



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:11 AM EDT

PDB ID : 9CQD / pdb_00009cqd
Title : Antibody 2B11 bound to the central conserved domain of RSV G
Authors : Juarez, M.G.; DuBois, R.M.
Deposited on : 2024-07-19
Resolution : 3.10 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

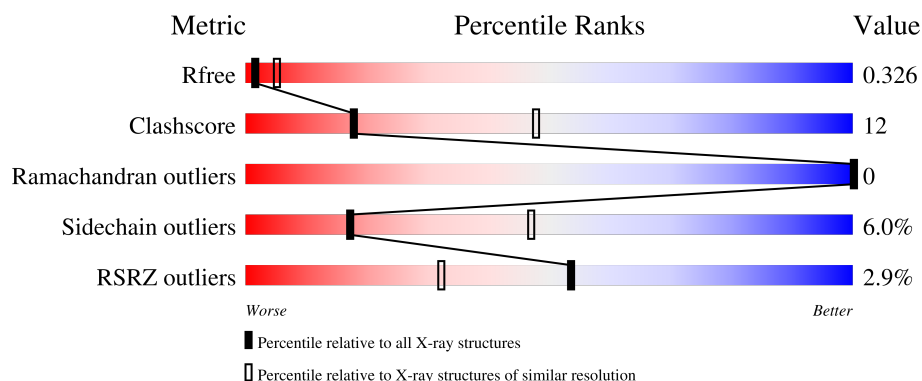
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	49	43% 16% • 37%
1	M	49	31% 20% • 45%
1	N	49	2% 51% 10% • 37%

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Mol	Chain	Length	Quality of chain
1	U	49	
1	V	49	
1	j	49	
2	B	261	
2	H	261	
2	J	261	
2	L	261	
2	P	261	
2	R	261	
2	X	261	
2	Z	261	
3	F	220	
3	G	220	
3	I	220	
3	K	220	
3	O	220	
3	Q	220	
3	W	220	
3	Y	220	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25772 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 Mature secreted glycoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	27	Total	C	N	O	S	0	0	0
			221	145	37	35	4			
1	N	31	Total	C	N	O	S	0	0	0
			253	164	43	42	4			
1	S	30	Total	C	N	O	S	0	0	0
			245	160	42	39	4			
1	T	30	Total	C	N	O	S	0	0	0
			245	160	42	39	4			
1	U	30	Total	C	N	O	S	0	0	0
			245	160	42	39	4			
1	V	29	Total	C	N	O	S	0	0	0
			236	154	40	38	4			
1	j	32	Total	C	N	O	S	0	0	0
			261	168	45	44	4			
1	A	31	Total	C	N	O	S	0	0	0
			254	166	44	40	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	155	MET	-	initiating methionine	UNP P03423
M	156	GLY	-	expression tag	UNP P03423
M	198	HIS	-	expression tag	UNP P03423
M	199	HIS	-	expression tag	UNP P03423
M	200	HIS	-	expression tag	UNP P03423
M	201	HIS	-	expression tag	UNP P03423
M	202	HIS	-	expression tag	UNP P03423
M	203	HIS	-	expression tag	UNP P03423
N	155	MET	-	initiating methionine	UNP P03423
N	156	GLY	-	expression tag	UNP P03423
N	198	HIS	-	expression tag	UNP P03423
N	199	HIS	-	expression tag	UNP P03423
N	200	HIS	-	expression tag	UNP P03423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	201	HIS	-	expression tag	UNP P03423
N	202	HIS	-	expression tag	UNP P03423
N	203	HIS	-	expression tag	UNP P03423
S	155	MET	-	initiating methionine	UNP P03423
S	156	GLY	-	expression tag	UNP P03423
S	198	HIS	-	expression tag	UNP P03423
S	199	HIS	-	expression tag	UNP P03423
S	200	HIS	-	expression tag	UNP P03423
S	201	HIS	-	expression tag	UNP P03423
S	202	HIS	-	expression tag	UNP P03423
S	203	HIS	-	expression tag	UNP P03423
T	155	MET	-	initiating methionine	UNP P03423
T	156	GLY	-	expression tag	UNP P03423
T	198	HIS	-	expression tag	UNP P03423
T	199	HIS	-	expression tag	UNP P03423
T	200	HIS	-	expression tag	UNP P03423
T	201	HIS	-	expression tag	UNP P03423
T	202	HIS	-	expression tag	UNP P03423
T	203	HIS	-	expression tag	UNP P03423
U	155	MET	-	initiating methionine	UNP P03423
U	156	GLY	-	expression tag	UNP P03423
U	198	HIS	-	expression tag	UNP P03423
U	199	HIS	-	expression tag	UNP P03423
U	200	HIS	-	expression tag	UNP P03423
U	201	HIS	-	expression tag	UNP P03423
U	202	HIS	-	expression tag	UNP P03423
U	203	HIS	-	expression tag	UNP P03423
V	155	MET	-	initiating methionine	UNP P03423
V	156	GLY	-	expression tag	UNP P03423
V	198	HIS	-	expression tag	UNP P03423
V	199	HIS	-	expression tag	UNP P03423
V	200	HIS	-	expression tag	UNP P03423
V	201	HIS	-	expression tag	UNP P03423
V	202	HIS	-	expression tag	UNP P03423
V	203	HIS	-	expression tag	UNP P03423
j	155	MET	-	initiating methionine	UNP P03423
j	156	GLY	-	expression tag	UNP P03423
j	198	HIS	-	expression tag	UNP P03423
j	199	HIS	-	expression tag	UNP P03423
j	200	HIS	-	expression tag	UNP P03423
j	201	HIS	-	expression tag	UNP P03423
j	202	HIS	-	expression tag	UNP P03423

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Chain	Residue	Modelled	Actual	Comment	Reference
j	203	HIS	-	expression tag	UNP P03423
A	155	MET	-	initiating methionine	UNP P03423
A	156	GLY	-	expression tag	UNP P03423
A	198	HIS	-	expression tag	UNP P03423
A	199	HIS	-	expression tag	UNP P03423
A	200	HIS	-	expression tag	UNP P03423
A	201	HIS	-	expression tag	UNP P03423
A	202	HIS	-	expression tag	UNP P03423
A	203	HIS	-	expression tag	UNP P03423

- Molecule 2 is a protein called Fab 2B11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1605	1021	267	309	8			
2	J	210	Total	C	N	O	S	0	0	0
			1566	998	260	300	8			
2	L	216	Total	C	N	O	S	0	0	0
			1601	1017	267	309	8			
2	P	214	Total	C	N	O	S	0	0	0
			1592	1014	265	305	8			
2	R	217	Total	C	N	O	S	0	0	0
			1611	1024	268	310	9			
2	X	219	Total	C	N	O	S	0	0	0
			1627	1033	271	315	8			
2	Z	215	Total	C	N	O	S	0	0	0
			1599	1018	266	307	8			
2	H	115	Total	C	N	O	S	0	0	0
			870	552	149	163	6			

- Molecule 3 is a protein called Fab 2B11 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	208	Total	C	N	O	S	0	0	0
			1578	984	267	323	4			
3	G	104	Total	C	N	O	S	0	0	0
			767	477	131	157	2			
3	I	199	Total	C	N	O	S	0	0	0
			1509	939	256	310	4			
3	K	209	Total	C	N	O	S	0	0	0
			1565	973	266	322	4			
3	O	206	Total	C	N	O	S	0	0	0
			1553	966	265	318	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	211	Total	C	N	O	S	0	0	0
			1584	985	267	328	4			
3	W	211	Total	C	N	O	S	0	0	0
			1593	993	270	326	4			
3	Y	212	Total	C	N	O	S	0	0	0
			1592	989	270	329	4			

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.

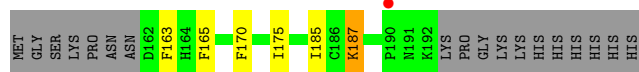
- Molecule 1: Mature secreted glycoprotein G

Chain M: 

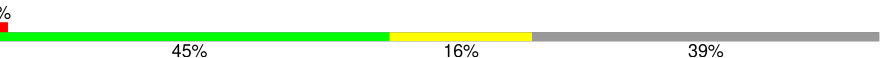


- Molecule 1: Mature secreted glycoprotein G

Chain N: 



- Molecule 1: Mature secreted glycoprotein G

Chain S: 

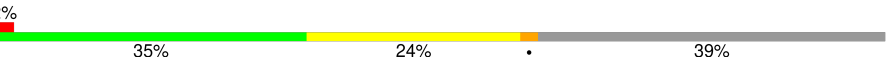


- Molecule 1: Mature secreted glycoprotein G

Chain T: 

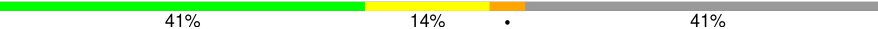


- Molecule 1: Mature secreted glycoprotein G

Chain U: 



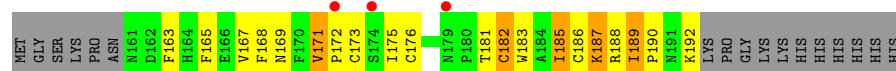
- Molecule 1: Mature secreted glycoprotein G

Chain V: 

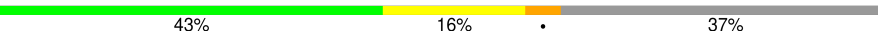


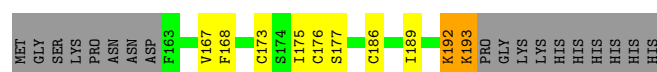
- Molecule 1: Mature secreted glycoprotein G

Chain j: 



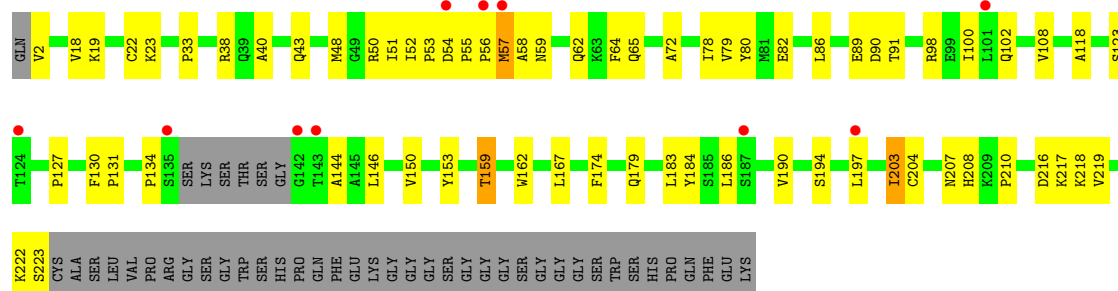
- Molecule 1: Mature secreted glycoprotein G

Chain A: 



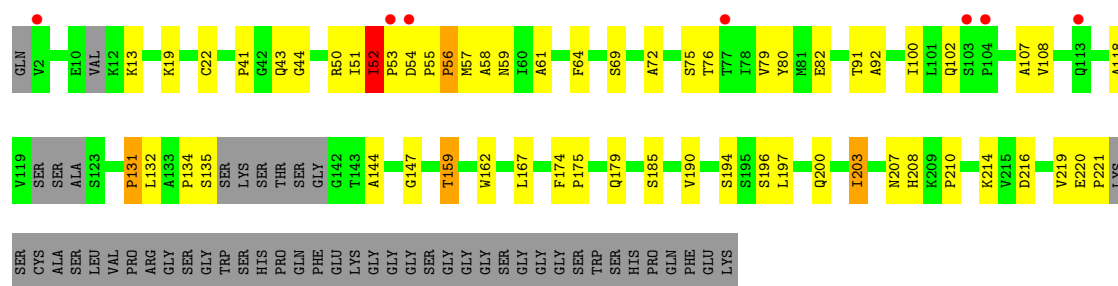
- Molecule 2: Fab 2B11 Heavy Chain

Chain B: 



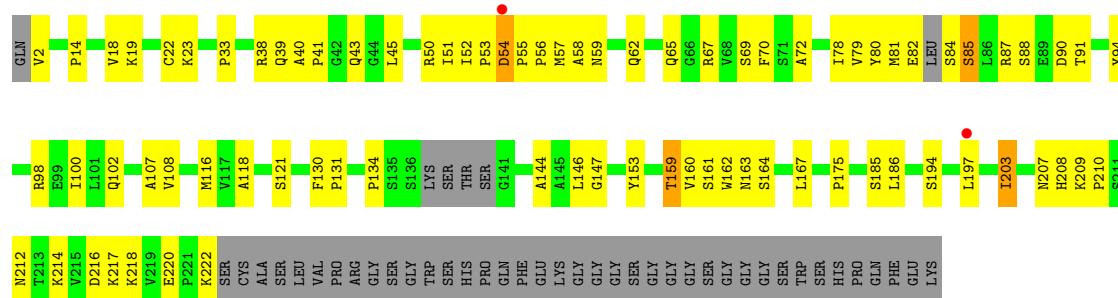
- Molecule 2: Fab 2B11 Heavy Chain

Chain J: 

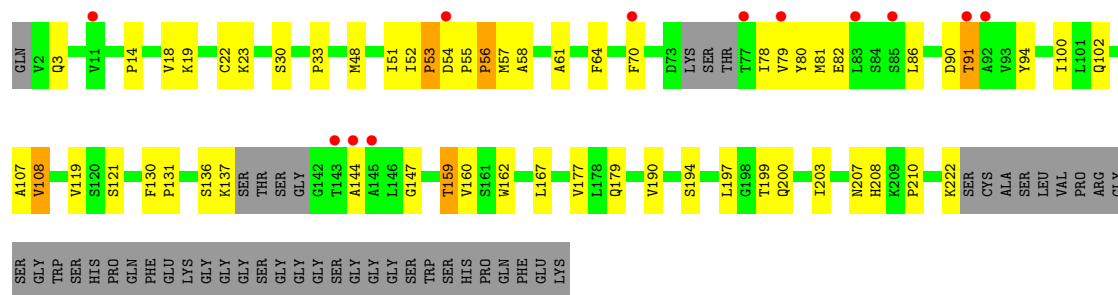


- Molecule 2: Fab 2B11 Heavy Chain

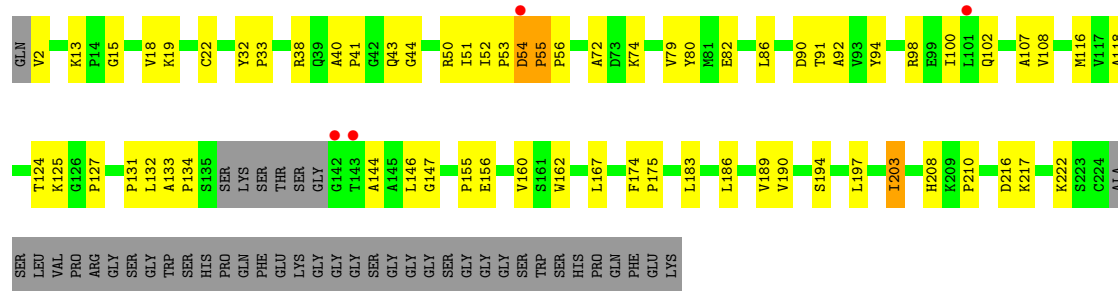
Chain L: 



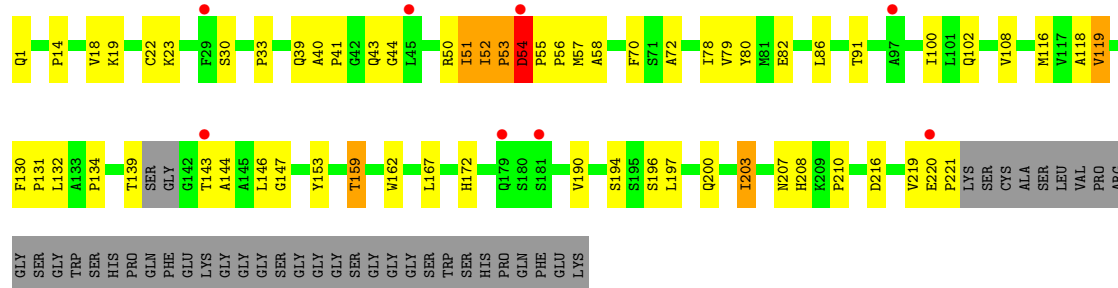
• Molecule 2: Fab 2B11 Heavy Chain



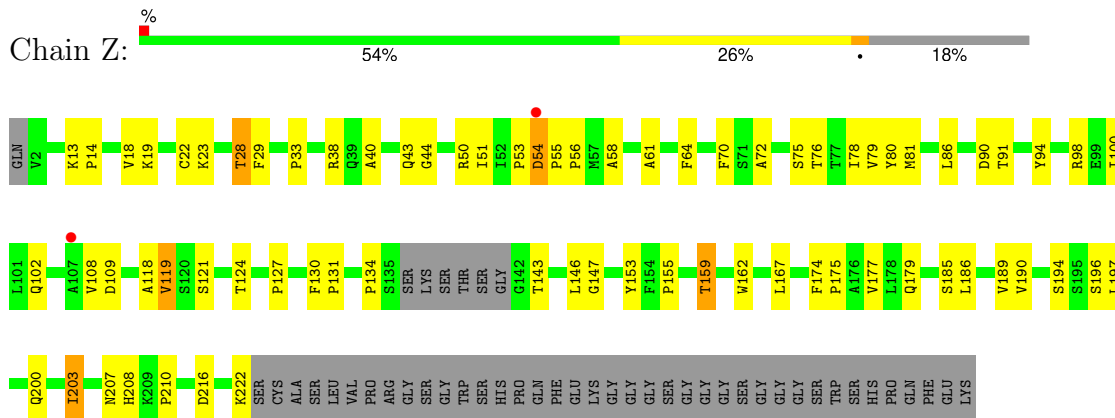
• Molecule 2: Fab 2B11 Heavy Chain



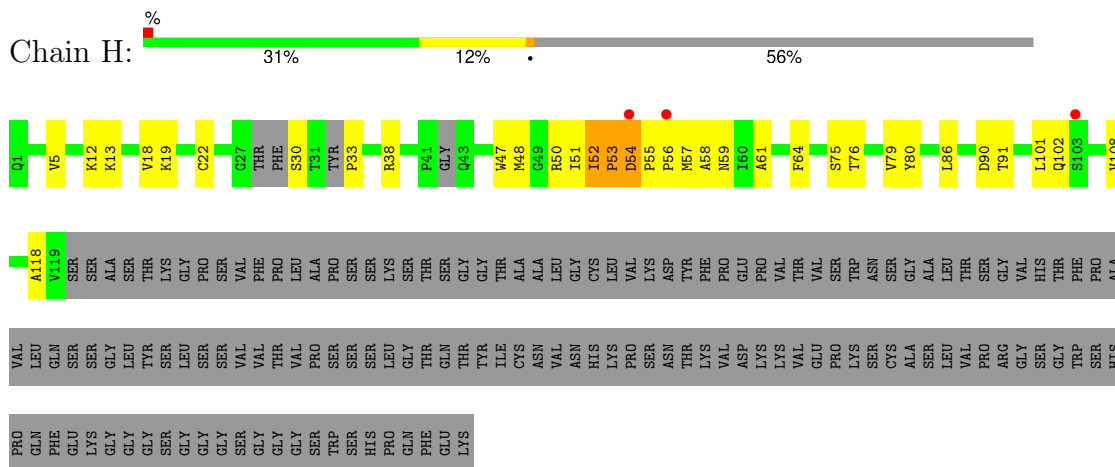
• Molecule 2: Fab 2B11 Heavy Chain



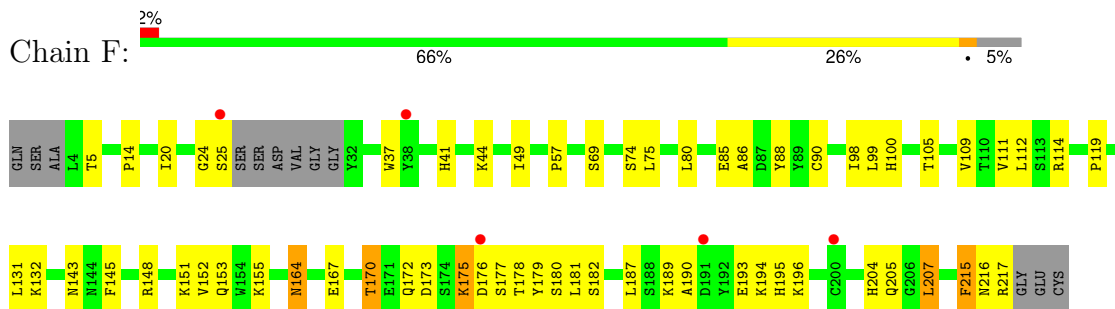
- Molecule 2: Fab 2B11 Heavy Chain



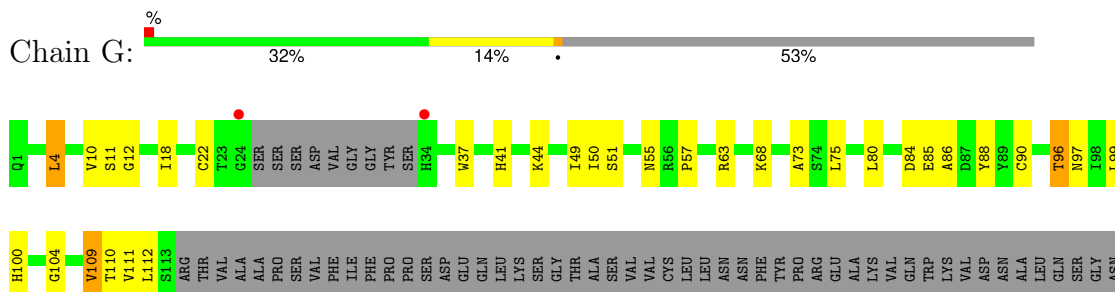
- Molecule 2: Fab 2B11 Heavy Chain



- Molecule 3: Fab 2B11 Light Chain



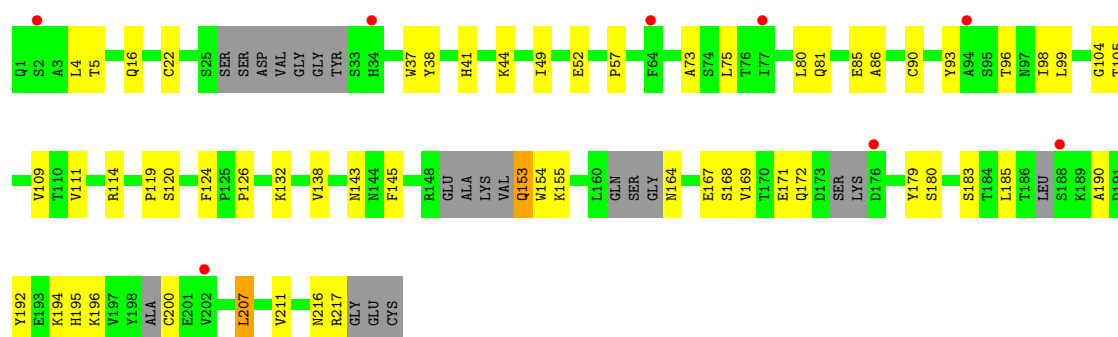
- Molecule 3: Fab 2B11 Light Chain



SER GLN GLU SER SER VAL THR GLU ASP SER LYS ASP SER THR TYR LEU SER SER THR LEU THR THR SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS VAL THR HIS THR GLN LEU SER SER SER PRO VAL THR SER PHE ASN ARG GLY GLU CYS

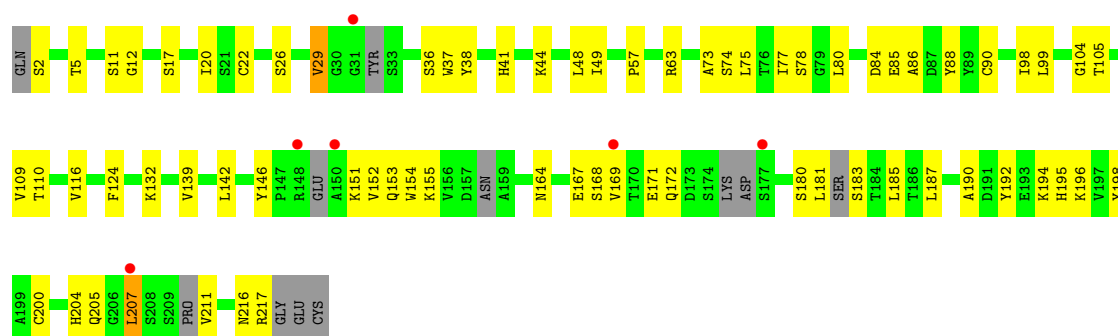
• Molecule 3: Fab 2B11 Light Chain

Chain I:  4% 64% 25% 10%



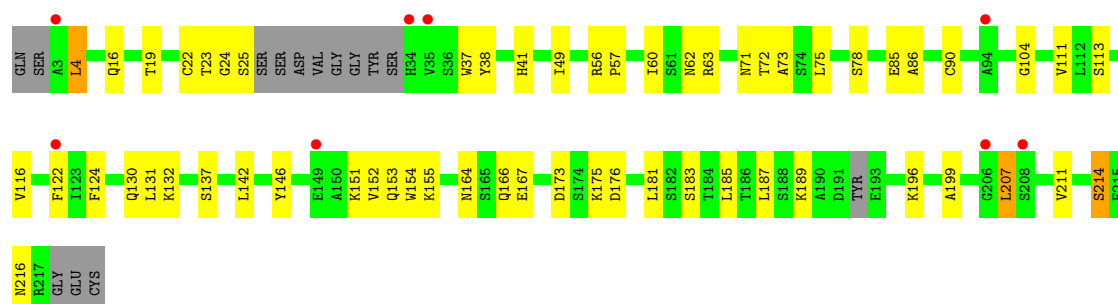
• Molecule 3: Fab 2B11 Light Chain

Chain K:  3% 63% 31% 5%



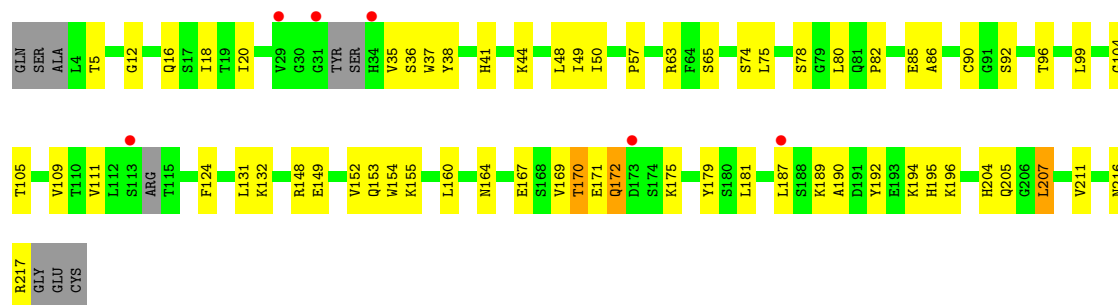
• Molecule 3: Fab 2B11 Light Chain

Chain O:  4% 67% 25% 6%

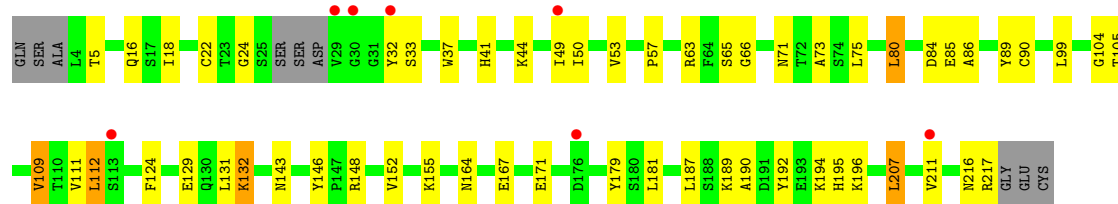


• Molecule 3: Fab 2B11 Light Chain

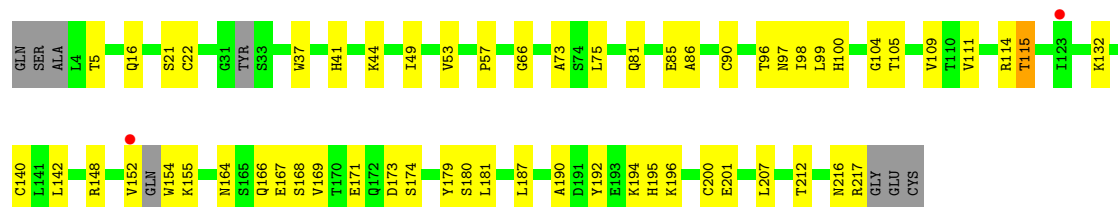
Chain Q:  3% 67% 28% 2%



• Molecule 3: Fab 2B11 Light Chain



• Molecule 3: Fab 2B11 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.65Å 184.34Å 161.24Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	80.04 – 3.10 80.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (80.04-3.10) 99.1 (80.04-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.292 , 0.324 0.291 , 0.326	Depositor DCC
R_{free} test set	2061 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	25772	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.55	0/263	0.80	0/356
1	M	0.45	0/229	0.58	0/311
1	N	0.44	0/262	0.67	0/356
1	S	0.48	0/254	0.66	0/345
1	T	0.67	0/254	0.88	0/345
1	U	0.74	0/254	0.93	0/345
1	V	0.42	0/245	0.70	0/334
1	j	0.52	0/270	0.69	0/367
2	B	0.39	0/1645	0.54	0/2243
2	H	0.48	1/887 (0.1%)	0.68	1/1199 (0.1%)
2	J	0.49	1/1604 (0.1%)	0.68	3/2185 (0.1%)
2	L	0.48	0/1640	0.68	1/2234 (0.0%)
2	P	0.38	0/1631	0.61	2/2222 (0.1%)
2	R	0.43	0/1651	0.60	1/2251 (0.0%)
2	X	0.39	0/1667	0.61	4/2273 (0.2%)
2	Z	0.44	0/1639	0.59	0/2235
3	F	0.29	0/1612	0.45	0/2192
3	G	0.32	0/783	0.44	0/1065
3	I	0.32	0/1537	0.47	0/2084
3	K	0.41	0/1592	0.57	0/2156
3	O	0.34	0/1584	0.50	0/2152
3	Q	0.26	0/1616	0.45	0/2196
3	W	0.28	0/1627	0.49	0/2212
3	Y	0.24	0/1624	0.43	1/2206 (0.0%)
All	All	0.39	2/26370 (0.0%)	0.57	13/35864 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	52	ILE	N-CA	5.15	1.50	1.46
2	H	52	ILE	N-CA	5.15	1.50	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	55	PRO	N-CA-C	-8.97	99.75	110.70
2	L	88	SER	N-CA-C	-8.29	102.25	111.28
2	P	56	PRO	N-CA-C	-6.48	101.05	111.03
2	H	53	PRO	N-CA-C	6.39	122.42	113.53
2	J	131	PRO	CB-CA-C	-5.92	106.90	111.87
2	X	51	ILE	CA-C-N	-5.83	117.02	123.43
2	X	51	ILE	C-N-CA	-5.83	117.02	123.43
2	X	53	PRO	N-CA-C	5.71	121.47	113.53
2	J	56	PRO	N-CA-C	-5.18	103.05	111.03
3	Y	115	THR	N-CA-C	-5.18	103.85	110.53
2	P	53	PRO	N-CA-C	5.17	120.72	113.53
2	X	54	ASP	N-CA-C	-5.12	105.64	112.55
2	J	53	PRO	N-CA-C	5.01	120.50	113.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	254	0	244	13	0
1	M	221	0	205	16	0
1	N	253	0	235	6	0
1	S	245	0	231	6	0
1	T	245	0	231	10	0
1	U	245	0	231	15	0
1	V	236	0	218	8	0
1	j	261	0	241	28	0
2	B	1605	0	1602	43	0
2	H	870	0	873	30	0
2	J	1566	0	1558	45	0
2	L	1601	0	1593	45	0
2	P	1592	0	1589	42	0
2	R	1611	0	1607	42	0
2	X	1627	0	1625	54	0
2	Z	1599	0	1597	45	0
3	F	1578	0	1528	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	767	0	745	22	0
3	I	1509	0	1452	34	0
3	K	1565	0	1512	44	0
3	O	1553	0	1509	38	0
3	Q	1584	0	1529	41	0
3	W	1593	0	1543	35	0
3	Y	1592	0	1539	36	0
All	All	25772	0	25237	629	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 12.

All (629) 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:j:190:PRO:HB3	2:X:56:PRO:HD2	1.40	1.02
1:j:190:PRO:HG2	2:X:57:MET:HG3	1.53	0.88
2:L:14:PRO:HG2	2:L:121:SER:HB3	1.60	0.83
3:O:85:GLU:HG2	3:O:111:VAL:H	1.45	0.81
2:Z:14:PRO:HG2	2:Z:121:SER:HB3	1.62	0.80
2:L:131:PRO:HG3	2:L:217:LYS:HE2	1.66	0.78
3:Q:171:GLU:HG3	3:Q:179:TYR:HE1	1.50	0.77
3:O:196:LYS:HE2	3:O:216:ASN:HB3	1.66	0.76
3:I:120:SER:HB2	3:I:143:ASN:HB3	1.67	0.75
2:L:40:ALA:HB3	2:L:43:GLN:HB2	1.69	0.75
3:W:89:TYR:HE2	2:X:44:GLY:HA2	1.51	0.75
2:Z:134:PRO:HB3	2:Z:146:LEU:HB3	1.69	0.75
3:I:85:GLU:HG2	3:I:111:VAL:H	1.51	0.74
2:R:134:PRO:HB3	2:R:146:LEU:HB3	1.69	0.74
2:B:134:PRO:HB3	2:B:146:LEU:HB3	1.70	0.74
1:j:183:TRP:HZ3	1:j:188:ARG:HH21	1.36	0.73
2:R:54:ASP:HB2	2:R:55:PRO:HD3	1.71	0.73
3:K:85:GLU:HA	3:K:109:VAL:HG23	1.71	0.73
2:B:203:ILE:HD11	2:B:216:ASP:HB3	1.70	0.72
2:X:134:PRO:HB3	2:X:146:LEU:HB3	1.72	0.72
3:Q:196:LYS:HE2	3:Q:216:ASN:HB3	1.72	0.72
3:F:196:LYS:HE2	3:F:216:ASN:HB3	1.70	0.72
1:U:171:VAL:HG13	1:U:175:ILE:HD11	1.74	0.70
3:F:85:GLU:HG2	3:F:111:VAL:H	1.56	0.70
3:I:192:TYR:O	3:I:217:ARG:NH2	2.25	0.70
3:Y:85:GLU:HG2	3:Y:111:VAL:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:33:PRO:HG3	2:X:52:ILE:HG23	1.74	0.69
3:O:62:ASN:ND2	3:Q:149:GLU:OE1	2.20	0.69
3:Y:192:TYR:O	3:Y:217:ARG:NH2	2.25	0.69
1:T:189:ILE:HD12	1:T:189:ILE:H	1.58	0.68
3:O:23:THR:HG23	3:O:72:THR:HG22	1.74	0.67
2:B:50:ARG:HH12	3:F:99:LEU:HB3	1.60	0.67
3:O:62:ASN:OD1	3:Q:205:GLN:NE2	2.26	0.67
2:P:136:SER:O	2:P:137:LYS:HG3	1.95	0.67
2:X:40:ALA:HB3	2:X:43:GLN:HB2	1.77	0.67
2:Z:167:LEU:HD21	2:Z:190:VAL:HG21	1.77	0.66
1:j:190:PRO:HG2	2:X:57:MET:CG	2.23	0.66
3:G:99:LEU:HD23	2:H:101:LEU:HD11	1.78	0.66
2:L:203:ILE:HD11	2:L:216:ASP:HB3	1.76	0.66
2:B:91:THR:HG23	2:B:118:ALA:HA	1.78	0.66
3:F:151:LYS:HE3	3:F:153:GLN:HG2	1.78	0.65
3:K:192:TYR:O	3:K:217:ARG:NH2	2.29	0.65
2:L:208:HIS:HD2	2:L:210:PRO:HD2	1.62	0.65
2:B:159:THR:HG23	2:B:207:ASN:HB3	1.78	0.65
1:U:189:ILE:HD12	1:U:190:PRO:HD2	1.80	0.64
3:F:175:LYS:HD2	3:F:176:ASP:H	1.62	0.64
2:X:30:SER:HA	2:X:53:PRO:HB3	1.79	0.64
3:G:85:GLU:HG2	3:G:111:VAL:H	1.62	0.64
2:R:203:ILE:HD11	2:R:216:ASP:HB3	1.80	0.64
2:R:41:PRO:HG3	2:R:116:MET:HE1	1.79	0.64
3:Q:170:THR:HG22	2:R:175:PRO:HD3	1.79	0.63
3:Y:167:GLU:HB3	3:Y:181:LEU:HD11	1.80	0.63
1:M:169:ASN:HB2	1:j:169:ASN:ND2	2.13	0.63
1:A:177:SER:HB3	2:H:102:GLN:HB2	1.79	0.63
2:B:167:LEU:HD21	2:B:190:VAL:HG21	1.80	0.63
2:J:41:PRO:HD3	2:J:92:ALA:HA	1.80	0.63
2:J:167:LEU:HD21	2:J:190:VAL:HG21	1.80	0.63
1:j:168:PHE:HD2	2:J:57:MET:HG2	1.64	0.63
2:L:91:THR:HG23	2:L:118:ALA:HA	1.79	0.62
2:L:134:PRO:HB3	2:L:146:LEU:HB3	1.79	0.62
3:Q:85:GLU:HG2	3:Q:111:VAL:H	1.64	0.62
3:F:131:LEU:O	3:F:189:LYS:NZ	2.27	0.62
1:S:163:PHE:HE2	2:P:56:PRO:HB3	1.64	0.62
3:Q:99:LEU:HB3	2:R:50:ARG:HH12	1.65	0.62
2:P:147:GLY:HA2	2:P:162:TRP:HZ2	1.65	0.61
3:W:192:TYR:O	3:W:217:ARG:NH2	2.32	0.61
2:H:13:LYS:H	2:H:13:LYS:HZ3	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:GLN:HB2	2:L:45:LEU:HD23	1.81	0.61
3:O:4:LEU:HA	3:O:24:GLY:HA2	1.82	0.61
2:Z:196:SER:HB2	2:Z:200:GLN:HB2	1.83	0.61
3:F:173:ASP:HA	3:F:177:SER:HA	1.82	0.61
1:V:182:CYS:O	1:V:186:CYS:HB3	2.00	0.61
3:O:124:PHE:CZ	2:P:137:LYS:HE2	2.36	0.61
3:Y:196:LYS:HE2	3:Y:216:ASN:HB3	1.82	0.60
1:M:163:PHE:N	2:X:72:ALA:O	2.33	0.60
1:j:175:ILE:HG21	2:J:52:ILE:HG21	1.83	0.60
2:X:91:THR:HG23	2:X:118:ALA:HA	1.82	0.60
2:B:55:PRO:HG2	2:B:57:MET:HB2	1.81	0.60
2:B:208:HIS:HD2	2:B:210:PRO:HD2	1.65	0.60
1:j:167:VAL:HA	2:J:58:ALA:HB3	1.84	0.60
3:G:10:VAL:O	3:G:110:THR:N	2.34	0.60
2:L:159:THR:HG23	2:L:207:ASN:HB3	1.83	0.60
3:Y:168:SER:HB2	2:Z:175:PRO:HD2	1.84	0.60
2:P:159:THR:HG23	2:P:207:ASN:HB3	1.83	0.59
2:R:91:THR:HG23	2:R:118:ALA:HA	1.83	0.59
2:Z:28:THR:O	2:Z:29:PHE:C	2.46	0.59
3:Q:167:GLU:HB3	3:Q:181:LEU:HD11	1.83	0.59
1:A:175:ILE:HD13	2:H:52:ILE:HD13	1.83	0.59
3:W:63:ARG:HH21	3:W:84:ASP:CG	2.11	0.59
1:M:175:ILE:HD13	2:X:52:ILE:HG21	1.85	0.59
3:O:122:PHE:HB3	2:P:137:LYS:CE	2.32	0.59
2:X:39:GLN:HG2	2:X:40:ALA:O	2.03	0.59
2:X:1:GLN:HB2	3:Y:212:THR:HG22	1.84	0.59
2:L:38:ARG:HH12	2:L:90:ASP:HA	1.68	0.58
2:L:153:TYR:HB2	2:L:208:HIS:CE1	2.38	0.58
3:W:196:LYS:HE2	3:W:216:ASN:HB3	1.84	0.58
1:T:170:PHE:HB2	1:T:187:LYS:HD2	1.86	0.58
2:Z:203:ILE:HD11	2:Z:216:ASP:HB3	1.86	0.58
2:Z:208:HIS:HD2	2:Z:210:PRO:HD2	1.68	0.58
2:B:62:GLN:HA	2:B:65:GLN:HB2	1.84	0.58
2:X:144:ALA:HB2	2:X:194:SER:HB3	1.84	0.58
1:j:190:PRO:CB	2:X:56:PRO:HD2	2.24	0.58
3:I:196:LYS:HE2	3:I:216:ASN:HB3	1.85	0.58
1:A:192:LYS:O	1:A:193:LYS:C	2.47	0.58
3:K:124:PHE:HB2	3:K:139:VAL:HB	1.85	0.58
3:Y:148:ARG:HG3	3:Y:179:TYR:CE2	2.39	0.57
1:T:175:ILE:HD13	2:B:52:ILE:HD13	1.87	0.57
3:O:151:LYS:HE3	3:O:153:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HA	2:H:58:ALA:HB3	1.87	0.57
3:K:168:SER:HB2	2:L:175:PRO:HD2	1.86	0.57
1:M:167:VAL:HA	2:X:58:ALA:O	2.05	0.57
1:j:172:PRO:HD3	2:J:57:MET:SD	2.45	0.57
2:Z:22:CYS:HB3	2:Z:79:VAL:HG13	1.85	0.57
1:A:167:VAL:HG22	2:H:58:ALA:CB	2.35	0.57
3:I:171:GLU:HG3	3:I:179:TYR:CE2	2.40	0.57
2:J:131:PRO:HB3	2:J:219:VAL:HG22	1.86	0.57
2:Z:61:ALA:HB3	2:Z:64:PHE:HD2	1.69	0.57
3:W:89:TYR:CE2	2:X:44:GLY:HA2	2.37	0.57
1:T:171:VAL:HG13	1:T:175:ILE:HD11	1.88	0.56
2:P:208:HIS:HD2	2:P:210:PRO:HD2	1.70	0.56
2:Z:98:ARG:NH2	2:Z:109:ASP:OD2	2.33	0.56
3:O:25:SER:C	3:O:71:ASN:HD22	2.14	0.56
3:O:90:CYS:O	3:O:104:GLY:N	2.38	0.56
3:O:122:PHE:HB3	2:P:137:LYS:HE3	1.87	0.56
3:I:99:LEU:HB3	2:J:50:ARG:HH12	1.70	0.56
2:P:147:GLY:HA2	2:P:162:TRP:CZ2	2.41	0.56
3:Y:41:HIS:CD2	3:Y:86:ALA:HB2	2.41	0.56
3:G:22:CYS:HB3	3:G:73:ALA:HB3	1.87	0.56
2:P:22:CYS:HB3	2:P:79:VAL:HG13	1.87	0.56
3:K:195:HIS:O	3:K:217:ARG:NH2	2.28	0.56
3:W:37:TRP:HB2	3:W:50:ILE:HB	1.88	0.56
3:Y:195:HIS:O	3:Y:217:ARG:NH2	2.31	0.56
1:M:169:ASN:HB2	1:j:169:ASN:CG	2.31	0.55
3:K:151:LYS:HE3	3:K:153:GLN:HG3	1.87	0.55
2:P:19:LYS:HG2	2:P:80:TYR:HB3	1.88	0.55
3:Q:49:ILE:O	3:Q:57:PRO:HD2	2.07	0.55
2:R:40:ALA:HB3	2:R:43:GLN:HB2	1.87	0.55
3:W:63:ARG:NH2	3:W:84:ASP:OD1	2.32	0.55
2:H:54:ASP:OD1	2:H:54:ASP:N	2.40	0.55
1:N:165:PHE:HE1	2:R:72:ALA:HB3	1.71	0.55
1:j:182:CYS:HB2	3:I:99:LEU:HD22	1.88	0.55
2:B:22:CYS:HB3	2:B:79:VAL:HG13	1.87	0.55
2:X:208:HIS:HD2	2:X:210:PRO:HD2	1.71	0.55
2:J:208:HIS:HD2	2:J:210:PRO:HD2	1.70	0.55
3:O:22:CYS:HB3	3:O:73:ALA:HB3	1.88	0.55
2:P:54:ASP:HB2	2:P:55:PRO:HD3	1.88	0.55
2:P:194:SER:HA	2:P:197:LEU:HG	1.88	0.55
2:J:203:ILE:HD11	2:J:216:ASP:HB3	1.87	0.55
3:Q:41:HIS:HB2	3:Q:44:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:194:SER:HA	2:J:197:LEU:HG	1.89	0.55
3:Q:192:TYR:O	3:Q:217:ARG:NH2	2.40	0.55
3:Q:148:ARG:HG3	3:Q:179:TYR:CD2	2.41	0.54
3:W:80:LEU:HD13	3:W:111:VAL:HG22	1.89	0.54
2:Z:54:ASP:N	2:Z:54:ASP:OD1	2.40	0.54
2:P:136:SER:O	2:P:137:LYS:CG	2.55	0.54
2:R:208:HIS:HD2	2:R:210:PRO:HD2	1.72	0.54
3:W:148:ARG:HG2	3:W:179:TYR:CE2	2.42	0.54
2:H:38:ARG:HH12	2:H:90:ASP:HA	1.71	0.54
2:J:43:GLN:HG2	2:J:44:GLY:H	1.72	0.54
1:M:175:ILE:HG21	2:X:52:ILE:HG21	1.90	0.54
1:U:165:PHE:HD2	2:L:57:MET:H	1.56	0.54
2:Z:159:THR:HG23	2:Z:207:ASN:HB3	1.88	0.54
1:j:175:ILE:HD13	2:J:52:ILE:HD13	1.89	0.54
3:F:164:ASN:OD1	3:F:164:ASN:N	2.40	0.54
3:K:2:SER:N	3:K:29:VAL:HG21	2.22	0.54
3:Y:99:LEU:HB3	2:Z:50:ARG:HH12	1.73	0.54
3:W:124:PHE:CD2	2:X:132:LEU:HB3	2.43	0.54
3:F:167:GLU:HB3	3:F:181:LEU:HD11	1.90	0.54
3:I:119:PRO:HB3	3:I:145:PHE:HB3	1.89	0.54
2:X:159:THR:HG23	2:X:207:ASN:HB3	1.88	0.54
3:G:49:ILE:HG22	3:G:50:ILE:HG12	1.90	0.54
3:W:167:GLU:HB3	3:W:181:LEU:HD11	1.89	0.53
2:X:18:VAL:HG12	2:X:86:LEU:HD11	1.88	0.53
3:Y:37:TRP:CE2	3:Y:75:LEU:HB2	2.42	0.53
3:Y:166:GLN:HB3	2:Z:177:VAL:HG11	1.91	0.53
3:G:99:LEU:HB3	2:H:50:ARG:HH12	1.73	0.53
1:S:167:VAL:HA	2:P:58:ALA:O	2.08	0.53
2:L:147:GLY:HA2	2:L:162:TRP:CZ2	2.42	0.53
2:Z:147:GLY:HA2	2:Z:162:TRP:HZ2	1.73	0.53
3:F:148:ARG:HG2	3:F:179:TYR:CE2	2.44	0.53
3:K:86:ALA:O	3:K:109:VAL:HG22	2.08	0.53
3:O:23:THR:HA	3:O:72:THR:HA	1.90	0.53
2:X:162:TRP:HB3	2:X:167:LEU:HD23	1.89	0.53
2:J:147:GLY:HA2	2:J:162:TRP:CZ2	2.44	0.53
3:O:173:ASP:HB3	3:O:175:LYS:HD2	1.90	0.53
2:B:19:LYS:HG2	2:B:80:TYR:HB3	1.88	0.53
1:V:185:ILE:HG12	3:Y:96:THR:O	2.08	0.53
2:H:12:LYS:HG3	2:H:18:VAL:HB	1.91	0.53
2:H:33:PRO:HG3	2:H:52:ILE:HG23	1.89	0.53
3:F:41:HIS:HB2	3:F:44:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:18:VAL:HG12	2:P:86:LEU:HD11	1.91	0.53
3:Y:148:ARG:HG3	3:Y:179:TYR:CD2	2.43	0.53
2:X:22:CYS:HB3	2:X:79:VAL:HG13	1.91	0.52
2:J:69:SER:OG	2:J:82:GLU:HB3	2.09	0.52
2:Z:75:SER:O	2:Z:76:THR:OG1	2.21	0.52
2:X:167:LEU:HD21	2:X:190:VAL:HG21	1.91	0.52
3:Q:37:TRP:CE2	3:Q:75:LEU:HB2	2.44	0.52
3:Y:5:THR:HA	3:Y:105:THR:HG23	1.90	0.52
3:F:193:GLU:O	3:F:217:ARG:NH2	2.43	0.52
2:J:50:ARG:HG2	2:J:59:ASN:HB2	1.92	0.52
2:Z:54:ASP:HB2	2:Z:55:PRO:HD3	1.90	0.52
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.92	0.52
2:J:159:THR:HG23	2:J:207:ASN:HB3	1.92	0.52
2:R:147:GLY:HA2	2:R:162:TRP:CZ2	2.45	0.52
3:W:99:LEU:HB3	2:X:50:ARG:HH12	1.75	0.52
2:X:54:ASP:OD1	2:X:54:ASP:N	2.43	0.52
2:Z:147:GLY:HA2	2:Z:162:TRP:CZ2	2.45	0.52
1:M:166:GLU:HB3	1:j:187:LYS:HZ2	1.74	0.52
3:W:195:HIS:O	3:W:217:ARG:NH2	2.31	0.52
2:R:127:PRO:HD3	2:R:208:HIS:ND1	2.25	0.51
3:K:41:HIS:HB2	3:K:44:LYS:HE2	1.93	0.51
2:L:54:ASP:HB2	2:L:55:PRO:HD3	1.91	0.51
2:X:153:TYR:HB2	2:X:208:HIS:CE1	2.45	0.51
2:H:50:ARG:HG2	2:H:59:ASN:HB2	1.91	0.51
3:G:80:LEU:HD13	3:G:111:VAL:HG22	1.93	0.51
3:I:98:ILE:HB	2:J:59:ASN:HB3	1.92	0.51
2:B:33:PRO:HA	2:B:53:PRO:HD3	1.93	0.51
3:G:12:GLY:O	3:G:112:LEU:N	2.29	0.51
3:K:63:ARG:HH21	3:K:84:ASP:CG	2.18	0.51
3:Q:148:ARG:HG3	3:Q:179:TYR:CE2	2.46	0.51
2:Z:19:LYS:HG2	2:Z:80:TYR:HB3	1.91	0.51
2:B:52:ILE:HD12	2:B:57:MET:HB3	1.92	0.51
2:L:54:ASP:OD1	2:L:54:ASP:N	2.43	0.51
3:W:65:SER:O	3:W:75:LEU:HD12	2.10	0.51
3:W:143:ASN:HD21	2:X:172:HIS:CE1	2.29	0.51
3:Y:201:GLU:HA	3:Y:212:THR:HB	1.93	0.51
1:j:168:PHE:CD2	2:J:57:MET:HG2	2.46	0.51
2:H:30:SER:HA	2:H:53:PRO:HB2	1.91	0.51
3:Q:37:TRP:CZ3	3:Q:90:CYS:HB3	2.46	0.51
3:Q:85:GLU:HA	3:Q:109:VAL:HG23	1.93	0.51
3:I:126:PRO:HG3	3:I:138:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:69:SER:HG	2:J:82:GLU:HB3	1.76	0.51
2:J:147:GLY:HA2	2:J:162:TRP:HZ2	1.76	0.51
2:X:131:PRO:HB3	2:X:219:VAL:HG22	1.93	0.50
1:M:188:ARG:HE	1:M:189:ILE:HG13	1.76	0.50
3:F:49:ILE:O	3:F:57:PRO:HD2	2.11	0.50
3:G:96:THR:HG22	3:G:97:ASN:H	1.76	0.50
1:M:188:ARG:NH1	1:M:188:ARG:HA	2.27	0.50
3:Y:85:GLU:HA	3:Y:109:VAL:HG23	1.94	0.50
3:Y:142:LEU:HB2	3:Y:181:LEU:HB3	1.92	0.50
3:G:90:CYS:O	3:G:104:GLY:N	2.45	0.50
2:J:134:PRO:O	2:J:135:SER:C	2.53	0.50
2:L:41:PRO:HG3	2:L:116:MET:HE1	1.94	0.50
2:L:194:SER:HA	2:L:197:LEU:HG	1.94	0.50
3:Y:41:HIS:HB2	3:Y:44:LYS:HE2	1.93	0.50
2:Z:38:ARG:HH12	2:Z:90:ASP:HA	1.77	0.50
1:j:163:PHE:HE2	2:J:56:PRO:HB3	1.76	0.50
2:B:2:VAL:HG21	2:B:98:ARG:NH1	2.27	0.50
2:L:163:ASN:HA	2:L:203:ILE:HG23	1.93	0.50
3:O:130:GLN:HE22	3:O:137:SER:HG	1.58	0.50
2:R:19:LYS:HG2	2:R:80:TYR:HB3	1.93	0.50
2:J:220:GLU:N	2:J:221:PRO:HD3	2.27	0.50
2:R:167:LEU:HD21	2:R:190:VAL:HG21	1.94	0.50
2:X:19:LYS:HG3	2:X:82:GLU:HB2	1.94	0.50
1:N:165:PHE:CE1	2:R:72:ALA:HB3	2.47	0.49
1:T:172:PRO:O	1:T:175:ILE:HG12	2.11	0.49
2:B:162:TRP:HB3	2:B:167:LEU:HD23	1.94	0.49
3:O:131:LEU:O	3:O:189:LYS:NZ	2.28	0.49
2:R:22:CYS:HB3	2:R:79:VAL:HG13	1.93	0.49
3:Q:41:HIS:CD2	3:Q:86:ALA:HB2	2.47	0.49
2:X:203:ILE:HD11	2:X:216:ASP:HB3	1.94	0.49
1:j:185:ILE:HD12	3:I:96:THR:O	2.13	0.49
3:K:169:VAL:HA	3:K:180:SER:O	2.11	0.49
3:W:22:CYS:HB3	3:W:73:ALA:HB3	1.95	0.49
3:W:131:LEU:O	3:W:189:LYS:NZ	2.33	0.49
2:B:59:ASN:HB3	3:F:98:ILE:HB	1.94	0.49
3:I:90:CYS:O	3:I:104:GLY:N	2.45	0.49
3:K:99:LEU:HB3	2:L:50:ARG:HH12	1.77	0.49
2:R:147:GLY:HA2	2:R:162:TRP:HZ2	1.77	0.49
1:U:175:ILE:HG21	2:L:52:ILE:HG21	1.93	0.49
2:J:61:ALA:HB3	2:J:64:PHE:HD2	1.76	0.49
3:Q:195:HIS:O	3:Q:217:ARG:NH2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:ASP:HB2	2:H:55:PRO:HD3	1.95	0.49
1:U:172:PRO:O	1:U:175:ILE:HG12	2.13	0.49
3:K:2:SER:N	3:K:26:SER:HG	2.10	0.49
3:K:98:ILE:HB	2:L:59:ASN:HB3	1.95	0.49
1:j:171:VAL:HG23	1:j:175:ILE:HD11	1.94	0.49
3:O:166:GLN:HB3	2:P:177:VAL:HG11	1.95	0.49
3:Q:36:SER:HB3	3:Q:48:LEU:HD11	1.94	0.49
1:M:189:ILE:HG23	1:j:189:ILE:HD13	1.94	0.49
3:I:180:SER:C	2:J:174:PHE:HE1	2.20	0.49
2:L:147:GLY:HA2	2:L:162:TRP:HZ2	1.77	0.49
3:F:215:PHE:CD1	3:F:215:PHE:C	2.91	0.49
3:W:112:LEU:HD12	3:W:146:TYR:CZ	2.48	0.49
3:G:41:HIS:HB2	3:G:44:LYS:HE2	1.94	0.48
3:K:90:CYS:O	3:K:104:GLY:N	2.45	0.48
3:O:166:GLN:HE22	2:P:179:GLN:HA	1.77	0.48
1:U:182:CYS:O	1:U:186:CYS:HB3	2.14	0.48
3:I:153:GLN:HE21	3:I:153:GLN:N	2.10	0.48
2:X:220:GLU:N	2:X:221:PRO:HD3	2.29	0.48
1:T:165:PHE:HB3	2:B:58:ALA:HB2	1.96	0.48
3:F:175:LYS:CD	3:F:176:ASP:H	2.25	0.48
3:K:167:GLU:HB3	3:K:181:LEU:HD11	1.95	0.48
2:L:33:PRO:HA	2:L:53:PRO:HD3	1.94	0.48
2:L:144:ALA:HB2	2:L:194:SER:HB3	1.94	0.48
1:V:177:SER:HB3	2:Z:102:GLN:HB2	1.96	0.48
3:K:49:ILE:O	3:K:57:PRO:HD2	2.12	0.48
2:L:55:PRO:O	2:L:56:PRO:C	2.55	0.48
3:W:53:VAL:O	3:W:66:GLY:HA3	2.13	0.48
1:A:167:VAL:HG22	2:H:58:ALA:HB3	1.96	0.48
2:J:91:THR:HG23	2:J:118:ALA:HA	1.95	0.48
3:Y:22:CYS:HB3	3:Y:73:ALA:HB3	1.95	0.48
2:J:22:CYS:HB3	2:J:79:VAL:HG13	1.94	0.48
2:R:144:ALA:HB2	2:R:194:SER:HB3	1.95	0.48
2:X:194:SER:HA	2:X:197:LEU:HG	1.95	0.48
1:A:192:LYS:HB3	1:A:192:LYS:HE2	1.36	0.48
1:S:168:PHE:CD2	2:P:57:MET:HG2	2.49	0.48
1:j:173:CYS:HA	1:j:176:CYS:SG	2.53	0.48
3:F:41:HIS:CD2	3:F:86:ALA:HB2	2.48	0.48
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.49	0.48
3:W:18:ILE:HD13	3:W:80:LEU:HD11	1.95	0.48
1:M:166:GLU:HB3	1:j:187:LYS:NZ	2.29	0.48
3:F:24:GLY:O	3:F:25:SER:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:142:LEU:HB2	3:O:181:LEU:HB3	1.95	0.48
2:P:167:LEU:HD21	2:P:190:VAL:HG21	1.95	0.48
2:X:54:ASP:HB2	2:X:55:PRO:HD3	1.96	0.48
3:O:175:LYS:HD3	3:O:176:ASP:H	1.79	0.47
2:P:14:PRO:HG2	2:P:121:SER:HB2	1.95	0.47
2:R:38:ARG:NH1	2:R:94:TYR:OH	2.47	0.47
1:V:173:CYS:HB2	1:V:188:ARG:NH1	2.29	0.47
2:B:19:LYS:HG3	2:B:82:GLU:HB2	1.95	0.47
3:I:86:ALA:O	3:I:109:VAL:HG22	2.14	0.47
3:Q:190:ALA:O	3:Q:194:LYS:HG2	2.14	0.47
2:X:14:PRO:HG3	2:X:119:VAL:HG13	1.96	0.47
2:X:19:LYS:HG2	2:X:80:TYR:HB3	1.96	0.47
3:K:196:LYS:HE2	3:K:216:ASN:HB3	1.96	0.47
1:M:168:PHE:CD2	2:X:57:MET:HG2	2.49	0.47
1:j:165:PHE:CE2	2:J:56:PRO:HA	2.50	0.47
1:A:167:VAL:HG22	2:H:58:ALA:HB1	1.95	0.47
3:I:207:LEU:HD22	3:I:211:VAL:HG21	1.95	0.47
3:K:20:ILE:O	3:K:74:SER:HA	2.14	0.47
3:Q:172:GLN:O	3:Q:175:LYS:HG2	2.14	0.47
2:Z:33:PRO:HA	2:Z:53:PRO:HD3	1.97	0.47
1:j:175:ILE:HD13	2:J:52:ILE:HG21	1.96	0.47
2:J:100:ILE:HG22	2:J:102:GLN:O	2.14	0.47
2:P:144:ALA:HB2	2:P:194:SER:HB3	1.95	0.47
3:Q:171:GLU:HG3	3:Q:179:TYR:CE1	2.40	0.47
1:M:165:PHE:HE1	2:X:72:ALA:HB3	1.80	0.47
3:K:5:THR:HA	3:K:105:THR:HG23	1.96	0.47
2:X:43:GLN:HG2	2:X:44:GLY:H	1.80	0.47
2:B:123:SER:HB3	2:B:183:LEU:HD21	1.97	0.47
3:F:80:LEU:HD22	3:F:111:VAL:HG22	1.97	0.47
3:F:85:GLU:HA	3:F:109:VAL:HG23	1.97	0.47
2:P:55:PRO:O	2:P:56:PRO:C	2.54	0.47
2:P:90:ASP:O	2:P:94:TYR:OH	2.33	0.47
2:B:38:ARG:HH12	2:B:90:ASP:HA	1.79	0.47
3:I:190:ALA:O	3:I:194:LYS:HG2	2.15	0.47
2:L:19:LYS:HG2	2:L:80:TYR:HB3	1.97	0.47
2:R:18:VAL:HG12	2:R:86:LEU:HD11	1.97	0.47
2:R:131:PRO:HG3	2:R:217:LYS:HE2	1.95	0.47
3:W:41:HIS:HB2	3:W:44:LYS:HE2	1.96	0.47
3:Y:166:GLN:HE22	2:Z:179:GLN:HA	1.78	0.47
3:I:22:CYS:HB3	3:I:73:ALA:HB3	1.97	0.47
3:I:49:ILE:O	3:I:57:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:192:TYR:HA	3:K:198:TYR:OH	2.15	0.47
3:Q:18:ILE:HG23	3:Q:80:LEU:HD11	1.96	0.47
2:R:194:SER:HA	2:R:197:LEU:HG	1.97	0.47
3:W:190:ALA:O	3:W:194:LYS:HG2	2.15	0.47
3:I:80:LEU:HD22	3:I:111:VAL:HG22	1.97	0.47
2:Z:194:SER:HA	2:Z:197:LEU:HG	1.97	0.46
2:J:19:LYS:HG2	2:J:80:TYR:HB3	1.96	0.46
2:R:125:LYS:HD3	2:R:183:LEU:HD13	1.97	0.46
3:I:168:SER:HB2	2:J:175:PRO:HD2	1.97	0.46
3:I:169:VAL:HA	3:I:180:SER:O	2.16	0.46
3:I:195:HIS:O	3:I:217:ARG:NH2	2.39	0.46
3:K:142:LEU:HB2	3:K:181:LEU:HB3	1.96	0.46
2:Z:55:PRO:O	2:Z:56:PRO:C	2.57	0.46
2:Z:100:ILE:HG22	2:Z:102:GLN:O	2.15	0.46
1:j:163:PHE:N	2:J:72:ALA:O	2.47	0.46
3:G:10:VAL:O	3:G:109:VAL:HA	2.16	0.46
2:R:100:ILE:HG22	2:R:102:GLN:O	2.15	0.46
3:W:129:GLU:HG3	3:W:132:LYS:HZ1	1.80	0.46
1:U:167:VAL:HA	2:L:58:ALA:O	2.15	0.46
2:L:100:ILE:HG22	2:L:102:GLN:O	2.15	0.46
2:P:14:PRO:HG3	2:P:119:VAL:HG12	1.98	0.46
2:R:54:ASP:N	2:R:54:ASP:OD1	2.48	0.46
2:Z:124:THR:HG22	2:Z:155:PRO:HD3	1.98	0.46
1:M:168:PHE:HB2	2:X:57:MET:HE3	1.96	0.46
3:K:190:ALA:O	3:K:194:LYS:HG2	2.16	0.46
3:Q:65:SER:O	3:Q:75:LEU:HD12	2.15	0.46
2:H:61:ALA:HB3	2:H:64:PHE:HD2	1.81	0.46
3:O:154:TRP:CE2	3:O:185:LEU:HB2	2.51	0.46
2:Z:179:GLN:OE1	2:Z:185:SER:HB3	2.16	0.46
2:H:19:LYS:HG2	2:H:80:TYR:HB3	1.97	0.46
1:A:167:VAL:CA	2:H:58:ALA:HB3	2.45	0.46
3:G:18:ILE:HD13	3:G:80:LEU:HD11	1.98	0.46
3:W:24:GLY:O	3:W:71:ASN:ND2	2.50	0.46
3:W:171:GLU:N	3:W:171:GLU:OE1	2.47	0.46
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.97	0.46
1:N:163:PHE:HE2	2:R:56:PRO:HB3	1.81	0.45
3:F:170:THR:CG2	3:F:180:SER:HB2	2.46	0.45
3:I:38:TYR:OH	2:J:107:ALA:HB1	2.16	0.45
3:I:93:TYR:HB3	3:I:99:LEU:HD11	1.98	0.45
2:L:70:PHE:HE1	2:L:81:MET:HG3	1.81	0.45
3:F:98:ILE:HG12	3:F:100:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:62:GLN:HA	2:L:65:GLN:HB2	1.98	0.45
2:X:147:GLY:HA2	2:X:162:TRP:CZ2	2.50	0.45
1:T:165:PHE:HE1	2:B:72:ALA:HB3	1.82	0.45
3:K:22:CYS:HB3	3:K:73:ALA:HB3	1.97	0.45
3:G:37:TRP:CE2	3:G:75:LEU:HB2	2.51	0.45
3:O:199:ALA:HB2	3:O:214:SER:HB3	1.98	0.45
2:X:30:SER:HA	2:X:53:PRO:CB	2.46	0.45
1:U:171:VAL:HG23	3:K:98:ILE:HA	1.98	0.45
3:K:63:ARG:HB3	3:K:78:SER:O	2.16	0.45
2:R:33:PRO:HA	2:R:53:PRO:HD3	1.98	0.45
1:N:165:PHE:CZ	2:R:74:LYS:HE3	2.51	0.45
3:I:41:HIS:HB2	3:I:44:LYS:HE2	1.99	0.45
2:X:1:GLN:HB2	3:Y:212:THR:CG2	2.46	0.45
2:B:100:ILE:HG22	2:B:102:GLN:O	2.17	0.45
2:Z:43:GLN:HG2	2:Z:44:GLY:H	1.82	0.45
2:Z:174:PHE:HE1	2:Z:189:VAL:HG22	1.82	0.45
3:I:37:TRP:CE2	3:I:75:LEU:HB2	2.52	0.45
3:Q:90:CYS:O	3:Q:104:GLY:N	2.50	0.45
3:Y:173:ASP:OD1	3:Y:174:SER:N	2.46	0.45
3:O:167:GLU:HB3	3:O:181:LEU:HD11	1.98	0.45
3:W:90:CYS:O	3:W:104:GLY:N	2.49	0.45
3:O:41:HIS:CD2	3:O:86:ALA:HB2	2.52	0.45
3:Y:81:GLN:O	3:Y:111:VAL:HG21	2.17	0.45
2:H:55:PRO:HD2	2:H:55:PRO:O	2.16	0.45
3:F:20:ILE:HD12	3:F:75:LEU:HD23	1.99	0.44
2:X:147:GLY:HA2	2:X:162:TRP:HZ2	1.81	0.44
1:T:175:ILE:HG21	2:B:52:ILE:HG21	1.98	0.44
3:F:5:THR:HA	3:F:105:THR:HG23	2.00	0.44
3:O:38:TYR:OH	2:P:107:ALA:HB1	2.17	0.44
3:O:207:LEU:HD22	3:O:211:VAL:HG21	1.99	0.44
3:W:5:THR:HA	3:W:105:THR:HG23	1.99	0.44
3:F:37:TRP:CZ3	3:F:90:CYS:HB3	2.52	0.44
2:R:18:VAL:O	2:R:82:GLU:HA	2.17	0.44
3:W:171:GLU:HG3	3:W:179:TYR:HE1	1.81	0.44
2:Z:40:ALA:HB3	2:Z:43:GLN:HB2	2.00	0.44
2:Z:162:TRP:HB3	2:Z:167:LEU:HD23	1.99	0.44
2:R:174:PHE:HE1	2:R:189:VAL:HG22	1.83	0.44
3:W:207:LEU:HD22	3:W:211:VAL:HG21	2.00	0.44
1:M:175:ILE:HD13	2:X:52:ILE:HD13	2.00	0.44
2:B:50:ARG:NH1	3:F:99:LEU:HB3	2.29	0.44
2:P:30:SER:HA	2:P:53:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:49:ILE:HG22	3:Q:50:ILE:HG12	1.99	0.44
3:Q:154:TRP:O	3:Q:160:LEU:HA	2.17	0.44
2:X:196:SER:HB2	2:X:200:GLN:HB2	2.00	0.44
3:Y:169:VAL:HA	3:Y:180:SER:O	2.18	0.44
3:Y:190:ALA:O	3:Y:194:LYS:HG2	2.18	0.44
1:M:182:CYS:O	1:M:186:CYS:HB3	2.18	0.44
1:N:170:PHE:HB2	1:N:187:LYS:HE2	1.99	0.44
1:U:168:PHE:HB2	2:L:57:MET:HE3	1.98	0.44
1:U:188:ARG:HH11	1:U:189:ILE:HG22	1.82	0.44
2:J:56:PRO:O	2:J:57:MET:HG3	2.18	0.44
3:Y:154:TRP:CZ3	3:Y:200:CYS:HB3	2.53	0.44
2:J:55:PRO:O	2:J:56:PRO:C	2.56	0.44
2:P:91:THR:OG1	2:P:119:VAL:HG23	2.18	0.44
2:Z:86:LEU:HB3	2:Z:119:VAL:HG11	2.00	0.44
2:H:22:CYS:HB3	2:H:79:VAL:HG13	1.99	0.44
2:H:48:MET:HA	2:H:64:PHE:CD2	2.53	0.44
1:A:176:CYS:SG	1:A:186:CYS:SG	3.16	0.44
2:P:162:TRP:HB3	2:P:167:LEU:HD23	2.00	0.44
3:Y:142:LEU:HD13	3:Y:181:LEU:HD23	2.00	0.44
3:Y:171:GLU:OE1	3:Y:171:GLU:N	2.51	0.44
3:F:195:HIS:O	3:F:217:ARG:NH2	2.50	0.44
2:L:67:ARG:NH1	2:L:87:ARG:NH2	2.66	0.44
3:O:49:ILE:O	3:O:57:PRO:HD2	2.18	0.44
2:P:130:PHE:HA	2:P:131:PRO:HD3	1.88	0.44
3:W:86:ALA:H	3:W:109:VAL:HG13	1.83	0.44
2:Z:18:VAL:HG12	2:Z:86:LEU:HD11	1.99	0.44
2:Z:91:THR:HG23	2:Z:118:ALA:HA	2.00	0.44
3:F:37:TRP:CE2	3:F:75:LEU:HB2	2.52	0.43
2:P:70:PHE:HE1	2:P:81:MET:HG3	1.83	0.43
3:I:154:TRP:CZ3	3:I:200:CYS:HB3	2.53	0.43
2:J:55:PRO:O	2:J:55:PRO:HD2	2.18	0.43
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.99	0.43
2:B:62:GLN:C	2:B:64:PHE:N	2.73	0.43
3:K:12:GLY:N	3:K:110:THR:O	2.50	0.43
3:K:36:SER:HB3	3:K:48:LEU:HD11	2.00	0.43
3:O:4:LEU:CD1	3:O:24:GLY:HA3	2.48	0.43
3:Q:5:THR:HA	3:Q:105:THR:HG23	1.99	0.43
2:H:55:PRO:O	2:H:56:PRO:C	2.58	0.43
3:F:20:ILE:O	3:F:74:SER:HA	2.19	0.43
3:K:171:GLU:N	3:K:171:GLU:OE1	2.52	0.43
2:L:2:VAL:HG21	2:L:98:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:163:PHE:HZ	2:B:56:PRO:HB3	1.84	0.43
3:I:124:PHE:CD2	2:J:132:LEU:HB3	2.54	0.43
2:L:84:SER:O	2:L:85:SER:C	2.59	0.43
2:P:136:SER:C	2:P:137:LYS:HG3	2.43	0.43
1:U:169:ASN:HA	3:K:98:ILE:CG2	2.49	0.43
3:F:170:THR:HG23	3:F:180:SER:HB2	2.01	0.43
3:F:172:GLN:O	3:F:178:THR:N	2.52	0.43
3:G:49:ILE:O	3:G:57:PRO:HD2	2.19	0.43
3:I:167:GLU:HG3	3:I:183:SER:HA	2.00	0.43
3:K:124:PHE:N	3:K:139:VAL:O	2.43	0.43
3:K:207:LEU:HD22	3:K:211:VAL:HG21	2.01	0.43
3:O:167:GLU:HG3	3:O:183:SER:HA	1.99	0.43
2:H:52:ILE:HB	2:H:57:MET:HB2	1.99	0.43
1:N:185:ILE:HG12	3:Q:96:THR:O	2.18	0.43
3:G:68:LYS:HE2	3:G:68:LYS:HB3	1.82	0.43
2:J:196:SER:HB2	2:J:200:GLN:HB2	2.01	0.43
3:K:63:ARG:NH2	3:K:84:ASP:OD1	2.46	0.43
3:W:41:HIS:CD2	3:W:86:ALA:HB2	2.54	0.43
3:W:148:ARG:HE	3:W:148:ARG:HB2	1.61	0.43
3:Y:49:ILE:O	3:Y:57:PRO:HD2	2.19	0.43
3:O:38:TYR:CE2	2:P:108:VAL:HG23	2.54	0.42
3:Q:207:LEU:HD22	3:Q:211:VAL:HG21	2.01	0.42
3:W:129:GLU:HG3	3:W:132:LYS:NZ	2.34	0.42
3:Y:90:CYS:O	3:Y:104:GLY:N	2.51	0.42
1:U:163:PHE:HB3	2:L:72:ALA:O	2.19	0.42
3:F:148:ARG:HE	3:F:148:ARG:HB2	1.59	0.42
3:K:37:TRP:CZ3	3:K:90:CYS:HB3	2.54	0.42
3:K:84:ASP:O	3:K:88:TYR:OH	2.26	0.42
3:Q:131:LEU:O	3:Q:189:LYS:NZ	2.38	0.42
2:R:38:ARG:HH22	2:R:90:ASP:HA	1.84	0.42
2:X:134:PRO:HD2	2:X:221:PRO:HD2	2.01	0.42
1:T:171:VAL:HG23	3:F:98:ILE:HA	2.00	0.42
1:V:167:VAL:HA	2:Z:58:ALA:O	2.19	0.42
3:F:69:SER:HB2	3:Q:82:PRO:HG2	2.02	0.42
3:I:81:GLN:O	3:I:111:VAL:HG21	2.18	0.42
2:J:75:SER:O	2:J:76:THR:OG1	2.31	0.42
2:L:81:MET:HE1	2:L:94:TYR:CD2	2.55	0.42
1:V:165:PHE:HE1	2:Z:72:ALA:HB3	1.84	0.42
1:A:168:PHE:HB2	2:H:57:MET:HE1	2.02	0.42
2:B:194:SER:HA	2:B:197:LEU:HG	2.00	0.42
2:P:48:MET:HA	2:P:64:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:140:CYS:HB2	3:Y:154:TRP:CH2	2.53	0.42
1:S:176:CYS:SG	1:S:186:CYS:SG	3.17	0.42
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.54	0.42
2:L:18:VAL:O	2:L:82:GLU:HA	2.19	0.42
3:Q:63:ARG:HB3	3:Q:78:SER:O	2.19	0.42
3:Q:148:ARG:HD2	3:Q:169:VAL:HG11	2.00	0.42
2:R:40:ALA:HA	2:R:92:ALA:HA	2.02	0.42
2:H:91:THR:HG23	2:H:118:ALA:HA	2.00	0.42
1:U:172:PRO:HD3	2:L:57:MET:HE1	2.01	0.42
1:j:173:CYS:SG	1:j:188:ARG:HD2	2.59	0.42
3:Q:20:ILE:O	3:Q:74:SER:HA	2.19	0.42
3:Q:124:PHE:CD2	2:R:132:LEU:HB3	2.54	0.42
2:R:43:GLN:HG2	2:R:44:GLY:H	1.85	0.42
3:F:14:PRO:HD3	3:F:112:LEU:O	2.20	0.42
3:G:100:HIS:HA	2:H:47:TRP:CZ3	2.55	0.42
2:L:22:CYS:HB3	2:L:79:VAL:HG13	2.01	0.42
2:L:130:PHE:HA	2:L:131:PRO:HD3	1.93	0.42
2:Z:130:PHE:HA	2:Z:131:PRO:HD3	1.92	0.42
3:F:119:PRO:HD2	3:F:207:LEU:HG	2.02	0.42
2:R:2:VAL:HG21	2:R:98:ARG:NH1	2.35	0.42
2:Z:153:TYR:OH	2:Z:186:LEU:HD23	2.20	0.42
1:U:168:PHE:HD2	2:L:57:MET:HG2	1.85	0.42
2:L:23:LYS:HG2	2:L:78:ILE:HG23	2.01	0.42
2:X:58:ALA:HB1	2:X:70:PHE:HD2	1.85	0.42
1:V:185:ILE:HG12	3:Y:97:ASN:HA	2.02	0.41
3:O:23:THR:O	3:O:24:GLY:C	2.63	0.41
2:P:19:LYS:HG3	2:P:82:GLU:HB2	2.02	0.41
1:A:173:CYS:HA	1:A:176:CYS:SG	2.61	0.41
2:B:38:ARG:NH2	2:B:89:GLU:O	2.52	0.41
3:I:154:TRP:CE2	3:I:185:LEU:HB2	2.54	0.41
3:K:154:TRP:CZ3	3:K:200:CYS:HB3	2.55	0.41
3:Q:99:LEU:O	2:R:50:ARG:NH2	2.49	0.41
1:V:163:PHE:CE2	2:Z:56:PRO:HB3	2.55	0.41
1:j:172:PRO:HD3	2:J:57:MET:CE	2.49	0.41
1:j:192:LYS:HB2	1:j:192:LYS:HE2	1.87	0.41
2:B:174:PHE:CE2	3:F:182:SER:HB3	2.54	0.41
3:F:86:ALA:HB3	3:F:88:TYR:CE1	2.55	0.41
3:O:19:THR:HA	3:O:75:LEU:O	2.20	0.41
2:R:133:ALA:HB1	2:R:222:LYS:HB2	2.01	0.41
3:W:33:SER:HA	3:W:53:VAL:CG2	2.50	0.41
2:J:144:ALA:HB2	2:J:194:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:86:ALA:HB3	3:K:88:TYR:HE1	1.85	0.41
3:O:113:SER:H	3:O:146:TYR:HE2	1.69	0.41
3:K:38:TYR:OH	2:L:107:ALA:HB1	2.20	0.41
2:P:61:ALA:HB3	2:P:64:PHE:HD2	1.86	0.41
3:Y:53:VAL:O	3:Y:66:GLY:HA3	2.20	0.41
3:K:116:VAL:HG23	3:K:146:TYR:O	2.19	0.41
2:L:67:ARG:NH1	2:L:87:ARG:HH22	2.17	0.41
3:O:63:ARG:HB3	3:O:78:SER:O	2.21	0.41
2:H:75:SER:O	2:H:76:THR:OG1	2.34	0.41
1:A:175:ILE:CD1	2:H:52:ILE:HD13	2.50	0.41
2:B:23:LYS:HG2	2:B:78:ILE:HG23	2.01	0.41
3:F:145:PHE:HE2	3:F:148:ARG:HA	1.85	0.41
3:G:4:LEU:HD13	3:G:4:LEU:HA	1.86	0.41
3:G:11:SER:HA	3:G:110:THR:O	2.21	0.41
3:G:51:SER:O	3:G:55:ASN:HB2	2.21	0.41
3:K:2:SER:N	3:K:26:SER:OG	2.53	0.41
2:P:23:LYS:HG2	2:P:78:ILE:HG23	2.02	0.41
2:X:100:ILE:HG22	2:X:102:GLN:O	2.20	0.41
2:Z:70:PHE:HE1	2:Z:81:MET:HG3	1.86	0.41
2:B:48:MET:HE3	2:B:64:PHE:CD1	2.56	0.41
2:B:127:PRO:HB2	2:B:150:VAL:HG13	2.02	0.41
2:B:146:LEU:HB2	2:B:219:VAL:HG11	2.03	0.41
3:K:154:TRP:CE2	3:K:185:LEU:HB2	2.56	0.41
2:P:14:PRO:HD3	2:P:121:SER:H	1.85	0.41
2:P:100:ILE:HG22	2:P:102:GLN:O	2.21	0.41
3:Q:38:TYR:OH	2:R:107:ALA:HB1	2.21	0.41
2:R:15:GLY:N	2:R:86:LEU:O	2.44	0.41
2:R:124:THR:HG22	2:R:155:PRO:HD3	2.03	0.41
3:W:49:ILE:O	3:W:57:PRO:HD2	2.19	0.41
2:Z:23:LYS:HG2	2:Z:78:ILE:HG23	2.02	0.41
1:S:173:CYS:HA	1:S:176:CYS:SG	2.61	0.41
2:B:134:PRO:HD3	2:B:219:VAL:HG12	2.02	0.41
2:B:144:ALA:HB2	2:B:194:SER:HB3	2.03	0.41
3:F:86:ALA:HB3	3:F:88:TYR:HE1	1.86	0.41
3:G:63:ARG:NH2	3:G:84:ASP:OD1	2.54	0.41
2:J:179:GLN:OE1	2:J:185:SER:HB3	2.20	0.41
3:K:204:HIS:CG	3:K:205:GLN:N	2.89	0.41
2:P:55:PRO:O	2:P:55:PRO:HD2	2.21	0.41
1:j:173:CYS:SG	1:j:188:ARG:NE	2.94	0.41
2:B:40:ALA:HB3	2:B:43:GLN:HB2	2.03	0.41
2:B:153:TYR:CE1	2:B:184:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:5:THR:HA	3:I:105:THR:HG23	2.03	0.41
3:K:17:SER:HA	3:K:77:ILE:O	2.20	0.41
3:O:56:ARG:HG2	3:O:60:ILE:HB	2.03	0.41
2:Z:127:PRO:HD3	2:Z:208:HIS:ND1	2.36	0.41
2:B:162:TRP:CH2	2:B:204:CYS:HB3	2.56	0.40
3:G:86:ALA:HB3	3:G:88:TYR:HE1	1.85	0.40
2:P:33:PRO:HG3	2:P:52:ILE:HG23	2.02	0.40
3:Q:35:VAL:HA	3:Q:92:SER:HB2	2.03	0.40
2:R:32:TYR:HA	2:R:33:PRO:HD3	1.98	0.40
2:R:127:PRO:HG3	2:R:208:HIS:HB2	2.04	0.40
3:Y:98:ILE:HG12	3:Y:100:HIS:CE1	2.56	0.40
1:S:175:ILE:HD13	2:P:52:ILE:HD13	2.03	0.40
3:F:190:ALA:O	3:F:194:LYS:HG2	2.21	0.40
3:I:171:GLU:N	3:I:171:GLU:OE1	2.53	0.40
3:O:22:CYS:N	3:O:73:ALA:O	2.52	0.40
2:X:55:PRO:O	2:X:57:MET:N	2.54	0.40
2:X:130:PHE:HA	2:X:131:PRO:HD3	1.93	0.40
2:B:50:ARG:NH2	3:F:99:LEU:O	2.51	0.40
3:F:204:HIS:CG	3:F:205:GLN:N	2.89	0.40
3:Q:12:GLY:O	3:Q:111:VAL:HA	2.21	0.40
2:X:41:PRO:HG3	2:X:116:MET:HE1	2.02	0.40
2:Z:81:MET:HE1	2:Z:94:TYR:CD2	2.56	0.40
1:U:188:ARG:O	1:U:189:ILE:C	2.64	0.40
2:B:130:PHE:HA	2:B:131:PRO:HD3	1.89	0.40
3:F:119:PRO:HD3	3:F:204:HIS:ND1	2.37	0.40
2:J:214:LYS:HE3	2:J:214:LYS:HB3	1.92	0.40
3:Q:204:HIS:CG	3:Q:205:GLN:N	2.89	0.40
2:X:23:LYS:HG2	2:X:78:ILE:HG23	2.02	0.40
3:Y:37:TRP:CZ3	3:Y:90:CYS:HB3	2.57	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	A	29/49 (59%)	27 (93%)	2 (7%)	0	100	100
1	M	25/49 (51%)	23 (92%)	2 (8%)	0	100	100
1	N	29/49 (59%)	26 (90%)	3 (10%)	0	100	100
1	S	28/49 (57%)	25 (89%)	3 (11%)	0	100	100
1	T	28/49 (57%)	28 (100%)	0	0	100	100
1	U	28/49 (57%)	24 (86%)	4 (14%)	0	100	100
1	V	27/49 (55%)	25 (93%)	2 (7%)	0	100	100
1	j	30/49 (61%)	28 (93%)	2 (7%)	0	100	100
2	B	212/261 (81%)	198 (93%)	14 (7%)	0	100	100
2	H	107/261 (41%)	99 (92%)	8 (8%)	0	100	100
2	J	202/261 (77%)	187 (93%)	15 (7%)	0	100	100
2	L	210/261 (80%)	195 (93%)	15 (7%)	0	100	100
2	P	208/261 (80%)	196 (94%)	12 (6%)	0	100	100
2	R	213/261 (82%)	197 (92%)	16 (8%)	0	100	100
2	X	215/261 (82%)	198 (92%)	17 (8%)	0	100	100
2	Z	211/261 (81%)	195 (92%)	16 (8%)	0	100	100
3	F	204/220 (93%)	194 (95%)	10 (5%)	0	100	100
3	G	100/220 (46%)	93 (93%)	7 (7%)	0	100	100
3	I	185/220 (84%)	176 (95%)	9 (5%)	0	100	100
3	K	195/220 (89%)	183 (94%)	12 (6%)	0	100	100
3	O	200/220 (91%)	192 (96%)	8 (4%)	0	100	100
3	Q	205/220 (93%)	192 (94%)	13 (6%)	0	100	100
3	W	207/220 (94%)	196 (95%)	11 (5%)	0	100	100
3	Y	206/220 (94%)	194 (94%)	12 (6%)	0	100	100
All	All	3304/4240 (78%)	3091 (94%)	213 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	30/46 (65%)	27 (90%)	3 (10%)	7	29
1	M	26/46 (56%)	23 (88%)	3 (12%)	5	23
1	N	30/46 (65%)	28 (93%)	2 (7%)	15	43
1	S	29/46 (63%)	28 (97%)	1 (3%)	32	63
1	T	29/46 (63%)	27 (93%)	2 (7%)	14	41
1	U	29/46 (63%)	28 (97%)	1 (3%)	32	63
1	V	28/46 (61%)	26 (93%)	2 (7%)	13	41
1	j	31/46 (67%)	24 (77%)	7 (23%)	1	4
2	B	183/215 (85%)	171 (93%)	12 (7%)	15	43
2	H	96/215 (45%)	92 (96%)	4 (4%)	26	58
2	J	178/215 (83%)	171 (96%)	7 (4%)	28	60
2	L	182/215 (85%)	163 (90%)	19 (10%)	7	27
2	P	181/215 (84%)	171 (94%)	10 (6%)	19	50
2	R	184/215 (86%)	175 (95%)	9 (5%)	22	53
2	X	186/215 (86%)	177 (95%)	9 (5%)	23	54
2	Z	182/215 (85%)	172 (94%)	10 (6%)	19	50
3	F	183/191 (96%)	172 (94%)	11 (6%)	17	47
3	G	88/191 (46%)	85 (97%)	3 (3%)	32	63
3	I	176/191 (92%)	166 (94%)	10 (6%)	18	49
3	K	181/191 (95%)	170 (94%)	11 (6%)	17	46
3	O	180/191 (94%)	170 (94%)	10 (6%)	19	49
3	Q	184/191 (96%)	174 (95%)	10 (5%)	20	50
3	W	184/191 (96%)	172 (94%)	12 (6%)	15	44
3	Y	185/191 (97%)	175 (95%)	10 (5%)	20	50
All	All	2965/3616 (82%)	2787 (94%)	178 (6%)	17	47

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	173	CYS
1	M	182	CYS
1	M	188	ARG
1	N	175	ILE

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Mol	Chain	Res	Type
1	N	187	LYS
1	S	189	ILE
1	T	178	ASN
1	T	188	ARG
1	U	188	ARG
1	V	186	CYS
1	V	188	ARG
1	j	171	VAL
1	j	181	THR
1	j	182	CYS
1	j	185	ILE
1	j	186	CYS
1	j	187	LYS
1	j	189	ILE
1	A	189	ILE
1	A	192	LYS
1	A	193	LYS
2	B	51	ILE
2	B	54	ASP
2	B	57	MET
2	B	108	VAL
2	B	159	THR
2	B	179	GLN
2	B	186	LEU
2	B	203	ILE
2	B	217	LYS
2	B	218	LYS
2	B	222	LYS
2	B	223	SER
3	F	114	ARG
3	F	132	LYS
3	F	143	ASN
3	F	152	VAL
3	F	155	LYS
3	F	164	ASN
3	F	170	THR
3	F	175	LYS
3	F	187	LEU
3	F	207	LEU
3	F	215	PHE
3	G	4	LEU
3	G	96	THR

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Mol	Chain	Res	Type
3	G	109	VAL
3	I	4	LEU
3	I	16	GLN
3	I	52	GLU
3	I	114	ARG
3	I	132	LYS
3	I	153	GLN
3	I	155	LYS
3	I	164	ASN
3	I	172	GLN
3	I	207	LEU
2	J	13	LYS
2	J	51	ILE
2	J	52	ILE
2	J	54	ASP
2	J	108	VAL
2	J	159	THR
2	J	203	ILE
3	K	11	SER
3	K	29	VAL
3	K	80	LEU
3	K	132	LYS
3	K	152	VAL
3	K	155	LYS
3	K	164	ASN
3	K	172	GLN
3	K	183	SER
3	K	187	LEU
3	K	207	LEU
2	L	51	ILE
2	L	54	ASP
2	L	69	SER
2	L	85	SER
2	L	108	VAL
2	L	159	THR
2	L	160	VAL
2	L	161	SER
2	L	164	SER
2	L	167	LEU
2	L	185	SER
2	L	186	LEU
2	L	203	ILE

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Mol	Chain	Res	Type
2	L	209	LYS
2	L	212	ASN
2	L	214	LYS
2	L	218	LYS
2	L	220	GLU
2	L	222	LYS
3	O	4	LEU
3	O	16	GLN
3	O	116	VAL
3	O	132	LYS
3	O	152	VAL
3	O	155	LYS
3	O	164	ASN
3	O	187	LEU
3	O	207	LEU
3	O	214	SER
2	P	3	GLN
2	P	51	ILE
2	P	91	THR
2	P	108	VAL
2	P	159	THR
2	P	160	VAL
2	P	199	THR
2	P	200	GLN
2	P	203	ILE
2	P	222	LYS
3	Q	16	GLN
3	Q	132	LYS
3	Q	152	VAL
3	Q	153	GLN
3	Q	155	LYS
3	Q	164	ASN
3	Q	170	THR
3	Q	172	GLN
3	Q	187	LEU
3	Q	207	LEU
2	R	13	LYS
2	R	51	ILE
2	R	52	ILE
2	R	54	ASP
2	R	108	VAL
2	R	156	GLU

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Mol	Chain	Res	Type
2	R	160	VAL
2	R	186	LEU
2	R	203	ILE
3	W	16	GLN
3	W	32	TYR
3	W	80	LEU
3	W	85	GLU
3	W	109	VAL
3	W	112	LEU
3	W	132	LYS
3	W	152	VAL
3	W	155	LYS
3	W	164	ASN
3	W	187	LEU
3	W	207	LEU
2	X	51	ILE
2	X	52	ILE
2	X	54	ASP
2	X	108	VAL
2	X	119	VAL
2	X	139	THR
2	X	143	THR
2	X	159	THR
2	X	203	ILE
3	Y	16	GLN
3	Y	21	SER
3	Y	114	ARG
3	Y	115	THR
3	Y	132	LYS
3	Y	152	VAL
3	Y	155	LYS
3	Y	164	ASN
3	Y	187	LEU
3	Y	207	LEU
2	Z	13	LYS
2	Z	28	THR
2	Z	51	ILE
2	Z	54	ASP
2	Z	108	VAL
2	Z	119	VAL
2	Z	143	THR
2	Z	159	THR

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Mol	Chain	Res	Type
2	Z	203	ILE
2	Z	222	LYS
2	H	5	VAL
2	H	51	ILE
2	H	54	ASP
2	H	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	169	ASN
1	S	169	ASN
1	T	191	ASN
1	U	191	ASN
1	V	178	ASN
3	F	16	GLN
3	F	39	GLN
3	F	161	GLN
3	G	39	GLN
3	G	41	HIS
3	G	81	GLN
3	I	143	ASN
3	I	153	GLN
3	I	164	ASN
3	I	195	HIS
2	J	172	HIS
3	K	172	GLN
2	L	172	HIS
3	O	39	GLN
3	Q	39	GLN
3	Q	161	GLN
3	Q	195	HIS
3	W	143	ASN
3	W	164	ASN
3	W	166	GLN
2	X	59	ASN
3	Y	39	GLN
3	Y	161	GLN
3	Y	166	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	31/49 (63%)	0.51	0 100 100	30, 66, 83, 85	0
1	M	27/49 (55%)	0.48	0 100 100	47, 65, 73, 93	0
1	N	31/49 (63%)	0.72	1 (3%) 50 30	43, 62, 85, 93	0
1	S	30/49 (61%)	0.35	1 (3%) 49 29	43, 66, 83, 85	0
1	T	30/49 (61%)	0.46	1 (3%) 49 29	49, 63, 75, 85	0
1	U	30/49 (61%)	0.49	1 (3%) 49 29	55, 75, 89, 96	0
1	V	29/49 (59%)	0.15	0 100 100	48, 68, 80, 86	0
1	j	32/49 (65%)	0.86	3 (9%) 14 8	40, 69, 93, 101	0
2	B	216/261 (82%)	0.36	10 (4%) 37 20	31, 68, 104, 125	0
2	H	115/261 (44%)	0.44	3 (2%) 57 36	47, 73, 96, 125	0
2	J	210/261 (80%)	0.52	7 (3%) 49 29	36, 84, 113, 121	0
2	L	216/261 (82%)	0.49	2 (0%) 81 63	39, 82, 109, 129	0
2	P	214/261 (81%)	0.64	12 (5%) 30 16	30, 85, 109, 120	0
2	R	217/261 (83%)	0.34	4 (1%) 67 47	32, 68, 104, 132	0
2	X	219/261 (83%)	0.35	8 (3%) 45 25	40, 69, 114, 137	0
2	Z	215/261 (82%)	0.39	2 (0%) 81 63	44, 80, 108, 128	0
3	F	208/220 (94%)	0.37	5 (2%) 59 38	29, 65, 91, 112	0
3	G	104/220 (47%)	0.25	2 (1%) 66 45	34, 62, 84, 91	0
3	I	199/220 (90%)	0.50	8 (4%) 42 23	30, 86, 120, 133	0
3	K	209/220 (95%)	0.48	6 (2%) 53 32	37, 81, 111, 136	0
3	O	206/220 (93%)	0.45	8 (3%) 43 24	24, 81, 122, 139	0
3	Q	211/220 (95%)	0.25	6 (2%) 55 34	27, 60, 102, 137	0
3	W	211/220 (95%)	0.38	7 (3%) 49 29	36, 75, 109, 126	0
3	Y	212/220 (96%)	0.43	2 (0%) 81 63	30, 73, 110, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3422/4240 (80%)	0.43	99 (2%) 53 32	24, 73, 112, 139	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	29	VAL	4.3
2	P	143	THR	4.2
3	Q	173	ASP	4.0
3	I	2	SER	3.9
2	B	56	PRO	3.7
2	P	54	ASP	3.7
2	B	135	SER	3.6
2	B	54	ASP	3.6
3	I	94	ALA	3.5
3	W	32	TYR	3.4
2	X	97	ALA	3.4
2	H	54	ASP	3.3
2	B	143	THR	3.3
3	O	149	GLU	3.3
3	O	206	GLY	3.3
2	P	83	LEU	3.2
3	I	77	ILE	3.2
2	R	143	THR	3.2
3	O	34	HIS	3.0
3	F	25	SER	3.0
1	N	190	PRO	3.0
2	X	29	PHE	3.0
1	j	172	PRO	3.0
3	I	34	HIS	3.0
3	I	64	PHE	3.0
2	H	103	SER	2.9
2	L	54	ASP	2.9
3	Q	31	GLY	2.8
3	O	35	VAL	2.8
2	R	101	LEU	2.7
2	J	54	ASP	2.7
2	P	92	ALA	2.7
3	Q	113	SER	2.7
2	P	91	THR	2.7
1	T	175	ILE	2.6
1	j	174	SER	2.6
2	J	2	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	J	77	THR	2.6
3	O	94	ALA	2.6
3	Q	29	VAL	2.6
2	H	56	PRO	2.6
2	P	85	SER	2.5
2	B	187	SER	2.5
1	U	190	PRO	2.5
3	F	38	TYR	2.5
3	Q	187	LEU	2.5
2	P	79	VAL	2.5
3	W	176	ASP	2.5
3	K	207	LEU	2.5
2	J	104	PRO	2.4
2	X	179	GLN	2.4
3	W	113	SER	2.4
2	P	70	PHE	2.4
2	B	197	LEU	2.4
2	X	45	LEU	2.4
2	P	11	VAL	2.4
3	Y	152	VAL	2.4
3	O	3	ALA	2.3
2	X	181	SER	2.3
3	Q	34	HIS	2.3
2	J	113	GLN	2.3
2	X	143	THR	2.3
2	Z	107	ALA	2.3
2	J	103	SER	2.3
3	W	211	VAL	2.3
3	Y	123	ILE	2.2
2	J	53	PRO	2.2
2	P	145	ALA	2.2
3	K	31	GLY	2.2
2	B	101	LEU	2.2
1	S	165	PHE	2.2
3	I	188	SER	2.2
3	F	176	ASP	2.2
3	I	202	VAL	2.2
3	K	169	VAL	2.2
2	B	142	GLY	2.2
3	G	34	HIS	2.2
1	j	179	ASN	2.2
2	P	144	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	W	30	GLY	2.2
2	Z	54	ASP	2.2
3	I	176	ASP	2.2
2	P	77	THR	2.1
3	W	49	ILE	2.1
2	B	57	MET	2.1
3	K	150	ALA	2.1
2	X	220	GLU	2.1
2	R	54	ASP	2.1
3	K	177	SER	2.1
3	F	191	ASP	2.1
2	R	142	GLY	2.1
3	K	148	ARG	2.1
2	X	54	ASP	2.1
2	B	124	THR	2.1
3	F	200	CYS	2.1
3	O	208	SER	2.0
3	G	24	GLY	2.0
3	O	122	PHE	2.0
2	L	197	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 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.