



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:07 PM UTC

PDB ID : 9D3J / pdb\_00009d3j  
Title : Structure of L9 Fab in complex with CSP\_Res5-Y\_mC2 Scaffold  
Authors : Jain, M.; Agrawal, S.; Wilson, I.A.  
Deposited on : 2024-08-10  
Resolution : 3.50 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](mailto: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>.

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

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

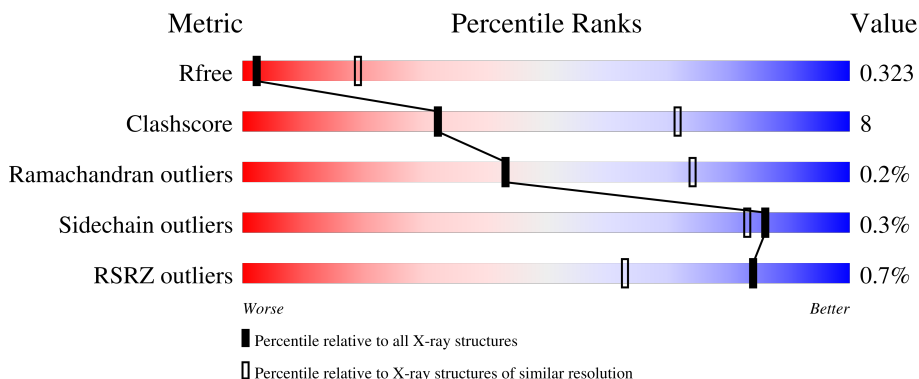
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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  $\geq 3$ , 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	C	64	<div> <div>77%</div> <div>11%</div> <div>12%</div> </div>
1	D	64	<div> <div>69%</div> <div>9%</div> <div>22%</div> </div>
2	A	224	<div> <div>56%</div> <div>24%</div> <div>20%</div> </div>
2	E	224	<div> <div>74%</div> <div>20%</div> <div>5%</div> </div>
3	B	214	<div> <div>61%</div> <div>14%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	214	<div><div><div>%</div><div><div></div></div><div>73%</div><div>17%</div><div>10%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6469 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 PfCSP\_Res5-Y\_mC2 Scaffold.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	56	Total	C	N	O	0	0	0
			395	249	68	78			
1	D	50	Total	C	N	O	0	0	0
			355	224	62	69			

- Molecule 2 is a protein called L9 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	180	Total	C	N	O	S	0	0	0
			1390	885	236	262	7			
2	E	212	Total	C	N	O	S	0	0	0
			1608	1021	271	309	7			

- Molecule 3 is a protein called L9 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	161	Total	C	N	O	S	0	0	0
			1251	786	210	252	3			
3	F	193	Total	C	N	O	S	0	0	0
			1470	909	251	304	6			



● Molecule 1: PfCSP Res5-Y mC2 Scaffold

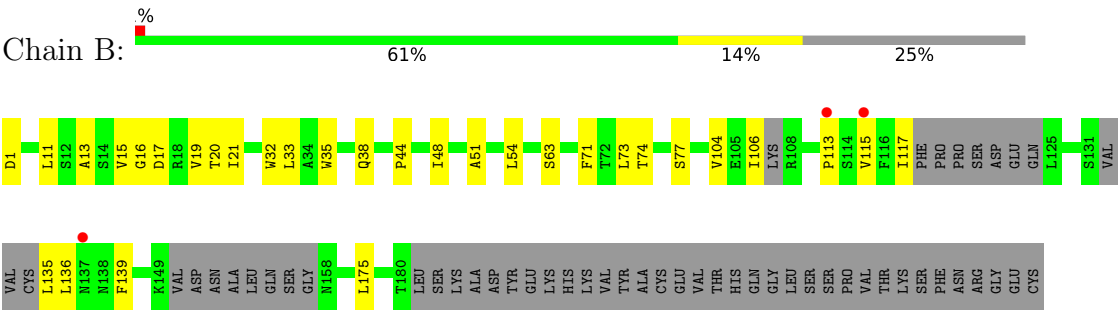


- |     |     |
|-----|-----|
| ALA | ALA |
| VAL | VAL |
| GLU | GLU |
| ASP | ASP |
| ALA | ALA |
| LEU | LEU |
| LYS | LYS |
| LYS | LYS |
| ALA | ALA |
| GLU | GLU |
| ALA | ALA |
| ALA | ALA |
| GLY | GLY |
| D14 | D14 |
| L24 | L24 |
| V28 | V28 |
| R32 | R32 |
| A43 | A43 |
| W46 | W46 |
| V52 | V52 |
| S63 | S63 |
| TYR | TYR |

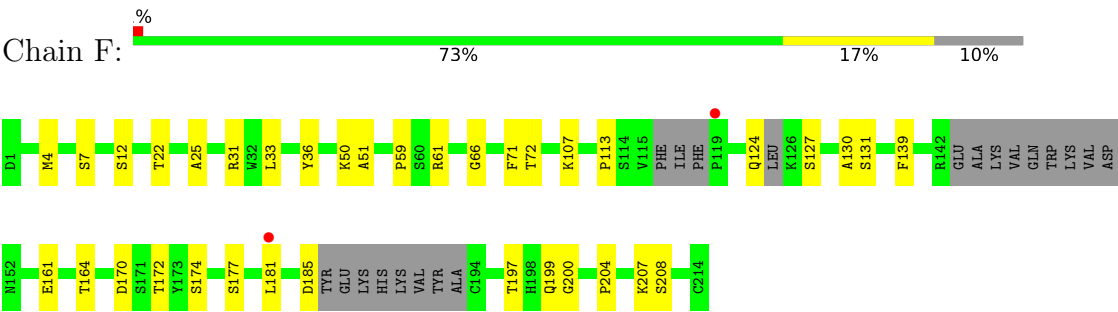
- |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |     |      |      |      |      |     |     |     |     |     |     |     |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | THR | GLN | THR | TYR | I202 | I203 | H204 | H205 | H206 | H207 | H208 | P209 | S210 | V214 | ASP | LYS | LYS | VAL | GLU | PRO | LYS | SER | CYS | ASP | N99 | F100 | F101 | D102 | G103 | L115 | V118 | P126 | SER | VAL | PHE | PRO | PRO | ALA | ALA | ALA | ALA | LEU | GLY | GLY | THR | ALA | ALA | LEU | GLY | V149 | K150 | E155 | P156 | V157 | T158 | V159 | N162 | L166 | THR | S168 | S184 | L185 | V188 | VAL | THR | VAL | PRO | SER | SER | SER | Q1 | S7 | Q13 | R16 | S21 | A24 | I28 | M34 | H35 | V36 | V37 | Q38 | Q39 | A40 | K43 | G44 | L45 | E46 | W47 | V50 | I51 | W52 | N57 | R67 | T70 | S71 | R72 | D73 | N74 | S75 | K76 | N77 | F80 | M83 | L86 | R87 | D90 | V93 | Y94 | Y95 | C96 | H97 |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |      |      |      |      |      |      |      |      |      |     |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |     |     |     |      |
|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|-----|-----|-----|------|
| T142 | G146 | P154 | G164 | A165 | L166 | V189 | P192 | S195 | LEU | G197 | T198 | Y201 | N204 | H207 | S210 | K213 | K216 | LYS | VAL | GLU | PRO | LYS | CYS | ASP |     |     |      |      |      |      |      |      |      |      |     |     |     |      |
| T1   | V2   | E6   | S7   | V12  | Q13  | R16  | S21  | G33  | M34 | A40  | K43  | V47  | V48  | A49  | V50  | I51  | W52  | V64 | T69 | N77 | Q82 | L86 | T91 | H97 | R98 | N99 | W110 | T117 | T123 | P130 | L131 | S134 | S135 | K136 | SER | THR | SER | G140 |

● Molecule 3: L9 Fab light chain



● Molecule 3: L9 Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.94Å 119.94Å 217.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.90 – 3.50 26.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.90-3.50) 91.0 (26.90-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 3.46Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.272 , 0.323 0.272 , 0.323	Depositor DCC
$R_{free}$ test set	2000 reflections (9.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.8	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 82.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	C	0.08	0/400	0.22	0/548
1	D	0.12	0/359	0.34	0/492
2	A	0.12	0/1426	0.34	1/1934 (0.1%)
2	E	0.09	0/1650	0.28	0/2243
3	B	0.09	0/1274	0.28	0/1723
3	F	0.10	0/1495	0.30	0/2022
All	All	0.10	0/6604	0.30	1/8962 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	75	SER	N-CA-C	-5.00	108.92	114.62

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	C	395	0	393	5	0
1	D	355	0	360	3	0
2	A	1390	0	1331	32	0
2	E	1608	0	1550	26	0
3	B	1251	0	1223	21	0
3	F	1470	0	1425	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6469	0	6282	102	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 8.

All (102) 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)
3:B:115:VAL:HG12	3:B:117:ILE:HG12	1.73	0.70
3:B:113:PRO:HB3	3:B:139:PHE:HB3	1.73	0.70
3:B:16:GLY:HA2	3:B:77:SER:HA	1.75	0.68
2:A:147:CYS:N	2:A:203:CYS:SG	2.67	0.67
2:A:207:HIS:HD1	2:A:210:SER:HG	1.42	0.67
2:E:123:THR:HG22	2:E:210:SER:HB2	1.78	0.66
2:A:72:ARG:HH21	2:A:74:ASN:HA	1.63	0.64
3:F:22:THR:HA	3:F:72:THR:HA	1.80	0.61
2:A:67:ARG:NH2	2:A:90:ASP:OD2	2.33	0.61
2:E:34:MET:HG3	2:E:98:ARG:HB2	1.82	0.61
2:A:40:ALA:HB3	2:A:43:LYS:HB2	1.83	0.60
3:F:31:ARG:HH21	3:F:50:LYS:HE3	1.66	0.59
1:C:40:VAL:HG22	2:A:101:TYR:HB2	1.83	0.59
2:E:204:ASN:HD21	2:E:213:LYS:HG2	1.67	0.59
2:A:45:LEU:HD21	3:B:44:PRO:HG3	1.83	0.59
1:D:24:LEU:HD21	1:D:52:VAL:HB	1.84	0.58
3:F:124:GLN:HA	3:F:127:SER:HA	1.84	0.58
2:A:155:GLU:O	2:A:157:VAL:HG12	2.05	0.57
2:E:130:PRO:HB3	2:E:216:LYS:HD3	1.87	0.56
3:B:63:SER:HG	3:B:74:THR:HG1	1.51	0.56
2:E:13:GLN:HG2	2:E:16:ARG:HB2	1.88	0.56
2:E:164:GLY:O	2:E:166:LEU:N	2.39	0.56
3:B:20:THR:HG22	3:B:74:THR:HG22	1.88	0.55
2:E:166:LEU:HD21	2:E:189:VAL:HG11	1.89	0.55
2:A:207:HIS:CD2	2:A:209:PRO:HD2	2.41	0.55
2:E:47:TRP:HZ2	2:E:50:VAL:HG12	1.71	0.54
3:F:66:GLY:HA3	3:F:71:PHE:HA	1.88	0.54
1:C:34:ILE:HG12	3:B:32:TRP:HH2	1.72	0.54
3:F:124:GLN:OE1	3:F:131:SER:N	2.42	0.53
3:F:113:PRO:HB3	3:F:139:PHE:HB3	1.90	0.53
2:E:7:SER:OG	2:E:21:SER:OG	2.28	0.52
2:E:91:THR:HG23	2:E:117:THR:HA	1.91	0.52
2:A:52:TRP:HB2	2:A:57:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:93:VAL:HG22	2:A:115:LEU:HG	1.90	0.52
2:E:131:LEU:HB2	2:E:146:GLY:HA3	1.92	0.51
2:A:37:VAL:O	2:A:95:TYR:N	2.44	0.51
2:A:83:MET:HE2	2:A:86:LEU:HD21	1.92	0.51
3:F:161:GLU:HA	3:F:177:SER:HA	1.92	0.50
3:B:15:VAL:HG22	3:B:106:ILE:HD11	1.92	0.50
2:A:73:ASP:HB2	2:A:80:PHE:HE2	1.77	0.50
2:E:110:TRP:HE1	3:F:36:TYR:HE2	1.59	0.49
2:A:7:SER:OG	2:A:21:SER:OG	2.25	0.49
2:A:97:HIS:CE1	2:A:99:ASN:HB3	2.47	0.49
2:E:195:SER:HB3	2:E:198:THR:OG1	2.11	0.49
2:A:102:ASP:OD1	2:A:103:GLY:N	2.39	0.49
3:B:1:ASP:OD1	3:B:1:ASP:N	2.46	0.49
3:B:136:LEU:HB2	3:B:175:LEU:HB3	1.94	0.48
2:A:150:LYS:HG3	2:A:184:SER:HB3	1.95	0.48
2:E:6:GLU:N	2:E:6:GLU:OE1	2.48	0.47
3:F:12:SER:HB2	3:F:107:LYS:HG3	1.95	0.47
3:F:170:ASP:OD1	3:F:170:ASP:N	2.43	0.47
2:A:87:ARG:O	2:A:118:VAL:HG21	2.14	0.47
2:E:12:VAL:HG11	2:E:86:LEU:HD22	1.97	0.47
3:B:13:ALA:HB1	3:B:17:ASP:HB2	1.96	0.47
2:A:149:VAL:HB	2:A:185:LEU:HG	1.97	0.46
2:A:28:ILE:HA	2:A:77:ASN:HD21	1.80	0.46
3:B:33:LEU:HB3	3:B:51:ALA:HB2	1.97	0.46
3:F:170:ASP:OD2	3:F:172:THR:OG1	2.28	0.46
2:A:24:ALA:HB3	2:A:77:ASN:HB3	1.96	0.46
3:F:7:SER:HB3	3:F:22:THR:HG23	1.98	0.45
2:A:13:GLN:HB2	2:A:16:ARG:HG3	1.99	0.45
3:B:48:ILE:HG12	3:B:54:LEU:HG	1.98	0.45
2:E:34:MET:HE2	2:E:98:ARG:HD2	1.97	0.45
1:D:28:VAL:O	1:D:32:ARG:HG3	2.17	0.45
2:E:69:THR:O	2:E:82:GLN:N	2.49	0.45
2:A:7:SER:HG	2:A:21:SER:HG	1.59	0.45
2:A:188:VAL:HG11	3:B:135:LEU:HD21	1.99	0.45
1:D:43:ALA:HA	1:D:46:TRP:HD1	1.83	0.44
2:A:36:TRP:HD1	2:A:70:ILE:HD11	1.82	0.44
1:C:43:ALA:HA	1:C:46:TRP:HD1	1.82	0.44
3:B:35:TRP:CD2	3:B:73:LEU:HD12	2.52	0.44
3:B:11:LEU:HD23	3:B:104:VAL:HG22	2.00	0.44
3:F:199:GLN:OE1	3:F:200:GLY:N	2.50	0.44
3:F:33:LEU:HB3	3:F:51:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:47:TRP:HZ2	2:A:50:VAL:HG12	1.82	0.43
2:E:40:ALA:HB3	2:E:43:LYS:HB2	2.01	0.43
2:A:159:VAL:HG13	2:A:205:VAL:HG12	2.01	0.42
3:F:4:MET:HE3	3:F:25:ALA:HB2	2.01	0.42
2:A:38:ARG:NH2	2:A:90:ASP:HA	2.35	0.42
1:C:24:LEU:O	1:C:28:VAL:HG23	2.20	0.42
2:E:97:HIS:CE1	2:E:99:ASN:HB3	2.55	0.42
2:E:33:GLY:HA2	2:E:52:TRP:HA	2.02	0.42
2:E:131:LEU:HD12	2:E:146:GLY:HA3	2.01	0.41
3:F:181:LEU:HD13	3:F:185:ASP:O	2.20	0.41
2:E:48:VAL:HG13	2:E:64:VAL:HG21	2.03	0.41
3:F:207:LYS:HG3	3:F:208:SER:H	1.84	0.41
3:B:35:TRP:CE3	3:B:73:LEU:HD12	2.56	0.41
1:C:38:PRO:HB2	2:A:52:TRP:CZ2	2.56	0.41
2:A:34:MET:HG2	2:A:98:ARG:HD2	2.02	0.41
3:B:11:LEU:HD22	3:B:21:ILE:HD11	2.02	0.41
3:B:38:GLN:HB2	3:B:44:PRO:HB3	2.03	0.41
2:E:77:ASN:OD1	2:E:77:ASN:N	2.54	0.41
2:E:154:PRO:O	2:E:207:HIS:NE2	2.50	0.41
3:F:164:THR:HG22	3:F:174:SER:H	1.84	0.41
2:E:134:SER:HB2	2:E:136:LYS:HE2	2.02	0.41
2:E:142:THR:HG22	2:E:192:PRO:HA	2.02	0.40
2:A:162:ASN:HD21	2:A:202:ILE:HG23	1.85	0.40
3:B:33:LEU:HD22	3:B:71:PHE:CG	2.57	0.40
3:F:59:PRO:HB2	3:F:61:ARG:HG2	2.04	0.40
3:B:11:LEU:HD21	3:B:19:VAL:HB	2.03	0.40
3:F:124:GLN:HG3	3:F:130:ALA:HA	2.04	0.40
3:F:197:THR:HB	3:F:204:PRO:HB3	2.04	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	C	54/64 (84%)	51 (94%)	3 (6%)	0	100	100
1	D	48/64 (75%)	43 (90%)	5 (10%)	0	100	100
2	A	172/224 (77%)	157 (91%)	14 (8%)	1 (1%)	21	54
2	E	206/224 (92%)	192 (93%)	13 (6%)	1 (0%)	24	57
3	B	151/214 (71%)	136 (90%)	15 (10%)	0	100	100
3	F	183/214 (86%)	171 (93%)	12 (7%)	0	100	100
All	All	814/1004 (81%)	750 (92%)	62 (8%)	2 (0%)	43	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	157	VAL
2	E	165	ALA

### 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	C	34/40 (85%)	34 (100%)	0	100	100
1	D	32/40 (80%)	32 (100%)	0	100	100
2	A	153/190 (80%)	153 (100%)	0	100	100
2	E	178/190 (94%)	176 (99%)	2 (1%)	65	74
3	B	142/189 (75%)	142 (100%)	0	100	100
3	F	170/189 (90%)	170 (100%)	0	100	100
All	All	709/838 (85%)	707 (100%)	2 (0%)	86	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	2	VAL
2	E	12	VAL

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

Mol	Chain	Res	Type
2	A	57	ASN
2	A	82	GLN
3	B	79	GLN
3	B	138	ASN
3	F	6	GLN
3	F	37	GLN
3	F	138	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	56/64 (87%)	-0.11	0 <span>100</span> <span>100</span>	72, 130, 189, 203	0
1	D	50/64 (78%)	0.05	0 <span>100</span> <span>100</span>	80, 132, 192, 212	0
2	A	180/224 (80%)	-0.06	0 <span>100</span> <span>100</span>	85, 132, 193, 212	0
2	E	212/224 (94%)	-0.10	1 (0%) <span>87</span> <span>68</span>	83, 138, 180, 219	0
3	B	161/214 (75%)	0.01	3 (1%) <span>66</span> <span>41</span>	90, 150, 203, 253	0
3	F	193/214 (90%)	0.07	2 (1%) <span>79</span> <span>56</span>	86, 135, 197, 230	0
All	All	852/1004 (84%)	-0.02	6 (0%) <span>84</span> <span>63</span>	72, 138, 198, 253	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	181	LEU	3.2
3	F	119	PRO	2.9
3	B	113	PRO	2.4
3	B	137	ASN	2.2
3	B	115	VAL	2.1
2	E	201	TYR	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.