2,2,2	0.07	0
3	EDO	BBB	309	-	3,3,3	0.08	0	2,2,2	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	JJJ	306	-	3,3,3	0.14	0	2,2,2	0.15	0
3	EDO	CCC	302	-	3,3,3	0.09	0	2,2,2	0.01	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	BBB	313	-	-	0/1/1/1	-
3	EDO	DDD	310	-	-	1/1/1/1	-
3	EDO	FFF	306	-	-	0/1/1/1	-
3	EDO	AAA	307	-	-	0/1/1/1	-
3	EDO	AAA	306	-	-	0/1/1/1	-
3	EDO	DDD	303	-	-	0/1/1/1	-
3	EDO	DDD	302	-	-	0/1/1/1	-
3	EDO	FFF	305	-	-	1/1/1/1	-
3	EDO	BBB	312	-	-	0/1/1/1	-
3	EDO	EEE	306	-	-	0/1/1/1	-
2	IMD	JJJ	301	-	-	-	0/1/1/1
3	EDO	AAA	302	-	-	0/1/1/1	-
3	EDO	GGG	311	-	-	0/1/1/1	-
3	EDO	CCC	307	-	-	1/1/1/1	-
3	EDO	GGG	312	-	-	1/1/1/1	-
3	EDO	III	302	-	-	0/1/1/1	-
3	EDO	GGG	310	-	-	0/1/1/1	-
3	EDO	GGG	306	-	-	0/1/1/1	-
3	EDO	HHH	310	-	-	0/1/1/1	-
3	EDO	EEE	304	-	-	0/1/1/1	-
3	EDO	DDD	309	-	-	1/1/1/1	-
3	EDO	III	304	-	-	0/1/1/1	-
3	EDO	HHH	301	-	-	0/1/1/1	-
3	EDO	CCC	310	-	-	0/1/1/1	-
3	EDO	DDD	311	-	-	1/1/1/1	-
3	EDO	DDD	306	-	-	0/1/1/1	-
3	EDO	GGG	301	-	-	0/1/1/1	-
3	EDO	BBB	305	-	-	0/1/1/1	-
3	EDO	III	305	-	-	1/1/1/1	-
3	EDO	EEE	308	-	-	0/1/1/1	-
3	EDO	JJJ	303	-	-	1/1/1/1	-
3	EDO	AAA	311	-	-	1/1/1/1	-
3	EDO	CCC	301	-	-	0/1/1/1	-
3	EDO	GGG	309	-	-	1/1/1/1	-

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	306	EDO	O1-C1-C2-O2
3	BBB	311	EDO	O1-C1-C2-O2
3	DDD	309	EDO	O1-C1-C2-O2
3	GGG	309	EDO	O1-C1-C2-O2
3	HHH	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	GGG	307	EDO	1	0
3	HHH	309	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.33	3 (1%) 78 82	4, 11, 23, 32	10 (3%)
1	BBB	265/287 (92%)	-0.36	2 (0%) 82 86	4, 11, 21, 35	8 (3%)
1	CCC	265/287 (92%)	-0.31	1 (0%) 88 91	5, 12, 20, 38	11 (4%)
1	DDD	265/287 (92%)	-0.26	1 (0%) 88 91	5, 12, 23, 36	9 (3%)
1	EEE	264/287 (91%)	-0.38	0 100 100	4, 11, 22, 33	8 (3%)
1	FFF	268/287 (93%)	-0.21	6 (2%) 62 65	4, 12, 29, 49	10 (3%)
1	GGG	267/287 (93%)	-0.35	6 (2%) 62 65	4, 10, 24, 45	10 (3%)
1	HHH	268/287 (93%)	-0.36	5 (1%) 66 68	4, 11, 20, 41	9 (3%)
1	III	267/287 (93%)	-0.25	3 (1%) 78 82	5, 11, 22, 42	10 (3%)
1	JJJ	264/287 (91%)	-0.25	6 (2%) 61 63	4, 11, 28, 45	8 (3%)
All	All	2658/2870 (92%)	-0.31	33 (1%) 76 80	4, 11, 23, 49	93 (3%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	22	GLY	7.7
1	GGG	21	GLY	5.8
1	FFF	21	GLY	5.0
1	FFF	19	HIS	4.1
1	DDD	22	GLY	3.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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	0.69	0.22	50,50,50,53	0
3	EDO	GGG	312	4/4	0.71	0.19	42,47,47,50	0
3	EDO	FFF	310	4/4	0.72	0.20	34,36,38,41	0
3	EDO	AAA	310	4/4	0.73	0.21	49,50,51,51	0
3	EDO	BBB	312	4/4	0.75	0.17	32,34,35,37	0
3	EDO	HHH	307	4/4	0.75	0.23	44,45,45,47	0
3	EDO	CCC	310	4/4	0.78	0.20	36,38,40,45	0
3	EDO	DDD	304	4/4	0.79	0.16	29,30,30,31	0
3	EDO	GGG	304	4/4	0.79	0.18	33,33,34,36	0
3	EDO	CCC	308	4/4	0.79	0.18	42,42,42,44	0
3	EDO	EEE	308	4/4	0.79	0.17	33,37,38,41	0
3	EDO	III	307	4/4	0.79	0.20	48,48,48,50	0
3	EDO	AAA	305	4/4	0.80	0.18	33,33,34,34	0
3	EDO	EEE	302	4/4	0.80	0.18	35,36,36,37	0
3	EDO	III	303	4/4	0.81	0.17	34,34,34,37	0
3	EDO	JJJ	303	4/4	0.81	0.18	28,28,29,33	0
3	EDO	BBB	313	4/4	0.82	0.17	36,38,38,41	0
3	EDO	III	306	4/4	0.82	0.15	32,36,37,39	0
3	EDO	FFF	304	4/4	0.82	0.16	30,31,32,34	0
3	EDO	BBB	311	4/4	0.82	0.17	33,33,33,36	0
3	EDO	FFF	309	4/4	0.83	0.20	50,50,52,52	0
3	EDO	HHH	303	4/4	0.83	0.15	28,28,30,32	0
3	EDO	GGG	309	4/4	0.83	0.14	40,41,42,43	0
3	EDO	HHH	309	4/4	0.83	0.15	30,31,32,33	0
3	EDO	JJJ	308	4/4	0.83	0.15	33,36,37,39	0
3	EDO	DDD	311	4/4	0.84	0.14	43,44,44,45	0
3	EDO	BBB	305	4/4	0.85	0.13	27,28,28,29	0
3	EDO	CCC	303	4/4	0.85	0.15	29,30,30,30	0
3	EDO	BBB	310	4/4	0.85	0.21	51,52,52,52	0
3	EDO	III	305	4/4	0.85	0.16	33,37,37,40	0
3	EDO	GGG	307	4/4	0.85	0.15	25,27,27,30	0
3	EDO	AAA	308	4/4	0.85	0.16	42,43,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	AAA	311	4/4	0.85	0.15	34,34,36,36	0
3	EDO	FFF	308	4/4	0.85	0.16	32,34,34,35	0
3	EDO	AAA	307	4/4	0.86	0.14	34,35,36,37	0
3	EDO	HHH	305	4/4	0.86	0.12	26,30,31,33	0
3	EDO	DDD	308	4/4	0.86	0.13	33,33,34,34	0
3	EDO	EEE	307	4/4	0.86	0.15	40,40,41,42	0
3	EDO	JJJ	307	4/4	0.86	0.18	46,50,50,51	0
3	EDO	CCC	307	4/4	0.86	0.16	42,42,43,44	0
3	EDO	HHH	310	4/4	0.87	0.13	34,36,37,40	0
3	EDO	GGG	311	4/4	0.87	0.15	31,35,36,41	0
3	EDO	DDD	309	4/4	0.87	0.14	42,44,44,45	0
3	EDO	BBB	306	4/4	0.87	0.13	21,23,25,29	0
3	EDO	CCC	304	4/4	0.87	0.14	26,29,31,34	0
3	EDO	III	308	4/4	0.87	0.14	38,38,40,41	0
3	EDO	III	309	4/4	0.87	0.14	47,48,48,49	0
3	EDO	FFF	307	4/4	0.87	0.13	30,30,31,31	0
3	EDO	HHH	308	4/4	0.87	0.13	31,31,31,32	0
3	EDO	CCC	309	4/4	0.87	0.19	47,49,50,50	0
3	EDO	EEE	306	4/4	0.88	0.14	27,31,32,32	0
3	EDO	GGG	305	4/4	0.88	0.13	25,26,27,31	0
3	EDO	DDD	307	4/4	0.88	0.13	31,32,32,34	0
3	EDO	GGG	308	4/4	0.88	0.12	26,28,29,29	0
3	EDO	BBB	307	4/4	0.88	0.13	28,29,29,30	0
3	EDO	EEE	303	4/4	0.88	0.14	28,29,31,34	0
3	EDO	JJJ	304	4/4	0.88	0.13	27,29,31,33	0
3	EDO	JJJ	306	4/4	0.88	0.14	31,31,33,35	0
3	EDO	III	302	4/4	0.88	0.13	24,25,26,27	0
3	EDO	GGG	303	4/4	0.88	0.13	25,25,27,27	0
3	EDO	BBB	309	4/4	0.89	0.11	34,35,35,36	0
3	EDO	CCC	306	4/4	0.89	0.15	30,30,30,32	0
3	EDO	HHH	304	4/4	0.89	0.14	24,26,28,31	0
3	EDO	EEE	305	4/4	0.89	0.11	26,27,28,29	0
3	EDO	HHH	306	4/4	0.89	0.14	37,38,39,41	0
3	EDO	FFF	305	4/4	0.89	0.13	25,26,27,31	0
3	EDO	BBB	308	4/4	0.89	0.14	28,30,32,32	0
3	EDO	AAA	306	4/4	0.90	0.11	25,25,26,29	0
3	EDO	DDD	303	4/4	0.90	0.12	24,24,25,27	0
3	EDO	JJJ	305	4/4	0.90	0.11	27,29,31,31	0
3	EDO	GGG	310	4/4	0.90	0.13	23,28,30,36	0
3	EDO	AAA	304	4/4	0.90	0.12	23,23,23,26	0
3	EDO	CCC	302	4/4	0.90	0.13	25,27,27,32	0
4	CL	AAA	313	1/1	0.90	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	HHH	312	1/1	0.90	0.11	45,45,45,45	0
3	EDO	AAA	312	4/4	0.91	0.11	31,32,33,37	0
3	EDO	DDD	306	4/4	0.91	0.11	24,26,26,27	0
4	CL	HHH	311	1/1	0.91	0.14	43,43,43,43	0
3	EDO	BBB	303	4/4	0.91	0.12	29,29,30,33	0
3	EDO	HHH	302	4/4	0.92	0.10	25,26,26,29	0
3	EDO	DDD	305	4/4	0.92	0.11	23,27,29,32	0
3	EDO	FFF	303	4/4	0.92	0.11	24,24,25,28	0
4	CL	GGG	313	1/1	0.92	0.15	42,42,42,42	0
3	EDO	GGG	301	4/4	0.92	0.09	13,13,14,17	0
3	EDO	AAA	309	4/4	0.92	0.11	19,24,27,29	0
3	EDO	III	304	4/4	0.93	0.12	23,25,26,29	0
3	EDO	JJJ	302	4/4	0.93	0.09	23,23,24,24	0
3	EDO	CCC	301	4/4	0.93	0.09	16,17,18,19	0
4	CL	CCC	311	1/1	0.93	0.13	46,46,46,46	0
4	CL	EEE	309	1/1	0.93	0.14	41,41,41,41	0
3	EDO	BBB	304	4/4	0.93	0.10	24,25,26,30	0
3	EDO	EEE	301	4/4	0.93	0.11	22,22,22,26	0
3	EDO	FFF	302	4/4	0.93	0.08	13,15,15,17	0
4	CL	III	310	1/1	0.93	0.18	43,43,43,43	0
4	CL	BBB	315	1/1	0.94	0.09	35,35,35,35	0
4	CL	FFF	311	1/1	0.94	0.12	40,40,40,40	0
4	CL	DDD	312	1/1	0.94	0.14	44,44,44,44	0
4	CL	III	311	1/1	0.94	0.08	37,37,37,37	0
3	EDO	FFF	306	4/4	0.95	0.09	24,26,29,30	0
3	EDO	GGG	302	4/4	0.95	0.07	12,14,14,17	0
2	IMD	BBB	301	5/5	0.95	0.06	11,11,12,12	0
2	IMD	JJJ	301	5/5	0.95	0.06	10,10,11,11	0
3	EDO	AAA	302	4/4	0.95	0.07	13,13,13,16	0
3	EDO	HHH	301	4/4	0.95	0.08	15,15,15,17	0
3	EDO	GGG	306	4/4	0.95	0.08	18,20,22,23	0
4	CL	BBB	314	1/1	0.95	0.12	42,42,42,42	0
3	EDO	BBB	302	4/4	0.95	0.08	15,16,16,19	0
4	CL	JJJ	309	1/1	0.95	0.08	40,40,40,40	0
4	CL	GGG	314	1/1	0.96	0.08	36,36,36,36	0
3	EDO	AAA	303	4/4	0.96	0.07	14,16,17,21	0
4	CL	DDD	313	1/1	0.96	0.07	40,40,40,40	0
3	EDO	DDD	302	4/4	0.96	0.07	15,15,16,16	0
2	IMD	DDD	301	5/5	0.96	0.05	10,11,11,11	0
2	IMD	III	301	5/5	0.96	0.05	10,10,10,10	0
3	EDO	EEE	304	4/4	0.97	0.06	19,22,25,26	0
4	CL	CCC	312	1/1	0.97	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	FFF	312	1/1	0.97	0.07	36,36,36,36	0
3	EDO	FFF	301	4/4	0.97	0.06	16,17,17,18	0
3	EDO	CCC	305	4/4	0.97	0.05	16,20,22,24	0
2	IMD	AAA	301	5/5	0.98	0.04	11,11,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.