



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:58 AM UTC

PDB ID : 7N9X / pdb_00007n9x
Title : CA-targeting nanobody is a tool for studying HIV-1 capsid lattice interactions
Authors : Gerber, E.E.; Digianantonio, K.M.; Tripler, T.N.; Smaga, S.S.; Summers, B.J.; Xiong, Y.
Deposited on : 2021-06-18
Resolution : 3.51 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

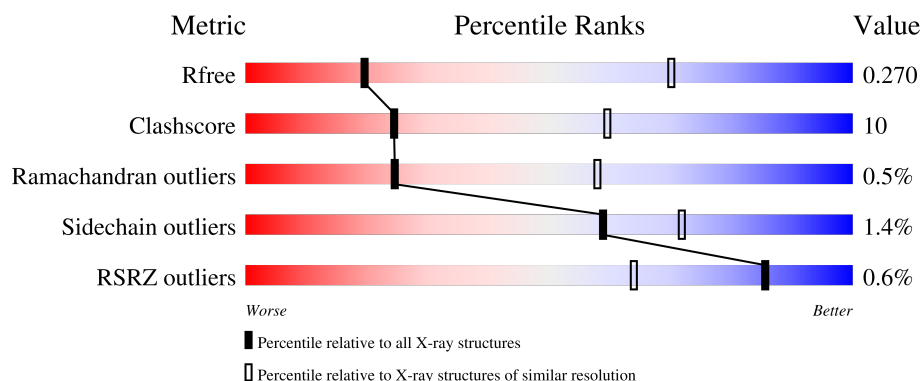
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	222	 81% 17% ..
1	BBB	222	 81% 17% ..
1	CCC	222	 80% 19%
2	FFF	115	 79% 17% . .
3	EEE	112	 70% 29% .

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Mol	Chain	Length	Quality of chain
4	DDD	114	3%58%39%
5	GGG	165	%76%22%
5	HHH	165	74%24%
5	III	165	%76%23%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11458 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	219	Total	C	N	O	S	0	9	0
			1700	1069	298	319	14			
1	CCC	222	Total	C	N	O	S	0	9	0
			1715	1078	301	322	14			
1	AAA	219	Total	C	N	O	S	0	8	0
			1700	1069	298	319	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	14	CYS	ALA	conflict	UNP B6DRA0
BBB	45	CYS	GLU	conflict	UNP B6DRA0
BBB	184	ALA	TRP	conflict	UNP B6DRA0
BBB	185	ALA	MET	conflict	UNP B6DRA0
CCC	14	CYS	ALA	conflict	UNP B6DRA0
CCC	45	CYS	GLU	conflict	UNP B6DRA0
CCC	184	ALA	TRP	conflict	UNP B6DRA0
CCC	185	ALA	MET	conflict	UNP B6DRA0
AAA	14	CYS	ALA	conflict	UNP B6DRA0
AAA	45	CYS	GLU	conflict	UNP B6DRA0
AAA	184	ALA	TRP	conflict	UNP B6DRA0
AAA	185	ALA	MET	conflict	UNP B6DRA0

- Molecule 2 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	FFF	113	Total	C	N	O	S	0	0	0
			857	538	151	164	4			

- Molecule 3 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	EEE	112	Total	C	N	O	S	0	0	0
			851	535	150	162	4			

- Molecule 4 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	112	Total	C	N	O	S	0	0	0
			852	535	153	161	3			

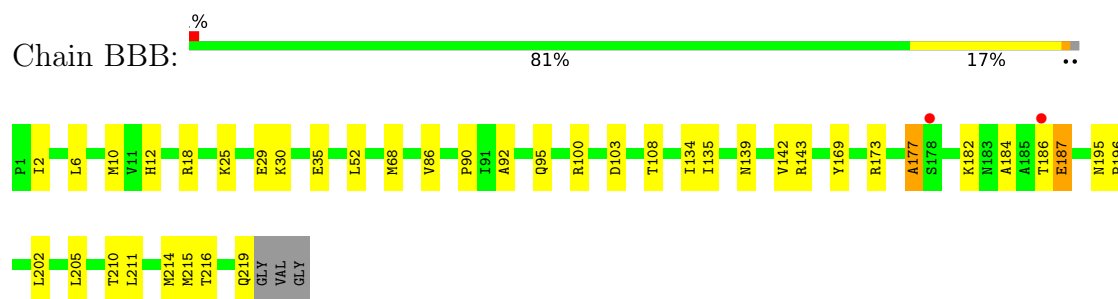
- Molecule 5 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	GGG	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
5	HHH	163	Total	C	N	O	S	12	0	0
			1251	792	216	235	8			
5	III	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			

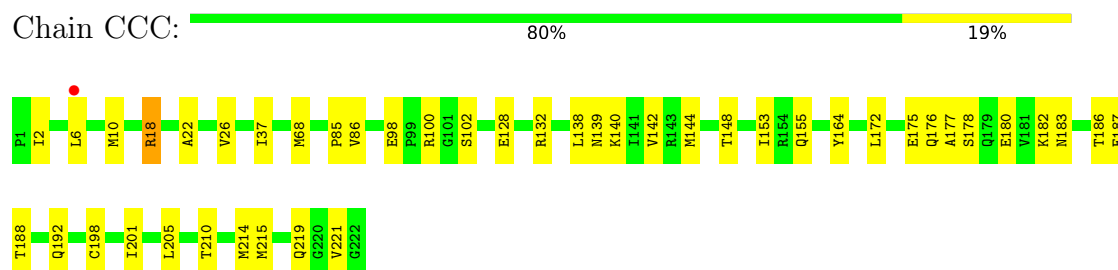
3 Residue-property plots

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.

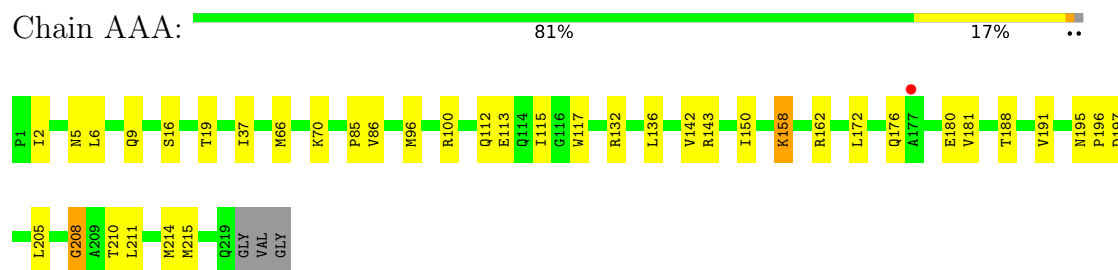
- Molecule 1: Capsid protein



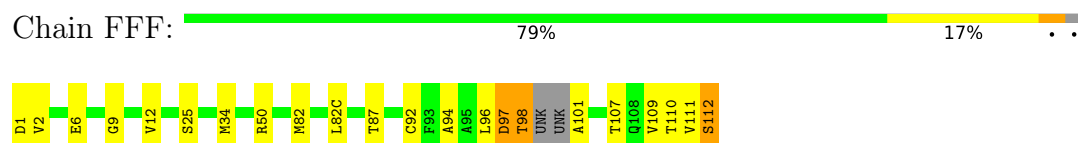
- Molecule 1: Capsid protein



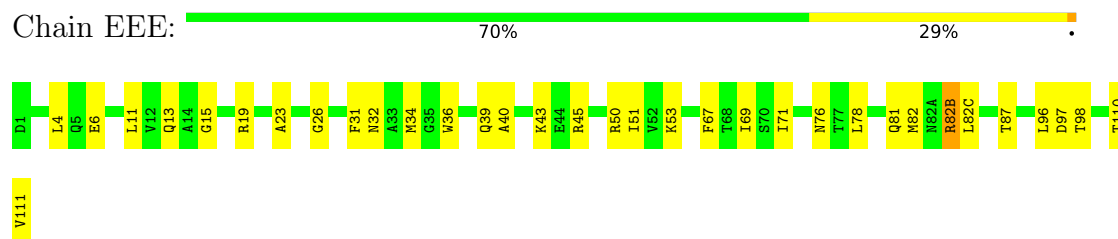
- Molecule 1: Capsid protein



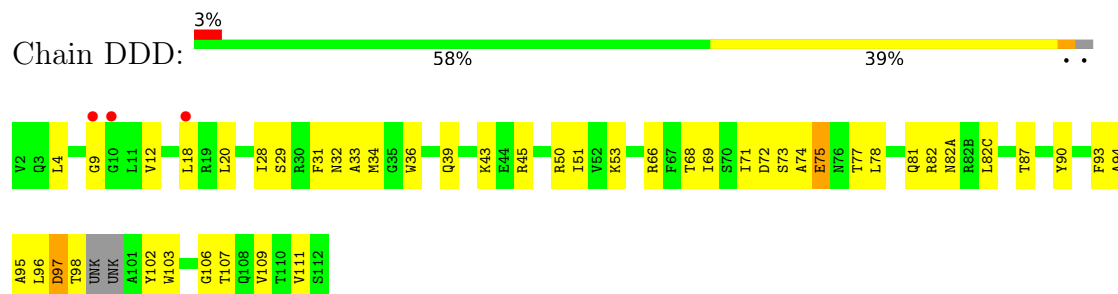
- Molecule 2: Nanobody



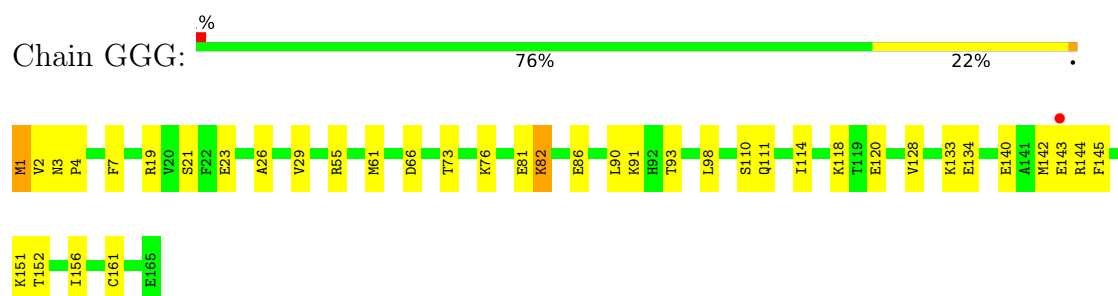
- Molecule 3: Nanobody



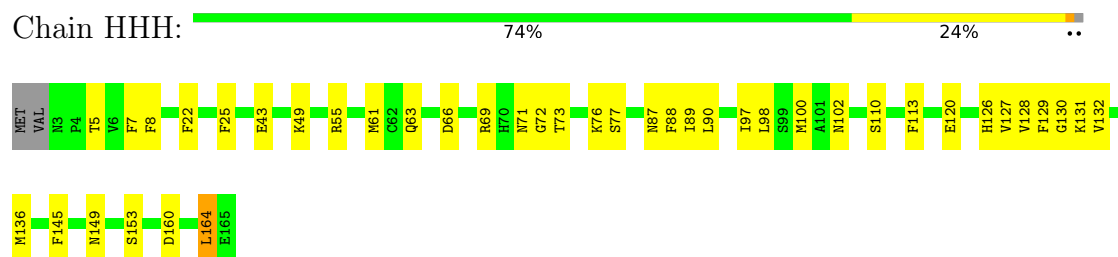
- Molecule 4: Nanobody



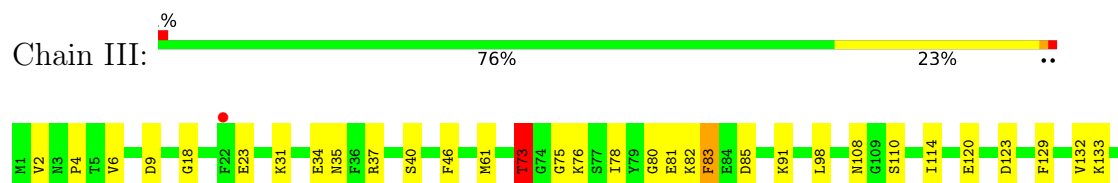
- Molecule 5: Peptidyl-prolyl cis-trans isomerase A



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M136	M137	I138	V139	E140	A141	R144	N149	C161	G162	E165
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.95Å 137.85Å 313.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.58 – 3.51 49.58 – 3.51	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.58-3.51) 94.4 (49.58-3.51)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.245 , 0.270 0.245 , 0.270	Depositor DCC
R_{free} test set	1668 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	94.4	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 115.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11458	wwPDB-VP
Average B, all atoms (Å ²)	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	AAA	0.23	0/1737	0.66	2/2361 (0.1%)
1	BBB	0.25	0/1737	0.61	0/2361
1	CCC	0.23	0/1752	0.60	0/2381
2	FFF	0.23	0/872	0.76	3/1178 (0.3%)
3	EEE	0.24	0/867	0.69	0/1173
4	DDD	0.38	0/867	1.00	2/1171 (0.2%)
5	GGG	0.29	0/1294	0.80	3/1733 (0.2%)
5	HHH	0.24	0/1279	0.71	0/1713
5	III	0.27	0/1294	0.89	8/1733 (0.5%)
All	All	0.26	0/11699	0.73	18/15804 (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
5	III	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	GGG	144	ARG	CB-CG-CD	-10.77	86.52	111.30
5	III	82	LYS	CA-C-N	-10.58	104.30	122.92
5	III	82	LYS	C-N-CA	-10.58	104.30	122.92
5	III	81	GLU	N-CA-C	-7.15	97.42	108.00
5	III	73	THR	CA-C-N	-6.92	117.28	122.33
5	III	73	THR	C-N-CA	-6.92	117.28	122.33
4	DDD	75	GLU	CA-CB-CG	6.55	127.21	114.10
5	III	82	LYS	CA-CB-CG	5.71	125.53	114.10
2	FFF	97	ASP	CA-C-N	5.40	131.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FFF	97	ASP	C-N-CA	5.40	131.42	121.70
5	GGG	144	ARG	CD-NE-CZ	-5.30	116.98	124.40
5	GGG	144	ARG	CB-CA-C	-5.16	99.64	110.17
2	FFF	98	THR	N-CA-CB	5.12	120.21	111.50
1	AAA	208	GLY	CA-C-N	-5.10	113.77	122.33
1	AAA	208	GLY	C-N-CA	-5.10	113.77	122.33
5	III	82	LYS	N-CA-C	5.04	118.55	111.90
5	III	75	GLY	N-CA-C	-5.04	101.25	113.18
4	DDD	75	GLU	CB-CA-C	-5.03	100.95	110.01

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	III	46	PHE	Mainchain

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	AAA	1700	0	1697	26	0
1	BBB	1700	0	1691	29	0
1	CCC	1715	0	1707	27	0
2	FFF	857	0	838	15	0
3	EEE	851	0	834	25	0
4	DDD	852	0	835	43	0
5	GGG	1266	0	1237	26	0
5	HHH	1251	0	1216	27	0
5	III	1266	0	1237	23	0
All	All	11458	0	11292	226	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 10.

All (226) 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)
4:DDD:9:GLY:HA3	4:DDD:107:THR:HG21	1.40	1.03
4:DDD:4:LEU:HD11	4:DDD:102:TYR:HB3	1.44	0.98
5:GGG:118:LYS:HE2	5:GGG:120:GLU:HG2	1.59	0.83
1:AAA:85:PRO:HB2	5:GGG:73:THR:HG21	1.61	0.81
5:GGG:1:MET:HE2	5:GGG:3:ASN:HB2	1.64	0.80
1:AAA:86:VAL:HG21	1:AAA:100:ARG:HG2	1.64	0.78
5:III:35:ASN:HD22	5:III:83:PHE:HE2	1.32	0.77
1:AAA:208:GLY:O	4:DDD:50:ARG:NH2	2.18	0.76
5:GGG:21:SER:HB2	5:GGG:134:GLU:H	1.51	0.75
4:DDD:39:GLN:HB2	4:DDD:45:ARG:HG3	1.67	0.74
1:BBB:68:MET:HG3	1:AAA:211:LEU:HD22	1.71	0.73
4:DDD:32:ASN:HA	4:DDD:53:LYS:HE2	1.71	0.73
5:III:76:LYS:O	5:III:110:SER:HB3	1.89	0.73
5:III:35:ASN:ND2	5:III:83:PHE:HE2	1.88	0.72
1:BBB:182:LYS:O	1:BBB:186:THR:OG1	2.05	0.72
4:DDD:96:LEU:O	4:DDD:98:THR:N	2.24	0.71
1:BBB:135:ILE:O	1:BBB:139:ASN:ND2	2.25	0.70
4:DDD:69:ILE:HD11	4:DDD:78:LEU:HD11	1.74	0.70
2:FFF:34:MET:HE3	2:FFF:94:ALA:HB2	1.76	0.68
4:DDD:51:ILE:HG21	4:DDD:71:ILE:CD1	2.25	0.66
5:III:76:LYS:NZ	5:III:80:GLY:HA2	2.11	0.66
1:CCC:86:VAL:HG21	1:CCC:100:ARG:HG2	1.78	0.66
4:DDD:33:ALA:HB3	4:DDD:95:ALA:HB3	1.77	0.65
5:GGG:7:PHE:CD2	5:GGG:19:ARG:HD3	2.32	0.64
3:EEE:96:LEU:O	3:EEE:98:THR:N	2.31	0.63
4:DDD:28:ILE:HG22	4:DDD:73:SER:HA	1.78	0.63
4:DDD:90:TYR:O	4:DDD:106:GLY:HA2	1.98	0.63
1:AAA:150[A]:ILE:HD12	1:AAA:172:LEU:HD13	1.79	0.62
1:BBB:68:MET:CG	1:AAA:211:LEU:HD22	2.29	0.62
1:BBB:139:ASN:O	1:BBB:143:ARG:HG3	2.00	0.62
3:EEE:36:TRP:HE1	3:EEE:78:LEU:HD22	1.65	0.61
1:AAA:188:THR:O	1:AAA:191:VAL:HG22	2.01	0.61
1:BBB:202:LEU:HD22	1:BBB:214[A]:MET:HE3	1.83	0.61
4:DDD:9:GLY:HA3	4:DDD:107:THR:CG2	2.25	0.61
5:HHH:5:THR:HB	5:HHH:164:LEU:HB2	1.82	0.60
5:III:2:VAL:HG22	5:III:4:PRO:HD3	1.84	0.59
4:DDD:36:TRP:HE1	4:DDD:78:LEU:HG	1.67	0.59
4:DDD:18:LEU:O	4:DDD:82:ARG:HG3	2.02	0.59
1:CCC:188:THR:O	1:CCC:192:GLN:NE2	2.35	0.59
2:FFF:97:ASP:O	2:FFF:98:THR:HG22	2.03	0.59
4:DDD:87:THR:HA	4:DDD:109:VAL:O	2.03	0.59
3:EEE:67:PHE:CE1	3:EEE:82:MET:HB3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DDD:34:MET:HA	4:DDD:94:ALA:HA	1.85	0.58
4:DDD:51:ILE:HG21	4:DDD:71:ILE:HD12	1.86	0.58
1:AAA:158:LYS:H	1:AAA:158:LYS:HD3	1.67	0.58
5:III:76:LYS:HZ2	5:III:80:GLY:HA2	1.69	0.58
3:EEE:26:GLY:O	3:EEE:76:ASN:ND2	2.37	0.57
4:DDD:66:ARG:O	4:DDD:82(A):ASN:HB2	2.04	0.57
1:BBB:2:ILE:HG22	1:BBB:10:MET:HE3	1.87	0.57
2:FFF:98:THR:HG1	2:FFF:101:ALA:N	2.03	0.56
3:EEE:87:THR:HG23	3:EEE:110:THR:HA	1.87	0.56
1:CCC:2:ILE:HG22	1:CCC:10:MET:HE3	1.88	0.56
4:DDD:72:ASP:OD2	4:DDD:74:ALA:HB3	2.05	0.56
1:AAA:132:ARG:O	1:AAA:136:LEU:HD23	2.07	0.55
4:DDD:36:TRP:NE1	4:DDD:78:LEU:HG	2.21	0.55
5:III:91:LYS:HE3	5:III:123:ASP:HB3	1.87	0.55
1:CCC:205:LEU:O	2:FFF:50:ARG:NH1	2.40	0.55
1:AAA:2:ILE:HD11	1:AAA:115:ILE:HG12	1.87	0.55
1:AAA:195:ASN:OD1	1:AAA:196[A]:PRO:HD2	2.06	0.55
4:DDD:68:THR:O	4:DDD:81:GLN:N	2.35	0.55
1:BBB:6:LEU:HB3	1:CCC:6:LEU:HD12	1.89	0.55
5:HHH:132:VAL:HG11	5:HHH:136:MET:HG2	1.89	0.55
5:HHH:102:ASN:OD1	5:HHH:126:HIS:ND1	2.39	0.55
2:FFF:6:GLU:HG3	2:FFF:92:CYS:SG	2.47	0.54
1:BBB:139:ASN:O	1:BBB:142:VAL:HG22	2.08	0.54
5:GGG:90:LEU:HB3	5:GGG:128:VAL:HB	1.90	0.54
5:III:40:SER:O	5:III:161:CYS:HB2	2.08	0.54
4:DDD:69:ILE:CD1	4:DDD:78:LEU:HD11	2.37	0.53
3:EEE:36:TRP:NE1	3:EEE:78:LEU:HD22	2.23	0.53
4:DDD:51:ILE:HG21	4:DDD:71:ILE:HD11	1.89	0.53
5:GGG:140:GLU:O	5:GGG:143:GLU:HG2	2.08	0.53
5:HHH:90:LEU:HB2	5:HHH:128:VAL:HB	1.91	0.52
5:GGG:23:GLU:HB2	5:GGG:133:LYS:HG2	1.91	0.52
4:DDD:9:GLY:CA	4:DDD:107:THR:HG21	2.28	0.51
1:CCC:210:THR:O	1:CCC:214[A]:MET:HG2	2.10	0.51
3:EEE:82(C):LEU:HB3	3:EEE:111:VAL:HG21	1.91	0.51
5:GGG:2:VAL:O	5:GGG:26:ALA:HB3	2.10	0.51
5:III:23:GLU:HB2	5:III:133:LYS:HD3	1.91	0.51
1:BBB:30:LYS:NZ	1:BBB:35:GLU:OE1	2.35	0.51
2:FFF:82:MET:HE2	2:FFF:82(C):LEU:HD21	1.92	0.51
5:III:120:GLU:CD	5:III:120:GLU:H	2.18	0.51
5:III:140:GLU:O	5:III:144:ARG:NH1	2.43	0.51
4:DDD:29:SER:HB3	4:DDD:73:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:HHH:55:ARG:HB3	5:HHH:63:GLN:HG2	1.93	0.51
5:HHH:69:ARG:HH12	5:HHH:71:ASN:HD21	1.57	0.51
3:EEE:13:GLN:OE1	3:EEE:13:GLN:N	2.34	0.51
3:EEE:69:ILE:HD11	3:EEE:78:LEU:HD21	1.93	0.51
5:HHH:76:LYS:O	5:HHH:110:SER:HB3	2.10	0.51
5:III:18:GLY:HA3	5:III:138:ILE:HG12	1.93	0.51
3:EEE:34:MET:HB3	3:EEE:78:LEU:HD12	1.91	0.51
3:EEE:51:ILE:HG21	3:EEE:71:ILE:HD11	1.92	0.51
4:DDD:4:LEU:CD1	4:DDD:102:TYR:HB3	2.30	0.51
5:HHH:88:PHE:HE1	5:HHH:127:VAL:HG22	1.75	0.51
5:GGG:76:LYS:O	5:GGG:110:SER:HB3	2.12	0.50
4:DDD:93:PHE:HB2	4:DDD:102:TYR:O	2.11	0.50
3:EEE:39:GLN:HB2	3:EEE:45:ARG:HG3	1.92	0.50
5:GGG:1:MET:HG2	5:GGG:2:VAL:N	2.26	0.50
1:BBB:86:VAL:HG21	1:BBB:100:ARG:HG2	1.92	0.50
1:BBB:210:THR:O	1:BBB:214[A]:MET:HG2	2.11	0.50
5:HHH:25:PHE:HD1	5:HHH:130:GLY:HA2	1.76	0.50
5:III:132:VAL:HG11	5:III:136:MET:HG2	1.94	0.50
5:HHH:145:PHE:O	5:HHH:153:SER:N	2.41	0.49
1:CCC:172:LEU:HD22	1:CCC:182:LYS:HG2	1.94	0.49
3:EEE:11:LEU:HA	3:EEE:110:THR:O	2.12	0.49
5:GGG:29:VAL:HG12	5:GGG:29:VAL:O	2.12	0.49
1:AAA:112:GLN:HG3	1:AAA:113:GLU:N	2.28	0.49
1:AAA:210:THR:O	1:AAA:214[A]:MET:HG2	2.13	0.49
1:AAA:162:ARG:HG3	1:AAA:215:MET:HE1	1.95	0.49
3:EEE:31:PHE:O	3:EEE:53:LYS:HE2	2.13	0.48
1:BBB:215:MET:HE2	1:CCC:68:MET:HE2	1.95	0.48
1:AAA:85:PRO:HB2	5:GGG:73:THR:CG2	2.39	0.48
1:CCC:201:ILE:HD11	2:FFF:98:THR:HA	1.96	0.48
5:III:6:VAL:HG13	5:III:162:GLY:O	2.13	0.48
5:HHH:87:ASN:HB3	5:HHH:89:ILE:HG13	1.96	0.48
4:DDD:51:ILE:HG23	4:DDD:51:ILE:O	2.14	0.48
1:AAA:96:MET:HG2	1:AAA:117:TRP:NE1	2.29	0.47
3:EEE:40:ALA:HB3	3:EEE:43:LYS:HB2	1.96	0.47
4:DDD:82:ARG:CB	4:DDD:82(C):LEU:HD21	2.44	0.47
5:GGG:7:PHE:O	5:GGG:161:CYS:HA	2.14	0.47
1:AAA:5:ASN:ND2	1:AAA:9:GLN:O	2.47	0.47
3:EEE:32:ASN:HA	3:EEE:53:LYS:HE2	1.95	0.47
1:BBB:18:ARG:HD3	1:CCC:18:ARG:HH11	1.79	0.47
1:BBB:52:LEU:HD23	1:BBB:134:ILE:HD12	1.97	0.47
1:AAA:16:SER:O	1:AAA:19:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FFF:9:GLY:HA3	2:FFF:107:THR:OG1	2.15	0.47
3:EEE:19:ARG:NH1	3:EEE:81:GLN:OE1	2.45	0.47
5:GGG:118:LYS:HG2	5:GGG:120:GLU:HG3	1.97	0.47
1:BBB:18:ARG:HD3	1:CCC:18:ARG:NH1	2.30	0.47
5:GGG:98:LEU:HD13	5:GGG:114:ILE:HG12	1.96	0.47
4:DDD:33:ALA:O	4:DDD:95:ALA:N	2.25	0.47
4:DDD:75:GLU:O	4:DDD:77:THR:HG23	2.15	0.47
5:HHH:22:PHE:CD2	5:HHH:98:LEU:HD22	2.51	0.46
1:CCC:86:VAL:HG13	1:CCC:98:GLU:HB2	1.97	0.46
1:AAA:205:LEU:O	4:DDD:50:ARG:NH1	2.49	0.46
5:III:98:LEU:HG	5:III:129:PHE:CZ	2.51	0.45
2:FFF:87:THR:HA	2:FFF:109:VAL:O	2.16	0.45
1:BBB:169:TYR:HE2	1:BBB:211:LEU:HD21	1.81	0.45
5:III:35:ASN:OD1	5:III:78:ILE:HG23	2.15	0.45
4:DDD:82:ARG:HB2	4:DDD:82(C):LEU:HD21	1.98	0.45
1:BBB:92:ALA:HB3	1:BBB:95:GLN:CG	2.46	0.45
5:HHH:49:LYS:HG2	5:HHH:160:ASP:HA	1.97	0.45
1:BBB:103:ASP:OD1	1:BBB:108:THR:HG23	2.17	0.45
4:DDD:43:LYS:HD3	4:DDD:43:LYS:HA	1.82	0.45
1:AAA:143:ARG:HD3	1:AAA:176:GLN:H	1.82	0.45
1:CCC:198:CYS:SG	1:CCC:221:VAL:HG21	2.57	0.45
4:DDD:93:PHE:HB3	4:DDD:103:TRP:CE3	2.52	0.45
5:III:91:LYS:HG3	5:III:123:ASP:CG	2.42	0.45
5:HHH:76:LYS:HG2	5:HHH:77:SER:O	2.17	0.44
5:III:31:LYS:NZ	5:III:83:PHE:HB2	2.31	0.44
5:III:85:ASP:OD1	5:III:108:ASN:ND2	2.28	0.44
1:CCC:85:PRO:HB2	5:III:73:THR:HG23	1.99	0.44
1:CCC:186:THR:C	1:CCC:188:THR:H	2.25	0.44
1:CCC:37:ILE:HD13	1:CCC:139:ASN:OD1	2.17	0.44
5:GGG:21:SER:OG	5:GGG:134:GLU:HB3	2.18	0.44
1:BBB:205:LEU:HD12	1:BBB:205:LEU:HA	1.83	0.44
5:HHH:43:GLU:H	5:HHH:43:GLU:HG2	1.64	0.44
5:HHH:120:GLU:H	5:HHH:120:GLU:CD	2.25	0.44
1:AAA:66:MET:O	1:AAA:70:LYS:HG2	2.18	0.44
1:CCC:178:SER:O	1:CCC:182:LYS:HG3	2.18	0.43
3:EEE:96:LEU:HA	3:EEE:96:LEU:HD12	1.74	0.43
5:HHH:87:ASN:O	5:HHH:127:VAL:HG13	2.17	0.43
5:HHH:69:ARG:NH1	5:HHH:71:ASN:HD21	2.15	0.43
1:CCC:175:GLU:O	1:CCC:177:ALA:N	2.52	0.43
3:EEE:6:GLU:OE1	3:EEE:6:GLU:N	2.48	0.43
5:HHH:100:MET:HE3	5:HHH:100:MET:HB3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:III:98:LEU:HD13	5:III:114:ILE:HG12	2.00	0.43
4:DDD:12:VAL:HG23	4:DDD:111:VAL:HG13	2.00	0.43
5:GGG:23:GLU:CB	5:GGG:133:LYS:HG2	2.49	0.43
1:BBB:184:ALA:HA	1:BBB:187:GLU:OE2	2.19	0.43
2:FFF:6:GLU:OE1	2:FFF:6:GLU:N	2.45	0.43
5:GGG:29:VAL:HG13	5:GGG:86:GLU:OE1	2.19	0.43
1:CCC:22:ALA:O	1:CCC:26:VAL:HG13	2.18	0.43
2:FFF:12:VAL:O	2:FFF:111:VAL:HA	2.18	0.43
1:BBB:92:ALA:HB3	1:BBB:95:GLN:HG3	2.00	0.43
5:GGG:66:ASP:HB2	5:GGG:111:GLN:NE2	2.34	0.43
1:BBB:25:LYS:HD2	1:BBB:29:GLU:OE2	2.18	0.43
1:BBB:195:ASN:HB2	1:BBB:196[A]:PRO:HD2	2.01	0.43
1:CCC:138:LEU:O	1:CCC:142:VAL:HG13	2.19	0.42
4:DDD:34:MET:CE	4:DDD:71:ILE:HD13	2.50	0.42
1:BBB:205:LEU:O	3:EEE:50:ARG:HD3	2.19	0.42
5:GGG:91:LYS:O	5:GGG:93:THR:HG23	2.19	0.42
1:CCC:139:ASN:O	1:CCC:142:VAL:HG22	2.20	0.42
1:CCC:180:GLU:HA	1:CCC:183:ASN:ND2	2.35	0.42
1:BBB:90:PRO:HG3	5:HHH:113:PHE:CD2	2.55	0.42
4:DDD:96:LEU:O	4:DDD:97:ASP:C	2.62	0.42
5:GGG:2:VAL:O	5:GGG:4:PRO:HD3	2.19	0.42
5:HHH:66:ASP:OD2	5:HHH:72:GLY:N	2.51	0.42
1:AAA:96:MET:HG2	1:AAA:117:TRP:HE1	1.84	0.42
2:FFF:96:LEU:HD23	2:FFF:97:ASP:OD2	2.20	0.42
5:GGG:81:GLU:HB3	5:GGG:82:LYS:H	1.62	0.42
5:GGG:145:PHE:O	5:GGG:152:THR:HA	2.19	0.42
1:BBB:216:THR:O	1:BBB:219:GLN:HG2	2.20	0.41
1:AAA:37:ILE:HD11	1:AAA:142:VAL:HG21	2.02	0.41
1:AAA:180:GLU:HG3	1:AAA:181:VAL:H	1.84	0.41
1:CCC:140:LYS:O	1:CCC:144:MET:HG2	2.21	0.41
4:DDD:69:ILE:CG1	4:DDD:78:LEU:HD11	2.50	0.41
5:HHH:25:PHE:HE1	5:HHH:131:LYS:HB3	1.85	0.41
5:HHH:88:PHE:CE1	5:HHH:127:VAL:HG22	2.53	0.41
5:HHH:69:ARG:HH11	5:HHH:73:THR:HB	1.85	0.41
5:HHH:97:ILE:HG23	5:HHH:128:VAL:HG13	2.01	0.41
5:III:34:GLU:OE1	5:III:37:ARG:NH2	2.53	0.41
2:FFF:1:ASP:HB3	2:FFF:2:VAL:H	1.57	0.41
2:FFF:87:THR:HG23	2:FFF:110:THR:HG23	2.03	0.41
3:EEE:4:LEU:HA	3:EEE:23:ALA:O	2.21	0.41
4:DDD:20:LEU:HB3	4:DDD:36:TRP:CH2	2.55	0.41
1:CCC:148:THR:OG1	1:CCC:153:ILE:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:215:MET:O	1:CCC:219:GLN:HG3	2.20	0.41
5:GGG:142:MET:HE3	5:GGG:156:ILE:HG21	2.03	0.41
1:AAA:215:MET:HE2	1:AAA:215:MET:HB3	1.95	0.41
3:EEE:15:GLY:HA2	3:EEE:82(B):ARG:HA	2.03	0.41
1:BBB:173:ARG:O	1:BBB:177:ALA:HA	2.21	0.41
1:CCC:155:GLN:HG3	1:CCC:164:TYR:HB2	2.03	0.41
4:DDD:28:ILE:HD12	4:DDD:31:PHE:CD1	2.55	0.41
5:III:141:ALA:HA	5:III:144:ARG:NE	2.36	0.41
2:FFF:111:VAL:O	2:FFF:112:SER:HB2	2.20	0.41
4:DDD:34:MET:HG3	4:DDD:94:ALA:HB1	2.02	0.41
5:HHH:7:PHE:C	5:HHH:8:PHE:HD1	2.28	0.41
5:HHH:98:LEU:HG	5:HHH:129:PHE:CZ	2.55	0.41
3:EEE:34:MET:HE3	3:EEE:34:MET:HB2	1.97	0.41
5:GGG:151:LYS:HD3	5:GGG:151:LYS:HA	1.70	0.40
3:EEE:96:LEU:O	3:EEE:98:THR:O	2.39	0.40
1:AAA:6:LEU:HD13	1:AAA:6:LEU:HA	1.89	0.40
1:BBB:2:ILE:HD13	1:BBB:12:HIS:HA	2.04	0.40
1:CCC:128:GLU:O	1:CCC:132:ARG:HG3	2.21	0.40
3:EEE:34:MET:HB3	3:EEE:78:LEU:CD1	2.51	0.40
4:DDD:34:MET:HE2	4:DDD:71:ILE:HD13	2.04	0.40

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	AAA	217/222 (98%)	208 (96%)	9 (4%)	0	100	100
1	BBB	217/222 (98%)	211 (97%)	4 (2%)	2 (1%)	14	48
1	CCC	220/222 (99%)	215 (98%)	3 (1%)	2 (1%)	14	48
2	FFF	109/115 (95%)	107 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EEE	110/112 (98%)	108 (98%)	1 (1%)	1 (1%)	14	48
4	DDD	108/114 (95%)	106 (98%)	1 (1%)	1 (1%)	14	48
5	GGG	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
5	HHH	161/165 (98%)	153 (95%)	7 (4%)	1 (1%)	21	55
5	III	163/165 (99%)	156 (96%)	6 (4%)	1 (1%)	21	55
All	All	1468/1502 (98%)	1420 (97%)	40 (3%)	8 (0%)	24	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	EEE	97	ASP
4	DDD	97	ASP
1	BBB	177	ALA
1	CCC	176	GLN
5	III	73	THR
5	HHH	164	LEU
1	CCC	187	GLU
1	BBB	187	GLU

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	186/187 (100%)	184 (99%)	2 (1%)	65	75
1	BBB	186/187 (100%)	186 (100%)	0	100	100
1	CCC	187/187 (100%)	185 (99%)	2 (1%)	65	75
2	FFF	88/88 (100%)	86 (98%)	2 (2%)	44	65
3	EEE	87/87 (100%)	86 (99%)	1 (1%)	65	75
4	DDD	87/87 (100%)	87 (100%)	0	100	100
5	GGG	133/133 (100%)	129 (97%)	4 (3%)	36	60
5	HHH	131/133 (98%)	129 (98%)	2 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	III	133/133 (100%)	129 (97%)	4 (3%)	36	60
All	All	1218/1222 (100%)	1201 (99%)	17 (1%)	59	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	18	ARG
1	CCC	102	SER
1	AAA	158	LYS
1	AAA	197	ASP
2	FFF	25	SER
2	FFF	112	SER
3	EEE	82(B)	ARG
5	GGG	1	MET
5	GGG	55	ARG
5	GGG	61	MET
5	GGG	82	LYS
5	HHH	61	MET
5	HHH	149	ASN
5	III	9	ASP
5	III	61	MET
5	III	83	PHE
5	III	149	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	219/222 (98%)	0.03	1 (0%) 87 67	78, 127, 235, 275	0
1	BBB	219/222 (98%)	0.04	2 (0%) 81 56	83, 119, 191, 304	0
1	CCC	222/222 (100%)	0.01	1 (0%) 87 67	80, 121, 177, 253	0
2	FFF	113/115 (98%)	0.09	0 100 100	116, 183, 257, 280	0
3	EEE	112/112 (100%)	0.14	0 100 100	134, 224, 291, 311	0
4	DDD	112/114 (98%)	0.43	3 (2%) 56 32	207, 299, 361, 423	0
5	GGG	165/165 (100%)	0.13	1 (0%) 85 64	122, 200, 289, 327	0
5	HHH	162/165 (98%)	0.13	0 100 100	94, 207, 289, 389	2 (1%)
5	III	165/165 (100%)	0.05	1 (0%) 85 64	121, 204, 295, 391	0
All	All	1489/1502 (99%)	0.10	9 (0%) 85 64	78, 169, 299, 423	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	6	LEU	3.0
1	BBB	186	THR	2.8
4	DDD	10	GLY	2.6
1	AAA	177	ALA	2.6
5	III	22	PHE	2.4
4	DDD	9	GLY	2.4
1	BBB	178	SER	2.3
5	GGG	143	GLU	2.2
4	DDD	18	LEU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no 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.