



wwPDB X-ray Structure Validation Summary Report

Feb 16, 2023 – 12:16 pm GMT

PDB ID : 8AH0
Title : BK Polyomavirus VP1 mutant VQQ
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 : 1.80 Å(reported)

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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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

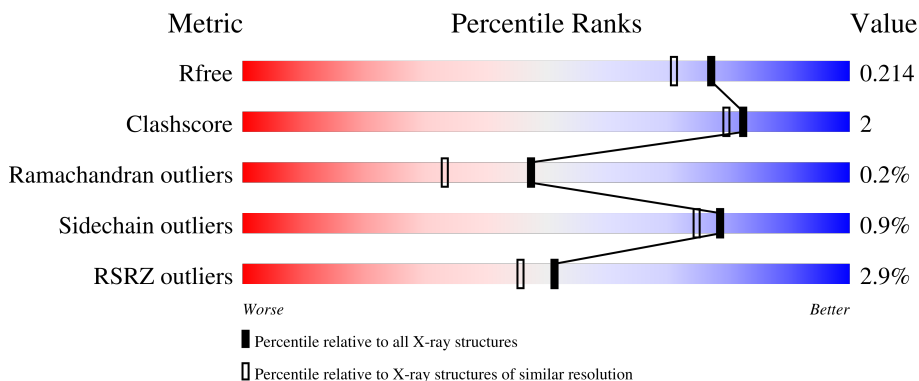
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	 2% 86% 9% .
1	BBB	271	 3% 90% 6%
1	CCC	271	 5% 87% 6% 7%
1	DDD	271	 3% 92% 6% .
1	EEE	271	 2% 86% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10626 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
			Total	C	N	O	S			
1	AAA	260	1989	1252	345	380	12	0	2	0
1	BBB	255	1956	1233	340	370	13	0	2	0
1	CCC	252	1920	1213	332	362	13	0	2	0
1	DDD	266	2012	1266	349	384	13	0	2	0
1	EEE	262	2030	1279	352	386	13	0	5	0

There are 20 discrepancies between the modelled and reference sequences:

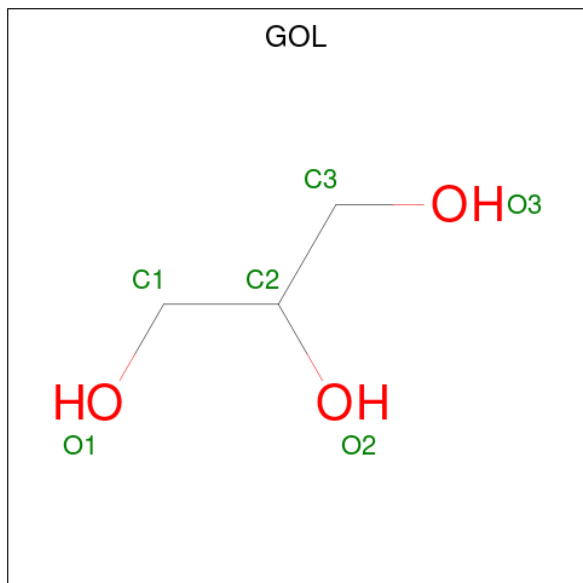
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	71	VAL	ALA	engineered mutation	UNP P03088
AAA	72	GLN	GLU	engineered mutation	UNP P03088
AAA	81	GLN	GLU	engineered mutation	UNP P03088
AAA	104	SER	CYS	engineered mutation	UNP P03088
BBB	71	VAL	ALA	engineered mutation	UNP P03088
BBB	72	GLN	GLU	engineered mutation	UNP P03088
BBB	81	GLN	GLU	engineered mutation	UNP P03088
BBB	104	SER	CYS	engineered mutation	UNP P03088
CCC	71	VAL	ALA	engineered mutation	UNP P03088
CCC	72	GLN	GLU	engineered mutation	UNP P03088
CCC	81	GLN	GLU	engineered mutation	UNP P03088
CCC	104	SER	CYS	engineered mutation	UNP P03088
DDD	71	VAL	ALA	engineered mutation	UNP P03088
DDD	72	GLN	GLU	engineered mutation	UNP P03088
DDD	81	GLN	GLU	engineered mutation	UNP P03088
DDD	104	SER	CYS	engineered mutation	UNP P03088
EEE	71	VAL	ALA	engineered mutation	UNP P03088
EEE	72	GLN	GLU	engineered mutation	UNP P03088
EEE	81	GLN	GLU	engineered mutation	UNP P03088

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	104	SER	CYS	engineered mutation	UNP P03088

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			6	3	3		
2	AAA	1	Total	C	O	0	0
			6	3	3		
2	BBB	1	Total	C	O	0	0
			6	3	3		
2	CCC	1	Total	C	O	0	0
			6	3	3		
2	CCC	1	Total	C	O	0	0
			6	3	3		
2	DDD	1	Total	C	O	0	0
			6	3	3		
2	DDD	1	Total	C	O	0	0
			6	3	3		
2	EEE	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	1	Total 1	Cl 1	0	0
3	CCC	1	Total 1	Cl 1	0	0
3	DDD	1	Total 1	Cl 1	0	0
3	EEE	1	Total 1	Cl 1	0	0

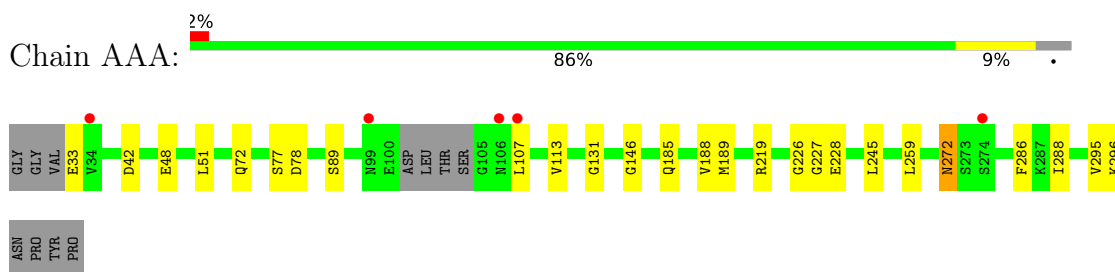
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	131	Total 131	O 131	0	0
4	BBB	127	Total 127	O 127	0	0
4	CCC	123	Total 123	O 123	0	0
4	DDD	132	Total 132	O 132	0	0
4	EEE	153	Total 153	O 153	0	0

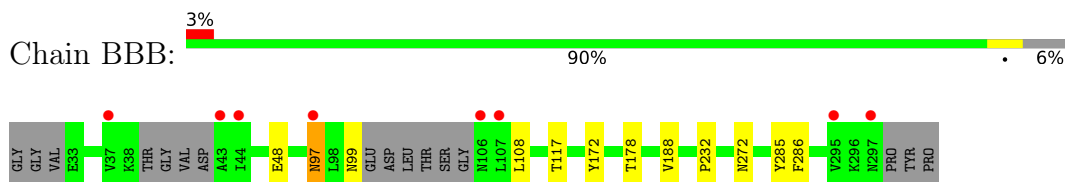
3 Residue-property plots [i](#)

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.

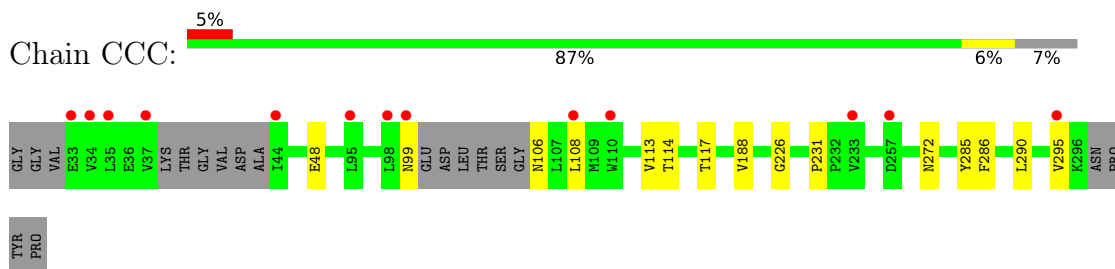
- Molecule 1: Major capsid protein VP1



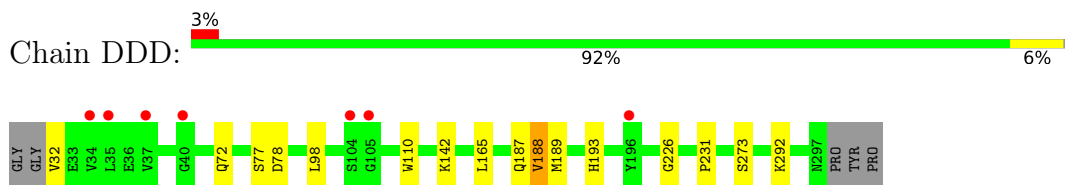
- Molecule 1: Major capsid protein VP1



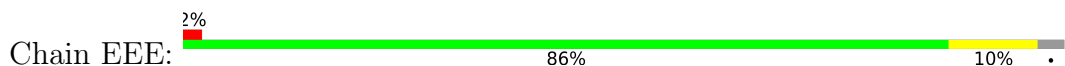
- Molecule 1: Major capsid protein VP1

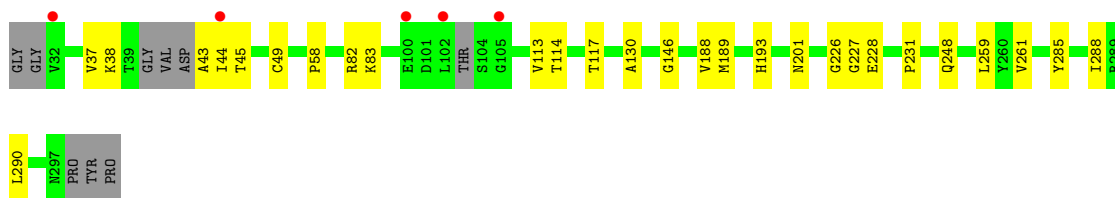


- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.69Å 152.60Å 62.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 1.80 48.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.46-1.80) 99.9 (48.46-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.210 0.180 , 0.214	Depositor DCC
R_{free} test set	6484 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10626	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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	0.72	0/2037	0.89	1/2772 (0.0%)
1	BBB	0.73	0/2003	0.89	0/2725
1	CCC	0.70	0/1970	0.87	0/2682
1	DDD	0.73	0/2064	0.91	0/2814
1	EEE	0.74	0/2086	0.87	0/2835
All	All	0.73	0/10160	0.89	1/13828 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	219	ARG	NE-CZ-NH1	5.34	122.97	120.30

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	AAA	1989	0	1914	14	0
1	BBB	1956	0	1880	6	0
1	CCC	1920	0	1826	7	0
1	DDD	2012	0	1920	10	0
1	EEE	2030	0	1965	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	12	0	16	0	0
2	BBB	6	0	8	0	0
2	CCC	12	0	16	0	0
2	DDD	12	0	16	0	0
2	EEE	6	0	8	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	1	0
3	EEE	1	0	0	1	0
4	AAA	131	0	0	2	0
4	BBB	127	0	0	0	0
4	CCC	123	0	0	0	0
4	DDD	132	0	0	1	0
4	EEE	153	0	0	0	0
All	All	10626	0	9569	48	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.

The worst 5 of 48 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:DDD:98:LEU:HD22	1:DDD:292:LYS:HD2	1.79	0.65
1:EEE:37:VAL:HG12	1:EEE:38:LYS:O	2.00	0.61
1:AAA:259:LEU:HD21	1:AAA:288:ILE:HD13	1.82	0.60
1:BBB:99:ASN:HD21	1:BBB:108:LEU:H	1.48	0.59
1:AAA:78:ASP:CG	1:EEE:130:ALA:HB2	2.26	0.56

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	258/271 (95%)	248 (96%)	10 (4%)	0	100	100
1	BBB	251/271 (93%)	242 (96%)	8 (3%)	1 (0%)	34	21
1	CCC	248/271 (92%)	238 (96%)	9 (4%)	1 (0%)	34	21
1	DDD	266/271 (98%)	258 (97%)	7 (3%)	1 (0%)	34	21
1	EEE	261/271 (96%)	252 (97%)	9 (3%)	0	100	100
All	All	1284/1355 (95%)	1238 (96%)	43 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	188	VAL
1	CCC	188	VAL
1	DDD	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	215/233 (92%)	213 (99%)	2 (1%)	78	75
1	BBB	211/233 (91%)	209 (99%)	2 (1%)	78	75
1	CCC	203/233 (87%)	201 (99%)	2 (1%)	76	71
1	DDD	215/233 (92%)	213 (99%)	2 (1%)	78	75
1	EEE	221/233 (95%)	220 (100%)	1 (0%)	88	87
All	All	1065/1165 (91%)	1056 (99%)	9 (1%)	78	78

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	273	SER
1	EEE	248	GLN
1	BBB	272	ASN
1	CCC	272	ASN
1	CCC	290	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
2	GOL	AAA	602	-	5,5,5	0.11	0	5,5,5	0.24	0
2	GOL	CCC	602	-	5,5,5	0.09	0	5,5,5	0.25	0
2	GOL	DDD	401	-	5,5,5	0.16	0	5,5,5	0.30	0
2	GOL	CCC	601	-	5,5,5	0.15	0	5,5,5	0.49	0
2	GOL	DDD	402	-	5,5,5	0.22	0	5,5,5	0.41	0
2	GOL	EEE	401	-	5,5,5	0.11	0	5,5,5	0.50	0
2	GOL	AAA	601	-	5,5,5	0.19	0	5,5,5	0.36	0
2	GOL	BBB	401	-	5,5,5	0.16	0	5,5,5	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
2	GOL	AAA	602	-	-	0/4/4/4	-
2	GOL	CCC	602	-	-	0/4/4/4	-
2	GOL	DDD	401	-	-	0/4/4/4	-
2	GOL	CCC	601	-	-	2/4/4/4	-
2	GOL	DDD	402	-	-	2/4/4/4	-
2	GOL	EEE	401	-	-	2/4/4/4	-
2	GOL	AAA	601	-	-	2/4/4/4	-
2	GOL	BBB	401	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	GOL	C1-C2-C3-O3
2	BBB	401	GOL	O1-C1-C2-C3
2	CCC	601	GOL	O1-C1-C2-C3
2	DDD	402	GOL	O1-C1-C2-C3
2	EEE	401	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	260/271 (95%)	-0.13	5 (1%) 66 63	17, 26, 48, 65	0
1	BBB	255/271 (94%)	-0.07	8 (3%) 49 43	18, 27, 48, 74	0
1	CCC	252/271 (92%)	0.16	13 (5%) 27 22	19, 29, 55, 80	0
1	DDD	266/271 (98%)	0.00	7 (2%) 56 51	16, 26, 49, 69	0
1	EEE	262/271 (96%)	-0.08	5 (1%) 66 63	16, 24, 46, 76	0
All	All	1295/1355 (95%)	-0.03	38 (2%) 51 46	16, 27, 50, 80	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	98	LEU	4.9
1	CCC	37	VAL	4.5
1	CCC	108	LEU	4.1
1	CCC	44	ILE	4.1
1	EEE	102	LEU	4.0

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 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, 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
2	GOL	BBB	401	6/6	0.77	0.20	44,52,61,62	0
2	GOL	AAA	601	6/6	0.78	0.17	38,53,58,62	0
2	GOL	EEE	401	6/6	0.78	0.21	37,57,63,63	0
2	GOL	DDD	402	6/6	0.82	0.16	34,50,53,55	0
2	GOL	CCC	601	6/6	0.85	0.16	48,53,58,59	0
2	GOL	CCC	602	6/6	0.91	0.12	38,42,44,46	0
2	GOL	AAA	602	6/6	0.92	0.14	38,42,43,44	0
2	GOL	DDD	401	6/6	0.93	0.10	37,43,49,50	0
3	CL	CCC	603	1/1	0.94	0.12	49,49,49,49	0
3	CL	DDD	403	1/1	0.95	0.05	41,41,41,41	0
3	CL	AAA	603	1/1	0.97	0.04	37,37,37,37	0
3	CL	EEE	402	1/1	0.97	0.11	41,41,41,41	0
3	CL	BBB	402	1/1	0.98	0.09	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.