



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:43 PM GMT

PDB ID : 4POQ
Title : Structure of unliganded VP1 pentamer of Human Polyomavirus 9
Authors : Khan, Z.M.; Stehle, T.
Deposited on : 2014-02-26
Resolution : 2.00 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

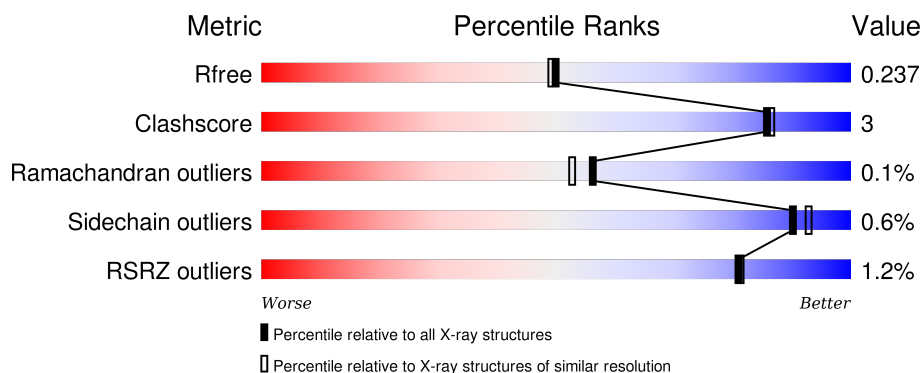
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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>3%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	B	278	<div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	C	278	<div> <div>%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	D	278	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	E	278	<div> <div>3%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	278	 91% 7% •
1	G	278	 91% 6% •
1	H	278	 93% 6% •
1	I	278	 91% 7% •
1	J	278	 90% 8% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	402	-	-	-	X
3	EDO	F	402	-	-	-	X
3	EDO	F	403	-	-	-	X
3	EDO	J	402	-	-	-	X
4	IPA	A	403	-	-	-	X
4	IPA	C	403	-	-	-	X
4	IPA	D	403	-	-	-	X
4	IPA	E	403	-	-	-	X
4	IPA	F	404	-	-	-	X
4	IPA	G	404	-	-	-	X
4	IPA	H	402	-	-	-	X
4	IPA	I	403	-	-	-	X
4	IPA	J	403	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22785 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	271	Total	C	N	O	S	0	1	0
			2077	1311	343	412	11			
1	B	270	Total	C	N	O	S	1	2	0
			2071	1306	344	410	11			
1	C	269	Total	C	N	O	S	1	5	0
			2085	1315	346	412	12			
1	D	271	Total	C	N	O	S	0	1	0
			2075	1309	342	413	11			
1	E	270	Total	C	N	O	S	0	1	0
			2064	1300	341	412	11			
1	F	272	Total	C	N	O	S	2	4	0
			2101	1327	344	418	12			
1	G	271	Total	C	N	O	S	3	0	0
			2071	1306	342	412	11			
1	H	274	Total	C	N	O	S	0	0	0
			2087	1315	345	416	11			
1	I	272	Total	C	N	O	S	0	1	0
			2075	1305	344	415	11			
1	J	273	Total	C	N	O	S	0	3	0
			2100	1324	345	420	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).

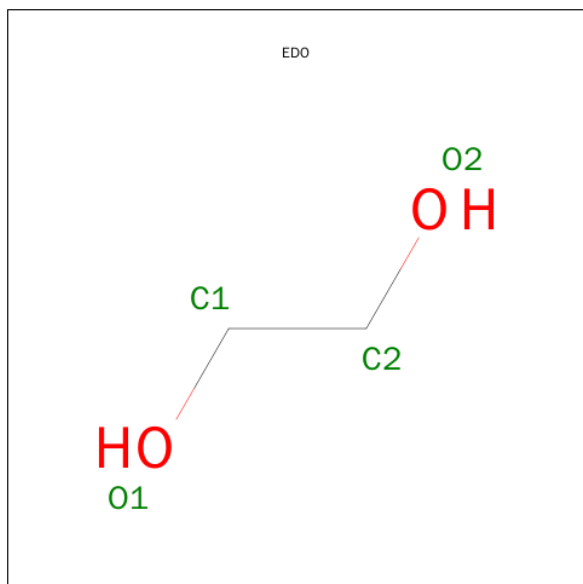
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0

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

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



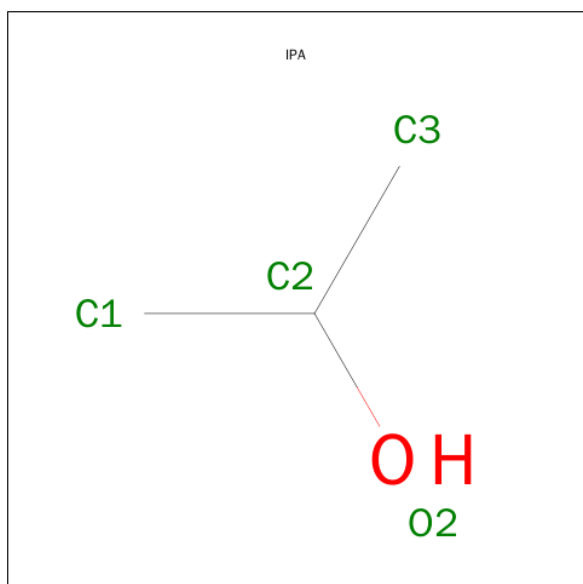
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	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: C₃H₈O).



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		
4	E	1	Total	C	O	0	0
			4	3	1		

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

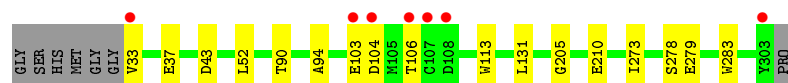
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	221	Total O 221 221	0	0
5	B	222	Total O 222 222	0	0
5	C	177	Total O 177 177	0	0
5	D	171	Total O 171 171	0	0
5	E	192	Total O 192 192	0	0
5	F	166	Total O 166 166	0	0
5	G	186	Total O 186 186	0	0
5	H	199	Total O 199 199	0	0
5	I	181	Total O 181 181	0	0
5	J	170	Total O 170 170	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 ($\text{RSRZ} > 2$). 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.

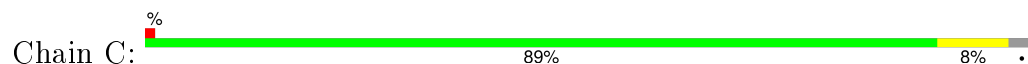
- Molecule 1: VP1



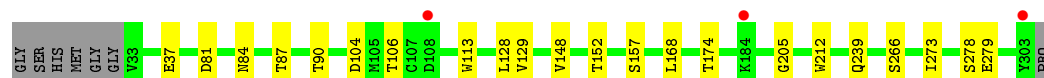
- Molecule 1: VP1



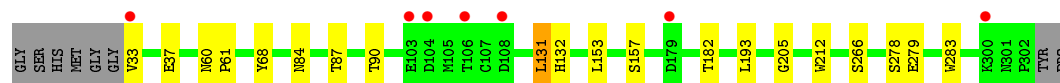
- Molecule 1: VP1



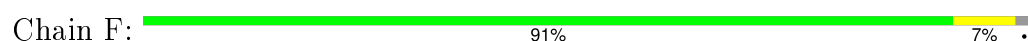
- Molecule 1: VP1



- Molecule 1: VP1

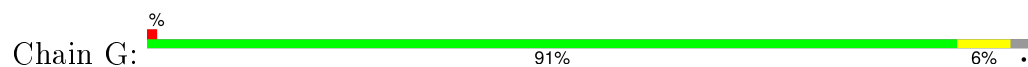


- Molecule 1: VP1





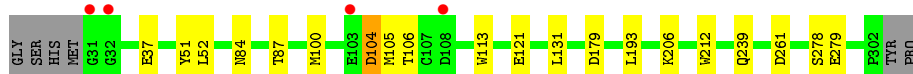
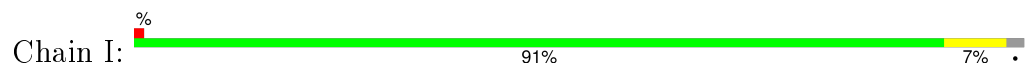
- Molecule 1: VP1



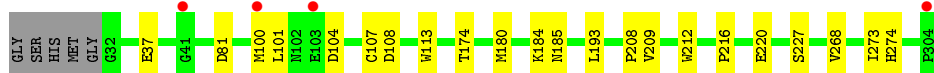
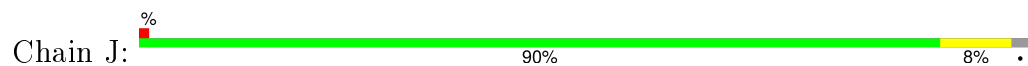
- Molecule 1: VP1



- 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	97.33Å 180.09Å 199.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	133.65 – 2.00 44.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (133.65-2.00) 96.2 (44.37-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0025	Depositor
R, R_{free}	0.196 , 0.236 0.198 , 0.237	Depositor DCC
R_{free} test set	11393 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 226820 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22785	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 2.75% 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: CA, IPA, EDO

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	0.55	2/2125 (0.1%)	0.65	0/2901
1	B	0.55	2/2121 (0.1%)	0.65	0/2896
1	C	0.52	1/2137 (0.0%)	0.64	0/2915
1	D	0.53	2/2123 (0.1%)	0.63	0/2900
1	E	0.54	1/2111 (0.0%)	0.63	0/2883
1	F	0.54	1/2156 (0.0%)	0.63	0/2943
1	G	0.56	1/2116 (0.0%)	0.64	0/2890
1	H	0.54	1/2133 (0.0%)	0.67	0/2912
1	I	0.53	2/2119 (0.1%)	0.63	0/2893
1	J	0.53	1/2155 (0.0%)	0.63	1/2942 (0.0%)
All	All	0.54	14/21296 (0.1%)	0.64	1/29075 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	212	TRP	CD2-CE2	5.59	1.48	1.41
1	E	212	TRP	CD2-CE2	5.49	1.48	1.41
1	C	113	TRP	CD2-CE2	5.47	1.48	1.41
1	A	283	TRP	CD2-CE2	5.46	1.47	1.41
1	F	113	TRP	CD2-CE2	5.46	1.48	1.41
1	J	212	TRP	CD2-CE2	5.44	1.47	1.41
1	B	113	TRP	CD2-CE2	5.42	1.47	1.41
1	D	113	TRP	CD2-CE2	5.42	1.47	1.41
1	B	212	TRP	CD2-CE2	5.36	1.47	1.41
1	D	212	TRP	CD2-CE2	5.35	1.47	1.41
1	I	113	TRP	CD2-CE2	5.22	1.47	1.41
1	H	113	TRP	CD2-CE2	5.21	1.47	1.41
1	G	212	TRP	CD2-CE2	5.17	1.47	1.41
1	A	113	TRP	CD2-CE2	5.02	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	100	MET	CB-CG-SD	5.61	129.22	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2077	0	2059	14	0
1	B	2071	0	2060	12	0
1	C	2085	0	2074	14	0
1	D	2075	0	2054	15	0
1	E	2064	0	2042	13	0
1	F	2101	0	2084	12	0
1	G	2071	0	2047	11	0
1	H	2087	0	2060	9	0
1	I	2075	0	2046	14	0
1	J	2100	0	2075	17	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	4	0	6	2	0
3	B	4	0	6	2	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
3	E	4	0	6	0	0
3	F	8	0	12	0	0
3	G	8	0	12	1	0
3	I	4	0	6	0	0
3	J	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	8	0	0
4	B	4	0	8	0	0
4	C	4	0	8	0	0
4	D	4	0	8	0	0
4	E	4	0	8	0	0
4	F	4	0	8	0	0
4	G	4	0	8	0	0
4	H	4	0	8	1	0
4	I	4	0	8	0	0
4	J	4	0	8	0	0
5	A	221	0	0	4	0
5	B	222	0	0	2	0
5	C	177	0	0	0	0
5	D	171	0	0	2	0
5	E	192	0	0	2	0
5	F	166	0	0	2	0
5	G	186	0	0	0	0
5	H	199	0	0	2	0
5	I	181	0	0	1	0
5	J	170	0	0	2	0
All	All	22785	0	20747	113	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 (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASP:OD1	1:A:106:THR:OG1	1.87	0.93
1:B:106:THR:HG23	5:H:672:HOH:O	1.75	0.86
1:I:104:ASP:OD2	1:I:106:THR:OG1	1.99	0.78
1:D:104:ASP:OD1	1:D:106:THR:HG22	1.85	0.77
1:C:131:LEU:HD11	1:D:273:ILE:HD13	1.70	0.73
3:B:402:EDO:H21	5:B:648:HOH:O	1.87	0.73
1:F:182:THR:HB	5:F:598:HOH:O	1.93	0.69
1:I:239:GLN:NE2	1:J:227:SER:HB3	2.13	0.63
1:C:131:LEU:HD11	1:D:273:ILE:CD1	2.29	0.62
1:D:128:LEU:HD22	1:D:148:VAL:HB	1.81	0.62
1:E:37:GLU:HG3	1:J:37:GLU:HG3	1.85	0.59
1:J:101:LEU:HD21	1:J:113:TRP:CZ2	2.39	0.58
1:B:223[A]:ARG:NH2	1:B:254:VAL:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:SER:O	1:A:279:GLU:HB2	2.04	0.57
3:A:402:EDO:H21	5:A:614:HOH:O	2.05	0.56
1:A:131:LEU:HD11	1:B:273:ILE:CD1	2.35	0.56
1:I:179[B]:ASP:N	1:I:179[B]:ASP:OD1	2.34	0.56
1:A:37:GLU:HG3	1:I:37:GLU:HG3	1.87	0.56
1:J:184:LYS:HG3	1:J:185:ASN:ND2	2.21	0.55
1:E:278:SER:O	1:E:279:GLU:HB2	2.07	0.55
1:E:33:VAL:N	5:E:564:HOH:O	2.40	0.54
1:G:157:SER:OG	1:G:266:SER:HB2	2.08	0.54
1:C:209:VAL:HG11	1:C:268:VAL:HG21	1.90	0.54
1:I:239:GLN:HE22	1:J:227:SER:HB3	1.74	0.53
1:J:220[A]:GLU:CD	1:J:220[A]:GLU:H	2.12	0.53
1:A:273:ILE:HD13	1:E:131:LEU:HD21	1.91	0.51
1:G:60:ASN:OD1	1:G:62:THR:HG22	2.11	0.51
1:G:64:GLU:HG2	1:H:78:LYS:HE2	1.93	0.50
1:J:180:MET:CE	1:J:208:PRO:HG3	2.41	0.50
1:F:84:ASN:HB2	1:F:87:THR:HG23	1.92	0.50
1:D:84:ASN:HB2	1:D:87:THR:HG23	1.93	0.50
1:H:182:THR:HB	5:H:502:HOH:O	2.11	0.49
1:F:84:ASN:HB3	5:F:521:HOH:O	2.12	0.49
1:C:72:ILE:HG12	1:C:281:GLN:O	2.12	0.49
1:E:182:THR:HB	5:E:513:HOH:O	2.13	0.49
1:B:239:GLN:OE1	1:C:227:SER:HB3	2.12	0.49
1:D:129:VAL:HG21	1:E:153:LEU:HD22	1.95	0.49
1:C:124:GLY:HA3	1:D:168:LEU:HD13	1.95	0.49
1:A:273:ILE:CD1	1:E:131:LEU:HD21	2.43	0.48
1:A:131:LEU:HD11	1:B:273:ILE:HD13	1.96	0.48
1:A:90:THR:OG1	1:A:205:GLY:HA2	2.14	0.48
3:A:402:EDO:C2	5:A:614:HOH:O	2.62	0.48
1:J:180:MET:HE2	1:J:208:PRO:HG3	1.96	0.47
1:D:157:SER:OG	1:D:266:SER:HB2	2.14	0.47
1:D:152[B]:THR:HG22	5:D:533:HOH:O	2.14	0.47
1:H:102:ASN:HB2	1:H:105:MET:CE	2.44	0.47
1:I:278:SER:O	1:I:279:GLU:HB2	2.15	0.47
1:B:209:VAL:HG11	1:B:268:VAL:HG21	1.96	0.46
1:J:184:LYS:HG3	1:J:185:ASN:HD22	1.81	0.46
1:G:278:SER:O	1:G:279:GLU:HB2	2.15	0.46
1:I:84:ASN:HB2	1:I:87:THR:HG23	1.98	0.46
1:A:43:ASP:HA	5:A:701:HOH:O	2.16	0.46
1:A:33:VAL:N	5:A:653:HOH:O	2.49	0.46
1:D:239:GLN:HG2	5:D:606:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:C	1:C:48:ILE:HD12	2.36	0.45
1:E:90:THR:OG1	1:E:205:GLY:HA2	2.17	0.45
1:G:239:GLN:O	3:G:403:EDO:H22	2.16	0.45
1:E:157:SER:OG	1:E:266:SER:HB2	2.17	0.45
1:I:121:GLU:HG3	1:J:216:PRO:HB3	1.97	0.45
1:J:209:VAL:HG11	1:J:268:VAL:HG21	1.99	0.45
1:F:153[B]:LEU:HD22	1:F:268:VAL:HG13	1.99	0.45
1:G:223:ARG:NH2	1:G:254:VAL:O	2.50	0.44
1:B:157:SER:OG	1:B:266:SER:HB2	2.16	0.44
1:G:60:ASN:CG	1:G:62:THR:HG22	2.38	0.44
1:D:90:THR:OG1	1:D:205:GLY:HA2	2.17	0.44
1:G:209:VAL:HG11	1:G:268:VAL:HG21	2.00	0.44
1:H:102:ASN:HB2	1:H:105:MET:HE1	2.00	0.44
1:D:278:SER:O	1:D:279:GLU:HB2	2.17	0.44
1:I:104:ASP:CG	1:I:106:THR:OG1	2.54	0.43
1:F:209:VAL:HG11	1:F:268:VAL:HG21	2.00	0.43
3:B:402:EDO:C2	5:B:648:HOH:O	2.56	0.43
1:J:81:ASP:HB3	1:J:174:THR:HA	2.00	0.43
1:A:131:LEU:HD11	1:B:273:ILE:HD11	1.99	0.43
1:G:60:ASN:OD1	1:G:61:PRO:HD2	2.19	0.43
1:E:68:TYR:HA	1:E:283:TRP:O	2.18	0.43
1:H:169:VAL:O	1:H:191:GLN:HA	2.19	0.42
1:B:132:HIS:HE2	1:C:210:GLU:CD	2.20	0.42
1:H:278:SER:O	1:H:279:GLU:HB2	2.19	0.42
1:F:300:LYS:O	1:F:302:PRO:HD3	2.20	0.42
1:F:161:GLU:HB2	1:F:162:PRO:CD	2.49	0.42
1:H:227:SER:HB2	4:H:402:IPA:H31	2.01	0.42
1:F:97:LYS:HE3	1:F:98:LEU:O	2.20	0.42
1:E:84:ASN:HB2	1:E:87:THR:HG23	2.01	0.42
1:C:121:GLU:OE2	1:C:240:PHE:HB2	2.19	0.42
1:A:210:GLU:CD	1:E:132:HIS:HE2	2.22	0.42
1:F:48:ILE:C	1:F:48:ILE:HD12	2.40	0.42
1:D:104:ASP:CG	1:D:106:THR:HG22	2.38	0.42
1:B:116[B]:VAL:HG12	1:B:249:LEU:HD21	2.02	0.42
1:B:223[B]:ARG:HD2	1:B:248:LEU:O	2.19	0.41
1:B:236:PRO:HD2	1:C:230:GLY:HA3	2.01	0.41
1:G:68:TYR:CE1	1:G:284:ARG:HD3	2.55	0.41
1:G:184:LYS:HA	1:G:184:LYS:HD3	1.76	0.41
1:C:75:ALA:HB2	1:C:81:ASP:OD1	2.20	0.41
1:D:81:ASP:HB3	1:D:174:THR:HA	2.02	0.41
1:F:278:SER:O	1:F:279:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:LYS:NZ	5:I:601:HOH:O	2.39	0.41
1:A:52:LEU:HD21	1:A:94:ALA:CB	2.51	0.41
1:F:90:THR:OG1	1:F:205:GLY:HA2	2.20	0.41
1:J:104:ASP:HB3	1:J:107:CYS:SG	2.61	0.41
1:J:274:HIS:HE1	5:J:649:HOH:O	2.03	0.41
1:I:51:TYR:C	1:I:52:LEU:HD12	2.40	0.41
1:H:128:LEU:HD11	1:H:286:LEU:HD11	2.03	0.41
1:I:131:LEU:HD11	1:J:273:ILE:CD1	2.51	0.41
1:C:60:ASN:HA	1:C:61:PRO:HD2	1.92	0.41
1:J:180:MET:HG2	5:J:580:HOH:O	2.20	0.41
1:C:155[A]:MET:HE1	1:C:163:LEU:HD21	2.02	0.41
1:D:37:GLU:HG3	1:F:37:GLU:HG3	2.04	0.40
1:A:37:GLU:CG	1:I:37:GLU:HG3	2.51	0.40
1:I:100:MET:HA	1:I:261:ASP:OD2	2.21	0.40
1:C:195:PRO:O	1:C:198:LYS:HE2	2.21	0.40
1:H:155:MET:HG2	1:H:156:PHE:N	2.36	0.40
1:E:60:ASN:HA	1:E:61:PRO:HD2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/278 (97%)	258 (96%)	11 (4%)	1 (0%)	39	33
1	B	270/278 (97%)	256 (95%)	14 (5%)	0	100	100
1	C	270/278 (97%)	256 (95%)	14 (5%)	0	100	100
1	D	270/278 (97%)	260 (96%)	10 (4%)	0	100	100
1	E	269/278 (97%)	256 (95%)	13 (5%)	0	100	100
1	F	274/278 (99%)	261 (95%)	13 (5%)	0	100	100
1	G	269/278 (97%)	255 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	272/278 (98%)	261 (96%)	11 (4%)	0	100	100
1	I	271/278 (98%)	259 (96%)	12 (4%)	0	100	100
1	J	274/278 (99%)	261 (95%)	12 (4%)	1 (0%)	39	33
All	All	2709/2780 (97%)	2583 (95%)	124 (5%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	J	108	ASP

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	237/240 (99%)	237 (100%)	0	100	100
1	B	237/240 (99%)	235 (99%)	2 (1%)	86	89
1	C	239/240 (100%)	238 (100%)	1 (0%)	93	95
1	D	237/240 (99%)	237 (100%)	0	100	100
1	E	236/240 (98%)	234 (99%)	2 (1%)	86	89
1	F	241/240 (100%)	240 (100%)	1 (0%)	93	95
1	G	236/240 (98%)	235 (100%)	1 (0%)	93	95
1	H	237/240 (99%)	235 (99%)	2 (1%)	86	89
1	I	236/240 (98%)	233 (99%)	3 (1%)	76	79
1	J	240/240 (100%)	239 (100%)	1 (0%)	93	95
All	All	2376/2400 (99%)	2363 (100%)	13 (0%)	90	94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	GLU

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Mol	Chain	Res	Type
1	B	193	LEU
1	C	104	ASP
1	E	131	LEU
1	E	193	LEU
1	F	193	LEU
1	G	193	LEU
1	H	121	GLU
1	H	193	LEU
1	I	104	ASP
1	I	105	MET
1	I	193	LEU
1	J	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	B	196	ASN
1	D	185	ASN
1	E	47	GLN
1	G	239	GLN
1	I	239	GLN
1	J	185	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 10 are monoatomic - leaving 21 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	0.49	0	2,2,2	0.21	0
4	IPA	A	403	-	3,3,3	0.52	0	3,3,3	0.41	0
3	EDO	B	402	-	3,3,3	0.43	0	2,2,2	0.35	0
4	IPA	B	403	-	3,3,3	0.47	0	3,3,3	0.42	0
3	EDO	C	402	-	3,3,3	0.42	0	2,2,2	0.55	0
4	IPA	C	403	-	3,3,3	0.48	0	3,3,3	0.43	0
3	EDO	D	402	-	3,3,3	0.41	0	2,2,2	0.87	0
4	IPA	D	403	-	3,3,3	0.46	0	3,3,3	0.35	0
3	EDO	E	402	-	3,3,3	0.63	0	2,2,2	0.29	0
4	IPA	E	403	-	3,3,3	0.51	0	3,3,3	0.34	0
3	EDO	F	402	-	3,3,3	0.42	0	2,2,2	0.72	0
3	EDO	F	403	-	3,3,3	0.48	0	2,2,2	0.36	0
4	IPA	F	404	-	3,3,3	0.56	0	3,3,3	0.23	0
3	EDO	G	402	-	3,3,3	0.51	0	2,2,2	0.38	0
3	EDO	G	403	-	3,3,3	0.50	0	2,2,2	0.15	0
4	IPA	G	404	-	3,3,3	0.50	0	3,3,3	0.40	0
4	IPA	H	402	-	3,3,3	0.45	0	3,3,3	0.52	0
3	EDO	I	402	-	3,3,3	0.46	0	2,2,2	0.59	0
4	IPA	I	403	-	3,3,3	0.47	0	3,3,3	0.38	0
3	EDO	J	402	-	3,3,3	0.38	0	2,2,2	0.66	0
4	IPA	J	403	-	3,3,3	0.47	0	3,3,3	0.36	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
4	IPA	A	403	-	-	0/0/0/0	0/0/0/0
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
4	IPA	B	403	-	-	0/0/0/0	0/0/0/0
3	EDO	C	402	-	-	0/1/1/1	0/0/0/0
4	IPA	C	403	-	-	0/0/0/0	0/0/0/0
3	EDO	D	402	-	-	0/1/1/1	0/0/0/0

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

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	EDO	2	0
3	B	402	EDO	2	0
3	G	403	EDO	1	0
4	H	402	IPA	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	271/278 (97%)	-0.07	7 (2%) 59 60	15, 22, 41, 82	0
1	B	270/278 (97%)	-0.32	1 (0%) 93 93	15, 21, 43, 58	1 (0%)
1	C	269/278 (96%)	-0.18	2 (0%) 89 89	17, 25, 42, 78	1 (0%)
1	D	271/278 (97%)	-0.11	3 (1%) 82 83	20, 28, 44, 73	0
1	E	270/278 (97%)	-0.04	7 (2%) 59 60	17, 26, 45, 73	0
1	F	272/278 (97%)	-0.18	0 100 100	20, 28, 42, 57	1 (0%)
1	G	271/278 (97%)	-0.25	2 (0%) 89 89	18, 25, 43, 53	1 (0%)
1	H	274/278 (98%)	-0.16	2 (0%) 89 89	15, 23, 44, 77	0
1	I	272/278 (97%)	-0.11	4 (1%) 76 77	18, 25, 44, 66	0
1	J	273/278 (98%)	-0.10	4 (1%) 76 77	19, 27, 46, 66	0
All	All	2713/2780 (97%)	-0.15	32 (1%) 81 81	15, 25, 44, 82	4 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	303	TYR	8.2
1	A	303	TYR	7.0
1	H	304	PRO	4.9
1	H	303	TYR	4.0
1	I	103	GLU	3.7
1	J	304	PRO	3.6
1	E	108	ASP	3.3
1	C	104	ASP	3.2
1	A	108	ASP	3.1
1	E	106	THR	3.1
1	A	106	THR	3.1
1	J	100	MET	2.7
1	G	303	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	32	GLY	2.6
1	E	104	ASP	2.5
1	E	179[A]	ASP	2.5
1	D	108	ASP	2.4
1	I	108	ASP	2.4
1	A	33	VAL	2.4
1	A	107	CYS	2.3
1	E	103	GLU	2.3
1	J	41	GLY	2.2
1	E	33	VAL	2.2
1	A	103	GLU	2.2
1	D	184	LYS	2.2
1	I	31	GLY	2.2
1	B	108	ASP	2.2
1	G	184	LYS	2.1
1	E	300	LYS	2.1
1	A	104	ASP	2.0
1	J	103	GLU	2.0
1	C	108	ASP	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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
4	IPA	G	404	4/4	0.91	0.19	10.94	37,38,38,41	0
4	IPA	H	402	4/4	0.93	0.20	9.26	26,27,29,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	IPA	A	403	4/4	0.89	0.23	5.57	30,30,31,32	0
3	EDO	F	403	4/4	0.90	0.25	5.52	35,35,37,39	0
4	IPA	E	403	4/4	0.92	0.19	5.41	29,29,29,32	0
3	EDO	F	402	4/4	0.93	0.17	4.65	27,27,29,29	0
4	IPA	F	404	4/4	0.84	0.18	4.53	35,38,40,41	0
4	IPA	C	403	4/4	0.90	0.19	3.30	33,33,34,35	0
4	IPA	D	403	4/4	0.96	0.18	2.84	31,31,32,33	0
4	IPA	I	403	4/4	0.91	0.14	2.82	25,28,30,30	0
3	EDO	J	402	4/4	0.95	0.15	2.75	32,35,37,41	0
4	IPA	J	403	4/4	0.94	0.16	2.38	29,30,31,32	0
3	EDO	A	402	4/4	0.84	0.18	2.30	36,37,41,42	0
4	IPA	B	403	4/4	0.92	0.16	1.37	28,29,29,31	0
3	EDO	B	402	4/4	0.89	0.14	1.17	40,40,42,43	0
3	EDO	D	402	4/4	0.93	0.16	0.83	36,37,37,43	0
3	EDO	G	403	4/4	0.91	0.11	0.52	29,32,33,35	0
3	EDO	E	402	4/4	0.90	0.14	-0.12	32,34,34,36	0
3	EDO	I	402	4/4	0.94	0.10	-0.79	30,33,33,36	0
3	EDO	C	402	4/4	0.96	0.10	-1.27	29,29,30,30	0
2	CA	I	401	1/1	0.96	0.07	-2.08	43,43,43,43	0
2	CA	B	401	1/1	0.97	0.04	-2.20	39,39,39,39	0
2	CA	J	401	1/1	0.96	0.05	-2.52	45,45,45,45	0
2	CA	H	401	1/1	0.97	0.06	-	33,33,33,33	0
2	CA	F	401	1/1	0.87	0.12	-	55,55,55,55	0
2	CA	D	401	1/1	0.97	0.03	-	51,51,51,51	0
2	CA	A	401	1/1	0.98	0.05	-	43,43,43,43	0
3	EDO	G	402	4/4	0.84	0.16	-	41,44,47,48	0
2	CA	E	401	1/1	0.99	0.04	-	36,36,36,36	0
2	CA	C	401	1/1	0.99	0.03	-	45,45,45,45	0
2	CA	G	401	1/1	0.99	0.04	-	39,39,39,39	0

6.5 Other polymers

There are no such residues in this entry.