



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:14 AM UTC

PDB ID : 9WRN / pdb_00009wrn
Title : Crystal structure of chimeric anti-Z-DNA Fab cZ22-Fab
Authors : Lee, C.C.; Hsu, S.F.; Wang, A.H.J.
Deposited on : 2025-09-12
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

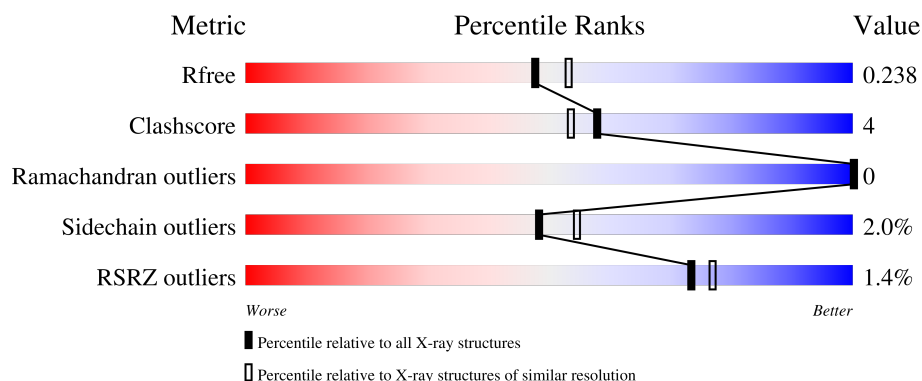
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	H	236	
1	I	236	
1	J	236	
1	K	236	
2	L	214	

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Mol	Chain	Length	Quality of chain
2	M	214	<div><div></div><div>89%</div><div>9% ..</div></div>
2	N	214	<div>%<div><div></div><div>86%</div><div>13%</div></div></div>
2	O	214	<div><div></div><div>92%</div><div>7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14204 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 cZ22-Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	217	Total	C	N	O	S	0	0	0
			1648	1041	276	321	10			
1	I	215	Total	C	N	O	S	0	0	0
			1628	1028	272	318	10			
1	J	213	Total	C	N	O	S	0	0	0
			1623	1027	271	315	10			
1	K	214	Total	C	N	O	S	0	0	0
			1627	1029	272	316	10			

- Molecule 2 is a protein called cZ22-Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1643	1029	273	336	5			
2	M	212	Total	C	N	O	S	0	0	0
			1643	1029	273	336	5			
2	N	213	Total	C	N	O	S	0	0	0
			1652	1034	274	339	5			
2	O	214	Total	C	N	O	S	0	0	0
			1659	1037	275	341	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	123	Total	O	0	0
			123	123		
3	I	133	Total	O	0	0
			133	133		
3	J	103	Total	O	0	0
			103	103		
3	K	142	Total	O	0	0
			142	142		

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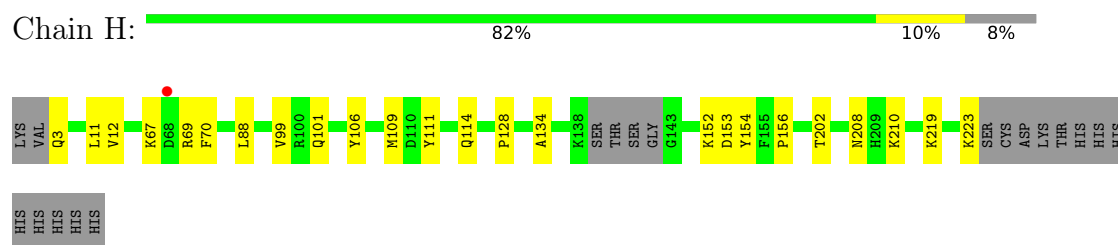
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	151	Total 151	O 151	0	0
3	M	174	Total 174	O 174	0	0
3	N	66	Total 66	O 66	0	0
3	O	189	Total 189	O 189	0	0

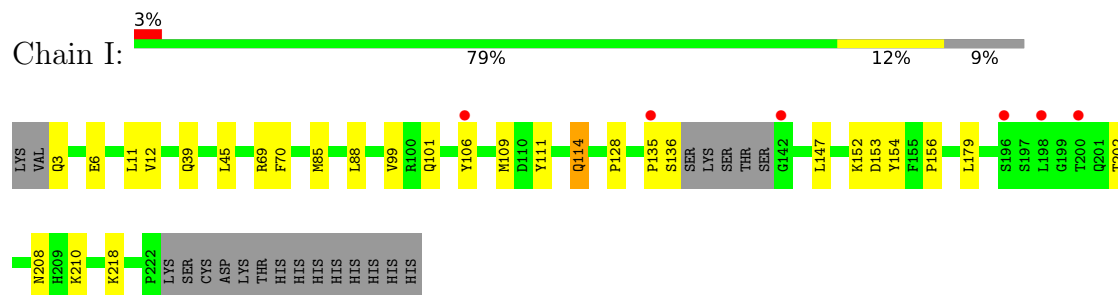
3 Residue-property plots [i](#)

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.

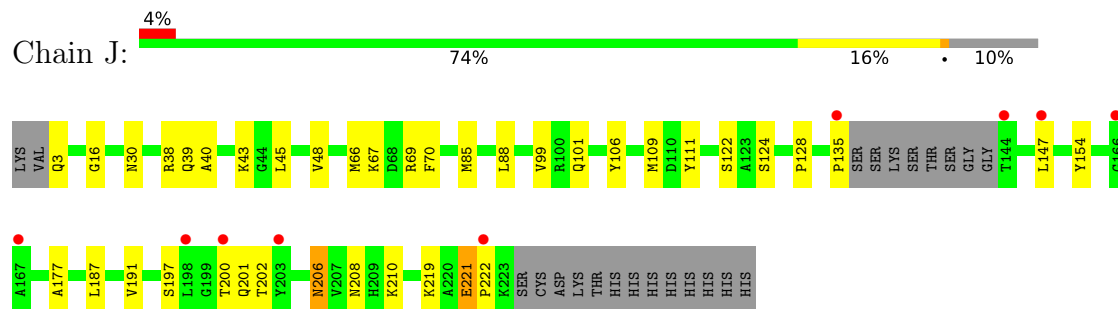
- Molecule 1: cZ22-Fab heavy chain



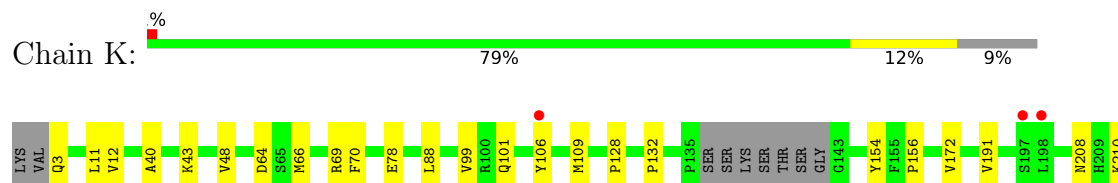
- Molecule 1: cZ22-Fab heavy chain

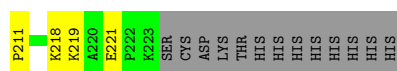


- Molecule 1: cZ22-Fab heavy chain

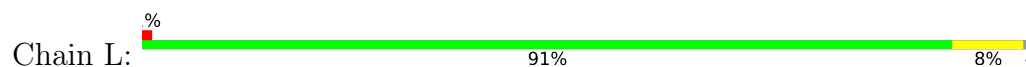


- Molecule 1: cZ22-Fab heavy chain





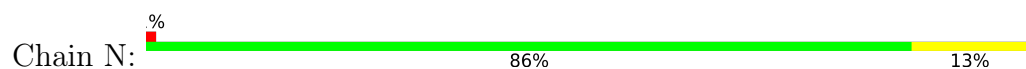
- Molecule 2: cZ22-Fab light chain



- Molecule 2: cZ22-Fab light chain



- Molecule 2: cZ22-Fab light chain



- Molecule 2: cZ22-Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.02Å 87.03Å 149.40Å 90.00° 95.47° 90.00°	Depositor
Resolution (Å)	18.02 – 2.15 18.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (18.02-2.15) 98.0 (18.02-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.15Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.192 , 0.238 0.192 , 0.238	Depositor DCC
R_{free} test set	5051 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14204	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6250e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	H	0.20	0/1679	0.44	0/2281
1	I	0.20	0/1659	0.44	0/2256
1	J	0.19	0/1654	0.43	0/2249
1	K	0.20	0/1658	0.44	0/2254
2	L	0.19	0/1678	0.43	0/2277
2	M	0.19	0/1678	0.43	0/2277
2	N	0.20	0/1687	0.42	0/2289
2	O	0.20	0/1694	0.44	0/2297
All	All	0.20	0/13387	0.43	0/18180

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	H	1648	0	1609	12	0
1	I	1628	0	1581	14	0
1	J	1623	0	1583	26	0
1	K	1627	0	1586	14	0
2	L	1643	0	1591	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1643	0	1591	12	0
2	N	1652	0	1597	16	0
2	O	1659	0	1602	12	0
3	H	123	0	0	2	0
3	I	133	0	0	0	0
3	J	103	0	0	2	0
3	K	142	0	0	2	0
3	L	151	0	0	3	0
3	M	174	0	0	3	0
3	N	66	0	0	0	0
3	O	189	0	0	4	0
All	All	14204	0	12740	116	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 4.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:ALA:HB3	1:K:43:LYS:HD2	1.60	0.83
1:I:208:ASN:HD21	1:I:210:LYS:HE3	1.45	0.79
1:J:48:VAL:HG22	1:J:66:MET:HE1	1.66	0.77
1:K:48:VAL:HG22	1:K:66:MET:HE1	1.70	0.74
2:N:142:ARG:NH2	2:N:163:VAL:HG11	2.02	0.72
1:J:201:GLN:NE2	3:J:303:HOH:O	2.24	0.71
2:N:2:ILE:HD11	2:N:93:LYS:HD3	1.75	0.69
2:N:145:LYS:HE2	2:N:197:THR:HB	1.74	0.68
2:N:4:MET:HE3	2:N:90:GLN:HG2	1.77	0.66
2:N:120:PRO:HD3	2:N:132:VAL:HG22	1.77	0.66
1:H:128:PRO:HB3	1:H:154:TYR:HB3	1.79	0.65
2:M:132:VAL:HG13	2:M:179:LEU:HB3	1.80	0.63
1:J:101:GLN:NE2	1:J:106:TYR:O	2.31	0.62
2:O:187:GLU:OE1	3:O:301:HOH:O	2.16	0.61
1:K:128:PRO:HB3	1:K:154:TYR:HB3	1.82	0.61
1:K:172:VAL:HG22	1:K:191:VAL:HG22	1.82	0.60
1:H:152:LYS:NZ	1:H:153:ASP:OD2	2.34	0.60
1:J:135:PRO:HD3	1:J:147:LEU:HD21	1.83	0.60
1:J:39:GLN:HB2	1:J:45:LEU:HD23	1.82	0.60
2:L:61:ARG:HH12	2:L:82:ASP:CG	2.09	0.59
2:O:185:ASP:HA	2:O:188:LYS:HD2	1.84	0.59
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:128:PRO:HB3	1:J:154:TYR:HB3	1.84	0.59
2:O:149:LYS:HG2	2:O:154:LEU:HD23	1.85	0.58
1:I:208:ASN:ND2	1:I:210:LYS:HE3	2.16	0.58
1:J:85:MET:HE2	1:J:88:LEU:HD11	1.85	0.58
1:J:202:THR:HG23	1:J:219:LYS:HE3	1.84	0.58
2:M:15:LEU:HD11	2:M:80:PRO:HD3	1.86	0.57
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.86	0.57
1:J:70:PHE:CZ	1:J:85:MET:HE3	2.40	0.56
1:I:101:GLN:NE2	1:I:106:TYR:O	2.39	0.56
1:I:39:GLN:HB2	1:I:45:LEU:HD23	1.87	0.56
2:O:142:ARG:NH1	3:O:306:HOH:O	2.34	0.55
1:I:12:VAL:HG11	1:I:88:LEU:HD13	1.88	0.55
1:K:101:GLN:NE2	1:K:106:TYR:O	2.40	0.55
2:O:132:VAL:HG13	2:O:179:LEU:HB3	1.88	0.55
1:K:219:LYS:HZ1	1:K:221:GLU:CD	2.16	0.54
1:J:221:GLU:HG2	1:J:222:PRO:HD2	1.90	0.54
1:H:134:ALA:O	3:H:301:HOH:O	2.19	0.53
2:O:56:SER:O	3:O:302:HOH:O	2.19	0.53
1:H:202:THR:HG23	1:H:219:LYS:HE3	1.90	0.53
1:J:208:ASN:HD21	1:J:210:LYS:HE3	1.73	0.53
2:L:210:ASN:ND2	3:L:307:HOH:O	2.40	0.53
2:N:33:LEU:HD21	2:N:88:CYS:HB2	1.91	0.53
2:N:145:LYS:HE2	2:N:197:THR:CB	2.39	0.52
2:L:125:LEU:O	2:L:183:LYS:HE2	2.09	0.52
1:K:12:VAL:HG11	1:K:88:LEU:HD13	1.91	0.52
1:H:12:VAL:HG11	1:H:88:LEU:HD13	1.90	0.52
1:I:85:MET:HE3	1:I:88:LEU:HD21	1.92	0.51
2:O:1:ASP:OD2	3:O:303:HOH:O	2.19	0.51
2:M:129:THR:HG23	3:M:449:HOH:O	2.10	0.50
1:J:135:PRO:CD	1:J:147:LEU:HD21	2.40	0.50
1:J:197:SER:HB2	1:J:201:GLN:HB3	1.93	0.50
1:J:40:ALA:HB3	1:J:43:LYS:HD3	1.93	0.50
1:H:208:ASN:ND2	1:H:210:LYS:HE3	2.27	0.49
1:H:11:LEU:HD22	1:H:156:PRO:HG3	1.94	0.49
2:O:149:LYS:HE2	2:O:154:LEU:HD21	1.95	0.49
1:H:101:GLN:NE2	1:H:106:TYR:O	2.46	0.49
1:J:16:GLY:O	1:J:88:LEU:HD23	2.13	0.48
1:J:30:ASN:ND2	3:J:308:HOH:O	2.45	0.48
1:H:67:LYS:O	3:H:302:HOH:O	2.20	0.48
2:L:18:ARG:NH1	3:L:308:HOH:O	2.44	0.48
2:M:33:LEU:HD21	2:M:88:CYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:17:ASP:OD2	3:M:301:HOH:O	2.20	0.46
2:N:36:TYR:HB2	2:N:87:PHE:CZ	2.50	0.46
2:N:183:LYS:NZ	2:N:187:GLU:OE2	2.33	0.46
1:H:223:LYS:HA	1:H:223:LYS:HD2	1.78	0.46
2:M:207:LYS:HD3	2:M:207:LYS:HA	1.76	0.46
2:M:4:MET:HE3	2:M:23:CYS:SG	2.54	0.46
1:K:69:ARG:C	1:K:70:PHE:HD1	2.24	0.46
2:L:184:ALA:O	2:L:188:LYS:HG3	2.16	0.45
2:N:142:ARG:CZ	2:N:163:VAL:HG11	2.46	0.45
1:J:99:VAL:CG1	1:J:109:MET:HB3	2.46	0.45
1:J:67:LYS:HB3	1:J:67:LYS:HE3	1.70	0.45
1:I:135:PRO:HD3	1:I:147:LEU:HB3	1.98	0.45
1:J:135:PRO:HG3	1:J:222:PRO:HG3	1.99	0.45
1:H:99:VAL:CG1	1:H:109:MET:HB3	2.48	0.44
1:J:147:LEU:HD23	1:J:147:LEU:HA	1.57	0.44
2:N:113:PRO:HB3	2:N:139:PHE:HB3	1.99	0.44
2:N:207:LYS:HD3	2:N:207:LYS:HA	1.82	0.44
1:H:69:ARG:C	1:H:70:PHE:HD1	2.26	0.44
1:I:69:ARG:C	1:I:70:PHE:HD1	2.26	0.43
1:K:99:VAL:CG1	1:K:109:MET:HB3	2.48	0.43
2:L:103:LYS:NZ	2:L:165:GLU:OE2	2.46	0.43
1:J:69:ARG:C	1:J:70:PHE:HD1	2.26	0.43
2:M:159:SER:HA	2:M:178:THR:O	2.18	0.43
1:I:6:GLU:OE1	1:I:114:GLN:HG3	2.19	0.43
1:I:128:PRO:HB3	1:I:154:TYR:HB3	2.00	0.43
1:J:221:GLU:HG2	1:J:222:PRO:CD	2.48	0.43
2:O:193:ALA:HB2	2:O:208:SER:HB3	2.00	0.43
2:N:79:GLU:HG3	2:N:80:PRO:HD2	2.01	0.43
2:M:83:ILE:HG13	2:M:106:ILE:HG13	1.99	0.43
1:K:11:LEU:HD11	1:K:156:PRO:HG3	2.01	0.42
1:J:206:ASN:OD1	1:J:206:ASN:N	2.51	0.42
2:M:36:TYR:HB2	2:M:87:PHE:CZ	2.55	0.42
2:N:193:ALA:HB2	2:N:208:SER:HB3	2.00	0.42
1:I:210:LYS:HD3	1:I:210:LYS:HA	1.89	0.42
1:J:177:ALA:HA	1:J:187:LEU:HB3	2.01	0.42
2:L:145:LYS:NZ	3:L:311:HOH:O	2.51	0.42
1:K:210:LYS:HB2	1:K:211:PRO:HD3	2.02	0.41
2:O:149:LYS:HG2	2:O:154:LEU:CD2	2.48	0.41
2:L:113:PRO:HB3	2:L:139:PHE:HB3	2.02	0.41
1:K:78:GLU:OE2	3:K:302:HOH:O	2.22	0.41
2:N:148:TRP:O	2:N:154:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:LYS:HG2	1:I:153:ASP:CG	2.46	0.41
2:O:158:ASN:HD22	2:O:181:LEU:HD21	1.86	0.41
1:K:64:ASP:OD2	3:K:301:HOH:O	2.22	0.41
1:I:99:VAL:CG1	1:I:109:MET:HB3	2.51	0.41
2:M:180:THR:HG23	3:M:357:HOH:O	2.20	0.41
1:I:11:LEU:HD22	1:I:156:PRO:HG3	2.02	0.41
1:J:38:ARG:CZ	1:J:66:MET:HE3	2.50	0.41
2:N:145:LYS:HE3	2:N:147:GLN:NE2	2.35	0.40
1:K:132:PRO:HD3	1:K:218:LYS:HE3	2.03	0.40
1:J:48:VAL:HG13	1:J:66:MET:HE2	2.03	0.40
2:O:145:LYS:HB3	2:O:197:THR:HB	2.03	0.40
2:M:140:TYR:CG	2:M:141:PRO:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	213/236 (90%)	212 (100%)	1 (0%)	0	100	100
1	I	211/236 (89%)	208 (99%)	3 (1%)	0	100	100
1	J	209/236 (89%)	206 (99%)	3 (1%)	0	100	100
1	K	210/236 (89%)	209 (100%)	1 (0%)	0	100	100
2	L	210/214 (98%)	204 (97%)	6 (3%)	0	100	100
2	M	210/214 (98%)	206 (98%)	4 (2%)	0	100	100
2	N	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
2	O	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
All	All	1686/1800 (94%)	1657 (98%)	29 (2%)	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	H	181/199 (91%)	179 (99%)	2 (1%)	65	72
1	I	178/199 (89%)	172 (97%)	6 (3%)	32	33
1	J	178/199 (89%)	171 (96%)	7 (4%)	28	28
1	K	178/199 (89%)	177 (99%)	1 (1%)	78	84
2	L	190/192 (99%)	187 (98%)	3 (2%)	55	61
2	M	190/192 (99%)	186 (98%)	4 (2%)	47	52
2	N	191/192 (100%)	187 (98%)	4 (2%)	47	52
2	O	192/192 (100%)	190 (99%)	2 (1%)	68	75
All	All	1478/1564 (94%)	1449 (98%)	29 (2%)	48	54

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	111	TYR
1	H	114	GLN
1	I	111	TYR
1	I	114	GLN
1	I	136	SER
1	I	179	LEU
1	I	202	THR
1	I	218	LYS
1	J	111	TYR
1	J	122	SER
1	J	124	SER
1	J	191	VAL
1	J	200	THR
1	J	206	ASN
1	J	221	GLU
1	K	208	ASN
2	L	105	GLU
2	L	180	THR
2	L	207	LYS

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Mol	Chain	Res	Type
2	M	15	LEU
2	M	105	GLU
2	M	129	THR
2	M	190	LYS
2	N	7	THR
2	N	27	GLN
2	N	79	GLU
2	N	129	THR
2	O	132	VAL
2	O	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	201	GLN
1	H	208	ASN
1	H	213	ASN
1	I	208	ASN
1	J	173	HIS
1	J	208	ASN
1	K	39	GLN
2	L	38	GLN
2	L	199	GLN
2	N	137	ASN
2	N	147	GLN
2	O	38	GLN
2	O	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PCA	K	3	1	7,8,9	1.95	1 (14%)	9,10,12	2.13	5 (55%)
1	PCA	I	3	1	7,8,9	1.90	1 (14%)	9,10,12	2.17	5 (55%)
1	PCA	H	3	1	7,8,9	1.89	1 (14%)	9,10,12	1.95	4 (44%)
1	PCA	J	3	1	7,8,9	1.93	1 (14%)	9,10,12	2.27	5 (55%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	K	3	1	-	0/0/11/13	0/1/1/1
1	PCA	I	3	1	-	0/0/11/13	0/1/1/1
1	PCA	H	3	1	-	0/0/11/13	0/1/1/1
1	PCA	J	3	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	3	PCA	CD-N	5.02	1.47	1.34
1	J	3	PCA	CD-N	5.00	1.46	1.34
1	I	3	PCA	CD-N	4.93	1.46	1.34
1	H	3	PCA	CD-N	4.91	1.46	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	3	PCA	CA-N-CD	-3.08	103.05	113.58
1	I	3	PCA	CA-N-CD	-2.99	103.35	113.58
1	K	3	PCA	CB-CA-C	-2.97	108.59	112.66
1	J	3	PCA	OE-CD-CG	-2.92	121.51	126.72
1	K	3	PCA	OE-CD-CG	-2.91	121.53	126.72
1	K	3	PCA	CA-N-CD	-2.81	103.96	113.58
1	H	3	PCA	CA-N-CD	-2.81	103.97	113.58
1	I	3	PCA	OE-CD-CG	-2.78	121.77	126.72
1	J	3	PCA	CB-CA-C	-2.76	108.87	112.66
1	J	3	PCA	CB-CA-N	2.74	110.79	103.24
1	I	3	PCA	CB-CA-N	2.72	110.72	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	3	PCA	CG-CD-N	2.70	115.00	108.39
1	I	3	PCA	CG-CD-N	2.60	114.74	108.39
1	H	3	PCA	OE-CD-CG	-2.59	122.10	126.72
1	H	3	PCA	CB-CA-N	2.47	110.03	103.24
1	H	3	PCA	CG-CD-N	2.45	114.38	108.39
1	K	3	PCA	CG-CD-N	2.44	114.36	108.39
1	I	3	PCA	CB-CA-C	-2.43	109.33	112.66
1	K	3	PCA	CB-CA-N	2.41	109.87	103.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	H	216/236 (91%)	-0.10	1 (0%) 87 89	17, 36, 62, 86	0
1	I	214/236 (90%)	-0.01	6 (2%) 55 59	17, 34, 80, 102	0
1	J	212/236 (89%)	0.23	9 (4%) 40 45	18, 44, 91, 112	0
1	K	213/236 (90%)	-0.10	3 (1%) 73 77	15, 34, 64, 84	0
2	L	212/214 (99%)	-0.18	2 (0%) 81 83	17, 35, 63, 72	0
2	M	212/214 (99%)	-0.27	0 100 100	17, 30, 48, 95	0
2	N	213/214 (99%)	0.21	2 (0%) 81 83	21, 52, 73, 102	0
2	O	214/214 (100%)	-0.35	1 (0%) 87 89	15, 30, 49, 81	0
All	All	1706/1800 (94%)	-0.07	24 (1%) 73 77	15, 35, 71, 112	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	200	THR	3.6
1	I	198	LEU	3.4
1	H	68	ASP	3.4
1	J	198	LEU	3.4
1	K	106	TYR	3.3
1	K	198	LEU	3.1
1	J	203	TYR	3.1
2	O	23	CYS	3.1
1	J	167	ALA	3.0
1	J	135	PRO	3.0
1	I	135	PRO	2.8
1	I	106	TYR	2.6
1	I	200	THR	2.4
2	L	87	PHE	2.3
2	N	94	PHE	2.3
1	K	197	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	147	LEU	2.3
2	N	212	ASN	2.3
1	J	166	GLY	2.3
1	I	196	SER	2.2
1	J	144	THR	2.2
2	L	212	ASN	2.1
1	J	222	PRO	2.1
1	I	142	GLY	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	H	3	8/9	0.90	0.09	36,43,52,53	0
1	PCA	K	3	8/9	0.91	0.07	34,36,45,48	0
1	PCA	J	3	8/9	0.96	0.05	26,30,34,36	0
1	PCA	I	3	8/9	0.97	0.04	19,24,28,28	0

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.