



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:16 PM UTC

PDB ID : 6T9D / pdb_00006t9d
Title : Crystal structure of a bispecific DutaFab in complex with human VEGF121
Authors : Kimbung, R.; Logan, D.T.; Beckmann, R.; Jensen, K.; Speck, J.; Fenn, S.; Kettenberger, H.
Deposited on : 2019-10-28
Resolution : 2.90 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

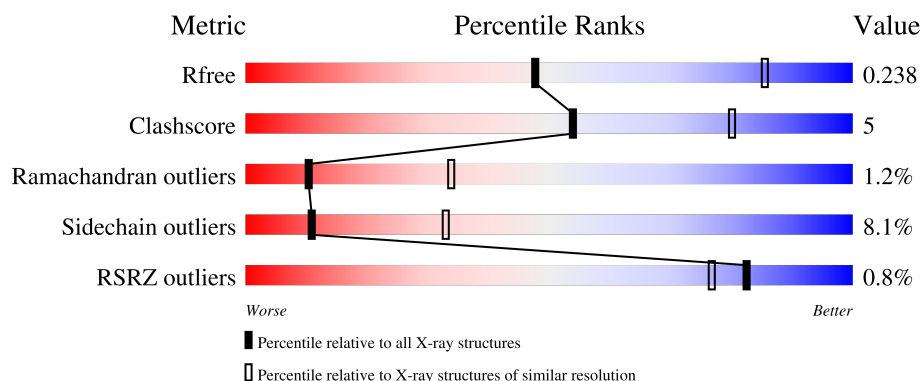
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	220	
1	HHH	220	
2	BBB	213	
2	LLL	213	
3	CCC	121	

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Mol	Chain	Length	Quality of chain
3	DDD	121	% 67% 9% •• 21%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8284 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 VP mat DutaFab VH chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	212	Total	C	N	O	S	0	0	0
			1597	1013	264	314	6			
1	HHH	210	Total	C	N	O	S	0	0	0
			1586	1007	262	311	6			

- Molecule 2 is a protein called VP mat DutaFab VL chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	213	Total	C	N	O	S	0	0	0
			1678	1056	283	334	5			
2	LLL	211	Total	C	N	O	S	0	2	0
			1677	1057	282	333	5			

- Molecule 3 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	91	Total	C	N	O	S	0	1	0
			747	468	124	141	14			
3	DDD	96	Total	C	N	O	S	0	1	0
			786	492	133	147	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	115	ASN	LYS	conflict	UNP P15692
DDD	115	ASN	LYS	conflict	UNP P15692

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	28	Total	O	0	0
			28	28		

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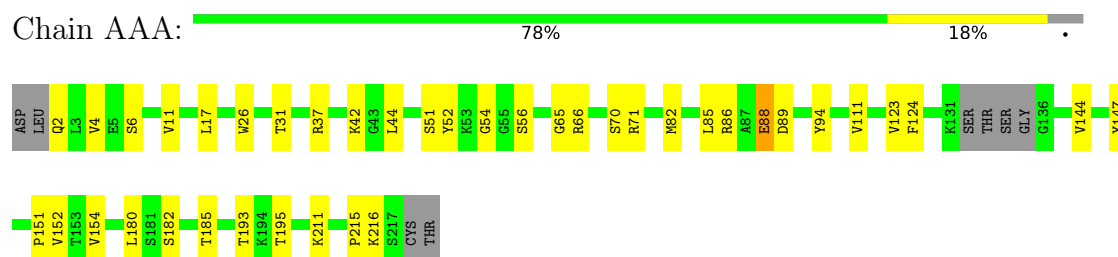
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	49	Total 49	O 49	0	0
4	CCC	25	Total 25	O 25	0	0
4	DDD	25	Total 25	O 25	0	0
4	HHH	40	Total 40	O 40	0	0
4	LLL	46	Total 46	O 46	0	0

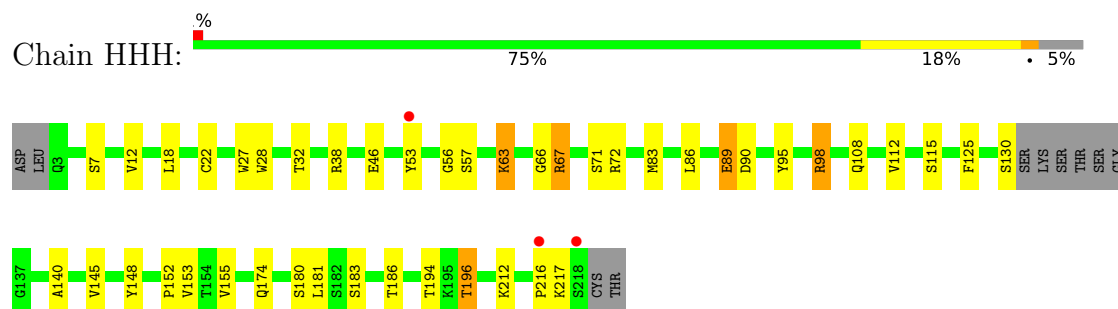
3 Residue-property plots [i](#)

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.

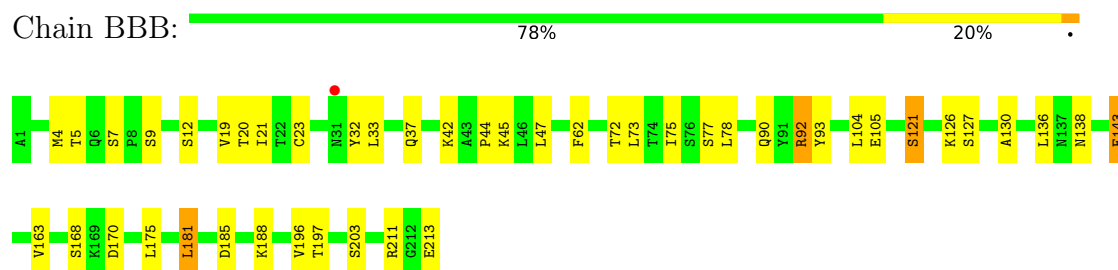
- Molecule 1: VP mat DutaFab VH chain



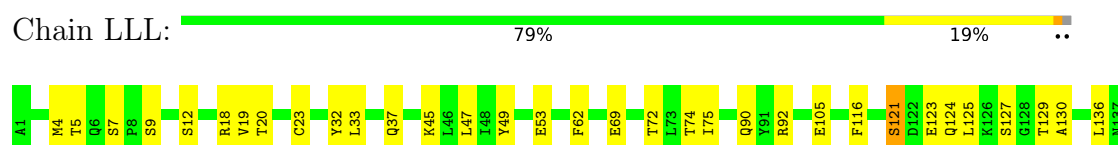
- Molecule 1: VP mat DutaFab VH chain

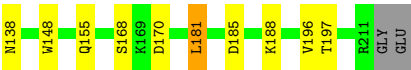


- Molecule 2: VP mat DutaFab VL chain



- Molecule 2: VP mat DutaFab VL chain





● Molecule 3: Vascular endothelial growth factor A



● Molecule 3: Vascular endothelial growth factor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.08Å 107.88Å 87.37Å 90.00° 95.34° 90.00°	Depositor
Resolution (Å)	29.29 – 2.90 29.29 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.29-2.90) 98.9 (29.29-2.90)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.212 , 0.280 (Not available) , 0.238	Depositor DCC
R_{free} test set	1416 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8284	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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	1.03	0/1638	1.35	5/2231 (0.2%)
1	HHH	1.04	0/1627	1.34	6/2216 (0.3%)
2	BBB	1.03	0/1721	1.33	1/2336 (0.0%)
2	LLL	1.03	0/1726	1.32	1/2343 (0.0%)
3	CCC	1.03	0/763	1.34	1/1027 (0.1%)
3	DDD	1.04	0/805	1.33	1/1085 (0.1%)
All	All	1.03	0/8280	1.33	15/11238 (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	1
1	HHH	0	1
All	All	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	215	PRO	N-CA-C	7.43	122.41	114.68
1	HHH	216	PRO	N-CA-C	6.88	121.83	114.68
3	DDD	41	ASP	CA-CB-CG	6.15	118.75	112.60
2	BBB	170	ASP	CA-CB-CG	5.56	118.16	112.60
1	HHH	95	TYR	CA-C-N	5.35	128.44	120.95
1	HHH	95	TYR	C-N-CA	5.35	128.44	120.95
1	AAA	94	TYR	CA-C-N	5.28	128.34	120.95
1	AAA	94	TYR	C-N-CA	5.28	128.34	120.95
2	LLL	170	ASP	CA-CB-CG	5.11	117.71	112.60
1	HHH	196	THR	CA-CB-OG1	-5.07	101.99	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HHH	28	TRP	CA-C-N	5.06	127.31	120.38
1	HHH	28	TRP	C-N-CA	5.06	127.31	120.38
1	AAA	54	GLY	CA-C-N	5.04	125.68	119.99
1	AAA	54	GLY	C-N-CA	5.04	125.68	119.99
3	CCC	59	GLY	CA-C-O	-5.02	118.04	122.16

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	65	GLY	Peptide
1	HHH	66	GLY	Peptide

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	1597	0	1541	19	0
1	HHH	1586	0	1534	19	0
2	BBB	1678	0	1609	19	0
2	LLL	1677	0	1614	20	0
3	CCC	747	0	704	4	0
3	DDD	786	0	742	9	0
4	AAA	28	0	0	2	0
4	BBB	49	0	0	2	0
4	CCC	25	0	0	0	0
4	DDD	25	0	0	0	0
4	HHH	40	0	0	1	0
4	LLL	46	0	0	0	0
All	All	8284	0	7744	78	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 5.

All (78) 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)
2:BBB:143:GLU:HB2	4:BBB:314:HOH:O	1.76	0.86
2:LLL:123[A]:GLU:H	2:LLL:123[A]:GLU:CD	2.08	0.62
2:BBB:4:MET:HE3	2:BBB:23:CYS:SG	2.40	0.61
1:AAA:88:GLU:HG3	4:AAA:305:HOH:O	1.99	0.61
2:LLL:4:MET:HE3	2:LLL:23:CYS:SG	2.42	0.60
1:HHH:32:THR:OG1	1:HHH:98:ARG:HD3	2.03	0.59
2:LLL:18:ARG:NH1	2:LLL:74:THR:HG21	2.19	0.57
1:HHH:125:PHE:HB3	2:LLL:121:SER:OG	2.07	0.55
1:HHH:155:VAL:HG11	1:HHH:183:SER:CB	2.37	0.54
1:AAA:154:VAL:HG11	1:AAA:182:SER:CB	2.38	0.54
1:AAA:44:LEU:HD11	2:BBB:44:PRO:HG2	1.91	0.53
1:AAA:56:SER:HA	3:DDD:103:GLU:OE2	2.09	0.52
1:AAA:31:THR:O	1:AAA:71:ARG:NH2	2.42	0.52
2:BBB:21:ILE:HD12	2:BBB:73:LEU:HD23	1.92	0.51
1:AAA:147:TYR:CE1	1:AAA:152:VAL:HG23	2.45	0.51
2:LLL:185:ASP:O	2:LLL:188:LYS:HB2	2.10	0.51
1:AAA:11:VAL:HG11	1:AAA:85:LEU:HD12	1.93	0.50
2:BBB:185:ASP:O	2:BBB:188:LYS:HB2	2.11	0.50
1:HHH:174:GLN:NE2	1:HHH:180:SER:HB2	2.26	0.49
1:AAA:2:GLN:NE2	4:AAA:301:HOH:O	2.31	0.49
1:HHH:32:THR:O	1:HHH:72:ARG:NH2	2.46	0.49
1:AAA:44:LEU:HD11	2:BBB:44:PRO:CG	2.42	0.49
1:HHH:12:VAL:HG11	1:HHH:86:LEU:HD12	1.94	0.48
2:BBB:163:VAL:HG22	2:BBB:175:LEU:HD12	1.95	0.48
1:AAA:85:LEU:O	1:AAA:86:ARG:NH1	2.47	0.48
3:CCC:61:CYS:O	3:CCC:62:ASN:CB	2.61	0.48
3:DDD:61:CYS:O	3:DDD:62:ASN:CB	2.61	0.48
2:BBB:12:SER:HA	2:BBB:105:GLU:O	2.14	0.47
1:AAA:42:LYS:N	1:AAA:42:LYS:HD3	2.29	0.47
2:BBB:92:ARG:HG2	2:BBB:93:TYR:CZ	2.49	0.47
2:BBB:92:ARG:HG2	2:BBB:93:TYR:CE2	2.50	0.47
1:HHH:148:TYR:CE2	1:HHH:153:VAL:HG23	2.50	0.47
3:DDD:23:ARG:NH2	2:LLL:69:GLU:OE2	2.44	0.47
2:LLL:12:SER:HA	2:LLL:105:GLU:O	2.15	0.47
1:HHH:145:VAL:HG11	1:HHH:153:VAL:HG11	1.97	0.46
1:AAA:37:ARG:NH1	1:AAA:89:ASP:HA	2.30	0.46
1:HHH:46:GLU:OE1	1:HHH:63:LYS:HD3	2.16	0.46
1:HHH:67:ARG:NH2	1:HHH:90:ASP:OD2	2.47	0.46
2:BBB:37:GLN:HB2	2:BBB:47:LEU:HD11	1.98	0.46
2:BBB:42:LYS:HD3	4:BBB:344:HOH:O	2.14	0.46
1:AAA:66:ARG:NH2	1:AAA:89:ASP:OD2	2.47	0.45
1:HHH:56:GLY:N	4:HHH:306:HOH:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:148:TRP:HB2	2:LLL:155:GLN:HB2	1.99	0.45
1:HHH:38:ARG:NH1	1:HHH:90:ASP:HA	2.31	0.45
1:HHH:83:MET:HB3	1:HHH:86:LEU:HD21	1.99	0.45
1:HHH:83:MET:HE1	1:HHH:112:VAL:HG21	1.99	0.45
1:AAA:82:MET:HE1	1:AAA:111:VAL:HG21	2.00	0.44
3:CCC:51:CYS:N	3:DDD:60[B]:CYS:SG	2.90	0.44
3:DDD:61:CYS:O	3:DDD:62:ASN:HB3	2.17	0.44
1:HHH:140:ALA:HB3	2:LLL:116:PHE:CD2	2.53	0.44
3:DDD:24:SER:HB2	3:DDD:60[A]:CYS:SG	2.58	0.44
1:HHH:12:VAL:HG22	1:HHH:18:LEU:HD13	2.00	0.44
2:LLL:33:LEU:C	2:LLL:33:LEU:HD13	2.42	0.44
2:LLL:37:GLN:HB2	2:LLL:47:LEU:HD11	1.99	0.43
2:LLL:62:PHE:CD1	2:LLL:75:ILE:HG12	2.53	0.43
1:AAA:180:LEU:HD23	1:AAA:180:LEU:C	2.43	0.43
2:BBB:78:LEU:HD11	2:BBB:104:LEU:HD21	2.01	0.43
1:AAA:123:VAL:O	1:AAA:211:LYS:HE3	2.19	0.42
2:BBB:32:TYR:HB2	2:BBB:92:ARG:HB2	2.01	0.42
2:BBB:130:ALA:HB3	2:BBB:181:LEU:HD12	2.01	0.42
3:CCC:103:GLU:OE2	1:HHH:57:SER:HA	2.19	0.42
2:BBB:33:LEU:HD13	2:BBB:33:LEU:C	2.43	0.42
2:LLL:32:TYR:HB2	2:LLL:92:ARG:HB2	2.00	0.42
2:BBB:62:PHE:CD1	2:BBB:75:ILE:HG12	2.54	0.42
2:LLL:130:ALA:HB3	2:LLL:181:LEU:HD12	2.02	0.42
1:AAA:11:VAL:HG22	1:AAA:17:LEU:HD13	2.02	0.42
1:HHH:181:LEU:C	1:HHH:181:LEU:HD23	2.43	0.42
2:LLL:136:LEU:HD21	2:LLL:196:VAL:HG13	2.02	0.42
3:DDD:40:PRO:C	3:DDD:42:GLU:H	2.27	0.41
1:HHH:212:LYS:NZ	2:LLL:123[B]:GLU:OE2	2.44	0.41
2:BBB:136:LEU:HD21	2:BBB:196:VAL:HG13	2.01	0.41
1:AAA:124:PHE:HB3	2:BBB:121:SER:OG	2.21	0.40
3:DDD:23:ARG:HH22	2:LLL:69:GLU:CD	2.29	0.40
1:AAA:144:VAL:HG11	1:AAA:152:VAL:HG11	2.02	0.40
3:CCC:51:CYS:SG	3:DDD:60[B]:CYS:N	2.95	0.40
2:LLL:49:TYR:O	2:LLL:53:GLU:HB2	2.22	0.40
2:LLL:124:GLN:HG2	2:LLL:129:THR:O	2.21	0.40
2:LLL:125:LEU:HD23	2:LLL:125:LEU:HA	1.95	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	208/220 (94%)	197 (95%)	8 (4%)	3 (1%)	9	30
1	HHH	206/220 (94%)	194 (94%)	9 (4%)	3 (2%)	8	28
2	BBB	211/213 (99%)	199 (94%)	11 (5%)	1 (0%)	24	54
2	LLL	211/213 (99%)	199 (94%)	11 (5%)	1 (0%)	24	54
3	CCC	88/121 (73%)	84 (96%)	3 (3%)	1 (1%)	11	36
3	DDD	95/121 (78%)	87 (92%)	5 (5%)	3 (3%)	3	13
All	All	1019/1108 (92%)	960 (94%)	47 (5%)	12 (1%)	10	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	DDD	41	ASP
1	HHH	27	TRP
1	AAA	26	TRP
1	AAA	88	GLU
3	CCC	62	ASN
3	DDD	62	ASN
1	HHH	89	GLU
1	HHH	217	LYS
3	DDD	89	GLN
1	AAA	216	LYS
2	LLL	138	ASN
2	BBB	138	ASN

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	176/184 (96%)	167 (95%)	9 (5%)	21	53
1	HHH	175/184 (95%)	160 (91%)	15 (9%)	10	30
2	BBB	188/188 (100%)	168 (89%)	20 (11%)	6	22
2	LLL	189/188 (100%)	176 (93%)	13 (7%)	14	41
3	CCC	88/110 (80%)	80 (91%)	8 (9%)	9	28
3	DDD	92/110 (84%)	83 (90%)	9 (10%)	7	25
All	All	908/964 (94%)	834 (92%)	74 (8%)	11	33

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	VAL
1	AAA	6	SER
1	AAA	51	SER
1	AAA	52	TYR
1	AAA	70	SER
1	AAA	151	PRO
1	AAA	185	THR
1	AAA	193	THR
1	AAA	195	THR
2	BBB	5	THR
2	BBB	7	SER
2	BBB	9	SER
2	BBB	19	VAL
2	BBB	20	THR
2	BBB	45	LYS
2	BBB	72	THR
2	BBB	77	SER
2	BBB	90	GLN
2	BBB	92	ARG
2	BBB	121	SER
2	BBB	126	LYS
2	BBB	127	SER
2	BBB	143	GLU
2	BBB	168	SER
2	BBB	181	LEU
2	BBB	197	THR
2	BBB	203	SER
2	BBB	211	ARG

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Mol	Chain	Res	Type
2	BBB	213	GLU
3	CCC	19	ASP
3	CCC	24	SER
3	CCC	46	ILE
3	CCC	50	SER
3	CCC	61	CYS
3	CCC	64	GLU
3	CCC	81	MET
3	CCC	105	ARG
3	DDD	19	ASP
3	DDD	41	ASP
3	DDD	46	ILE
3	DDD	50	SER
3	DDD	60[A]	CYS
3	DDD	60[B]	CYS
3	DDD	61	CYS
3	DDD	81	MET
3	DDD	105	ARG
1	HHH	7	SER
1	HHH	22	CYS
1	HHH	53	TYR
1	HHH	63	LYS
1	HHH	67	ARG
1	HHH	71	SER
1	HHH	89	GLU
1	HHH	98	ARG
1	HHH	108	GLN
1	HHH	115	SER
1	HHH	130	SER
1	HHH	152	PRO
1	HHH	186	THR
1	HHH	194	THR
1	HHH	196	THR
2	LLL	5	THR
2	LLL	7	SER
2	LLL	9	SER
2	LLL	19	VAL
2	LLL	20	THR
2	LLL	45	LYS
2	LLL	72	THR
2	LLL	90	GLN
2	LLL	121	SER

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Mol	Chain	Res	Type
2	LLL	127	SER
2	LLL	168	SER
2	LLL	181	LEU
2	LLL	197	THR

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](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	212/220 (96%)	0.02	0 100 100	22, 38, 63, 81	0
1	HHH	210/220 (95%)	0.01	3 (1%) 73 65	20, 35, 60, 75	0
2	BBB	213/213 (100%)	-0.06	1 (0%) 87 83	20, 36, 51, 72	0
2	LLL	211/213 (99%)	-0.09	0 100 100	13, 34, 50, 61	2 (0%)
3	CCC	91/121 (75%)	0.22	3 (3%) 49 40	22, 42, 68, 78	1 (1%)
3	DDD	96/121 (79%)	0.17	1 (1%) 79 73	24, 42, 66, 75	1 (1%)
All	All	1033/1108 (93%)	0.01	8 (0%) 82 77	13, 36, 60, 81	4 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	HHH	53	TYR	2.6
3	CCC	43	ILE	2.5
1	HHH	216	PRO	2.4
3	DDD	86	HIS	2.4
2	BBB	31	ASN	2.2
3	CCC	57	CYS	2.2
1	HHH	218	SER	2.0
3	CCC	62	ASN	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.