



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:56 PM UTC

PDB ID : 8RTX / pdb_00008rtx
Title : Crystal Structure of an Anti-idiotypic Fab Fragment
Authors : Eronen, V.; Parkkinen, T.; Hakulinen, N.; Rouvinen, J.
Deposited on : 2024-01-29
Resolution : 2.70 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
Xtrriage (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

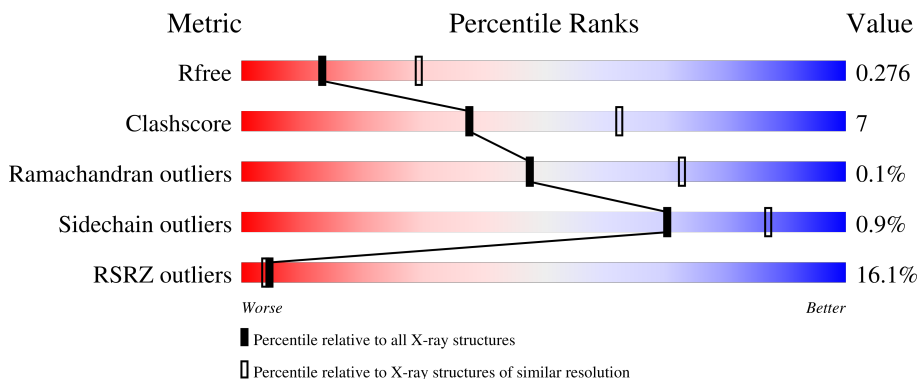
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



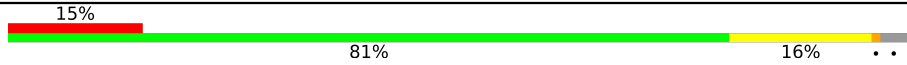
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	214	
1	C	214	
1	E	214	
2	B	227	
2	D	227	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	227	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '15%', a large green segment in the middle labeled '81%', and a yellow segment on the right labeled '16%'. The bar ends with a grey segment and two dots '••'.</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9738 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 Anti-IC Fab fragment B12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	Total 1625	C 1016	N 273	O 330	S 6	0	0	0
1	C	214	Total 1625	C 1016	N 273	O 330	S 6	0	0	0
1	E	214	Total 1625	C 1016	N 273	O 330	S 6	0	0	0

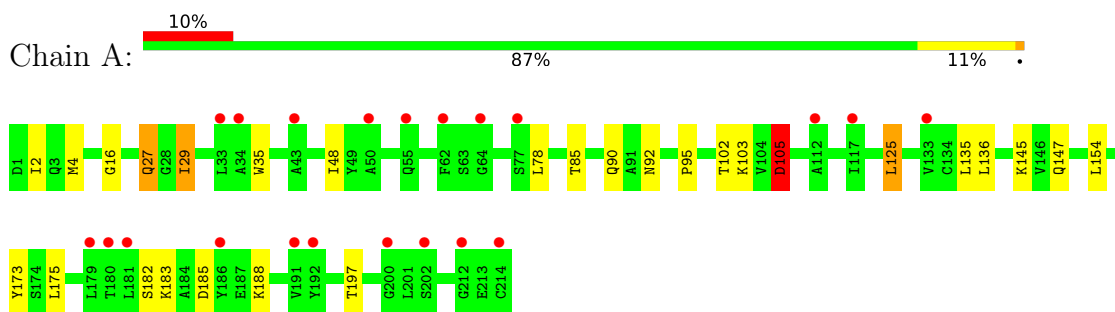
- Molecule 2 is a protein called Anti-IC Fab fragment B12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	221	Total 1621	C 1013	N 277	O 324	S 7	0	0	0
2	D	221	Total 1621	C 1013	N 277	O 324	S 7	0	0	0
2	F	221	Total 1621	C 1013	N 277	O 324	S 7	0	0	0

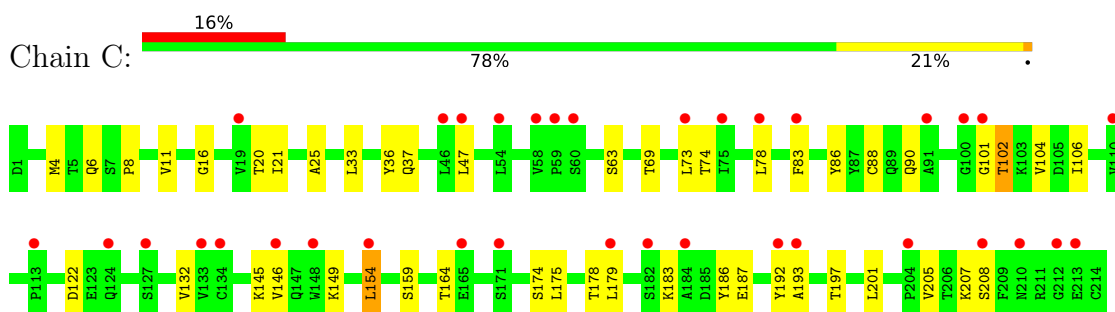
3 Residue-property plots [i](#)

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.

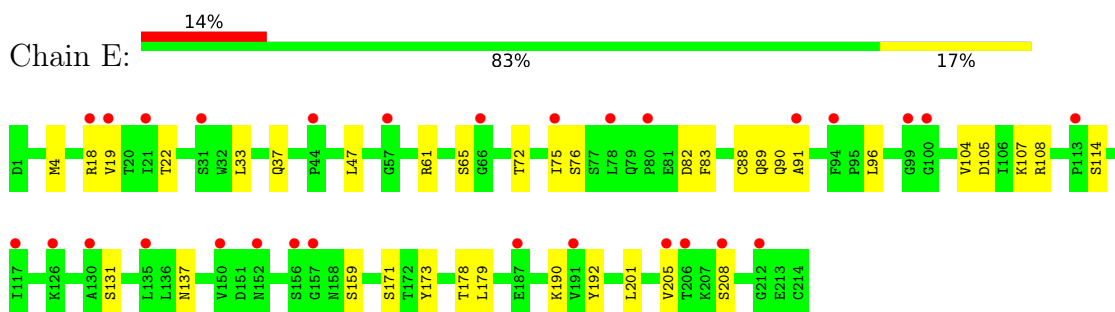
- Molecule 1: Anti-IC Fab fragment B12 light chain



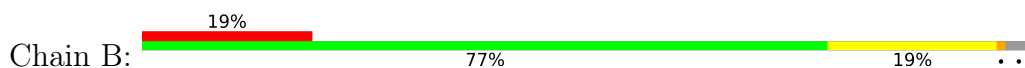
- Molecule 1: Anti-IC Fab fragment B12 light chain

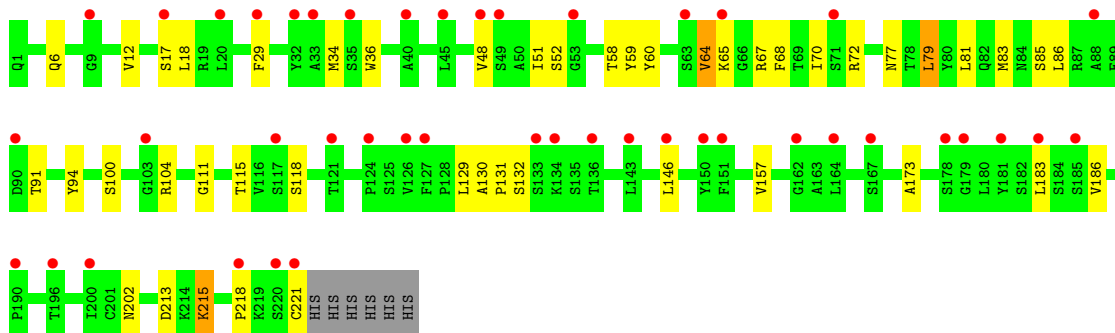


- Molecule 1: Anti-IC Fab fragment B12 light chain

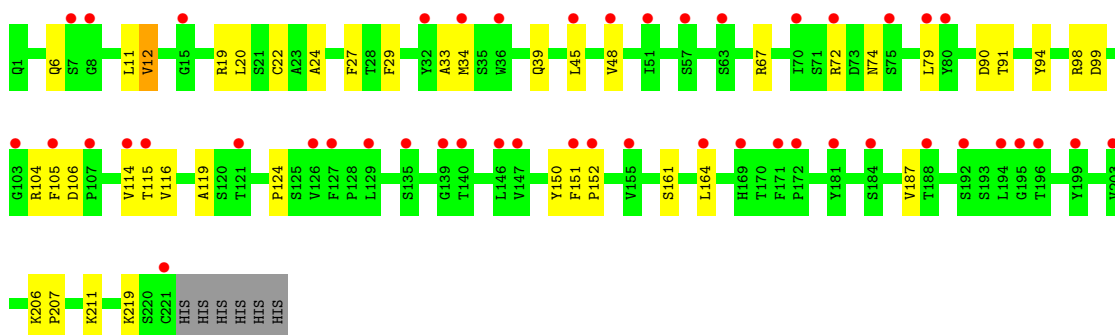
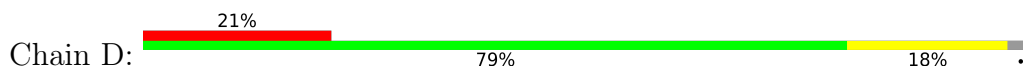


- Molecule 2: Anti-IC Fab fragment B12 heavy chain

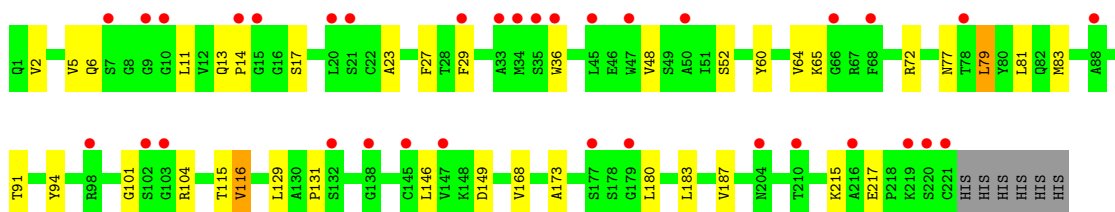
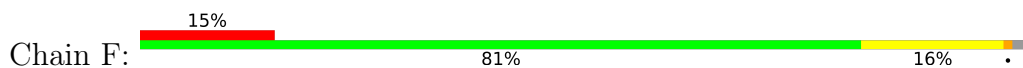




- Molecule 2: Anti-IC Fab fragment B12 heavy chain



- Molecule 2: Anti-IC Fab fragment B12 heavy chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	81.86Å 81.86Å 181.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.93 – 2.70 40.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.5 (40.93-2.70) 85.0 (40.93-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.247 , 0.269 0.250 , 0.276	Depositor DCC
R_{free} test set	2020 reflections (5.69%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtrriage
Anisotropy	0.508	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 173.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,l 0.459 for h,-h-k,-l 0.023 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	9738	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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 [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	0/1660	0.92	4/2254 (0.2%)
1	C	0.44	0/1660	0.86	2/2254 (0.1%)
1	E	0.46	0/1660	0.88	0/2254
2	B	0.53	0/1658	1.09	6/2255 (0.3%)
2	D	0.48	0/1658	0.98	4/2255 (0.2%)
2	F	0.43	0/1658	0.94	1/2255 (0.0%)
All	All	0.47	0/9954	0.95	17/13527 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	19	ARG	CA-CB-CG	6.78	127.66	114.10
1	A	29	ILE	CA-CB-CG2	6.77	122.01	110.50
1	C	102	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	29	ILE	CG1-CB-CG2	-6.16	92.23	110.70
2	B	118	SER	CA-C-N	-6.01	112.48	122.21
2	B	118	SER	C-N-CA	-6.01	112.48	122.21
2	B	64	VAL	N-CA-CB	-5.66	105.59	112.33
2	F	79	LEU	CA-CB-CG	5.61	135.93	116.30
2	B	68	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	154	LEU	CD1-CG-CD2	-5.55	98.59	110.80
2	D	119	ALA	CA-C-N	5.34	131.21	122.07
2	D	119	ALA	C-N-CA	5.34	131.21	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CB-CA-C	-5.18	101.48	110.45
2	D	34	MET	CA-CB-CG	5.13	124.36	114.10
2	B	131	PRO	CA-C-N	-5.11	113.82	122.67
2	B	131	PRO	C-N-CA	-5.11	113.82	122.67
1	A	103	LYS	CB-CG-CD	5.02	122.84	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	104	ARG	Sidechain

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	1625	0	1579	18	0
1	C	1625	0	1579	29	0
1	E	1625	0	1580	20	0
2	B	1621	0	1585	30	0
2	D	1621	0	1585	21	0
2	F	1621	0	1586	20	0
All	All	9738	0	9494	134	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 7.

All (134) 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:130:ALA:HB1	2:B:218:PRO:HA	1.74	0.68
1:C:63:SER:HG	1:C:74:THR:HG1	1.42	0.68
2:D:11:LEU:HA	2:D:115:THR:O	1.95	0.67
1:E:4:MET:HE2	1:E:90:GLN:HB3	1.77	0.67
1:C:6:GLN:HG2	1:C:21:ILE:HD11	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:SER:HA	2:F:83:MET:O	1.95	0.65
2:F:13:GLN:HG3	2:F:14:PRO:HD2	1.81	0.63
1:A:4:MET:HE2	1:A:90:GLN:HB3	1.82	0.62
2:B:67:ARG:NH2	2:B:85:SER:O	2.33	0.62
2:B:52:SER:O	2:B:72:ARG:NH1	2.33	0.62
1:C:33:LEU:HD11	1:C:88:CYS:HB2	1.82	0.61
2:D:91:THR:HG22	2:D:115:THR:HA	1.82	0.61
1:C:36:TYR:OH	2:D:105:PHE:HB2	2.02	0.59
1:A:2:ILE:HD13	1:A:29:ILE:HD11	1.84	0.59
2:B:17:SER:HA	2:B:83:MET:O	2.02	0.59
1:E:201:LEU:HD21	1:E:205:VAL:HG22	1.84	0.59
2:B:29:PHE:HE1	2:B:34:MET:HG3	1.68	0.59
2:B:51:ILE:HG12	2:B:58:THR:HG22	1.85	0.58
1:C:20:THR:HG22	1:C:74:THR:HG22	1.85	0.57
2:D:12:VAL:HG13	2:D:116:VAL:HG22	1.87	0.57
2:D:211:LYS:HB2	1:E:107:LYS:HE2	1.85	0.56
2:F:48:VAL:HG22	2:F:64:VAL:HG11	1.87	0.56
2:D:29:PHE:O	2:D:72:ARG:NH2	2.39	0.56
2:B:202:ASN:ND2	2:B:213:ASP:OD1	2.37	0.56
2:B:60:TYR:HD2	2:B:65:LYS:HA	1.71	0.56
1:C:192:TYR:O	1:C:208:SER:HA	2.06	0.56
1:A:136:LEU:HD23	1:A:175:LEU:HD22	1.89	0.56
1:C:193:ALA:HA	1:C:207:LYS:O	2.06	0.55
2:F:60:TYR:HD2	2:F:65:LYS:HA	1.71	0.55
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.21	0.55
1:C:201:LEU:HD13	1:C:205:VAL:HG13	1.88	0.54
1:C:4:MET:HE2	1:C:90:GLN:HB3	1.89	0.54
1:A:2:ILE:HG12	1:A:27:GLN:HG3	1.89	0.54
2:D:161:SER:O	2:D:161:SER:OG	2.26	0.53
1:C:21:ILE:HG23	1:C:73:LEU:HB3	1.90	0.53
1:C:25:ALA:O	1:C:69:THR:OG1	2.27	0.53
2:F:215:LYS:HD2	2:F:217:GLU:HG3	1.91	0.53
1:A:105:ASP:OD1	1:A:173:TYR:OH	2.27	0.52
2:D:6:GLN:NE2	2:D:94:TYR:O	2.40	0.52
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.90	0.52
1:A:90:GLN:NE2	1:A:95:PRO:O	2.43	0.52
2:B:12:VAL:HG11	2:B:18:LEU:HB2	1.91	0.52
2:B:34:MET:CG	2:B:79:LEU:HD11	2.40	0.51
1:C:11:VAL:HG13	1:C:104:VAL:HG23	1.92	0.51
1:A:16:GLY:N	1:A:78:LEU:O	2.37	0.51
2:F:173:ALA:HA	2:F:183:LEU:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:HG3	2:B:79:LEU:HD11	1.94	0.50
1:C:183:LYS:NZ	1:C:187:GLU:OE2	2.41	0.50
1:E:61:ARG:NE	1:E:82:ASP:OD2	2.37	0.50
1:E:65:SER:OG	1:E:72:THR:OG1	2.30	0.50
1:C:186:TYR:O	1:C:192:TYR:OH	2.31	0.49
1:E:22:THR:HG22	1:E:72:THR:HG22	1.94	0.49
2:B:48:VAL:HG13	2:B:64:VAL:HG21	1.95	0.49
2:D:98:ARG:NE	2:D:106:ASP:O	2.45	0.49
2:F:11:LEU:HA	2:F:115:THR:O	2.12	0.49
1:E:114:SER:HB2	1:E:137:ASN:HB3	1.94	0.48
1:A:136:LEU:HB2	1:A:175:LEU:HB3	1.96	0.48
2:B:132:SER:HB2	2:B:221:CYS:HB2	1.95	0.48
2:D:124:PRO:HB3	2:D:150:TYR:HB3	1.96	0.47
1:E:83:PHE:HA	1:E:104:VAL:HG23	1.97	0.47
1:E:91:ALA:HA	1:E:96:LEU:HD23	1.96	0.47
2:D:22:CYS:HB3	2:D:79:LEU:HB3	1.97	0.47
2:B:77:ASN:OD1	2:B:77:ASN:N	2.46	0.47
2:B:215:LYS:HB3	2:B:215:LYS:HE3	1.63	0.47
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.47	0.47
2:F:149:ASP:HA	2:F:180:LEU:HB3	1.97	0.47
1:A:135:LEU:HD12	2:B:186:VAL:HG11	1.96	0.47
1:C:16:GLY:N	1:C:78:LEU:O	2.34	0.47
1:A:35:TRP:HB2	1:A:48:ILE:HB	1.97	0.46
2:F:29:PHE:HZ	2:F:79:LEU:HB2	1.80	0.46
2:F:52:SER:O	2:F:72:ARG:NH1	2.48	0.46
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.96	0.46
2:F:36:TRP:NE1	2:F:81:LEU:HB2	2.31	0.46
2:B:94:TYR:O	2:B:111:GLY:HA2	2.16	0.46
2:F:6:GLN:NE2	2:F:94:TYR:O	2.41	0.46
1:A:147:GLN:NE2	1:A:154:LEU:HD21	2.31	0.46
2:F:29:PHE:HD2	2:F:77:ASN:HA	1.79	0.46
1:A:27:GLN:O	1:A:29:ILE:HD13	2.16	0.46
1:E:105:ASP:OD1	1:E:173:TYR:OH	2.34	0.45
1:C:146:VAL:HG21	1:C:175:LEU:HD22	1.98	0.45
1:A:182:SER:OG	1:A:185:ASP:OD1	2.34	0.45
1:C:132:VAL:HG23	1:C:179:LEU:HB3	1.97	0.45
1:C:83:PHE:HA	1:C:104:VAL:HG13	1.98	0.45
2:F:2:VAL:HG23	2:F:27:PHE:CD1	2.51	0.45
1:C:122:ASP:OD1	2:D:219:LYS:NZ	2.50	0.45
2:B:51:ILE:HD12	2:B:70:ILE:HG12	2.00	0.44
2:F:91:THR:HG22	2:F:116:VAL:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PHE:HD1	1:C:104:VAL:HG13	1.81	0.44
2:F:168:VAL:HG22	2:F:187:VAL:HG12	1.99	0.44
2:D:151:PHE:HD1	2:D:152:PRO:HA	1.82	0.44
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.98	0.44
1:C:159:SER:HA	1:C:178:THR:O	2.18	0.44
1:C:164:THR:HG22	1:C:174:SER:H	1.82	0.44
2:B:173:ALA:HA	2:B:183:LEU:HB3	2.00	0.44
1:E:18:ARG:HG3	1:E:76:SER:HA	2.00	0.44
2:D:206:LYS:HG2	2:D:207:PRO:HD3	2.00	0.44
1:E:19:VAL:HG13	1:E:75:ILE:HB	2.00	0.43
1:E:33:LEU:HD11	1:E:88:CYS:HB2	2.00	0.43
1:E:131:SER:HA	1:E:179:LEU:O	2.17	0.43
1:E:192:TYR:O	1:E:208:SER:HA	2.18	0.43
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.99	0.43
2:B:129:LEU:HD21	2:B:146:LEU:HB2	2.00	0.43
2:B:51:ILE:HD13	2:B:51:ILE:HG21	1.83	0.43
2:D:164:LEU:HD21	2:D:187:VAL:HG21	1.99	0.43
2:F:129:LEU:HD21	2:F:146:LEU:HB2	2.00	0.43
2:B:83:MET:SD	2:B:86:LEU:HD21	2.58	0.43
1:C:149:LYS:HE2	1:C:154:LEU:HD13	2.00	0.43
2:B:34:MET:HB2	2:B:79:LEU:HD21	2.01	0.42
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.54	0.42
1:C:83:PHE:CE2	1:C:106:ILE:HB	2.55	0.42
1:A:125:LEU:O	1:A:183:LYS:HD2	2.20	0.42
2:F:5:VAL:HG22	2:F:23:ALA:HB3	2.01	0.42
1:C:8:PRO:O	1:C:102:THR:OG1	2.37	0.42
2:D:20:LEU:HD11	2:D:114:VAL:HG21	2.02	0.42
2:F:91:THR:HG23	2:F:116:VAL:HG13	2.01	0.42
1:E:33:LEU:HD12	1:E:89:GLN:O	2.20	0.42
1:E:33:LEU:HD12	1:E:89:GLN:C	2.45	0.41
1:A:29:ILE:HG23	1:A:92:ASN:HB2	2.02	0.41
2:B:59:TYR:C	2:B:60:TYR:HD1	2.28	0.41
1:E:159:SER:HA	1:E:178:THR:O	2.21	0.41
1:A:145:LYS:HB3	1:A:197:THR:HB	2.02	0.41
2:B:157:VAL:HA	2:B:202:ASN:O	2.21	0.41
1:E:108:ARG:HD3	1:E:171:SER:HB2	2.03	0.41
1:A:85:THR:HA	1:A:102:THR:O	2.20	0.41
2:B:100:SER:HB2	2:B:104:ARG:HE	1.86	0.41
2:D:72:ARG:NE	2:D:74:ASN:OD1	2.51	0.41
1:C:86:TYR:O	1:C:101:GLY:HA2	2.21	0.40
1:A:147:GLN:HE21	1:A:154:LEU:HD21	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:HB3	1:C:197:THR:HB	2.02	0.40
2:B:6:GLN:NE2	2:B:94:TYR:O	2.43	0.40
1:C:78:LEU:HD21	1:C:83:PHE:HE1	1.86	0.40
2:F:101:GLY:O	2:F:104:ARG:HG2	2.21	0.40
2:B:91:THR:HG23	2:B:115:THR:HA	2.03	0.40
2:D:33:ALA:HB3	2:D:99:ASP: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	A	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
1	C	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
1	E	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
2	D	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
2	F	219/227 (96%)	215 (98%)	3 (1%)	1 (0%)	24	48
All	All	1293/1323 (98%)	1259 (97%)	33 (3%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	131	PRO

5.3.2 Protein sidechains [i](#)

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	185/185 (100%)	181 (98%)	4 (2%)	45	74
1	C	185/185 (100%)	185 (100%)	0	100	100
1	E	185/185 (100%)	184 (100%)	1 (0%)	81	92
2	B	182/188 (97%)	180 (99%)	2 (1%)	65	85
2	D	182/188 (97%)	180 (99%)	2 (1%)	65	85
2	F	182/188 (97%)	181 (100%)	1 (0%)	81	92
All	All	1101/1119 (98%)	1091 (99%)	10 (1%)	70	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	105	ASP
1	A	125	LEU
1	A	188	LYS
2	B	79	LEU
2	B	215	LYS
2	D	12	VAL
2	D	48	VAL
1	E	190	LYS
2	F	116	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	38	GLN
2	B	39	GLN
2	B	82	GLN
2	B	176	GLN
1	C	55	GLN
1	C	79	GLN
1	E	55	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	0.97	21 (9%) 13 11	67, 87, 108, 136	0
1	C	214/214 (100%)	1.10	35 (16%) 4 4	68, 88, 107, 164	0
1	E	214/214 (100%)	1.07	29 (13%) 7 6	65, 89, 110, 154	0
2	B	221/227 (97%)	1.29	44 (19%) 3 2	77, 101, 133, 169	0
2	D	221/227 (97%)	1.28	47 (21%) 2 2	75, 95, 116, 188	0
2	F	221/227 (97%)	1.18	34 (15%) 5 4	69, 93, 119, 214	0
All	All	1305/1323 (98%)	1.15	210 (16%) 4 4	65, 92, 117, 214	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	CYS	5.2
2	F	35	SER	5.0
1	A	50	ALA	4.9
1	E	113	PRO	4.6
2	B	133	SER	4.4
1	C	213	GLU	4.2
2	B	126	VAL	4.0
1	C	47	LEU	4.0
2	D	171	PHE	4.0
2	B	183	LEU	3.9
2	D	127	PHE	3.9
2	D	194	LEU	3.8
1	E	80	PRO	3.8
2	F	78	THR	3.8
1	E	130	ALA	3.7
1	E	208	SER	3.7
1	C	148	TRP	3.7
2	D	105	PHE	3.7
1	A	212	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	126	VAL	3.5
2	F	102	SER	3.5
1	A	77	SER	3.4
1	C	208	SER	3.4
2	B	20	LEU	3.4
1	E	66	GLY	3.4
2	F	33	ALA	3.4
2	B	48	VAL	3.4
2	D	147	VAL	3.4
2	D	121	THR	3.3
1	E	212	GLY	3.3
2	D	75	SER	3.2
2	D	135	SER	3.2
1	A	214	CYS	3.2
2	F	10	GLY	3.2
2	D	196	THR	3.2
1	A	200	GLY	3.2
2	B	103	GLY	3.1
2	D	34	MET	3.1
1	A	133	VAL	3.1
2	D	129	LEU	3.1
2	B	190	PRO	3.1
2	D	139	GLY	3.1
2	B	218	PRO	3.0
2	F	14	PRO	3.0
2	B	63	SER	3.0
2	D	221	CYS	3.0
1	E	191	VAL	3.0
2	B	178	SER	3.0
2	B	29	PHE	3.0
2	F	145	CYS	2.9
1	E	18	ARG	2.9
2	F	50	ALA	2.9
2	B	185	SER	2.9
2	D	63	SER	2.9
1	A	64	GLY	2.9
2	D	169	HIS	2.9
2	B	49	SER	2.9
2	B	117	SER	2.9
2	F	221	CYS	2.9
2	B	162	GLY	2.9
2	B	134	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	72	ARG	2.8
2	F	177	SER	2.8
1	C	184	ALA	2.8
2	B	33	ALA	2.8
1	E	94	PHE	2.8
2	B	146	LEU	2.8
1	E	91	ALA	2.8
2	D	114	VAL	2.8
2	F	29	PHE	2.8
2	D	152	PRO	2.8
1	C	19	VAL	2.8
2	D	103	GLY	2.7
2	B	127	PHE	2.7
2	F	179	GLY	2.7
2	B	40	ALA	2.7
2	B	143	LEU	2.7
2	B	220	SER	2.7
2	F	36	TRP	2.7
1	E	19	VAL	2.7
2	B	179	GLY	2.7
2	D	8	GLY	2.7
2	F	9	GLY	2.7
1	C	182	SER	2.7
2	D	151	PHE	2.7
2	F	219	LYS	2.7
1	A	192	TYR	2.6
1	A	43	ALA	2.6
2	B	35	SER	2.6
1	E	206	THR	2.6
2	B	136	THR	2.6
2	B	181	TYR	2.6
1	C	78	LEU	2.6
2	D	155	VAL	2.6
1	C	59	PRO	2.6
1	A	112	ALA	2.6
2	F	216	ALA	2.6
1	C	60	SER	2.5
1	C	127	SER	2.5
1	E	117	ILE	2.5
1	A	33	LEU	2.5
2	D	146	LEU	2.5
1	C	101	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	58	VAL	2.5
1	C	204	PRO	2.5
1	E	44	PRO	2.5
1	E	75	ILE	2.5
1	C	154	LEU	2.5
1	E	187	GLU	2.5
1	C	146	VAL	2.5
1	E	99	GLY	2.5
2	F	15	GLY	2.5
1	E	152	ASN	2.5
1	C	46	LEU	2.5
2	B	9	GLY	2.5
1	E	205	VAL	2.5
1	C	75	ILE	2.4
1	C	192	TYR	2.4
2	D	48	VAL	2.4
1	E	135	LEU	2.4
2	B	17	SER	2.4
2	F	220	SER	2.4
2	F	47	TRP	2.4
1	A	117	ILE	2.4
1	E	31	SER	2.4
1	C	133	VAL	2.4
2	D	199	TYR	2.4
2	B	164	LEU	2.4
2	D	79	LEU	2.4
1	C	193	ALA	2.4
1	E	78	LEU	2.3
1	E	21	ILE	2.3
2	B	167	SER	2.3
2	B	124	PRO	2.3
2	B	150	TYR	2.3
2	D	57	SER	2.3
2	F	132	SER	2.3
2	D	172	PRO	2.3
1	A	55	GLN	2.3
1	A	180	THR	2.3
1	E	126	LYS	2.3
1	E	156	SER	2.3
2	D	15	GLY	2.3
2	F	103	GLY	2.3
1	A	62	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	88	ALA	2.3
2	F	210	THR	2.3
2	B	90	ASP	2.3
2	D	36	TRP	2.3
2	D	195	GLY	2.3
2	B	151	PHE	2.3
2	F	68	PHE	2.3
2	F	88	ALA	2.2
2	B	121	THR	2.2
2	D	181	TYR	2.2
1	C	124	GLN	2.2
2	F	7	SER	2.2
1	A	191	VAL	2.2
1	C	179	LEU	2.2
2	D	45	LEU	2.2
2	D	164	LEU	2.2
1	C	83	PHE	2.2
2	D	80	TYR	2.2
2	D	203	VAL	2.2
2	F	147	VAL	2.2
1	E	57	GLY	2.2
2	B	45	LEU	2.2
2	F	21	SER	2.2
2	D	70	ILE	2.2
1	C	210	ASN	2.2
2	D	107	PRO	2.2
1	C	54	LEU	2.2
1	C	212	GLY	2.2
1	E	157	GLY	2.2
2	F	138	GLY	2.2
2	F	34	MET	2.2
1	C	110	VAL	2.2
1	C	91	ALA	2.1
1	A	181	LEU	2.1
2	F	66	GLY	2.1
1	A	202	SER	2.1
2	B	71	SER	2.1
2	D	184	SER	2.1
1	C	165	GLU	2.1
2	D	140	THR	2.1
2	D	188	THR	2.1
1	C	134	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	186	TYR	2.1
2	F	45	LEU	2.1
2	D	7	SER	2.1
2	F	98	ARG	2.1
2	B	65	LYS	2.1
1	C	100	GLY	2.1
1	E	100	GLY	2.1
2	B	32	TYR	2.1
2	D	32	TYR	2.1
2	B	200	ILE	2.1
1	A	179	LEU	2.1
1	E	150	VAL	2.1
1	A	34	ALA	2.0
2	D	192	SER	2.0
2	F	20	LEU	2.0
2	B	53	GLY	2.0
1	C	171	SER	2.0
1	C	113	PRO	2.0
2	B	196	THR	2.0
2	D	115	THR	2.0
1	C	73	LEU	2.0
2	D	51	ILE	2.0
2	F	204	ASN	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.