



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:43 PM GMT

PDB ID : 4POR
Title : Structure of Human Polyomavirus 9 VP1 pentamer in complex with 3'-sialyllactose
Authors : Khan, Z.M.; Stehle, T.
Deposited on : 2014-02-26
Resolution : 2.09 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

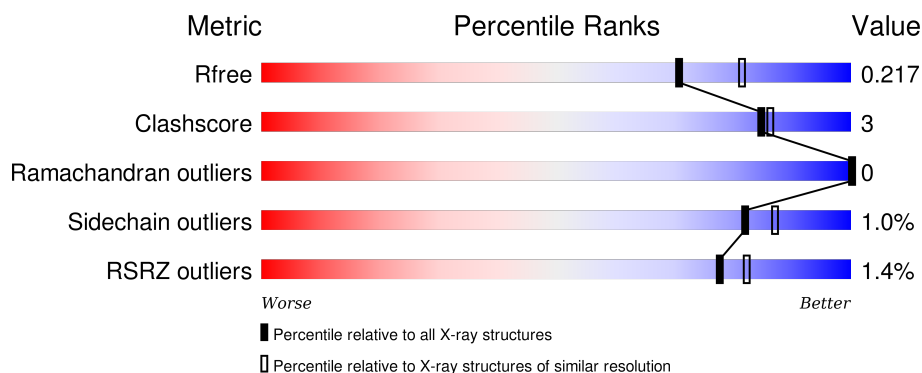
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	278	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	B	278	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	C	278	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	278	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	E	278	<div> <div>%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	278	
1	G	278	
1	H	278	
1	I	278	
1	J	278	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	403	-	-	-	X
3	EDO	A	404	-	-	-	X
3	EDO	B	403	-	-	-	X
3	EDO	B	404	-	-	-	X
3	EDO	C	403	-	-	X	X
3	EDO	C	404	-	-	-	X
3	EDO	C	405	-	-	-	X
3	EDO	D	403	-	-	-	X
3	EDO	D	405	-	-	-	X
3	EDO	E	404	-	-	-	X
3	EDO	F	403	-	-	-	X
3	EDO	F	404	-	-	-	X
3	EDO	G	403	-	-	-	X
3	EDO	G	405	-	-	-	X
3	EDO	H	404	-	-	X	-
3	EDO	I	403	-	-	X	-
3	EDO	I	404	-	-	-	X
4	IPA	A	405	-	-	-	X
4	IPA	C	406	-	-	-	X
4	IPA	D	406	-	-	-	X
4	IPA	E	406	-	-	-	X
4	IPA	F	405	-	-	-	X
4	IPA	G	406	-	-	-	X
4	IPA	H	406	-	-	-	X
4	IPA	I	405	-	-	-	X
4	IPA	J	403	-	-	-	X
5	GAL	B	408	-	-	-	X
5	BGC	D	408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GAL	D	409	-	-	-	X
5	GAL	G	409	-	-	-	X
5	GAL	I	408	-	-	-	X
5	GAL	J	406	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23567 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2059	1297	341	410	11			
1	B	270	Total	C	N	O	S	0	2	0
			2070	1304	341	414	11			
1	C	269	Total	C	N	O	S	0	0	0
			2050	1292	340	407	11			
1	D	270	Total	C	N	O	S	0	0	0
			2059	1297	341	410	11			
1	E	269	Total	C	N	O	S	0	2	0
			2066	1302	342	411	11			
1	F	272	Total	C	N	O	S	0	3	0
			2101	1324	346	420	11			
1	G	266	Total	C	N	O	S	0	1	0
			2035	1283	338	404	10			
1	H	270	Total	C	N	O	S	0	0	0
			2059	1297	341	410	11			
1	I	269	Total	C	N	O	S	0	0	0
			2052	1293	340	408	11			
1	J	273	Total	C	N	O	S	0	0	0
			2083	1313	344	415	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
A	28	SER	-	EXPRESSION TAG	UNP E9NQ90
A	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
A	30	MET	-	EXPRESSION TAG	UNP E9NQ90
B	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
B	28	SER	-	EXPRESSION TAG	UNP E9NQ90
B	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
B	30	MET	-	EXPRESSION TAG	UNP E9NQ90
C	27	GLY	-	EXPRESSION TAG	UNP E9NQ90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	SER	-	EXPRESSION TAG	UNP E9NQ90
C	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
C	30	MET	-	EXPRESSION TAG	UNP E9NQ90
D	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
D	28	SER	-	EXPRESSION TAG	UNP E9NQ90
D	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
D	30	MET	-	EXPRESSION TAG	UNP E9NQ90
E	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
E	28	SER	-	EXPRESSION TAG	UNP E9NQ90
E	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
E	30	MET	-	EXPRESSION TAG	UNP E9NQ90
F	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
F	28	SER	-	EXPRESSION TAG	UNP E9NQ90
F	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
F	30	MET	-	EXPRESSION TAG	UNP E9NQ90
G	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
G	28	SER	-	EXPRESSION TAG	UNP E9NQ90
G	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
G	30	MET	-	EXPRESSION TAG	UNP E9NQ90
H	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
H	28	SER	-	EXPRESSION TAG	UNP E9NQ90
H	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
H	30	MET	-	EXPRESSION TAG	UNP E9NQ90
I	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
I	28	SER	-	EXPRESSION TAG	UNP E9NQ90
I	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
I	30	MET	-	EXPRESSION TAG	UNP E9NQ90
J	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
J	28	SER	-	EXPRESSION TAG	UNP E9NQ90
J	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
J	30	MET	-	EXPRESSION TAG	UNP E9NQ90

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

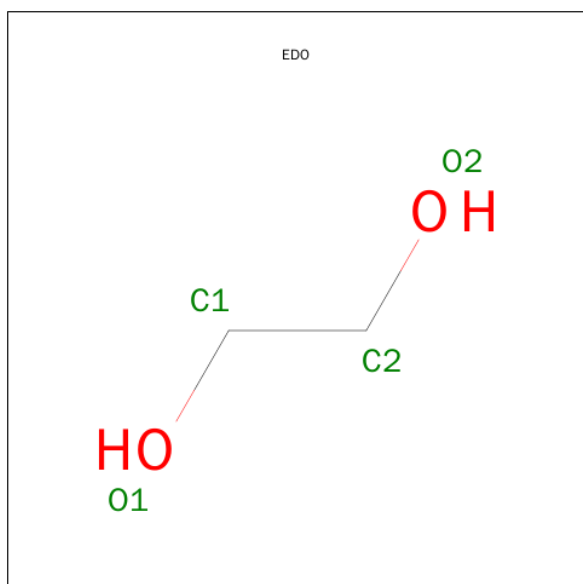
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	I	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	A	1	Total 1	Ca 1	0	0
2	F	1	Total 1	Ca 1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

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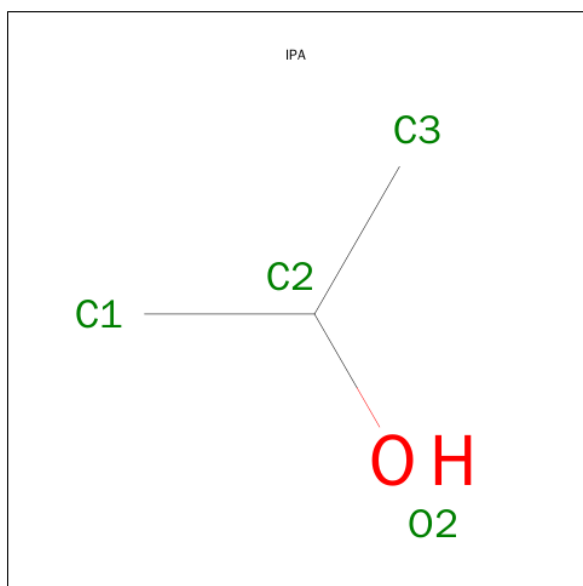
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	C	1	Total	C	O	0	0
			4	3	1		
4	D	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	3	1		
4	F	1	Total	C	O	0	0
			4	3	1		
4	G	1	Total	C	O	0	0
			4	3	1		
4	H	1	Total	C	O	0	0
			4	3	1		
4	I	1	Total	C	O	0	0
			4	3	1		
4	J	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			43	23	1	19		
5	B	3	Total	C	N	O	0	0
			43	23	1	19		
5	D	3	Total	C	N	O	0	0
			43	23	1	19		
5	E	3	Total	C	N	O	0	0
			43	23	1	19		
5	F	3	Total	C	N	O	0	0
			43	23	1	19		
5	G	3	Total	C	N	O	0	0
			43	23	1	19		
5	H	3	Total	C	N	O	0	0
			43	23	1	19		
5	I	3	Total	C	N	O	0	0
			43	23	1	19		
5	J	3	Total	C	N	O	0	0
			43	23	1	19		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	250	Total	O	0	0
			250	250		
6	B	259	Total	O	0	0
			259	259		

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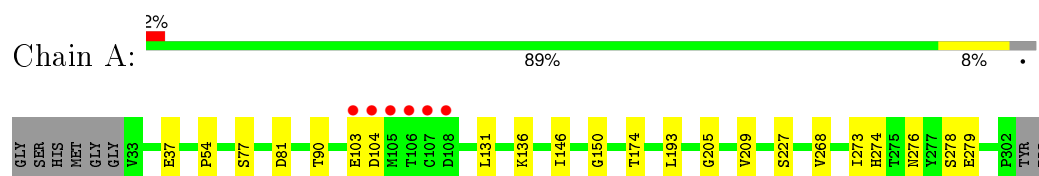
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	216	Total 216	O 216	0	0
6	D	207	Total 207	O 207	0	0
6	E	241	Total 241	O 241	0	0
6	F	230	Total 230	O 230	0	0
6	G	236	Total 236	O 236	0	0
6	H	250	Total 250	O 250	0	0
6	I	260	Total 260	O 260	0	0
6	J	215	Total 215	O 215	0	0

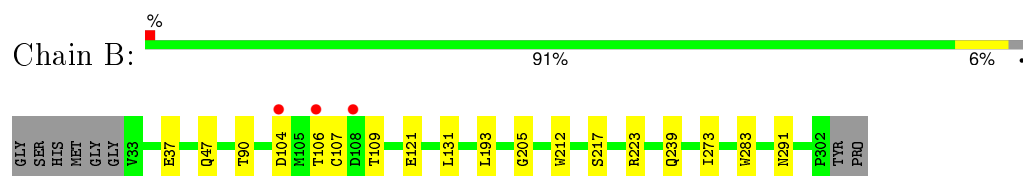
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

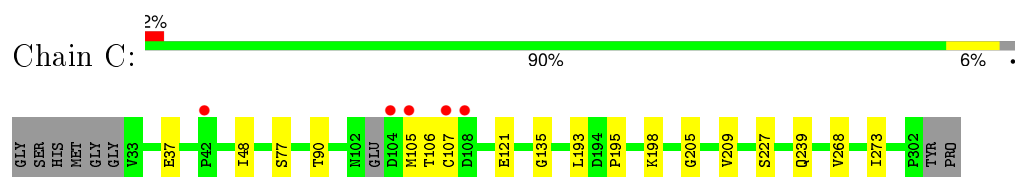
- Molecule 1: VP1



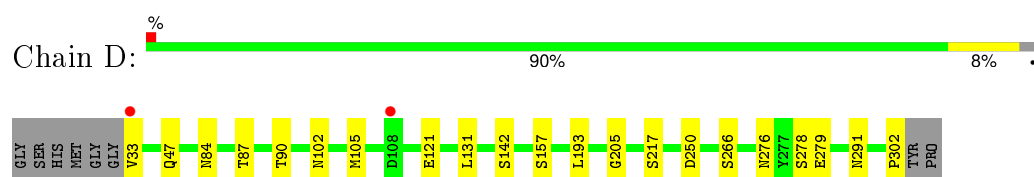
- Molecule 1: VP1



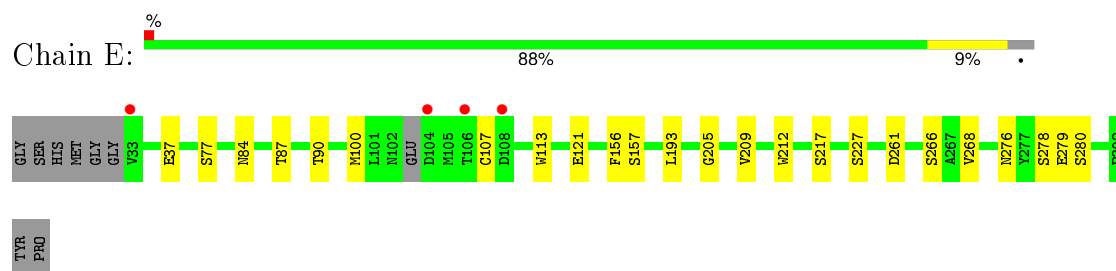
- Molecule 1: VP1



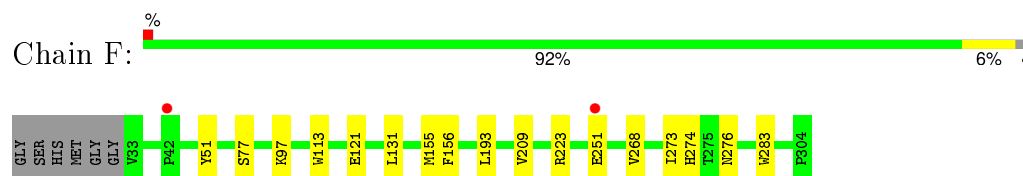
- Molecule 1: VP1



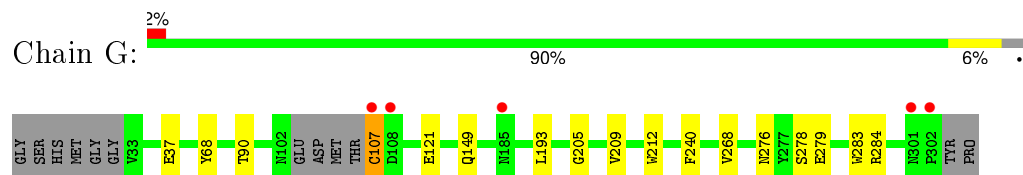
- Molecule 1: VP1



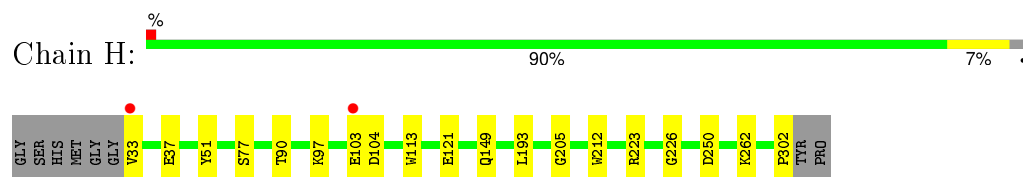
- Molecule 1: VP1



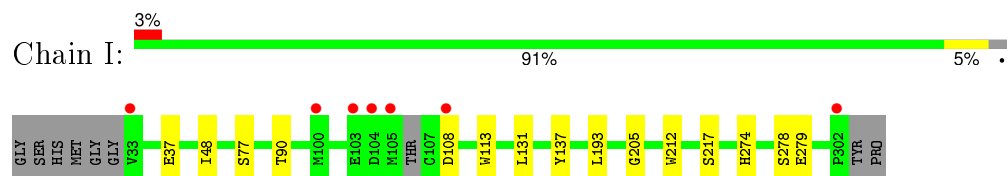
- Molecule 1: VP1



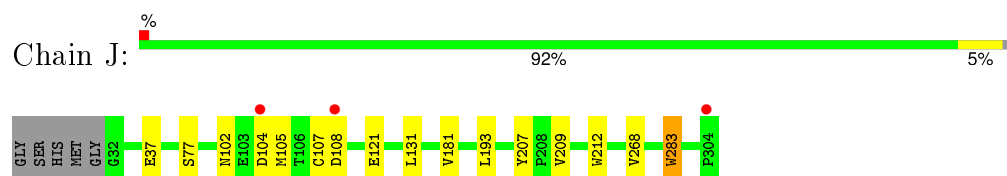
- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 1: VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.01Å 180.40Å 199.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	133.85 – 2.09 48.11 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.9 (133.85-2.09) 99.0 (48.11-2.09)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0025	Depositor
R, R_{free}	0.178 , 0.216 0.180 , 0.217	Depositor DCC
R_{free} test set	10219 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 204785 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23567	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BGC, IPA, CA, EDO, SIA, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	1/2103 (0.0%)	0.65	0/2872
1	B	0.53	2/2120 (0.1%)	0.61	0/2895
1	C	0.50	0/2093	0.59	0/2857
1	D	0.51	0/2103	0.61	0/2872
1	E	0.52	2/2109 (0.1%)	0.61	0/2879
1	F	0.52	2/2147 (0.1%)	0.60	0/2932
1	G	0.50	1/2078 (0.0%)	0.60	0/2837
1	H	0.55	2/2103 (0.1%)	0.62	0/2872
1	I	0.52	2/2095 (0.1%)	0.61	0/2859
1	J	0.54	2/2129 (0.1%)	0.62	0/2907
All	All	0.53	14/21080 (0.1%)	0.61	0/28782

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	PRO	C-N	-8.00	1.15	1.34
1	F	113	TRP	CD2-CE2	5.65	1.48	1.41
1	F	283	TRP	CD2-CE2	5.56	1.48	1.41
1	J	212	TRP	CD2-CE2	5.48	1.48	1.41
1	E	113	TRP	CD2-CE2	5.44	1.47	1.41
1	H	113	TRP	CD2-CE2	5.35	1.47	1.41
1	E	212	TRP	CD2-CE2	5.30	1.47	1.41
1	B	212	TRP	CD2-CE2	5.20	1.47	1.41
1	G	212	TRP	CD2-CE2	5.20	1.47	1.41
1	B	283	TRP	CD2-CE2	5.18	1.47	1.41
1	H	212	TRP	CD2-CE2	5.08	1.47	1.41
1	I	212	TRP	CD2-CE2	5.08	1.47	1.41
1	J	283	TRP	CD2-CE2	5.05	1.47	1.41
1	I	113	TRP	CD2-CE2	5.03	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2059	0	2036	14	0
1	B	2070	0	2047	14	0
1	C	2050	0	2031	19	0
1	D	2059	0	2038	11	0
1	E	2066	0	2044	15	0
1	F	2101	0	2071	14	0
1	G	2035	0	2012	11	0
1	H	2059	0	2037	16	0
1	I	2052	0	2029	11	0
1	J	2083	0	2057	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	12	0	18	0	0
3	B	12	0	18	4	0
3	C	16	0	24	8	0
3	D	16	0	24	2	0
3	E	16	0	24	1	0
3	F	12	0	18	1	0
3	G	16	0	24	2	0
3	H	16	0	24	6	0
3	I	12	0	18	5	0
3	J	4	0	6	0	0
4	A	4	0	8	0	0
4	B	4	0	8	0	0
4	C	4	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	4	0	8	0	0
4	E	4	0	8	2	0
4	F	4	0	8	2	0
4	G	4	0	8	0	0
4	H	4	0	8	0	0
4	I	4	0	8	0	0
4	J	4	0	8	0	0
5	A	43	0	37	2	0
5	B	43	0	37	1	0
5	D	43	0	37	3	0
5	E	43	0	37	2	0
5	F	43	0	37	2	0
5	G	43	0	37	2	0
5	H	43	0	37	1	0
5	I	43	0	37	2	0
5	J	43	0	37	1	0
6	A	250	0	0	0	0
6	B	259	0	0	2	0
6	C	216	0	0	0	0
6	D	207	0	0	1	0
6	E	241	0	0	0	0
6	F	230	0	0	1	0
6	G	236	0	0	1	0
6	H	250	0	0	2	0
6	I	260	0	0	0	0
6	J	215	0	0	1	0
All	All	23567	0	21013	121	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.

All (121) 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:H:223:ARG:HD2	3:H:404:EDO:H22	1.19	1.12
1:H:223:ARG:CD	3:H:404:EDO:H22	2.03	0.86
1:B:104:ASP:OD1	1:B:106:THR:OG1	1.95	0.85
1:B:223:ARG:HD2	3:B:404:EDO:H21	1.60	0.83
1:F:51:TYR:CD2	3:G:403:EDO:H12	2.16	0.80
1:H:103:GLU:HG2	1:H:104:ASP:H	1.48	0.78
1:F:251:GLU:HG2	6:F:730:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLY:H	3:C:404:EDO:H12	1.55	0.72
1:B:107:CYS:HB3	6:B:567:HOH:O	1.91	0.69
1:E:107:CYS:HG	1:J:107:CYS:HG	1.41	0.69
1:F:51:TYR:HD2	3:G:403:EDO:H12	1.53	0.69
1:J:108:ASP:HB2	6:J:612:HOH:O	1.94	0.67
1:C:239:GLN:H	3:C:402:EDO:H21	1.58	0.67
1:B:239:GLN:OE1	1:C:227:SER:HB3	1.95	0.65
1:D:276:ASN:HB3	5:D:407:SIA:O1B	1.97	0.65
1:D:217:SER:HB3	3:D:403:EDO:H21	1.79	0.65
1:H:223:ARG:HD2	3:H:404:EDO:C2	2.11	0.63
1:H:51:TYR:HD2	3:I:403:EDO:H22	1.63	0.62
1:C:239:GLN:H	3:C:402:EDO:C2	2.10	0.62
1:A:131:LEU:HD11	1:B:273:ILE:HD13	1.82	0.60
1:A:103:GLU:HG2	1:A:104:ASP:H	1.66	0.60
5:G:409:GAL:H2	1:H:77:SER:HB2	1.85	0.59
1:C:198:LYS:HZ1	3:C:403:EDO:H21	1.67	0.58
1:H:51:TYR:CD2	3:I:403:EDO:H22	2.39	0.58
1:F:156:PHE:CE2	4:F:405:IPA:H12	2.39	0.58
1:A:131:LEU:HD11	1:B:273:ILE:CD1	2.34	0.58
6:B:567:HOH:O	3:H:405:EDO:H12	2.04	0.57
1:C:107:CYS:CB	1:G:107:CYS:SG	2.94	0.56
1:A:274:HIS:CD2	5:A:406:SIA:H113	2.41	0.56
1:A:37:GLU:HG3	1:I:37:GLU:HG3	1.86	0.56
1:A:136:LYS:HD3	1:A:146:ILE:HD12	1.87	0.56
1:F:77:SER:HB2	5:J:406:GAL:H2	1.88	0.55
1:H:103:GLU:HG2	1:H:104:ASP:N	2.19	0.55
1:E:156:PHE:HE2	4:E:406:IPA:H12	1.71	0.55
1:C:107:CYS:HB2	1:G:107:CYS:SG	2.47	0.55
1:C:37:GLU:HG3	1:G:37:GLU:HG3	1.89	0.55
1:H:97:LYS:HD3	6:H:737:HOH:O	2.08	0.54
1:C:239:GLN:N	3:C:402:EDO:H21	2.23	0.54
1:H:33:VAL:HG12	1:H:302:PRO:HG3	1.89	0.53
1:I:274:HIS:CD2	5:I:406:SIA:H113	2.43	0.53
1:J:102:ASN:HB2	1:J:105:MET:CE	2.39	0.53
1:J:102:ASN:HB2	1:J:105:MET:HE2	1.93	0.51
5:I:408:GAL:H2	1:J:77:SER:HB2	1.93	0.51
1:B:223:ARG:HD2	3:B:404:EDO:C2	2.38	0.49
1:B:109:THR:OG1	3:H:405:EDO:H11	2.12	0.49
1:B:217:SER:HB3	3:B:403:EDO:H11	1.93	0.49
1:I:48:ILE:HD12	1:I:48:ILE:C	2.33	0.49
5:B:408:GAL:H2	1:C:77:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ARG:HD2	3:F:404:EDO:H11	1.95	0.49
1:D:90:THR:OG1	1:D:205:GLY:HA2	2.13	0.49
1:I:278:SER:O	1:I:279:GLU:HB2	2.13	0.49
1:G:90:THR:OG1	1:G:205:GLY:HA2	2.12	0.48
1:D:157:SER:OG	1:D:266:SER:HB2	2.13	0.48
1:A:278:SER:O	1:A:279:GLU:HB2	2.13	0.48
1:B:37:GLU:HG3	1:H:37:GLU:HG3	1.96	0.48
6:D:691:HOH:O	1:E:227:SER:HB2	2.14	0.48
1:B:223:ARG:CD	3:B:404:EDO:H21	2.39	0.47
1:E:100:MET:HA	1:E:261:ASP:OD2	2.14	0.47
1:C:198:LYS:NZ	3:C:403:EDO:H21	2.28	0.47
1:H:250:ASP:HA	3:H:404:EDO:H11	1.96	0.47
5:D:409:GAL:H2	1:E:77:SER:HB2	1.97	0.47
1:E:217:SER:HB3	3:E:404:EDO:H12	1.96	0.47
1:C:48:ILE:C	1:C:48:ILE:HD12	2.35	0.47
1:D:278:SER:O	1:D:279:GLU:HB2	2.14	0.47
1:A:37:GLU:HG3	1:I:37:GLU:CG	2.45	0.46
1:E:156:PHE:CE2	4:E:406:IPA:H12	2.49	0.46
1:E:209:VAL:HG11	1:E:268:VAL:HG21	1.97	0.46
1:G:68:TYR:CE1	1:G:284:ARG:HD3	2.50	0.46
1:I:137:TYR:OH	3:I:404:EDO:H12	2.15	0.46
1:G:276:ASN:HB3	5:G:407:SIA:O1B	2.17	0.45
1:A:90:THR:OG1	1:A:205:GLY:HA2	2.16	0.45
1:A:81:ASP:HB3	1:A:174:THR:HA	1.98	0.45
1:E:90:THR:OG1	1:E:205:GLY:HA2	2.16	0.45
1:G:209:VAL:HG11	1:G:268:VAL:HG21	1.98	0.45
1:I:217:SER:OG	3:I:403:EDO:H11	2.17	0.45
1:F:276:ASN:HB3	5:F:406:SIA:O1B	2.15	0.45
1:I:131:LEU:HG	1:J:283:TRP:CZ2	2.51	0.45
1:H:97:LYS:HG2	1:H:262:LYS:HG2	1.98	0.44
1:B:131:LEU:HD11	1:C:273:ILE:HD13	1.99	0.44
5:H:409:GAL:H2	1:I:77:SER:HB2	1.99	0.44
1:D:142:SER:O	1:E:280:SER:HA	2.18	0.44
1:B:47:GLN:HE21	1:B:291:ASN:HD21	1.64	0.44
1:I:90:THR:OG1	1:I:205:GLY:HA2	2.17	0.44
1:E:37:GLU:HG3	1:J:37:GLU:HG3	2.00	0.44
1:C:198:LYS:HZ1	3:C:403:EDO:C2	2.31	0.44
1:D:84:ASN:HB2	1:D:87:THR:HG23	1.99	0.44
1:E:278:SER:O	1:E:279:GLU:HB2	2.17	0.44
1:E:84:ASN:HB2	1:E:87:THR:HG23	1.99	0.44
1:A:276:ASN:HB3	5:A:406:SIA:O1B	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ASN:HB3	5:E:407:SIA:O1B	2.18	0.44
1:F:209:VAL:HG11	1:F:268:VAL:HG21	2.00	0.44
1:F:155:MET:HG2	1:F:156:PHE:N	2.32	0.43
1:J:209:VAL:HG11	1:J:268:VAL:HG21	2.00	0.43
1:F:97:LYS:HA	1:F:97:LYS:HD2	1.76	0.43
1:H:149:GLN:HA	6:H:743:HOH:O	2.18	0.43
1:E:157:SER:OG	1:E:266:SER:HB2	2.18	0.43
1:D:102:ASN:HB2	1:D:105:MET:HE1	1.99	0.43
1:D:33:VAL:HG12	1:D:302:PRO:HG3	2.00	0.43
1:C:209:VAL:HG11	1:C:268:VAL:HG21	1.98	0.43
1:C:195:PRO:O	1:C:198:LYS:HE2	2.17	0.43
1:C:105:MET:O	1:C:105:MET:HG3	2.19	0.43
1:F:274:HIS:CD2	5:F:406:SIA:H113	2.54	0.42
1:C:198:LYS:NZ	3:C:403:EDO:C2	2.82	0.42
1:D:250:ASP:HA	3:D:404:EDO:H11	2.01	0.42
1:A:209:VAL:HG11	1:A:268:VAL:HG21	2.01	0.42
1:I:217:SER:CB	3:I:403:EDO:H11	2.49	0.42
5:D:407:SIA:C1	5:D:409:GAL:H4	2.50	0.42
1:D:47:GLN:HE21	1:D:291:ASN:HD21	1.66	0.42
1:C:90:THR:OG1	1:C:205:GLY:HA2	2.20	0.42
1:B:90:THR:OG1	1:B:205:GLY:HA2	2.20	0.41
1:G:240:PHE:O	1:H:226:GLY:N	2.53	0.41
1:A:150:GLY:HA3	1:A:273:ILE:HD12	2.02	0.41
1:J:104:ASP:HB3	1:J:107:CYS:SG	2.61	0.41
1:F:131:LEU:HG	1:G:283:TRP:CZ2	2.56	0.41
1:F:156:PHE:HE2	4:F:405:IPA:H12	1.82	0.41
1:G:149:GLN:HA	6:G:730:HOH:O	2.21	0.41
1:G:278:SER:O	1:G:279:GLU:HB2	2.22	0.40
1:J:181:VAL:HG11	1:J:207:TYR:CE1	2.56	0.40
1:H:90:THR:OG1	1:H:205:GLY:HA2	2.21	0.40
1:F:273:ILE:CD1	1:J:131:LEU:HD11	2.51	0.40
1:A:77:SER:HB2	5:E:409:GAL:H2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/278 (96%)	257 (96%)	11 (4%)	0	100	100
1	B	270/278 (97%)	256 (95%)	14 (5%)	0	100	100
1	C	265/278 (95%)	254 (96%)	11 (4%)	0	100	100
1	D	268/278 (96%)	257 (96%)	11 (4%)	0	100	100
1	E	267/278 (96%)	258 (97%)	9 (3%)	0	100	100
1	F	273/278 (98%)	263 (96%)	10 (4%)	0	100	100
1	G	263/278 (95%)	254 (97%)	9 (3%)	0	100	100
1	H	268/278 (96%)	253 (94%)	15 (6%)	0	100	100
1	I	265/278 (95%)	252 (95%)	13 (5%)	0	100	100
1	J	271/278 (98%)	258 (95%)	13 (5%)	0	100	100
All	All	2678/2780 (96%)	2562 (96%)	116 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/240 (98%)	233 (99%)	2 (1%)	84	89
1	B	237/240 (99%)	235 (99%)	2 (1%)	86	91
1	C	234/240 (98%)	231 (99%)	3 (1%)	76	82
1	D	235/240 (98%)	232 (99%)	3 (1%)	76	82
1	E	236/240 (98%)	234 (99%)	2 (1%)	86	91
1	F	240/240 (100%)	238 (99%)	2 (1%)	86	91
1	G	232/240 (97%)	229 (99%)	3 (1%)	76	82
1	H	235/240 (98%)	233 (99%)	2 (1%)	84	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	234/240 (98%)	232 (99%)	2 (1%)	84	89
1	J	237/240 (99%)	235 (99%)	2 (1%)	86	91
All	All	2355/2400 (98%)	2332 (99%)	23 (1%)	82	87

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LEU
1	A	227	SER
1	B	121	GLU
1	B	193	LEU
1	C	106	THR
1	C	121	GLU
1	C	193	LEU
1	D	121	GLU
1	D	131	LEU
1	D	193	LEU
1	E	121	GLU
1	E	193	LEU
1	F	121	GLU
1	F	193	LEU
1	G	107	CYS
1	G	121	GLU
1	G	193	LEU
1	H	121	GLU
1	H	193	LEU
1	I	108	ASP
1	I	193	LEU
1	J	121	GLU
1	J	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	B	47	GLN
1	D	47	GLN
1	D	274	HIS
1	F	47	GLN
1	F	274	HIS

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Mol	Chain	Res	Type
1	H	60	ASN
1	H	239	GLN

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 ⓘ

27 carbohydrates 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	$\# Z > 2$
5	SIA	A	406	5	16,20,21	0.65	0	18,28,31	0.88	0
5	BGC	A	407	5	12,12,12	0.53	0	17,17,17	1.16	2 (11%)
5	GAL	A	408	5	11,11,12	0.56	0	14,15,17	0.94	1 (7%)
5	SIA	B	406	5	16,20,21	0.74	0	18,28,31	0.69	0
5	BGC	B	407	5	12,12,12	0.40	0	17,17,17	0.80	0
5	GAL	B	408	5	11,11,12	0.57	0	14,15,17	1.13	1 (7%)
5	SIA	D	407	5	16,20,21	0.54	0	18,28,31	0.85	0
5	BGC	D	408	5	12,12,12	0.46	0	17,17,17	0.64	0
5	GAL	D	409	5	11,11,12	0.51	0	14,15,17	1.69	2 (14%)
5	SIA	E	407	5	16,20,21	0.59	0	18,28,31	0.94	0
5	BGC	E	408	5	12,12,12	0.48	0	17,17,17	1.32	3 (17%)
5	GAL	E	409	5	11,11,12	0.56	0	14,15,17	1.28	1 (7%)
5	SIA	F	406	5	16,20,21	0.52	0	18,28,31	0.67	0
5	BGC	F	407	5	12,12,12	0.48	0	17,17,17	0.70	0
5	GAL	F	408	5	11,11,12	0.61	0	14,15,17	0.97	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SIA	G	407	5	16,20,21	0.48	0	18,28,31	0.68	0
5	BGC	G	408	5	12,12,12	0.42	0	17,17,17	0.61	0
5	GAL	G	409	5	11,11,12	0.53	0	14,15,17	1.43	2 (14%)
5	SIA	H	407	5	16,20,21	0.57	0	18,28,31	0.61	0
5	BGC	H	408	5	12,12,12	0.41	0	17,17,17	0.99	1 (5%)
5	GAL	H	409	5	11,11,12	0.64	0	14,15,17	1.36	2 (14%)
5	SIA	I	406	5	16,20,21	0.65	0	18,28,31	0.82	0
5	BGC	I	407	5	12,12,12	0.42	0	17,17,17	0.93	0
5	GAL	I	408	5	11,11,12	0.60	0	14,15,17	0.83	1 (7%)
5	SIA	J	404	5	16,20,21	0.64	0	18,28,31	0.95	0
5	BGC	J	405	5	12,12,12	0.49	0	17,17,17	1.15	1 (5%)
5	GAL	J	406	5	11,11,12	0.65	0	14,15,17	1.08	2 (14%)

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	A	406	5	-	0/14/34/38	0/1/1/1
5	BGC	A	407	5	-	0/2/22/22	0/1/1/1
5	GAL	A	408	5	-	0/2/19/22	0/1/1/1
5	SIA	B	406	5	-	0/14/34/38	0/1/1/1
5	BGC	B	407	5	-	0/2/22/22	0/1/1/1
5	GAL	B	408	5	-	0/2/19/22	0/1/1/1
5	SIA	D	407	5	-	0/14/34/38	0/1/1/1
5	BGC	D	408	5	-	0/2/22/22	0/1/1/1
5	GAL	D	409	5	-	0/2/19/22	0/1/1/1
5	SIA	E	407	5	-	0/14/34/38	0/1/1/1
5	BGC	E	408	5	-	0/2/22/22	0/1/1/1
5	GAL	E	409	5	-	0/2/19/22	0/1/1/1
5	SIA	F	406	5	-	0/14/34/38	0/1/1/1
5	BGC	F	407	5	-	0/2/22/22	0/1/1/1
5	GAL	F	408	5	-	0/2/19/22	0/1/1/1
5	SIA	G	407	5	-	0/14/34/38	0/1/1/1
5	BGC	G	408	5	-	0/2/22/22	0/1/1/1
5	GAL	G	409	5	-	0/2/19/22	0/1/1/1
5	SIA	H	407	5	-	0/14/34/38	0/1/1/1
5	BGC	H	408	5	-	0/2/22/22	0/1/1/1
5	GAL	H	409	5	-	0/2/19/22	0/1/1/1
5	SIA	I	406	5	-	0/14/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BGC	I	407	5	-	0/2/22/22	0/1/1/1
5	GAL	I	408	5	-	0/2/19/22	0/1/1/1
5	SIA	J	404	5	-	0/14/34/38	0/1/1/1
5	BGC	J	405	5	-	0/2/22/22	0/1/1/1
5	GAL	J	406	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	408	BGC	C1-O5-C5	-2.75	108.39	113.47
5	H	408	BGC	O4-C4-C3	-2.20	105.37	110.34
5	E	408	BGC	O4-C4-C3	-2.05	105.71	110.34
5	J	406	GAL	C1-O5-C5	2.02	114.81	112.25
5	G	409	GAL	O5-C1-C2	2.02	114.13	110.86
5	I	408	GAL	C1-C2-C3	2.04	111.95	109.54
5	D	409	GAL	O5-C1-C2	2.14	114.33	110.86
5	E	408	BGC	C4-C3-C2	2.15	114.81	110.79
5	A	408	GAL	C1-O5-C5	2.18	115.02	112.25
5	J	405	BGC	C1-C2-C3	2.18	113.67	110.43
5	J	406	GAL	C1-C2-C3	2.21	112.16	109.54
5	A	407	BGC	O5-C1-C2	2.23	113.35	109.80
5	H	409	GAL	C1-C2-C3	2.42	112.41	109.54
5	F	408	GAL	C1-O5-C5	2.71	115.68	112.25
5	A	407	BGC	C1-C2-C3	2.79	114.58	110.43
5	E	409	GAL	C1-O5-C5	2.84	115.85	112.25
5	B	408	GAL	C1-O5-C5	3.06	116.14	112.25
5	H	409	GAL	C1-O5-C5	3.63	116.85	112.25
5	G	409	GAL	C1-O5-C5	4.01	117.34	112.25
5	D	409	GAL	C1-O5-C5	4.97	118.55	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	SIA	2	0
5	B	408	GAL	1	0
5	D	407	SIA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	409	GAL	2	0
5	E	407	SIA	1	0
5	E	409	GAL	1	0
5	F	406	SIA	2	0
5	G	407	SIA	1	0
5	G	409	GAL	1	0
5	H	409	GAL	1	0
5	I	406	SIA	1	0
5	I	408	GAL	1	0
5	J	406	GAL	1	0

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 10 are monoatomic - leaving 43 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	A	402	-	3,3,3	0.48	0	2,2,2	0.41	0
3	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.41	0
3	EDO	A	404	-	3,3,3	0.38	0	2,2,2	0.77	0
4	IPA	A	405	-	3,3,3	0.55	0	3,3,3	0.39	0
3	EDO	B	402	-	3,3,3	0.51	0	2,2,2	0.65	0
3	EDO	B	403	-	3,3,3	0.53	0	2,2,2	0.42	0
3	EDO	B	404	-	3,3,3	0.39	0	2,2,2	0.59	0
4	IPA	B	405	-	3,3,3	0.47	0	3,3,3	0.47	0
3	EDO	C	402	-	3,3,3	0.50	0	2,2,2	0.19	0
3	EDO	C	403	-	3,3,3	0.55	0	2,2,2	0.26	0
3	EDO	C	404	-	3,3,3	0.57	0	2,2,2	0.26	0
3	EDO	C	405	-	3,3,3	0.49	0	2,2,2	0.36	0
4	IPA	C	406	-	3,3,3	0.45	0	3,3,3	0.58	0
3	EDO	D	402	-	3,3,3	0.36	0	2,2,2	0.84	0
3	EDO	D	403	-	3,3,3	0.54	0	2,2,2	0.44	0
3	EDO	D	404	-	3,3,3	0.53	0	2,2,2	0.33	0
3	EDO	D	405	-	3,3,3	0.48	0	2,2,2	0.45	0
4	IPA	D	406	-	3,3,3	0.48	0	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	E	402	-	3,3,3	0.53	0	2,2,2	0.28	0
3	EDO	E	403	-	3,3,3	0.51	0	2,2,2	0.38	0
3	EDO	E	404	-	3,3,3	0.54	0	2,2,2	0.39	0
3	EDO	E	405	-	3,3,3	0.69	0	2,2,2	0.17	0
4	IPA	E	406	-	3,3,3	0.51	0	3,3,3	0.42	0
3	EDO	F	402	-	3,3,3	0.60	0	2,2,2	0.32	0
3	EDO	F	403	-	3,3,3	0.51	0	2,2,2	0.40	0
3	EDO	F	404	-	3,3,3	0.46	0	2,2,2	0.53	0
4	IPA	F	405	-	3,3,3	0.47	0	3,3,3	0.49	0
3	EDO	G	402	-	3,3,3	0.43	0	2,2,2	0.61	0
3	EDO	G	403	-	3,3,3	0.53	0	2,2,2	0.21	0
3	EDO	G	404	-	3,3,3	0.52	0	2,2,2	0.51	0
3	EDO	G	405	-	3,3,3	0.45	0	2,2,2	0.70	0
4	IPA	G	406	-	3,3,3	0.54	0	3,3,3	0.50	0
3	EDO	H	402	-	3,3,3	0.52	0	2,2,2	0.38	0
3	EDO	H	403	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	H	404	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	H	405	-	3,3,3	0.48	0	2,2,2	0.46	0
4	IPA	H	406	-	3,3,3	0.48	0	3,3,3	0.51	0
3	EDO	I	402	-	3,3,3	0.42	0	2,2,2	0.54	0
3	EDO	I	403	-	3,3,3	0.43	0	2,2,2	0.33	0
3	EDO	I	404	-	3,3,3	0.54	0	2,2,2	0.43	0
4	IPA	I	405	-	3,3,3	0.49	0	3,3,3	0.33	0
3	EDO	J	402	-	3,3,3	0.38	0	2,2,2	0.76	0
4	IPA	J	403	-	3,3,3	0.50	0	3,3,3	0.42	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	A	402	-	-	0/1/1/1	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
3	EDO	A	404	-	-	0/1/1/1	0/0/0/0
4	IPA	A	405	-	-	0/0/0/0	0/0/0/0
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	403	-	-	0/1/1/1	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
4	IPA	B	405	-	-	0/0/0/0	0/0/0/0
3	EDO	C	402	-	-	0/1/1/1	0/0/0/0
3	EDO	C	403	-	-	0/1/1/1	0/0/0/0
3	EDO	C	404	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	405	-	-	0/1/1/1	0/0/0/0
4	IPA	C	406	-	-	0/0/0/0	0/0/0/0
3	EDO	D	402	-	-	0/1/1/1	0/0/0/0
3	EDO	D	403	-	-	0/1/1/1	0/0/0/0
3	EDO	D	404	-	-	0/1/1/1	0/0/0/0
3	EDO	D	405	-	-	0/1/1/1	0/0/0/0
4	IPA	D	406	-	-	0/0/0/0	0/0/0/0
3	EDO	E	402	-	-	0/1/1/1	0/0/0/0
3	EDO	E	403	-	-	0/1/1/1	0/0/0/0
3	EDO	E	404	-	-	0/1/1/1	0/0/0/0
3	EDO	E	405	-	-	0/1/1/1	0/0/0/0
4	IPA	E	406	-	-	0/0/0/0	0/0/0/0
3	EDO	F	402	-	-	0/1/1/1	0/0/0/0
3	EDO	F	403	-	-	0/1/1/1	0/0/0/0
3	EDO	F	404	-	-	0/1/1/1	0/0/0/0
4	IPA	F	405	-	-	0/0/0/0	0/0/0/0
3	EDO	G	402	-	-	0/1/1/1	0/0/0/0
3	EDO	G	403	-	-	0/1/1/1	0/0/0/0
3	EDO	G	404	-	-	0/1/1/1	0/0/0/0
3	EDO	G	405	-	-	0/1/1/1	0/0/0/0
4	IPA	G	406	-	-	0/0/0/0	0/0/0/0
3	EDO	H	402	-	-	0/1/1/1	0/0/0/0
3	EDO	H	403	-	-	0/1/1/1	0/0/0/0
3	EDO	H	404	-	-	0/1/1/1	0/0/0/0
3	EDO	H	405	-	-	0/1/1/1	0/0/0/0
4	IPA	H	406	-	-	0/0/0/0	0/0/0/0
3	EDO	I	402	-	-	0/1/1/1	0/0/0/0
3	EDO	I	403	-	-	0/1/1/1	0/0/0/0
3	EDO	I	404	-	-	0/1/1/1	0/0/0/0
4	IPA	I	405	-	-	0/0/0/0	0/0/0/0
3	EDO	J	402	-	-	0/1/1/1	0/0/0/0
4	IPA	J	403	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	EDO	1	0
3	B	404	EDO	3	0
3	C	402	EDO	3	0
3	C	403	EDO	4	0
3	C	404	EDO	1	0
3	D	403	EDO	1	0
3	D	404	EDO	1	0
3	E	404	EDO	1	0
4	E	406	IPA	2	0
3	F	404	EDO	1	0
4	F	405	IPA	2	0
3	G	403	EDO	2	0
3	H	404	EDO	4	0
3	H	405	EDO	2	0
3	I	403	EDO	4	0
3	I	404	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	A	270/278 (97%)	-0.38	6 (2%) 65 71	15, 21, 46, 82	2 (0%)
1	B	270/278 (97%)	-0.64	3 (1%) 82 86	16, 22, 43, 78	0
1	C	269/278 (96%)	-0.40	5 (1%) 70 75	19, 26, 49, 90	0
1	D	270/278 (97%)	-0.48	2 (0%) 89 91	18, 26, 46, 68	0
1	E	269/278 (96%)	-0.50	4 (1%) 76 81	15, 23, 45, 87	0
1	F	272/278 (97%)	-0.47	2 (0%) 89 91	21, 28, 41, 61	0
1	G	266/278 (95%)	-0.42	5 (1%) 70 75	18, 25, 44, 78	0
1	H	270/278 (97%)	-0.39	2 (0%) 89 91	14, 22, 43, 84	0
1	I	269/278 (96%)	-0.41	7 (2%) 59 66	18, 24, 46, 91	0
1	J	273/278 (98%)	-0.49	3 (1%) 82 86	20, 26, 48, 80	0
All	All	2698/2780 (97%)	-0.46	39 (1%) 78 82	14, 24, 46, 91	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	THR	5.1
1	I	105	MET	4.7
1	G	108	ASP	4.6
1	H	103	GLU	4.0
1	I	103	GLU	3.7
1	A	108	ASP	3.7
1	A	104	ASP	3.7
1	A	103	GLU	3.6
1	I	302	PRO	3.6
1	C	104	ASP	3.5
1	C	108	ASP	3.5
1	I	104	ASP	3.5
1	D	108	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	108	ASP	2.9
1	E	106	THR	2.8
1	E	108	ASP	2.8
1	A	107	CYS	2.7
1	I	108	ASP	2.7
1	A	105	MET	2.6
1	B	106	THR	2.6
1	E	104	ASP	2.6
1	G	301	ASN	2.5
1	C	107	CYS	2.5
1	E	33	VAL	2.4
1	B	104	ASP	2.4
1	I	33	VAL	2.4
1	B	108	ASP	2.4
1	H	33	VAL	2.3
1	G	107	CYS	2.3
1	F	42	PRO	2.3
1	D	33	VAL	2.3
1	C	105	MET	2.3
1	C	42	PRO	2.2
1	G	185	ASN	2.2
1	J	104	ASP	2.1
1	J	304	PRO	2.1
1	I	100	MET	2.1
1	F	251	GLU	2.0
1	G	302	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	GAL	D	409	11/12	0.78	0.24	6.15	45,48,54,58	0
5	GAL	G	409	11/12	0.93	0.14	4.62	31,35,39,41	0
5	BGC	D	408	12/12	0.80	0.31	4.10	60,70,81,89	0
5	GAL	I	408	11/12	0.96	0.11	3.40	27,32,35,41	0
5	GAL	B	408	11/12	0.94	0.14	2.67	24,27,36,41	0
5	GAL	J	406	11/12	0.92	0.15	2.21	30,34,38,43	0
5	GAL	H	409	11/12	0.95	0.10	1.88	23,27,29,32	0
5	SIA	D	407	20/21	0.89	0.15	1.64	27,38,40,40	0
5	GAL	A	408	11/12	0.93	0.13	1.31	31,38,42,43	0
5	SIA	B	406	20/21	0.96	0.10	1.26	19,22,26,26	0
5	SIA	J	404	20/21	0.94	0.13	1.11	23,27,29,30	0
5	SIA	G	407	20/21	0.93	0.10	0.97	22,28,31,32	0
5	GAL	F	408	11/12	0.94	0.09	0.76	31,34,37,42	0
5	SIA	I	406	20/21	0.96	0.09	0.21	19,24,29,30	0
5	SIA	A	406	20/21	0.94	0.09	0.13	28,31,33,33	0
5	SIA	E	407	20/21	0.95	0.08	-0.20	16,23,25,27	0
5	GAL	E	409	11/12	0.95	0.09	-0.40	24,27,32,33	0
5	SIA	F	406	20/21	0.94	0.08	-0.42	25,28,31,32	0
5	SIA	H	407	20/21	0.97	0.07	-1.23	15,20,23,23	0
5	BGC	B	407	12/12	0.88	0.15	-	34,41,47,51	0
5	BGC	G	408	12/12	0.86	0.23	-	47,53,62,71	0
5	BGC	H	408	12/12	0.90	0.14	-	29,36,45,50	0
5	BGC	F	407	12/12	0.89	0.17	-	39,48,52,57	0
5	BGC	E	408	12/12	0.87	0.16	-	36,45,48,53	0
5	BGC	I	407	12/12	0.93	0.19	-	37,45,57,59	0
5	BGC	A	407	12/12	0.84	0.20	-	46,55,66,69	0
5	BGC	J	405	12/12	0.89	0.22	-	44,48,53,65	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	D	403	4/4	0.88	0.20	13.17	41,43,43,45	0
3	EDO	I	404	4/4	0.89	0.17	10.56	31,32,34,40	0
3	EDO	C	405	4/4	0.92	0.24	8.23	41,41,41,48	0
3	EDO	B	403	4/4	0.94	0.14	6.58	28,30,30,37	0
4	IPA	C	406	4/4	0.88	0.23	6.37	32,33,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	IPA	E	406	4/4	0.90	0.17	6.03	35,38,40,41	0
3	EDO	A	404	4/4	0.94	0.14	5.92	30,32,33,45	0
4	IPA	F	405	4/4	0.93	0.19	5.08	32,34,35,36	0
4	IPA	G	406	4/4	0.86	0.20	4.65	30,32,35,38	0
3	EDO	C	403	4/4	0.86	0.14	4.57	33,36,38,41	0
3	EDO	E	404	4/4	0.93	0.13	4.46	35,40,41,45	0
4	IPA	J	403	4/4	0.94	0.13	4.35	34,34,35,35	0
3	EDO	D	405	4/4	0.95	0.17	4.22	29,34,39,46	0
4	IPA	A	405	4/4	0.92	0.16	3.99	28,31,31,32	0
3	EDO	B	404	4/4	0.94	0.17	3.78	31,31,32,34	0
4	IPA	H	406	4/4	0.92	0.18	3.75	31,31,31,33	0
4	IPA	D	406	4/4	0.95	0.16	3.30	29,30,31,33	0
3	EDO	C	404	4/4	0.86	0.15	2.98	36,36,39,41	0
3	EDO	G	405	4/4	0.96	0.12	2.98	29,29,32,38	0
3	EDO	A	403	4/4	0.92	0.15	2.65	26,27,33,36	0
3	EDO	G	403	4/4	0.89	0.13	2.65	34,35,38,39	0
3	EDO	F	403	4/4	0.93	0.11	2.36	41,42,43,45	0
3	EDO	F	404	4/4	0.90	0.26	2.32	41,42,45,46	0
4	IPA	I	405	4/4	0.89	0.15	2.24	29,30,32,33	0
3	EDO	H	404	4/4	0.80	0.20	1.82	38,39,39,50	0
3	EDO	E	403	4/4	0.89	0.14	1.80	35,37,37,38	0
4	IPA	B	405	4/4	0.94	0.13	1.64	26,27,28,29	0
3	EDO	D	404	4/4	0.91	0.15	1.64	39,40,40,41	0
3	EDO	I	403	4/4	0.96	0.11	0.65	26,28,31,36	0
3	EDO	G	402	4/4	0.97	0.12	0.48	28,29,30,30	0
3	EDO	H	403	4/4	0.95	0.09	0.42	31,32,34,40	0
3	EDO	H	405	4/4	0.92	0.14	0.36	38,41,43,43	0
3	EDO	J	402	4/4	0.94	0.09	-0.12	32,34,35,35	0
3	EDO	D	402	4/4	0.97	0.10	-0.16	23,26,26,29	0
3	EDO	E	402	4/4	0.96	0.10	-0.17	27,28,29,29	0
3	EDO	A	402	4/4	0.96	0.11	-0.24	29,31,31,34	0
3	EDO	C	402	4/4	0.97	0.11	-0.93	26,27,27,28	0
3	EDO	G	404	4/4	0.95	0.07	-1.02	29,31,32,35	0
3	EDO	B	402	4/4	0.96	0.07	-1.55	26,27,29,29	0
3	EDO	F	402	4/4	0.93	0.10	-1.59	31,31,32,34	0
3	EDO	I	402	4/4	0.98	0.08	-1.94	24,25,29,33	0
3	EDO	H	402	4/4	0.96	0.09	-2.88	25,27,27,28	0
2	CA	I	401	1/1	0.99	0.04	-	37,37,37,37	0
2	CA	J	401	1/1	0.98	0.06	-	43,43,43,43	0
2	CA	B	401	1/1	0.97	0.04	-	39,39,39,39	0
2	CA	E	401	1/1	0.97	0.04	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	D	401	1/1	0.98	0.05	-	37,37,37,37	0
2	CA	A	401	1/1	1.00	0.03	-	38,38,38,38	0
3	EDO	E	405	4/4	0.86	0.15	-	28,32,32,33	0
2	CA	H	401	1/1	0.99	0.03	-	31,31,31,31	0
2	CA	F	401	1/1	0.94	0.04	-	42,42,42,42	0
2	CA	C	401	1/1	0.96	0.03	-	41,41,41,41	0
2	CA	G	401	1/1	0.96	0.05	-	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.