



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 PM UTC

PDB ID : 6J6Y / pdb_00006j6y
Title : FGFR4 D2 - Fab complex
Authors : Takahashi, M.; Hanzawa, H.
Deposited on : 2019-01-16
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:

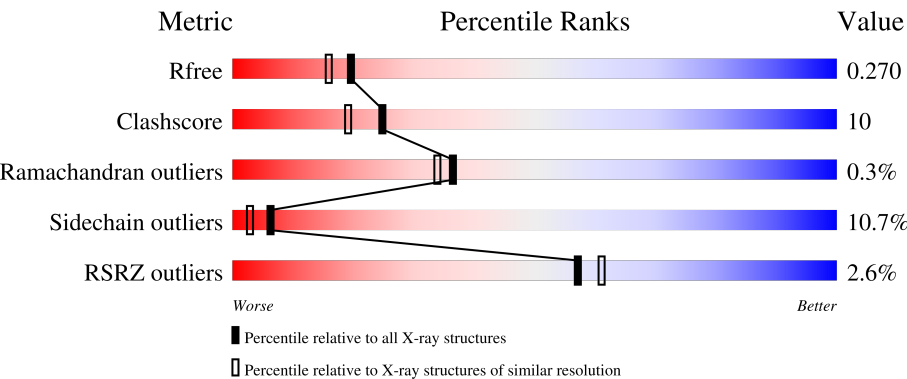
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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	A	104	5% 78%17% . .
1	D	104	6% 62%31% . .
2	B	249	% 67%16% . 14%
2	E	249	3% 69%16% . 13%
3	C	243	% 72%14% . 12%

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Mol	Chain	Length	Quality of chain
3	F	243	2% 60% 23% • 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8410 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 Fibroblast growth factor receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			793	504	144	141	4			
1	D	101	Total	C	N	O	S	0	0	0
			798	510	146	138	4			

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1598	1006	269	317	6			
2	E	216	Total	C	N	O	S	0	0	0
			1600	1006	269	318	7			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1587	991	268	324	4			
3	F	213	Total	C	N	O	S	0	0	0
			1579	987	268	320	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	113	Total	O	0	0
			113	113		
4	C	76	Total	O	0	0
			76	76		
4	D	44	Total	O	0	0
			44	44		

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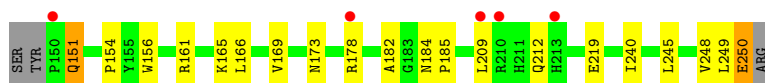
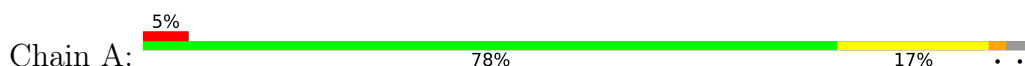
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	116	Total 116	O 116	0	0
4	F	69	Total 69	O 69	0	0

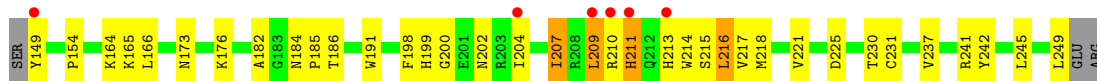
3 Residue-property plots [i](#)

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: Fibroblast growth factor receptor 4



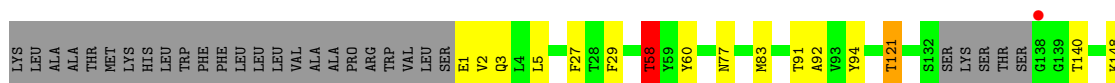
- Molecule 1: Fibroblast growth factor receptor 4



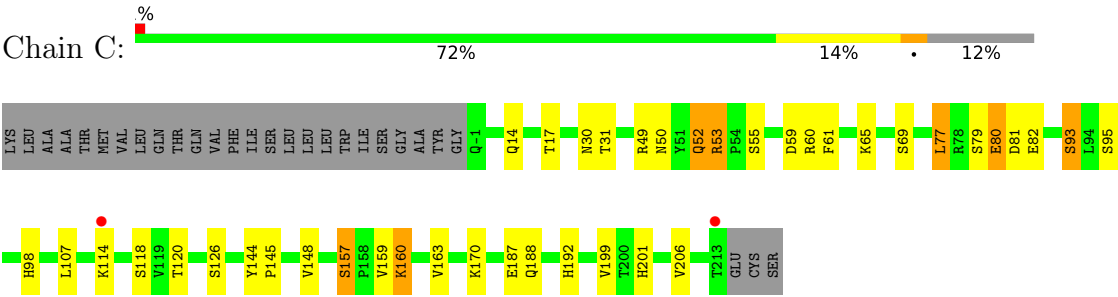
- Molecule 2: Fab Heavy chain



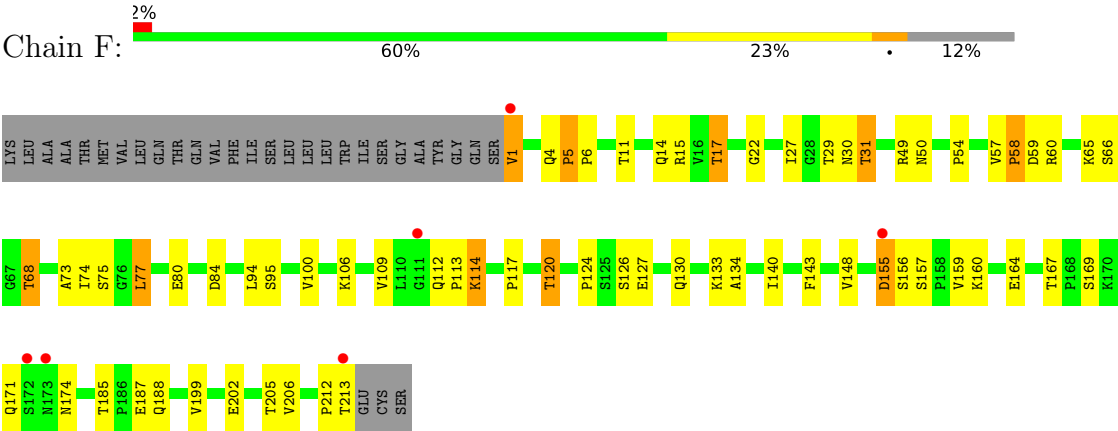
- Molecule 2: Fab Heavy chain



- Molecule 3: Fab light chain



● Molecule 3: Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.22Å 119.17Å 105.10Å 90.00° 97.29° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 20.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.15) 99.7 (20.00-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.193 , 0.258 0.207 , 0.270	Depositor DCC
R_{free} test set	3449 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8410	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/816	1.06	0/1112
1	D	0.76	0/823	1.06	2/1123 (0.2%)
2	B	0.80	0/1635	1.04	2/2226 (0.1%)
2	E	0.78	0/1637	1.03	1/2230 (0.0%)
3	C	0.75	0/1627	1.05	2/2226 (0.1%)
3	F	0.77	0/1619	1.07	5/2214 (0.2%)
All	All	0.77	0/8157	1.05	12/11131 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	58	THR	CB-CA-C	6.25	122.07	109.38
3	C	157	SER	CA-C-N	6.07	126.09	119.90
3	C	157	SER	C-N-CA	6.07	126.09	119.90
1	D	186	THR	CA-C-N	-5.85	114.57	120.31
1	D	186	THR	C-N-CA	-5.85	114.57	120.31
2	B	217	GLU	CA-C-N	5.67	125.69	119.90
2	B	217	GLU	C-N-CA	5.67	125.69	119.90
3	F	17	THR	CB-CA-C	5.37	119.08	110.16
3	F	5	PRO	CA-C-N	5.36	125.00	119.05
3	F	5	PRO	C-N-CA	5.36	125.00	119.05
3	F	58	PRO	N-CA-CB	5.15	107.89	103.31
3	F	120	THR	CB-CA-C	5.01	118.88	109.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	793	0	769	14	0
1	D	798	0	774	27	0
2	B	1598	0	1559	33	0
2	E	1600	0	1553	38	0
3	C	1587	0	1535	19	0
3	F	1579	0	1535	41	0
4	A	37	0	0	0	0
4	B	113	0	0	3	0
4	C	76	0	0	0	0
4	D	44	0	0	1	0
4	E	116	0	0	7	0
4	F	69	0	0	3	0
All	All	8410	0	7725	154	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 10.

All (154) 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:E:148:LYS:NZ	3:F:133:LYS:HE2	1.73	1.02
2:B:83:MET:HE2	2:B:86:LEU:HD21	1.47	0.97
2:E:148:LYS:HZ1	3:F:133:LYS:HE2	1.30	0.91
2:E:161:SER:H	2:E:202:ASN:HD21	1.20	0.87
1:D:198:PHE:CE2	1:D:207:ILE:HD11	2.12	0.85
2:B:58:THR:HG23	2:B:60:TYR:CE2	2.11	0.84
2:E:174:VAL:HG21	3:F:164:GLU:HB3	1.59	0.82
2:E:58:THR:HG23	2:E:60:TYR:CE2	2.20	0.75
2:E:148:LYS:HZ3	3:F:133:LYS:HE2	1.52	0.73
2:B:190:PRO:O	2:B:193:SER:HB2	1.89	0.72
2:E:58:THR:HG23	2:E:60:TYR:HE2	1.55	0.72
3:C:187:GLU:OE2	3:C:187:GLU:N	2.20	0.71
2:B:193:SER:O	2:B:196:THR:HB	1.89	0.71
1:D:165:LYS:NZ	3:F:30:ASN:HD21	1.89	0.71
3:F:112:GLN:HG2	3:F:113:PRO:HD2	1.73	0.71
2:B:196:THR:HG22	4:E:353:HOH:O	1.91	0.70
1:A:165:LYS:HE2	3:C:30:ASN:ND2	2.08	0.68
1:A:151:GLN:HB2	1:A:184:ASN:O	1.94	0.67
2:B:156:THR:HG21	4:E:346:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:VAL:CG2	3:F:164:GLU:HB3	2.24	0.67
2:B:197:GLN:HG2	4:B:344:HOH:O	1.95	0.66
2:B:196:THR:CG2	4:E:353:HOH:O	2.44	0.66
2:B:58:THR:HG21	4:B:338:HOH:O	1.96	0.66
2:E:200:ILE:HD13	2:E:213:ASP:HB3	1.78	0.66
2:B:161:SER:O	2:E:156:THR:HG21	1.97	0.65
1:D:176:LYS:HG3	1:D:217:VAL:HG22	1.79	0.65
1:D:184:ASN:HA	1:D:185:PRO:C	2.21	0.65
2:B:139:GLY:O	2:B:191:SER:HB2	1.97	0.65
2:E:200:ILE:HD11	2:E:202:ASN:OD1	1.97	0.65
2:B:58:THR:HG23	2:B:60:TYR:HE2	1.58	0.65
3:F:133:LYS:HE3	4:F:305:HOH:O	1.97	0.65
3:C:53:ARG:HD3	3:C:61:PHE:O	1.99	0.63
3:C:93:SER:OG	3:C:98:HIS:NE2	2.31	0.62
3:F:84:ASP:OD1	3:F:106:LYS:HD2	1.99	0.62
3:F:112:GLN:CG	3:F:113:PRO:HD2	2.29	0.62
1:D:210:ARG:HB2	1:D:213:HIS:HB2	1.81	0.62
3:F:155:ASP:O	3:F:156:SER:HB3	1.99	0.61
3:C:188:GLN:O	3:C:192:HIS:HD2	1.83	0.61
2:E:194:LEU:HG	2:E:218:PRO:HG3	1.81	0.61
2:E:197:GLN:HB3	4:E:367:HOH:O	1.98	0.61
3:C:82:GLU:OE1	3:C:170:LYS:HE3	2.02	0.60
2:E:161:SER:N	2:E:202:ASN:HD21	1.98	0.59
3:F:22:GLY:C	3:F:68:THR:HG23	2.29	0.58
1:A:165:LYS:HE2	3:C:30:ASN:HD21	1.68	0.57
2:E:58:THR:HG21	4:E:379:HOH:O	2.05	0.57
2:B:58:THR:CG2	2:B:60:TYR:HE2	2.17	0.57
2:B:190:PRO:HD2	2:B:193:SER:OG	2.05	0.56
2:E:121:THR:HG22	2:E:208:SER:HB3	1.88	0.56
2:E:91:THR:O	2:E:92:ALA:HB2	2.06	0.56
2:B:124:PRO:HB3	2:B:150:TYR:HB3	1.87	0.56
3:C:80:GLU:HG2	3:C:80:GLU:O	2.05	0.56
1:A:161:ARG:NH1	1:A:178:ARG:NH2	2.54	0.55
2:B:12:VAL:CG2	2:B:18:LEU:HD22	2.37	0.55
2:E:183:LEU:HD12	2:E:183:LEU:C	2.31	0.55
1:D:165:LYS:HZ2	3:F:30:ASN:HD21	1.53	0.55
3:F:11:THR:O	3:F:14:GLN:HG2	2.06	0.54
1:D:210:ARG:CB	1:D:213:HIS:HB2	2.38	0.54
2:B:183:LEU:HD12	2:B:183:LEU:C	2.32	0.54
2:E:1:GLU:HG2	2:E:2:VAL:N	2.23	0.54
1:D:210:ARG:O	1:D:214:TRP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:LEU:HD11	2:E:188:THR:HG22	1.90	0.53
3:C:77:LEU:HD21	3:C:107:LEU:HD21	1.90	0.53
3:F:11:THR:O	3:F:14:GLN:CG	2.57	0.53
1:A:166:LEU:HD22	1:A:245:LEU:HD22	1.90	0.52
3:F:68:THR:HG22	4:F:335:HOH:O	2.09	0.52
2:B:206:LYS:HD2	2:E:163:ALA:O	2.09	0.52
2:E:193:SER:HB3	2:E:199:TYR:OH	2.10	0.52
2:E:121:THR:HG21	2:E:207:PRO:O	2.10	0.51
2:B:110:GLN:H	2:B:110:GLN:HE21	1.58	0.51
1:D:165:LYS:HZ3	3:F:30:ASN:HD21	1.59	0.50
1:D:209:LEU:HD12	1:D:216:LEU:HA	1.93	0.50
3:C:160:LYS:HA	3:C:160:LYS:HE2	1.94	0.50
2:B:105:VAL:HG11	2:B:108:TRP:CE2	2.47	0.49
1:D:242:TYR:HD1	3:F:29:THR:CG2	2.25	0.49
2:E:215:ARG:HD3	2:E:217:GLU:HG3	1.94	0.49
3:F:54:PRO:HD2	3:F:57:VAL:HG21	1.95	0.49
3:F:49:ARG:O	3:F:50:ASN:HB2	2.12	0.49
2:E:1:GLU:HG2	2:E:2:VAL:H	1.76	0.48
2:E:83:MET:HE1	2:E:94:TYR:CZ	2.49	0.48
1:D:166:LEU:HD22	1:D:245:LEU:HD22	1.96	0.48
1:D:241:ARG:HD2	4:D:320:HOH:O	2.14	0.48
3:F:126:SER:O	3:F:130:GLN:HG2	2.13	0.47
2:E:200:ILE:CD1	2:E:213:ASP:HB3	2.43	0.47
2:B:6:GLU:OE2	2:B:95:TYR:HA	2.14	0.47
3:F:1:VAL:HG12	3:F:100:VAL:HG11	1.97	0.47
1:D:204:ILE:HD12	1:D:204:ILE:H	1.79	0.47
3:F:27:ILE:O	3:F:65:LYS:HE3	2.14	0.47
3:C:144:TYR:O	3:C:201:HIS:HE1	1.97	0.47
1:D:200:GLY:CA	1:D:207:ILE:HD12	2.45	0.47
2:E:161:SER:H	2:E:202:ASN:ND2	2.01	0.47
2:E:200:ILE:C	2:E:200:ILE:HD12	2.40	0.47
2:E:189:VAL:HG11	2:E:199:TYR:CE1	2.50	0.47
2:B:129:LEU:HD21	2:B:146:LEU:HB2	1.97	0.47
3:C:144:TYR:CG	3:C:145:PRO:HA	2.50	0.47
2:E:155:VAL:HG23	2:E:183:LEU:HD21	1.97	0.46
3:F:17:THR:HG22	3:F:73:ALA:HA	1.97	0.46
3:F:185:THR:OG1	3:F:188:GLN:HG3	2.15	0.46
1:D:173:ASN:O	1:D:221:VAL:HG13	2.15	0.46
1:D:218:MET:HE1	1:D:225:ASP:HB3	1.98	0.46
2:B:12:VAL:HG21	2:B:18:LEU:HD22	1.98	0.46
2:B:13:GLN:HG2	4:B:343:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:60:ARG:HB2	3:F:75:SER:O	2.16	0.46
3:F:30:ASN:O	3:F:65:LYS:NZ	2.47	0.45
2:B:68:PHE:CZ	2:B:83:MET:HE3	2.52	0.45
1:D:149:TYR:CD1	1:D:149:TYR:C	2.95	0.45
1:D:154:PRO:HA	1:D:182:ALA:O	2.17	0.45
3:F:22:GLY:O	3:F:68:THR:CG2	2.64	0.45
3:F:77:LEU:HD11	3:F:109:VAL:HG22	1.97	0.45
1:A:250:GLU:OE2	1:A:250:GLU:HA	2.17	0.45
2:B:167:GLY:O	2:B:187:VAL:HA	2.16	0.45
3:F:54:PRO:HD2	3:F:57:VAL:CG2	2.47	0.44
1:D:211:HIS:ND1	1:D:211:HIS:O	2.49	0.44
3:C:49:ARG:HB2	3:C:52:GLN:HG3	2.00	0.44
2:E:58:THR:HG22	4:E:364:HOH:O	2.17	0.44
2:E:148:LYS:HZ3	3:F:133:LYS:CE	2.25	0.43
1:D:242:TYR:CD1	3:F:29:THR:HG22	2.52	0.43
3:F:14:GLN:O	3:F:77:LEU:HB2	2.18	0.43
1:A:165:LYS:CE	3:C:30:ASN:HD21	2.32	0.43
3:C:60:ARG:NH2	3:C:81:ASP:OD1	2.51	0.43
2:B:140:THR:CG2	2:B:188:THR:HG23	2.49	0.43
3:F:31:THR:HG22	4:F:303:HOH:O	2.19	0.43
1:A:184:ASN:HA	1:A:185:PRO:C	2.43	0.43
3:F:117:PRO:HB3	3:F:143:PHE:HB3	2.00	0.43
2:B:194:LEU:HD12	2:B:194:LEU:HA	1.89	0.43
3:F:15:ARG:HA	3:F:74:ILE:O	2.19	0.43
1:A:156:TRP:CE2	1:A:240:ILE:HD12	2.54	0.42
1:D:209:LEU:CD1	1:D:216:LEU:HA	2.48	0.42
1:D:242:TYR:HD1	3:F:29:THR:HG22	1.85	0.42
2:E:155:VAL:HG12	2:E:205:HIS:CD2	2.54	0.42
3:F:5:PRO:HA	3:F:6:PRO:HD2	1.80	0.42
2:B:51:ILE:HD11	2:B:55:GLY:HA2	2.01	0.42
1:D:200:GLY:N	1:D:207:ILE:HD12	2.34	0.42
1:A:169:VAL:O	1:A:248:VAL:HA	2.20	0.42
2:B:219:LYS:O	2:B:220:SER:HB3	2.20	0.42
3:C:50:ASN:OD1	3:C:65:LYS:HD3	2.20	0.42
2:E:164:LEU:C	2:E:164:LEU:CD2	2.92	0.42
2:E:155:VAL:CG2	2:E:183:LEU:HD21	2.49	0.42
3:C:144:TYR:O	3:C:201:HIS:CE1	2.73	0.41
1:A:173:ASN:N	1:A:173:ASN:HD22	2.18	0.41
2:B:132:SER:O	2:B:219:LYS:HD3	2.20	0.41
3:F:58:PRO:HB2	3:F:60:ARG:HG2	2.01	0.41
2:B:58:THR:CG2	2:B:60:TYR:CE2	2.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:GLN:O	3:C:77:LEU:HB2	2.21	0.41
1:D:191:TRP:CZ3	1:D:231:CYS:HB3	2.56	0.41
1:A:154:PRO:HA	1:A:182:ALA:O	2.20	0.41
1:D:149:TYR:C	1:D:149:TYR:HD1	2.28	0.41
1:A:212:GLN:HA	1:A:212:GLN:OE1	2.20	0.41
1:D:198:PHE:HE2	1:D:207:ILE:HD11	1.77	0.41
2:E:27:PHE:CE2	2:E:29:PHE:HA	2.56	0.41
1:A:161:ARG:HH11	1:A:178:ARG:NH2	2.18	0.40
3:F:124:PRO:HG3	3:F:134:ALA:HB1	2.04	0.40
3:F:114:LYS:HG2	3:F:202:GLU:HG3	2.04	0.40
3:C:31:THR:HB	3:C:49:ARG:HA	2.03	0.40
2:E:206:LYS:HE3	4:E:409:HOH:O	2.20	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	99/104 (95%)	97 (98%)	2 (2%)	0	100	100
1	D	99/104 (95%)	96 (97%)	3 (3%)	0	100	100
2	B	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
2	E	212/249 (85%)	202 (95%)	9 (4%)	1 (0%)	24	20
3	C	213/243 (88%)	205 (96%)	7 (3%)	1 (0%)	24	20
3	F	211/243 (87%)	204 (97%)	6 (3%)	1 (0%)	24	20
All	All	1045/1192 (88%)	1010 (97%)	32 (3%)	3 (0%)	36	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	59	ASP

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Mol	Chain	Res	Type
3	C	59	ASP
2	E	195	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/89 (93%)	78 (94%)	5 (6%)	17	13
1	D	83/89 (93%)	72 (87%)	11 (13%)	4	1
2	B	178/208 (86%)	164 (92%)	14 (8%)	11	7
2	E	178/208 (86%)	163 (92%)	15 (8%)	10	6
3	C	178/203 (88%)	157 (88%)	21 (12%)	5	2
3	F	177/203 (87%)	149 (84%)	28 (16%)	2	1
All	All	877/1000 (88%)	783 (89%)	94 (11%)	6	3

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	209	LEU
1	A	219	GLU
1	A	249	LEU
1	A	250	GLU
2	B	3	GLN
2	B	7	SER
2	B	12	VAL
2	B	22	CYS
2	B	58	THR
2	B	87	ARG
2	B	99	LEU
2	B	110	GLN
2	B	120	SER
2	B	156	THR
2	B	194	LEU

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Mol	Chain	Res	Type
2	B	196	THR
2	B	211	LYS
2	B	216	VAL
3	C	17	THR
3	C	52	GLN
3	C	53	ARG
3	C	55	SER
3	C	69	SER
3	C	77	LEU
3	C	79	SER
3	C	80	GLU
3	C	93	SER
3	C	95	SER
3	C	114	LYS
3	C	118	SER
3	C	120	THR
3	C	126	SER
3	C	148	VAL
3	C	157	SER
3	C	159	VAL
3	C	160	LYS
3	C	163	VAL
3	C	199	VAL
3	C	206	VAL
1	D	164	LYS
1	D	199	HIS
1	D	202	ASN
1	D	207	ILE
1	D	209	LEU
1	D	211	HIS
1	D	215	SER
1	D	216	LEU
1	D	230	THR
1	D	237	VAL
1	D	249	LEU
2	E	3	GLN
2	E	5	LEU
2	E	58	THR
2	E	77	ASN
2	E	121	THR
2	E	140	THR
2	E	164	LEU

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Mol	Chain	Res	Type
2	E	192	SER
2	E	194	LEU
2	E	200	ILE
2	E	211	LYS
2	E	214	LYS
2	E	215	ARG
2	E	216	VAL
2	E	221	CYS
3	F	1	VAL
3	F	4	GLN
3	F	31	THR
3	F	66	SER
3	F	68	THR
3	F	77	LEU
3	F	80	GLU
3	F	94	LEU
3	F	95	SER
3	F	114	LYS
3	F	120	THR
3	F	127	GLU
3	F	140	ILE
3	F	148	VAL
3	F	155	ASP
3	F	157	SER
3	F	159	VAL
3	F	160	LYS
3	F	167	THR
3	F	169	SER
3	F	171	GLN
3	F	174	ASN
3	F	187	GLU
3	F	199	VAL
3	F	205	THR
3	F	206	VAL
3	F	212	PRO
3	F	213	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	211	HIS
1	A	243	ASN
2	B	39	GLN
2	B	110	GLN
3	C	30	ASN
3	C	37	GLN
3	C	52	GLN
3	C	112	GLN
3	C	130	GLN
3	C	192	HIS
3	C	198	GLN
3	C	201	HIS
1	D	158	HIS
1	D	243	ASN
2	E	77	ASN
2	E	82	GLN
2	E	197	GLN
2	E	202	ASN
2	E	204	ASN
3	F	30	ASN
3	F	171	GLN
3	F	198	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	101/104 (97%)	0.24	5 (4%)	34 38	56, 66, 107, 122	0
1	D	101/104 (97%)	0.29	6 (5%)	28 32	55, 66, 97, 133	0
2	B	215/249 (86%)	-0.04	2 (0%)	81 83	51, 62, 81, 132	0
2	E	216/249 (86%)	0.00	7 (3%)	50 54	49, 62, 91, 145	0
3	C	215/243 (88%)	0.17	2 (0%)	81 83	53, 69, 94, 118	0
3	F	213/243 (87%)	0.40	6 (2%)	55 59	53, 73, 98, 133	0
All	All	1061/1192 (89%)	0.16	28 (2%)	57 61	49, 66, 96, 145	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	PRO	3.8
1	D	211	HIS	3.5
2	E	195	GLY	3.4
3	C	114	LYS	3.3
1	A	213	HIS	3.3
1	D	149	TYR	3.2
2	B	132	SER	3.1
1	D	209	LEU	3.1
1	A	209	LEU	3.0
1	D	204	ILE	3.0
3	F	173	ASN	2.8
2	E	138	GLY	2.7
2	E	221	CYS	2.7
2	E	220	SER	2.6
1	D	213	HIS	2.6
2	E	194	LEU	2.5
1	A	210	ARG	2.4
3	F	111	GLY	2.4
2	E	219	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	213	THR	2.4
3	F	1	VAL	2.3
1	D	210	ARG	2.2
2	E	193	SER	2.2
3	F	172	SER	2.2
1	A	178	ARG	2.1
3	F	155	ASP	2.1
3	C	213	THR	2.0
2	B	138	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.