



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:41 PM UTC

PDB ID : 6GAP / pdb_00006gap
Title : Crystal structure of the T3D reovirus sigma1 coiled coil tail and body
Authors : Dietrich, M.H.; Stehle, T.
Deposited on : 2018-04-11
Resolution : 2.15 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

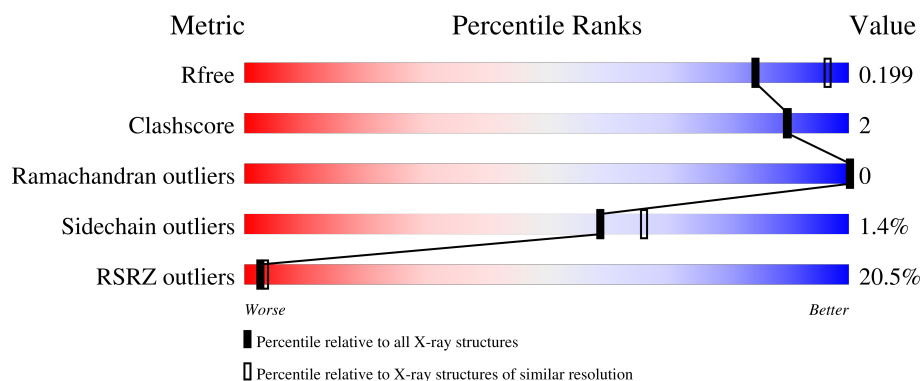
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	A	261	18% 79% 5% 16%
1	B	261	16% 78% • • 18%
1	C	261	16% 76% 5% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5186 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	1	0
			1606	983	295	326	2			
1	B	214	Total	C	N	O	S	0	0	0
			1586	965	295	324	2			
1	C	213	Total	C	N	O	S	0	0	0
			1579	962	290	325	2			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP P03528
A	3	GLY	-	expression tag	UNP P03528
A	4	SER	-	expression tag	UNP P03528
A	5	SER	-	expression tag	UNP P03528
A	6	HIS	-	expression tag	UNP P03528
A	7	HIS	-	expression tag	UNP P03528
A	8	HIS	-	expression tag	UNP P03528
A	9	HIS	-	expression tag	UNP P03528
A	10	HIS	-	expression tag	UNP P03528
A	11	HIS	-	expression tag	UNP P03528
A	12	SER	-	expression tag	UNP P03528
A	13	SER	-	expression tag	UNP P03528
A	14	GLY	-	expression tag	UNP P03528
A	15	LEU	-	expression tag	UNP P03528
A	16	VAL	-	expression tag	UNP P03528
A	17	PRO	-	expression tag	UNP P03528
A	18	ARG	-	expression tag	UNP P03528
A	19	GLY	-	expression tag	UNP P03528
A	20	SER	-	expression tag	UNP P03528
A	21	HIS	-	expression tag	UNP P03528
A	22	MET	-	expression tag	UNP P03528
A	23	ALA	-	expression tag	UNP P03528
A	24	SER	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP P03528
B	3	GLY	-	expression tag	UNP P03528
B	4	SER	-	expression tag	UNP P03528
B	5	SER	-	expression tag	UNP P03528
B	6	HIS	-	expression tag	UNP P03528
B	7	HIS	-	expression tag	UNP P03528
B	8	HIS	-	expression tag	UNP P03528
B	9	HIS	-	expression tag	UNP P03528
B	10	HIS	-	expression tag	UNP P03528
B	11	HIS	-	expression tag	UNP P03528
B	12	SER	-	expression tag	UNP P03528
B	13	SER	-	expression tag	UNP P03528
B	14	GLY	-	expression tag	UNP P03528
B	15	LEU	-	expression tag	UNP P03528
B	16	VAL	-	expression tag	UNP P03528
B	17	PRO	-	expression tag	UNP P03528
B	18	ARG	-	expression tag	UNP P03528
B	19	GLY	-	expression tag	UNP P03528
B	20	SER	-	expression tag	UNP P03528
B	21	HIS	-	expression tag	UNP P03528
B	22	MET	-	expression tag	UNP P03528
B	23	ALA	-	expression tag	UNP P03528
B	24	SER	-	expression tag	UNP P03528
C	2	MET	-	initiating methionine	UNP P03528
C	3	GLY	-	expression tag	UNP P03528
C	4	SER	-	expression tag	UNP P03528
C	5	SER	-	expression tag	UNP P03528
C	6	HIS	-	expression tag	UNP P03528
C	7	HIS	-	expression tag	UNP P03528
C	8	HIS	-	expression tag	UNP P03528
C	9	HIS	-	expression tag	UNP P03528
C	10	HIS	-	expression tag	UNP P03528
C	11	HIS	-	expression tag	UNP P03528
C	12	SER	-	expression tag	UNP P03528
C	13	SER	-	expression tag	UNP P03528
C	14	GLY	-	expression tag	UNP P03528
C	15	LEU	-	expression tag	UNP P03528
C	16	VAL	-	expression tag	UNP P03528
C	17	PRO	-	expression tag	UNP P03528
C	18	ARG	-	expression tag	UNP P03528
C	19	GLY	-	expression tag	UNP P03528
C	20	SER	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	HIS	-	expression tag	UNP P03528
C	22	MET	-	expression tag	UNP P03528
C	23	ALA	-	expression tag	UNP P03528
C	24	SER	-	expression tag	UNP P03528

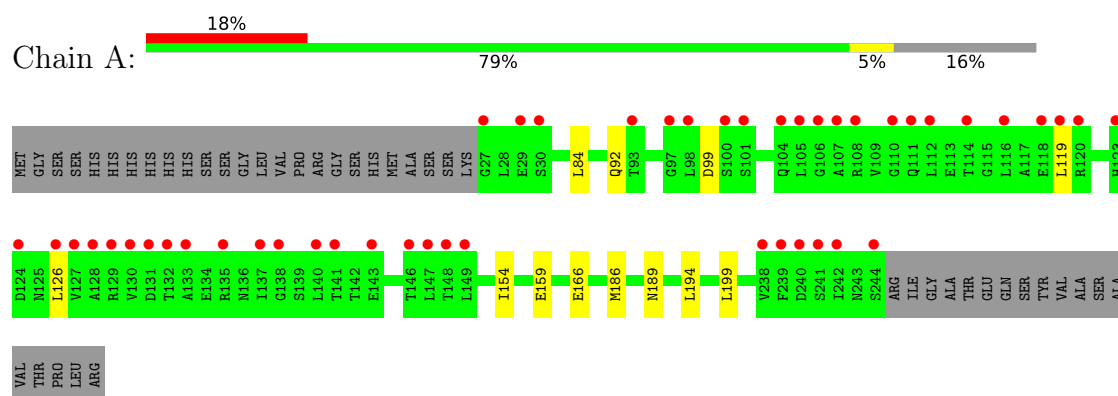
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total 148	O 148	0	0
2	B	119	Total 119	O 119	0	0
2	C	148	Total 148	O 148	0	0

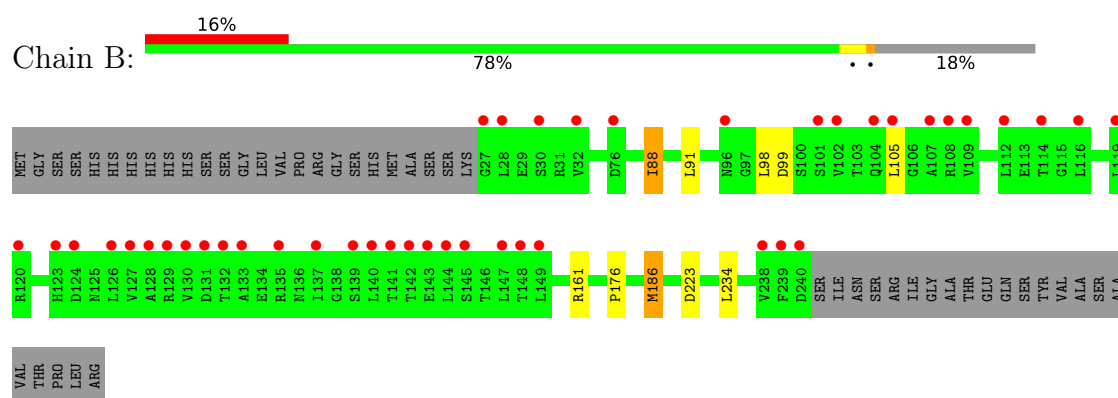
3 Residue-property plots [i](#)

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.

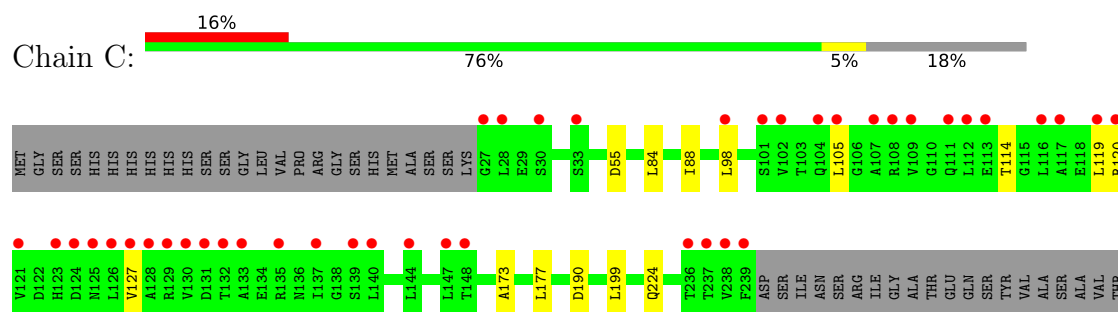
• Molecule 1: Outer capsid protein sigma-1



• Molecule 1: Outer capsid protein sigma-1



• Molecule 1: Outer capsid protein sigma-1



PRO
LEU
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	350.71Å 41.53Å 63.32Å 90.00° 94.98° 90.00°	Depositor
Resolution (Å)	49.15 – 2.15 49.15 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-2.15) 99.9 (49.15-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.208 , 0.249 (Not available) , 0.199	Depositor DCC
R_{free} test set	2513 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.5	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	0.94	EDS
Total number of atoms	5186	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.83% 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

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	A	0.84	0/1617	1.39	0/2194
1	B	0.84	1/1593 (0.1%)	1.38	0/2161
1	C	0.82	0/1586	1.36	3/2151 (0.1%)
All	All	0.84	1/4796 (0.0%)	1.37	3/6506 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	MET	SD-CE	-8.59	1.58	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	THR	CA-C-N	5.35	125.92	119.98
1	C	114	THR	C-N-CA	5.35	125.92	119.98
1	C	190	ASP	CA-CB-CG	5.14	117.74	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1606	0	1597	11	0
1	B	1586	0	1581	11	0
1	C	1579	0	1584	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	148	0	0	0	0
2	B	119	0	0	0	0
2	C	148	0	0	1	0
All	All	5186	0	4762	17	0

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

All (17) 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:A:194:LEU:HD21	1:B:176:PRO:HD3	1.85	0.59
1:B:88:ILE:HD11	1:C:88:ILE:HD11	1.88	0.55
1:B:234:LEU:HD12	1:C:224:GLN:HB3	1.90	0.51
1:C:55:ASP:HB3	2:C:413:HOH:O	2.10	0.51
1:A:84:LEU:HD22	1:C:88:ILE:HD12	1.92	0.49
1:A:199:LEU:HD22	1:B:186:MET:CE	2.42	0.48
1:A:194:LEU:CD2	1:B:176:PRO:HD3	2.42	0.48
1:B:99:ASP:HA	1:C:98:LEU:HD21	1.96	0.47
1:A:99:ASP:HA	1:B:98:LEU:HD21	1.97	0.46
1:A:119:LEU:HD13	1:C:120:ARG:HD2	1.98	0.45
1:B:88:ILE:HD13	1:C:84:LEU:HD22	1.99	0.44
1:A:159:GLU:OE2	1:B:161:ARG:NH2	2.44	0.44
1:A:166:GLU:OE2	1:B:161:ARG:HD2	2.19	0.42
1:A:126:LEU:HD13	1:C:127:VAL:HG22	2.00	0.42
1:A:92:GLN:HG2	1:B:91:LEU:HD13	2.02	0.42
1:A:186:MET:CE	1:C:199:LEU:HD22	2.50	0.41
1:C:173:ALA:HB1	1:C:177:LEU:HB2	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	217/261 (83%)	217 (100%)	0	0	100	100
1	B	212/261 (81%)	211 (100%)	1 (0%)	0	100	100
1	C	211/261 (81%)	209 (99%)	2 (1%)	0	100	100
All	All	640/783 (82%)	637 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	A	172/221 (78%)	170 (99%)	2 (1%)	63	70
1	B	171/221 (77%)	168 (98%)	3 (2%)	51	58
1	C	173/221 (78%)	171 (99%)	2 (1%)	63	70
All	All	516/663 (78%)	509 (99%)	7 (1%)	59	66

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ILE
1	A	189	ASN
1	B	88	ILE
1	B	105	LEU
1	B	223	ASP
1	C	105	LEU
1	C	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	198	ASN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	226	GLN
1	B	42	HIS
1	B	189	ASN
1	B	206	ASN
1	B	213	ASN

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](#)

There are no ligands in this entry.

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	A	218/261 (83%)	0.83	47 (21%) 2 3	18, 40, 83, 112	1 (0%)
1	B	214/261 (81%)	0.88	43 (20%) 3 3	21, 43, 87, 102	0
1	C	213/261 (81%)	0.84	42 (19%) 3 4	21, 42, 87, 102	0
All	All	645/783 (82%)	0.85	132 (20%) 2 3	18, 42, 86, 112	1 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	PHE	8.6
1	A	244	SER	7.7
1	C	121	VAL	5.2
1	A	242	ILE	5.0
1	B	238	VAL	4.6
1	B	239	PHE	4.6
1	B	127	VAL	4.4
1	C	130	VAL	4.4
1	A	241	SER	4.4
1	C	236	THR	4.3
1	A	130	VAL	4.2
1	C	238	VAL	4.1
1	A	148	THR	4.0
1	C	132	THR	4.0
1	C	28	LEU	4.0
1	C	116	LEU	3.9
1	B	112	LEU	3.9
1	B	128	ALA	3.9
1	B	240	ASP	3.8
1	C	117	ALA	3.8
1	A	119	LEU	3.8
1	B	126	LEU	3.7
1	A	116	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	105	LEU	3.7
1	A	127	VAL	3.7
1	C	129	ARG	3.7
1	B	119	LEU	3.6
1	C	112	LEU	3.6
1	C	102	VAL	3.5
1	B	130	VAL	3.5
1	C	126	LEU	3.5
1	B	132	THR	3.5
1	B	133	ALA	3.5
1	B	137	ILE	3.4
1	C	27	GLY	3.4
1	A	112	LEU	3.4
1	A	123	HIS	3.4
1	C	237	THR	3.4
1	B	116	LEU	3.4
1	C	119	LEU	3.4
1	C	124	ASP	3.3
1	A	238	VAL	3.3
1	C	128	ALA	3.2
1	A	131	ASP	3.2
1	A	132	THR	3.2
1	B	27	GLY	3.2
1	B	143	GLU	3.2
1	B	104	GLN	3.2
1	C	133	ALA	3.1
1	A	126	LEU	3.1
1	B	149	LEU	3.1
1	A	120	ARG	3.1
1	A	240	ASP	3.1
1	C	127	VAL	3.1
1	A	98	LEU	3.1
1	A	29	GLU	3.1
1	B	109	VAL	3.1
1	B	145	SER	3.0
1	C	104	GLN	3.0
1	C	107	ALA	3.0
1	A	108	ARG	3.0
1	B	131	ASP	3.0
1	B	144	LEU	3.0
1	B	139	SER	2.9
1	B	123	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	96	ASN	2.9
1	C	111	GLN	2.9
1	B	140	LEU	2.8
1	A	128	ALA	2.8
1	B	76	ASP	2.8
1	C	120	ARG	2.8
1	C	131	ASP	2.8
1	B	105	LEU	2.8
1	A	143	GLU	2.8
1	A	239	PHE	2.8
1	A	27	GLY	2.8
1	C	140	LEU	2.8
1	B	120	ARG	2.8
1	C	109	VAL	2.8
1	A	105	LEU	2.7
1	C	123	HIS	2.7
1	A	118	GLU	2.7
1	C	135	ARG	2.7
1	B	129	ARG	2.7
1	A	135	ARG	2.6
1	A	93	THR	2.6
1	A	149	LEU	2.6
1	A	147	LEU	2.6
1	B	108	ARG	2.6
1	C	144	LEU	2.6
1	A	97	GLY	2.5
1	C	98	LEU	2.5
1	B	114	THR	2.5
1	C	148	THR	2.5
1	A	101	SER	2.5
1	A	107	ALA	2.5
1	C	30	SER	2.5
1	A	30	SER	2.4
1	B	30	SER	2.4
1	C	108	ARG	2.4
1	A	100	SER	2.4
1	B	135	ARG	2.4
1	A	106	GLY	2.4
1	B	124	ASP	2.4
1	B	32	VAL	2.4
1	A	114	THR	2.4
1	A	141	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	133	ALA	2.4
1	B	142	THR	2.4
1	A	138	GLY	2.3
1	C	101	SER	2.3
1	C	137	ILE	2.3
1	A	146	THR	2.3
1	C	139	SER	2.3
1	B	101	SER	2.3
1	C	147	LEU	2.3
1	A	104	GLN	2.2
1	A	124	ASP	2.2
1	B	107	ALA	2.2
1	C	33	SER	2.2
1	C	125	ASN	2.2
1	C	113	GLU	2.1
1	A	110	GLY	2.1
1	B	28	LEU	2.1
1	A	129	ARG	2.1
1	B	148	THR	2.1
1	A	137	ILE	2.1
1	B	102	VAL	2.1
1	B	147	LEU	2.0
1	A	111	GLN	2.0
1	A	140	LEU	2.0
1	B	141	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.