



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:33 am BST

PDB ID : 1F11
Title : F124 FAB FRAGMENT FROM A MONOCLONAL ANTI-PRES2 ANTI-BODY
Authors : Saul, F.A.; Vulliez-Le Normand, B.; Passafiume, M.; Riottot, M.M.; Bentley, G.A.
Deposited on : 2000-05-18
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

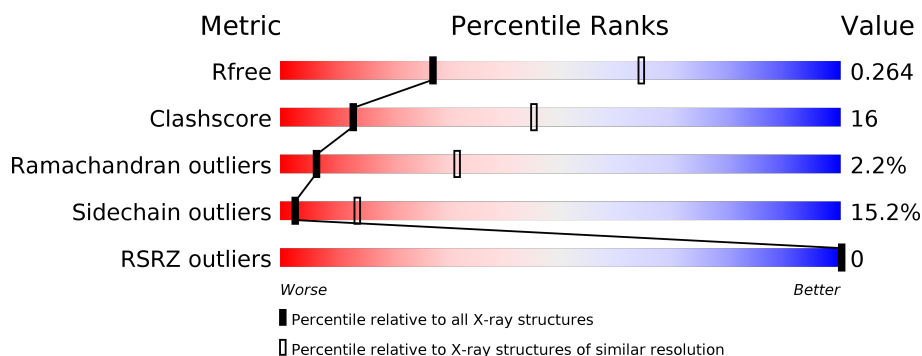
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	218	
1	C	218	
2	B	221	
2	D	221	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6598 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 F124 IMMUNOGLOBULIN (KAPPA LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	29	0	0
			1668	1037	279	345	7			
1	C	216	Total	C	N	O	S	29	0	0
			1668	1037	279	345	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	ILE	conflict	UNP P01665
A	50	VAL	ALA	conflict	UNP P01665
A	55	LYS	GLU	conflict	UNP P01665
A	108	ARG	-	linker	UNP P01665
C	2	MET	ILE	conflict	UNP P01665
C	50	VAL	ALA	conflict	UNP P01665
C	55	LYS	GLU	conflict	UNP P01665
C	108	ARG	-	linker	UNP P01665

- Molecule 2 is a protein called F124 IMMUNOGLOBULIN (IGG1 HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	64	0	0
			1631	1032	264	327	8			
2	D	218	Total	C	N	O	S	64	0	0
			1631	1032	264	327	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	HIS	PRO	conflict	UNP Q65ZR6
B	58	GLY	SER	conflict	UNP Q65ZR6
B	94	ASN	ARG	conflict	UNP Q65ZR6
B	97	GLY	-	insertion	UNP Q65ZR6

Continued on next page...

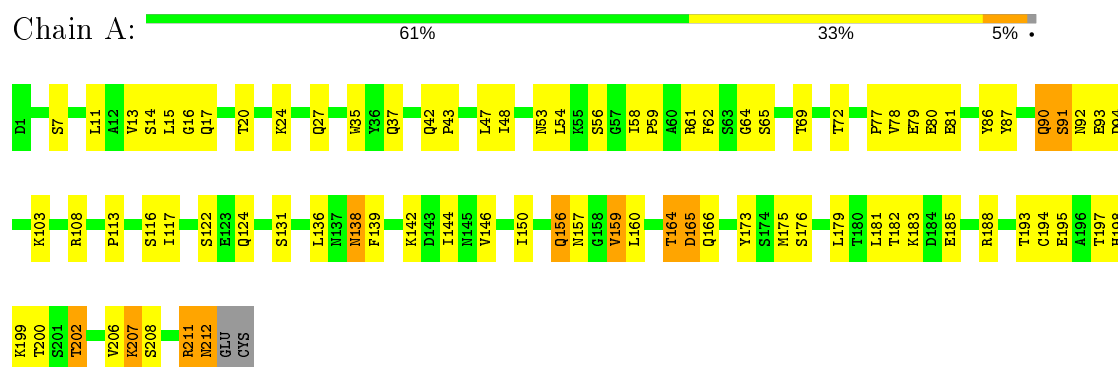
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	SER	-	insertion	UNP Q65ZR6
B	99	THR	SER	conflict	UNP Q65ZR6
B	100A	GLY	VAL	conflict	UNP Q65ZR6
B	101	ALA	ASP	conflict	UNP Q65ZR6
B	108	LEU	THR	conflict	UNP Q65ZR6
B	109	VAL	LEU	conflict	UNP Q65ZR6
B	113	ALA	SER	conflict	UNP Q65ZR6
B	114	ALA	-	linker	UNP Q65ZR6
D	41	HIS	PRO	conflict	UNP Q65ZR6
D	58	GLY	SER	conflict	UNP Q65ZR6
D	94	ASN	ARG	conflict	UNP Q65ZR6
D	97	GLY	-	insertion	UNP Q65ZR6
D	98	SER	-	insertion	UNP Q65ZR6
D	99	THR	SER	conflict	UNP Q65ZR6
D	100A	GLY	VAL	conflict	UNP Q65ZR6
D	101	ALA	ASP	conflict	UNP Q65ZR6
D	108	LEU	THR	conflict	UNP Q65ZR6
D	109	VAL	LEU	conflict	UNP Q65ZR6
D	113	ALA	SER	conflict	UNP Q65ZR6
D	114	ALA	-	linker	UNP Q65ZR6

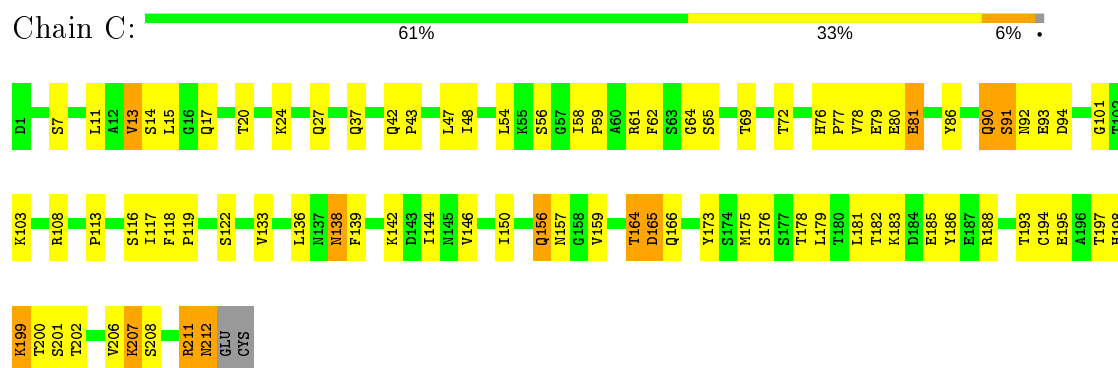
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

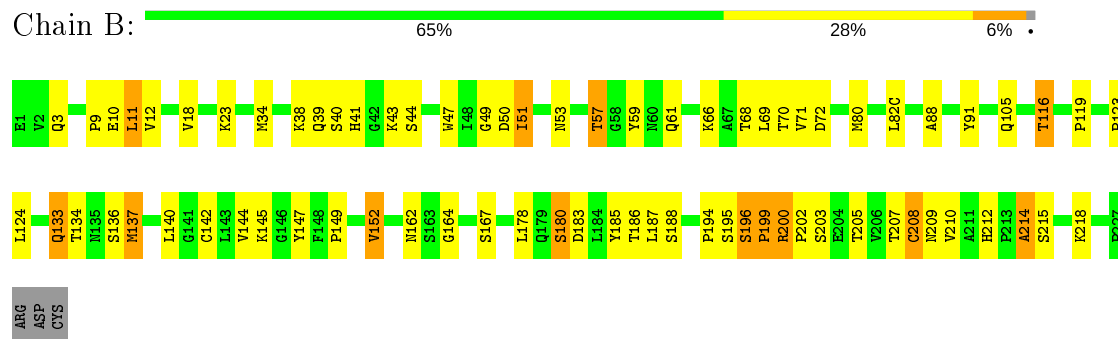
• Molecule 1: F124 IMMUNOGLOBULIN (KAPPA LIGHT CHAIN)



• Molecule 1: F124 IMMUNOGLOBULIN (KAPPA LIGHT CHAIN)



• Molecule 2: F124 IMMUNOGLOBULIN (IGG1 HEAVY CHAIN)



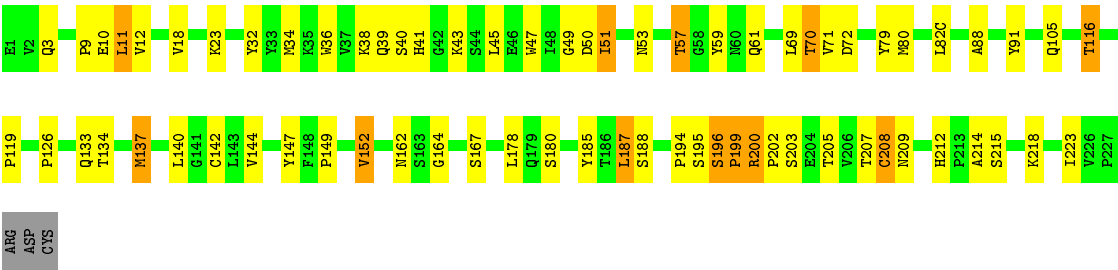
● Molecule 2: F124 IMMUNOGLOBULIN (IGG1 HEAVY CHAIN)

Chain D:

67%

26%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.70Å 54.00Å 120.00Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-3.00) 99.2 (29.87-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.184 , 0.271 0.184 , 0.264	Depositor DCC
R_{free} test set	878 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6598	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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	0.45	0/1706	0.64	0/2318
1	C	0.46	0/1706	0.65	0/2318
2	B	0.43	0/1674	0.70	0/2287
2	D	0.42	0/1674	0.70	0/2287
All	All	0.44	0/6760	0.67	0/9210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1668	0	1586	54	0
1	C	1668	0	1586	53	0
2	B	1631	0	1589	52	0
2	D	1631	0	1589	50	0
All	All	6598	0	6350	207	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 16.

All (207) 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:D:200:ARG:HG2	2:D:202:PRO:HA	1.32	1.11
2:B:200:ARG:HG2	2:B:202:PRO:HA	1.37	1.05
2:B:194:PRO:HD2	2:B:199:PRO:HG2	1.40	1.01
2:D:194:PRO:HD2	2:D:199:PRO:HG2	1.43	1.00
1:A:195:GLU:HB3	1:A:206:VAL:HG12	1.49	0.93
2:B:200:ARG:HB3	2:B:200:ARG:HH11	1.38	0.88
1:C:195:GLU:HB3	1:C:206:VAL:HG12	1.54	0.88
1:A:146:VAL:HG21	1:A:175:MET:HE3	1.55	0.85
2:D:200:ARG:HH11	2:D:200:ARG:HB3	1.45	0.81
1:A:27:GLN:O	1:A:69:THR:HG22	1.82	0.78
1:C:54:LEU:HD21	1:C:58:ILE:O	1.86	0.76
1:C:146:VAL:HG21	1:C:175:MET:HE3	1.68	0.76
1:A:54:LEU:HD21	1:A:58:ILE:O	1.86	0.76
2:D:70:THR:HG22	2:D:79:TYR:HB2	1.68	0.75
1:A:195:GLU:CB	1:A:206:VAL:HG12	2.17	0.74
1:C:13:VAL:HG11	1:C:78:VAL:HG21	1.70	0.73
2:D:196:SER:HB2	2:D:199:PRO:HD3	1.72	0.72
1:C:27:GLN:O	1:C:69:THR:HG22	1.90	0.71
1:A:90:GLN:HG2	1:A:92:ASN:H	1.55	0.71
1:C:90:GLN:HG2	1:C:92:ASN:H	1.56	0.70
1:C:195:GLU:CB	1:C:206:VAL:HG12	2.20	0.70
2:D:140:LEU:HD11	2:D:200:ARG:HD3	1.72	0.70
1:A:13:VAL:HG11	1:A:78:VAL:HG21	1.74	0.69
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.74	0.69
1:A:61:ARG:HD2	1:A:77:PRO:HD2	1.75	0.69
2:D:200:ARG:CG	2:D:202:PRO:HA	2.18	0.69
2:B:194:PRO:O	2:B:199:PRO:HD2	1.92	0.68
2:D:194:PRO:O	2:D:199:PRO:HD2	1.94	0.68
2:B:140:LEU:HD11	2:B:200:ARG:HD3	1.74	0.68
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.78	0.66
1:C:182:THR:OG1	1:C:185:GLU:HG3	1.96	0.65
1:C:61:ARG:HD2	1:C:77:PRO:HD2	1.78	0.65
2:D:149:PRO:HD2	2:D:214:ALA:CB	2.28	0.64
1:A:182:THR:OG1	1:A:185:GLU:HG3	1.98	0.64
2:B:194:PRO:HB2	2:B:199:PRO:HD2	1.80	0.64
2:D:18:VAL:HG12	2:D:82(C):LEU:HD11	1.80	0.63
2:B:12:VAL:HG11	2:B:82(C):LEU:HD12	1.81	0.63
1:C:188:ARG:O	1:C:188:ARG:HG3	1.97	0.63
2:D:178:LEU:HD13	2:D:185:TYR:CE1	2.33	0.63
2:B:196:SER:HB2	2:B:199:PRO:HD3	1.81	0.62
1:A:47:LEU:HD23	1:A:58:ILE:HD12	1.82	0.61
2:D:194:PRO:HB2	2:D:199:PRO:HD2	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:PRO:CD	2:B:199:PRO:HG2	2.24	0.61
1:C:146:VAL:HG21	1:C:175:MET:CE	2.31	0.60
2:D:57:THR:HG21	2:D:59:TYR:CE2	2.36	0.60
2:B:178:LEU:HD13	2:B:185:TYR:CE1	2.36	0.60
1:C:113:PRO:HG3	1:C:144:ILE:HD11	1.82	0.60
2:D:12:VAL:HG11	2:D:82(C):LEU:HD12	1.84	0.59
2:D:194:PRO:CD	2:D:199:PRO:HG2	2.26	0.59
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.84	0.59
2:D:212:HIS:HD1	2:D:215:SER:HG	1.49	0.59
2:B:18:VAL:HG12	2:B:82(C):LEU:HD11	1.85	0.59
2:B:207:THR:HG22	2:B:208:CYS:N	2.16	0.59
2:D:12:VAL:HG21	2:D:18:VAL:HB	1.85	0.59
1:C:164:THR:HG23	1:C:165:ASP:O	2.02	0.59
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.85	0.59
2:B:12:VAL:HG21	2:B:18:VAL:HB	1.85	0.59
2:B:200:ARG:HB3	2:B:200:ARG:NH1	2.16	0.59
2:B:59:TYR:CE1	2:B:69:LEU:HG	2.37	0.58
1:C:166:GLN:HG3	1:C:173:TYR:CZ	2.38	0.58
1:A:164:THR:HG23	1:A:165:ASP:O	2.03	0.58
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.87	0.57
1:A:48:ILE:HD13	1:A:64:GLY:N	2.20	0.56
1:C:61:ARG:CZ	1:C:79:GLU:HG3	2.35	0.56
1:A:206:VAL:O	1:A:207:LYS:HD3	2.05	0.56
1:C:206:VAL:O	1:C:207:LYS:HD3	2.06	0.56
1:A:15:LEU:HD21	1:A:80:GLU:HG3	1.86	0.56
2:D:207:THR:HG22	2:D:208:CYS:N	2.21	0.56
1:A:193:THR:OG1	1:A:208:SER:HB3	2.06	0.56
1:C:59:PRO:HG2	1:C:62:PHE:CE2	2.40	0.56
2:D:196:SER:HB2	2:D:199:PRO:CD	2.35	0.56
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.86	0.56
1:C:15:LEU:HD21	1:C:80:GLU:HG3	1.88	0.55
2:D:187:LEU:HD12	2:D:188:SER:N	2.21	0.55
1:C:47:LEU:HD23	1:C:58:ILE:HD12	1.89	0.55
2:B:149:PRO:HD2	2:B:214:ALA:CB	2.36	0.55
2:B:68:THR:O	2:B:68:THR:HG22	2.07	0.53
1:C:142:LYS:HD2	1:C:173:TYR:CE2	2.43	0.53
1:A:136:LEU:HD13	1:A:175:MET:CE	2.38	0.53
1:A:136:LEU:HD22	1:A:175:MET:HE1	1.91	0.53
1:A:61:ARG:CZ	1:A:79:GLU:HG3	2.37	0.53
2:B:200:ARG:CG	2:B:202:PRO:HA	2.25	0.53
1:C:14:SER:O	1:C:17:GLN:HB2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:PRO:HG2	1:C:62:PHE:HE2	1.74	0.53
2:B:145:LYS:CB	2:B:186:THR:HG23	2.39	0.52
2:D:57:THR:CG2	2:D:59:TYR:CE2	2.92	0.52
1:A:146:VAL:HG21	1:A:175:MET:CE	2.35	0.52
2:B:57:THR:HG21	2:B:59:TYR:CE2	2.45	0.52
1:A:37:GLN:HG3	1:A:86:TYR:CE2	2.44	0.52
1:C:37:GLN:HG3	1:C:86:TYR:CE2	2.44	0.52
2:D:207:THR:HG22	2:D:208:CYS:H	1.74	0.52
2:B:212:HIS:HD1	2:B:215:SER:HG	1.57	0.52
1:C:166:GLN:HG3	1:C:173:TYR:CE1	2.44	0.52
2:B:39:GLN:O	2:B:88:ALA:HB1	2.10	0.52
2:D:9:PRO:C	2:D:10:GLU:HG2	2.30	0.51
1:A:14:SER:O	1:A:17:GLN:HB2	2.10	0.51
1:C:48:ILE:HD13	1:C:64:GLY:N	2.25	0.51
1:C:136:LEU:HD13	1:C:175:MET:CE	2.40	0.51
2:B:194:PRO:C	2:B:199:PRO:HD2	2.31	0.50
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.92	0.50
2:B:194:PRO:HB2	2:B:199:PRO:CD	2.42	0.50
2:D:59:TYR:CE1	2:D:69:LEU:HG	2.46	0.50
2:B:123:PRO:O	2:B:124:LEU:HD23	2.11	0.50
2:B:71:VAL:HG22	2:B:72:ASP:N	2.26	0.50
1:C:136:LEU:N	1:C:136:LEU:HD12	2.26	0.50
2:D:194:PRO:C	2:D:199:PRO:HD2	2.33	0.49
1:A:59:PRO:HG2	1:A:62:PHE:CE2	2.47	0.49
1:A:117:ILE:HD12	1:A:194:CYS:HB3	1.94	0.49
1:A:142:LYS:HD2	1:A:173:TYR:CE2	2.48	0.49
2:B:11:LEU:HD12	2:B:116:THR:HG22	1.95	0.49
1:A:188:ARG:O	1:A:188:ARG:HG3	2.12	0.49
1:A:156:GLN:CD	1:A:156:GLN:H	2.16	0.49
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.95	0.49
1:C:90:GLN:NE2	1:C:93:GLU:H	2.11	0.48
2:B:11:LEU:CD1	2:B:116:THR:HG22	2.43	0.48
1:C:20:THR:HG23	1:C:72:THR:HG23	1.96	0.48
2:B:59:TYR:HE1	2:B:69:LEU:HG	1.77	0.48
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.49	0.48
2:D:71:VAL:HG22	2:D:72:ASP:N	2.27	0.48
1:A:90:GLN:NE2	1:A:93:GLU:H	2.11	0.48
2:D:119:PRO:HB2	2:D:144:VAL:HG13	1.96	0.48
1:A:124:GLN:HE22	1:A:131:SER:CB	2.27	0.47
1:C:138:ASN:N	1:C:138:ASN:OD1	2.48	0.47
2:D:11:LEU:HD12	2:D:116:THR:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:N	1:A:138:ASN:OD1	2.47	0.47
1:C:61:ARG:HD2	1:C:77:PRO:O	2.14	0.47
1:C:211:ARG:C	1:C:212:ASN:ND2	2.67	0.47
2:B:187:LEU:HD12	2:B:188:SER:N	2.30	0.47
2:B:57:THR:CG2	2:B:59:TYR:CE2	2.97	0.47
1:C:156:GLN:CD	1:C:156:GLN:H	2.18	0.47
2:D:194:PRO:HB2	2:D:199:PRO:CD	2.45	0.47
1:C:20:THR:HG23	1:C:72:THR:CG2	2.45	0.46
1:A:136:LEU:HD13	1:A:175:MET:HE2	1.97	0.46
2:B:196:SER:HB2	2:B:199:PRO:CD	2.43	0.46
2:B:9:PRO:C	2:B:10:GLU:HG2	2.35	0.46
1:A:159:VAL:O	1:A:160:LEU:HD23	2.16	0.46
2:B:144:VAL:HG22	2:B:210:VAL:HG21	1.97	0.46
2:D:69:LEU:HD23	2:D:69:LEU:N	2.30	0.46
1:A:166:GLN:HG3	1:A:173:TYR:CZ	2.51	0.46
1:C:79:GLU:HB3	1:C:81:GLU:OE2	2.16	0.45
1:A:211:ARG:C	1:A:212:ASN:ND2	2.70	0.45
1:C:193:THR:OG1	1:C:208:SER:HB3	2.15	0.45
2:D:47:TRP:NE1	2:D:50:ASP:OD1	2.46	0.45
2:D:39:GLN:O	2:D:88:ALA:HB1	2.17	0.45
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.82	0.45
1:A:117:ILE:HD12	1:A:194:CYS:CB	2.47	0.45
1:A:113:PRO:HG3	1:A:144:ILE:HD11	1.99	0.45
1:A:136:LEU:HD12	1:A:136:LEU:N	2.32	0.45
1:C:13:VAL:CG1	1:C:78:VAL:HG21	2.44	0.45
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.52	0.44
1:C:136:LEU:HD22	1:C:175:MET:HE1	1.98	0.44
1:C:61:ARG:CD	1:C:77:PRO:HD2	2.47	0.44
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.00	0.44
1:C:76:HIS:HA	1:C:77:PRO:HA	1.82	0.44
2:D:152:VAL:HG23	2:D:187:LEU:HD21	2.00	0.44
1:C:43:PRO:HB3	2:D:91:TYR:CE1	2.53	0.44
2:D:34:MET:HB3	2:D:51:ILE:HG22	1.99	0.44
2:D:200:ARG:HB3	2:D:200:ARG:NH1	2.22	0.43
1:A:136:LEU:HD21	1:A:146:VAL:HG22	2.00	0.43
2:D:11:LEU:CD1	2:D:116:THR:HG22	2.48	0.43
1:C:118:PHE:HA	1:C:119:PRO:HD3	1.89	0.43
2:D:126:PRO:HD3	2:D:140:LEU:CD2	2.48	0.43
2:B:47:TRP:NE1	2:B:50:ASP:OD1	2.46	0.43
2:D:32:TYR:N	2:D:32:TYR:CD1	2.87	0.43
2:B:207:THR:HG22	2:B:208:CYS:H	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:TYR:CE2	1:C:211:ARG:HD3	2.54	0.43
1:A:61:ARG:HD2	1:A:77:PRO:O	2.19	0.43
1:A:48:ILE:HD13	1:A:64:GLY:H	1.82	0.43
2:B:178:LEU:HD13	2:B:185:TYR:CZ	2.54	0.43
1:A:59:PRO:HG2	1:A:62:PHE:HE2	1.84	0.43
2:B:207:THR:CG2	2:B:208:CYS:N	2.82	0.43
2:B:34:MET:HB3	2:B:51:ILE:HG22	2.01	0.43
2:B:71:VAL:CG2	2:B:72:ASP:N	2.82	0.43
1:A:61:ARG:CD	1:A:77:PRO:HD2	2.46	0.42
1:A:35:TRP:HA	1:A:87:TYR:O	2.19	0.42
2:D:36:TRP:CD1	2:D:69:LEU:HD13	2.53	0.42
1:A:90:GLN:HG2	1:A:91:SER:N	2.30	0.42
2:B:69:LEU:N	2:B:69:LEU:HD23	2.34	0.42
1:C:113:PRO:HG3	1:C:144:ILE:CD1	2.49	0.42
1:C:86:TYR:O	1:C:101:GLY:HA2	2.20	0.42
1:A:48:ILE:HA	1:A:53:ASN:O	2.19	0.42
2:D:162:ASN:C	2:D:164:GLY:H	2.23	0.42
2:B:11:LEU:HG	2:B:149:PRO:HG3	2.02	0.42
1:A:90:GLN:HE21	1:A:93:GLU:H	1.66	0.41
2:B:162:ASN:C	2:B:164:GLY:H	2.24	0.41
2:B:144:VAL:CG2	2:B:210:VAL:HG21	2.50	0.41
2:B:152:VAL:HG23	2:B:187:LEU:HD21	2.02	0.41
1:C:133:VAL:HG22	1:C:178:THR:HG23	2.02	0.41
2:D:137:MET:HE1	2:D:194:PRO:HG3	2.01	0.41
2:D:140:LEU:HD22	2:D:223:ILE:HG21	2.02	0.41
2:B:137:MET:HE1	2:B:194:PRO:CA	2.51	0.41
2:B:119:PRO:HB2	2:B:144:VAL:HG13	2.02	0.41
2:B:66:LYS:HB2	2:B:66:LYS:HE2	1.93	0.41
1:A:43:PRO:HB3	2:B:91:TYR:CE1	2.56	0.41
1:A:166:GLN:HG3	1:A:173:TYR:CE1	2.56	0.41
1:A:37:GLN:HB2	1:A:47:LEU:CD1	2.48	0.41
1:C:117:ILE:HD12	1:C:194:CYS:HB3	2.02	0.41
1:C:90:GLN:HE21	1:C:93:GLU:H	1.68	0.41
2:D:140:LEU:CD1	2:D:200:ARG:HD3	2.46	0.41
1:C:90:GLN:HG2	1:C:91:SER:N	2.35	0.41
2:D:59:TYR:HE1	2:D:69:LEU:HG	1.85	0.41
1:A:20:THR:HG23	1:A:72:THR:CG2	2.51	0.40
2:D:71:VAL:CG2	2:D:72:ASP:N	2.83	0.40
2:B:180:SER:HB2	2:B:183:ASP:H	1.66	0.40
1:C:54:LEU:CD2	1:C:58:ILE:HB	2.52	0.40
1:A:16:GLY:HA2	1:A:77:PRO:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:SER:CB	2:D:199:PRO:CD	3.00	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	214/218 (98%)	193 (90%)	19 (9%)	2 (1%)	17	55
1	C	214/218 (98%)	199 (93%)	11 (5%)	4 (2%)	8	36
2	B	216/221 (98%)	190 (88%)	19 (9%)	7 (3%)	4	22
2	D	216/221 (98%)	189 (88%)	21 (10%)	6 (3%)	5	25
All	All	860/878 (98%)	771 (90%)	70 (8%)	19 (2%)	6	31

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	41	HIS
2	D	41	HIS
2	B	137	MET
1	C	199	LYS
1	C	201	SER
2	D	134	THR
1	A	202	THR
1	A	211	ARG
2	B	133	GLN
2	B	199	PRO
2	B	203	SER
1	C	211	ARG
2	D	137	MET
2	D	199	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	203	SER
2	B	43	LYS
2	B	214	ALA
1	C	200	THR
2	D	43	LYS

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	190/192 (99%)	160 (84%)	30 (16%)	2	12
1	C	190/192 (99%)	160 (84%)	30 (16%)	2	12
2	B	185/188 (98%)	157 (85%)	28 (15%)	3	14
2	D	185/188 (98%)	159 (86%)	26 (14%)	3	16
All	All	750/760 (99%)	636 (85%)	114 (15%)	3	14

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	11	LEU
1	A	24	LYS
1	A	42	GLN
1	A	56	SER
1	A	65	SER
1	A	81	GLU
1	A	90	GLN
1	A	91	SER
1	A	94	ASP
1	A	103	LYS
1	A	108	ARG
1	A	116	SER
1	A	122	SER
1	A	138	ASN
1	A	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	157	ASN
1	A	159	VAL
1	A	164	THR
1	A	165	ASP
1	A	176	SER
1	A	181	LEU
1	A	183	LYS
1	A	197	THR
1	A	198	HIS
1	A	199	LYS
1	A	200	THR
1	A	202	THR
1	A	207	LYS
1	A	212	ASN
2	B	3	GLN
2	B	11	LEU
2	B	23	LYS
2	B	38	LYS
2	B	40	SER
2	B	44	SER
2	B	51	ILE
2	B	53	ASN
2	B	57	THR
2	B	61	GLN
2	B	70	THR
2	B	80	MET
2	B	105	GLN
2	B	116	THR
2	B	133	GLN
2	B	134	THR
2	B	136	SER
2	B	142	CYS
2	B	152	VAL
2	B	167	SER
2	B	180	SER
2	B	195	SER
2	B	196	SER
2	B	200	ARG
2	B	205	THR
2	B	208	CYS
2	B	209	ASN
2	B	218	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	7	SER
1	C	11	LEU
1	C	13	VAL
1	C	24	LYS
1	C	42	GLN
1	C	56	SER
1	C	65	SER
1	C	81	GLU
1	C	90	GLN
1	C	91	SER
1	C	94	ASP
1	C	103	LYS
1	C	108	ARG
1	C	116	SER
1	C	122	SER
1	C	138	ASN
1	C	156	GLN
1	C	157	ASN
1	C	159	VAL
1	C	164	THR
1	C	165	ASP
1	C	176	SER
1	C	181	LEU
1	C	183	LYS
1	C	197	THR
1	C	198	HIS
1	C	199	LYS
1	C	202	THR
1	C	207	LYS
1	C	212	ASN
2	D	3	GLN
2	D	11	LEU
2	D	23	LYS
2	D	38	LYS
2	D	40	SER
2	D	51	ILE
2	D	53	ASN
2	D	57	THR
2	D	61	GLN
2	D	70	THR
2	D	80	MET
2	D	105	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	116	THR
2	D	133	GLN
2	D	142	CYS
2	D	152	VAL
2	D	167	SER
2	D	180	SER
2	D	187	LEU
2	D	195	SER
2	D	196	SER
2	D	200	ARG
2	D	205	THR
2	D	208	CYS
2	D	209	ASN
2	D	218	LYS

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

Mol	Chain	Res	Type
1	A	17	GLN
1	A	53	ASN
1	A	90	GLN
1	A	157	ASN
1	A	212	ASN
2	B	53	ASN
2	B	172	HIS
1	C	17	GLN
1	C	90	GLN
1	C	157	ASN
1	C	212	ASN
2	D	53	ASN
2	D	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	212/218 (97%)	-0.74	0 100 100	3, 17, 42, 62	0
1	C	212/218 (97%)	-0.67	0 100 100	6, 21, 47, 66	0
2	B	209/221 (94%)	-0.65	0 100 100	2, 20, 54, 73	1 (0%)
2	D	209/221 (94%)	-0.66	0 100 100	4, 23, 49, 82	1 (0%)
All	All	842/878 (95%)	-0.68	0 100 100	2, 20, 49, 82	2 (0%)

There are no RSRZ outliers to report.

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 carbohydrates 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.