



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:55 PM UTC

PDB ID : 7B6A / pdb_00007b6a
Title : BK Polyomavirus VP1 pentamer core (residues 30-299)
Authors : Osipov, E.M.; Munawar, A.; Beelen, S.; Strelkov, S.V.
Deposited on : 2020-12-07
Resolution : 1.44 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

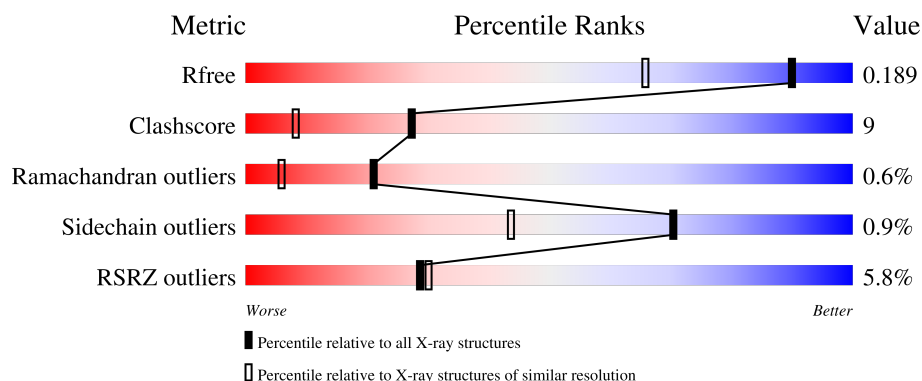
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	270	7% 80% 16% ..
1	BBB	270	3% 87% 9% .
1	CCC	270	7% 86% 10% .
1	DDD	270	5% 84% 13% ..
1	EEE	270	7% 89% 10% .

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
4	IOD	CCC	307	-	-	X	-
4	IOD	CCC	308	-	-	X	-
4	IOD	DDD	308	-	-	X	-
5	NA	AAA	311	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11960 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	265	Total	C	N	O	S	0	13	0
			2106	1333	358	397	18			
1	BBB	261	Total	C	N	O	S	0	5	0
			2031	1279	353	385	14			
1	CCC	261	Total	C	N	O	S	0	6	0
			2061	1302	358	388	13			
1	DDD	265	Total	C	N	O	S	0	8	0
			2080	1312	356	398	14			
1	EEE	266	Total	C	N	O	S	0	5	0
			2080	1306	359	402	13			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	5	Total	Ca	0	0
			5	5		
2	BBB	2	Total	Ca	0	0
			2	2		
2	CCC	2	Total	Ca	0	0
			2	2		
2	DDD	3	Total	Ca	0	0
			3	3		
2	EEE	1	Total	Ca	0	0
			1	1		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	3	Total I 3 3	0	0
4	BBB	2	Total I 2 2	0	0
4	CCC	5	Total I 5 5	0	0
4	DDD	3	Total I 3 3	0	0
4	EEE	3	Total I 3 3	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Na 1 1	0	0
5	DDD	1	Total Na 1 1	0	0

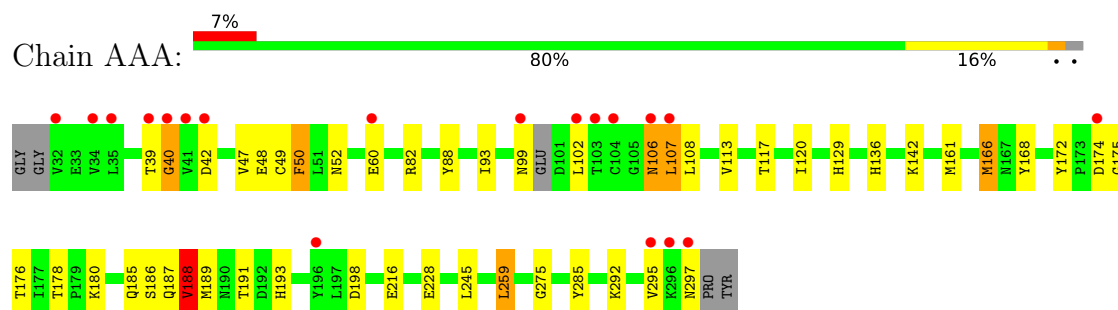
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	305	Total O 305 305	0	0
6	BBB	309	Total O 309 309	0	0
6	CCC	285	Total O 285 285	0	0
6	DDD	307	Total O 307 307	0	0
6	EEE	317	Total O 317 317	0	0

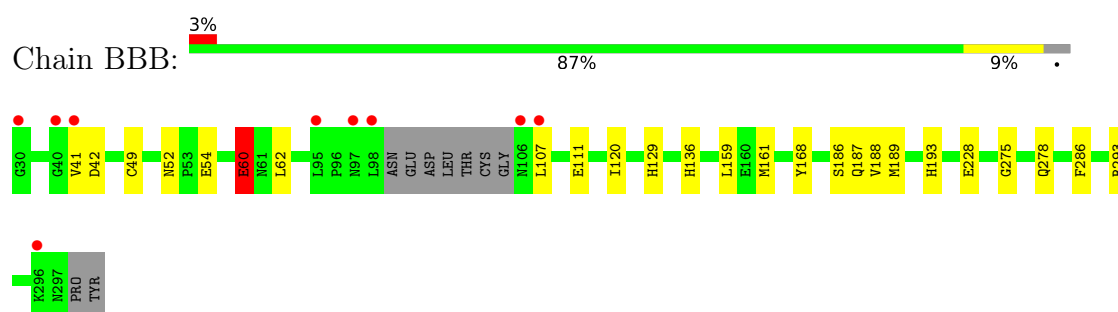
3 Residue-property plots [i](#)

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.

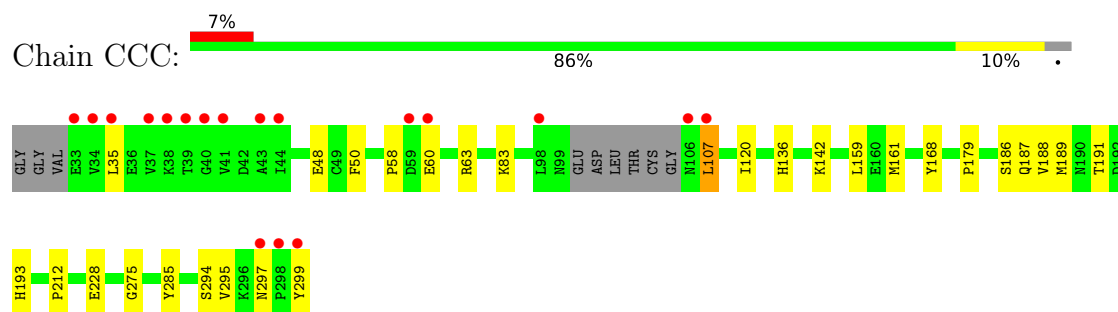
- Molecule 1: Major capsid protein VP1



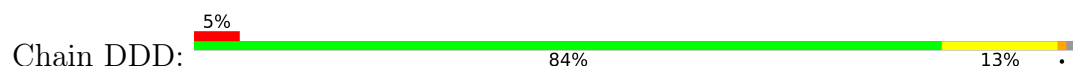
- Molecule 1: Major capsid protein VP1

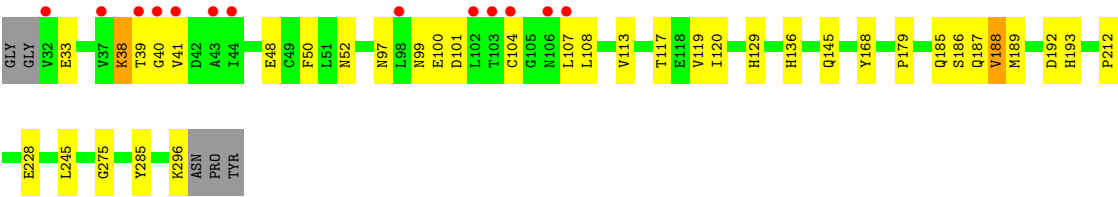


- Molecule 1: Major capsid protein VP1

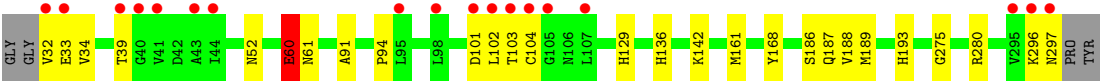
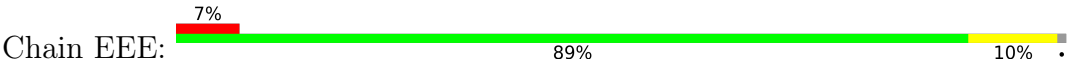


- Molecule 1: Major capsid protein VP1





- 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	138.62Å 149.72Å 65.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.44 50.00 – 1.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.44) 100.0 (50.00-1.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.162 , 0.186 0.168 , 0.189	Depositor DCC
R_{free} test set	4820 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11960	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, IOD, 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	1.05	2/2189 (0.1%)	1.11	1/2971 (0.0%)
1	BBB	1.01	1/2092 (0.0%)	1.11	2/2841 (0.1%)
1	CCC	1.03	0/2128	1.10	1/2888 (0.0%)
1	DDD	1.00	0/2156	1.12	2/2930 (0.1%)
1	EEE	1.00	1/2139 (0.0%)	1.12	2/2910 (0.1%)
All	All	1.02	4/10704 (0.0%)	1.11	8/14540 (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	AAA	0	2
1	BBB	0	1
1	DDD	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	94	PRO	CA-C	6.23	1.59	1.52
1	AAA	50[A]	PHE	C-O	5.70	1.31	1.23
1	AAA	50[B]	PHE	C-O	5.70	1.31	1.23
1	BBB	60	GLU	CD-OE2	5.22	1.35	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	161	MET	CG-SD-CE	-10.38	78.06	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	60	GLU	CB-CG-CD	9.03	127.94	112.60
1	EEE	60	GLU	CB-CG-CD	8.07	126.31	112.60
1	DDD	38	LYS	CA-C-N	6.28	133.54	121.54
1	DDD	38	LYS	C-N-CA	6.28	133.54	121.54
1	BBB	228	GLU	CB-CA-C	-6.04	100.77	110.79
1	CCC	228	GLU	CB-CA-C	-5.66	101.40	110.79
1	AAA	259	LEU	N-CA-CB	-5.49	102.07	110.85

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	174[B]	ASP	Mainchain
1	AAA	188	VAL	Mainchain
1	BBB	60	GLU	Mainchain
1	DDD	38	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	2106	0	2087	79	0
1	BBB	2031	0	1991	25	0
1	CCC	2061	0	2026	39	1
1	DDD	2080	0	2035	42	0
1	EEE	2080	0	2025	33	0
2	AAA	5	0	0	0	0
2	BBB	2	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	3	0	0	0	0
2	EEE	1	0	0	0	0
3	AAA	8	0	12	0	0
3	BBB	8	0	12	3	0
3	CCC	12	0	18	0	0
3	DDD	12	0	18	1	0
3	EEE	8	0	12	0	0
4	AAA	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	2	0	0	2	0
4	CCC	5	0	0	6	0
4	DDD	3	0	0	5	0
4	EEE	3	0	0	2	0
5	AAA	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	305	0	0	13	1
6	BBB	309	0	0	4	0
6	CCC	285	0	0	5	2
6	DDD	307	0	0	5	1
6	EEE	317	0	0	10	0
All	All	11960	0	10236	189	3

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 9.

All (189) 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:CCC:50[B]:PHE:CD2	1:CCC:120[B]:ILE:CD1	2.35	1.09
1:AAA:189[B]:MET:HA	1:AAA:189[B]:MET:HE2	1.36	1.05
1:AAA:60:GLU:HG3	6:AAA:667:HOH:O	1.55	1.02
1:AAA:50[B]:PHE:CD2	1:AAA:120:ILE:CD1	2.44	1.00
1:AAA:50[B]:PHE:HD2	1:AAA:120:ILE:CD1	1.74	1.00
1:CCC:50[B]:PHE:HD2	1:CCC:120[B]:ILE:CD1	1.69	1.00
1:DDD:50[B]:PHE:CE2	1:EEE:189:MET:HE2	1.98	0.99
1:AAA:185:GLN:NE2	1:EEE:33:GLU:OE2	1.94	0.98
1:CCC:50[B]:PHE:CD2	1:CCC:120[B]:ILE:HD11	1.97	0.98
1:EEE:168:TYR:H	1:EEE:187:GLN:HE21	1.16	0.91
1:AAA:50[B]:PHE:CD2	1:AAA:120:ILE:HD11	2.03	0.90
1:BBB:168:TYR:H	1:BBB:187:GLN:HE21	1.19	0.89
1:CCC:168:TYR:H	1:CCC:187:GLN:HE21	1.17	0.89
1:AAA:168:TYR:H	1:AAA:187:GLN:HE21	1.20	0.88
1:AAA:99:ASN:HD21	1:AAA:108:LEU:H	1.21	0.87
1:DDD:50[B]:PHE:CZ	1:EEE:189:MET:HE2	2.09	0.87
1:DDD:168:TYR:H	1:DDD:187:GLN:HE21	1.17	0.86
1:CCC:50[B]:PHE:CE2	1:CCC:120[B]:ILE:CD1	2.59	0.86
1:CCC:50[B]:PHE:CE2	1:CCC:120[B]:ILE:HD13	2.12	0.85
1:DDD:99:ASN:HD21	1:DDD:108:LEU:H	1.23	0.85
1:CCC:142:LYS:HE3	1:DDD:228:GLU:OE1	1.77	0.85
1:DDD:145:GLN:OE1	6:DDD:401:HOH:O	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:50[B]:PHE:CD2	1:CCC:120[B]:ILE:HD13	2.13	0.81
1:AAA:82[B]:ARG:HH11	1:AAA:176:THR:HG22	1.47	0.79
4:CCC:308:IOD:I	6:CCC:652:HOH:O	2.69	0.79
1:AAA:50[B]:PHE:CD2	1:AAA:120:ILE:HD13	2.18	0.78
1:AAA:186:SER:OG	1:AAA:193:HIS:HE1	1.65	0.78
1:CCC:136:HIS:HD2	6:CCC:634:HOH:O	1.66	0.78
1:AAA:50[B]:PHE:CE2	1:AAA:120:ILE:HD13	2.19	0.77
1:AAA:166[A]:MET:HE3	6:EEE:533:HOH:O	1.86	0.76
1:AAA:189[B]:MET:HA	1:AAA:189[B]:MET:CE	2.14	0.75
1:AAA:50[B]:PHE:CE2	1:AAA:120:ILE:CD1	2.70	0.75
1:BBB:186:SER:OG	1:BBB:193:HIS:HE1	1.69	0.74
1:AAA:185:GLN:HG3	6:EEE:620:HOH:O	1.86	0.74
1:AAA:185:GLN:NE2	1:EEE:33:GLU:CD	2.46	0.73
1:BBB:136:HIS:HD2	6:BBB:657:HOH:O	1.70	0.73
1:AAA:275:GLY:O	1:EEE:136:HIS:HE1	1.72	0.72
1:CCC:50[B]:PHE:CE2	1:CCC:120[B]:ILE:HD11	2.23	0.72
1:EEE:186:SER:OG	1:EEE:193:HIS:HE1	1.72	0.72
1:AAA:60:GLU:HG3	6:AAA:408:HOH:O	1.90	0.71
1:DDD:186:SER:OG	1:DDD:193:HIS:HE1	1.73	0.71
1:AAA:136:HIS:HE1	1:BBB:275:GLY:O	1.74	0.71
1:AAA:102:LEU:HD21	1:AAA:107[B]:LEU:HD21	1.72	0.71
1:CCC:63[B]:ARG:NH2	1:DDD:185:GLN:OE1	2.24	0.70
1:DDD:136:HIS:HE1	1:EEE:275:GLY:O	1.74	0.70
1:AAA:198:ASP:CG	6:AAA:403:HOH:O	2.33	0.70
1:CCC:186:SER:OG	1:CCC:193:HIS:HE1	1.77	0.68
1:AAA:185:GLN:HG3	6:EEE:405:HOH:O	1.93	0.67
1:CCC:193:HIS:HA	4:CCC:307:IOD:I	2.64	0.67
1:AAA:50[B]:PHE:HD2	1:AAA:120:ILE:HD11	1.44	0.67
1:AAA:216:GLU:OE1	6:AAA:402:HOH:O	2.12	0.67
1:DDD:52:ASN:HD21	1:EEE:189:MET:H	1.44	0.66
1:AAA:166[A]:MET:HE3	1:AAA:166[A]:MET:HA	1.77	0.66
1:AAA:52:ASN:HD21	1:BBB:189:MET:H	1.44	0.65
1:DDD:117:THR:O	6:DDD:402:HOH:O	2.15	0.65
1:AAA:50[B]:PHE:CE2	1:BBB:189:MET:HE2	2.31	0.65
1:EEE:136:HIS:HD2	6:EEE:665:HOH:O	1.78	0.65
1:AAA:102:LEU:CD2	1:AAA:107[B]:LEU:HD21	2.27	0.65
1:AAA:107[B]:LEU:HD12	1:AAA:107[B]:LEU:H	1.61	0.64
1:DDD:50[B]:PHE:CD2	1:EEE:189:MET:HE2	2.32	0.64
1:CCC:48:GLU:HG2	4:CCC:308:IOD:I	2.68	0.64
1:AAA:166[A]:MET:CE	6:EEE:533:HOH:O	2.45	0.63
1:AAA:82[B]:ARG:NH1	1:AAA:176:THR:HG22	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:107:LEU:HD12	1:CCC:295:VAL:CG2	2.28	0.62
1:DDD:50[B]:PHE:CZ	1:EEE:189:MET:CE	2.81	0.62
1:BBB:136:HIS:HE1	1:CCC:275:GLY:O	1.83	0.62
1:EEE:32:VAL:HG23	1:EEE:91:ALA:CB	2.30	0.61
1:AAA:189[B]:MET:HE2	1:AAA:189[B]:MET:CA	2.22	0.61
1:AAA:136:HIS:HD2	6:AAA:657:HOH:O	1.81	0.61
1:CCC:136:HIS:HE1	1:DDD:275:GLY:O	1.84	0.61
1:DDD:129:HIS:HB3	6:EEE:518:HOH:O	2.01	0.60
1:DDD:193:HIS:HD2	4:DDD:308:IOD:I	2.54	0.60
1:AAA:50[B]:PHE:CZ	1:BBB:189:MET:HE2	2.37	0.60
1:AAA:99:ASN:ND2	1:AAA:107[A]:LEU:HA	2.17	0.59
1:CCC:193:HIS:HD2	4:CCC:307:IOD:I	2.55	0.59
1:CCC:299:TYR:OXT	6:CCC:403:HOH:O	2.16	0.58
1:AAA:99:ASN:ND2	1:AAA:107[B]:LEU:HA	2.18	0.58
1:DDD:193:HIS:HA	4:DDD:308:IOD:I	2.75	0.57
1:AAA:193:HIS:HD2	6:AAA:404:HOH:O	1.87	0.57
1:DDD:50[B]:PHE:CE2	1:EEE:189:MET:CE	2.83	0.56
1:CCC:189:MET:HE3	1:CCC:191:THR:HG22	1.86	0.56
1:CCC:297:ASN:HB3	1:CCC:299:TYR:CE2	2.40	0.56
4:EEE:306:IOD:I	6:EEE:423:HOH:O	2.88	0.56
1:AAA:185:GLN:CG	6:EEE:405:HOH:O	2.53	0.56
1:BBB:62:LEU:HD21	3:BBB:304:DMS:H22	1.88	0.56
1:AAA:50[B]:PHE:CE2	1:AAA:120:ILE:HD11	2.37	0.56
1:DDD:136:HIS:HD2	6:DDD:665:HOH:O	1.89	0.55
1:BBB:52:ASN:HD21	1:CCC:189:MET:H	1.53	0.55
1:DDD:119:VAL:C	1:DDD:120[B]:ILE:HD13	2.32	0.55
1:EEE:193:HIS:HA	4:EEE:305:IOD:I	2.77	0.55
1:AAA:60:GLU:CG	6:AAA:408:HOH:O	2.51	0.54
6:AAA:442:HOH:O	1:EEE:129:HIS:HB3	2.08	0.54
1:DDD:168:TYR:N	1:DDD:187:GLN:HE21	1.98	0.54
1:AAA:166[A]:MET:CE	1:EEE:280:ARG:HE	2.20	0.54
1:CCC:107:LEU:HD21	1:CCC:297:ASN:ND2	2.23	0.53
1:AAA:185:GLN:HE21	1:EEE:33:GLU:CD	2.16	0.53
1:DDD:39:THR:HA	6:DDD:464:HOH:O	2.09	0.53
1:AAA:99:ASN:HD21	1:AAA:108:LEU:N	1.97	0.53
1:BBB:41:VAL:HG13	1:BBB:42:ASP:OD1	2.07	0.53
1:CCC:168:TYR:N	1:CCC:187:GLN:HE21	1.97	0.53
1:DDD:185:GLN:NE2	1:DDD:188:VAL:HG23	2.24	0.52
1:AAA:180:LYS:O	6:AAA:404:HOH:O	2.19	0.52
1:AAA:50[B]:PHE:CD2	1:BBB:189:MET:HE2	2.45	0.52
1:AAA:113[B]:VAL:HG12	1:AAA:245:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:168:TYR:N	1:EEE:187:GLN:HE21	1.98	0.52
1:DDD:33:GLU:HB3	1:DDD:296:LYS:HB2	1.92	0.51
1:CCC:120[A]:ILE:HD11	1:DDD:212:PRO:HG3	1.91	0.51
1:EEE:39:THR:HG21	6:EEE:664:HOH:O	2.10	0.51
1:AAA:198:ASP:OD1	6:AAA:403:HOH:O	2.18	0.51
1:AAA:168:TYR:N	1:AAA:187:GLN:HE21	2.00	0.51
1:BBB:54:GLU:OE2	6:BBB:402:HOH:O	2.19	0.51
1:AAA:166[A]:MET:HA	1:AAA:166[A]:MET:CE	2.41	0.50
1:AAA:47:VAL:HG21	1:AAA:259:LEU:HD23	1.94	0.50
1:AAA:39:THR:O	1:AAA:40:GLY:O	2.30	0.49
1:EEE:101:ASP:OD1	1:EEE:103:THR:CG2	2.60	0.49
1:DDD:113[B]:VAL:HG12	1:DDD:245:LEU:HD21	1.94	0.49
1:DDD:99:ASN:ND2	1:DDD:108:LEU:H	2.00	0.49
1:CCC:58:PRO:HA	1:CCC:83:LYS:HD3	1.94	0.49
1:CCC:107:LEU:HD21	1:CCC:297:ASN:CG	2.38	0.49
1:BBB:168:TYR:N	1:BBB:187:GLN:HE21	1.99	0.49
1:EEE:104:CYS:O	1:EEE:297:ASN:ND2	2.40	0.48
1:DDD:179:PRO:HA	4:DDD:308:IOD:I	2.83	0.48
1:CCC:50[B]:PHE:HE2	1:CCC:120[B]:ILE:CD1	2.19	0.48
1:DDD:100[B]:GLU:OE1	6:DDD:403:HOH:O	2.20	0.48
1:BBB:60:GLU:HB2	6:BBB:520:HOH:O	2.12	0.48
1:AAA:106:ASN:ND2	1:AAA:106:ASN:H	2.11	0.48
1:BBB:186:SER:OG	1:BBB:193:HIS:CE1	2.60	0.47
1:EEE:60:GLU:HG2	1:EEE:61:ASN:N	2.30	0.47
1:AAA:275:GLY:O	1:EEE:136:HIS:CE1	2.62	0.47
1:AAA:297:ASN:N	1:AAA:297:ASN:OD1	2.46	0.47
1:AAA:117:THR:O	6:AAA:405:HOH:O	2.20	0.47
1:AAA:188:VAL:HG23	1:AAA:189[A]:MET:H	1.80	0.47
1:AAA:188:VAL:HG23	1:AAA:189[B]:MET:H	1.80	0.47
1:CCC:48:GLU:HG3	1:CCC:285:TYR:CE1	2.50	0.47
1:CCC:50[B]:PHE:HE2	1:CCC:120[B]:ILE:HD13	1.72	0.46
1:CCC:159:LEU:HD23	1:CCC:161[B]:MET:SD	2.55	0.46
1:AAA:198:ASP:OD2	6:AAA:403:HOH:O	2.20	0.46
3:BBB:303:DMS:H11	4:BBB:305:IOD:I	2.85	0.46
1:CCC:120[A]:ILE:CD1	1:DDD:212:PRO:HG3	2.46	0.46
1:AAA:60:GLU:CD	6:AAA:408:HOH:O	2.58	0.46
1:DDD:97:ASN:HD22	1:DDD:100[B]:GLU:HG3	1.80	0.46
1:AAA:191:THR:HG21	1:EEE:34:VAL:HG11	1.98	0.45
1:DDD:193:HIS:CD2	4:DDD:308:IOD:I	3.38	0.45
1:AAA:49:CYS:SG	1:AAA:93:ILE:HD11	2.57	0.45
1:BBB:111:GLU:OE1	1:BBB:293:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:101:ASP:CG	1:DDD:104:CYS:HB3	2.41	0.45
1:EEE:168:TYR:H	1:EEE:187:GLN:NE2	1.99	0.45
1:AAA:48:GLU:HG3	1:AAA:285:TYR:CE1	2.52	0.45
1:AAA:42:ASP:CG	1:AAA:42:ASP:O	2.60	0.45
1:BBB:193:HIS:HA	4:BBB:306:IOD:I	2.87	0.44
1:BBB:278:GLN:OE1	3:BBB:304:DMS:H12	2.17	0.44
1:CCC:35:LEU:HB2	1:CCC:294:SER:OG	2.17	0.44
1:CCC:107:LEU:HD12	1:CCC:295:VAL:HG23	1.97	0.44
1:AAA:142[B]:LYS:HB2	1:AAA:142[B]:LYS:HE2	1.78	0.44
3:DDD:304:DMS:H13	6:EEE:585:HOH:O	2.16	0.44
1:DDD:52:ASN:ND2	1:EEE:189:MET:H	2.14	0.44
1:AAA:228:GLU:OE1	1:EEE:142:LYS:HE3	2.18	0.43
1:AAA:107[B]:LEU:HD13	1:AAA:295:VAL:O	2.18	0.43
1:AAA:129:HIS:HB3	6:BBB:445:HOH:O	2.18	0.43
1:AAA:50[B]:PHE:CZ	1:BBB:189:MET:CE	3.02	0.43
1:BBB:159:LEU:HD23	1:BBB:161[B]:MET:SD	2.59	0.43
1:EEE:101:ASP:OD1	1:EEE:103:THR:HG22	2.18	0.43
1:AAA:50[B]:PHE:HE2	1:AAA:120:ILE:HD13	1.80	0.42
1:CCC:193:HIS:CD2	4:CCC:307:IOD:I	3.40	0.42
1:BBB:49[A]:CYS:SG	1:BBB:286:PHE:HB2	2.59	0.42
1:BBB:120[B]:ILE:HD11	1:CCC:212:PRO:HG3	2.01	0.42
1:AAA:99:ASN:HD21	1:AAA:107[A]:LEU:HA	1.83	0.42
1:DDD:99:ASN:HD21	1:DDD:108:LEU:N	2.04	0.42
1:DDD:188:VAL:HG23	1:DDD:189:MET:H	1.85	0.42
1:DDD:48:GLU:HG2	4:DDD:309:IOD:I	2.90	0.41
1:DDD:50[B]:PHE:CE1	1:EEE:189:MET:HE2	2.52	0.41
1:AAA:50[B]:PHE:CE1	1:BBB:189:MET:HE2	2.55	0.41
1:DDD:39:THR:HG22	1:DDD:40:GLY:N	2.35	0.41
1:EEE:101:ASP:OD1	1:EEE:103:THR:HG23	2.19	0.41
1:AAA:42:ASP:O	1:AAA:292:LYS:HE3	2.20	0.41
1:CCC:50[B]:PHE:HD2	1:CCC:120[B]:ILE:HD12	1.73	0.41
1:CCC:189:MET:HE2	6:CCC:662:HOH:O	2.21	0.41
1:AAA:88:TYR:CZ	1:AAA:161[A]:MET:HE1	2.56	0.40
1:AAA:99:ASN:HD21	1:AAA:107[B]:LEU:HA	1.84	0.40
1:AAA:172:TYR:CG	1:AAA:178:THR:HG21	2.57	0.40
1:AAA:191:THR:HG21	1:EEE:34:VAL:CG1	2.51	0.40
1:DDD:48:GLU:HG3	1:DDD:285:TYR:CE1	2.56	0.40
1:AAA:107[B]:LEU:HB2	1:AAA:295:VAL:O	2.20	0.40
1:DDD:186:SER:OG	1:DDD:193:HIS:CE1	2.64	0.40
1:EEE:52:ASN:HD22	1:EEE:52:ASN:HA	1.77	0.40
1:BBB:129:HIS:HB3	6:CCC:484:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:179:PRO:HA	4:CCC:307:IOD:I	2.91	0.40

All (3) 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)
1:CCC:60:GLU:N	1:CCC:60:GLU:N[2_875]	2.14	0.06
6:CCC:645:HOH:O	6:DDD:556:HOH:O[2_875]	2.14	0.06
6:AAA:422:HOH:O	6:CCC:490:HOH:O[4_476]	2.17	0.03

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	274/270 (102%)	262 (96%)	9 (3%)	3 (1%)	11	2
1	BBB	262/270 (97%)	251 (96%)	10 (4%)	1 (0%)	30	11
1	CCC	263/270 (97%)	253 (96%)	9 (3%)	1 (0%)	30	11
1	DDD	271/270 (100%)	261 (96%)	8 (3%)	2 (1%)	18	4
1	EEE	269/270 (100%)	261 (97%)	7 (3%)	1 (0%)	30	11
All	All	1339/1350 (99%)	1288 (96%)	43 (3%)	8 (1%)	21	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	40	GLY
1	AAA	175	GLY
1	DDD	41	VAL
1	CCC	188	VAL
1	BBB	188	VAL
1	DDD	188	VAL

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Mol	Chain	Res	Type
1	EEE	188	VAL
1	AAA	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	238/231 (103%)	233 (98%)	5 (2%)	47	13
1	BBB	225/231 (97%)	224 (100%)	1 (0%)	84	69
1	CCC	229/231 (99%)	228 (100%)	1 (0%)	84	69
1	DDD	233/231 (101%)	231 (99%)	2 (1%)	70	44
1	EEE	232/231 (100%)	229 (99%)	3 (1%)	61	29
All	All	1157/1155 (100%)	1145 (99%)	12 (1%)	70	39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	106	ASN
1	AAA	107[A]	LEU
1	AAA	107[B]	LEU
1	AAA	166[A]	MET
1	AAA	166[B]	MET
1	BBB	107	LEU
1	CCC	107	LEU
1	DDD	107	LEU
1	DDD	192	ASP
1	EEE	60	GLU
1	EEE	102	LEU
1	EEE	296	LYS

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 43 ligands modelled in this entry, 31 are monoatomic - leaving 12 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	DMS	DDD	306	-	3,3,3	0.22	0	3,3,3	1.23	1 (33%)
3	DMS	EEE	303	-	3,3,3	0.14	0	3,3,3	0.15	0
3	DMS	AAA	306	-	3,3,3	0.27	0	3,3,3	1.01	0
3	DMS	CCC	304	-	3,3,3	0.25	0	3,3,3	0.17	0
3	DMS	CCC	303	-	3,3,3	0.59	0	3,3,3	0.56	0
3	DMS	AAA	307	-	3,3,3	0.22	0	3,3,3	0.14	0
3	DMS	DDD	304	-	3,3,3	0.18	0	3,3,3	0.17	0
3	DMS	CCC	305	-	3,3,3	0.23	0	3,3,3	0.10	0
3	DMS	BBB	304	-	3,3,3	0.22	0	3,3,3	0.20	0
3	DMS	DDD	305	-	3,3,3	0.15	0	3,3,3	0.46	0
3	DMS	EEE	302	-	3,3,3	0.27	0	3,3,3	0.98	0
3	DMS	BBB	303	-	3,3,3	0.32	0	3,3,3	0.84	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DDD	306	DMS	O-S-C2	-2.08	96.07	106.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	304	DMS	1	0
3	BBB	304	DMS	2	0
3	BBB	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, 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	265/270 (98%)	0.05	19 (7%)	21 23	10, 18, 43, 63	13 (4%)
1	BBB	261/270 (96%)	-0.05	9 (3%)	48 51	9, 19, 39, 74	5 (1%)
1	CCC	261/270 (96%)	0.12	18 (6%)	23 24	9, 18, 53, 96	6 (2%)
1	DDD	265/270 (98%)	0.05	13 (4%)	35 37	10, 18, 44, 81	8 (3%)
1	EEE	266/270 (98%)	0.11	18 (6%)	23 25	9, 20, 52, 103	5 (1%)
All	All	1318/1350 (97%)	0.06	77 (5%)	29 30	9, 19, 49, 103	37 (2%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	41	VAL	6.7
1	CCC	41	VAL	6.0
1	BBB	41	VAL	5.7
1	EEE	43	ALA	5.7
1	CCC	299	TYR	5.1
1	EEE	102	LEU	5.1
1	AAA	104[A]	CYS	5.1
1	EEE	41	VAL	4.7
1	AAA	107[A]	LEU	4.7
1	EEE	44	ILE	4.5
1	AAA	32	VAL	4.4
1	DDD	39	THR	4.4
1	CCC	60	GLU	4.4
1	DDD	102	LEU	4.3
1	EEE	107	LEU	4.3
1	EEE	32	VAL	4.2
1	CCC	37	VAL	4.1
1	CCC	39	THR	4.0
1	CCC	298	PRO	3.9
1	DDD	40	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	DDD	103	THR	3.7
1	CCC	44	ILE	3.7
1	DDD	32	VAL	3.6
1	AAA	297	ASN	3.5
1	EEE	103	THR	3.5
1	EEE	104	CYS	3.5
1	AAA	106	ASN	3.4
1	CCC	40	GLY	3.3
1	AAA	102	LEU	3.3
1	DDD	107	LEU	3.2
1	EEE	105	GLY	3.2
1	AAA	99	ASN	3.2
1	EEE	295	VAL	3.2
1	CCC	106	ASN	3.2
1	AAA	103	THR	3.2
1	BBB	40	GLY	3.1
1	EEE	33	GLU	3.1
1	CCC	107	LEU	3.0
1	CCC	34	VAL	2.9
1	EEE	95	LEU	2.9
1	AAA	39	THR	2.9
1	BBB	95	LEU	2.9
1	BBB	30	GLY	2.9
1	BBB	107	LEU	2.8
1	AAA	42	ASP	2.7
1	AAA	174[A]	ASP	2.7
1	AAA	60	GLU	2.7
1	CCC	59	ASP	2.7
1	EEE	296	LYS	2.6
1	AAA	34	VAL	2.6
1	DDD	44	ILE	2.6
1	AAA	40	GLY	2.6
1	CCC	35	LEU	2.6
1	BBB	296	LYS	2.5
1	BBB	97	ASN	2.5
1	AAA	295	VAL	2.5
1	CCC	98	LEU	2.5
1	DDD	106	ASN	2.4
1	DDD	98	LEU	2.4
1	AAA	41	VAL	2.4
1	DDD	104	CYS	2.4
1	EEE	297	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	43	ALA	2.3
1	DDD	43	ALA	2.3
1	CCC	297	ASN	2.3
1	DDD	37	VAL	2.3
1	EEE	40	GLY	2.3
1	EEE	101	ASP	2.2
1	AAA	35	LEU	2.2
1	CCC	38	LYS	2.2
1	CCC	33	GLU	2.2
1	EEE	98	LEU	2.1
1	EEE	39	THR	2.1
1	BBB	106	ASN	2.1
1	AAA	296	LYS	2.1
1	BBB	98	LEU	2.0
1	AAA	196	TYR	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
5	NA	AAA	311	1/1	0.73	0.58	52,52,52,52	0
2	CA	CCC	302	1/1	0.80	0.23	76,76,76,76	0
3	DMS	CCC	304	4/4	0.81	0.19	50,55,57,58	0
5	NA	DDD	310	1/1	0.82	0.29	62,62,62,62	0
3	DMS	CCC	305	4/4	0.84	0.22	75,76,78,79	0
3	DMS	BBB	304	4/4	0.85	0.23	61,62,65,65	0
3	DMS	DDD	306	4/4	0.85	0.16	26,33,39,39	0
2	CA	DDD	302	1/1	0.86	0.23	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMS	AAA	306	4/4	0.88	0.14	28,31,37,39	0
3	DMS	EEE	303	4/4	0.88	0.20	54,57,57,59	0
3	DMS	AAA	307	4/4	0.89	0.19	59,60,64,66	0
4	IOD	AAA	310	1/1	0.89	0.14	42,42,42,42	1
4	IOD	CCC	307	1/1	0.90	0.12	33,33,33,33	1
3	DMS	DDD	305	4/4	0.90	0.15	33,38,40,44	0
3	DMS	DDD	304	4/4	0.90	0.15	50,51,53,55	0
4	IOD	CCC	309	1/1	0.91	0.12	43,43,43,43	1
3	DMS	BBB	303	4/4	0.92	0.11	29,30,36,38	0
4	IOD	BBB	305	1/1	0.92	0.14	39,39,39,39	1
2	CA	DDD	303	1/1	0.92	0.21	35,35,35,35	1
2	CA	AAA	304	1/1	0.92	0.10	31,31,31,31	1
4	IOD	DDD	308	1/1	0.92	0.09	27,27,27,27	1
3	DMS	EEE	302	4/4	0.92	0.12	29,30,36,39	0
2	CA	BBB	302	1/1	0.92	0.19	33,33,33,33	1
4	IOD	EEE	304	1/1	0.93	0.15	38,38,38,38	1
4	IOD	EEE	306	1/1	0.93	0.11	43,43,43,43	1
2	CA	AAA	303	1/1	0.93	0.15	28,28,28,28	1
3	DMS	CCC	303	4/4	0.93	0.12	29,32,40,41	0
4	IOD	EEE	305	1/1	0.94	0.09	35,35,35,35	1
4	IOD	AAA	309	1/1	0.94	0.09	29,29,29,29	1
4	IOD	BBB	306	1/1	0.94	0.09	39,39,39,39	1
2	CA	DDD	301	1/1	0.94	0.14	28,28,28,28	1
2	CA	AAA	302	1/1	0.95	0.16	31,31,31,31	1
2	CA	CCC	301	1/1	0.95	0.07	26,26,26,26	1
4	IOD	DDD	307	1/1	0.95	0.06	22,22,22,22	1
4	IOD	CCC	306	1/1	0.96	0.06	24,24,24,24	1
2	CA	AAA	305	1/1	0.96	0.11	25,25,25,25	1
4	IOD	CCC	308	1/1	0.97	0.06	30,30,30,30	1
2	CA	BBB	301	1/1	0.97	0.06	21,21,21,21	1
4	IOD	CCC	310	1/1	0.97	0.07	17,17,17,17	1
2	CA	EEE	301	1/1	0.97	0.08	24,24,24,24	1
4	IOD	AAA	308	1/1	0.97	0.05	23,23,23,23	1
4	IOD	DDD	309	1/1	0.98	0.07	27,27,27,27	1
2	CA	AAA	301	1/1	0.98	0.04	19,19,19,19	1

6.5 Other polymers

There are no such residues in this entry.