Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 10:48 pm GMT

PDB ID	:	6T9E
Title	:	Crystal structure of a bispecific DutaFab in complex with human PDGF
Authors	:	Kimbung, R.; Logan, D.T.; Beckmann, R.; Jensen, K.; Speck, J.; Fenn, S.; Kettenberger, H.
Deposited on	:	2019-10-28
Resolution	:	2.99 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:

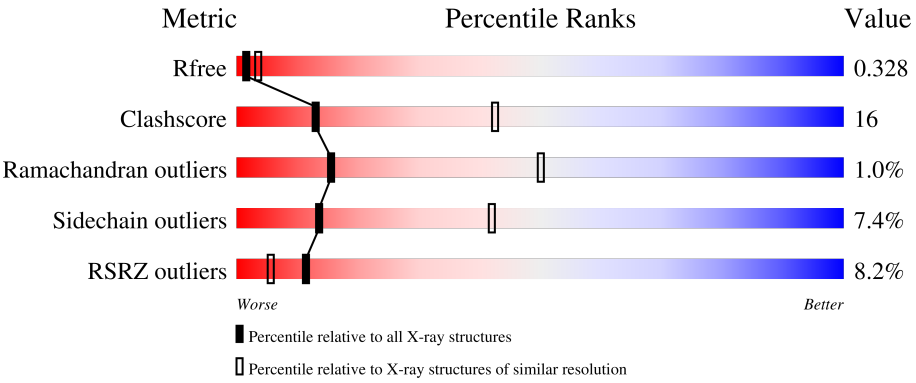
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.99 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	7% 60% 32% • 5%
1	HHH	220	6% 62% 30% • 5%
2	BBB	214	11% 61% 34% • •
2	LLL	214	9% 64% 32% • •
3	CCC	109	7% 61% 24% •• 13%

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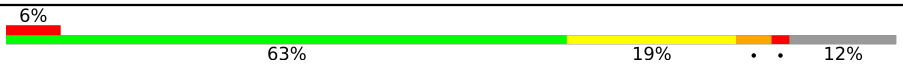
Mol	Chain	Length	Quality of chain
3	DDD	109	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7935 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 DutaFab mat VH chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	209	Total	C	N	O	S	0	0	0
			1578	1001	260	311	6			
1	HHH	209	Total	C	N	O	S	0	0	0
			1578	1001	260	311	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	207	Total	C	N	O	S	0	0	0
			1626	1023	273	325	5			
2	LLL	208	Total	C	N	O	S	0	0	0
			1628	1025	273	325	5			

- Molecule 3 is a protein called Platelet-derived growth factor subunit B.

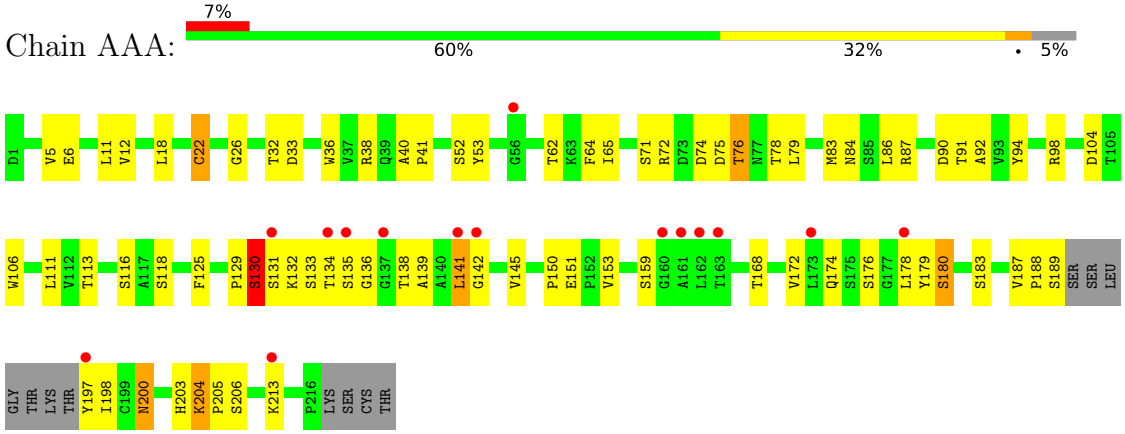
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	95	Total	C	N	O	S	0	0	0
			759	471	145	134	9			
3	DDD	96	Total	C	N	O	S	0	0	0
			766	476	146	135	9			

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.

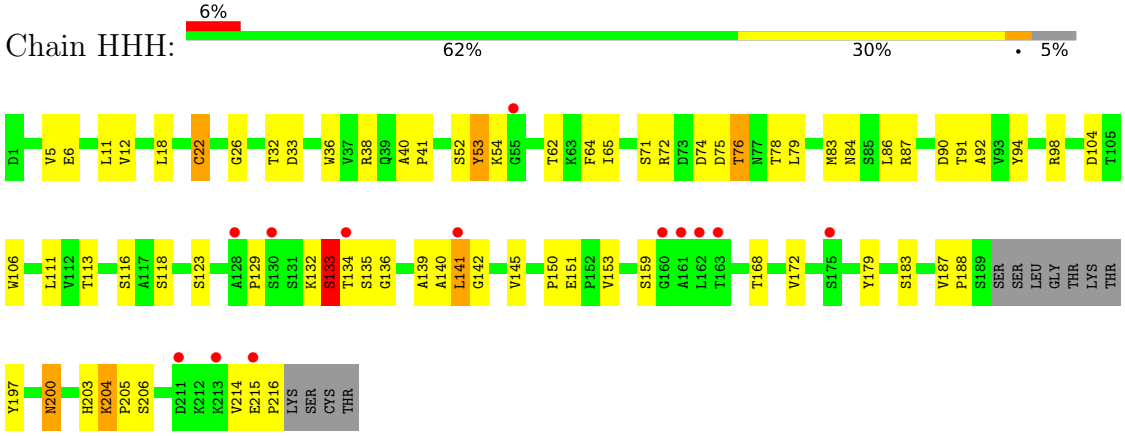
• Molecule 1: DutaFab mat VH chain

Chain AAA:



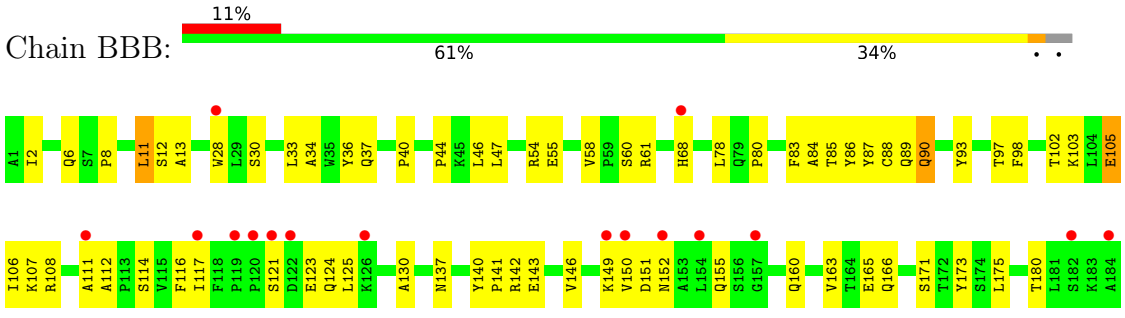
• Molecule 1: DutaFab mat VH chain

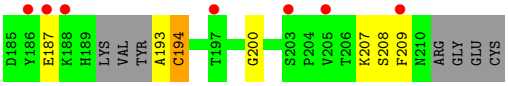
Chain HHH:



• Molecule 2: DutaFab mat VL chain

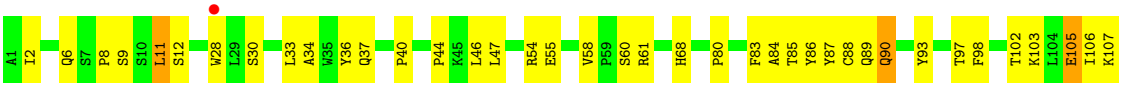
Chain BBB:

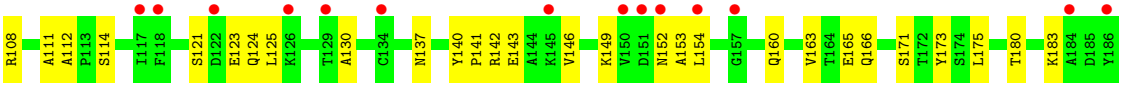


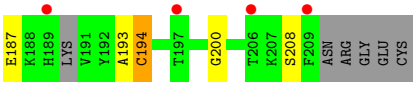


• Molecule 2: DutaFab mat VL chain

Chain LLL:

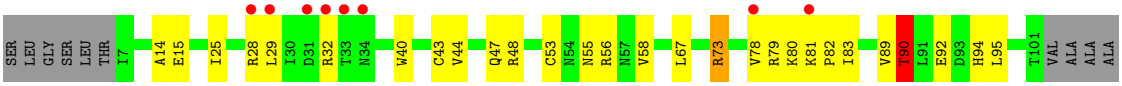






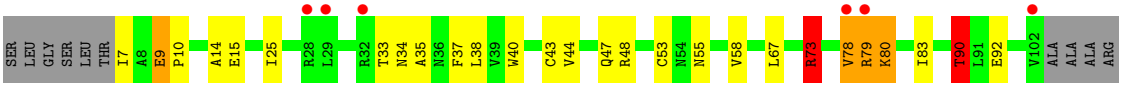
• Molecule 3: Platelet-derived growth factor subunit B

Chain CCC:



• Molecule 3: Platelet-derived growth factor subunit B

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.30Å 75.47Å 116.50Å 90.00° 110.58° 90.00°	Depositor
Resolution (Å)	29.73 – 2.99 29.73 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.73-2.99) 97.9 (29.73-2.99)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.253 , 0.304 0.279 , 0.328	Depositor DCC
R_{free} test set	1451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	7935	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.41	0/1619	0.77	0/2206
1	HHH	0.39	0/1618	0.78	0/2202
2	BBB	0.38	0/1667	0.75	0/2263
2	LLL	0.38	0/1669	0.74	0/2266
3	CCC	0.34	0/770	0.91	2/1040 (0.2%)
3	DDD	0.34	0/777	0.88	2/1050 (0.2%)
All	All	0.38	0/8120	0.79	4/11027 (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
3	DDD	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CCC	90	THR	CA-CB-OG1	-5.64	97.16	109.00
3	CCC	80	LYS	CB-CA-C	5.55	121.50	110.40
3	DDD	90	THR	CA-CB-OG1	-5.53	97.38	109.00
3	DDD	73	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	DDD	7	ILE	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	1578	0	1521	71	0
1	HHH	1578	0	1521	56	0
2	BBB	1626	0	1555	71	0
2	LLL	1628	0	1553	51	0
3	CCC	759	0	778	25	0
3	DDD	766	0	787	20	0
All	All	7935	0	7715	256	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 16.

All (256) 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:HHH:197:TYR:CD2	1:HHH:214:VAL:O	2.00	1.13
1:AAA:132:LYS:HE2	2:BBB:207:LYS:HD2	1.30	1.12
3:CCC:78:VAL:CG1	3:CCC:83:ILE:HD13	1.83	1.07
1:HHH:197:TYR:CE2	1:HHH:214:VAL:O	2.11	1.02
1:AAA:132:LYS:HZ1	2:BBB:208:SER:C	1.62	1.02
1:HHH:132:LYS:O	1:HHH:133:SER:HB2	1.54	1.02
1:AAA:132:LYS:NZ	2:BBB:117:ILE:HG21	1.73	1.02
1:HHH:215:GLU:C	1:HHH:216:PRO:N	2.15	0.99
3:CCC:78:VAL:HG11	3:CCC:83:ILE:HD13	1.46	0.95
1:HHH:197:TYR:HD2	1:HHH:214:VAL:O	1.52	0.92
2:BBB:150:VAL:HG22	2:BBB:193:ALA:N	1.86	0.90
1:AAA:132:LYS:HZ3	2:BBB:117:ILE:HG21	1.35	0.87
2:LLL:125:LEU:HD22	2:LLL:183:LYS:HG3	1.57	0.86
1:AAA:132:LYS:CE	2:BBB:207:LYS:HD2	2.05	0.84
3:CCC:78:VAL:HG13	3:CCC:83:ILE:HD13	1.61	0.82
1:AAA:132:LYS:HD3	2:BBB:209:PHE:CZ	2.14	0.81
1:AAA:132:LYS:NZ	2:BBB:117:ILE:CG2	2.46	0.79
2:BBB:193:ALA:HB2	2:BBB:208:SER:HB3	1.65	0.77
1:AAA:132:LYS:HE2	2:BBB:207:LYS:CD	2.13	0.76
1:HHH:62:THR:HG22	1:HHH:65:ILE:HD11	1.65	0.76
1:AAA:132:LYS:HZ2	2:BBB:117:ILE:HG21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:149:LYS:HE2	2:LLL:154:LEU:HD21	1.70	0.74
2:BBB:117:ILE:HG23	2:BBB:209:PHE:CE2	2.23	0.73
1:AAA:62:THR:HG22	1:AAA:65:ILE:HD11	1.69	0.73
2:LLL:37:GLN:HB2	2:LLL:47:LEU:HD11	1.69	0.73
1:AAA:187:VAL:CG1	1:AAA:188:PRO:HD2	2.19	0.73
2:LLL:149:LYS:CE	2:LLL:154:LEU:HD21	2.19	0.72
2:LLL:193:ALA:HB2	2:LLL:208:SER:HB3	1.70	0.72
2:BBB:37:GLN:HB2	2:BBB:47:LEU:HD11	1.70	0.72
1:AAA:187:VAL:HG12	1:AAA:188:PRO:HD2	1.73	0.70
1:HHH:133:SER:O	1:HHH:139:ALA:HA	1.92	0.70
2:BBB:33:LEU:HD11	2:BBB:88:CYS:HB2	1.76	0.68
2:LLL:149:LYS:HG2	2:LLL:154:LEU:HD23	1.74	0.68
1:HHH:83:MET:HB3	1:HHH:86:LEU:HD21	1.75	0.68
1:AAA:133:SER:O	1:AAA:139:ALA:HA	1.94	0.67
1:AAA:132:LYS:NZ	2:BBB:208:SER:C	2.45	0.67
1:HHH:197:TYR:HE2	1:HHH:214:VAL:O	1.76	0.66
1:AAA:83:MET:HB3	1:AAA:86:LEU:HD21	1.76	0.66
2:LLL:33:LEU:HD11	2:LLL:88:CYS:HB2	1.78	0.66
1:AAA:132:LYS:HZ2	2:BBB:117:ILE:CG2	2.08	0.66
1:AAA:187:VAL:HG11	1:AAA:197:TYR:OH	1.96	0.65
1:HHH:215:GLU:C	1:HHH:216:PRO:C	2.56	0.65
1:AAA:132:LYS:HG2	2:BBB:207:LYS:HE3	1.79	0.64
1:AAA:132:LYS:HD3	2:BBB:209:PHE:CE2	2.34	0.63
2:BBB:103:LYS:NZ	2:BBB:142:ARG:HH22	1.96	0.62
1:HHH:98:ARG:NH1	1:HHH:104:ASP:OD1	2.31	0.62
1:HHH:168:THR:HG22	1:HHH:183:SER:OG	1.99	0.62
3:CCC:55:ASN:ND2	1:HHH:75:ASP:O	2.30	0.62
1:HHH:133:SER:OG	1:HHH:140:ALA:HB3	1.99	0.62
2:BBB:193:ALA:CB	2:BBB:208:SER:HB3	2.30	0.62
1:AAA:168:THR:HG22	1:AAA:183:SER:OG	1.99	0.61
3:DDD:40:TRP:CH2	1:HHH:26:GLY:HA2	2.36	0.61
1:AAA:26:GLY:HA2	3:CCC:40:TRP:CH2	2.36	0.61
2:LLL:125:LEU:CD2	2:LLL:183:LYS:HG3	2.29	0.61
2:BBB:166:GLN:HG2	2:BBB:171:SER:HA	1.83	0.61
1:HHH:62:THR:HG22	1:HHH:65:ILE:CD1	2.31	0.60
1:HHH:187:VAL:HG23	1:HHH:188:PRO:HD2	1.82	0.60
2:LLL:103:LYS:NZ	2:LLL:142:ARG:HH22	1.99	0.60
2:LLL:193:ALA:CB	2:LLL:208:SER:HB3	2.31	0.60
1:AAA:62:THR:HG22	1:AAA:65:ILE:CD1	2.32	0.59
2:LLL:166:GLN:HG2	2:LLL:171:SER:HA	1.84	0.59
1:HHH:215:GLU:C	1:HHH:216:PRO:CA	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:132:LYS:HB3	2:BBB:207:LYS:HE2	1.85	0.58
3:CCC:78:VAL:O	3:CCC:78:VAL:HG23	2.03	0.58
2:LLL:125:LEU:O	2:LLL:183:LYS:HD2	2.03	0.58
1:HHH:145:VAL:HG11	1:HHH:153:VAL:HG11	1.85	0.58
3:CCC:29:LEU:HD22	3:CCC:89:VAL:HG22	1.84	0.58
1:AAA:145:VAL:HG11	1:AAA:153:VAL:HG11	1.85	0.58
3:DDD:40:TRP:CH2	1:HHH:26:GLY:CA	2.86	0.57
3:DDD:47:GLN:O	3:DDD:48:ARG:HD2	2.05	0.57
2:BBB:112:ALA:HB2	2:BBB:200:GLY:O	2.04	0.57
3:DDD:37:PHE:C	3:DDD:38:LEU:HD12	2.24	0.57
2:BBB:152:ASN:ND2	2:BBB:155:GLN:OE1	2.38	0.56
1:AAA:98:ARG:NH1	1:AAA:104:ASP:OD1	2.34	0.56
1:AAA:132:LYS:CD	2:BBB:209:PHE:CZ	2.86	0.56
2:LLL:112:ALA:HB2	2:LLL:200:GLY:O	2.05	0.56
3:CCC:78:VAL:O	3:CCC:78:VAL:CG2	2.54	0.56
3:DDD:53:CYS:HB3	3:DDD:58:VAL:HG23	1.88	0.55
1:AAA:132:LYS:HZ1	2:BBB:208:SER:CA	2.19	0.55
2:LLL:149:LYS:CG	2:LLL:154:LEU:HD23	2.35	0.55
1:AAA:172:VAL:HG21	2:BBB:160:GLN:HB3	1.89	0.55
2:LLL:6:GLN:HG3	2:LLL:88:CYS:SG	2.47	0.55
1:AAA:130:SER:O	1:AAA:132:LYS:N	2.40	0.54
1:AAA:132:LYS:NZ	2:BBB:208:SER:N	2.56	0.54
3:DDD:78:VAL:O	3:DDD:78:VAL:HG13	2.06	0.54
2:LLL:149:LYS:HE3	2:LLL:154:LEU:HD21	1.90	0.54
3:CCC:47:GLN:O	3:CCC:48:ARG:HD2	2.06	0.54
2:BBB:8:PRO:O	2:BBB:102:THR:HG23	2.08	0.54
3:DDD:9:GLU:HG2	3:DDD:10:PRO:HD3	1.90	0.54
2:LLL:90:GLN:NE2	2:LLL:97:THR:OG1	2.41	0.54
2:LLL:149:LYS:HE2	2:LLL:154:LEU:CD2	2.36	0.54
3:CCC:53:CYS:HB3	3:CCC:58:VAL:HG23	1.88	0.54
1:HHH:11:LEU:HB2	1:HHH:150:PRO:HG3	1.89	0.54
2:LLL:146:VAL:HG13	2:LLL:194:CYS:SG	2.47	0.54
1:HHH:204:LYS:N	1:HHH:205:PRO:HD2	2.23	0.54
2:LLL:8:PRO:O	2:LLL:102:THR:HG23	2.07	0.54
1:AAA:132:LYS:HB3	2:BBB:207:LYS:CE	2.38	0.53
1:AAA:198:ILE:HG12	1:AAA:213:LYS:HG2	1.91	0.53
1:HHH:62:THR:HA	1:HHH:65:ILE:HG13	1.90	0.53
2:BBB:105:GLU:CG	2:BBB:173:TYR:OH	2.57	0.53
2:BBB:146:VAL:HG13	2:BBB:194:CYS:SG	2.49	0.53
2:BBB:6:GLN:HG3	2:BBB:88:CYS:SG	2.48	0.53
3:CCC:73:ARG:HH11	3:CCC:73:ARG:CG	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:78:VAL:O	3:DDD:78:VAL:CG1	2.56	0.53
1:AAA:26:GLY:CA	3:CCC:40:TRP:CH2	2.92	0.53
1:AAA:204:LYS:N	1:AAA:205:PRO:HD2	2.24	0.53
3:DDD:79:ARG:O	3:DDD:80:LYS:CB	2.57	0.53
1:HHH:40:ALA:HB1	1:HHH:41:PRO:HD2	1.91	0.52
2:LLL:105:GLU:CG	2:LLL:173:TYR:OH	2.57	0.52
1:AAA:11:LEU:HB2	1:AAA:150:PRO:HG3	1.90	0.52
2:LLL:33:LEU:HD12	2:LLL:89:GLN:O	2.10	0.52
3:DDD:92:GLU:HG2	3:DDD:92:GLU:O	2.10	0.52
1:AAA:203:HIS:NE2	1:AAA:205:PRO:HG2	2.24	0.52
3:CCC:43:CYS:SG	3:DDD:14:ALA:HB3	2.50	0.52
1:HHH:91:THR:HG23	1:HHH:113:THR:HA	1.92	0.52
1:AAA:62:THR:HA	1:AAA:65:ILE:HG13	1.90	0.51
3:CCC:92:GLU:O	3:CCC:92:GLU:HG2	2.10	0.51
3:DDD:78:VAL:HB	3:DDD:83:ILE:HD13	1.91	0.51
1:AAA:125:PHE:CE2	2:BBB:124:GLN:HG3	2.44	0.51
2:BBB:90:GLN:NE2	2:BBB:97:THR:OG1	2.42	0.51
1:AAA:91:THR:HG23	1:AAA:113:THR:HA	1.92	0.51
1:AAA:134:THR:HG22	1:AAA:189:SER:HB3	1.92	0.51
1:AAA:40:ALA:HB1	1:AAA:41:PRO:HD2	1.93	0.50
2:BBB:40:PRO:HB3	2:BBB:165:GLU:HG3	1.94	0.50
3:DDD:79:ARG:O	3:DDD:80:LYS:HB2	2.12	0.50
2:BBB:33:LEU:HG	2:BBB:34:ALA:N	2.26	0.50
1:HHH:132:LYS:O	1:HHH:133:SER:CB	2.41	0.50
2:BBB:33:LEU:HD12	2:BBB:89:GLN:O	2.11	0.50
2:BBB:117:ILE:HG23	2:BBB:209:PHE:HE2	1.74	0.50
3:CCC:29:LEU:HD23	3:CCC:29:LEU:O	2.11	0.50
1:AAA:132:LYS:O	2:BBB:116:PHE:HD1	1.95	0.50
2:LLL:108:ARG:HH12	2:LLL:111:ALA:HB2	1.77	0.50
1:HHH:203:HIS:NE2	1:HHH:205:PRO:HG2	2.25	0.49
1:AAA:132:LYS:NZ	2:BBB:208:SER:CA	2.76	0.49
3:DDD:73:ARG:HH11	3:DDD:73:ARG:CG	2.25	0.49
1:AAA:32:THR:O	1:AAA:72:ARG:NH2	2.44	0.49
1:HHH:187:VAL:CG2	1:HHH:188:PRO:HD2	2.41	0.49
2:LLL:40:PRO:CB	2:LLL:165:GLU:HG3	2.42	0.48
1:AAA:129:PRO:HD3	1:AAA:141:LEU:HB2	1.95	0.48
1:AAA:12:VAL:HG21	1:AAA:18:LEU:HD22	1.96	0.48
1:AAA:200:ASN:N	1:AAA:200:ASN:OD1	2.47	0.48
2:LLL:33:LEU:HG	2:LLL:34:ALA:N	2.27	0.48
2:LLL:40:PRO:HB3	2:LLL:165:GLU:HG3	1.96	0.48
1:HHH:12:VAL:HG21	1:HHH:18:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:28:ARG:HG2	3:CCC:32:ARG:HG3	1.96	0.47
2:BBB:140:TYR:CG	2:BBB:141:PRO:HA	2.49	0.47
1:HHH:32:THR:O	1:HHH:72:ARG:NH2	2.47	0.47
1:AAA:187:VAL:HG13	1:AAA:188:PRO:HD2	1.96	0.47
3:DDD:40:TRP:CH2	1:HHH:26:GLY:HA3	2.49	0.47
2:BBB:40:PRO:CB	2:BBB:165:GLU:HG3	2.45	0.47
2:BBB:108:ARG:HH12	2:BBB:111:ALA:HB2	1.78	0.47
3:DDD:67:LEU:HD13	3:DDD:90:THR:HG21	1.97	0.47
1:HHH:200:ASN:OD1	1:HHH:200:ASN:N	2.47	0.47
1:AAA:76:THR:HB	1:AAA:78:THR:OG1	2.15	0.47
1:HHH:76:THR:HB	1:HHH:78:THR:OG1	2.14	0.46
2:LLL:140:TYR:CG	2:LLL:141:PRO:HA	2.50	0.46
1:HHH:33:ASP:OD1	1:HHH:33:ASP:N	2.48	0.46
1:HHH:92:ALA:HB3	1:HHH:94:TYR:CE1	2.50	0.46
2:LLL:143:GLU:OE1	2:LLL:143:GLU:N	2.49	0.46
1:AAA:33:ASP:OD1	1:AAA:33:ASP:N	2.47	0.46
1:AAA:72:ARG:NH1	1:AAA:74:ASP:OD1	2.37	0.46
1:AAA:132:LYS:HZ3	2:BBB:208:SER:N	2.11	0.46
2:LLL:54:ARG:HG2	2:LLL:58:VAL:HB	1.98	0.46
2:LLL:149:LYS:CE	2:LLL:154:LEU:CD2	2.90	0.46
1:HHH:172:VAL:HG21	2:LLL:160:GLN:HB3	1.97	0.46
2:BBB:143:GLU:N	2:BBB:143:GLU:OE1	2.48	0.46
1:HHH:38:ARG:NH1	1:HHH:90:ASP:HA	2.31	0.46
1:AAA:6:GLU:HG3	1:AAA:22:CYS:HB2	1.98	0.46
1:AAA:38:ARG:NH1	1:AAA:90:ASP:HA	2.31	0.46
1:AAA:134:THR:O	1:AAA:136:GLY:O	2.34	0.46
2:LLL:61:ARG:HH11	2:LLL:61:ARG:HG2	1.80	0.45
1:HHH:6:GLU:HG3	1:HHH:22:CYS:HB2	1.97	0.45
1:HHH:134:THR:O	1:HHH:136:GLY:O	2.34	0.45
1:AAA:92:ALA:HB3	1:AAA:94:TYR:CE1	2.51	0.45
2:BBB:84:ALA:HB3	2:BBB:86:TYR:CE1	2.50	0.45
1:AAA:132:LYS:CG	2:BBB:207:LYS:HE3	2.44	0.45
1:HHH:134:THR:HA	1:HHH:139:ALA:HB2	1.98	0.45
2:LLL:84:ALA:HB3	2:LLL:86:TYR:CE1	2.51	0.45
2:BBB:121:SER:HB3	2:BBB:123:GLU:HG2	1.98	0.45
3:CCC:56:ARG:HH21	1:HHH:75:ASP:CG	2.19	0.45
2:LLL:2:ILE:HD11	2:LLL:93:TYR:HD2	1.82	0.45
1:HHH:111:LEU:CD2	1:HHH:151:GLU:HB2	2.47	0.45
2:LLL:85:THR:HG22	2:LLL:87:TYR:CE1	2.52	0.45
2:BBB:55:GLU:HB3	2:BBB:58:VAL:CG2	2.47	0.45
1:HHH:129:PRO:HD3	1:HHH:141:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:107:LYS:HA	2:BBB:140:TYR:OH	2.17	0.45
1:HHH:72:ARG:NH1	1:HHH:74:ASP:OD1	2.38	0.44
2:LLL:107:LYS:HA	2:LLL:140:TYR:OH	2.17	0.44
1:HHH:203:HIS:CE1	1:HHH:206:SER:HB3	2.52	0.44
1:HHH:111:LEU:HD21	1:HHH:151:GLU:HB2	2.00	0.44
3:CCC:79:ARG:HA	3:CCC:79:ARG:HD3	1.60	0.44
2:BBB:124:GLN:O	2:BBB:124:GLN:HG2	2.18	0.44
1:HHH:106:TRP:CZ3	2:LLL:44:PRO:HG2	2.53	0.44
1:AAA:36:TRP:NE1	1:AAA:79:LEU:HD21	2.33	0.43
3:CCC:56:ARG:H	3:CCC:56:ARG:HG2	1.60	0.43
2:LLL:55:GLU:HB3	2:LLL:58:VAL:CG2	2.48	0.43
2:LLL:125:LEU:HD21	2:LLL:130:ALA:HB2	2.00	0.43
1:HHH:62:THR:CG2	1:HHH:65:ILE:HD11	2.43	0.43
2:LLL:149:LYS:HA	2:LLL:153:ALA:O	2.18	0.43
2:BBB:54:ARG:HG2	2:BBB:58:VAL:HB	2.01	0.43
1:HHH:62:THR:C	1:HHH:64:PHE:H	2.22	0.43
3:CCC:67:LEU:HD13	3:CCC:90:THR:HG21	2.00	0.43
2:BBB:61:ARG:HG2	2:BBB:61:ARG:HH11	1.83	0.43
2:BBB:105:GLU:HG3	2:BBB:173:TYR:OH	2.19	0.43
2:LLL:28:TRP:CD1	2:LLL:68:HIS:HB3	2.53	0.43
1:AAA:134:THR:HA	1:AAA:139:ALA:HB2	2.00	0.43
1:AAA:174:GLN:NE2	1:AAA:180:SER:HB2	2.34	0.42
1:AAA:106:TRP:CZ3	2:BBB:44:PRO:HG2	2.54	0.42
1:AAA:203:HIS:CE1	1:AAA:206:SER:HB3	2.54	0.42
1:AAA:75:ASP:O	3:DDD:55:ASN:ND2	2.46	0.42
2:BBB:85:THR:HG22	2:BBB:87:TYR:CE1	2.54	0.42
3:DDD:67:LEU:HD23	3:DDD:67:LEU:HA	1.88	0.42
2:BBB:125:LEU:HD21	2:BBB:130:ALA:HB2	2.01	0.42
3:CCC:78:VAL:HG11	3:CCC:83:ILE:CD1	2.34	0.42
2:LLL:124:GLN:O	2:LLL:124:GLN:HG2	2.18	0.42
2:BBB:28:TRP:CD1	2:BBB:68:HIS:HB3	2.55	0.42
2:LLL:55:GLU:O	2:LLL:58:VAL:HG23	2.20	0.42
1:HHH:151:GLU:OE1	1:HHH:179:TYR:CD1	2.73	0.41
1:HHH:203:HIS:CE1	1:HHH:206:SER:HG	2.33	0.41
2:BBB:11:LEU:HD12	2:BBB:12:SER:O	2.20	0.41
2:LLL:80:PRO:HA	2:LLL:106:ILE:HG13	2.02	0.41
1:AAA:111:LEU:HD21	1:AAA:151:GLU:HB2	2.03	0.41
1:AAA:62:THR:C	1:AAA:64:PHE:H	2.22	0.41
3:DDD:25:ILE:HD11	3:DDD:44:VAL:HG23	2.02	0.41
2:LLL:12:SER:HB3	2:LLL:107:LYS:HB2	2.01	0.41
2:BBB:2:ILE:HD11	2:BBB:93:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:13:ALA:HB3	2:BBB:78:LEU:CD2	2.51	0.41
2:BBB:103:LYS:HZ2	2:BBB:142:ARG:HH22	1.69	0.41
1:HHH:53:TYR:CE2	1:HHH:54:LYS:HG3	2.55	0.41
2:LLL:121:SER:HB3	2:LLL:123:GLU:HG2	2.03	0.41
1:AAA:132:LYS:HD2	2:BBB:209:PHE:CE1	2.56	0.41
1:HHH:36:TRP:NE1	1:HHH:79:LEU:HD21	2.36	0.41
2:LLL:36:TYR:CD1	2:LLL:46:LEU:HA	2.56	0.41
1:AAA:136:GLY:C	1:AAA:138:THR:H	2.24	0.41
1:AAA:141:LEU:HD12	1:AAA:142:GLY:N	2.36	0.41
3:CCC:94:HIS:O	3:CCC:95:LEU:HD23	2.21	0.41
1:AAA:151:GLU:OE1	1:AAA:179:TYR:CD1	2.74	0.41
2:BBB:12:SER:HB3	2:BBB:107:LYS:HB2	2.02	0.41
2:BBB:36:TYR:CD1	2:BBB:46:LEU:HA	2.56	0.41
2:BBB:89:GLN:HB2	2:BBB:98:PHE:CD1	2.56	0.41
2:BBB:90:GLN:HE21	2:BBB:90:GLN:HB3	1.72	0.41
2:BBB:193:ALA:CA	2:BBB:208:SER:HB3	2.51	0.41
3:CCC:81:LYS:HA	3:CCC:82:PRO:HD3	1.96	0.41
3:CCC:14:ALA:HB3	3:DDD:43:CYS:SG	2.61	0.41
2:LLL:89:GLN:HB2	2:LLL:98:PHE:CD1	2.56	0.41
1:HHH:141:LEU:HD12	1:HHH:142:GLY:N	2.36	0.40
1:HHH:134:THR:HA	1:HHH:139:ALA:CB	2.51	0.40
2:BBB:80:PRO:HA	2:BBB:106:ILE:HG13	2.04	0.40
3:CCC:25:ILE:HD11	3:CCC:44:VAL:HG23	2.03	0.40
2:LLL:163:VAL:HG22	2:LLL:175:LEU:HD12	2.04	0.40
1:AAA:151:GLU:OE1	1:AAA:179:TYR:CG	2.75	0.40
2:BBB:163:VAL:HG22	2:BBB:175:LEU:HD12	2.04	0.40
1:HHH:151:GLU:OE1	1:HHH:179:TYR:CG	2.75	0.40
2:LLL:89:GLN:HG3	2:LLL:98:PHE:CE1	2.57	0.40
1:AAA:176:SER:HB3	1:AAA:178:LEU:HD12	2.04	0.40
2:LLL:11:LEU:HD12	2:LLL:12:SER:O	2.21	0.40

There are no symmetry-related clashes.

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	205/220 (93%)	189 (92%)	13 (6%)	3 (2%)	10 39
1	HHH	204/220 (93%)	190 (93%)	12 (6%)	2 (1%)	15 50
2	BBB	203/214 (95%)	190 (94%)	12 (6%)	1 (0%)	29 66
2	LLL	204/214 (95%)	193 (95%)	11 (5%)	0	100 100
3	CCC	93/109 (85%)	84 (90%)	9 (10%)	0	100 100
3	DDD	94/109 (86%)	84 (89%)	6 (6%)	4 (4%)	2 14
All	All	1003/1086 (92%)	930 (93%)	63 (6%)	10 (1%)	15 50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	131	SER
3	DDD	35	ALA
3	DDD	79	ARG
3	DDD	80	LYS
1	AAA	135	SER
2	BBB	149	LYS
3	DDD	33	THR
1	HHH	133	SER
1	AAA	130	SER
1	HHH	135	SER

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	174/184 (95%)	158 (91%)	16 (9%)	9 32
1	HHH	174/184 (95%)	158 (91%)	16 (9%)	9 32
2	BBB	183/189 (97%)	171 (93%)	12 (7%)	16 47
2	LLL	182/189 (96%)	169 (93%)	13 (7%)	14 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	CCC	87/98 (89%)	84 (97%)	3 (3%)	37 70
3	DDD	88/98 (90%)	82 (93%)	6 (7%)	16 46
All	All	888/942 (94%)	822 (93%)	66 (7%)	13 42

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	5	VAL
1	AAA	22	CYS
1	AAA	52	SER
1	AAA	53	TYR
1	AAA	71	SER
1	AAA	76	THR
1	AAA	84	ASN
1	AAA	87	ARG
1	AAA	116	SER
1	AAA	118	SER
1	AAA	130	SER
1	AAA	141	LEU
1	AAA	159	SER
1	AAA	180	SER
1	AAA	200	ASN
1	AAA	204	LYS
2	BBB	11	LEU
2	BBB	30	SER
2	BBB	60	SER
2	BBB	83	PHE
2	BBB	90	GLN
2	BBB	105	GLU
2	BBB	114	SER
2	BBB	137	ASN
2	BBB	151	ASP
2	BBB	180	THR
2	BBB	187	GLU
2	BBB	194	CYS
3	CCC	15	GLU
3	CCC	73	ARG
3	CCC	90	THR
3	DDD	9	GLU
3	DDD	15	GLU
3	DDD	34	ASN

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Mol	Chain	Res	Type
3	DDD	73	ARG
3	DDD	78	VAL
3	DDD	90	THR
1	HHH	5	VAL
1	HHH	22	CYS
1	HHH	52	SER
1	HHH	53	TYR
1	HHH	71	SER
1	HHH	76	THR
1	HHH	84	ASN
1	HHH	87	ARG
1	HHH	116	SER
1	HHH	118	SER
1	HHH	123	SER
1	HHH	133	SER
1	HHH	141	LEU
1	HHH	159	SER
1	HHH	200	ASN
1	HHH	204	LYS
2	LLL	9	SER
2	LLL	11	LEU
2	LLL	30	SER
2	LLL	60	SER
2	LLL	83	PHE
2	LLL	90	GLN
2	LLL	105	GLU
2	LLL	114	SER
2	LLL	137	ASN
2	LLL	152	ASN
2	LLL	180	THR
2	LLL	187	GLU
2	LLL	194	CYS

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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	HHH	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	HHH	215:GLU	C	216:PRO	N	2.15

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, 95^{th} 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	209/220 (95%)	0.36	15 (7%) 15 8	27, 52, 111, 157	0
1	HHH	209/220 (95%)	0.34	13 (6%) 20 11	22, 52, 109, 146	0
2	BBB	207/214 (96%)	0.52	23 (11%) 5 3	21, 57, 131, 159	1 (0%)
2	LLL	208/214 (97%)	0.47	19 (9%) 9 5	23, 59, 119, 134	0
3	CCC	95/109 (87%)	0.32	8 (8%) 11 5	28, 51, 107, 141	0
3	DDD	96/109 (88%)	0.27	6 (6%) 20 10	29, 51, 110, 130	0
All	All	1024/1086 (94%)	0.40	84 (8%) 11 5	21, 54, 118, 159	1 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	HHH	161	ALA	5.9
2	LLL	157	GLY	5.5
1	AAA	161	ALA	4.9
2	BBB	122	ASP	4.6
1	HHH	163	THR	4.6
2	LLL	151	ASP	4.5
2	BBB	184	ALA	4.4
1	AAA	135	SER	4.4
1	AAA	163	THR	4.2
1	HHH	175	SER	4.2
1	AAA	134	THR	4.2
3	CCC	28	ARG	4.1
2	LLL	152	ASN	3.9
2	BBB	152	ASN	3.9
2	LLL	126	LYS	3.7
2	BBB	209	PHE	3.7
2	BBB	119	PRO	3.7
1	HHH	162	LEU	3.6
1	AAA	56	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	BBB	186	TYR	3.4
2	BBB	182	SER	3.3
2	LLL	189	HIS	3.3
2	LLL	209	PHE	3.2
3	DDD	79	ARG	3.1
3	DDD	29	LEU	3.1
2	LLL	122	ASP	3.1
1	HHH	134	THR	3.1
2	BBB	203	SER	3.1
2	BBB	111	ALA	3.0
2	BBB	197	THR	3.0
3	DDD	32	ARG	2.9
3	CCC	29	LEU	2.9
1	AAA	160	GLY	2.9
1	AAA	162	LEU	2.8
2	BBB	157	GLY	2.8
1	HHH	130	SER	2.8
1	HHH	160	GLY	2.8
3	DDD	102	VAL	2.8
3	CCC	34	ASN	2.7
2	BBB	120	PRO	2.7
3	DDD	28	ARG	2.6
2	BBB	121	SER	2.6
2	LLL	150	VAL	2.6
2	LLL	28	TRP	2.6
1	AAA	213	LYS	2.6
3	CCC	32	ARG	2.6
3	CCC	33	THR	2.5
2	BBB	150	VAL	2.5
1	HHH	211	ASP	2.5
2	BBB	149	LYS	2.5
2	BBB	126	LYS	2.4
2	BBB	117	ILE	2.4
1	AAA	197	TYR	2.4
3	DDD	78	VAL	2.4
2	BBB	187	GLU	2.3
2	LLL	118	PHE	2.3
1	AAA	173	LEU	2.3
2	LLL	206	THR	2.3
2	LLL	197	THR	2.3
1	HHH	215	GLU	2.3
2	LLL	154	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	LLL	186	TYR	2.3
2	LLL	117	ILE	2.2
2	LLL	134	CYS	2.2
1	HHH	128	ALA	2.2
3	CCC	78	VAL	2.2
2	BBB	188	LYS	2.2
2	LLL	145	LYS	2.2
1	AAA	142	GLY	2.2
2	BBB	205	VAL	2.2
1	HHH	213	LYS	2.1
2	BBB	154	LEU	2.1
1	AAA	131	SER	2.1
2	BBB	68	HIS	2.1
2	LLL	129	THR	2.1
1	HHH	55	GLY	2.1
1	HHH	141	LEU	2.1
2	LLL	184	ALA	2.1
1	AAA	137	GLY	2.0
1	AAA	178	LEU	2.0
3	CCC	31	ASP	2.0
2	BBB	28	TRP	2.0
3	CCC	81	LYS	2.0
1	AAA	141	LEU	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 monosaccharides 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.