



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:09 AM UTC

PDB ID : 4EVN / pdb_00004evn
Title : Crystal Structure of Fab CR6261 (somatic heavy chain with germline-reverted light chain)
Authors : Whittle, J.R.R.
Deposited on : 2012-04-26
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

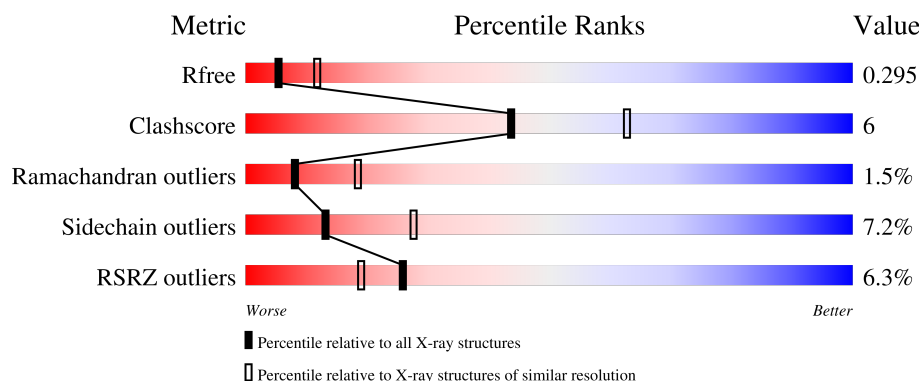
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	242	5% 71% 18% • 9%
1	C	242	6% 69% 19% • 9%
1	E	242	9% 70% 17% • 9%
1	G	242	9% 72% 16% • 9%
1	I	242	5% 71% 17% • 9%

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Mol	Chain	Length	Quality of chain
1	K	242	
1	M	242	
1	O	242	
2	B	217	
2	D	217	
2	F	217	
2	H	217	
2	J	217	
2	L	217	
2	N	217	
2	P	217	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25293 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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	C	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	E	221	Total	C	N	O	S	0	0	0
			1625	1029	269	318	9			
1	G	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	I	221	Total	C	N	O	S	0	0	0
			1625	1029	269	318	9			
1	K	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	M	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	O	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			

- Molecule 2 is a protein called Fab Lambda Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1541	972	251	314	4			
2	D	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	F	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	H	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	J	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	L	213	Total	C	N	O	S	0	0	0
			1540	970	251	315	4			

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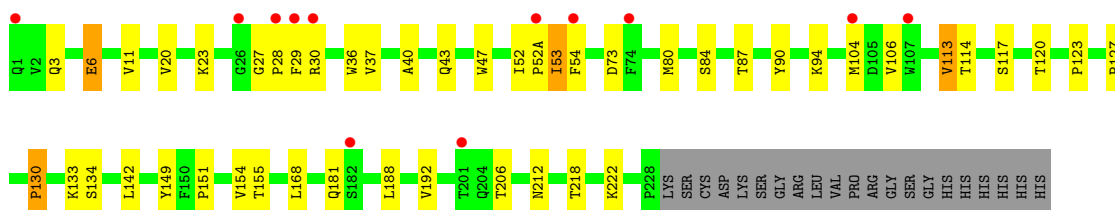
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	P	213	Total	C	N	O	S	0	0	0
			1539	970	251	314	4			

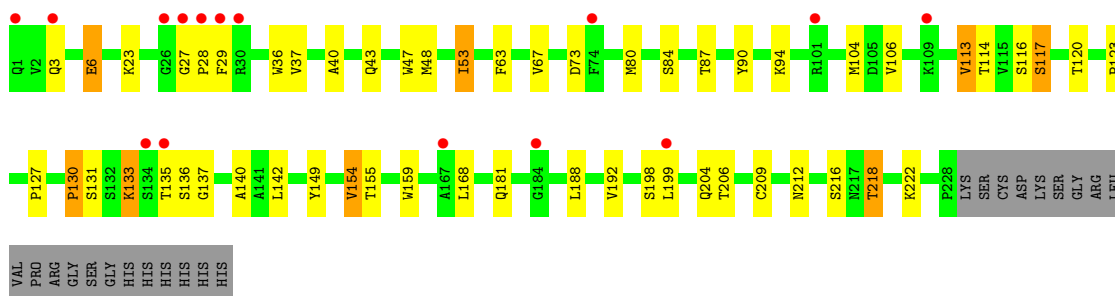
3 Residue-property plots [i](#)

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.

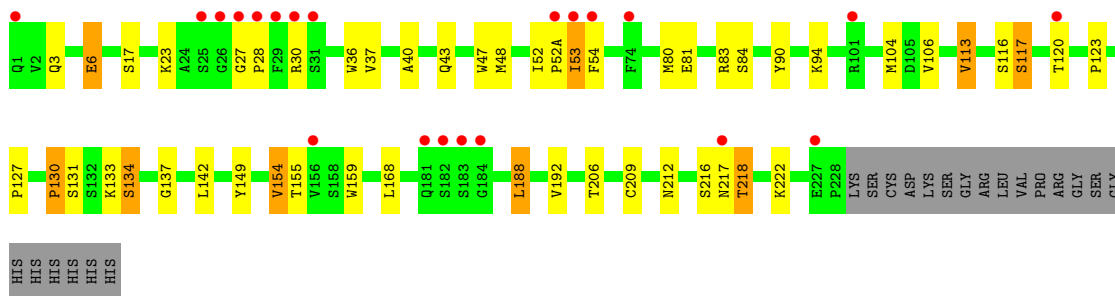
• Molecule 1: Fab Heavy Chain



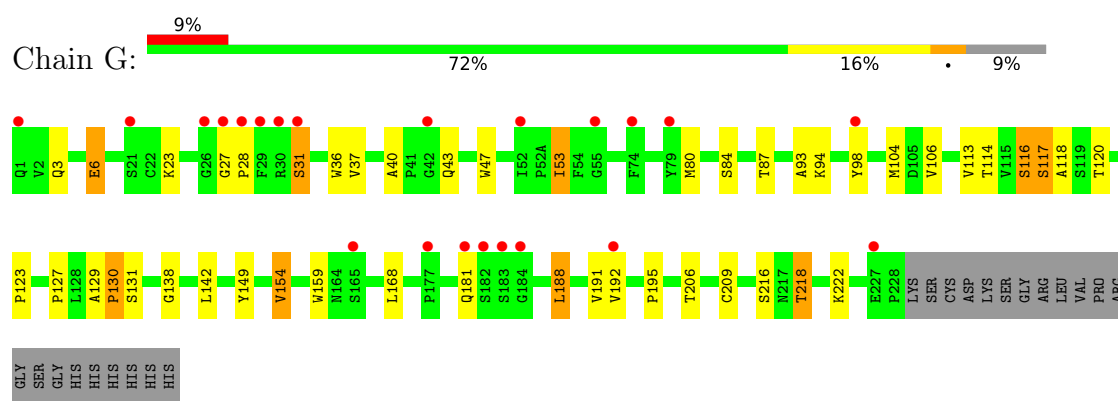
• Molecule 1: Fab Heavy Chain



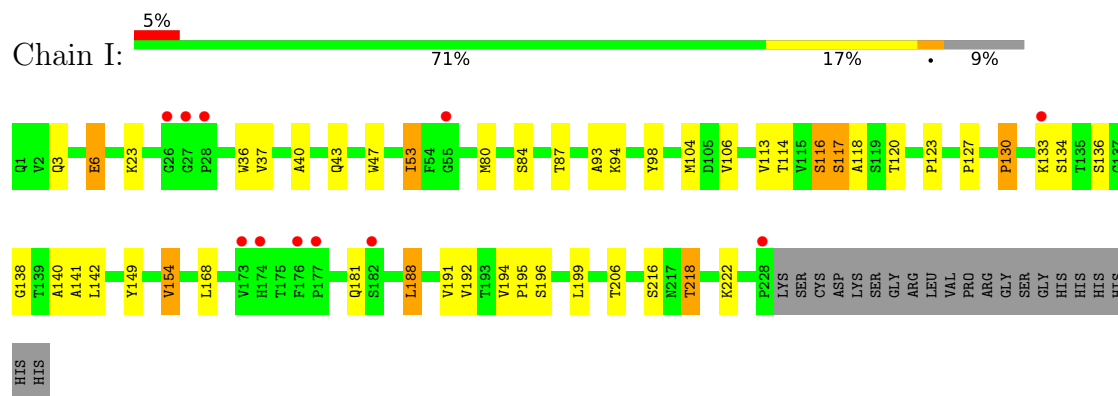
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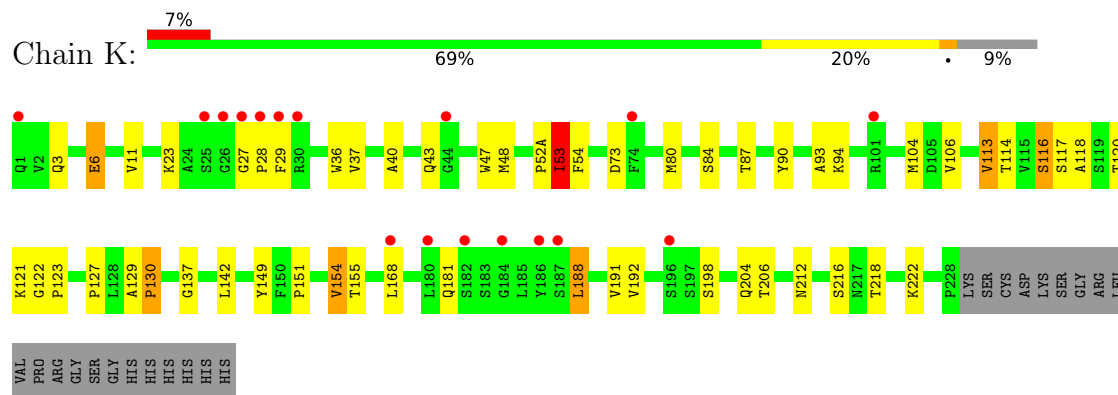
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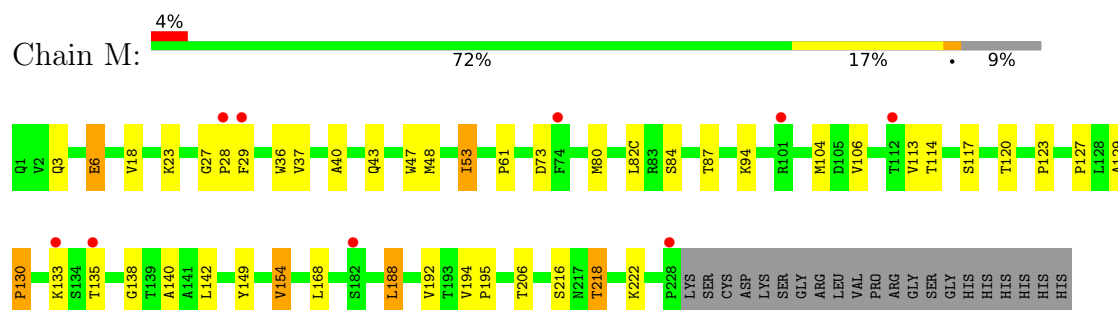
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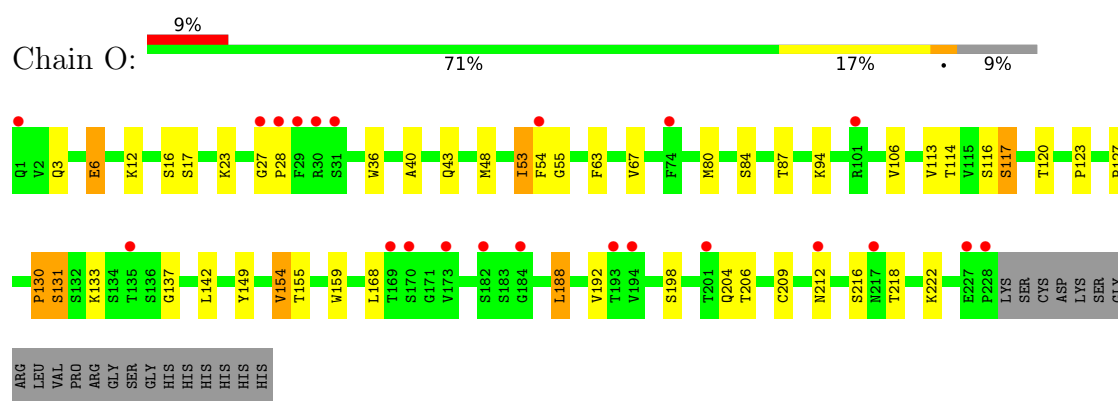
• Molecule 1: Fab Heavy Chain



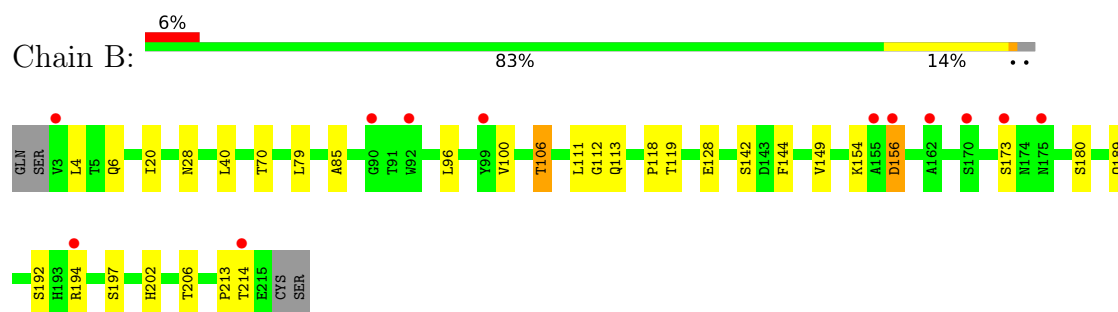
• Molecule 1: Fab Heavy Chain



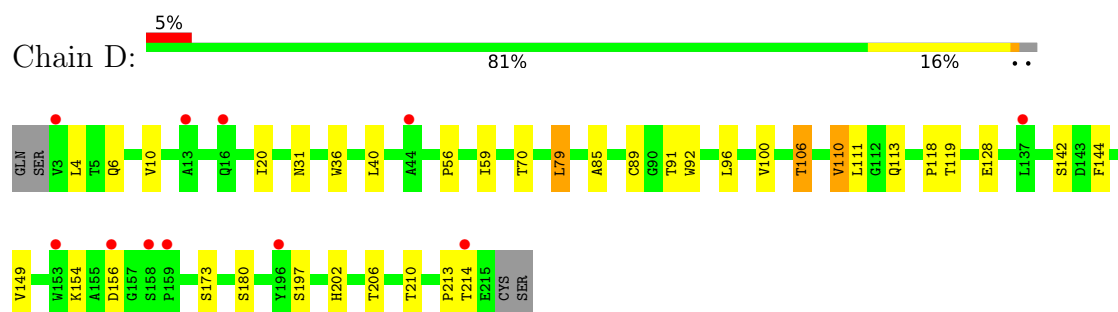
• Molecule 1: Fab Heavy Chain



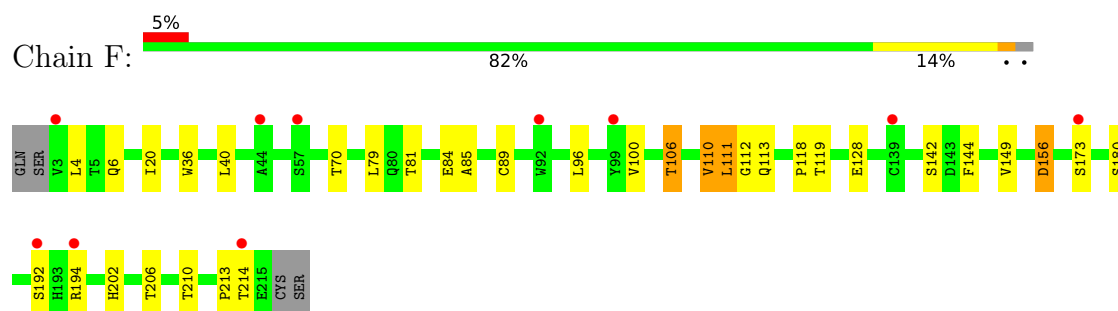
• Molecule 2: Fab Lambda Light Chain



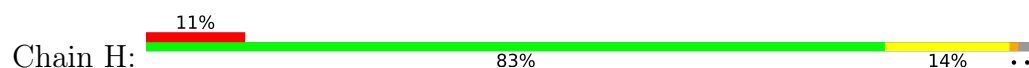
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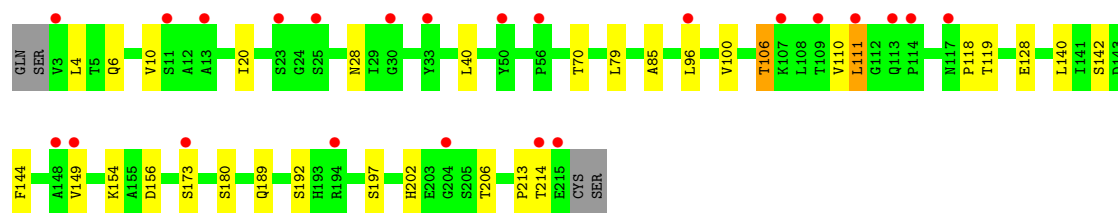


• Molecule 2: Fab Lambda Light Chain

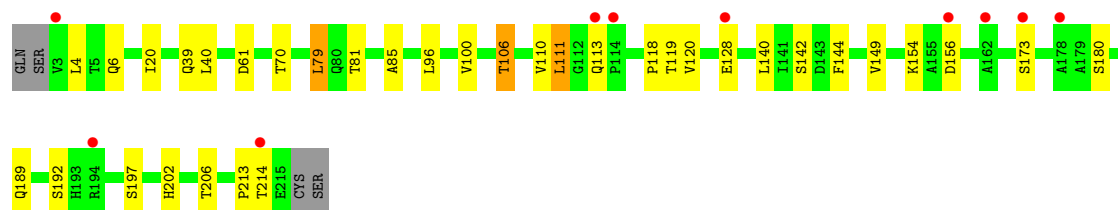
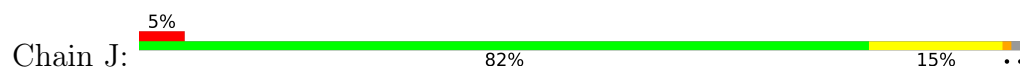


• Molecule 2: Fab Lambda Light Chain

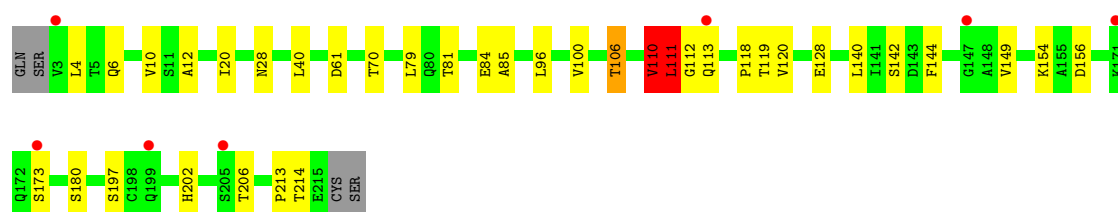
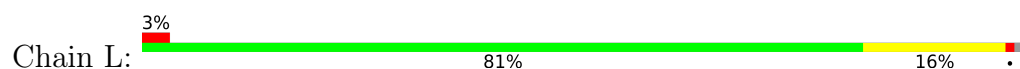




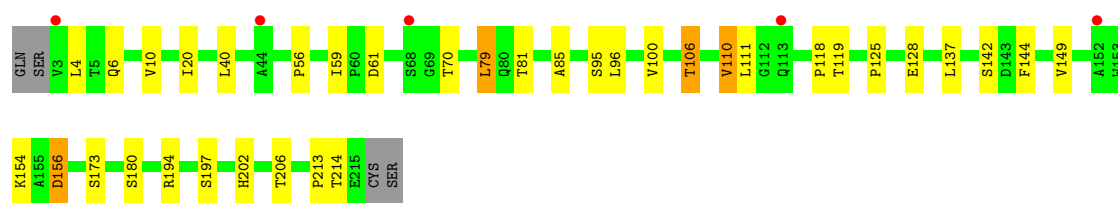
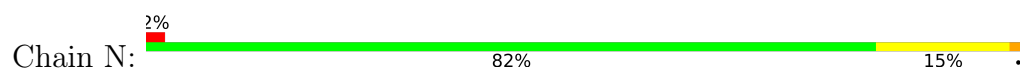
• Molecule 2: Fab Lambda Light Chain



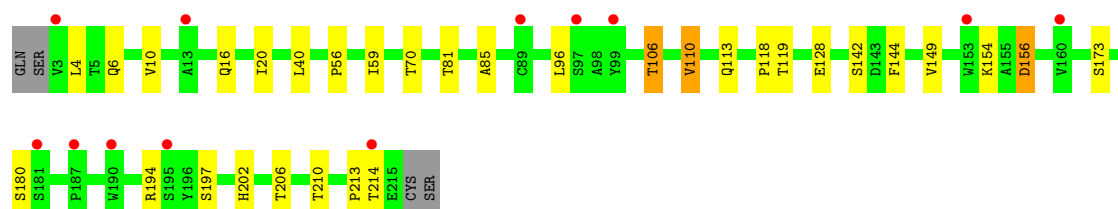
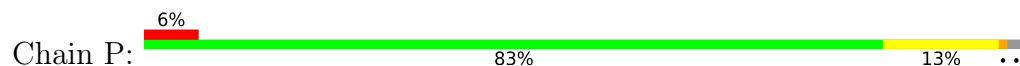
• Molecule 2: Fab Lambda Light Chain



• Molecule 2: Fab Lambda Light Chain



• Molecule 2: Fab Lambda 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	70.11Å 159.27Å 176.44Å 90.00° 89.73° 90.00°	Depositor
Resolution (Å)	55.01 – 2.85 55.01 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (55.01-2.85) 93.4 (55.01-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.230 , 0.293 0.227 , 0.295	Depositor DCC
R_{free} test set	2024 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25293	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.09% 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	0.60	0/1664	0.88	0/2270
1	C	0.70	3/1664 (0.2%)	0.94	0/2270
1	E	0.73	2/1666 (0.1%)	0.96	0/2272
1	G	0.63	1/1664 (0.1%)	0.89	2/2270 (0.1%)
1	I	0.67	2/1666 (0.1%)	0.90	1/2272 (0.0%)
1	K	0.67	1/1664 (0.1%)	0.93	1/2270 (0.0%)
1	M	0.61	0/1664	0.86	0/2270
1	O	0.69	2/1664 (0.1%)	0.92	1/2270 (0.0%)
2	B	0.61	1/1580 (0.1%)	0.90	1/2168 (0.0%)
2	D	0.64	0/1576	0.91	2/2164 (0.1%)
2	F	0.63	0/1576	0.91	1/2164 (0.0%)
2	H	0.60	1/1576 (0.1%)	0.85	0/2164
2	J	0.61	0/1576	0.91	1/2164 (0.0%)
2	L	0.62	1/1579 (0.1%)	0.91	3/2168 (0.1%)
2	N	0.60	0/1576	0.85	0/2164
2	P	0.59	0/1578	0.88	1/2166 (0.0%)
All	All	0.64	14/25933 (0.1%)	0.90	14/35486 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLN	CD-NE2	7.46	1.49	1.33
1	E	116	SER	CA-C	7.24	1.61	1.52
2	L	28	ASN	CA-C	6.51	1.56	1.52
1	O	116	SER	CA-C	6.24	1.60	1.52
2	H	28	ASN	CA-C	6.23	1.56	1.52
1	O	117	SER	N-CA	6.09	1.54	1.46
1	E	117	SER	N-CA	5.91	1.53	1.46
2	B	28	ASN	CA-C	5.62	1.55	1.52
1	I	116	SER	CA-C	-5.60	1.46	1.52
1	K	116	SER	CA-C	-5.21	1.46	1.52
1	I	117	SER	N-CA	-5.20	1.39	1.46
1	G	117	SER	N-CA	-5.14	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	SER	N-CA	5.09	1.52	1.46
1	C	116	SER	CA-C	5.04	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	GLN	N-CA-C	-7.74	95.69	108.23
2	F	113	GLN	N-CA-C	-6.47	101.98	110.39
2	J	120	VAL	N-CA-C	6.01	116.52	107.75
2	L	110	VAL	CB-CA-C	-6.01	104.74	111.23
1	G	116	SER	CA-C-O	5.92	126.89	120.32
1	I	116	SER	CA-C-O	5.81	126.40	120.24
1	G	31	SER	N-CA-C	-5.76	103.99	111.71
2	P	113	GLN	N-CA-C	-5.75	102.81	109.93
1	O	116	SER	CA-C-O	-5.46	115.43	121.33
2	D	110	VAL	N-CA-C	5.40	116.35	108.58
2	L	28	ASN	N-CA-C	5.25	117.15	108.48
2	D	113	GLN	N-CA-C	-5.24	102.99	109.64
2	L	120	VAL	N-CA-C	5.19	115.33	107.75
1	K	116	SER	CA-C-O	5.14	126.02	120.32

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	1623	0	1580	22	0
1	C	1623	0	1580	25	0
1	E	1625	0	1587	35	0
1	G	1623	0	1580	31	0
1	I	1625	0	1587	26	0
1	K	1623	0	1580	32	0
1	M	1623	0	1580	21	1
1	O	1623	0	1580	25	0
2	B	1541	0	1444	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1537	0	1433	18	0
2	F	1537	0	1433	15	0
2	H	1537	0	1433	11	0
2	J	1537	0	1433	16	0
2	L	1540	0	1437	16	0
2	N	1537	0	1433	18	0
2	P	1539	0	1440	12	1
All	All	25293	0	24140	303	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (303) 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:B:192:SER:HB2	2:P:96:LEU:HD12	1.49	0.94
1:E:81:GLU:OE2	1:O:12:LYS:NZ	2.02	0.93
2:P:81:THR:HA	2:P:110:VAL:HG21	1.52	0.91
1:I:138:GLY:O	1:I:196:SER:N	2.06	0.89
2:D:96:LEU:HD12	2:F:192:SER:HB2	1.51	0.88
1:K:11:VAL:HG21	1:K:151:PRO:HG3	1.54	0.86
1:E:217:ASN:ND2	1:O:55:GLY:O	2.13	0.82
1:O:127:PRO:HD3	1:O:222:LYS:HE2	1.66	0.78
1:M:127:PRO:HD3	1:M:222:LYS:HE2	1.65	0.78
1:E:127:PRO:HD3	1:E:222:LYS:HE2	1.65	0.78
1:A:127:PRO:HD3	1:A:222:LYS:HE2	1.66	0.76
1:E:52:ILE:HG21	1:G:98:TYR:CZ	2.20	0.76
1:I:127:PRO:HD3	1:I:222:LYS:HE2	1.68	0.74
1:K:127:PRO:HD3	1:K:222:LYS:HE2	1.69	0.74
2:P:40:LEU:HD23	2:P:85:ALA:HB2	1.70	0.73
1:G:127:PRO:HD3	1:G:222:LYS:HE2	1.69	0.72
2:B:40:LEU:HD23	2:B:85:ALA:HB2	1.71	0.72
2:H:40:LEU:HD23	2:H:85:ALA:HB2	1.71	0.72
1:C:127:PRO:HD3	1:C:222:LYS:HE2	1.72	0.70
2:J:40:LEU:HD23	2:J:85:ALA:HB2	1.73	0.70
2:B:149:VAL:HG12	2:B:202:HIS:HB2	1.74	0.70
2:D:40:LEU:HD23	2:D:85:ALA:HB2	1.73	0.69
2:N:40:LEU:HD23	2:N:85:ALA:HB2	1.72	0.69
2:F:40:LEU:HD23	2:F:85:ALA:HB2	1.76	0.69
2:L:40:LEU:HD23	2:L:85:ALA:HB2	1.74	0.68
2:F:149:VAL:HG12	2:F:202:HIS:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:123:PRO:HB3	1:M:149:TYR:HB3	1.76	0.67
2:N:149:VAL:HG12	2:N:202:HIS:HB2	1.78	0.66
1:A:123:PRO:HB3	1:A:149:TYR:HB3	1.78	0.65
1:E:40:ALA:HB3	1:E:43:GLN:HG3	1.79	0.64
1:C:123:PRO:HB3	1:C:149:TYR:HB3	1.79	0.64
1:O:40:ALA:HB3	1:O:43:GLN:HG3	1.80	0.64
1:I:140:ALA:N	1:I:194:VAL:O	2.31	0.64
1:I:123:PRO:HB3	1:I:149:TYR:HB3	1.80	0.63
1:O:123:PRO:HB3	1:O:149:TYR:HB3	1.78	0.63
1:E:54:PHE:CZ	1:G:98:TYR:HB3	2.34	0.63
2:F:84:GLU:HB2	2:F:110:VAL:HG23	1.81	0.63
1:E:123:PRO:HB3	1:E:149:TYR:HB3	1.80	0.62
1:M:40:ALA:HB3	1:M:43:GLN:HG3	1.81	0.61
2:P:149:VAL:HG12	2:P:202:HIS:HB2	1.81	0.61
2:D:149:VAL:HG12	2:D:202:HIS:HB2	1.81	0.61
2:H:149:VAL:HG12	2:H:202:HIS:HB2	1.83	0.61
1:G:40:ALA:HB3	1:G:43:GLN:HG3	1.83	0.61
2:L:84:GLU:HB2	2:L:110:VAL:HG23	1.83	0.60
1:C:40:ALA:HB3	1:C:43:GLN:HG3	1.83	0.60
1:E:54:PHE:CE2	1:G:98:TYR:HB3	2.36	0.60
2:J:149:VAL:HG12	2:J:202:HIS:HB2	1.84	0.60
1:C:140:ALA:HB2	1:C:199:LEU:HD11	1.85	0.58
1:G:123:PRO:HB3	1:G:149:TYR:HB3	1.84	0.58
2:F:118:PRO:HB3	2:F:144:PHE:HB3	1.86	0.58
2:L:149:VAL:HG12	2:L:202:HIS:HB2	1.86	0.58
1:A:40:ALA:HB3	1:A:43:GLN:HG3	1.85	0.57
1:K:37:VAL:HG21	1:K:104:MET:HE1	1.85	0.57
2:N:79:LEU:HD11	2:N:110:VAL:HG13	1.86	0.57
1:E:133:LYS:HE2	2:F:210:THR:O	2.04	0.57
2:H:189:GLN:O	2:H:192:SER:HB3	2.05	0.56
1:I:40:ALA:HB3	1:I:43:GLN:HG3	1.87	0.56
1:K:123:PRO:HB3	1:K:149:TYR:HB3	1.87	0.56
1:M:140:ALA:N	1:M:194:VAL:O	2.36	0.56
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.41	0.56
2:D:31:ASN:CG	2:N:95:SER:HA	2.30	0.56
1:E:17:SER:HB2	1:O:17:SER:H	1.71	0.56
1:G:138:GLY:O	1:G:195:PRO:HA	2.06	0.55
1:E:52:ILE:HG21	1:G:98:TYR:OH	2.05	0.55
1:I:36:TRP:CE2	1:I:80:MET:HB2	2.41	0.55
2:J:6:GLN:HB3	2:J:106:THR:HG22	1.89	0.55
1:E:54:PHE:HE2	1:G:31:SER:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:TRP:CE2	1:G:80:MET:HB2	2.42	0.54
2:H:6:GLN:HB3	2:H:106:THR:HG22	1.90	0.54
1:O:36:TRP:CE2	1:O:80:MET:HB2	2.43	0.54
1:K:40:ALA:HB3	1:K:43:GLN:HG3	1.90	0.54
1:A:54:PHE:CE2	1:I:98:TYR:HB3	2.43	0.54
1:K:37:VAL:CG2	1:K:104:MET:HE1	2.39	0.53
2:P:118:PRO:HB3	2:P:144:PHE:HB3	1.90	0.53
1:A:87:THR:HG23	1:A:114:THR:HA	1.91	0.53
2:N:6:GLN:HB3	2:N:106:THR:HG22	1.91	0.53
1:C:131:SER:O	1:C:135:THR:OG1	2.24	0.53
1:I:87:THR:HG23	1:I:114:THR:HA	1.91	0.53
1:I:94:LYS:HG2	1:I:106:VAL:HB	1.90	0.53
2:F:6:GLN:HB3	2:F:106:THR:HG22	1.91	0.52
1:K:93:ALA:HB3	1:K:104:MET:HE2	1.91	0.52
1:O:87:THR:HG23	1:O:114:THR:HA	1.92	0.52
2:D:154:LYS:HB2	2:D:197:SER:HB2	1.92	0.52
1:C:36:TRP:CE2	1:C:80:MET:HB2	2.45	0.52
2:L:6:GLN:HB3	2:L:106:THR:HG22	1.91	0.52
2:L:154:LYS:HB2	2:L:197:SER:HB2	1.90	0.52
1:K:87:THR:HG23	1:K:114:THR:HA	1.91	0.52
2:D:6:GLN:HB3	2:D:106:THR:HG22	1.90	0.51
2:J:79:LEU:CD1	2:J:110:VAL:HG12	2.40	0.51
2:N:81:THR:HA	2:N:110:VAL:HG21	1.91	0.51
2:L:81:THR:HA	2:L:110:VAL:HG21	1.93	0.51
1:K:168:LEU:HD13	1:K:192:VAL:HG21	1.91	0.51
1:M:37:VAL:HG21	1:M:104:MET:HE1	1.93	0.51
2:B:118:PRO:HB3	2:B:144:PHE:HB3	1.93	0.51
1:I:134:SER:HB2	1:I:141:ALA:HB3	1.93	0.51
1:M:36:TRP:CE2	1:M:80:MET:HB2	2.45	0.51
2:D:118:PRO:HB3	2:D:144:PHE:HB3	1.91	0.51
1:E:54:PHE:CZ	1:G:98:TYR:CB	2.94	0.51
1:M:94:LYS:HG2	1:M:106:VAL:HB	1.92	0.50
1:I:37:VAL:HG21	1:I:104:MET:HE1	1.94	0.50
2:P:6:GLN:HB3	2:P:106:THR:HG22	1.93	0.50
2:H:20:ILE:HG23	2:H:106:THR:HG21	1.94	0.50
2:H:118:PRO:HB3	2:H:144:PHE:HB3	1.93	0.50
1:K:54:PHE:HE1	1:O:54:PHE:CE1	2.30	0.50
1:K:54:PHE:CE1	1:O:54:PHE:HE1	2.30	0.49
2:B:20:ILE:HG23	2:B:106:THR:HG21	1.94	0.49
1:K:116:SER:C	1:K:118:ALA:N	2.70	0.49
2:P:20:ILE:HG23	2:P:106:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:TRP:CE2	1:E:80:MET:HB2	2.47	0.49
2:F:81:THR:HA	2:F:110:VAL:HG21	1.94	0.49
1:G:94:LYS:HG2	1:G:106:VAL:HB	1.93	0.49
1:I:168:LEU:HD13	1:I:192:VAL:HG21	1.95	0.49
1:A:11:VAL:HG21	1:A:151:PRO:HG3	1.93	0.49
1:I:130:PRO:HG3	1:I:142:LEU:HB3	1.95	0.49
1:M:130:PRO:HG3	1:M:142:LEU:HB3	1.95	0.49
1:G:116:SER:C	1:G:118:ALA:N	2.70	0.49
1:M:47:TRP:CG	2:N:100:VAL:HB	2.48	0.48
2:P:154:LYS:HB2	2:P:197:SER:HB2	1.94	0.48
1:G:168:LEU:HD13	1:G:192:VAL:HG21	1.95	0.48
1:M:87:THR:HG23	1:M:114:THR:HA	1.96	0.48
1:E:54:PHE:CE2	1:G:31:SER:O	2.66	0.48
1:M:37:VAL:CG2	1:M:104:MET:HE1	2.44	0.48
1:G:37:VAL:HG21	1:G:104:MET:HE1	1.94	0.48
1:C:94:LYS:HG2	1:C:106:VAL:HB	1.96	0.48
1:O:94:LYS:HG2	1:O:106:VAL:HB	1.94	0.48
1:I:130:PRO:O	1:I:134:SER:OG	2.31	0.48
1:A:94:LYS:HG2	1:A:106:VAL:HB	1.95	0.47
2:B:6:GLN:HB3	2:B:106:THR:HG22	1.95	0.47
1:G:47:TRP:CG	2:H:100:VAL:HB	2.48	0.47
1:E:94:LYS:HG2	1:E:106:VAL:HB	1.95	0.47
1:I:116:SER:C	1:I:118:ALA:N	2.70	0.47
2:J:20:ILE:HG23	2:J:106:THR:HG21	1.96	0.47
2:N:6:GLN:NE2	2:N:106:THR:HG23	2.29	0.47
2:B:189:GLN:O	2:B:192:SER:HB3	2.15	0.47
1:C:130:PRO:HG3	1:C:142:LEU:HB3	1.96	0.47
2:L:111:LEU:O	2:L:113:GLN:N	2.46	0.47
2:H:154:LYS:HB2	2:H:197:SER:HB2	1.96	0.47
2:D:96:LEU:HD23	2:D:96:LEU:HA	1.74	0.47
1:E:37:VAL:HG21	1:E:104:MET:HE1	1.97	0.47
1:M:154:VAL:HG12	1:M:188:LEU:HD21	1.95	0.47
2:L:118:PRO:HD3	2:L:202:HIS:ND1	2.30	0.47
2:N:56:PRO:HG2	2:N:59:ILE:HG13	1.97	0.47
2:N:79:LEU:CD1	2:N:110:VAL:HG13	2.44	0.47
2:D:20:ILE:HG23	2:D:106:THR:HG21	1.97	0.46
1:G:154:VAL:HG12	1:G:188:LEU:HD21	1.95	0.46
1:C:90:TYR:CD2	1:C:113:VAL:HG13	2.50	0.46
1:G:130:PRO:HG3	1:G:142:LEU:HB3	1.97	0.46
1:E:159:TRP:CH2	1:E:209:CYS:HB3	2.51	0.46
1:K:130:PRO:HG3	1:K:142:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:TRP:CG	2:F:100:VAL:HB	2.50	0.46
2:F:156:ASP:OD1	2:F:194:ARG:HB3	2.15	0.46
2:L:20:ILE:HG23	2:L:106:THR:HG21	1.97	0.46
1:M:138:GLY:O	1:M:195:PRO:HA	2.16	0.46
2:B:96:LEU:HD23	2:B:96:LEU:HA	1.78	0.46
1:C:6:GLU:H	1:C:6:GLU:HG2	1.58	0.46
2:P:96:LEU:HD23	2:P:96:LEU:HA	1.71	0.46
2:J:111:LEU:C	2:J:113:GLN:N	2.68	0.46
1:K:36:TRP:CE2	1:K:80:MET:HB2	2.50	0.46
1:K:47:TRP:CG	2:L:100:VAL:HB	2.51	0.46
2:N:20:ILE:HG23	2:N:106:THR:HG21	1.97	0.46
2:P:56:PRO:HG2	2:P:59:ILE:HG13	1.98	0.46
1:C:133:LYS:HE3	2:D:210:THR:O	2.16	0.46
2:D:6:GLN:HE21	2:D:106:THR:HG23	1.81	0.46
1:G:216:SER:OG	1:G:218:THR:HG23	2.16	0.46
2:L:118:PRO:HB3	2:L:144:PHE:HB3	1.96	0.46
1:M:168:LEU:HD13	1:M:192:VAL:HG21	1.97	0.46
2:N:6:GLN:HE21	2:N:106:THR:HG23	1.80	0.46
1:C:37:VAL:HG21	1:C:104:MET:HE1	1.98	0.45
2:F:20:ILE:HG23	2:F:106:THR:HG21	1.97	0.45
2:J:81:THR:HA	2:J:110:VAL:HG11	1.98	0.45
1:K:48:MET:HE2	1:K:48:MET:HB3	1.83	0.45
1:E:130:PRO:O	1:E:134:SER:HB3	2.16	0.45
1:E:154:VAL:HG12	1:E:188:LEU:HD21	1.98	0.45
2:F:111:LEU:HD22	2:F:112:GLY:N	2.31	0.45
1:A:36:TRP:NE1	1:A:80:MET:HB2	2.32	0.45
1:K:94:LYS:HG2	1:K:106:VAL:HB	1.98	0.45
1:A:37:VAL:HG21	1:A:104:MET:HE1	1.97	0.45
1:E:130:PRO:HG3	1:E:142:LEU:HB3	1.98	0.45
2:F:81:THR:HA	2:F:110:VAL:HG11	1.98	0.45
1:C:155:THR:HB	1:C:212:ASN:HB3	1.99	0.45
1:K:216:SER:OG	1:K:218:THR:HG23	2.17	0.45
2:L:12:ALA:C	2:L:111:LEU:HB2	2.42	0.45
1:O:48:MET:HE2	1:O:48:MET:HB3	1.82	0.45
1:O:168:LEU:HD13	1:O:192:VAL:HG21	1.98	0.45
1:K:198:SER:HB2	1:K:204:GLN:HB2	1.98	0.44
1:O:130:PRO:O	1:O:131:SER:OG	2.29	0.44
1:A:30:ARG:NH2	1:A:52(A):PRO:HA	2.31	0.44
1:A:130:PRO:HG3	1:A:142:LEU:HB3	1.99	0.44
2:L:81:THR:HA	2:L:110:VAL:HG11	1.99	0.44
2:N:154:LYS:HB2	2:N:197:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:SER:OG	1:I:218:THR:HG23	2.18	0.44
1:K:54:PHE:CE1	1:O:54:PHE:CE1	3.05	0.44
1:O:27:GLY:HA3	1:O:28:PRO:HA	1.85	0.44
1:E:130:PRO:O	1:E:131:SER:OG	2.31	0.44
1:G:159:TRP:CH2	1:G:209:CYS:HB3	2.53	0.44
1:E:155:THR:HB	1:E:212:ASN:HB3	2.00	0.44
2:J:118:PRO:HB3	2:J:144:PHE:HB3	1.99	0.44
2:J:154:LYS:HB2	2:J:197:SER:HB2	1.98	0.44
1:C:48:MET:HE2	1:C:48:MET:HB3	1.77	0.44
2:J:189:GLN:O	2:J:192:SER:HB3	2.18	0.44
1:E:48:MET:HE2	1:E:48:MET:HB3	1.79	0.44
1:G:27:GLY:HA3	1:G:28:PRO:HA	1.86	0.44
1:I:138:GLY:O	1:I:195:PRO:HA	2.18	0.44
2:N:118:PRO:HB3	2:N:144:PHE:HB3	1.99	0.44
2:D:6:GLN:NE2	2:D:106:THR:HG23	2.33	0.44
1:G:37:VAL:CG2	1:G:104:MET:HE1	2.48	0.44
1:G:87:THR:HG23	1:G:114:THR:HA	2.00	0.44
1:G:93:ALA:HB3	1:G:104:MET:HE2	1.99	0.44
1:E:27:GLY:HA3	1:E:28:PRO:HA	1.89	0.43
1:O:130:PRO:HG3	1:O:142:LEU:HB3	2.00	0.43
1:A:52:ILE:HG21	1:I:98:TYR:OH	2.18	0.43
2:B:154:LYS:HB2	2:B:197:SER:HB2	2.00	0.43
1:C:47:TRP:CG	2:D:100:VAL:HB	2.53	0.43
2:D:79:LEU:HD11	2:D:110:VAL:HG12	2.00	0.43
1:E:90:TYR:CD2	1:E:113:VAL:HG13	2.52	0.43
1:G:36:TRP:NE1	1:G:80:MET:HB2	2.32	0.43
1:K:27:GLY:HA3	1:K:28:PRO:HA	1.84	0.43
1:K:155:THR:HB	1:K:212:ASN:HB3	2.00	0.43
1:M:129:ALA:HA	1:M:130:PRO:HD3	1.92	0.43
1:M:216:SER:OG	1:M:218:THR:HG23	2.18	0.43
1:E:216:SER:OG	1:E:218:THR:HG23	2.19	0.43
2:D:56:PRO:HG2	2:D:59:ILE:HG13	2.01	0.43
1:G:6:GLU:H	1:G:6:GLU:HG2	1.66	0.43
1:C:168:LEU:HD13	1:C:192:VAL:HG21	2.01	0.43
1:I:47:TRP:CG	2:J:100:VAL:HB	2.54	0.43
1:I:6:GLU:H	1:I:6:GLU:HG2	1.63	0.43
2:J:6:GLN:NE2	2:J:106:THR:HG23	2.34	0.43
1:M:27:GLY:HA3	1:M:28:PRO:HA	1.87	0.43
1:A:155:THR:HB	1:A:212:ASN:HB3	2.01	0.42
1:C:216:SER:OG	1:C:218:THR:HG23	2.19	0.42
1:G:130:PRO:HB2	1:G:131:SER:H	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:198:SER:HB2	1:O:204:GLN:HB2	2.01	0.42
1:A:27:GLY:HA3	1:A:28:PRO:HA	1.87	0.42
2:J:61:ASP:OD1	2:J:61:ASP:N	2.48	0.42
1:I:36:TRP:NE1	1:I:80:MET:HB2	2.34	0.42
1:K:90:TYR:CD2	1:K:113:VAL:HG13	2.54	0.42
2:N:96:LEU:HD23	2:N:96:LEU:HA	1.74	0.42
1:O:6:GLU:H	1:O:6:GLU:HG2	1.52	0.42
1:A:181:GLN:HE21	1:A:181:GLN:HB2	1.70	0.42
1:G:181:GLN:HE21	1:G:181:GLN:HB2	1.63	0.42
2:J:39:GLN:O	2:J:85:ALA:HB1	2.19	0.42
2:J:96:LEU:HA	2:J:96:LEU:HD23	1.80	0.42
1:K:181:GLN:HE21	1:K:181:GLN:HB2	1.60	0.42
2:L:61:ASP:OD1	2:L:61:ASP:N	2.46	0.42
1:O:155:THR:HB	1:O:212:ASN:HB3	2.00	0.42
2:B:156:ASP:OD1	2:B:194:ARG:HB3	2.20	0.42
1:C:87:THR:HG23	1:C:114:THR:HA	2.02	0.42
2:F:36:TRP:CZ3	2:F:89:CYS:HB3	2.54	0.42
1:I:37:VAL:CG2	1:I:104:MET:HE1	2.49	0.42
1:K:154:VAL:HG12	1:K:188:LEU:HD21	2.00	0.42
2:D:36:TRP:CZ3	2:D:89:CYS:HB3	2.55	0.42
1:E:159:TRP:CZ3	1:E:209:CYS:HB3	2.55	0.42
1:I:93:ALA:HB3	1:I:104:MET:HE2	2.02	0.42
2:D:111:LEU:HD23	2:D:111:LEU:HA	1.86	0.42
1:E:17:SER:HB2	1:O:16:SER:HB2	2.01	0.42
1:E:52:ILE:CG2	1:E:52(A):PRO:HD2	2.49	0.42
1:K:129:ALA:HA	1:K:130:PRO:HD3	1.94	0.42
2:F:96:LEU:HD23	2:F:96:LEU:HA	1.85	0.41
1:E:30:ARG:NH2	1:E:52(A):PRO:HA	2.35	0.41
1:G:129:ALA:HA	1:G:130:PRO:HD3	1.95	0.41
1:A:168:LEU:HD13	1:A:192:VAL:HG21	2.02	0.41
1:I:181:GLN:HE21	1:I:181:GLN:HB2	1.61	0.41
1:K:6:GLU:H	1:K:6:GLU:HG2	1.59	0.41
2:L:96:LEU:HD23	2:L:96:LEU:HA	1.77	0.41
1:O:154:VAL:HG12	1:O:188:LEU:HD21	2.03	0.41
1:E:37:VAL:CG2	1:E:104:MET:HE1	2.50	0.41
1:G:191:VAL:HG21	2:H:140:LEU:HD13	2.01	0.41
1:K:121:LYS:HG2	1:K:122:GLY:O	2.21	0.41
1:M:48:MET:HE2	1:M:48:MET:HB3	1.92	0.41
2:N:156:ASP:OD1	2:N:194:ARG:HB3	2.20	0.41
1:O:216:SER:OG	1:O:218:THR:HG23	2.20	0.41
1:C:63:PHE:O	1:C:67:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:125:PRO:HD3	2:N:137:LEU:HD12	2.02	0.41
1:O:63:PHE:O	1:O:67:VAL:HG12	2.20	0.41
1:O:159:TRP:CH2	1:O:209:CYS:HB3	2.56	0.41
1:C:27:GLY:HA3	1:C:28:PRO:HA	1.85	0.41
1:E:168:LEU:HD13	1:E:192:VAL:HG21	2.02	0.41
1:I:154:VAL:HG12	1:I:188:LEU:HD21	2.01	0.41
1:K:29:PHE:HD1	1:K:73:ASP:HB3	1.84	0.41
1:K:52(A):PRO:C	1:K:53:ILE:HG12	2.46	0.41
2:P:118:PRO:HD3	2:P:202:HIS:ND1	2.36	0.41
1:A:29:PHE:HD1	1:A:73:ASP:HB3	1.86	0.41
1:C:154:VAL:HG12	1:C:188:LEU:HD21	2.03	0.41
2:H:118:PRO:HD3	2:H:202:HIS:ND1	2.36	0.41
1:M:6:GLU:H	1:M:6:GLU:HG2	1.62	0.41
1:A:20:VAL:HG12	1:A:36:TRP:CH2	2.57	0.40
1:C:36:TRP:NE1	1:C:80:MET:HB2	2.36	0.40
1:C:159:TRP:CH2	1:C:209:CYS:HB3	2.56	0.40
1:E:6:GLU:H	1:E:6:GLU:HG2	1.55	0.40
1:M:18:VAL:HG12	1:M:82(C):LEU:HD11	2.02	0.40
1:A:47:TRP:CG	2:B:100:VAL:HB	2.57	0.40
1:A:90:TYR:CD2	1:A:113:VAL:HG13	2.57	0.40
1:C:29:PHE:HD1	1:C:73:ASP:HB3	1.86	0.40
2:H:96:LEU:HD23	2:H:96:LEU:HA	1.82	0.40
2:N:61:ASP:OD1	2:N:61:ASP:N	2.48	0.40
1:A:6:GLU:H	1:A:6:GLU:HG2	1.53	0.40
1:C:198:SER:HB2	1:C:204:GLN:HB2	2.03	0.40
1:I:191:VAL:HG21	2:J:140:LEU:HD13	2.02	0.40
1:K:36:TRP:NE1	1:K:80:MET:HB2	2.36	0.40
1:K:191:VAL:HG21	2:L:140:LEU:HD13	2.03	0.40
1:M:29:PHE:HD1	1:M:73:ASP:HB3	1.86	0.40
2:D:91:THR:OG1	2:D:92:TRP:N	2.54	0.40
2:P:156:ASP:OD1	2:P:194:ARG:HB3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:PRO:O	2:P:16:GLN:NE2[2_555]	2.08	0.12

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	219/242 (90%)	211 (96%)	6 (3%)	2 (1%)	14	28
1	C	219/242 (90%)	210 (96%)	6 (3%)	3 (1%)	9	19
1	E	219/242 (90%)	207 (94%)	9 (4%)	3 (1%)	9	19
1	G	219/242 (90%)	207 (94%)	10 (5%)	2 (1%)	14	28
1	I	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	9	19
1	K	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	9	19
1	M	219/242 (90%)	209 (95%)	8 (4%)	2 (1%)	14	28
1	O	219/242 (90%)	208 (95%)	7 (3%)	4 (2%)	6	15
2	B	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	6	14
2	D	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	9	19
2	F	211/217 (97%)	201 (95%)	7 (3%)	3 (1%)	9	19
2	H	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	6	14
2	J	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	6	14
2	L	211/217 (97%)	199 (94%)	7 (3%)	5 (2%)	4	10
2	N	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	6	14
2	P	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	9	19
All	All	3440/3672 (94%)	3272 (95%)	116 (3%)	52 (2%)	8	18

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	130	PRO
2	J	111	LEU
2	L	111	LEU
2	N	111	LEU
2	B	214	THR
1	C	137	GLY

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Mol	Chain	Res	Type
2	D	214	THR
1	E	137	GLY
2	F	214	THR
1	G	53	ILE
2	H	111	LEU
2	H	214	THR
1	I	130	PRO
2	J	214	THR
1	K	130	PRO
2	L	214	THR
2	N	214	THR
1	O	131	SER
2	P	214	THR
1	A	53	ILE
2	B	112	GLY
2	B	156	ASP
2	B	213	PRO
1	C	130	PRO
2	D	213	PRO
1	E	53	ILE
2	F	156	ASP
2	F	213	PRO
2	H	213	PRO
1	I	53	ILE
2	J	156	ASP
2	J	213	PRO
1	K	53	ILE
2	L	112	GLY
2	L	156	ASP
2	L	213	PRO
1	M	53	ILE
2	N	156	ASP
2	N	213	PRO
1	O	53	ILE
1	O	130	PRO
2	P	213	PRO
1	C	53	ILE
2	D	156	ASP
2	H	156	ASP
1	M	130	PRO
2	P	156	ASP
1	A	130	PRO

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Mol	Chain	Res	Type
1	I	199	LEU
1	O	137	GLY
1	E	130	PRO
1	K	137	GLY

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	178/202 (88%)	164 (92%)	14 (8%)	11	24
1	C	178/202 (88%)	165 (93%)	13 (7%)	13	27
1	E	179/202 (89%)	165 (92%)	14 (8%)	11	25
1	G	178/202 (88%)	166 (93%)	12 (7%)	15	31
1	I	179/202 (89%)	165 (92%)	14 (8%)	11	25
1	K	178/202 (88%)	167 (94%)	11 (6%)	16	34
1	M	178/202 (88%)	164 (92%)	14 (8%)	11	24
1	O	178/202 (88%)	166 (93%)	12 (7%)	15	31
2	B	164/182 (90%)	153 (93%)	11 (7%)	15	31
2	D	163/182 (90%)	152 (93%)	11 (7%)	15	31
2	F	163/182 (90%)	151 (93%)	12 (7%)	13	26
2	H	163/182 (90%)	150 (92%)	13 (8%)	11	24
2	J	163/182 (90%)	153 (94%)	10 (6%)	17	35
2	L	164/182 (90%)	151 (92%)	13 (8%)	11	24
2	N	163/182 (90%)	151 (93%)	12 (7%)	13	26
2	P	164/182 (90%)	152 (93%)	12 (7%)	13	27
All	All	2733/3072 (89%)	2535 (93%)	198 (7%)	13	28

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLU
1	A	23	LYS
1	A	53	ILE
1	A	84	SER
1	A	113	VAL
1	A	117	SER
1	A	120	THR
1	A	133	LYS
1	A	134	SER
1	A	154	VAL
1	A	188	LEU
1	A	206	THR
1	A	218	THR
2	B	4	LEU
2	B	70	THR
2	B	79	LEU
2	B	106	THR
2	B	111	LEU
2	B	119	THR
2	B	128	GLU
2	B	142	SER
2	B	173	SER
2	B	180	SER
2	B	206	THR
1	C	3	GLN
1	C	6	GLU
1	C	23	LYS
1	C	53	ILE
1	C	84	SER
1	C	113	VAL
1	C	117	SER
1	C	120	THR
1	C	133	LYS
1	C	136	SER
1	C	154	VAL
1	C	206	THR
1	C	218	THR
2	D	4	LEU
2	D	10	VAL
2	D	70	THR
2	D	79	LEU
2	D	106	THR

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Mol	Chain	Res	Type
2	D	119	THR
2	D	128	GLU
2	D	142	SER
2	D	173	SER
2	D	180	SER
2	D	206	THR
1	E	3	GLN
1	E	6	GLU
1	E	23	LYS
1	E	53	ILE
1	E	83	ARG
1	E	84	SER
1	E	113	VAL
1	E	117	SER
1	E	120	THR
1	E	134	SER
1	E	154	VAL
1	E	188	LEU
1	E	206	THR
1	E	218	THR
2	F	4	LEU
2	F	70	THR
2	F	79	LEU
2	F	106	THR
2	F	110	VAL
2	F	111	LEU
2	F	119	THR
2	F	128	GLU
2	F	142	SER
2	F	173	SER
2	F	180	SER
2	F	206	THR
1	G	3	GLN
1	G	6	GLU
1	G	23	LYS
1	G	53	ILE
1	G	84	SER
1	G	113	VAL
1	G	117	SER
1	G	120	THR
1	G	154	VAL
1	G	188	LEU

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Mol	Chain	Res	Type
1	G	206	THR
1	G	218	THR
2	H	4	LEU
2	H	10	VAL
2	H	70	THR
2	H	79	LEU
2	H	106	THR
2	H	110	VAL
2	H	111	LEU
2	H	119	THR
2	H	128	GLU
2	H	142	SER
2	H	173	SER
2	H	180	SER
2	H	206	THR
1	I	3	GLN
1	I	6	GLU
1	I	23	LYS
1	I	53	ILE
1	I	84	SER
1	I	113	VAL
1	I	117	SER
1	I	120	THR
1	I	133	LYS
1	I	136	SER
1	I	154	VAL
1	I	188	LEU
1	I	206	THR
1	I	218	THR
2	J	4	LEU
2	J	70	THR
2	J	79	LEU
2	J	106	THR
2	J	119	THR
2	J	128	GLU
2	J	142	SER
2	J	173	SER
2	J	180	SER
2	J	206	THR
1	K	3	GLN
1	K	6	GLU
1	K	23	LYS

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Mol	Chain	Res	Type
1	K	53	ILE
1	K	84	SER
1	K	113	VAL
1	K	117	SER
1	K	120	THR
1	K	154	VAL
1	K	188	LEU
1	K	206	THR
2	L	4	LEU
2	L	10	VAL
2	L	70	THR
2	L	79	LEU
2	L	106	THR
2	L	110	VAL
2	L	111	LEU
2	L	119	THR
2	L	128	GLU
2	L	142	SER
2	L	173	SER
2	L	180	SER
2	L	206	THR
1	M	3	GLN
1	M	6	GLU
1	M	23	LYS
1	M	53	ILE
1	M	84	SER
1	M	113	VAL
1	M	117	SER
1	M	120	THR
1	M	133	LYS
1	M	135	THR
1	M	154	VAL
1	M	188	LEU
1	M	206	THR
1	M	218	THR
2	N	4	LEU
2	N	10	VAL
2	N	70	THR
2	N	79	LEU
2	N	106	THR
2	N	110	VAL
2	N	119	THR

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Mol	Chain	Res	Type
2	N	128	GLU
2	N	142	SER
2	N	173	SER
2	N	180	SER
2	N	206	THR
1	O	3	GLN
1	O	6	GLU
1	O	23	LYS
1	O	53	ILE
1	O	84	SER
1	O	113	VAL
1	O	117	SER
1	O	120	THR
1	O	133	LYS
1	O	154	VAL
1	O	188	LEU
1	O	206	THR
2	P	4	LEU
2	P	10	VAL
2	P	70	THR
2	P	106	THR
2	P	110	VAL
2	P	119	THR
2	P	128	GLU
2	P	142	SER
2	P	173	SER
2	P	180	SER
2	P	206	THR
2	P	210	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	99	GLN
2	B	193	HIS
1	C	43	GLN
1	C	99	GLN
2	D	32	ASN
1	E	43	GLN
1	E	99	GLN
1	E	217	ASN

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Mol	Chain	Res	Type
2	F	32	ASN
2	F	38	GLN
2	H	32	ASN
2	H	38	GLN
1	I	43	GLN
2	J	32	ASN
1	K	43	GLN
2	L	32	ASN
2	L	38	GLN
1	M	43	GLN
1	M	99	GLN
1	O	43	GLN
2	P	32	ASN

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	221/242 (91%)	0.34	12 (5%) 31 23	35, 65, 111, 200	0
1	C	221/242 (91%)	0.30	15 (6%) 23 17	32, 60, 132, 231	0
1	E	221/242 (91%)	0.50	21 (9%) 14 11	24, 57, 123, 199	0
1	G	221/242 (91%)	0.63	22 (9%) 12 10	52, 75, 130, 200	0
1	I	221/242 (91%)	0.37	11 (4%) 34 27	38, 72, 122, 200	0
1	K	221/242 (91%)	0.55	17 (7%) 19 14	31, 64, 111, 198	0
1	M	221/242 (91%)	0.44	9 (4%) 41 32	48, 76, 133, 200	0
1	O	221/242 (91%)	0.53	22 (9%) 12 10	28, 68, 146, 199	0
2	B	213/217 (98%)	0.45	12 (5%) 30 22	38, 75, 107, 163	0
2	D	213/217 (98%)	0.35	11 (5%) 33 25	30, 64, 104, 165	0
2	F	213/217 (98%)	0.36	10 (4%) 36 28	31, 65, 105, 162	0
2	H	213/217 (98%)	0.93	23 (10%) 11 8	55, 92, 141, 207	0
2	J	213/217 (98%)	0.52	10 (4%) 36 28	42, 76, 114, 161	0
2	L	213/217 (98%)	0.38	7 (3%) 49 40	34, 71, 118, 163	0
2	N	213/217 (98%)	0.34	5 (2%) 61 52	40, 77, 113, 183	0
2	P	213/217 (98%)	0.52	12 (5%) 30 22	32, 73, 114, 164	0
All	All	3472/3672 (94%)	0.47	219 (6%) 26 19	24, 72, 123, 231	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	29	PHE	5.4
2	J	173	SER	5.1
1	C	29	PHE	5.0
1	K	28	PRO	4.9
1	O	29	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	K	182	SER	4.8
1	G	28	PRO	4.4
2	P	3	VAL	4.3
1	A	28	PRO	4.1
2	B	155	ALA	4.1
2	J	214	THR	4.1
1	E	28	PRO	4.1
1	K	180	LEU	4.0
1	O	74	PHE	3.9
2	D	159	PRO	3.8
1	K	74	PHE	3.8
2	D	3	VAL	3.7
2	H	214	THR	3.7
1	C	28	PRO	3.6
2	B	194	ARG	3.5
1	E	27	GLY	3.5
1	O	28	PRO	3.5
1	K	101	ARG	3.5
1	E	184	GLY	3.5
1	O	173	VAL	3.5
2	H	3	VAL	3.4
1	E	52(A)	PRO	3.4
1	K	27	GLY	3.4
1	E	101	ARG	3.4
1	C	134	SER	3.4
1	G	31	SER	3.4
1	M	74	PHE	3.3
1	G	182	SER	3.3
1	M	28	PRO	3.2
1	O	1	GLN	3.2
1	I	28	PRO	3.2
1	M	133	LYS	3.2
1	I	55	GLY	3.2
1	G	98	TYR	3.2
2	D	13	ALA	3.2
1	C	74	PHE	3.1
2	H	173	SER	3.1
1	A	29	PHE	3.1
1	E	217	ASN	3.1
1	E	182	SER	3.1
1	A	54	PHE	3.0
1	O	101	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	194	VAL	3.0
2	D	153	TRP	3.0
1	A	26	GLY	3.0
2	J	113	GLN	3.0
1	G	27	GLY	3.0
2	F	214	THR	3.0
1	E	29	PHE	3.0
2	B	3	VAL	3.0
1	I	133	LYS	2.9
1	G	184	GLY	2.9
1	E	30	ARG	2.9
1	O	31	SER	2.9
2	P	153	TRP	2.9
1	I	176	PHE	2.9
2	B	214	THR	2.9
2	N	3	VAL	2.8
1	O	217	ASN	2.8
2	F	139	CYS	2.8
1	I	177	PRO	2.8
2	H	113	GLN	2.8
1	I	27	GLY	2.8
1	K	1	GLN	2.8
2	B	92	TRP	2.8
2	D	196	TYR	2.7
1	E	26	GLY	2.7
1	K	184	GLY	2.7
1	A	30	ARG	2.7
1	C	184	GLY	2.7
2	H	114	PRO	2.7
2	F	44	ALA	2.7
2	H	111	LEU	2.7
2	F	99	TYR	2.7
1	I	182	SER	2.7
2	D	214	THR	2.6
1	C	199	LEU	2.6
1	G	29	PHE	2.6
1	C	101	ARG	2.6
1	G	30	ARG	2.6
1	K	44	GLY	2.6
1	O	201	THR	2.6
1	O	135	THR	2.6
1	O	169	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	1	GLN	2.6
1	K	26	GLY	2.6
1	G	74	PHE	2.6
1	M	29	PHE	2.6
2	L	205	SER	2.5
2	H	107	LYS	2.5
1	M	135	THR	2.5
1	M	101	ARG	2.5
2	B	173	SER	2.5
2	D	158	SER	2.5
2	H	96	LEU	2.5
1	O	193	THR	2.5
2	F	194	ARG	2.5
1	M	228	PRO	2.5
2	D	137	LEU	2.5
2	H	30	GLY	2.5
1	C	135	THR	2.5
1	E	183	SER	2.5
1	O	182	SER	2.5
2	B	90	GLY	2.5
2	L	3	VAL	2.5
2	J	128	GLU	2.5
1	E	53	ILE	2.4
2	P	187	PRO	2.4
2	H	13	ALA	2.4
2	N	113	GLN	2.4
2	H	117	ASN	2.4
1	G	177	PRO	2.4
1	G	55	GLY	2.4
2	F	3	VAL	2.4
2	P	195	SER	2.4
1	A	74	PHE	2.4
1	E	74	PHE	2.4
1	O	212	ASN	2.4
1	E	54	PHE	2.4
1	G	165	SER	2.4
2	F	57	SER	2.4
1	G	1	GLN	2.4
2	L	171	LYS	2.4
1	A	1	GLN	2.4
1	G	181	GLN	2.4
2	F	173	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	33	TYR	2.4
2	H	50	TYR	2.4
1	O	27	GLY	2.3
1	O	227	GLU	2.3
2	H	25	SER	2.3
2	P	97	SER	2.3
1	M	112	THR	2.3
1	K	30	ARG	2.3
1	O	30	ARG	2.3
1	K	25	SER	2.3
1	K	196	SER	2.3
1	M	182	SER	2.3
2	P	99	TYR	2.3
1	G	192	VAL	2.3
2	P	13	ALA	2.3
1	I	174	HIS	2.3
1	E	156	VAL	2.3
1	C	26	GLY	2.3
1	G	42	GLY	2.3
1	O	184	GLY	2.3
2	D	16	GLN	2.3
1	E	120	THR	2.3
1	K	187	SER	2.3
2	N	68	SER	2.3
1	I	173	VAL	2.3
2	P	160	VAL	2.3
1	C	167	ALA	2.2
1	G	227	GLU	2.2
2	B	162	ALA	2.2
2	B	175	ASN	2.2
1	C	3	GLN	2.2
1	C	109	LYS	2.2
1	O	228	PRO	2.2
2	J	114	PRO	2.2
1	E	227	GLU	2.2
2	H	109	THR	2.2
1	A	182	SER	2.2
1	A	104	MET	2.2
1	C	1	GLN	2.2
1	C	30	ARG	2.2
1	A	201	THR	2.2
1	C	27	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	21	SER	2.2
1	G	183	SER	2.2
1	I	26	GLY	2.2
2	H	215	GLU	2.2
1	G	52	ILE	2.2
1	E	181	GLN	2.2
1	A	107	TRP	2.2
2	L	147	GLY	2.2
2	H	11	SER	2.2
2	J	162	ALA	2.2
1	I	228	PRO	2.1
2	B	156	ASP	2.1
1	E	25	SER	2.1
1	O	170	SER	2.1
2	B	170	SER	2.1
2	P	89	CYS	2.1
2	N	44	ALA	2.1
2	N	152	ALA	2.1
2	P	181	SER	2.1
2	H	56	PRO	2.1
2	J	156	ASP	2.1
1	G	26	GLY	2.1
1	G	79	TYR	2.1
2	J	194	ARG	2.1
2	F	192	SER	2.1
2	L	199	GLN	2.1
2	F	92	TRP	2.1
2	P	190	TRP	2.1
2	D	44	ALA	2.1
1	E	31	SER	2.1
2	H	23	SER	2.1
2	J	3	VAL	2.1
1	A	52(A)	PRO	2.1
1	O	54	PHE	2.1
2	D	156	ASP	2.1
2	H	194	ARG	2.1
2	P	214	THR	2.1
2	B	99	TYR	2.1
2	L	173	SER	2.0
2	H	148	ALA	2.0
2	J	178	ALA	2.0
1	K	186	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	149	VAL	2.0
2	L	113	GLN	2.0
1	K	168	LEU	2.0
2	H	204	GLY	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.