



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 03:56 AM UTC

PDB ID : 7PA8 / pdb_00007pa8
Title : JC polyomavirus VP1 in complex with Fab 27C2
Authors : Stroeh, L.J.; Harprecht, C.; Freytag, J.; Stehle, T.
Deposited on : 2021-07-29
Resolution : 3.15 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

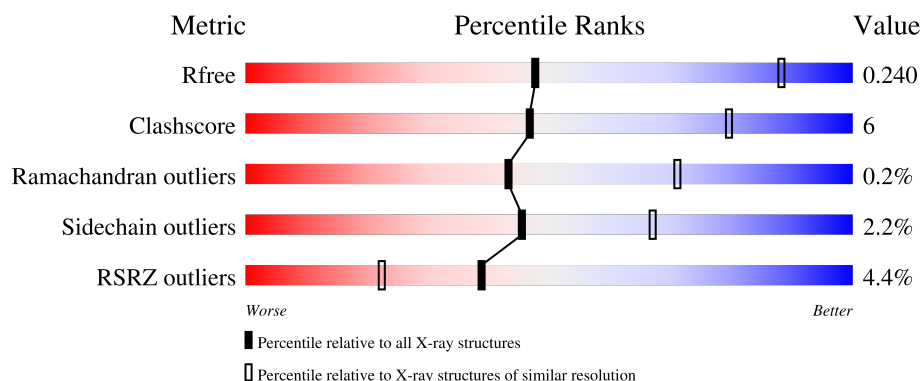
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	272	% 79% 16% .
1	BBB	272	% 83% 11% 5%
1	CCC	272	85% 10% 6%
1	DDD	272	% 83% 12% .
1	EEE	272	% 81% 15% .

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Mol	Chain	Length	Quality of chain
2	FFF	212	
2	GGG	212	
2	III	212	
2	KKK	212	
2	MMM	212	
3	HHH	398	
3	JJJ	398	
3	LLL	398	
3	NNN	398	
3	YYY	398	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21266 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	260	Total	C	N	O	S	0	0	0
			1997	1263	343	380	11			
1	BBB	258	Total	C	N	O	S	0	0	0
			2004	1263	344	386	11			
1	CCC	257	Total	C	N	O	S	0	0	0
			1989	1255	340	383	11			
1	DDD	261	Total	C	N	O	S	0	0	0
			2010	1268	344	387	11			
1	EEE	262	Total	C	N	O	S	0	0	0
			2014	1268	346	389	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	GLY	-	expression tag	UNP P03089
AAA	19	SER	-	expression tag	UNP P03089
AAA	20	HIS	-	expression tag	UNP P03089
AAA	21	MET	-	expression tag	UNP P03089
BBB	18	GLY	-	expression tag	UNP P03089
BBB	19	SER	-	expression tag	UNP P03089
BBB	20	HIS	-	expression tag	UNP P03089
BBB	21	MET	-	expression tag	UNP P03089
CCC	18	GLY	-	expression tag	UNP P03089
CCC	19	SER	-	expression tag	UNP P03089
CCC	20	HIS	-	expression tag	UNP P03089
CCC	21	MET	-	expression tag	UNP P03089
DDD	18	GLY	-	expression tag	UNP P03089
DDD	19	SER	-	expression tag	UNP P03089
DDD	20	HIS	-	expression tag	UNP P03089
DDD	21	MET	-	expression tag	UNP P03089
EEE	18	GLY	-	expression tag	UNP P03089
EEE	19	SER	-	expression tag	UNP P03089
EEE	20	HIS	-	expression tag	UNP P03089

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	21	MET	-	expression tag	UNP P03089

- Molecule 2 is a protein called Fab 27C2 light chain.

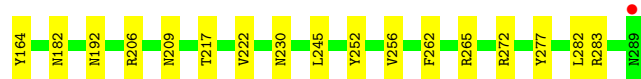
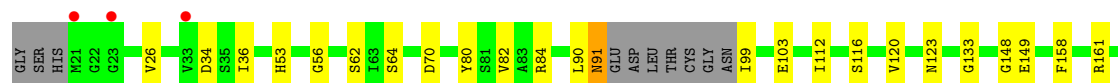
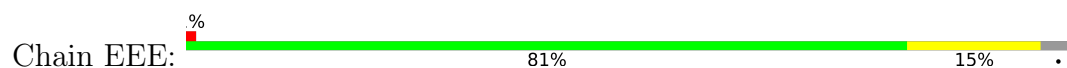
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	FFF	191	Total	C	N	O	S	0	0	0
			1329	827	223	275	4			
2	GGG	176	Total	C	N	O	S	0	0	0
			1213	755	208	246	4			
2	III	136	Total	C	N	O	S	0	0	0
			952	594	163	192	3			
2	KKK	134	Total	C	N	O	S	0	0	0
			952	597	162	191	2			
2	MMM	108	Total	C	N	O	S	0	0	0
			779	485	133	159	2			

- Molecule 3 is a protein called Fab 27C2 heavy chain.

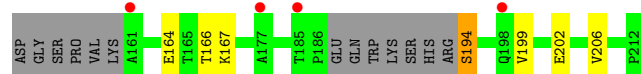
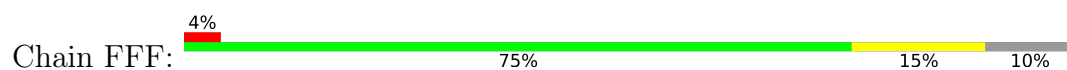
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	HHH	149	Total	C	N	O	S	0	0	0
			1125	714	186	220	5			
3	JJJ	177	Total	C	N	O	S	0	0	0
			1310	827	219	257	7			
3	LLL	170	Total	C	N	O	S	0	0	0
			1267	796	214	251	6			
3	NNN	118	Total	C	N	O	S	0	0	0
			906	571	155	175	5			
3	YYY	189	Total	C	N	O	S	0	0	0
			1419	902	239	271	7			



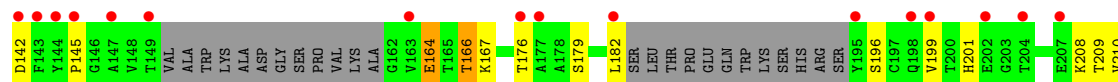
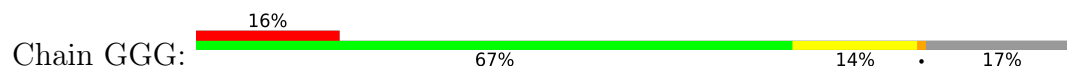
- Molecule 1: Major capsid protein VP1



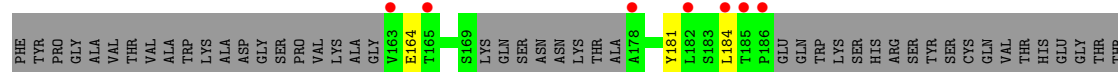
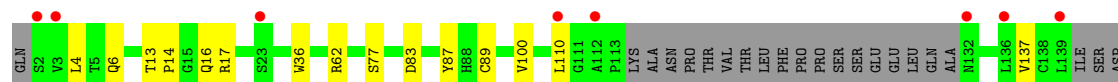
- Molecule 2: Fab 27C2 light chain



- Molecule 2: Fab 27C2 light chain

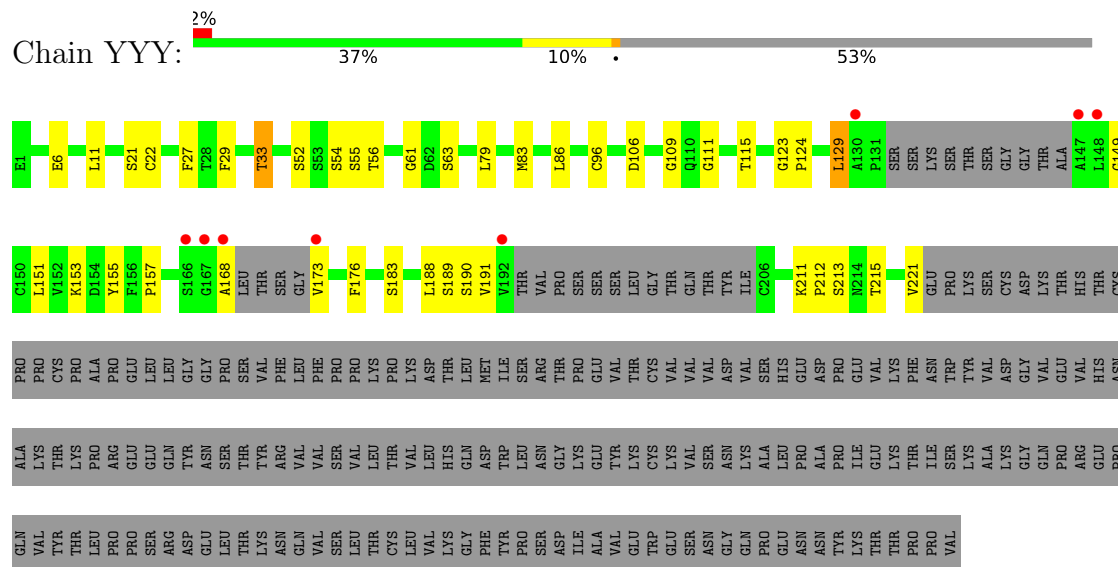


- Molecule 2: Fab 27C2 light chain





- Molecule 3: Fab 27C2 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.07Å 110.44Å 158.21Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	49.01 – 3.15 49.01 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.01-3.15) 99.7 (49.01-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.212 , 0.241 0.213 , 0.240	Depositor DCC
R_{free} test set	4079 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21266	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	1.05	1/2042 (0.0%)	1.33	3/2777 (0.1%)
1	BBB	1.03	0/2049	1.31	2/2784 (0.1%)
1	CCC	1.02	0/2034	1.34	1/2765 (0.0%)
1	DDD	1.05	0/2055	1.35	5/2794 (0.2%)
1	EEE	1.03	0/2059	1.35	1/2799 (0.0%)
2	FFF	1.17	1/1359 (0.1%)	1.41	3/1867 (0.2%)
2	GGG	1.19	0/1240	1.41	0/1701
2	III	1.15	0/972	1.34	0/1325
2	KKK	1.09	0/974	1.34	0/1327
2	MMM	1.13	0/799	1.37	0/1089
3	HHH	1.04	0/1153	1.37	2/1568 (0.1%)
3	JJJ	1.11	0/1342	1.34	2/1832 (0.1%)
3	LLL	1.09	0/1296	1.37	4/1768 (0.2%)
3	NNN	1.04	1/928 (0.1%)	1.35	2/1259 (0.2%)
3	YYY	1.09	0/1454	1.40	7/1980 (0.4%)
All	All	1.08	3/21756 (0.0%)	1.36	32/29635 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	FFF	88	HIS	CE1-NE2	5.58	1.38	1.32
1	AAA	135	PRO	C-O	-5.24	1.17	1.23
3	NNN	109	GLY	C-O	5.04	1.28	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LLL	62	ASP	N-CA-C	-6.10	104.63	111.28
3	YYY	61	GLY	N-CA-C	-6.07	104.95	111.93
1	BBB	180	VAL	O-C-N	6.05	126.64	121.98
3	LLL	64	VAL	N-CA-CB	-5.91	104.47	112.16
3	LLL	111	GLY	CA-C-O	-5.91	117.10	122.24
1	BBB	164	TYR	CB-CA-C	5.84	118.60	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	HHH	157	PRO	N-CA-C	5.80	124.42	112.47
3	YYY	106	ASP	CA-CB-CG	5.78	118.38	112.60
3	YYY	111	GLY	CA-C-O	-5.75	117.23	122.24
3	YYY	63	SER	N-CA-C	-5.61	105.26	111.71
1	AAA	164	TYR	CB-CA-C	5.53	118.10	109.42
3	YYY	109	GLY	CA-C-O	-5.46	116.83	122.28
3	JJJ	106	ASP	CA-CB-CG	5.43	118.03	112.60
1	EEE	164	TYR	CB-CA-C	5.41	117.91	109.42
3	NNN	33	THR	CB-CA-C	5.39	118.88	109.65
2	FFF	132	ASN	CA-CB-CG	5.35	117.95	112.60
3	YYY	33	THR	CB-CA-C	5.35	118.79	109.65
3	NNN	106	ASP	CA-CB-CG	5.33	117.93	112.60
1	CCC	180	VAL	O-C-N	5.27	126.04	121.98
3	HHH	189	SER	CA-C-O	5.26	129.74	120.80
3	JJJ	111	GLY	CA-C-O	-5.24	117.68	122.24
1	AAA	180	VAL	O-C-N	5.23	126.00	121.98
1	DDD	48	GLY	CA-C-N	5.16	128.40	122.83
1	DDD	48	GLY	C-N-CA	5.16	128.40	122.83
1	AAA	49	ASP	CA-CB-CG	5.15	117.75	112.60
3	YYY	56	THR	CA-CB-OG1	-5.11	101.93	109.60
3	LLL	218	ASP	CA-CB-CG	5.10	117.70	112.60
2	FFF	194	SER	CA-C-N	5.07	128.05	120.95
2	FFF	194	SER	C-N-CA	5.07	128.05	120.95
1	DDD	126	ALA	N-CA-CB	5.07	117.00	109.19
1	DDD	126	ALA	N-CA-C	-5.02	103.21	110.64
1	DDD	164	TYR	CB-CA-C	5.01	117.29	109.42

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	AAA	1997	0	1935	38	0
1	BBB	2004	0	1945	20	0
1	CCC	1989	0	1928	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DDD	2010	0	1944	17	0
1	EEE	2014	0	1942	30	0
2	FFF	1329	0	1234	18	0
2	GGG	1213	0	1119	27	0
2	III	952	0	894	12	0
2	KKK	952	0	897	6	0
2	MMM	779	0	734	7	0
3	HHH	1125	0	1048	12	0
3	JJJ	1310	0	1186	19	0
3	LLL	1267	0	1167	12	0
3	NNN	906	0	850	9	0
3	YYY	1419	0	1346	22	0
All	All	21266	0	20169	238	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 6.

All (238) 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:AAA:161:ARG:HH22	1:EEE:53:HIS:HB3	1.16	1.02
1:AAA:53:HIS:HB3	1:BBB:161:ARG:HH22	1.29	0.95
3:NNN:87:ARG:O	3:NNN:116:VAL:HG11	1.66	0.95
1:CCC:36:ILE:HD12	1:CCC:282:LEU:O	1.65	0.93
2:III:6:GLN:OE1	2:III:89:CYS:SG	2.27	0.92
3:JJJ:91:THR:HG22	3:JJJ:116:VAL:H	1.36	0.90
3:YYY:129:LEU:HD21	3:YYY:151:LEU:HB2	1.55	0.88
1:AAA:120:VAL:HG23	1:AAA:133:GLY:O	1.73	0.87
1:EEE:120:VAL:HG23	1:EEE:133:GLY:O	1.75	0.86
3:NNN:91:THR:HG22	3:NNN:116:VAL:H	1.45	0.80
2:GGG:145:PRO:CG	2:GGG:176:THR:HG21	2.12	0.80
3:NNN:87:ARG:O	3:NNN:116:VAL:CG1	2.30	0.80
1:AAA:161:ARG:HH22	1:EEE:53:HIS:CB	1.97	0.77
2:III:14:PRO:HD3	2:III:110:LEU:O	1.85	0.75
2:GGG:145:PRO:CB	2:GGG:176:THR:HG21	2.20	0.72
3:YYY:129:LEU:HD21	3:YYY:151:LEU:CB	2.20	0.72
2:GGG:145:PRO:HB3	2:GGG:176:THR:HG21	1.72	0.70
2:III:164:GLU:CB	2:III:181:TYR:O	2.42	0.67
1:AAA:123:ASN:OD1	1:AAA:265:ARG:NH1	2.28	0.67
1:DDD:123:ASN:OD1	1:DDD:265:ARG:NH1	2.29	0.66
3:LLL:121:THR:HG21	3:LLL:212:PRO:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:161:ARG:NH2	1:EEE:53:HIS:HB3	2.01	0.65
1:BBB:123:ASN:OD1	1:BBB:265:ARG:NH1	2.30	0.64
1:EEE:123:ASN:OD1	1:EEE:265:ARG:NH1	2.30	0.64
3:JJJ:11:LEU:HD12	3:JJJ:157:PRO:HG3	1.80	0.64
2:GGG:25:GLY:H	2:GGG:28:ASN:ND2	1.95	0.64
3:JJJ:121:THR:HG21	3:JJJ:212:PRO:O	1.98	0.64
1:AAA:264:ASN:OD1	1:AAA:270:GLN:NE2	2.31	0.63
1:AAA:120:VAL:CG2	1:AAA:133:GLY:O	2.46	0.63
3:JJJ:162:VAL:HG21	3:JJJ:190:SER:OG	1.99	0.63
3:YYY:149:GLY:HA3	3:YYY:190:SER:O	1.98	0.63
1:CCC:123:ASN:OD1	1:CCC:265:ARG:NH1	2.32	0.62
2:III:13:THR:HG22	2:III:16:GLN:CD	2.25	0.62
2:GGG:145:PRO:CD	2:GGG:176:THR:HG21	2.29	0.61
2:KKK:13:THR:HG22	2:KKK:16:GLN:CD	2.26	0.61
3:JJJ:152:VAL:HB	3:JJJ:188:LEU:HD23	1.83	0.60
3:LLL:162:VAL:C	3:LLL:207:ASN:O	2.45	0.60
2:MMM:6:GLN:OE1	2:MMM:89:CYS:HB3	2.02	0.60
1:BBB:149:GLU:HG2	1:BBB:209:ASN:HD22	1.66	0.60
2:FFF:6:GLN:OE1	2:FFF:89:CYS:HB3	2.02	0.60
1:CCC:149:GLU:HG2	1:CCC:209:ASN:HD22	1.68	0.59
1:DDD:36:ILE:HG13	1:DDD:282:LEU:O	2.03	0.59
2:GGG:145:PRO:HB3	2:GGG:176:THR:CG2	2.32	0.59
1:BBB:36:ILE:HG13	1:BBB:282:LEU:O	2.02	0.59
1:AAA:149:GLU:HG2	1:AAA:209:ASN:HD22	1.68	0.59
1:EEE:91:ASN:HD21	1:EEE:99:ILE:HA	1.66	0.59
1:AAA:53:HIS:HB3	1:BBB:161:ARG:NH2	2.09	0.58
1:AAA:90:LEU:O	1:AAA:99:ILE:HD11	2.03	0.58
1:DDD:149:GLU:HG2	1:DDD:209:ASN:HD22	1.68	0.58
1:AAA:36:ILE:HG13	1:AAA:282:LEU:O	2.04	0.58
1:AAA:217:THR:CG2	1:AAA:222:VAL:HG11	2.34	0.58
1:EEE:36:ILE:HG13	1:EEE:282:LEU:O	2.04	0.58
2:GGG:145:PRO:HB3	2:GGG:176:THR:CB	2.33	0.58
3:JJJ:79:LEU:HD23	3:JJJ:96:CYS:SG	2.43	0.57
1:EEE:120:VAL:CG2	1:EEE:133:GLY:O	2.49	0.57
3:YYY:155:TYR:OH	3:YYY:188:LEU:HD23	2.04	0.57
2:FFF:166:THR:HG22	2:FFF:167:LYS:O	2.05	0.56
1:BBB:112:ILE:HD11	1:BBB:277:TYR:HB2	1.86	0.56
1:BBB:217:THR:CG2	1:BBB:222:VAL:HG11	2.36	0.56
1:EEE:149:GLU:HG2	1:EEE:209:ASN:HD22	1.69	0.56
2:FFF:144:TYR:N	2:FFF:145:PRO:CD	2.69	0.56
1:DDD:112:ILE:HD11	1:DDD:277:TYR:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:112:ILE:HD11	1:EEE:277:TYR:HB2	1.88	0.55
2:GGG:164:GLU:CD	3:HHH:181:GLN:HA	2.31	0.55
3:HHH:79:LEU:HD23	3:HHH:96:CYS:SG	2.47	0.55
3:NNN:83:MET:HE2	3:NNN:86:LEU:HD21	1.87	0.55
2:III:137:VAL:HG21	3:JJJ:151:LEU:HD12	1.88	0.55
3:JJJ:127:PHE:CD1	3:JJJ:150:CYS:HA	2.43	0.54
1:AAA:112:ILE:HD11	1:AAA:277:TYR:HB2	1.88	0.54
1:AAA:161:ARG:NH2	1:EEE:53:HIS:CG	2.75	0.54
3:HHH:83:MET:HE2	3:HHH:86:LEU:HD21	1.87	0.54
1:EEE:90:LEU:C	1:EEE:91:ASN:OD1	2.51	0.54
3:JJJ:83:MET:HE2	3:JJJ:86:LEU:HD21	1.89	0.54
3:LLL:83:MET:HE2	3:LLL:86:LEU:HD21	1.90	0.54
1:EEE:217:THR:CG2	1:EEE:222:VAL:HG11	2.38	0.54
2:GGG:145:PRO:HG3	2:GGG:176:THR:HG21	1.90	0.54
3:LLL:79:LEU:HD23	3:LLL:96:CYS:SG	2.47	0.54
2:MMM:90:ALA:HB2	2:MMM:101:PHE:CD2	2.43	0.54
3:YYY:83:MET:HE2	3:YYY:86:LEU:HD21	1.89	0.54
2:GGG:145:PRO:HD3	2:GGG:176:THR:HG21	1.91	0.53
2:GGG:166:THR:HG22	2:GGG:179:SER:H	1.73	0.53
1:CCC:217:THR:CG2	1:CCC:222:VAL:HG11	2.38	0.53
2:FFF:90:ALA:HB2	2:FFF:101:PHE:CD2	2.45	0.52
1:CCC:112:ILE:HD11	1:CCC:277:TYR:HB2	1.91	0.52
1:AAA:53:HIS:CB	1:BBB:161:ARG:HH22	2.14	0.52
3:NNN:12:VAL:HG11	3:NNN:86:LEU:HD13	1.91	0.51
2:MMM:2:SER:HB2	2:MMM:93:ASP:OD2	2.10	0.51
1:AAA:120:VAL:HG22	1:AAA:120:VAL:O	2.10	0.51
1:DDD:217:THR:CG2	1:DDD:222:VAL:HG11	2.40	0.51
1:EEE:120:VAL:HG22	1:EEE:120:VAL:O	2.10	0.51
1:AAA:52:GLU:OE2	3:LLL:52:SER:HB2	2.12	0.50
3:JJJ:160:VAL:HG11	3:JJJ:188:LEU:HD22	1.94	0.49
3:HHH:89:GLU:H	3:HHH:89:GLU:CD	2.21	0.49
2:FFF:107:LEU:HD13	2:FFF:107:LEU:C	2.39	0.48
1:EEE:91:ASN:ND2	1:EEE:99:ILE:HA	2.26	0.48
2:GGG:90:ALA:HB2	2:GGG:101:PHE:CD2	2.49	0.48
3:JJJ:88:VAL:O	3:JJJ:91:THR:HG23	2.13	0.48
1:AAA:99:ILE:HG13	1:AAA:100:LEU:N	2.28	0.48
1:DDD:148:GLY:HA3	1:DDD:245:LEU:O	2.14	0.48
2:III:36:TRP:CZ3	2:III:89:CYS:HB3	2.48	0.48
1:EEE:80:TYR:HA	1:EEE:256:VAL:HG22	1.96	0.48
2:KKK:140:ILE:H	2:KKK:140:ILE:HG12	1.31	0.48
2:MMM:55:ARG:HD3	2:MMM:63:PHE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:52:GLU:OE2	3:JJJ:52:SER:HB2	2.15	0.47
2:GGG:55:ARG:HD3	2:GGG:63:PHE:O	2.15	0.47
1:CCC:137:GLN:HE21	1:CCC:221:ASN:HA	1.78	0.47
2:FFF:55:ARG:HD3	2:FFF:63:PHE:O	2.14	0.47
2:KKK:55:ARG:HD3	2:KKK:63:PHE:O	2.14	0.47
1:DDD:82:VAL:O	1:DDD:192:ASN:ND2	2.46	0.47
2:GGG:210:VAL:HG12	2:GGG:212:PRO:HD3	1.96	0.47
1:CCC:148:GLY:HA3	1:CCC:245:LEU:O	2.16	0.46
2:GGG:196:SER:OG	2:GGG:209:THR:HG23	2.15	0.46
2:III:184:LEU:C	2:III:184:LEU:HD12	2.41	0.46
3:YYY:22:CYS:HB3	3:YYY:79:LEU:HB3	1.97	0.46
1:AAA:116:SER:O	1:BBB:158:PHE:HB2	2.15	0.46
1:EEE:84:ARG:HD3	1:EEE:252:TYR:OH	2.16	0.46
2:GGG:62:ARG:NH2	2:GGG:83:ASP:OD2	2.48	0.46
3:YYY:129:LEU:N	3:YYY:129:LEU:CD2	2.79	0.46
1:AAA:84:ARG:HD3	1:AAA:252:TYR:OH	2.15	0.46
1:AAA:217:THR:HG21	1:AAA:222:VAL:HG11	1.98	0.46
3:JJJ:27:PHE:CE2	3:JJJ:29:PHE:HA	2.51	0.46
2:FFF:149:THR:HG22	2:FFF:150:VAL:H	1.81	0.46
3:LLL:27:PHE:CE2	3:LLL:29:PHE:HA	2.51	0.46
1:AAA:158:PHE:HB2	1:EEE:116:SER:O	2.16	0.45
1:AAA:80:TYR:HA	1:AAA:256:VAL:HG22	1.98	0.45
2:FFF:139:LEU:HB3	3:YYY:176:PHE:CZ	2.52	0.45
2:FFF:62:ARG:NH2	2:FFF:83:ASP:OD2	2.50	0.45
1:AAA:148:GLY:HA3	1:AAA:245:LEU:O	2.16	0.45
1:DDD:80:TYR:HA	1:DDD:256:VAL:HG22	1.99	0.45
2:KKK:62:ARG:NH2	2:KKK:83:ASP:OD2	2.49	0.45
3:YYY:11:LEU:CD1	3:YYY:157:PRO:HB3	2.47	0.45
1:BBB:148:GLY:HA3	1:BBB:245:LEU:O	2.17	0.45
1:DDD:103:GLU:OE1	1:DDD:283:ARG:NE	2.41	0.45
1:CCC:56:GLY:O	1:CCC:272:ARG:HD2	2.15	0.45
1:CCC:80:TYR:HA	1:CCC:256:VAL:HG22	1.98	0.45
1:EEE:56:GLY:O	1:EEE:272:ARG:HD2	2.17	0.45
3:HHH:18:LEU:HD23	3:HHH:18:LEU:HA	1.83	0.45
2:MMM:90:ALA:HB2	2:MMM:101:PHE:CE2	2.52	0.45
1:AAA:99:ILE:CG1	1:AAA:100:LEU:H	2.30	0.45
1:DDD:262:PHE:CD1	1:EEE:158:PHE:HZ	2.36	0.45
1:EEE:161:ARG:HE	1:EEE:161:ARG:HB2	1.64	0.45
1:EEE:148:GLY:HA3	1:EEE:245:LEU:O	2.17	0.44
3:YYY:27:PHE:CE2	3:YYY:29:PHE:HA	2.51	0.44
3:YYY:33:THR:HG22	3:YYY:52:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:64:SER:HB3	1:BBB:70:ASP:HA	1.99	0.44
2:III:17:ARG:HD2	2:III:77:SER:HB3	1.99	0.44
3:YYY:6:GLU:HA	3:YYY:21:SER:O	2.17	0.44
1:AAA:99:ILE:HG13	1:AAA:100:LEU:H	1.82	0.44
3:HHH:29:PHE:CE1	3:HHH:34:MET:HG3	2.52	0.44
1:DDD:84:ARG:HD3	1:DDD:252:TYR:OH	2.17	0.44
1:EEE:64:SER:HB3	1:EEE:70:ASP:HA	1.99	0.44
1:AAA:56:GLY:O	1:AAA:272:ARG:HD2	2.18	0.44
1:BBB:80:TYR:HA	1:BBB:256:VAL:HG22	1.99	0.44
2:FFF:90:ALA:HB2	2:FFF:101:PHE:CE2	2.52	0.44
2:MMM:62:ARG:NH2	2:MMM:83:ASP:OD2	2.51	0.44
3:NNN:6:GLU:HA	3:NNN:21:SER:O	2.17	0.44
3:NNN:33:THR:HG22	3:NNN:52:SER:HA	2.00	0.44
1:DDD:56:GLY:O	1:DDD:272:ARG:HD2	2.18	0.44
3:YYY:168:ALA:HA	3:YYY:173:VAL:HG11	1.99	0.44
1:BBB:56:GLY:O	1:BBB:272:ARG:HD2	2.17	0.43
1:AAA:63:ILE:HD11	1:EEE:133:GLY:N	2.32	0.43
3:JJJ:163:SER:HB2	3:JJJ:207:ASN:HB2	2.00	0.43
3:NNN:79:LEU:HD23	3:NNN:96:CYS:SG	2.58	0.43
3:HHH:6:GLU:HA	3:HHH:21:SER:O	2.18	0.43
3:LLL:6:GLU:HA	3:LLL:21:SER:O	2.18	0.43
2:III:62:ARG:NH2	2:III:83:ASP:OD2	2.51	0.43
2:FFF:206:VAL:HG12	2:FFF:206:VAL:O	2.18	0.43
2:GGG:199:VAL:HG23	2:GGG:199:VAL:O	2.18	0.43
3:JJJ:6:GLU:HA	3:JJJ:21:SER:O	2.18	0.43
1:DDD:116:SER:O	1:EEE:158:PHE:HB2	2.19	0.43
2:FFF:145:PRO:HB3	2:FFF:202:GLU:OE2	2.18	0.43
1:AAA:82:VAL:O	1:AAA:192:ASN:ND2	2.46	0.42
1:AAA:217:THR:HG22	1:AAA:222:VAL:HG11	2.00	0.42
3:HHH:158:GLU:O	3:HHH:159:PRO:C	2.61	0.42
3:JJJ:211:LYS:N	3:JJJ:212:PRO:CD	2.82	0.42
1:BBB:217:THR:HG22	1:BBB:222:VAL:HG11	2.00	0.42
1:EEE:182:ASN:C	1:EEE:182:ASN:OD1	2.62	0.42
3:HHH:155:TYR:HE1	3:HHH:158:GLU:H	1.67	0.42
3:LLL:208:VAL:HG12	3:LLL:217:VAL:O	2.19	0.42
1:AAA:262:PHE:CD1	1:BBB:158:PHE:HZ	2.37	0.42
1:BBB:84:ARG:HD3	1:BBB:252:TYR:OH	2.18	0.42
3:JJJ:99:TYR:CD1	3:JJJ:99:TYR:C	2.98	0.42
3:NNN:88:VAL:O	3:NNN:91:THR:HG23	2.19	0.42
3:YYY:149:GLY:CA	3:YYY:190:SER:O	2.64	0.42
1:DDD:182:ASN:OD1	1:DDD:182:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:HHH:180:LEU:HD12	3:HHH:186:TYR:CZ	2.54	0.42
2:KKK:139:LEU:HB3	2:KKK:140:ILE:H	1.64	0.42
2:GGG:6:GLN:OE1	2:GGG:89:CYS:SG	2.77	0.42
2:GGG:182:LEU:HD12	2:GGG:182:LEU:C	2.45	0.42
2:III:14:PRO:CD	2:III:110:LEU:O	2.63	0.42
2:MMM:4:LEU:HG	2:MMM:100:VAL:HG23	2.02	0.42
1:BBB:264:ASN:HB3	3:JJJ:102:ASP:CG	2.45	0.42
1:BBB:82:VAL:O	1:BBB:192:ASN:ND2	2.46	0.42
3:YYY:211:LYS:N	3:YYY:212:PRO:CD	2.83	0.42
3:HHH:99:TYR:CD1	3:HHH:99:TYR:C	2.98	0.42
2:GGG:112:ALA:HB1	2:GGG:113:PRO:HD2	2.00	0.41
3:HHH:22:CYS:HB3	3:HHH:79:LEU:HB3	2.01	0.41
1:CCC:103:GLU:OE1	1:CCC:283:ARG:NE	2.42	0.41
2:GGG:145:PRO:HD3	2:GGG:176:THR:CG2	2.50	0.41
2:III:4:LEU:HG	2:III:100:VAL:HG23	2.02	0.41
1:AAA:120:VAL:HG22	1:AAA:132:ALA:HB1	2.02	0.41
1:CCC:217:THR:HG22	1:CCC:222:VAL:HG11	2.01	0.41
1:DDD:194:ALA:O	1:DDD:196:PRO:HD3	2.21	0.41
1:AAA:103:GLU:OE1	1:AAA:283:ARG:NE	2.42	0.41
1:AAA:182:ASN:OD1	1:AAA:182:ASN:C	2.63	0.41
1:CCC:224:PRO:O	1:DDD:217:THR:HA	2.21	0.41
2:FFF:139:LEU:HD12	3:YYY:191:VAL:HG11	2.02	0.41
3:LLL:22:CYS:HB3	3:LLL:79:LEU:HB3	2.02	0.41
1:AAA:99:ILE:CG1	1:AAA:100:LEU:N	2.83	0.41
1:EEE:103:GLU:OE1	1:EEE:283:ARG:NE	2.42	0.41
2:GGG:121:LEU:HG	2:GGG:121:LEU:O	2.20	0.41
2:GGG:36:TRP:CZ3	2:GGG:89:CYS:HB3	2.55	0.41
2:FFF:14:PRO:HD3	2:FFF:110:LEU:O	2.21	0.41
2:GGG:201:HIS:CD2	2:GGG:201:HIS:C	2.97	0.41
3:YYY:123:GLY:HA3	3:YYY:213:SER:OG	2.20	0.41
3:YYY:124:PRO:HG2	3:YYY:215:THR:HG21	2.03	0.41
1:CCC:64:SER:HB3	1:CCC:70:ASP:HA	2.02	0.41
1:EEE:82:VAL:O	1:EEE:192:ASN:ND2	2.45	0.41
2:FFF:6:GLN:NE2	2:FFF:87:TYR:O	2.54	0.41
2:FFF:114:LYS:HA	2:FFF:145:PRO:HG3	2.03	0.41
2:FFF:139:LEU:HD21	3:YYY:189:SER:OG	2.21	0.41
3:LLL:126:VAL:HA	3:LLL:151:LEU:O	2.21	0.41
3:YYY:149:GLY:O	3:YYY:221:VAL:HG11	2.21	0.41
1:AAA:158:PHE:HZ	1:EEE:262:PHE:CD1	2.38	0.41
2:FFF:36:TRP:HB2	2:FFF:49:ILE:HB	2.03	0.41
2:GGG:20:ILE:HD12	2:GGG:105:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KKK:6:GLN:NE2	2:KKK:87:TYR:O	2.54	0.41
3:LLL:99:TYR:CD1	3:LLL:99:TYR:C	2.99	0.41
3:YYY:151:LEU:HD11	3:YYY:153:LYS:HB2	2.02	0.40
3:YYY:168:ALA:O	3:YYY:173:VAL:HG21	2.22	0.40
1:BBB:194:ALA:O	1:BBB:196:PRO:HD3	2.21	0.40
1:DDD:64:SER:HB3	1:DDD:70:ASP:HA	2.02	0.40
2:GGG:166:THR:HG23	2:GGG:167:LYS:O	2.21	0.40
3:JJJ:22:CYS:HB3	3:JJJ:79:LEU:HB3	2.03	0.40
3:LLL:211:LYS:N	3:LLL:212:PRO:CD	2.85	0.40
1:AAA:212:TYR:CE2	1:EEE:230:ASN:HB3	2.57	0.40
2:GGG:121:LEU:HD22	2:GGG:208:LYS:CB	2.52	0.40
2:III:6:GLN:NE2	2:III:87:TYR:O	2.54	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	256/272 (94%)	247 (96%)	9 (4%)	0	100	100
1	BBB	254/272 (93%)	244 (96%)	10 (4%)	0	100	100
1	CCC	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
1	DDD	257/272 (94%)	244 (95%)	13 (5%)	0	100	100
1	EEE	258/272 (95%)	244 (95%)	14 (5%)	0	100	100
2	FFF	183/212 (86%)	166 (91%)	16 (9%)	1 (0%)	24	55
2	GGG	168/212 (79%)	155 (92%)	12 (7%)	1 (1%)	21	52
2	III	128/212 (60%)	122 (95%)	6 (5%)	0	100	100
2	KKK	126/212 (59%)	116 (92%)	10 (8%)	0	100	100
2	MMM	106/212 (50%)	102 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	HHH	143/398 (36%)	133 (93%)	8 (6%)	2 (1%)	9	34
3	JJJ	169/398 (42%)	157 (93%)	11 (6%)	1 (1%)	21	52
3	LLL	162/398 (41%)	149 (92%)	12 (7%)	1 (1%)	21	52
3	NNN	116/398 (29%)	110 (95%)	6 (5%)	0	100	100
3	YYY	181/398 (46%)	167 (92%)	14 (8%)	0	100	100
All	All	2760/4410 (63%)	2595 (94%)	159 (6%)	6 (0%)	43	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	HHH	157	PRO
2	GGG	142	ASP
3	HHH	158	GLU
3	JJJ	104	ASN
3	LLL	104	ASN
2	FFF	124	PRO

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	219/237 (92%)	218 (100%)	1 (0%)	81	82
1	BBB	223/237 (94%)	222 (100%)	1 (0%)	84	84
1	CCC	221/237 (93%)	219 (99%)	2 (1%)	70	77
1	DDD	222/237 (94%)	220 (99%)	2 (1%)	70	77
1	EEE	222/237 (94%)	217 (98%)	5 (2%)	44	66
2	FFF	144/175 (82%)	138 (96%)	6 (4%)	26	55
2	GGG	127/175 (73%)	122 (96%)	5 (4%)	28	57
2	III	102/175 (58%)	102 (100%)	0	100	100
2	KKK	102/175 (58%)	98 (96%)	4 (4%)	28	57
2	MMM	86/175 (49%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	HHH	121/352 (34%)	114 (94%)	7 (6%)	18	46
3	JJJ	139/352 (40%)	135 (97%)	4 (3%)	37	63
3	LLL	138/352 (39%)	133 (96%)	5 (4%)	31	59
3	NNN	97/352 (28%)	94 (97%)	3 (3%)	35	61
3	YYY	155/352 (44%)	149 (96%)	6 (4%)	28	57
All	All	2318/3820 (61%)	2267 (98%)	51 (2%)	45	67

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	62	SER
1	BBB	62	SER
1	CCC	28	GLU
1	CCC	62	SER
1	DDD	62	SER
1	DDD	285	ARG
1	EEE	26	VAL
1	EEE	34	ASP
1	EEE	62	SER
1	EEE	91	ASN
1	EEE	206	ARG
2	FFF	61	ASP
2	FFF	84	GLU
2	FFF	136	LEU
2	FFF	164	GLU
2	FFF	194	SER
2	FFF	199	VAL
2	GGG	27	SER
2	GGG	28	ASN
2	GGG	135	THR
2	GGG	164	GLU
2	GGG	166	THR
3	HHH	28	THR
3	HHH	55	SER
3	HHH	152	VAL
3	HHH	154	ASP
3	HHH	155	TYR
3	HHH	156	PHE
3	HHH	175	THR
3	JJJ	54	SER

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Mol	Chain	Res	Type
3	JJJ	55	SER
3	JJJ	115	THR
3	JJJ	188	LEU
2	KKK	139	LEU
2	KKK	140	ILE
2	KKK	145	PRO
2	KKK	148	VAL
3	LLL	3	GLN
3	LLL	54	SER
3	LLL	55	SER
3	LLL	115	THR
3	LLL	218	ASP
3	NNN	54	SER
3	NNN	55	SER
3	NNN	118	SER
3	YYY	54	SER
3	YYY	55	SER
3	YYY	96	CYS
3	YYY	115	THR
3	YYY	129	LEU
3	YYY	183	SER

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

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	260/272 (95%)	-0.23	4 (1%) 72 52	21, 34, 70, 115	0
1	BBB	258/272 (94%)	-0.22	4 (1%) 70 50	20, 36, 74, 101	0
1	CCC	257/272 (94%)	-0.34	1 (0%) 88 78	18, 33, 54, 71	0
1	DDD	261/272 (95%)	-0.37	4 (1%) 72 52	18, 31, 57, 116	0
1	EEE	262/272 (96%)	-0.23	4 (1%) 72 52	20, 33, 77, 131	0
2	FFF	191/212 (90%)	0.33	9 (4%) 36 21	24, 60, 101, 121	0
2	GGG	176/212 (83%)	1.02	33 (18%) 3 2	30, 74, 142, 165	0
2	III	136/212 (64%)	0.64	15 (11%) 10 6	35, 69, 110, 124	0
2	KKK	134/212 (63%)	0.37	9 (6%) 24 13	29, 52, 103, 123	0
2	MMM	108/212 (50%)	0.29	5 (4%) 37 21	28, 55, 87, 97	0
3	HHH	149/398 (37%)	0.26	12 (8%) 18 10	26, 45, 110, 140	0
3	JJJ	177/398 (44%)	0.77	12 (6%) 23 13	29, 80, 127, 146	0
3	LLL	170/398 (42%)	0.26	6 (3%) 47 28	23, 49, 103, 121	0
3	NNN	118/398 (29%)	-0.09	0 100 100	24, 43, 60, 81	0
3	YYY	189/398 (47%)	0.08	8 (4%) 40 23	22, 40, 93, 104	0
All	All	2846/4410 (64%)	0.10	126 (4%) 39 22	18, 42, 105, 165	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	GGG	145	PRO	6.0
2	GGG	212	PRO	4.7
1	DDD	97	GLY	4.4
3	HHH	154	ASP	4.4
2	GGG	176	THR	4.3
2	III	186	PRO	4.3
1	DDD	289	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	GGG	144	TYR	4.1
2	III	139	LEU	4.0
2	KKK	182	LEU	4.0
3	YYY	147	ALA	4.0
2	GGG	24	GLY	4.0
2	GGG	122	PHE	3.9
3	HHH	177	PRO	3.8
2	KKK	113	PRO	3.7
3	YYY	167	GLY	3.7
2	III	185	THR	3.5
3	YYY	168	ALA	3.5
2	GGG	135	THR	3.4
2	GGG	182	LEU	3.4
3	HHH	156	PHE	3.4
2	III	182	LEU	3.4
2	GGG	149	THR	3.4
2	GGG	198	GLN	3.4
2	MMM	109	VAL	3.4
2	KKK	139	LEU	3.4
3	YYY	173	VAL	3.4
2	GGG	142	ASP	3.3
2	GGG	81	SER	3.3
1	AAA	289	ASN	3.3
2	KKK	140	ILE	3.2
2	GGG	124	PRO	3.2
2	III	184	LEU	3.2
3	JJJ	175	THR	3.2
1	BBB	24	VAL	3.1
2	FFF	144	TYR	3.1
3	HHH	157	PRO	3.1
2	FFF	177	ALA	3.0
1	AAA	91	ASN	3.0
1	EEE	23	GLY	3.0
2	III	165	THR	2.9
2	GGG	177	ALA	2.9
2	FFF	143	PHE	2.9
3	JJJ	162	VAL	2.9
1	EEE	33	VAL	2.9
1	DDD	98	ASN	2.8
2	GGG	211	ALA	2.8
2	GGG	204	THR	2.8
2	III	110	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	HHH	155	TYR	2.7
2	III	136	LEU	2.7
3	JJJ	176	PHE	2.7
2	FFF	198	GLN	2.7
2	III	132	ASN	2.7
1	AAA	33	VAL	2.7
2	GGG	123	PRO	2.7
3	HHH	126	VAL	2.7
3	LLL	162	VAL	2.7
3	HHH	159	PRO	2.6
2	GGG	119	VAL	2.6
2	GGG	61	ASP	2.6
2	GGG	115	ALA	2.6
2	III	2	SER	2.6
2	FFF	126	SER	2.6
2	GGG	134	ALA	2.6
2	GGG	23	SER	2.5
3	YYY	192	VAL	2.5
1	DDD	91	ASN	2.5
2	GGG	121	LEU	2.5
3	JJJ	151	LEU	2.5
2	KKK	148	VAL	2.5
1	BBB	91	ASN	2.5
2	GGG	139	LEU	2.5
2	GGG	199	VAL	2.5
3	HHH	189	SER	2.5
3	LLL	174	HIS	2.5
1	BBB	33	VAL	2.5
3	JJJ	147	ALA	2.4
3	JJJ	1	GLU	2.4
2	KKK	165	THR	2.4
2	GGG	195	TYR	2.4
2	FFF	112	ALA	2.4
3	YYY	130	ALA	2.4
1	BBB	161	ARG	2.4
1	EEE	21	MET	2.4
3	JJJ	180	LEU	2.4
2	FFF	161	ALA	2.4
3	YYY	148	LEU	2.4
2	GGG	120	THR	2.4
2	GGG	163	VAL	2.4
2	III	178	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	JJJ	154	ASP	2.3
2	III	163	VAL	2.3
1	CCC	65	ASP	2.3
2	GGG	202	GLU	2.3
2	KKK	179	SER	2.3
2	FFF	146	GLY	2.3
3	LLL	217	VAL	2.3
1	EEE	289	ASN	2.3
3	LLL	1	GLU	2.2
2	III	112	ALA	2.2
3	HHH	188	LEU	2.2
2	FFF	185	THR	2.2
2	GGG	113	PRO	2.2
3	HHH	121	THR	2.2
2	III	23	SER	2.2
3	LLL	188	LEU	2.2
2	MMM	108	THR	2.2
2	GGG	147	ALA	2.2
3	HHH	152	VAL	2.1
2	KKK	111	GLY	2.1
3	LLL	189	SER	2.1
3	YYY	166	SER	2.1
2	III	3	VAL	2.1
3	JJJ	191	VAL	2.1
3	JJJ	217	VAL	2.1
2	KKK	110	LEU	2.1
2	MMM	17	ARG	2.1
2	GGG	143	PHE	2.1
2	MMM	14	PRO	2.1
3	HHH	158	GLU	2.1
1	AAA	98	ASN	2.0
3	JJJ	127	PHE	2.0
2	GGG	207	GLU	2.0
3	JJJ	50	SER	2.0
2	MMM	12	GLY	2.0

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.