



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:10 PM UTC

PDB ID : 8AH1 / pdb_00008ah1
Title : BK Polyomavirus VP1 mutant N-Q
Authors : Sorin, M.N.; Di Maio, A.; Silva, L.M.; Ebert, D.; Delannoy, C.; Nguyen, N.-K.; Guerardel, Y.; Chai, W.; Halary, F.; Renaudin-Autain, K.; Liu, Y.; Bressollette-Bodin, C.; Stehle, T.; McIlroy, D.
Deposited on : 2022-07-20
Resolution : 2.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

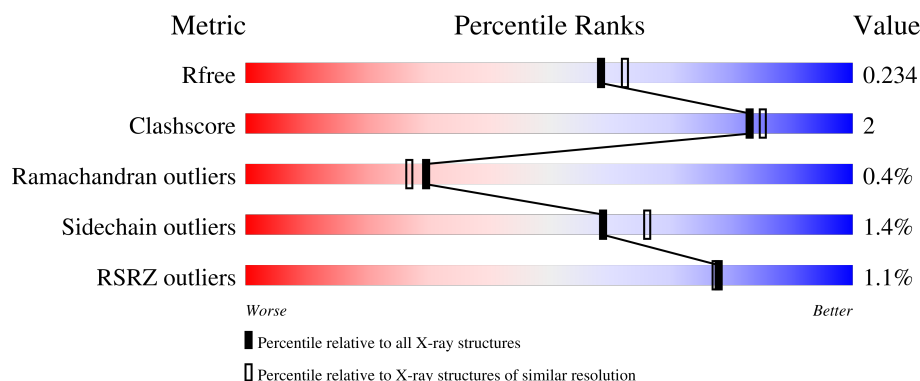
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	271	88% 7% 5%
1	BBB	271	83% 11% 6%
1	CCC	271	90% 7% . .
1	DDD	271	87% 7% 6%
1	EEE	271	88% 6% 5%

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Mol	Chain	Length	Quality of chain
1	FFF	271	% 87% 7%5%
1	GGG	271	% 87% 7%5%
1	HHH	271	87% 8%5%
1	III	271	% 89% 9%.
1	JJJ	271	% 87% 9%..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20804 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	258	Total	C	N	O	S	0	0	0
			1954	1231	339	372	12			
1	BBB	256	Total	C	N	O	S	0	1	0
			1955	1229	339	374	13			
1	CCC	264	Total	C	N	O	S	0	1	0
			2001	1258	348	383	12			
1	DDD	256	Total	C	N	O	S	0	1	0
			1932	1216	332	371	13			
1	EEE	258	Total	C	N	O	S	0	1	0
			1971	1240	344	375	12			
1	FFF	258	Total	C	N	O	S	0	1	0
			1959	1232	339	376	12			
1	GGG	257	Total	C	N	O	S	0	0	0
			1947	1225	340	370	12			
1	HHH	257	Total	C	N	O	S	0	1	0
			1963	1233	343	375	12			
1	III	265	Total	C	N	O	S	0	1	0
			2010	1262	348	387	13			
1	JJJ	264	Total	C	N	O	S	0	3	0
			2019	1268	352	386	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	68	ASN	LYS	engineered mutation	UNP P03088
AAA	81	GLN	GLU	engineered mutation	UNP P03088
AAA	104	SER	CYS	engineered mutation	UNP P03088
BBB	68	ASN	LYS	engineered mutation	UNP P03088
BBB	81	GLN	GLU	engineered mutation	UNP P03088
BBB	104	SER	CYS	engineered mutation	UNP P03088
CCC	68	ASN	LYS	engineered mutation	UNP P03088
CCC	81	GLN	GLU	engineered mutation	UNP P03088
CCC	104	SER	CYS	engineered mutation	UNP P03088

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	68	ASN	LYS	engineered mutation	UNP P03088
DDD	81	GLN	GLU	engineered mutation	UNP P03088
DDD	104	SER	CYS	engineered mutation	UNP P03088
EEE	68	ASN	LYS	engineered mutation	UNP P03088
EEE	81	GLN	GLU	engineered mutation	UNP P03088
EEE	104	SER	CYS	engineered mutation	UNP P03088
FFF	68	ASN	LYS	engineered mutation	UNP P03088
FFF	81	GLN	GLU	engineered mutation	UNP P03088
FFF	104	SER	CYS	engineered mutation	UNP P03088
GGG	68	ASN	LYS	engineered mutation	UNP P03088
GGG	81	GLN	GLU	engineered mutation	UNP P03088
GGG	104	SER	CYS	engineered mutation	UNP P03088
HHH	68	ASN	LYS	engineered mutation	UNP P03088
HHH	81	GLN	GLU	engineered mutation	UNP P03088
HHH	104	SER	CYS	engineered mutation	UNP P03088
III	68	ASN	LYS	engineered mutation	UNP P03088
III	81	GLN	GLU	engineered mutation	UNP P03088
III	104	SER	CYS	engineered mutation	UNP P03088
JJJ	68	ASN	LYS	engineered mutation	UNP P03088
JJJ	81	GLN	GLU	engineered mutation	UNP P03088
JJJ	104	SER	CYS	engineered mutation	UNP P03088

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	JJJ	1	Total	Cl	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

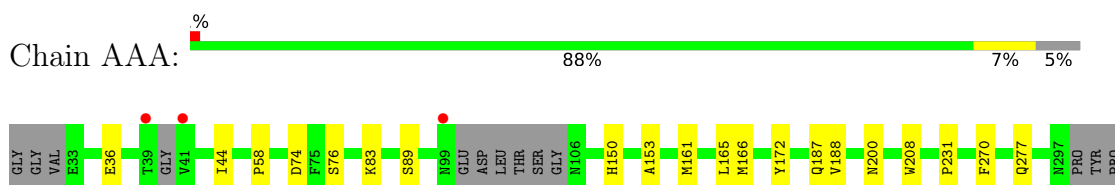
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	107	Total 107	O 107	0	0
4	BBB	92	Total 92	O 92	0	0
4	CCC	96	Total 96	O 96	0	0
4	DDD	79	Total 79	O 79	0	0
4	EEE	91	Total 91	O 91	0	0
4	FFF	99	Total 99	O 99	0	0
4	GGG	119	Total 119	O 119	0	0
4	HHH	104	Total 104	O 104	0	0
4	III	119	Total 119	O 119	0	0
4	JJJ	117	Total 117	O 117	0	0

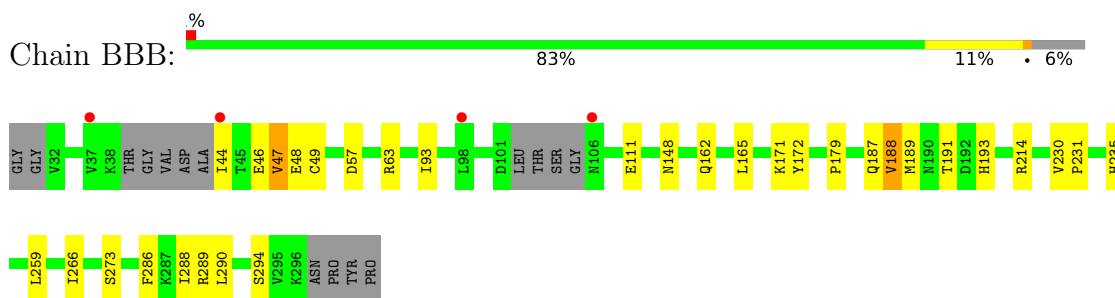
3 Residue-property plots

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.

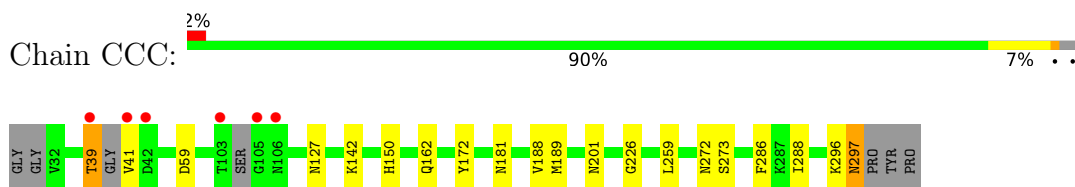
- Molecule 1: Major capsid protein VP1



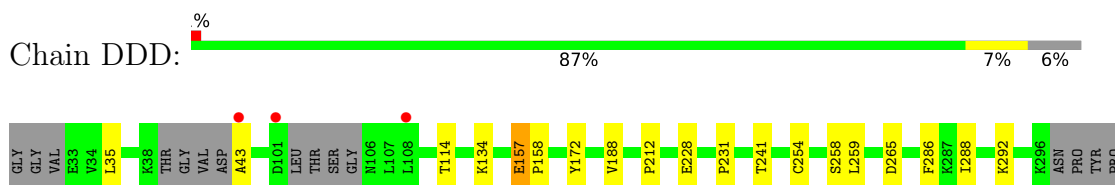
- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1

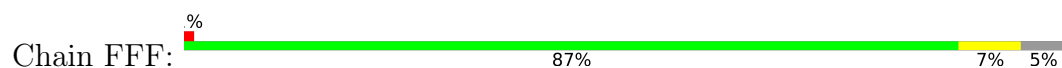


- Molecule 1: Major capsid protein VP1

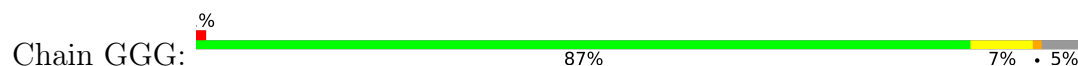




- Molecule 1: Major capsid protein VP1



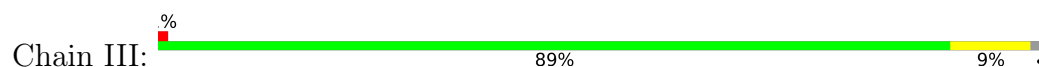
- Molecule 1: Major capsid protein VP1



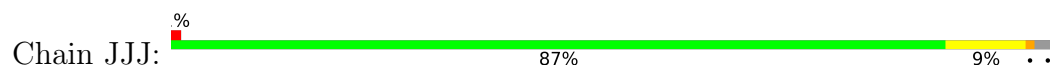
- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.46Å 155.96Å 141.32Å 90.00° 92.64° 90.00°	Depositor
Resolution (Å)	48.78 – 2.01 48.78 – 2.01	Depositor EDS
% Data completeness (in resolution range)	94.5 (48.78-2.01) 94.6 (48.78-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.232 0.188 , 0.234	Depositor DCC
R_{free} test set	8246 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20804	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL

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	1.15	2/1998 (0.1%)	1.37	2/2719 (0.1%)
1	BBB	1.15	1/1999 (0.1%)	1.34	2/2720 (0.1%)
1	CCC	1.15	0/2045	1.38	8/2784 (0.3%)
1	DDD	1.17	1/1979 (0.1%)	1.38	5/2697 (0.2%)
1	EEE	1.18	2/2019 (0.1%)	1.36	2/2748 (0.1%)
1	FFF	1.20	2/2007 (0.1%)	1.40	8/2734 (0.3%)
1	GGG	1.18	2/1991 (0.1%)	1.35	8/2708 (0.3%)
1	HHH	1.16	0/2008	1.37	5/2733 (0.2%)
1	III	1.16	1/2059 (0.0%)	1.37	1/2804 (0.0%)
1	JJJ	1.14	2/2073 (0.1%)	1.36	0/2821
All	All	1.16	13/20178 (0.1%)	1.37	41/27468 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	129	HIS	CE1-NE2	6.98	1.39	1.32
1	EEE	164	VAL	C-O	6.09	1.30	1.23
1	DDD	212	PRO	C-O	-6.00	1.17	1.24
1	GGG	35	LEU	N-CA	5.86	1.49	1.46
1	GGG	58	PRO	C-O	-5.64	1.17	1.24
1	FFF	178	THR	N-CA	5.24	1.50	1.45
1	JJJ	78	ASP	C-O	5.22	1.29	1.23
1	JJJ	178	THR	N-CA	5.22	1.50	1.45
1	AAA	153	ALA	C-O	5.18	1.30	1.23
1	AAA	150	HIS	CE1-NE2	5.13	1.37	1.32
1	BBB	235	HIS	CE1-NE2	5.05	1.37	1.32
1	III	70	SER	CA-CB	-5.02	1.45	1.53
1	FFF	129	HIS	CE1-NE2	5.01	1.37	1.32

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GGG	198	ASP	CA-CB-CG	7.82	120.42	112.60
1	BBB	172	TYR	CB-CA-C	7.59	120.49	109.11
1	AAA	172	TYR	CB-CA-C	7.05	118.81	108.87
1	FFF	183	THR	CA-CB-OG1	-6.67	99.59	109.60
1	CCC	181	ASN	O-C-N	-6.27	118.65	121.53
1	HHH	172	TYR	CB-CA-C	6.23	117.84	108.86
1	EEE	181	ASN	CB-CA-C	-6.14	105.66	111.00
1	DDD	286	PHE	CA-CB-CG	6.03	119.83	113.80
1	FFF	233	VAL	CA-C-O	-5.82	114.61	120.31
1	FFF	59	ASP	CA-C-N	5.79	128.61	120.28
1	FFF	59	ASP	C-N-CA	5.79	128.61	120.28
1	FFF	40	GLY	CA-C-O	-5.72	118.33	122.45
1	CCC	273	SER	CA-C-N	5.68	128.94	120.31
1	CCC	273	SER	C-N-CA	5.68	128.94	120.31
1	CCC	150	HIS	CB-CA-C	5.60	119.76	110.74
1	HHH	59	ASP	CA-C-N	5.47	127.62	120.28
1	HHH	59	ASP	C-N-CA	5.47	127.62	120.28
1	FFF	172	TYR	CB-CA-C	5.44	116.70	108.86
1	FFF	59	ASP	CA-C-O	-5.41	115.63	121.36
1	CCC	286	PHE	CA-CB-CG	5.40	119.20	113.80
1	GGG	295	VAL	CA-C-N	5.39	129.40	120.94
1	GGG	295	VAL	C-N-CA	5.39	129.40	120.94
1	GGG	178	THR	O-C-N	-5.34	118.29	121.71
1	GGG	188	VAL	CA-C-O	-5.33	114.12	120.78
1	EEE	59	ASP	CA-CB-CG	5.26	117.86	112.60
1	III	172	TYR	CB-CA-C	5.23	116.62	108.61
1	DDD	172	TYR	CB-CA-C	5.23	116.39	108.86
1	AAA	150	HIS	CB-CA-C	5.21	118.81	110.16
1	CCC	172	TYR	CB-CA-C	5.20	116.34	108.86
1	DDD	254	CYS	CA-C-N	5.17	127.16	120.44
1	DDD	254	CYS	C-N-CA	5.17	127.16	120.44
1	HHH	156	GLY	CA-C-N	5.16	129.55	122.06
1	HHH	156	GLY	C-N-CA	5.16	129.55	122.06
1	FFF	150	HIS	CB-CA-C	5.12	118.34	110.62
1	BBB	191	THR	CA-CB-OG1	-5.11	101.94	109.60
1	GGG	242	THR	CA-CB-OG1	-5.10	101.95	109.60
1	GGG	183	THR	CA-CB-OG1	-5.09	101.97	109.60
1	GGG	150	HIS	CB-CA-C	5.09	118.93	110.74
1	CCC	272	ASN	CA-C-N	5.05	128.39	120.82
1	CCC	272	ASN	C-N-CA	5.05	128.39	120.82
1	DDD	265	ASP	CB-CA-C	5.02	119.27	112.09

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	1954	0	1866	8	0
1	BBB	1955	0	1857	19	0
1	CCC	2001	0	1900	10	0
1	DDD	1932	0	1814	6	0
1	EEE	1971	0	1891	7	0
1	FFF	1959	0	1860	8	0
1	GGG	1947	0	1855	7	0
1	HHH	1963	0	1876	9	0
1	III	2010	0	1922	11	0
1	JJJ	2019	0	1935	17	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
2	EEE	1	0	0	0	0
2	FFF	1	0	0	0	0
2	GGG	1	0	0	0	0
2	HHH	1	0	0	0	0
2	III	1	0	0	1	0
2	JJJ	1	0	0	0	0
3	BBB	6	0	8	0	0
3	DDD	6	0	8	0	0
3	EEE	6	0	8	1	0
3	FFF	12	0	16	1	0
3	HHH	6	0	8	0	0
3	III	18	0	24	0	0
3	JJJ	6	0	8	0	0
4	AAA	107	0	0	1	0
4	BBB	92	0	0	1	0
4	CCC	96	0	0	1	0
4	DDD	79	0	0	0	0
4	EEE	91	0	0	0	0
4	FFF	99	0	0	0	0
4	GGG	119	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	HHH	104	0	0	1	0
4	III	119	0	0	0	0
4	JJJ	117	0	0	0	0
All	All	20804	0	18856	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (94) 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:JJJ:49[B]:CYS:SG	1:JJJ:93:ILE:HD11	2.25	0.76
1:JJJ:259:LEU:HD12	1:JJJ:259:LEU:C	2.11	0.75
1:BBB:49[A]:CYS:SG	1:BBB:93:ILE:HD11	2.34	0.68
1:JJJ:99:ASN:HD21	1:JJJ:108:LEU:H	1.39	0.67
1:DDD:259:LEU:HD21	1:DDD:288:ILE:HD13	1.76	0.67
1:AAA:166:MET:HE2	1:AAA:166:MET:HA	1.81	0.63
1:CCC:162:GLN:OE1	1:CCC:189:MET:HE1	2.01	0.61
1:HHH:43:ALA:HA	1:HHH:292:LYS:HD2	1.86	0.58
4:HHH:531:HOH:O	1:III:185:GLN:HG3	2.03	0.56
1:III:185:GLN:NE2	1:III:189:MET:O	2.38	0.56
1:GGG:34:VAL:HA	1:GGG:295:VAL:HG12	1.87	0.56
1:BBB:259:LEU:HD12	1:BBB:259:LEU:C	2.32	0.55
1:BBB:162:GLN:OE1	1:BBB:189:MET:HE1	2.07	0.55
1:EEE:188:VAL:HG23	1:EEE:189:MET:H	1.72	0.54
1:JJJ:82[B]:ARG:NH2	1:JJJ:201:ASN:O	2.41	0.54
1:BBB:49[A]:CYS:SG	1:BBB:93:ILE:CD1	2.98	0.52
1:HHH:44:ILE:HD12	1:HHH:289:ARG:NH1	2.26	0.51
1:DDD:157:GLU:HB2	1:DDD:158:PRO:CD	2.41	0.51
1:AAA:161:MET:HE3	1:AAA:208:TRP:HB3	1.93	0.51
1:BBB:57:ASP:OD2	1:BBB:63:ARG:NH1	2.44	0.51
1:DDD:231:PRO:HB3	1:EEE:226:GLY:O	2.10	0.51
1:EEE:165:LEU:O	1:EEE:187:GLN:HA	2.11	0.49
1:CCC:296:LYS:O	1:CCC:297:ASN:HB2	2.12	0.49
1:HHH:188:VAL:HG23	1:HHH:189:MET:H	1.77	0.49
1:BBB:165:LEU:O	1:BBB:187:GLN:HA	2.12	0.49
1:GGG:113:VAL:HG12	1:GGG:114:THR:HG23	1.94	0.48
1:BBB:47:VAL:HG23	1:BBB:288:ILE:HB	1.96	0.47
1:CCC:142:LYS:NZ	1:DDD:228:GLU:OE1	2.36	0.47
1:EEE:91:ALA:HA	3:EEE:401:GOL:H12	1.96	0.47
1:JJJ:188:VAL:HG23	1:JJJ:189:MET:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:59:ASP:OD1	1:CCC:59:ASP:C	2.57	0.47
1:HHH:233:VAL:HG22	1:III:225:THR:HG23	1.96	0.47
1:JJJ:259:LEU:C	1:JJJ:259:LEU:CD1	2.84	0.47
1:BBB:148:ASN:HB2	1:BBB:266:ILE:O	2.15	0.47
1:DDD:43:ALA:HA	1:DDD:292:LYS:HD2	1.97	0.47
1:FFF:179:PRO:HB3	1:FFF:193:HIS:CG	2.50	0.46
1:GGG:165:LEU:O	1:GGG:187:GLN:HA	2.15	0.46
1:CCC:201:ASN:O	1:CCC:201:ASN:CG	2.58	0.46
1:FFF:270:PHE:O	1:FFF:277:GLN:HA	2.16	0.46
1:BBB:46:GLU:HG3	1:BBB:289:ARG:HG2	1.97	0.46
1:FFF:224:PHE:CE2	1:JJJ:125:MET:HE3	2.51	0.46
1:CCC:39:THR:O	1:CCC:41:VAL:HA	2.16	0.45
1:BBB:162:GLN:CD	1:BBB:189:MET:HE1	2.41	0.45
1:AAA:231:PRO:HB3	1:BBB:230:VAL:CG2	2.47	0.45
1:CCC:127:ASN:OD1	1:CCC:127:ASN:C	2.58	0.45
1:HHH:113:VAL:HG12	1:HHH:114:THR:HG23	1.98	0.45
1:FFF:82[A]:ARG:NH2	1:FFF:201:ASN:O	2.49	0.45
1:EEE:113:VAL:HG23	1:EEE:114:THR:HG23	1.99	0.45
1:BBB:47:VAL:HG22	1:BBB:290:LEU:HD11	1.99	0.44
1:III:259:LEU:HD21	1:III:288:ILE:HD13	1.98	0.44
1:HHH:111:GLU:O	1:HHH:290:LEU:HA	2.17	0.44
1:III:117:THR:HA	1:III:285:TYR:O	2.17	0.44
1:BBB:188:VAL:HG23	1:BBB:189:MET:H	1.81	0.44
1:FFF:98:LEU:O	1:FFF:99:ASN:C	2.60	0.44
1:AAA:270:PHE:O	1:AAA:277:GLN:HA	2.17	0.43
1:HHH:51:LEU:HD12	1:HHH:51:LEU:HA	1.81	0.43
1:GGG:48:GLU:HA	1:GGG:286:PHE:O	2.18	0.43
1:JJJ:246:ASP:OD1	1:JJJ:246:ASP:C	2.61	0.43
1:JJJ:59:ASP:OD1	1:JJJ:59:ASP:C	2.62	0.43
1:AAA:74:ASP:OD2	1:AAA:76:SER:OG	2.29	0.43
1:AAA:58:PRO:HA	1:AAA:83:LYS:HD3	2.00	0.43
1:BBB:179:PRO:HB3	1:BBB:193:HIS:CG	2.54	0.43
1:III:42:ASP:O	1:III:292:LYS:HE3	2.19	0.43
1:III:146:GLY:HA2	1:III:227:GLY:O	2.19	0.43
1:HHH:270:PHE:O	1:HHH:277:GLN:HA	2.19	0.43
1:GGG:117:THR:HA	1:GGG:285:TYR:O	2.19	0.42
1:BBB:214:ARG:HD2	4:BBB:544:HOH:O	2.19	0.42
1:FFF:63:ARG:HH21	1:GGG:185:GLN:HE22	1.67	0.42
1:III:88:TYR:CE2	1:III:205:VAL:HA	2.54	0.42
1:GGG:146:GLY:HA2	1:GGG:227:GLY:O	2.19	0.42
1:JJJ:114:THR:HB	1:JJJ:241:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:165:LEU:O	1:AAA:187:GLN:HA	2.19	0.41
1:DDD:114:THR:HB	1:DDD:241:THR:HG23	2.02	0.41
1:JJJ:117:THR:HA	1:JJJ:285:TYR:O	2.20	0.41
1:JJJ:160:GLU:OE2	1:JJJ:214[A]:ARG:HD2	2.19	0.41
1:FFF:172:TYR:H	3:FFF:401:GOL:C1	2.33	0.41
1:CCC:259:LEU:HD21	1:CCC:288:ILE:HD13	2.02	0.41
1:JJJ:38:LYS:CG	1:JJJ:108:LEU:HD22	2.51	0.41
4:AAA:549:HOH:O	1:EEE:129:HIS:HB3	2.20	0.41
1:BBB:231:PRO:HB3	1:CCC:226:GLY:O	2.21	0.41
1:EEE:172:TYR:CG	1:EEE:178:THR:HG21	2.55	0.41
1:HHH:75:PHE:HA	1:HHH:167:ASN:ND2	2.36	0.41
1:FFF:225:THR:HG23	1:JJJ:233:VAL:HG22	2.01	0.41
1:III:113:VAL:HG12	1:III:114:THR:HG23	2.02	0.41
1:III:270:PHE:O	1:III:277:GLN:HA	2.20	0.41
1:III:193:HIS:HA	2:III:504:CL:CL	2.58	0.40
1:JJJ:259:LEU:HD12	1:JJJ:259:LEU:O	2.21	0.40
1:BBB:44:ILE:HA	1:BBB:290:LEU:O	2.22	0.40
1:JJJ:127:ASN:OD1	1:JJJ:127:ASN:C	2.65	0.40
1:AAA:89:SER:HA	1:AAA:200:ASN:OD1	2.21	0.40
1:CCC:142:LYS:HE2	4:CCC:557:HOH:O	2.21	0.40
1:JJJ:234:LEU:HD23	1:JJJ:234:LEU:HA	1.97	0.40
1:BBB:48:GLU:HA	1:BBB:286:PHE:O	2.22	0.40
1:BBB:111:GLU:O	1:BBB:290:LEU:HA	2.21	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	AAA	252/271 (93%)	239 (95%)	12 (5%)	1 (0%)	30 27
1	BBB	251/271 (93%)	239 (95%)	11 (4%)	1 (0%)	30 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	259/271 (96%)	248 (96%)	10 (4%)	1 (0%)	30	27
1	DDD	251/271 (93%)	238 (95%)	11 (4%)	2 (1%)	16	11
1	EEE	255/271 (94%)	243 (95%)	11 (4%)	1 (0%)	30	27
1	FFF	255/271 (94%)	247 (97%)	7 (3%)	1 (0%)	30	27
1	GGG	251/271 (93%)	237 (94%)	13 (5%)	1 (0%)	30	27
1	HHH	254/271 (94%)	240 (94%)	14 (6%)	0	100	100
1	III	264/271 (97%)	256 (97%)	7 (3%)	1 (0%)	30	27
1	JJJ	263/271 (97%)	248 (94%)	13 (5%)	2 (1%)	16	11
All	All	2555/2710 (94%)	2435 (95%)	109 (4%)	11 (0%)	30	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	JJJ	41	VAL
1	AAA	188	VAL
1	BBB	188	VAL
1	CCC	188	VAL
1	DDD	188	VAL
1	FFF	188	VAL
1	GGG	188	VAL
1	III	188	VAL
1	DDD	35	LEU
1	EEE	188	VAL
1	JJJ	188	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	208/232 (90%)	206 (99%)	2 (1%)	68	75
1	BBB	209/232 (90%)	205 (98%)	4 (2%)	50	56
1	CCC	212/232 (91%)	210 (99%)	2 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DDD	203/232 (88%)	200 (98%)	3 (2%)	57	64
1	EEE	211/232 (91%)	205 (97%)	6 (3%)	38	41
1	FFF	208/232 (90%)	207 (100%)	1 (0%)	81	87
1	GGG	206/232 (89%)	205 (100%)	1 (0%)	81	87
1	HHH	210/232 (90%)	207 (99%)	3 (1%)	59	66
1	III	216/232 (93%)	212 (98%)	4 (2%)	50	56
1	JJJ	217/232 (94%)	214 (99%)	3 (1%)	59	66
All	All	2100/2320 (90%)	2071 (99%)	29 (1%)	59	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	36	GLU
1	AAA	44	ILE
1	BBB	47	VAL
1	BBB	171	LYS
1	BBB	273	SER
1	BBB	294	SER
1	CCC	39	THR
1	CCC	297	ASN
1	DDD	134	LYS
1	DDD	157	GLU
1	DDD	258	SER
1	EEE	39	THR
1	EEE	99	ASN
1	EEE	113	VAL
1	EEE	174	ASP
1	EEE	230	VAL
1	EEE	287	LYS
1	FFF	45	THR
1	GGG	273	SER
1	HHH	171	LYS
1	HHH	287	LYS
1	HHH	293	ARG
1	III	39	THR
1	III	241	THR
1	III	273	SER
1	III	294	SER
1	JJJ	39	THR
1	JJJ	258	SER

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Mol	Chain	Res	Type
1	JJJ	259	LEU

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

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	GOL	III	502	-	5,5,5	0.38	0	5,5,5	0.73	0
3	GOL	III	503	-	5,5,5	0.17	0	5,5,5	0.41	0
3	GOL	FFF	402	-	5,5,5	0.12	0	5,5,5	0.22	0
3	GOL	III	501	-	5,5,5	0.13	0	5,5,5	0.32	0
3	GOL	JJJ	401	-	5,5,5	0.25	0	5,5,5	0.63	0
3	GOL	EEE	401	-	5,5,5	0.15	0	5,5,5	0.39	0
3	GOL	HHH	401	-	5,5,5	0.15	0	5,5,5	0.28	0
3	GOL	BBB	401	-	5,5,5	0.13	0	5,5,5	0.34	0
3	GOL	DDD	401	-	5,5,5	0.16	0	5,5,5	0.31	0
3	GOL	FFF	401	-	5,5,5	0.12	0	5,5,5	0.44	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	GOL	III	502	-	-	1/4/4/4	-
3	GOL	III	503	-	-	3/4/4/4	-
3	GOL	FFF	402	-	-	1/4/4/4	-
3	GOL	III	501	-	-	2/4/4/4	-
3	GOL	JJJ	401	-	-	2/4/4/4	-
3	GOL	EEE	401	-	-	2/4/4/4	-
3	GOL	HHH	401	-	-	2/4/4/4	-
3	GOL	BBB	401	-	-	1/4/4/4	-
3	GOL	DDD	401	-	-	4/4/4/4	-
3	GOL	FFF	401	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	DDD	401	GOL	O1-C1-C2-C3
3	FFF	401	GOL	O1-C1-C2-C3
3	III	503	GOL	O1-C1-C2-C3
3	JJJ	401	GOL	O1-C1-C2-C3
3	DDD	401	GOL	O1-C1-C2-O2
3	FFF	401	GOL	O1-C1-C2-O2
3	III	501	GOL	O2-C2-C3-O3
3	BBB	401	GOL	O1-C1-C2-C3
3	DDD	401	GOL	C1-C2-C3-O3
3	EEE	401	GOL	C1-C2-C3-O3
3	FFF	401	GOL	C1-C2-C3-O3
3	HHH	401	GOL	C1-C2-C3-O3
3	III	501	GOL	C1-C2-C3-O3
3	III	502	GOL	O1-C1-C2-C3
3	EEE	401	GOL	O2-C2-C3-O3
3	III	503	GOL	O1-C1-C2-O2
3	DDD	401	GOL	O2-C2-C3-O3
3	JJJ	401	GOL	O1-C1-C2-O2
3	FFF	401	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	HHH	401	GOL	O2-C2-C3-O3
3	FFF	402	GOL	O1-C1-C2-O2
3	III	503	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	EEE	401	GOL	1	0
3	FFF	401	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	258/271 (95%)	-0.20	3 (1%) 76 76	21, 29, 49, 75	0
1	BBB	256/271 (94%)	-0.15	4 (1%) 70 70	18, 30, 49, 72	1 (0%)
1	CCC	264/271 (97%)	-0.14	6 (2%) 61 60	16, 30, 51, 70	1 (0%)
1	DDD	256/271 (94%)	0.00	3 (1%) 76 76	22, 32, 57, 72	1 (0%)
1	EEE	258/271 (95%)	-0.17	1 (0%) 88 88	16, 31, 50, 69	1 (0%)
1	FFF	258/271 (95%)	-0.30	3 (1%) 76 76	15, 26, 48, 70	1 (0%)
1	GGG	257/271 (94%)	-0.30	2 (0%) 82 82	19, 26, 50, 71	0
1	HHH	257/271 (94%)	-0.26	1 (0%) 88 88	11, 27, 47, 69	1 (0%)
1	III	265/271 (97%)	-0.36	2 (0%) 82 82	18, 26, 40, 68	1 (0%)
1	JJJ	264/271 (97%)	-0.25	3 (1%) 78 77	13, 27, 47, 63	3 (1%)
All	All	2593/2710 (95%)	-0.21	28 (1%) 78 77	11, 28, 50, 75	10 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	43	ALA	3.9
1	CCC	41	VAL	3.5
1	HHH	41	VAL	3.5
1	BBB	106	ASN	3.2
1	CCC	39	THR	3.1
1	AAA	41	VAL	3.1
1	BBB	44	ILE	2.9
1	GGG	40	GLY	2.8
1	DDD	101	ASP	2.7
1	BBB	98	LEU	2.7
1	EEE	32	VAL	2.7
1	GGG	99	ASN	2.6
1	BBB	37	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	99	ASN	2.6
1	DDD	108	LEU	2.6
1	JJJ	41	VAL	2.5
1	CCC	42	ASP	2.5
1	CCC	105	GLY	2.4
1	JJJ	105	GLY	2.4
1	FFF	32	VAL	2.3
1	FFF	41	VAL	2.3
1	III	39	THR	2.3
1	III	41	VAL	2.3
1	CCC	103	THR	2.2
1	JJJ	32	VAL	2.1
1	FFF	39	THR	2.1
1	AAA	39	THR	2.1
1	CCC	106	ASN	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 oligosaccharides 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. 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	GOL	III	502	6/6	0.79	0.18	25,46,48,49	0
3	GOL	III	503	6/6	0.79	0.14	49,57,67,71	0
3	GOL	EEE	401	6/6	0.80	0.15	51,62,62,65	0
3	GOL	III	501	6/6	0.81	0.14	63,69,70,71	0
3	GOL	DDD	401	6/6	0.83	0.14	46,50,54,56	0
3	GOL	JJJ	401	6/6	0.83	0.17	48,57,62,68	0
3	GOL	FFF	401	6/6	0.85	0.15	47,53,63,76	0
3	GOL	HHH	401	6/6	0.87	0.11	42,51,53,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	BBB	401	6/6	0.89	0.11	48,54,58,61	0
3	GOL	FFF	402	6/6	0.90	0.11	51,54,58,58	0
2	CL	DDD	402	1/1	0.91	0.12	47,47,47,47	0
2	CL	EEE	402	1/1	0.92	0.16	47,47,47,47	0
2	CL	III	504	1/1	0.93	0.12	42,42,42,42	0
2	CL	CCC	401	1/1	0.94	0.10	49,49,49,49	0
2	CL	GGG	401	1/1	0.95	0.11	48,48,48,48	0
2	CL	JJJ	402	1/1	0.95	0.09	36,36,36,36	0
2	CL	BBB	402	1/1	0.96	0.09	44,44,44,44	0
2	CL	FFF	403	1/1	0.97	0.05	38,38,38,38	0
2	CL	HHH	402	1/1	0.98	0.04	36,36,36,36	0
2	CL	AAA	401	1/1	0.99	0.08	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.