



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 02:36 AM EDT

PDB ID : 6J6Y
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:

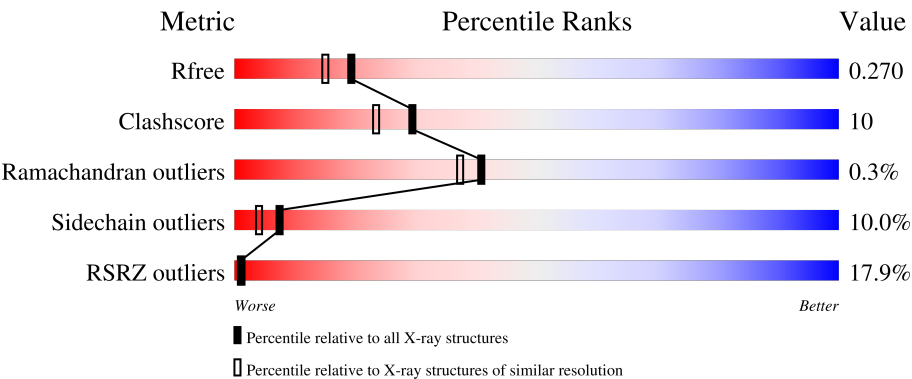
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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	<div><div>22%</div><div><div></div><div>78%</div><div>17%</div><div>• •</div></div></div>
1	D	104	<div><div>15%</div><div><div></div><div>64%</div><div>30%</div><div>• •</div></div></div>
2	B	249	<div><div>11%</div><div><div></div><div>68%</div><div>16%</div><div>• 14%</div></div></div>
2	E	249	<div><div>12%</div><div><div></div><div>69%</div><div>16%</div><div>• 13%</div></div></div>
3	C	243	<div><div>16%</div><div><div></div><div>72%</div><div>14%</div><div>• 12%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	243	<div><div></div><div>23%</div><div>61%</div><div>24%</div><div>•</div><div>12%</div></div>

2 Entry composition

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		

Continued on next page...

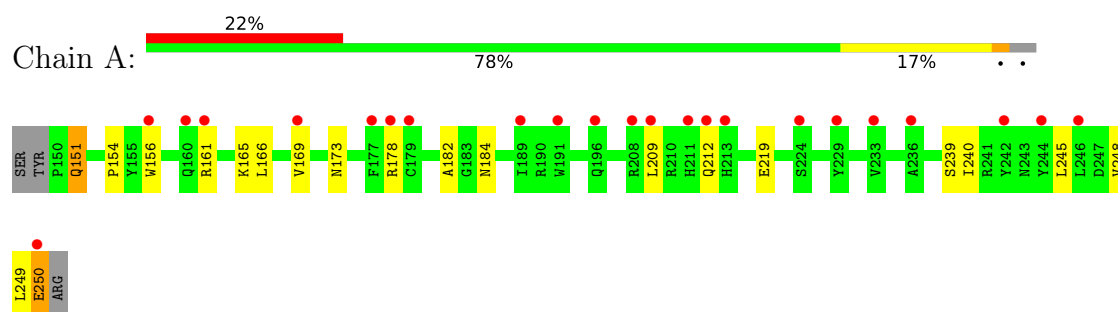
Continued from previous page...

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

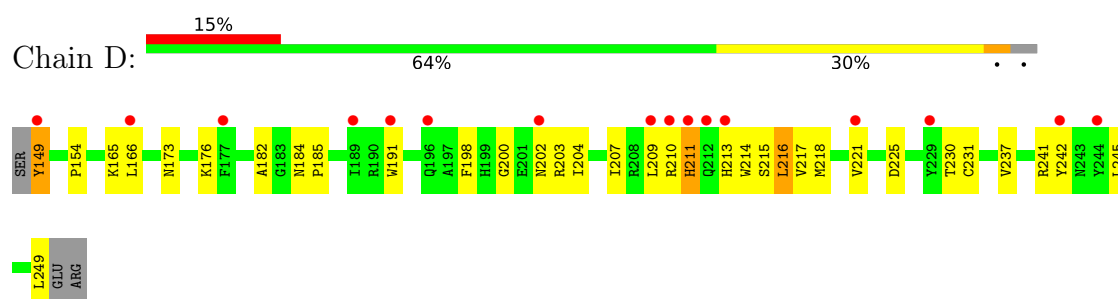
3 Residue-property plots [i](#)

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.

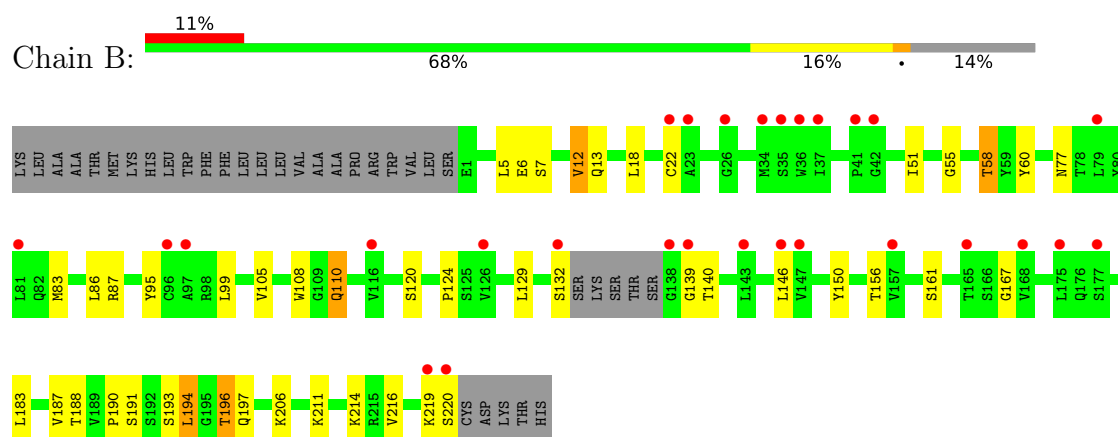
- Molecule 1: Fibroblast growth factor receptor 4



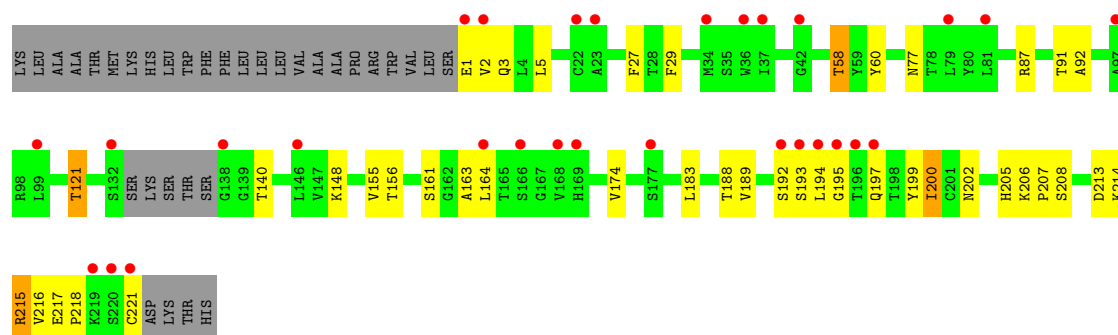
- Molecule 1: Fibroblast growth factor receptor 4



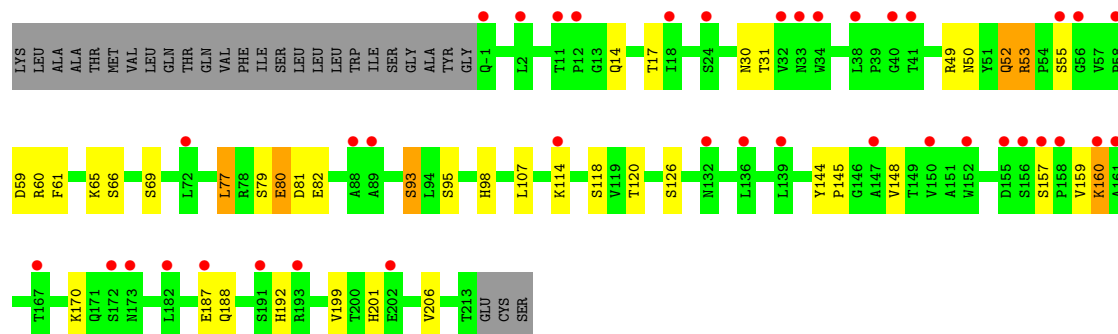
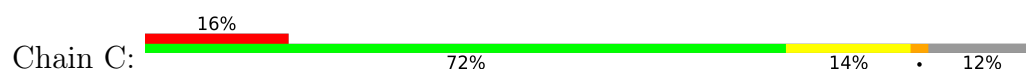
- Molecule 2: Fab Heavy chain



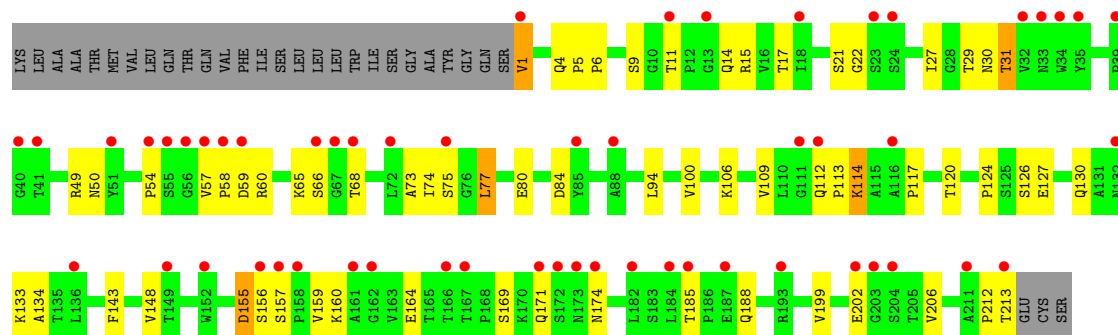
- Molecule 2: Fab Heavy chain



• 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 19.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.15) 99.8 (19.94-2.15)	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)	0.38 , 66.3	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	0.96	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 [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	0.49	0/816	0.74	0/1112
1	D	0.47	0/823	0.76	0/1123
2	B	0.53	0/1635	0.74	0/2226
2	E	0.52	0/1637	0.74	0/2230
3	C	0.50	0/1627	0.73	0/2226
3	F	0.50	0/1619	0.75	0/2214
All	All	0.51	0/8157	0.74	0/11131

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	793	0	769	13	0
1	D	798	0	774	26	0
2	B	1598	0	1559	33	0
2	E	1600	0	1553	35	0
3	C	1587	0	1535	19	0
3	F	1579	0	1535	40	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	116	0	0	7	0
4	F	69	0	0	3	0
All	All	8410	0	7725	149	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 (149) 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:HZ1	3:F:133:LYS:HE2	1.17	1.07
2:E:148:LYS:NZ	3:F:133:LYS:HE2	1.73	1.02
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:B:83:MET:HE2	2:B:86:LEU:HD21	1.68	0.74
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
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
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:93:SER:OG	3:C:98:HIS:NE2	2.31	0.63
3:C:53:ARG:HD3	3:C:61:PHE:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:184:ASN:HA	1:D:185:PRO:C	2.21	0.60
2:E:161:SER:N	2:E:202:ASN:HD21	1.98	0.59
2:E:148:LYS:HZ3	3:F:133:LYS:HE2	1.66	0.59
1:A:165:LYS:HE2	3:C:30:ASN:HD21	1.68	0.57
1:D:165:LYS:HZ3	3:F:30:ASN:HD21	1.52	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
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:E:1:GLU:HG2	2:E:2:VAL:N	2.23	0.54
3:F:22:GLY:C	3:F:68:THR:HG23	2.29	0.53
1:D:210:ARG:O	1:D:214:TRP:N	2.42	0.53
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
2:E:183:LEU:HD12	2:E:183:LEU:C	2.31	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
2:B:183:LEU:HD12	2:B:183:LEU:C	2.32	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:83:MET:CE	2:B:86:LEU:HD21	2.41	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
1:D:165:LYS:HZ2	3:F:30:ASN:HD21	1.60	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: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	1.97	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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:200:ILE:C	2:E:200:ILE:HD12	2.40	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: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
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: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
1:D:149:TYR:CD1	1:D:149:TYR:C	2.95	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	29	22
3	C	213/243 (88%)	205 (96%)	7 (3%)	1 (0%)	29	22
3	F	211/243 (87%)	204 (97%)	6 (3%)	1 (0%)	29	22
All	All	1045/1192 (88%)	1010 (97%)	32 (3%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	59	ASP
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%)	77 (93%)	6 (7%)	14	9
1	D	83/89 (93%)	74 (89%)	9 (11%)	6	3
2	B	178/208 (86%)	164 (92%)	14 (8%)	12	7
2	E	178/208 (86%)	164 (92%)	14 (8%)	12	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	178/203 (88%)	157 (88%)	21 (12%)	5	2
3	F	177/203 (87%)	153 (86%)	24 (14%)	3	1
All	All	877/1000 (88%)	789 (90%)	88 (10%)	7	4

All (88) 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	239	SER
1	A	249	LEU
1	A	250	GLU
2	B	7	SER
2	B	12	VAL
2	B	22	CYS
2	B	58	THR
2	B	77	ASN
2	B	87	ARG
2	B	99	LEU
2	B	110	GLN
2	B	120	SER
2	B	194	LEU
2	B	196	THR
2	B	211	LYS
2	B	214	LYS
2	B	216	VAL
3	C	17	THR
3	C	52	GLN
3	C	53	ARG
3	C	55	SER
3	C	66	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	126	SER
3	C	148	VAL
3	C	157	SER
3	C	159	VAL
3	C	160	LYS
3	C	199	VAL
3	C	206	VAL
1	D	149	TYR
1	D	202	ASN
1	D	203	ARG
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	87	ARG
2	E	121	THR
2	E	140	THR
2	E	164	LEU
2	E	192	SER
2	E	200	ILE
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	9	SER
3	F	21	SER
3	F	31	THR
3	F	66	SER
3	F	77	LEU
3	F	80	GLU
3	F	94	LEU
3	F	114	LYS
3	F	120	THR
3	F	127	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	148	VAL
3	F	155	ASP
3	F	157	SER
3	F	159	VAL
3	F	160	LYS
3	F	169	SER
3	F	171	GLN
3	F	174	ASN
3	F	199	VAL
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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	173	ASN
1	A	184	ASN
1	A	211	HIS
1	A	243	ASN
2	B	77	ASN
2	B	110	GLN
3	C	30	ASN
3	C	112	GLN
3	C	192	HIS
3	C	198	GLN
3	C	201	HIS
1	D	243	ASN
2	E	77	ASN
2	E	84	ASN
2	E	110	GLN
2	E	202	ASN
3	F	30	ASN
3	F	52	GLN
3	F	112	GLN
3	F	171	GLN
3	F	198	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 monosaccharides 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	101/104 (97%)	1.14	23 (22%) 0 0	56, 66, 107, 122	0
1	D	101/104 (97%)	1.06	16 (15%) 2 2	55, 66, 97, 133	0
2	B	215/249 (86%)	0.93	28 (13%) 3 4	51, 62, 81, 132	0
2	E	216/249 (86%)	0.90	29 (13%) 3 4	49, 62, 91, 145	0
3	C	215/243 (88%)	1.06	39 (18%) 1 1	53, 69, 94, 118	0
3	F	213/243 (87%)	1.32	55 (25%) 0 0	53, 73, 98, 133	0
All	All	1061/1192 (89%)	1.06	190 (17%) 1 1	49, 66, 96, 145	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	221	CYS	9.8
3	F	172	SER	8.4
1	D	213	HIS	8.3
2	B	132	SER	8.0
1	D	209	LEU	7.5
2	E	138	GLY	7.0
2	B	220	SER	6.6
3	F	213	THR	6.6
2	E	194	LEU	6.3
2	E	220	SER	6.0
3	C	172	SER	5.9
2	E	132	SER	5.7
2	B	177	SER	5.6
1	D	149	TYR	5.4
3	F	158	PRO	5.1
2	B	219	LYS	5.0
3	F	55	SER	4.9
2	B	138	GLY	4.8
3	C	72	LEU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	58	PRO	4.4
3	C	-1	GLN	4.2
3	F	193	ARG	4.2
2	E	79	LEU	4.1
2	B	79	LEU	4.1
3	F	39	PRO	4.1
1	D	211	HIS	4.0
2	E	219	LYS	4.0
1	A	213	HIS	4.0
3	F	174	ASN	4.0
1	A	212	GLN	4.0
2	E	195	GLY	3.9
3	F	111	GLY	3.9
3	C	160	LYS	3.9
3	F	34	TRP	3.9
3	F	1	VAL	3.8
3	F	149	THR	3.8
1	A	161	ARG	3.8
3	C	173	ASN	3.8
3	C	202	GLU	3.7
3	F	132	ASN	3.7
3	F	203	GLY	3.7
3	C	34	TRP	3.6
1	A	208	ARG	3.6
2	B	26	GLY	3.6
2	E	42	GLY	3.6
2	B	42	GLY	3.6
3	F	59	ASP	3.5
3	C	132	ASN	3.5
2	E	196	THR	3.5
3	C	193	ARG	3.4
3	F	18	ILE	3.4
1	A	246	LEU	3.4
3	C	40	GLY	3.4
3	F	162	GLY	3.4
3	C	32	VAL	3.4
3	C	88	ALA	3.4
3	F	72	LEU	3.4
1	A	209	LEU	3.3
3	C	167	THR	3.3
2	E	177	SER	3.3
3	C	157	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	58	PRO	3.3
1	A	178	ARG	3.2
2	B	165	THR	3.2
3	F	185	THR	3.2
3	C	114	LYS	3.2
3	F	68	THR	3.2
2	E	192	SER	3.2
3	F	112	GLN	3.2
2	E	193	SER	3.1
3	C	55	SER	3.1
3	F	167	THR	3.1
1	D	210	ARG	3.1
2	B	81	LEU	3.1
3	F	136	LEU	3.1
3	F	202	GLU	3.1
3	C	161	ALA	3.0
3	F	40	GLY	3.0
3	C	41	THR	3.0
2	E	1	GLU	3.0
3	F	187	GLU	3.0
3	F	88	ALA	3.0
3	C	182	LEU	2.9
3	F	56	GLY	2.9
3	F	35	TYR	2.9
3	F	24	SER	2.9
3	F	173	ASN	2.9
1	D	166	LEU	2.9
2	E	81	LEU	2.9
3	C	150	VAL	2.9
1	D	202	ASN	2.9
3	F	33	ASN	2.9
3	C	156	SER	2.9
1	D	244	TYR	2.9
1	D	212	GLN	2.9
3	C	136	LEU	2.9
3	F	13	GLY	2.9
2	B	41	PRO	2.9
3	C	187	GLU	2.8
1	A	229	TYR	2.8
3	C	24	SER	2.8
3	F	156	SER	2.8
3	F	54	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	196	GLN	2.7
2	B	96	CYS	2.7
3	C	38	LEU	2.7
2	B	147	VAL	2.7
3	F	171	GLN	2.7
1	A	244	TYR	2.7
3	F	23	SER	2.7
1	A	160	GLN	2.7
1	A	191	TRP	2.6
1	D	242	TYR	2.6
2	B	157	VAL	2.6
3	F	182	LEU	2.6
3	F	66	SER	2.6
3	C	56	GLY	2.6
1	A	177	PHE	2.6
3	C	155	ASP	2.6
3	C	18	ILE	2.6
2	B	36	TRP	2.6
3	F	85	TYR	2.5
1	A	236	ALA	2.5
3	F	57	VAL	2.5
3	F	152	TRP	2.5
3	F	51	TYR	2.5
3	F	157	SER	2.5
3	F	67	GLY	2.5
2	B	23	ALA	2.5
2	E	23	ALA	2.5
3	F	75	SER	2.4
3	F	11	THR	2.4
2	B	175	LEU	2.4
1	A	242	TYR	2.4
1	D	177	PHE	2.4
2	B	126	VAL	2.4
3	C	147	ALA	2.4
1	A	224	SER	2.4
1	D	189	ILE	2.4
1	D	229	TYR	2.3
1	A	156	TRP	2.3
2	E	146	LEU	2.3
2	E	34	MET	2.3
3	C	11	THR	2.3
3	F	41	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	197	GLN	2.3
2	E	2	VAL	2.3
3	C	89	ALA	2.3
2	E	166	SER	2.3
1	A	169	VAL	2.2
1	A	233	VAL	2.2
2	E	168	VAL	2.2
1	A	179	CYS	2.2
2	E	164	LEU	2.2
3	C	139	LEU	2.2
2	E	36	TRP	2.2
2	B	34	MET	2.2
3	F	116	ALA	2.2
3	F	161	ALA	2.2
3	C	33	ASN	2.2
2	B	168	VAL	2.2
3	C	158	PRO	2.2
3	C	191	SER	2.2
2	B	139	GLY	2.2
2	B	97	ALA	2.2
2	E	37	ILE	2.2
3	F	204	SER	2.2
1	D	221	VAL	2.2
1	A	211	HIS	2.2
3	F	211	ALA	2.2
3	F	32	VAL	2.1
3	F	166	THR	2.1
3	C	2	LEU	2.1
3	C	152	TRP	2.1
2	E	22	CYS	2.1
2	E	97	ALA	2.1
2	E	169	HIS	2.1
2	B	116	VAL	2.1
1	A	189	ILE	2.1
2	E	99	LEU	2.1
1	D	191	TRP	2.1
2	B	146	LEU	2.0
3	C	12	PRO	2.0
3	F	184	LEU	2.0
1	A	196	GLN	2.0
2	B	22	CYS	2.0
2	B	37	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	143	LEU	2.0
2	B	35	SER	2.0
1	A	250	GLU	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 monosaccharides 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.