



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:00 AM UTC

PDB ID : 7B69 / pdb_00007b69
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 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:

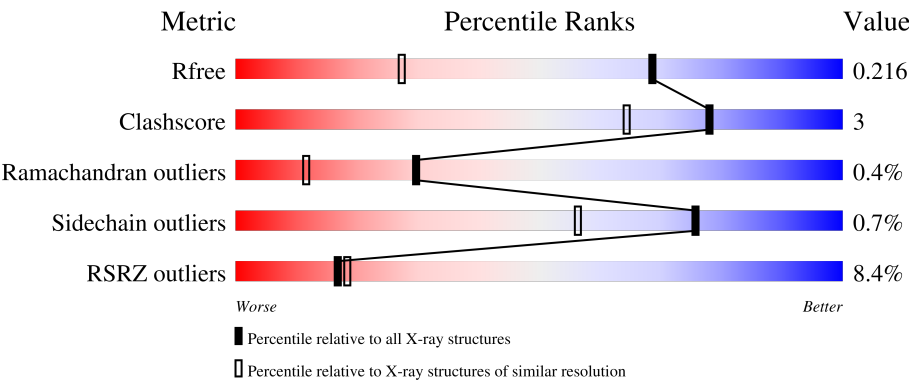
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (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 $\leq 5\%$. 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	275	7% 92% 5%
1	BBB	275	8% 90% 6%
1	CCC	275	4% 90% 7%
1	DDD	275	8% 88% 9%
1	EEE	275	15% 85% 7% 8%

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Mol	Chain	Length	Quality of chain
1	FFF	275	9% 89% 6%
1	GGG	275	8% 93% 7%
1	HHH	275	8% 87% 7% 5%
1	III	275	10% 91% 7%
1	JJJ	275	4% 91% 8%

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:

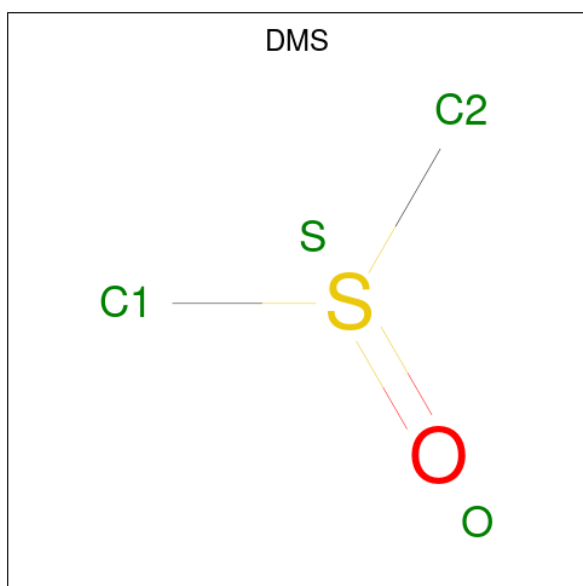
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	25	GLY	-	expression tag	UNP P03088
AAA	104	SER	CYS	engineered mutation	UNP P03088
BBB	25	GLY	-	expression tag	UNP P03088
BBB	104	SER	CYS	engineered mutation	UNP P03088
CCC	25	GLY	-	expression tag	UNP P03088
CCC	104	SER	CYS	engineered mutation	UNP P03088
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 (CCD ID: DMS) (formula: C₂H₆OS).



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 4	C 2	O 1	S 1	0	0
2	DDD	1	Total 4	C 2	O 1	S 1	0	0
2	DDD	1	Total 4	C 2	O 1	S 1	0	0
2	EEE	1	Total 4	C 2	O 1	S 1	0	0
2	EEE	1	Total 4	C 2	O 1	S 1	0	0
2	EEE	1	Total 4	C 2	O 1	S 1	0	0
2	EEE	1	Total 4	C 2	O 1	S 1	0	0
2	FFF	1	Total 4	C 2	O 1	S 1	0	0
2	FFF	1	Total 4	C 2	O 1	S 1	0	0
2	GGG	1	Total 4	C 2	O 1	S 1	0	0
2	GGG	1	Total 4	C 2	O 1	S 1	0	0
2	GGG	1	Total 4	C 2	O 1	S 1	0	0
2	HHH	1	Total 4	C 2	O 1	S 1	0	0
2	HHH	1	Total 4	C 2	O 1	S 1	0	0
2	III	1	Total 4	C 2	O 1	S 1	0	0
2	III	1	Total 4	C 2	O 1	S 1	0	0
2	JJJ	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 3 is water.

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

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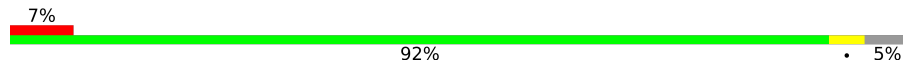
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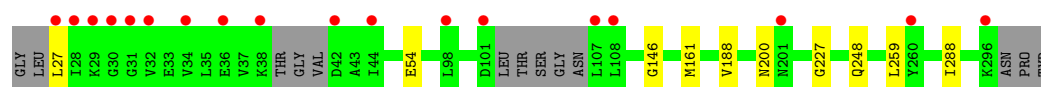
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CCC	244	Total 244	O 244	0	0
3	DDD	204	Total 204	O 204	0	0
3	EEE	179	Total 179	O 179	0	0
3	FFF	194	Total 194	O 194	0	0
3	GGG	184	Total 184	O 184	0	0
3	HHH	179	Total 179	O 179	0	0
3	III	205	Total 205	O 205	0	0
3	JJJ	205	Total 205	O 205	0	0

3 Residue-property plots [i](#)

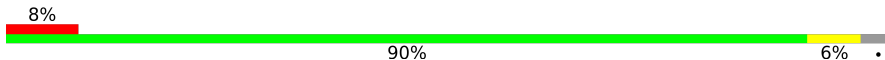
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

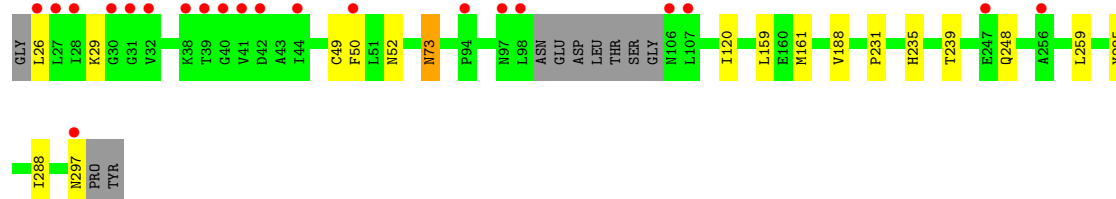
- Molecule 1: Major capsid protein VP1

Chain AAA: 

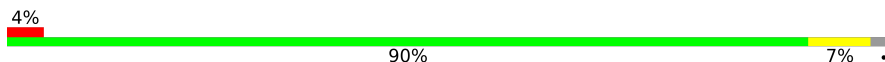


- Molecule 1: Major capsid protein VP1

Chain BBB: 

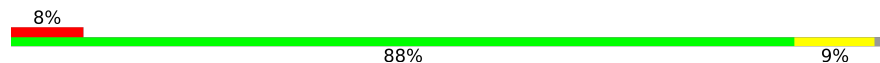


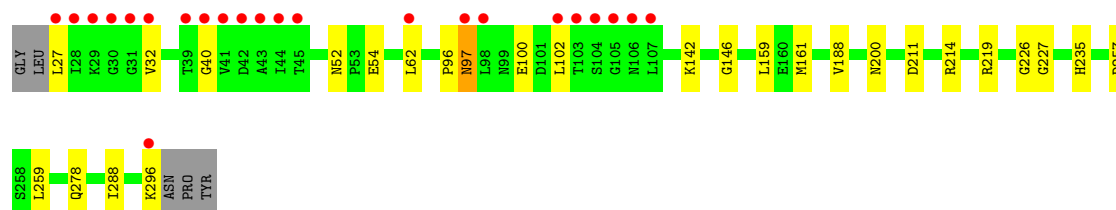
- Molecule 1: Major capsid protein VP1

Chain CCC: 

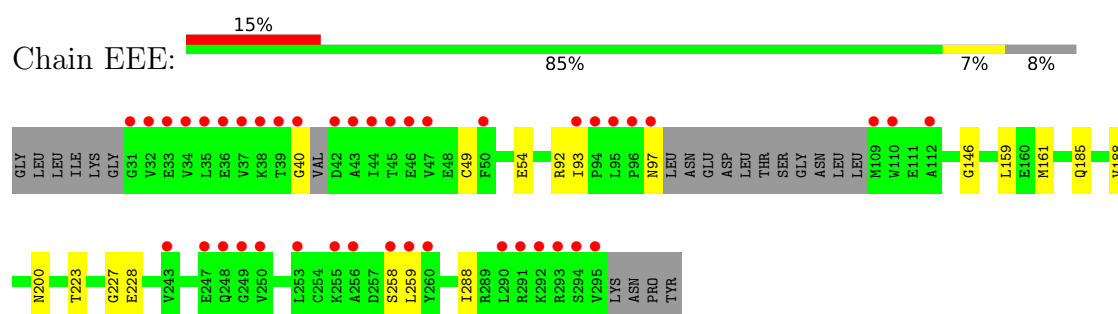


- Molecule 1: Major capsid protein VP1

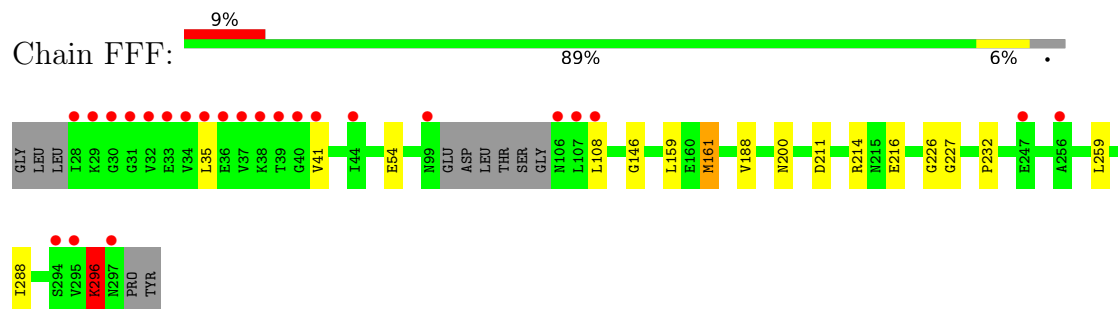
Chain DDD: 



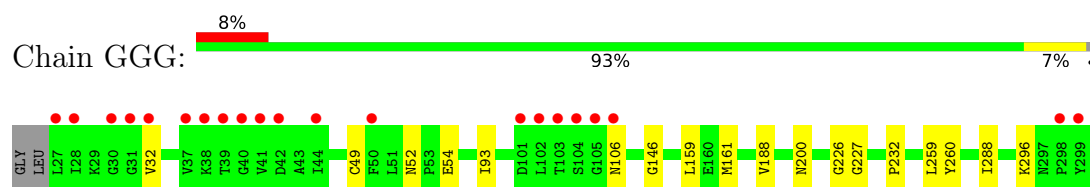
- Molecule 1: Major capsid protein VP1



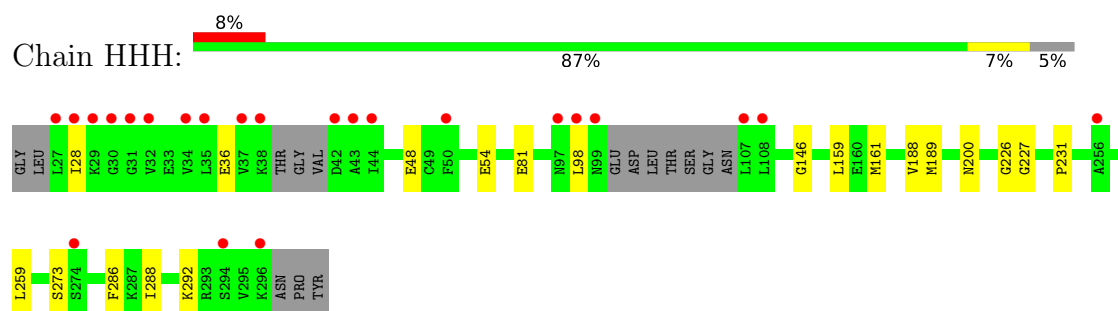
- Molecule 1: Major capsid protein VP1



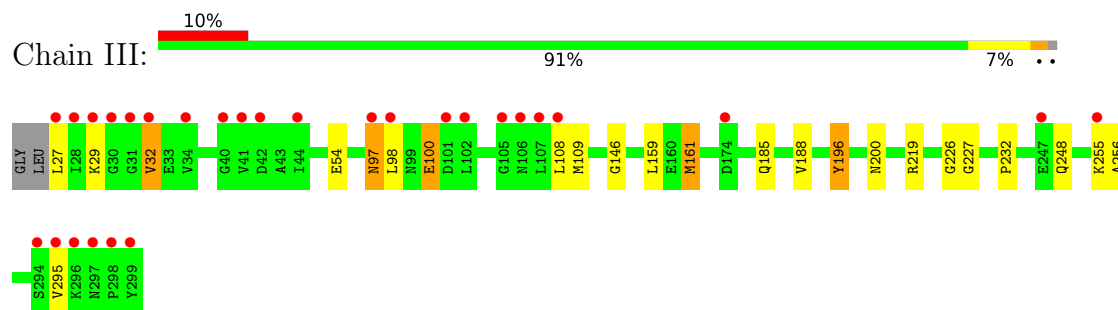
- Molecule 1: Major capsid protein VP1



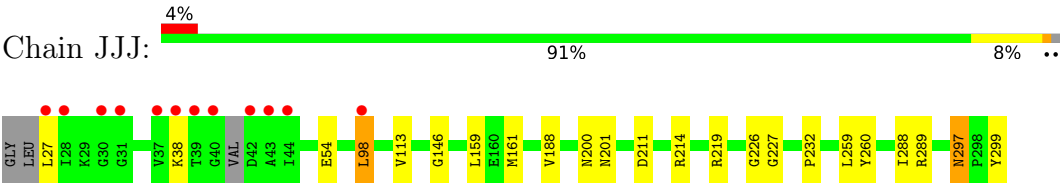
- Molecule 1: Major capsid protein VP1



- 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	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
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.197 (Not available) , 0.216	Depositor DCC
R_{free} test set	20576 reflections (4.75%)	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)	0.34 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.*

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: 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	0.88	0/2099	1.06	1/2848 (0.0%)
1	BBB	0.93	1/2117 (0.0%)	1.08	1/2875 (0.0%)
1	CCC	0.91	0/2141	1.05	1/2910 (0.0%)
1	DDD	0.94	1/2167 (0.0%)	1.09	3/2942 (0.1%)
1	EEE	0.89	0/2017	1.01	0/2738
1	FFF	0.91	0/2129	1.06	2/2889 (0.1%)
1	GGG	0.93	0/2171	1.04	0/2955
1	HHH	0.89	0/2104	1.03	0/2855
1	III	0.95	2/2160 (0.1%)	1.10	3/2937 (0.1%)
1	JJJ	0.91	0/2180	1.04	0/2961
All	All	0.92	4/21285 (0.0%)	1.06	11/28910 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	III	32	VAL	C-O	6.31	1.30	1.23
1	DDD	96	PRO	C-O	-5.81	1.17	1.23
1	III	100	GLU	C-O	5.51	1.30	1.23
1	BBB	49	CYS	C-N	-5.06	1.26	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	III	161	MET	CG-SD-CE	-10.67	77.43	100.90
1	FFF	161	MET	CG-SD-CE	-10.15	78.58	100.90
1	AAA	161	MET	CG-SD-CE	-10.12	78.63	100.90
1	DDD	100	GLU	CB-CA-C	-6.28	100.77	110.81
1	BBB	73	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	CCC	40	GLY	CA-C-O	-5.60	118.28	122.37
1	DDD	40	GLY	CA-C-O	-5.57	118.44	122.45
1	DDD	97	ASN	CA-CB-CG	5.26	117.86	112.60
1	III	196	TYR	CA-CB-CG	5.25	123.36	113.90
1	III	219	ARG	CG-CD-NE	-5.13	100.71	112.00
1	FFF	41	VAL	CA-C-O	-5.13	115.42	120.85

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	17	0
1	DDD	2105	0	2062	17	0
1	EEE	1960	0	1906	10	0
1	FFF	2068	0	2029	11	0
1	GGG	2109	0	2033	11	0
1	HHH	2039	0	1994	12	0
1	III	2105	0	2030	16	0
1	JJJ	2113	0	2054	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
3	DDD	204	0	0	4	1
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	114	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.

All (114) 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:III:109:MET:HE3	1:III:255:LYS:HA	1.56	0.86
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
1:BBB:50:PHE:O	3:BBB:402:HOH:O	2.01	0.79
1:JJJ:98:LEU:H	1:JJJ:98:LEU:HD23	1.49	0.76
1:FFF:216:GLU:OE2	3:FFF:401:HOH:O	2.08	0.72
1:HHH:81:GLU:OE1	3:HHH:403:HOH:O	2.10	0.69
1:FFF:211:ASP:OD2	1:FFF:214[B]:ARG:CD	2.41	0.68
1:III:97:ASN:HB3	3:III:403:HOH:O	1.92	0.68
1:DDD:211:ASP:OD2	1:DDD:214[B]:ARG:CD	2.42	0.67
1:JJJ:211:ASP:OD2	1:JJJ:214[A]:ARG:CD	2.43	0.66
1:GGG:52:ASN:HD21	1:HHH:189:MET:H	1.43	0.66
1:EEE:54[B]:GLU:OE2	1:EEE:200:ASN:OD1	2.15	0.64
1:FFF:108:LEU:O	3:FFF:402:HOH:O	2.16	0.61
1:GGG:49[A]:CYS:SG	1:GGG:93:ILE:HD11	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:32:VAL:CG2	1:DDD:296:LYS:O	2.53	0.57
1:BBB:52:ASN:HD21	1:CCC:189:MET:H	1.53	0.56
1:JJJ:297:ASN:C	1:JJJ:297:ASN:HD22	2.14	0.56
1:BBB:29:LYS:NZ	1:BBB:248:GLN:OE1	2.37	0.56
1:AAA:54[B]:GLU:OE2	1:AAA:200[B]:ASN:OD1	2.23	0.56
1:CCC:235[B]:HIS:HE1	3:DDD:419:HOH:O	1.89	0.55
1:III:97:ASN:CB	3:III:403:HOH:O	2.51	0.55
1:JJJ:113:VAL:HG22	1:JJJ:289:ARG:O	2.07	0.55
1:FFF:35:LEU:HD11	1:FFF:296:LYS:HG2	1.89	0.54
1:DDD:32:VAL:HG22	1:DDD:296:LYS:O	2.08	0.54
1:III:100:GLU:HG2	1:III:108:LEU:H	1.73	0.54
1:HHH:54[B]:GLU:OE2	1:HHH:200:ASN:OD1	2.27	0.53
1:EEE:40:GLY:C	3:EEE:409:HOH:O	2.52	0.53
1:DDD:102:LEU:O	3:DDD:403:HOH:O	2.18	0.52
1:III:256:ALA:N	3:III:401:HOH:O	2.04	0.52
1:CCC:260:TYR:HE1	3:CCC:480:HOH:O	1.94	0.51
1:DDD:54[B]:GLU:OE2	1:DDD:200:ASN:OD1	2.29	0.51
1:JJJ:98:LEU:HD23	1:JJJ:98:LEU:N	2.21	0.51
1:HHH:36:GLU:HB2	3:HHH:549:HOH:O	2.11	0.50
1:III:185:GLN:HG2	3:III:576:HOH:O	2.11	0.50
1:HHH:81:GLU:OE2	3:HHH:404:HOH:O	2.20	0.49
1:III:98:LEU:HD13	1:III:108:LEU:C	2.38	0.49
1:CCC:38:LYS:HD3	1:CCC:294[B]:SER:OG	2.11	0.49
1:DDD:219[A]:ARG:NH1	3:DDD:408:HOH:O	2.46	0.48
1:JJJ:219[A]:ARG:NH1	3:JJJ:413:HOH:O	2.46	0.48
1:III:29:LYS:NZ	1:III:248:GLN:OE1	2.42	0.48
1:EEE:49[B]:CYS:SG	1:EEE:93:ILE:HD11	2.54	0.48
1:III:98:LEU:HD13	1:III:108:LEU:O	2.14	0.47
1:FFF:54[B]:GLU:OE2	1:FFF:200:ASN:OD1	2.32	0.47
1:DDD:97:ASN:HA	1:DDD:257:ASP:OD2	2.14	0.47
1:HHH:98:LEU:CD2	1:HHH:292:LYS:HE2	2.44	0.47
1:GGG:232:PRO:HD2	1:HHH:226:GLY:O	2.14	0.47
1:GGG:32:VAL:HG22	1:GGG:296:LYS:O	2.15	0.47
1:CCC:259:LEU:HD21	1:CCC:288:ILE:HD13	1.97	0.47
1:DDD:142:LYS:NZ	1:EEE:228:GLU:OE1	2.29	0.47
1:JJJ:297:ASN:HD22	1:JJJ:299:TYR:H	1.61	0.47
1:GGG:32:VAL:CG2	1:GGG:296:LYS:O	2.63	0.47
1:CCC:235[B]:HIS:HD2	2:CCC:303:DMS:O	1.97	0.46
1:III:54[B]:GLU:OE2	1:III:200:ASN:OD1	2.33	0.46
1:III:232:PRO:HD2	1:JJJ:226:GLY:O	2.15	0.46
1:DDD:62:LEU:HD13	1:DDD:278:GLN:HE22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:219[B]:ARG:HD2	1:CCC:244:LEU:O	2.15	0.46
1:EEE:159:LEU:HD23	1:EEE:161[A]:MET:SD	2.56	0.46
1:HHH:231:PRO:HB3	1:III:226:GLY:O	2.15	0.46
1:EEE:92:ARG:NE	1:EEE:258:SER:OG	2.49	0.46
1:HHH:259:LEU:HD21	1:HHH:288:ILE:HD13	1.99	0.45
1:HHH:159:LEU:HD23	1:HHH:161[A]:MET:SD	2.57	0.44
1:JJJ:54[A]:GLU:CD	3:JJJ:404:HOH:O	2.59	0.44
1:EEE:259:LEU:HD21	1:EEE:288:ILE:HD13	1.99	0.44
1:BBB:120:ILE:HD11	1:BBB:285:TYR:HB2	1.99	0.44
1:FFF:259:LEU:HD21	1:FFF:288:ILE:HD13	1.98	0.44
1:AAA:259:LEU:HD21	1:AAA:288:ILE:HD13	1.99	0.44
1:BBB:159:LEU:HD23	1:BBB:161[A]:MET:SD	2.58	0.43
1:JJJ:54[B]:GLU:OE2	1:JJJ:200:ASN:OD1	2.36	0.43
1:CCC:219[B]:ARG:HD3	3:CCC:471:HOH:O	2.19	0.43
1:DDD:235[B]:HIS:HD2	1:EEE:223:THR:OG1	2.00	0.43
1:JJJ:54[B]:GLU:OE1	1:JJJ:201:ASN:N	2.50	0.43
1:FFF:159:LEU:HD23	1:FFF:161:MET:SD	2.59	0.43
1:GGG:159:LEU:HD23	1:GGG:161[A]:MET:SD	2.58	0.43
1:JJJ:159:LEU:HD23	1:JJJ:161[A]:MET:SD	2.58	0.43
1:FFF:146:GLY:HA2	1:FFF:227:GLY:O	2.19	0.42
1:CCC:185:GLN:HG2	3:CCC:609:HOH:O	2.19	0.42
1:JJJ:98:LEU:N	1:JJJ:98:LEU:CD2	2.82	0.42
1:HHH:146:GLY:HA2	1:HHH:227:GLY:O	2.19	0.42
1:GGG:54:GLU:OE1	1:GGG:200:ASN:OD1	2.38	0.42
1:CCC:231:PRO:HB3	1:DDD:226:GLY:O	2.20	0.42
1:JJJ:259:LEU:HD21	1:JJJ:288:ILE:HD13	2.01	0.42
1:CCC:219[B]:ARG:CD	3:CCC:471:HOH:O	2.68	0.42
1:EEE:146:GLY:HA2	1:EEE:227:GLY:O	2.20	0.41
1:GGG:259:LEU:HD21	1:GGG:288:ILE:HD13	2.02	0.41
1:JJJ:146:GLY:HA2	1:JJJ:227:GLY:O	2.20	0.41
1:DDD:159:LEU:HD23	1:DDD:161[A]:MET:SD	2.59	0.41
1:BBB:235[B]:HIS:HE1	3:BBB:576:HOH:O	2.03	0.41
1:BBB:239:THR:HG22	1:CCC:219[B]:ARG:HD3	2.02	0.41
1:GGG:146:GLY:HA2	1:GGG:227:GLY:O	2.19	0.41
1:AAA:248:GLN:OE1	1:AAA:248:GLN:N	2.53	0.41
1:DDD:142:LYS:HE2	3:DDD:550:HOH:O	2.21	0.41
1:FFF:226:GLY:O	1:JJJ:232:PRO:HD2	2.21	0.41
1:III:146:GLY:HA2	1:III:227:GLY:O	2.21	0.41
1:BBB:231:PRO:HB3	1:CCC:226:GLY:O	2.21	0.41
1:CCC:146:GLY:HA2	1:CCC:227:GLY:O	2.21	0.41
1:CCC:159:LEU:HD23	1:CCC:161[B]:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:297:ASN:ND2	1:JJJ:299:TYR:H	2.19	0.41
1:BBB:259:LEU:HD21	1:BBB:288:ILE:HD13	2.03	0.41
1:DDD:259:LEU:HD21	1:DDD:288:ILE:HD13	2.02	0.41
1:GGG:260:TYR:HE1	3:GGG:410:HOH:O	2.03	0.41
1:III:159:LEU:HD23	1:III:161:MET:SD	2.61	0.41
1:FFF:232:PRO:HD2	1:GGG:226:GLY:O	2.22	0.40
1:HHH:48:GLU:HA	1:HHH:286:PHE:O	2.21	0.40
1:DDD:52:ASN:ND2	1:EEE:185:GLN:HE22	2.19	0.40
1:JJJ:260:TYR:OH	3:JJJ:403:HOH:O	2.21	0.40
1:AAA:146:GLY:HA2	1:AAA:227:GLY:O	2.21	0.40
1:BBB:52:ASN:HD22	1:BBB:52:ASN:HA	1.73	0.40
1:CCC:116:GLN:CD	3:CCC:414:HOH:O	2.64	0.40
1:DDD:146:GLY:HA2	1:DDD:227:GLY:O	2.21	0.40
1:III:32:VAL:CG1	1:III:295:VAL:HB	2.52	0.40

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%)	30	11
1	BBB	265/275 (96%)	254 (96%)	10 (4%)	1 (0%)	30	11
1	CCC	270/275 (98%)	260 (96%)	9 (3%)	1 (0%)	30	11
1	DDD	274/275 (100%)	263 (96%)	10 (4%)	1 (0%)	30	11
1	EEE	251/275 (91%)	241 (96%)	9 (4%)	1 (0%)	30	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FFF	265/275 (96%)	254 (96%)	10 (4%)	1 (0%)	30	11
1	GGG	276/275 (100%)	267 (97%)	8 (3%)	1 (0%)	30	11
1	HHH	261/275 (95%)	251 (96%)	9 (3%)	1 (0%)	30	11
1	III	274/275 (100%)	262 (96%)	11 (4%)	1 (0%)	30	11
1	JJJ	274/275 (100%)	263 (96%)	10 (4%)	1 (0%)	30	11
All	All	2670/2750 (97%)	2564 (96%)	96 (4%)	10 (0%)	30	11

All (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
1	FFF	188	VAL
1	GGG	188	VAL
1	HHH	188	VAL
1	III	188	VAL
1	JJJ	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%)	84	70
1	BBB	227/235 (97%)	225 (99%)	2 (1%)	70	48
1	CCC	228/235 (97%)	228 (100%)	0	100	100
1	DDD	232/235 (99%)	231 (100%)	1 (0%)	84	70
1	EEE	216/235 (92%)	215 (100%)	1 (0%)	81	65
1	FFF	230/235 (98%)	229 (100%)	1 (0%)	84	70
1	GGG	231/235 (98%)	230 (100%)	1 (0%)	84	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HHH	225/235 (96%)	223 (99%)	2 (1%)	70	48
1	III	229/235 (97%)	226 (99%)	3 (1%)	61	33
1	JJJ	232/235 (99%)	228 (98%)	4 (2%)	53	24
All	All	2275/2350 (97%)	2259 (99%)	16 (1%)	76	56

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	27	LEU
1	BBB	26	LEU
1	BBB	297	ASN
1	DDD	27	LEU
1	EEE	97	ASN
1	FFF	296	LYS
1	GGG	106	ASN
1	HHH	28	ILE
1	HHH	273	SER
1	III	27	LEU
1	III	97	ASN
1	III	196	TYR
1	JJJ	27	LEU
1	JJJ	38	LYS
1	JJJ	98	LEU
1	JJJ	297	ASN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.25	0	3,3,3	0.04	0
2	DMS	EEE	304	-	3,3,3	0.33	0	3,3,3	0.23	0
2	DMS	DDD	302	-	3,3,3	0.33	0	3,3,3	0.19	0
2	DMS	III	301	-	3,3,3	0.52	0	3,3,3	0.89	0
2	DMS	BBB	302	-	3,3,3	0.39	0	3,3,3	0.35	0
2	DMS	FFF	302	-	3,3,3	0.28	0	3,3,3	0.12	0
2	DMS	CCC	303	-	3,3,3	0.54	0	3,3,3	0.19	0
2	DMS	BBB	301	-	3,3,3	0.65	0	3,3,3	1.17	0
2	DMS	CCC	302	-	3,3,3	0.38	0	3,3,3	0.40	0
2	DMS	JJJ	301	-	3,3,3	0.45	0	3,3,3	1.02	0
2	DMS	CCC	301	-	3,3,3	0.67	0	3,3,3	1.49	1 (33%)
2	DMS	HHH	302	-	3,3,3	0.40	0	3,3,3	0.16	0
2	DMS	GGG	302	-	3,3,3	0.44	0	3,3,3	0.26	0
2	DMS	HHH	301	-	3,3,3	0.39	0	3,3,3	1.12	0
2	DMS	III	302	-	3,3,3	0.42	0	3,3,3	0.41	0
2	DMS	AAA	302	-	3,3,3	0.32	0	3,3,3	0.19	0
2	DMS	EEE	303	-	3,3,3	0.47	0	3,3,3	0.32	0
2	DMS	EEE	302	-	3,3,3	0.44	0	3,3,3	0.29	0
2	DMS	DDD	301	-	3,3,3	0.43	0	3,3,3	1.01	0
2	DMS	EEE	301	-	3,3,3	0.49	0	3,3,3	1.10	0
2	DMS	FFF	301	-	3,3,3	0.42	0	3,3,3	0.97	0
2	DMS	AAA	301	-	3,3,3	0.60	0	3,3,3	1.19	0
2	DMS	GGG	301	-	3,3,3	0.33	0	3,3,3	0.85	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	301	DMS	O-S-C1	-2.57	93.64	106.49

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, 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	262/275 (95%)	0.37	18 (6%)	23 25	8, 19, 44, 63	4 (1%)
1	BBB	265/275 (96%)	0.24	21 (7%)	18 20	9, 17, 44, 77	4 (1%)
1	CCC	268/275 (97%)	0.00	11 (4%)	41 45	8, 16, 33, 85	6 (2%)
1	DDD	270/275 (98%)	0.35	23 (8%)	16 18	9, 19, 40, 70	6 (2%)
1	EEE	253/275 (92%)	0.69	42 (16%)	4 4	10, 20, 71, 95	4 (1%)
1	FFF	264/275 (96%)	0.55	24 (9%)	15 16	10, 20, 47, 67	5 (1%)
1	GGG	273/275 (99%)	0.36	21 (7%)	19 21	9, 19, 45, 76	5 (1%)
1	HHH	260/275 (94%)	0.37	23 (8%)	15 17	10, 19, 48, 71	7 (2%)
1	III	273/275 (99%)	0.38	28 (10%)	12 12	9, 18, 42, 66	3 (1%)
1	JJJ	272/275 (98%)	0.30	12 (4%)	39 43	9, 20, 36, 79	6 (2%)
All	All	2660/2750 (96%)	0.36	223 (8%)	17 18	8, 19, 45, 95	50 (1%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EEE	295	VAL	9.3
1	BBB	26	LEU	8.4
1	EEE	37	VAL	8.1
1	EEE	35	LEU	7.9
1	BBB	41	VAL	6.9
1	AAA	27	LEU	6.7
1	FFF	32	VAL	6.5
1	FFF	41	VAL	6.5
1	CCC	102	LEU	6.5
1	FFF	28	ILE	6.5
1	HHH	28	ILE	6.5
1	EEE	31	GLY	6.5
1	EEE	44	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
1	III	41	VAL	6.3
1	EEE	294	SER	6.1
1	EEE	43	ALA	6.1
1	BBB	31	GLY	6.0
1	III	27	LEU	5.8
1	CCC	41	VAL	5.6
1	EEE	32	VAL	5.4
1	DDD	41	VAL	5.2
1	EEE	40	GLY	5.2
1	HHH	27	LEU	5.2
1	EEE	39	THR	5.1
1	JJJ	40	GLY	5.0
1	EEE	34	VAL	5.0
1	GGG	28	ILE	5.0
1	FFF	39	THR	5.0
1	HHH	107	LEU	5.0
1	CCC	103	THR	4.9
1	CCC	27	LEU	4.9
1	BBB	28	ILE	4.9
1	HHH	38	LYS	4.8
1	FFF	35	LEU	4.6
1	BBB	30	GLY	4.5
1	GGG	41	VAL	4.5
1	EEE	36	GLU	4.5
1	AAA	107	LEU	4.5
1	HHH	42	ASP	4.4
1	III	108	LEU	4.2
1	EEE	38	LYS	4.2
1	DDD	40	GLY	4.2
1	III	32	VAL	4.2
1	III	107	LEU	4.2
1	AAA	28	ILE	4.0
1	GGG	27	LEU	4.0
1	HHH	98	LEU	4.0
1	DDD	102	LEU	4.0
1	III	31	GLY	3.9
1	EEE	110	TRP	3.9
1	GGG	299	TYR	3.9
1	DDD	44	ILE	3.9
1	JJJ	44	ILE	3.9
1	GGG	298	PRO	3.9
1	DDD	39	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	JJJ	39	THR	3.9
1	GGG	102	LEU	3.9
1	JJJ	27	LEU	3.9
1	FFF	44	ILE	3.9
1	FFF	30	GLY	3.8
1	FFF	295	VAL	3.8
1	FFF	31	GLY	3.8
1	EEE	97	ASN	3.7
1	BBB	32	VAL	3.7
1	DDD	31	GLY	3.7
1	BBB	27	LEU	3.7
1	FFF	297	ASN	3.6
1	HHH	44	ILE	3.6
1	EEE	42	ASP	3.6
1	HHH	34	VAL	3.6
1	HHH	97	ASN	3.6
1	FFF	38	LYS	3.6
1	FFF	107	LEU	3.6
1	AAA	42	ASP	3.6
1	HHH	29	LYS	3.6
1	III	30	GLY	3.5
1	DDD	27	LEU	3.5
1	EEE	109	MET	3.5
1	EEE	95	LEU	3.5
1	BBB	44	ILE	3.5
1	GGG	32	VAL	3.5
1	FFF	40	GLY	3.4
1	HHH	30	GLY	3.4
1	III	299	TYR	3.4
1	CCC	28	ILE	3.4
1	III	40	GLY	3.3
1	JJJ	42	ASP	3.3
1	DDD	103	THR	3.3
1	GGG	39	THR	3.3
1	EEE	50	PHE	3.3
1	AAA	98	LEU	3.2
1	DDD	104	SER	3.2
1	GGG	104	SER	3.2
1	EEE	250	VAL	3.2
1	FFF	37	VAL	3.2
1	HHH	37	VAL	3.2
1	GGG	31	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	GGG	40	GLY	3.2
1	AAA	44	ILE	3.2
1	EEE	256	ALA	3.2
1	GGG	30	GLY	3.2
1	III	98	LEU	3.2
1	HHH	32	VAL	3.2
1	GGG	38	LYS	3.1
1	III	28	ILE	3.1
1	EEE	249	GLY	3.1
1	AAA	31	GLY	3.1
1	EEE	255	LYS	3.1
1	GGG	106	ASN	3.1
1	EEE	290	LEU	3.1
1	III	102	LEU	3.1
1	AAA	38	LYS	3.1
1	FFF	256	ALA	3.1
1	DDD	32	VAL	3.0
1	III	295	VAL	3.0
1	HHH	31	GLY	3.0
1	III	105	GLY	3.0
1	EEE	96	PRO	3.0
1	BBB	40	GLY	3.0
1	EEE	247	GLU	3.0
1	AAA	260	TYR	3.0
1	III	255	LYS	2.9
1	AAA	32	VAL	2.9
1	BBB	98	LEU	2.9
1	EEE	45	THR	2.9
1	DDD	28	ILE	2.8
1	III	247	GLU	2.8
1	EEE	292	LYS	2.8
1	HHH	256	ALA	2.7
1	HHH	99	ASN	2.7
1	III	297	ASN	2.7
1	BBB	94	PRO	2.7
1	EEE	253	LEU	2.7
1	JJJ	31	GLY	2.7
1	III	298	PRO	2.7
1	EEE	33	GLU	2.7
1	HHH	43	ALA	2.7
1	DDD	30	GLY	2.7
1	III	34	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	BBB	297	ASN	2.7
1	FFF	99	ASN	2.7
1	GGG	101	ASP	2.7
1	GGG	44	ILE	2.7
1	JJJ	28	ILE	2.7
1	FFF	294	SER	2.6
1	DDD	29	LYS	2.6
1	III	29	LYS	2.6
1	BBB	97	ASN	2.6
1	FFF	106	ASN	2.6
1	AAA	30	GLY	2.6
1	HHH	50	PHE	2.6
1	BBB	107	LEU	2.6
1	III	296	LYS	2.6
1	III	97	ASN	2.6
1	AAA	108	LEU	2.5
1	DDD	107	LEU	2.5
1	FFF	33	GLU	2.5
1	BBB	256	ALA	2.5
1	III	106	ASN	2.5
1	EEE	260	TYR	2.5
1	GGG	105	GLY	2.5
1	FFF	34	VAL	2.5
1	JJJ	43	ALA	2.5
1	EEE	47	VAL	2.5
1	III	174	ASP	2.5
1	III	44	ILE	2.4
1	AAA	201	ASN	2.4
1	HHH	35	LEU	2.4
1	CCC	101	ASP	2.4
1	EEE	46	GLU	2.4
1	DDD	97	ASN	2.4
1	BBB	247	GLU	2.4
1	AAA	296	LYS	2.4
1	EEE	258	SER	2.4
1	III	42	ASP	2.4
1	III	101	ASP	2.4
1	FFF	29	LYS	2.4
1	AAA	29	LYS	2.3
1	BBB	38	LYS	2.3
1	DDD	106	ASN	2.3
1	GGG	42	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	EEE	112	ALA	2.3
1	HHH	296	LYS	2.3
1	AAA	34	VAL	2.3
1	AAA	101	ASP	2.3
1	DDD	62	LEU	2.3
1	FFF	108	LEU	2.3
1	JJJ	98	LEU	2.3
1	CCC	99	ASN	2.3
1	EEE	243	VAL	2.3
1	DDD	42	ASP	2.3
1	EEE	291	ARG	2.3
1	JJJ	30	GLY	2.3
1	CCC	296	LYS	2.3
1	AAA	36	GLU	2.3
1	CCC	106	ASN	2.2
1	EEE	248	GLN	2.2
1	GGG	50[A]	PHE	2.2
1	HHH	274	SER	2.2
1	DDD	45	THR	2.2
1	JJJ	38	LYS	2.2
1	DDD	105	GLY	2.2
1	BBB	106	ASN	2.2
1	EEE	259	LEU	2.2
1	EEE	93	ILE	2.2
1	GGG	103	THR	2.2
1	EEE	293	ARG	2.2
1	BBB	50	PHE	2.2
1	III	294	SER	2.1
1	CCC	100	GLU	2.1
1	FFF	247	GLU	2.1
1	JJJ	37	VAL	2.1
1	DDD	43	ALA	2.1
1	DDD	296	LYS	2.1
1	BBB	42	ASP	2.1
1	DDD	98	LEU	2.1
1	CCC	30	GLY	2.1
1	HHH	108	LEU	2.0
1	FFF	36	GLU	2.0
1	HHH	294	SER	2.0
1	BBB	39	THR	2.0
1	EEE	94	PRO	2.0
1	GGG	37	VAL	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($\text{\AA}^2$)	Q<0.9
2	DMS	GGG	302	4/4	0.80	0.19	32,42,43,43	0
2	DMS	FFF	302	4/4	0.86	0.15	31,38,38,39	0
2	DMS	DDD	302	4/4	0.86	0.17	34,34,36,37	0
2	DMS	GGG	303	4/4	0.86	0.18	37,40,48,49	0
2	DMS	III	302	4/4	0.86	0.17	31,32,37,38	0
2	DMS	AAA	302	4/4	0.87	0.16	36,36,36,39	0
2	DMS	EEE	304	4/4	0.87	0.16	37,37,42,42	0
2	DMS	CCC	303	4/4	0.88	0.17	30,35,36,36	0
2	DMS	HHH	302	4/4	0.89	0.15	33,35,37,38	0
2	DMS	GGG	301	4/4	0.89	0.15	24,27,29,30	0
2	DMS	AAA	301	4/4	0.90	0.15	24,27,30,30	0
2	DMS	EEE	303	4/4	0.92	0.14	25,32,32,33	0
2	DMS	BBB	302	4/4	0.92	0.13	25,28,30,31	0
2	DMS	DDD	301	4/4	0.92	0.13	25,27,28,28	0
2	DMS	CCC	301	4/4	0.92	0.13	23,23,29,30	0
2	DMS	BBB	301	4/4	0.93	0.15	19,22,24,25	0
2	DMS	HHH	301	4/4	0.93	0.12	24,26,31,32	0
2	DMS	EEE	301	4/4	0.93	0.12	24,25,30,30	0
2	DMS	FFF	301	4/4	0.93	0.12	25,26,29,30	0
2	DMS	III	301	4/4	0.94	0.11	24,27,28,30	0
2	DMS	EEE	302	4/4	0.95	0.12	31,32,32,35	0
2	DMS	CCC	302	4/4	0.95	0.12	24,25,26,27	0
2	DMS	JJJ	301	4/4	0.95	0.11	22,24,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.