wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2022 – 04:18 pm BST

PDB ID	:	7B69
Title	:	BK Polyomavirus VP1 pentamer core(residues 26-299) mutant C104S
Authors	:	Osipov, E.M.; Beelen, S.; Strelkov, S.V.
Deposited on	:	2020-12-07
Resolution	:	1.47 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

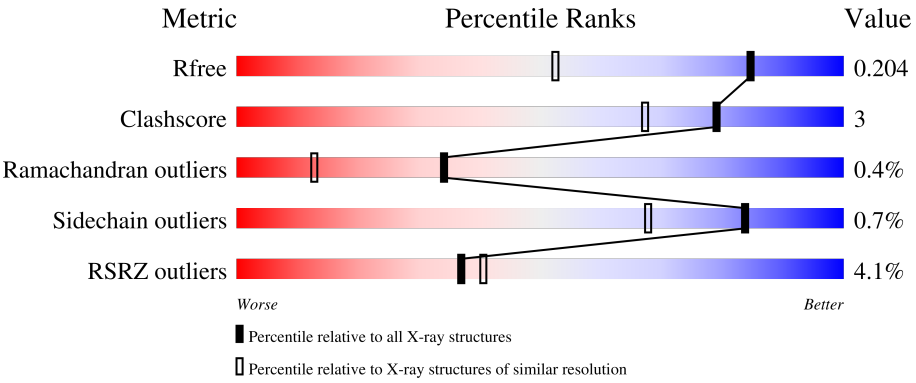
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	275	2% 91% · 5%
1	BBB	275	4% 90% 6% ·
1	CCC	275	2% 91% 7% ·
1	DDD	275	4% 89% 8% ·
1	EEE	275	7% 85% 7% 8%

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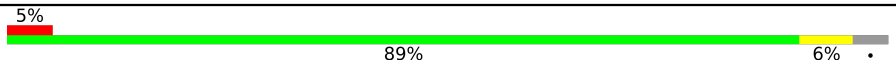
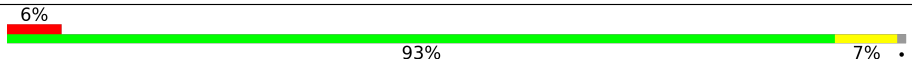
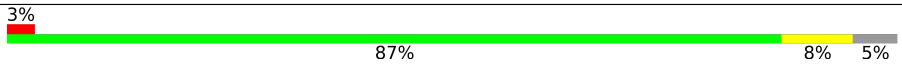
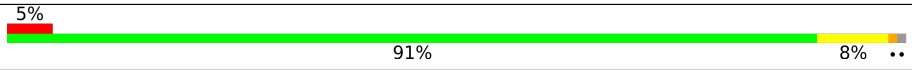
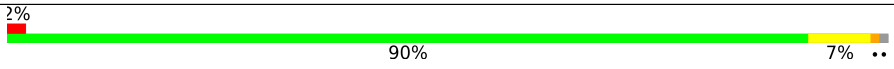
Mol	Chain	Length	Quality of chain
1	FFF	275	
1	GGG	275	
1	HHH	275	
1	III	275	
1	JJJ	275	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22750 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	262	Total	C	N	O	S	0	4	0
			2045	1287	356	390	12			
1	BBB	265	Total	C	N	O	S	0	4	0
			2059	1298	357	391	13			
1	CCC	268	Total	C	N	O	S	0	6	0
			2077	1309	359	396	13			
1	DDD	270	Total	C	N	O	S	0	6	0
			2105	1323	367	401	14			
1	EEE	253	Total	C	N	O	S	0	4	0
			1960	1233	340	373	14			
1	FFF	264	Total	C	N	O	S	0	5	0
			2068	1299	361	395	13			
1	GGG	273	Total	C	N	O	S	0	5	0
			2109	1329	360	406	14			
1	HHH	260	Total	C	N	O	S	0	7	0
			2039	1284	354	387	14			
1	III	273	Total	C	N	O	S	0	3	0
			2105	1324	361	407	13			
1	JJJ	272	Total	C	N	O	S	0	6	0
			2113	1329	367	404	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	25	GLY	-	expression tag	UNP P03088
AAA	104	SER	CYS	engineered mutation	UNP P03088
BBB	25	GLY	-	expression tag	UNP P03088
BBB	104	SER	CYS	engineered mutation	UNP P03088
CCC	25	GLY	-	expression tag	UNP P03088
CCC	104	SER	CYS	engineered mutation	UNP P03088
DDD	25	GLY	-	expression tag	UNP P03088
DDD	104	SER	CYS	engineered mutation	UNP P03088
EEE	25	GLY	-	expression tag	UNP P03088

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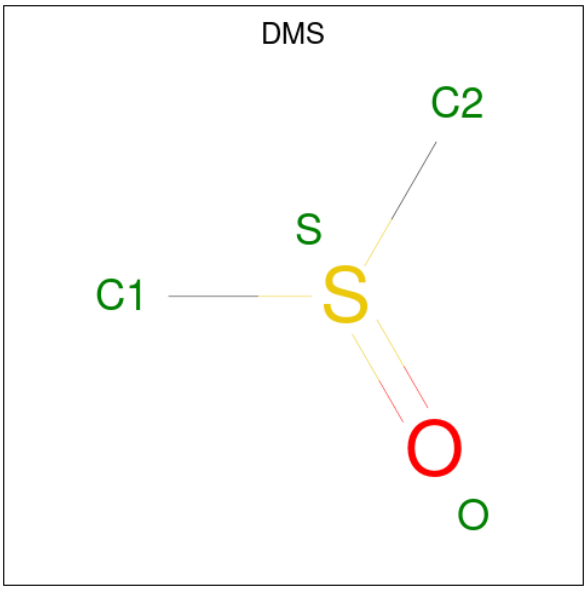
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	104	SER	CYS	engineered mutation	UNP P03088
FFF	25	GLY	-	expression tag	UNP P03088
FFF	104	SER	CYS	engineered mutation	UNP P03088
GGG	25	GLY	-	expression tag	UNP P03088
GGG	104	SER	CYS	engineered mutation	UNP P03088
HHH	25	GLY	-	expression tag	UNP P03088
HHH	104	SER	CYS	engineered mutation	UNP P03088
III	25	GLY	-	expression tag	UNP P03088
III	104	SER	CYS	engineered mutation	UNP P03088
JJJ	25	GLY	-	expression tag	UNP P03088
JJJ	104	SER	CYS	engineered mutation	UNP P03088

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	CCC	1	Total	C	O	S	0	0
			4	2	1	1		
2	DDD	1	Total	C	O	S	0	0
			4	2	1	1		
2	DDD	1	Total	C	O	S	0	0
			4	2	1	1		
2	EEE	1	Total	C	O	S	0	0
			4	2	1	1		
2	EEE	1	Total	C	O	S	0	0
			4	2	1	1		
2	EEE	1	Total	C	O	S	0	0
			4	2	1	1		
2	EEE	1	Total	C	O	S	0	0
			4	2	1	1		
2	FFF	1	Total	C	O	S	0	0
			4	2	1	1		
2	FFF	1	Total	C	O	S	0	0
			4	2	1	1		
2	GGG	1	Total	C	O	S	0	0
			4	2	1	1		
2	GGG	1	Total	C	O	S	0	0
			4	2	1	1		
2	GGG	1	Total	C	O	S	0	0
			4	2	1	1		
2	HHH	1	Total	C	O	S	0	0
			4	2	1	1		
2	HHH	1	Total	C	O	S	0	0
			4	2	1	1		
2	III	1	Total	C	O	S	0	0
			4	2	1	1		
2	III	1	Total	C	O	S	0	0
			4	2	1	1		
2	JJJ	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	183	Total	O	0	0
			183	183		
3	BBB	201	Total	O	0	0
			201	201		

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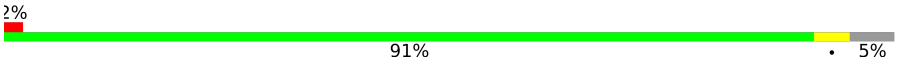
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	CCC	244	Total O 244 244	0	0
3	DDD	204	Total O 204 204	0	0
3	EEE	179	Total O 179 179	0	0
3	FFF	194	Total O 194 194	0	0
3	GGG	184	Total O 184 184	0	0
3	HHH	179	Total O 179 179	0	0
3	III	205	Total O 205 205	0	0
3	JJJ	205	Total O 205 205	0	0

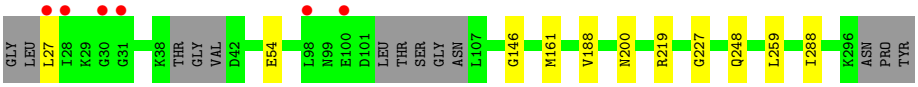
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Major capsid protein VP1

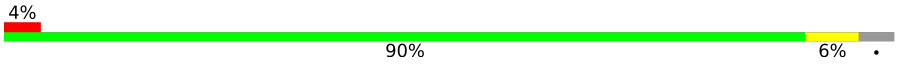
Chain AAA:

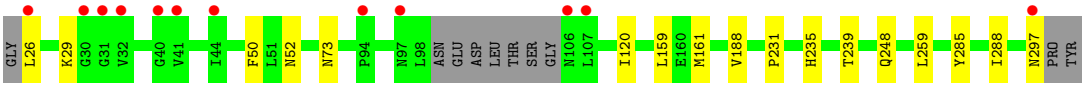




• Molecule 1: Major capsid protein VP1

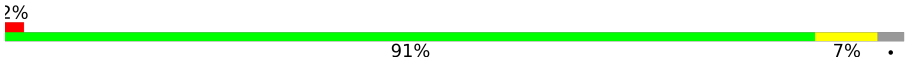
Chain BBB:

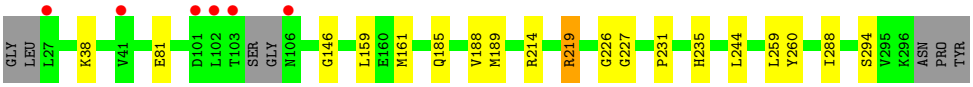




• Molecule 1: Major capsid protein VP1

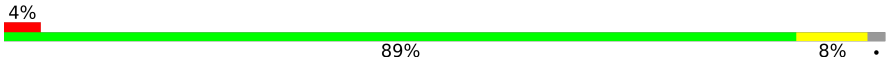
Chain CCC:

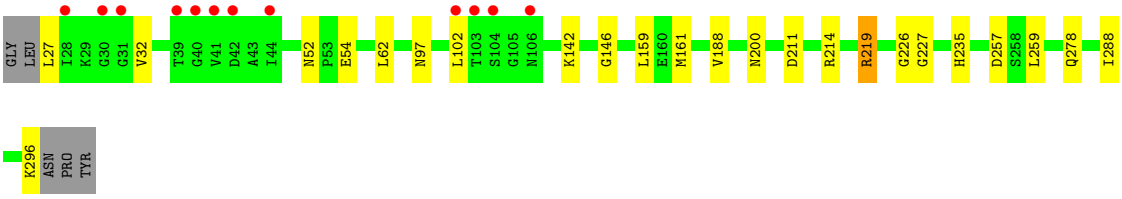




• Molecule 1: Major capsid protein VP1

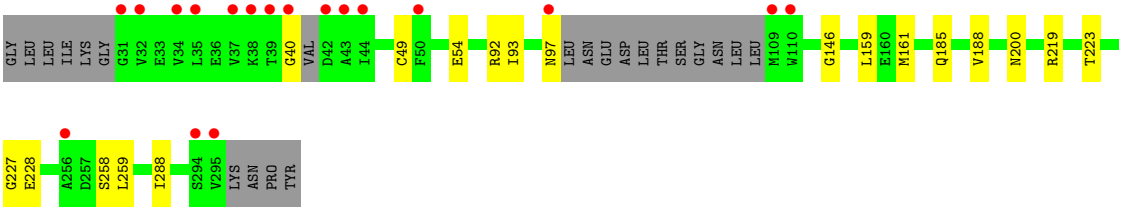
Chain DDD:



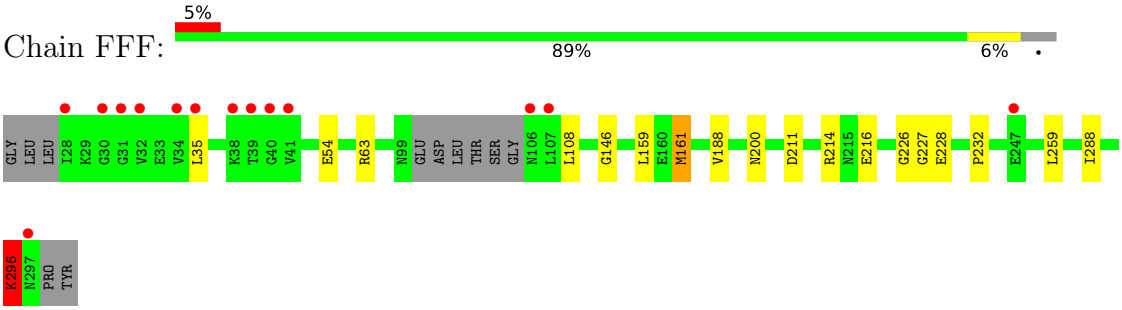


• Molecule 1: Major capsid protein VP1

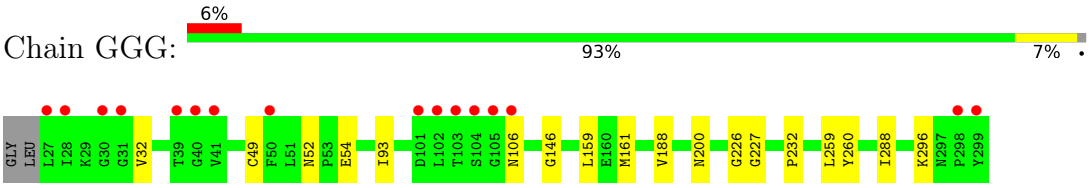
Chain EEE:



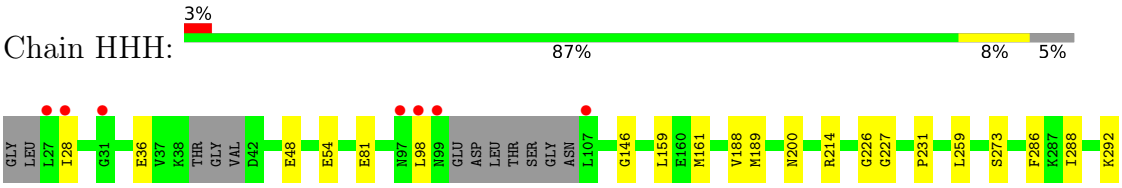
• Molecule 1: Major capsid protein VP1



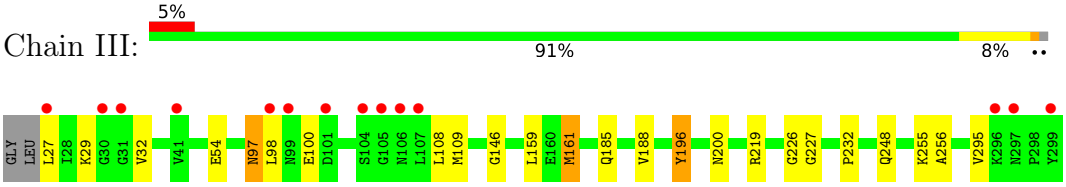
• Molecule 1: Major capsid protein VP1



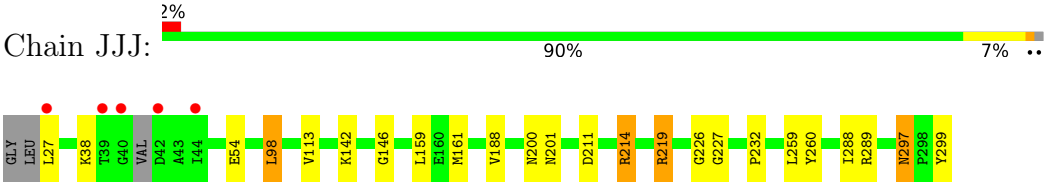
• Molecule 1: Major capsid protein VP1



• Molecule 1: Major capsid protein VP1



• Molecule 1: Major capsid protein VP1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.07Å 135.72Å 156.43Å 90.00° 94.98° 90.00°	Depositor
Resolution (Å)	102.35 – 1.47 102.35 – 1.47	Depositor EDS
% Data completeness (in resolution range)	96.6 (102.35-1.47) 96.6 (102.35-1.47)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.197 0.191 , 0.204	Depositor DCC
R_{free} test set	20576 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22750	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AAA	0.64	0/2099	0.89	5/2848 (0.2%)
1	BBB	0.67	0/2117	0.86	0/2875
1	CCC	0.69	0/2141	0.90	10/2910 (0.3%)
1	DDD	0.68	0/2167	0.87	6/2942 (0.2%)
1	EEE	0.65	0/2017	0.81	1/2738 (0.0%)
1	FFF	0.65	0/2129	0.88	2/2889 (0.1%)
1	GGG	0.66	0/2171	0.82	0/2955
1	HHH	0.63	0/2104	0.85	4/2855 (0.1%)
1	III	0.70	0/2160	0.93	5/2937 (0.2%)
1	JJJ	0.66	0/2180	0.93	8/2961 (0.3%)
All	All	0.66	0/21285	0.88	41/28910 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BBB	0	1
1	FFF	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	III	161	MET	CG-SD-CE	-14.23	77.43	100.20
1	FFF	161	MET	CG-SD-CE	-13.51	78.58	100.20
1	AAA	161	MET	CG-SD-CE	-13.48	78.63	100.20
1	JJJ	214[A]	ARG	NE-CZ-NH1	-11.38	114.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	JJJ	214[B]	ARG	NE-CZ-NH1	-11.38	114.61	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	73	ASN	Sidechain
1	FFF	296	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2045	0	1995	4	0
1	BBB	2059	0	2019	10	0
1	CCC	2077	0	2026	16	0
1	DDD	2105	0	2062	18	0
1	EEE	1960	0	1906	10	0
1	FFF	2068	0	2029	12	0
1	GGG	2109	0	2033	11	0
1	HHH	2039	0	1994	12	0
1	III	2105	0	2030	17	0
1	JJJ	2113	0	2054	20	0
2	AAA	8	0	12	0	0
2	BBB	8	0	12	0	0
2	CCC	12	0	18	1	0
2	DDD	8	0	12	0	0
2	EEE	16	0	24	0	0
2	FFF	8	0	12	0	0
2	GGG	12	0	18	0	0
2	HHH	8	0	12	0	0
2	III	8	0	12	0	0
2	JJJ	4	0	6	0	0
3	AAA	183	0	0	0	0
3	BBB	201	0	0	2	1
3	CCC	244	0	0	5	0
3	DDD	204	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	EEE	179	0	0	1	0
3	FFF	194	0	0	2	0
3	GGG	184	0	0	1	0
3	HHH	179	0	0	3	0
3	III	205	0	0	4	0
3	JJJ	205	0	0	3	0
All	All	22750	0	20286	116	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 116 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:III:109:MET:CE	1:III:255:LYS:HA	2.04	0.87
1:FFF:211:ASP:OD2	1:FFF:214[B]:ARG:HD3	1.73	0.87
1:JJJ:211:ASP:OD2	1:JJJ:214[A]:ARG:HD3	1.75	0.85
1:DDD:211:ASP:OD2	1:DDD:214[B]:ARG:HD3	1.76	0.84
1:CCC:81:GLU:OE1	3:CCC:403:HOH:O	2.00	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BBB:402:HOH:O	3:DDD:487:HOH:O[2_446]	2.06	0.14

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	260/275 (94%)	249 (96%)	10 (4%)	1 (0%)	34 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	265/275 (96%)	254 (96%)	10 (4%)	1 (0%)	34	13
1	CCC	270/275 (98%)	260 (96%)	9 (3%)	1 (0%)	34	13
1	DDD	274/275 (100%)	263 (96%)	10 (4%)	1 (0%)	34	13
1	EEE	251/275 (91%)	241 (96%)	9 (4%)	1 (0%)	34	13
1	FFF	265/275 (96%)	254 (96%)	10 (4%)	1 (0%)	34	13
1	GGG	276/275 (100%)	267 (97%)	8 (3%)	1 (0%)	34	13
1	HHH	261/275 (95%)	251 (96%)	9 (3%)	1 (0%)	34	13
1	III	274/275 (100%)	262 (96%)	11 (4%)	1 (0%)	34	13
1	JJJ	274/275 (100%)	263 (96%)	10 (4%)	1 (0%)	34	13
All	All	2670/2750 (97%)	2564 (96%)	96 (4%)	10 (0%)	34	13

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	188	VAL
1	BBB	188	VAL
1	CCC	188	VAL
1	DDD	188	VAL
1	EEE	188	VAL

5.3.2 Protein sidechains (i)

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	225/235 (96%)	224 (100%)	1 (0%)	91	81
1	BBB	227/235 (97%)	225 (99%)	2 (1%)	78	59
1	CCC	228/235 (97%)	228 (100%)	0	100	100
1	DDD	232/235 (99%)	231 (100%)	1 (0%)	91	81
1	EEE	216/235 (92%)	215 (100%)	1 (0%)	88	77
1	FFF	230/235 (98%)	229 (100%)	1 (0%)	91	81
1	GGG	231/235 (98%)	230 (100%)	1 (0%)	91	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	HHH	225/235 (96%)	223 (99%)	2 (1%)	78 59
1	III	229/235 (97%)	226 (99%)	3 (1%)	69 42
1	JJJ	232/235 (99%)	228 (98%)	4 (2%)	60 31
All	All	2275/2350 (97%)	2259 (99%)	16 (1%)	84 68

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	JJJ	98	LEU
1	JJJ	38	LYS
1	HHH	273	SER
1	JJJ	27	LEU
1	HHH	28	ILE

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

23 ligands 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	$\#\|Z\| > 2$
2	DMS	GGG	303	-	3,3,3	0.26	0	3,3,3	0.04	0
2	DMS	AAA	301	-	3,3,3	0.60	0	3,3,3	1.17	0
2	DMS	EEE	301	-	3,3,3	0.49	0	3,3,3	1.09	0
2	DMS	DDD	302	-	3,3,3	0.34	0	3,3,3	0.19	0
2	DMS	HHH	302	-	3,3,3	0.40	0	3,3,3	0.17	0
2	DMS	EEE	303	-	3,3,3	0.46	0	3,3,3	0.31	0
2	DMS	CCC	303	-	3,3,3	0.54	0	3,3,3	0.19	0
2	DMS	EEE	302	-	3,3,3	0.44	0	3,3,3	0.29	0
2	DMS	CCC	301	-	3,3,3	0.66	0	3,3,3	1.47	1 (33%)
2	DMS	GGG	302	-	3,3,3	0.44	0	3,3,3	0.26	0
2	DMS	EEE	304	-	3,3,3	0.34	0	3,3,3	0.23	0
2	DMS	JJJ	301	-	3,3,3	0.45	0	3,3,3	1.01	0
2	DMS	FFF	301	-	3,3,3	0.42	0	3,3,3	0.96	0
2	DMS	CCC	302	-	3,3,3	0.38	0	3,3,3	0.40	0
2	DMS	HHH	301	-	3,3,3	0.39	0	3,3,3	1.11	0
2	DMS	III	301	-	3,3,3	0.52	0	3,3,3	0.88	0
2	DMS	DDD	301	-	3,3,3	0.43	0	3,3,3	1.00	0
2	DMS	III	302	-	3,3,3	0.42	0	3,3,3	0.41	0
2	DMS	BBB	301	-	3,3,3	0.64	0	3,3,3	1.15	0
2	DMS	FFF	302	-	3,3,3	0.28	0	3,3,3	0.12	0
2	DMS	BBB	302	-	3,3,3	0.39	0	3,3,3	0.35	0
2	DMS	GGG	301	-	3,3,3	0.34	0	3,3,3	0.84	0
2	DMS	AAA	302	-	3,3,3	0.32	0	3,3,3	0.19	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CCC	301	DMS	O-S-C1	-2.53	93.64	106.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	303	DMS	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, 95^{th} 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	262/275 (95%)	0.01	6 (2%) 60 65	12, 19, 44, 63	0
1	BBB	265/275 (96%)	0.04	12 (4%) 33 36	12, 17, 44, 77	0
1	CCC	268/275 (97%)	-0.08	6 (2%) 62 66	11, 16, 33, 85	0
1	DDD	270/275 (98%)	0.03	12 (4%) 34 37	13, 19, 40, 70	0
1	EEE	253/275 (92%)	0.23	18 (7%) 16 17	14, 20, 71, 95	0
1	FFF	264/275 (96%)	0.15	14 (5%) 26 29	14, 20, 47, 67	0
1	GGG	273/275 (99%)	0.09	16 (5%) 22 24	13, 19, 45, 76	0
1	HHH	260/275 (94%)	0.00	7 (2%) 54 58	13, 19, 48, 71	0
1	III	273/275 (99%)	0.06	14 (5%) 28 30	13, 19, 42, 66	0
1	JJJ	272/275 (98%)	-0.05	5 (1%) 68 72	14, 20, 36, 79	0
All	All	2660/2750 (96%)	0.05	110 (4%) 37 40	11, 19, 45, 95	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	102	LEU	10.5
1	BBB	30	GLY	8.2
1	BBB	31	GLY	7.9
1	BBB	41	VAL	7.6
1	FFF	41	VAL	6.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
2	DMS	GGG	302	4/4	0.85	0.16	32,42,43,43	0
2	DMS	FFF	302	4/4	0.87	0.18	31,38,38,39	0
2	DMS	GGG	303	4/4	0.88	0.19	37,40,48,49	0
2	DMS	III	302	4/4	0.89	0.17	31,32,37,38	0
2	DMS	GGG	301	4/4	0.90	0.13	24,27,29,30	0
2	DMS	HHH	301	4/4	0.90	0.12	24,26,31,32	0
2	DMS	CCC	301	4/4	0.90	0.14	23,23,29,30	0
2	DMS	AAA	301	4/4	0.91	0.12	24,27,30,30	0
2	DMS	BBB	301	4/4	0.92	0.14	19,22,24,25	0
2	DMS	DDD	302	4/4	0.92	0.14	34,34,36,37	0
2	DMS	HHH	302	4/4	0.93	0.11	33,35,37,38	0
2	DMS	EEE	301	4/4	0.93	0.11	24,25,30,30	0
2	DMS	BBB	302	4/4	0.94	0.12	25,28,30,31	0
2	DMS	CCC	303	4/4	0.94	0.12	30,35,36,36	0
2	DMS	DDD	301	4/4	0.94	0.11	25,27,28,28	0
2	DMS	EEE	304	4/4	0.95	0.11	37,37,42,42	0
2	DMS	FFF	301	4/4	0.95	0.10	25,26,29,30	0
2	DMS	III	301	4/4	0.95	0.09	24,27,28,30	0
2	DMS	AAA	302	4/4	0.95	0.12	36,36,36,39	0
2	DMS	EEE	302	4/4	0.96	0.13	31,32,32,35	0
2	DMS	EEE	303	4/4	0.96	0.12	25,32,32,33	0
2	DMS	CCC	302	4/4	0.96	0.12	24,25,26,27	0
2	DMS	JJJ	301	4/4	0.96	0.08	22,24,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.