Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2025 – 10:06 AM EST

PDB ID	:	9CQD
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.

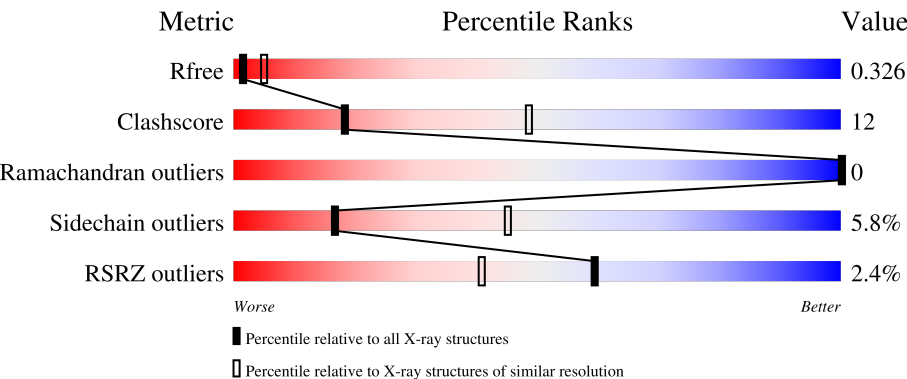The following versions of software and data (see references ⓘ) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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	Percentile Ranks	Value
Rfree		0.326
Clashscore		12
Ramachandran outliers		0
Sidechain outliers		5.8%
RSRZ outliers		2.4%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (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 <=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	47% 12% • 37%
1	M	49	35% 16% • 45%
1	N	49	2% 51% 10% • 37%
1	S	49	2% 45% 16% 39%
1	T	49	2% 41% 20% 39%

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Mol	Chain	Length	Quality of chain
1	U	49	2% 35% 24% 39%
1	V	49	41% 14% 41%
1	j	49	6% 53% 12% 35%
2	B	261	3% 57% 24% 17%
2	H	261	% 31% 13% 56%
2	J	261	3% 59% 20% 20%
2	L	261	54% 26% 17%
2	P	261	4% 59% 21% 18%
2	R	261	% 59% 23% 17%
2	X	261	2% 60% 23% 16%
2	Z	261	% 54% 26% 18%
3	F	220	% 67% 25% 5%
3	G	220	32% 14% 53%
3	I	220	4% 66% 24% 10%
3	K	220	% 64% 30% 5%
3	O	220	3% 69% 23% 6%
3	Q	220	3% 68% 26%
3	W	220	3% 70% 24%
3	Y	220	% 71% 25%

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

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

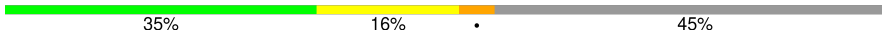| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	208	Total 1578	C 984	N 267	O 323	S 4	0	0	0
3	G	104	Total 767	C 477	N 131	O 157	S 2	0	0	0
3	I	199	Total 1509	C 939	N 256	O 310	S 4	0	0	0
3	K	209	Total 1565	C 973	N 266	O 322	S 4	0	0	0
3	O	206	Total 1553	C 966	N 265	O 318	S 4	0	0	0

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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 ⓘ

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:
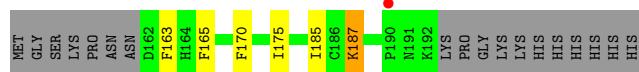
• Molecule 1: Mature secreted glycoprotein G

Chain S:

• Molecule 1: Mature secreted glycoprotein G

Chain T:

• Molecule 1: Mature secreted glycoprotein G

Chain U:

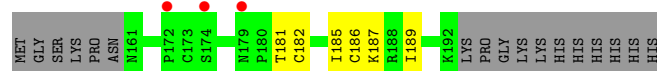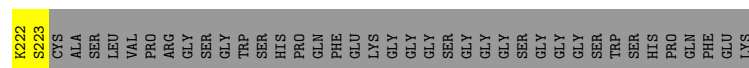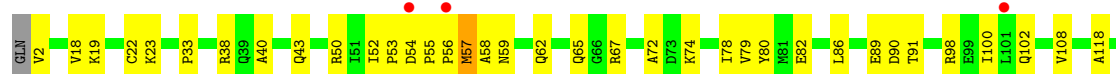• Molecule 1: Mature secreted glycoprotein G

Chain V:

41% 14% • 41%

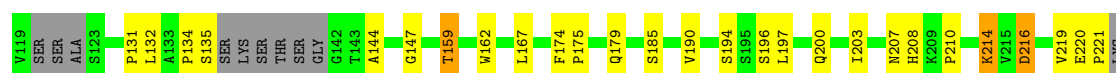MET GLY SER LYS PRO ASN ASN ASP F163 H164 F165 E166 V167 C173 S177 C182 I185 C186 K187 R188 N191 LYS LYS PRO GLY LYS LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: Mature secreted glycoprotein G

6%

Chain j:

53% 12% 35%

MET GLY SER LYS PRO ASN N161 P172 C173 S174 N179 P180 T181 C182 I185 C186 K187 R188 I189 K192 LYS PRO GLY LYS LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: Mature secreted glycoprotein G

Chain A:

47% 12% • 37%

MET GLY SER LYS PRO ASN ASN ASP F163 V167 C173 S174 I175 C176 S177 C186 K192 K193 PRO GLY LYS LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Fab 2B11 Heavy Chain

3%

Chain B:

57% 24% • 17%

GLN V2 V18 K19 C22 K23 P33 R38 Q39 A40 Q43 R50 I51 I52 P53 D54 P55 P56 M57 A58 N59 Q62 Q65 G66 R67 A72 D73 K74 I78 V79 Y80 M81 E82 L86 E89 D90 T91 R98 E99 I100 L101 Q102 V108 A118

S123 P127 F130 P131 P134 S135 SER LYS SER THR SER GLY G142 T143 A144 A145 L146 V150 Y153 T159 W162 L167 F174 L183 Y184 S185 L186 S187 V190 S194 L197 I203 C204 N207 H208 K209 P210 K214 V215 D216 K217 K218 V219

K222 S223 CYS ALA SER LEU VAL PRO ARG GLY SER GLY TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 2: Fab 2B11 Heavy Chain

3%

Chain J:

59% 20% • 20%

GLN V2 E10 VAL K12 K13 K19 C22 P41 G42 Q43 G44 R50 P53 D54 P55 P56 M57 A58 N59 I60 A61 F64 R67 V68 S69 K74 S75 T76 T77 I78 V79 Y80 M81 E82 T91 A92 I100 L101 Q102 S103 P104 A107 V108 Q113 A118

V119 SER SER ALA S123 P131 L132 A133 P134 S135 SER LYS SER THR SER GLY G142 T143 A144 G147 T159 W162 L167 F174 P175 Q179 S185 V190 S194 S195 S196 L197 Q200 I203 N207 H208 K209 P210 K214 V215 D216 V219 E220 P221 LYS

SER CYS ALA SER LEU VAL PRO ARG GLY SER GLY TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 2: Fab 2B11 Heavy Chain

Chain L:

54% 26% • 17%

- Molecule 2: Fab 2B11 Heavy Chain

- Molecule 2: Fab 2B11 Heavy Chain
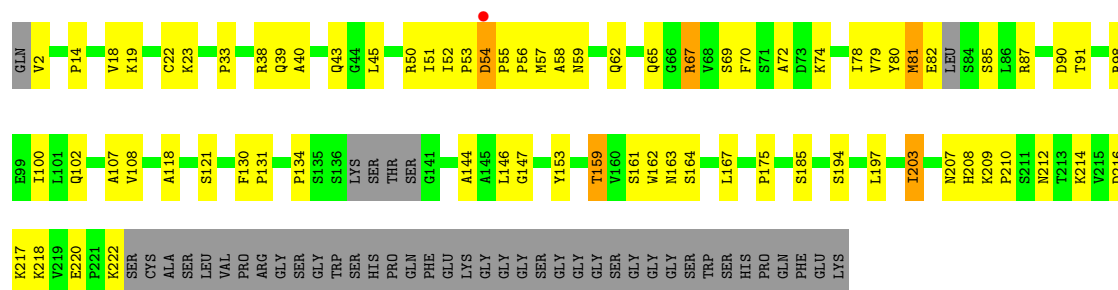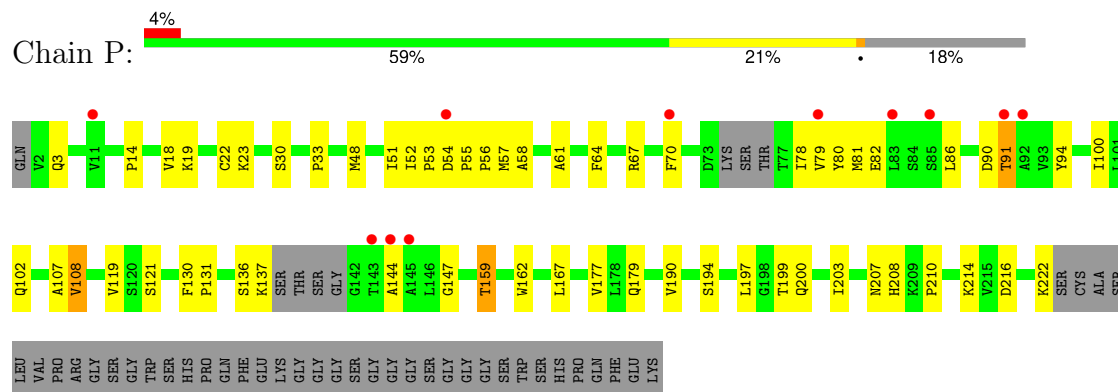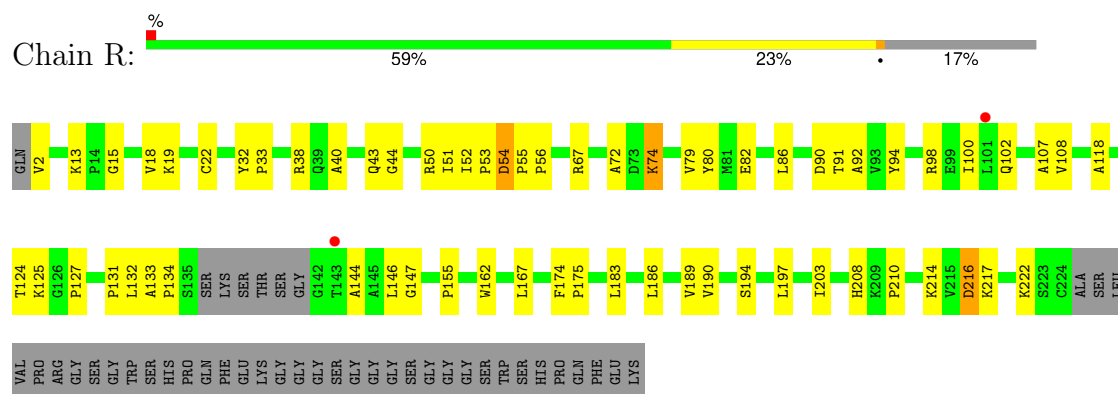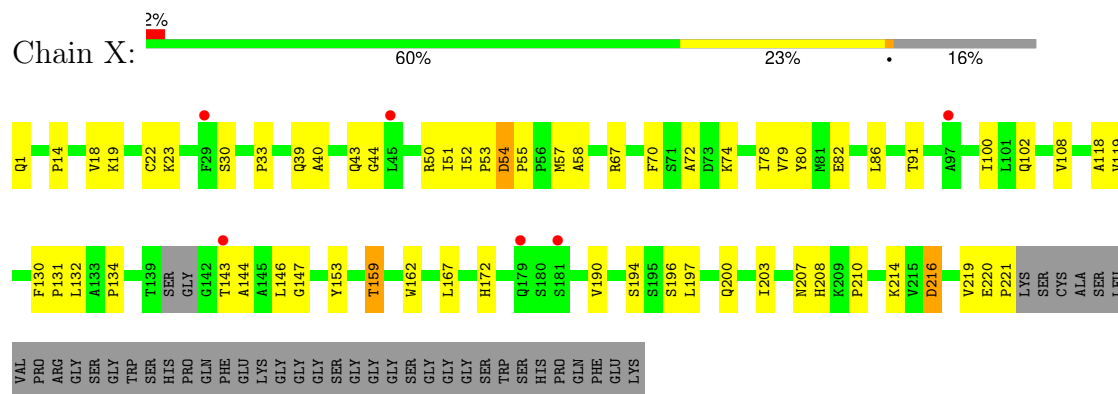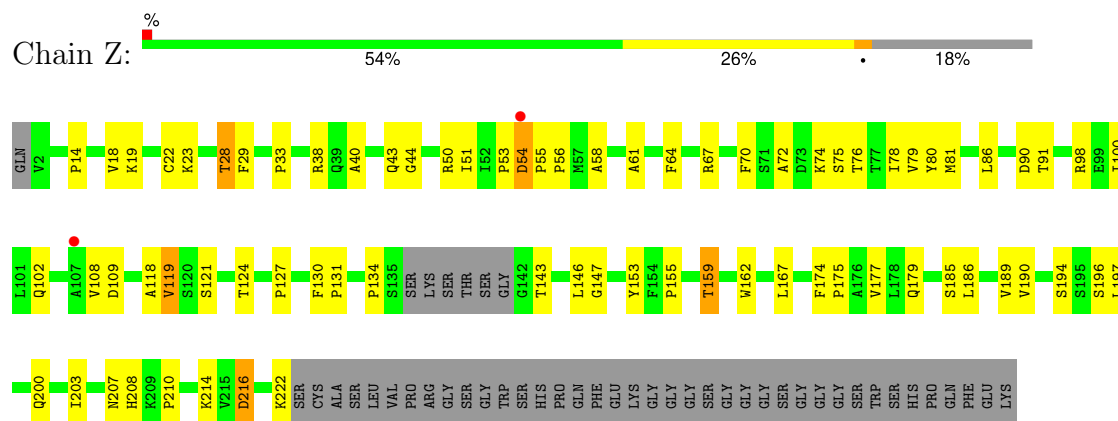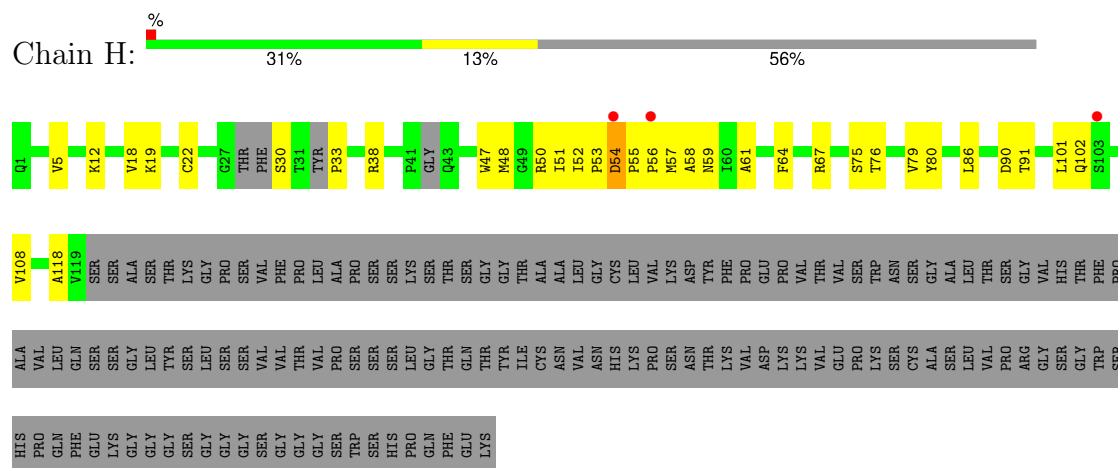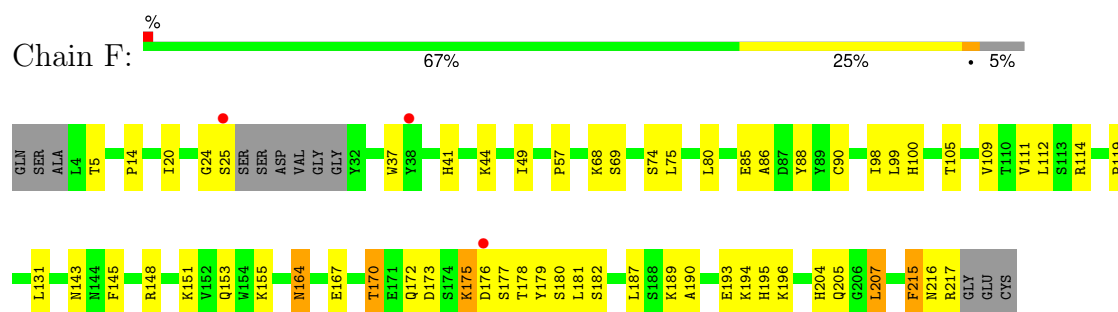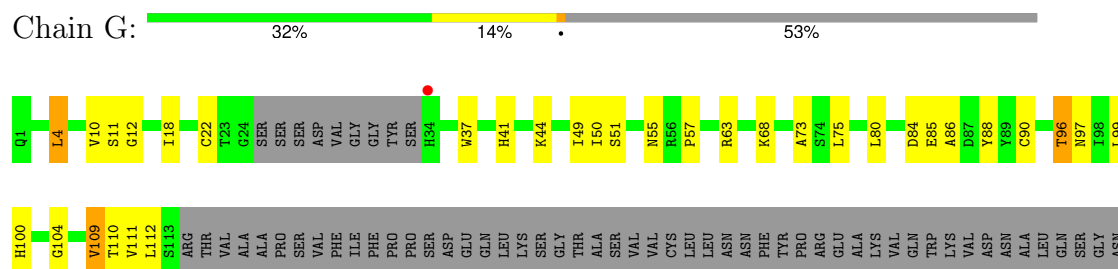

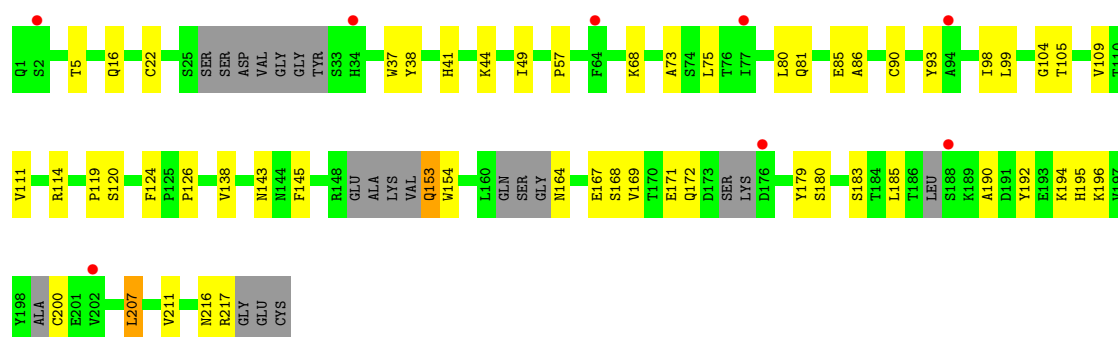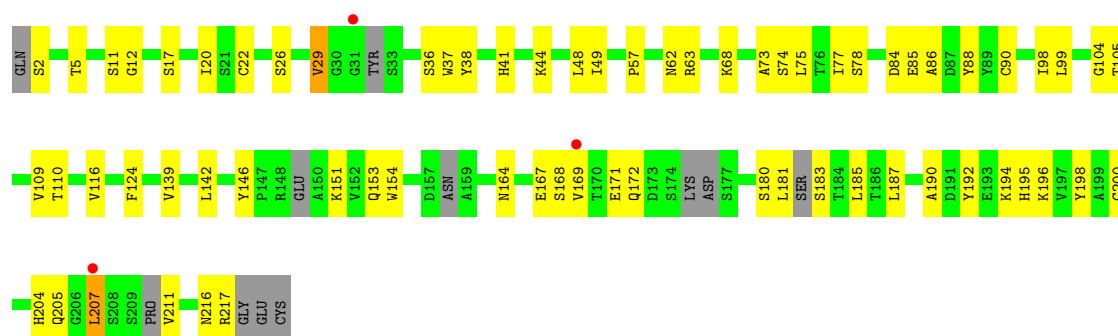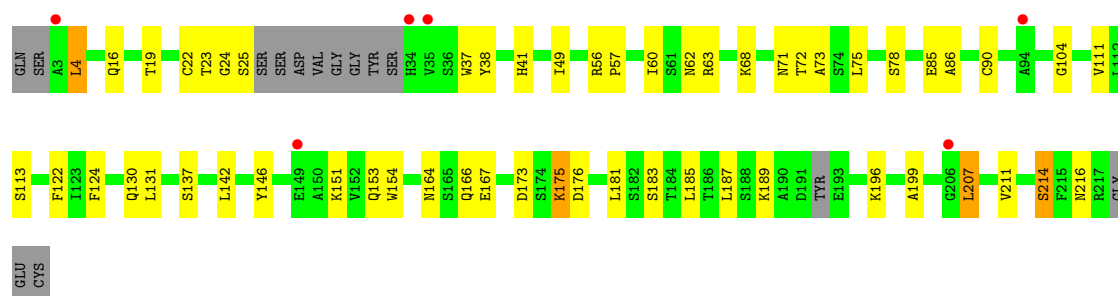- Molecule 2: Fab 2B11 Heavy Chain

- Molecule 2: Fab 2B11 Heavy Chain

Chain Z:

• Molecule 2: Fab 2B11 Heavy Chain

Chain H:

• Molecule 3: Fab 2B11 Light Chain

Chain F:

• Molecule 3: Fab 2B11 Light Chain

Chain G:

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

• Molecule 3: Fab 2B11 Light Chain
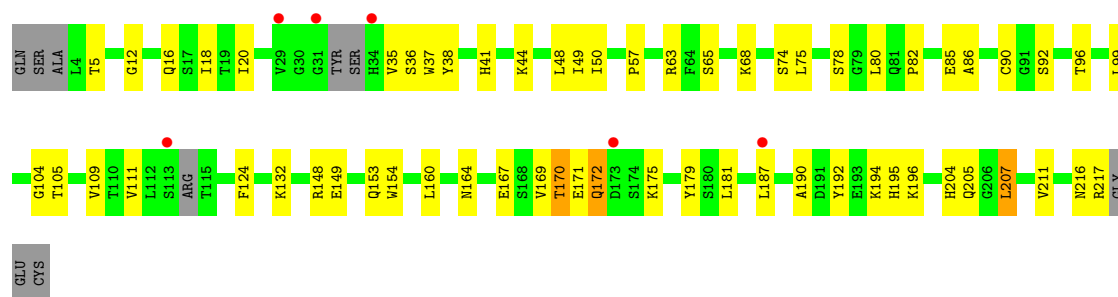
Chain I:

• Molecule 3: Fab 2B11 Light Chain

Chain K:

• Molecule 3: Fab 2B11 Light Chain

Chain O:

• Molecule 3: Fab 2B11 Light Chain

Chain Q:

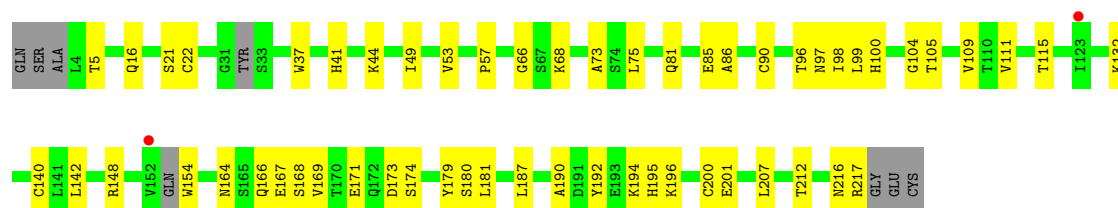GLN SER ALA L4 T5 G12 Q16 S17 I18 T19 I20 V29 G30 G31 TYR SER H34 V35 S36 W37 Y38 H41 K44 L48 I49 I50 P57 R63 F64 S65 K68 S74 L75 S78 G79 L80 Q81 P82 E85 A86 C90 G91 S92 T96 L99

G104 T105 V109 T110 V111 L112 S113 ARG T115 F124 K132 R148 E149 Q153 W154 L160 N164 E167 S168 V169 T170 E171 Q172 D173 S174 K175 Y179 S180 L181 L187 A190 D191 Y192 E193 K194 H195 K196 H204 Q205 G206 L207 V211 N216 R217 GLY

GLU CYS

• Molecule 3: Fab 2B11 Light Chain

Chain W:

3%

70%   24%   • •

GLN SER ALA L4 T5 Q16 S17 I18 C22 T23 G24 S25 SER SER ASP V29 G30 G31 Y32 S33 W37 H41 K44 I49 I50 V53 P57 R63 F64 S65 G66 S67 K68 N71 T72 A73 S74 L75 L80 D84 E85 A86 Y89 C90 L99

G104 T105 V109 T110 V111 L112 S113 F124 E129 Q130 L131 K132 N143 Y146 P147 R148 K155 N164 E167 E171 D176 Y179 S180 L181 L187 S188 K189 A190 D191 Y192 E193 K194 H195 K196 L207 V211 N216 R217 GLY GLU CYS

• Molecule 3: Fab 2B11 Light Chain

Chain Y:

%

71%   25%   •

GLN SER ALA L4 T5 Q16 S21 C22 G31 TYR S33 W37 H41 K44 I49 V53 P57 G66 S67 K68 A73 S74 L75 Q81 E85 A86 C90 T96 N97 I98 L99 H100 G104 T105 V109 T110 V111 T115 I123 K132

C140 L141 L142 R148 V152 GLN W154 N164 S165 Q166 E167 S168 V169 T170 E171 Q172 D173 S174 Y179 S180 L181 L187 A190 D191 Y192 E193 K194 H195 K196 C200 E201 L207 T212 N216 R217 GLY GLU CYS

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
$< I/\sigma(I) >$ [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 (2.64%)	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 , 61.2	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.21$	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.*

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[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 (i)

5.1 Standard geometry (i)

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	0.47	0/263	0.64	0/356
1	M	0.42	0/229	0.57	0/311
1	N	0.42	0/262	0.61	0/356
1	S	0.43	0/254	0.61	0/345
1	T	0.51	0/254	0.71	0/345
1	U	0.54	0/254	0.66	0/345
1	V	0.42	0/245	0.67	0/334
1	j	0.51	0/270	0.62	0/367
2	B	0.35	0/1645	0.54	0/2243
2	H	0.37	0/887	0.58	0/1199
2	J	0.39	0/1604	0.57	0/2185
2	L	0.40	0/1640	0.55	0/2234
2	P	0.35	0/1631	0.56	0/2222
2	R	0.37	0/1651	0.53	0/2251
2	X	0.35	0/1667	0.56	0/2273
2	Z	0.36	0/1639	0.53	0/2235
3	F	0.33	0/1612	0.52	0/2192
3	G	0.33	0/783	0.50	0/1065
3	I	0.32	0/1537	0.51	0/2084
3	K	0.38	0/1592	0.55	0/2156
3	O	0.34	0/1584	0.51	0/2152
3	Q	0.31	0/1616	0.54	0/2196
3	W	0.32	0/1627	0.54	0/2212
3	Y	0.31	0/1624	0.52	0/2206
All	All	0.36	0/26370	0.55	0/35864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	254	0	244	12	0
1	M	221	0	205	10	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	12	0
1	V	236	0	218	8	0
1	j	261	0	241	0	0
2	B	1605	0	1602	41	0
2	H	870	0	873	28	0
2	J	1566	0	1558	32	0
2	L	1601	0	1593	40	0
2	P	1592	0	1589	41	0
2	R	1611	0	1607	41	0
2	X	1627	0	1625	48	0
2	Z	1599	0	1597	44	0
3	F	1578	0	1528	44	0
3	G	767	0	745	22	0
3	I	1509	0	1452	32	0
3	K	1565	0	1512	44	0
3	O	1553	0	1509	37	0
3	Q	1584	0	1529	40	0
3	W	1593	0	1543	35	0
3	Y	1592	0	1539	36	0
All	All	25772	0	25237	582	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 (582) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:203:ILE:HD11	2:R:216:ASP:HB3	1.80	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: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
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
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: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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:196:LYS:HE2	3:I:216:ASN:HB3	1.85	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
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
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Z:28:THR:O	2:Z:29:PHE:C	2.46	0.55
3:Q:41:HIS:HB2	3:Q:44:LYS:HE2	1.88	0.55
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:63:ARG:HH21	3:W:84:ASP:CG	2.11	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
3:F:131:LEU:O	3:F:189:LYS:NZ	2.27	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
1:A:192:LYS:O	1:A:193:LYS:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:O:25:SER:C	3:O:71:ASN:HD22	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:201:GLU:HA	3:Y:212:THR:HB	1.93	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
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: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
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
3:W:129:GLU:HG3	3:W:132:LYS:HZ1	1.76	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
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
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:98:ILE:HB	2:L:59:ASN:HB3	1.95	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
2:L:147:GLY:HA2	2:L:162:TRP:HZ2	1.77	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
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
3:F:41:HIS:CD2	3:F:86:ALA:HB2	2.48	0.48
3:K:2:SER:N	3:K:26:SER:HG	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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
3:K:63:ARG:HH21	3:K:84:ASP:CG	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:100:ILE:HG22	2:Z:102:GLN:O	2.15	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
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
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:131:LEU:O	3:W:189:LYS:NZ	2.33	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
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
2:J:134:PRO:O	2:J:135:SER:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:180:SER:C	2:J:174:PHE:HE1	2.20	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
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:188:ARG:HH11	1:U:189:ILE:HG22	1.82	0.44
3:F:215:PHE:CD1	3:F:215:PHE:C	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:55:PRO:O	2:L:56:PRO:C	2.55	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:HD2	2:J:55:PRO:O	2.18	0.43
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.99	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
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
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
3:F:24:GLY:O	3:F:25:SER:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:V:165:PHE:HE1	2:Z:72:ALA:HB3	1.84	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
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
2:P:55:PRO:O	2:P:56:PRO:C	2.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:19:LYS:HG3	2:P:82:GLU:HB2	2.02	0.41
2:Z:55:PRO:O	2:Z:56:PRO:C	2.57	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
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
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
2:H:55:PRO:O	2:H:56:PRO:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:B:130:PHE:HA	2:B:131:PRO:HD3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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   (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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	28 (93%)	2 (7%)	13	40
1	M	26/46 (56%)	23 (88%)	3 (12%)	4	19
1	N	30/46 (65%)	28 (93%)	2 (7%)	13	40
1	S	29/46 (63%)	28 (97%)	1 (3%)	32	62
1	T	29/46 (63%)	27 (93%)	2 (7%)	13	39
1	U	29/46 (63%)	28 (97%)	1 (3%)	32	62
1	V	28/46 (61%)	26 (93%)	2 (7%)	12	39
1	j	31/46 (67%)	25 (81%)	6 (19%)	1	5
2	B	183/215 (85%)	171 (93%)	12 (7%)	14	41
2	H	96/215 (45%)	91 (95%)	5 (5%)	19	48
2	J	178/215 (83%)	170 (96%)	8 (4%)	23	53
2	L	182/215 (85%)	162 (89%)	20 (11%)	5	21
2	P	181/215 (84%)	169 (93%)	12 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	184/215 (86%)	174 (95%)	10 (5%)	18	47
2	X	186/215 (86%)	177 (95%)	9 (5%)	21	51
2	Z	182/215 (85%)	170 (93%)	12 (7%)	14	41
3	F	183/191 (96%)	173 (94%)	10 (6%)	18	47
3	G	88/191 (46%)	85 (97%)	3 (3%)	32	62
3	I	176/191 (92%)	169 (96%)	7 (4%)	27	58
3	K	181/191 (95%)	172 (95%)	9 (5%)	20	50
3	O	180/191 (94%)	172 (96%)	8 (4%)	24	54
3	Q	184/191 (96%)	175 (95%)	9 (5%)	21	51
3	W	184/191 (96%)	172 (94%)	12 (6%)	14	41
3	Y	185/191 (97%)	177 (96%)	8 (4%)	25	55
All	All	2965/3616 (82%)	2792 (94%)	173 (6%)	17	45

All (173) 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
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	181	THR
1	j	182	CYS
1	j	185	ILE
1	j	186	CYS
1	j	187	LYS
1	j	189	ILE
1	A	192	LYS
1	A	193	LYS
2	B	54	ASP
2	B	57	MET
2	B	67	ARG

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Mol	Chain	Res	Type
2	B	74	LYS
2	B	108	VAL
2	B	159	THR
2	B	186	LEU
2	B	214	LYS
2	B	216	ASP
2	B	217	LYS
2	B	222	LYS
2	B	223	SER
3	F	68	LYS
3	F	114	ARG
3	F	143	ASN
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
3	G	109	VAL
3	I	16	GLN
3	I	68	LYS
3	I	114	ARG
3	I	153	GLN
3	I	164	ASN
3	I	172	GLN
3	I	207	LEU
2	J	13	LYS
2	J	54	ASP
2	J	67	ARG
2	J	74	LYS
2	J	108	VAL
2	J	159	THR
2	J	214	LYS
2	J	216	ASP
3	K	11	SER
3	K	29	VAL
3	K	62	ASN
3	K	68	LYS
3	K	164	ASN

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Mol	Chain	Res	Type
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	67	ARG
2	L	69	SER
2	L	74	LYS
2	L	81	MET
2	L	85	SER
2	L	108	VAL
2	L	159	THR
2	L	161	SER
2	L	164	SER
2	L	167	LEU
2	L	185	SER
2	L	203	ILE
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	68	LYS
3	O	164	ASN
3	O	175	LYS
3	O	187	LEU
3	O	207	LEU
3	O	214	SER
2	P	3	GLN
2	P	51	ILE
2	P	67	ARG
2	P	91	THR
2	P	108	VAL
2	P	159	THR
2	P	199	THR
2	P	200	GLN
2	P	203	ILE
2	P	214	LYS

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Mol	Chain	Res	Type
2	P	216	ASP
2	P	222	LYS
3	Q	16	GLN
3	Q	68	LYS
3	Q	132	LYS
3	Q	153	GLN
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	67	ARG
2	R	74	LYS
2	R	108	VAL
2	R	186	LEU
2	R	214	LYS
2	R	216	ASP
3	W	16	GLN
3	W	32	TYR
3	W	68	LYS
3	W	80	LEU
3	W	85	GLU
3	W	109	VAL
3	W	112	LEU
3	W	132	LYS
3	W	155	LYS
3	W	164	ASN
3	W	187	LEU
3	W	207	LEU
2	X	51	ILE
2	X	54	ASP
2	X	67	ARG
2	X	74	LYS
2	X	108	VAL
2	X	143	THR
2	X	159	THR
2	X	214	LYS
2	X	216	ASP

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Mol	Chain	Res	Type
3	Y	16	GLN
3	Y	21	SER
3	Y	68	LYS
3	Y	115	THR
3	Y	132	LYS
3	Y	164	ASN
3	Y	187	LEU
3	Y	207	LEU
2	Z	28	THR
2	Z	51	ILE
2	Z	54	ASP
2	Z	67	ARG
2	Z	74	LYS
2	Z	108	VAL
2	Z	119	VAL
2	Z	143	THR
2	Z	159	THR
2	Z	214	LYS
2	Z	216	ASP
2	Z	222	LYS
2	H	5	VAL
2	H	51	ILE
2	H	54	ASP
2	H	67	ARG
2	H	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	169	ASN
1	V	178	ASN
3	F	16	GLN
3	I	40	GLN
2	J	39	GLN
3	Q	39	GLN
3	W	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	31/49 (63%)	0.36	0	100	100	30, 66, 83, 85	0
1	M	27/49 (55%)	0.33	0	100	100	47, 65, 73, 93	0
1	N	31/49 (63%)	0.56	1 (3%)	50	31	43, 62, 85, 93	0
1	S	30/49 (61%)	0.20	1 (3%)	49	30	43, 66, 83, 85	0
1	T	30/49 (61%)	0.31	1 (3%)	49	30	49, 63, 75, 85	0
1	U	30/49 (61%)	0.34	1 (3%)	49	30	55, 75, 89, 96	0
1	V	29/49 (59%)	-0.00	0	100	100	48, 68, 80, 86	0
1	j	32/49 (65%)	0.70	3 (9%)	15	9	40, 69, 93, 101	0
2	B	216/261 (82%)	0.21	8 (3%)	45	27	31, 68, 104, 125	0
2	H	115/261 (44%)	0.29	3 (2%)	57	38	47, 73, 96, 125	0
2	J	210/261 (80%)	0.37	7 (3%)	49	30	36, 84, 113, 121	0
2	L	216/261 (82%)	0.34	1 (0%)	87	75	39, 82, 109, 129	0
2	P	214/261 (81%)	0.49	11 (5%)	34	20	30, 85, 109, 120	0
2	R	217/261 (83%)	0.19	2 (0%)	81	66	32, 68, 104, 132	0
2	X	219/261 (83%)	0.20	6 (2%)	56	36	40, 69, 114, 137	0
2	Z	215/261 (82%)	0.24	2 (0%)	81	66	44, 80, 108, 128	0
3	F	208/220 (94%)	0.22	3 (1%)	73	56	29, 65, 91, 112	0
3	G	104/220 (47%)	0.10	1 (0%)	79	64	34, 62, 84, 91	0
3	I	199/220 (90%)	0.35	8 (4%)	43	25	30, 86, 120, 133	0
3	K	209/220 (95%)	0.33	3 (1%)	73	56	37, 81, 111, 136	0
3	O	206/220 (93%)	0.30	6 (2%)	54	34	24, 81, 122, 139	0
3	Q	211/220 (95%)	0.10	6 (2%)	55	35	27, 60, 102, 137	0
3	W	211/220 (95%)	0.23	6 (2%)	55	35	36, 75, 109, 126	0
3	Y	212/220 (96%)	0.28	2 (0%)	81	66	30, 73, 110, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
All	All	3422/4240 (80%)	0.28	82 (2%)	59	41	24, 73, 112, 139	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	29	VAL	4.1
2	P	143	THR	4.0
3	Q	173	ASP	3.8
3	I	2	SER	3.7
2	P	54	ASP	3.5
2	B	56	PRO	3.5
2	B	135	SER	3.4
2	B	54	ASP	3.4
3	I	94	ALA	3.3
3	W	32	TYR	3.3
2	X	97	ALA	3.2
2	B	143	THR	3.2
2	H	54	ASP	3.2
3	O	149	GLU	3.1
3	O	206	GLY	3.1
2	P	83	LEU	3.1
2	R	143	THR	3.0
3	I	77	ILE	3.0
3	O	34	HIS	2.9
1	N	190	PRO	2.9
3	F	25	SER	2.8
2	X	29	PHE	2.8
2	H	103	SER	2.8
3	I	34	HIS	2.8
1	j	172	PRO	2.8
2	L	54	ASP	2.8
3	I	64	PHE	2.7
3	Q	31	GLY	2.7
3	O	35	VAL	2.6
2	R	101	LEU	2.6
2	P	92	ALA	2.6
2	J	54	ASP	2.6
2	P	91	THR	2.5
3	Q	113	SER	2.5
1	T	175	ILE	2.5
2	J	2	VAL	2.5
3	O	94	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	29	VAL	2.5
2	J	77	THR	2.4
1	j	174	SER	2.4
2	H	56	PRO	2.4
2	P	85	SER	2.4
3	F	38	TYR	2.3
3	Q	187	LEU	2.3
2	B	187	SER	2.3
2	P	79	VAL	2.3
3	K	207	LEU	2.3
1	U	190	PRO	2.3
3	W	176	ASP	2.3
2	J	104	PRO	2.3
3	O	3	ALA	2.3
2	X	179	GLN	2.2
2	P	11	VAL	2.2
3	W	113	SER	2.2
3	Y	152	VAL	2.2
2	P	70	PHE	2.2
2	B	197	LEU	2.2
2	X	45	LEU	2.2
2	J	113	GLN	2.2
3	Q	34	HIS	2.2
2	X	181	SER	2.2
2	X	143	THR	2.1
3	W	211	VAL	2.1
2	P	145	ALA	2.1
2	Z	107	ALA	2.1
2	B	101	LEU	2.1
3	Y	123	ILE	2.1
3	K	31	GLY	2.1
1	S	165	PHE	2.1
2	J	53	PRO	2.1
3	K	169	VAL	2.1
2	J	103	SER	2.1
3	I	188	SER	2.1
1	j	179	ASN	2.1
2	B	142	GLY	2.0
3	F	176	ASP	2.0
3	I	202	VAL	2.0
3	G	34	HIS	2.0
2	P	144	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	W	30	GLY	2.0
2	Z	54	ASP	2.0
3	I	176	ASP	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.