Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 11:14 AM EDT

PDB ID	:	3U9U
Title	:	Crystal Structure of Extracellular Domain of Human ErbB4/Her4 in complex with the Fab fragment of mAb1479
Authors	:	Hollmen, M.; Liu, P.; Wildiers, H.; Reinvall, I.; Vandorpe, T.; Smeets, A.; Deraedt, K.; Vahlberg, T.; Joensuu, H.; Leahy, D.J.; Schoffski, P.; Elenius, K.
Deposited on	:	2011-10-19
Resolution	:	3.42 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:

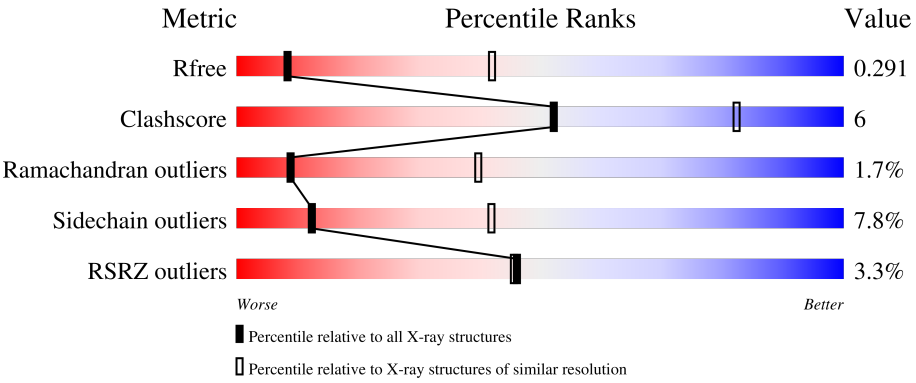
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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 <=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	224	71% 25%
1	C	224	75% 20%
2	B	219	2% 81% 16%
2	D	219	78% 19%
3	E	625	5% 79% 14% 6%

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Mol	Chain	Length	Quality of chain
3	F	625	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15819 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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1675	1069	275	326	5			
1	C	215	Total	C	N	O	S	0	0	0
			1644	1048	270	321	5			

- Molecule 2 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1701	1064	288	342	7			
2	D	219	Total	C	N	O	S	0	0	0
			1701	1064	288	342	7			

- Molecule 3 is a protein called Receptor tyrosine-protein kinase erbB-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	585	Total	C	N	O	S	0	0	0
			4563	2835	795	878	55			
3	F	580	Total	C	N	O	S	0	0	0
			4535	2827	784	870	54			

There are 2 discrepancies between the modelled and reference sequences:

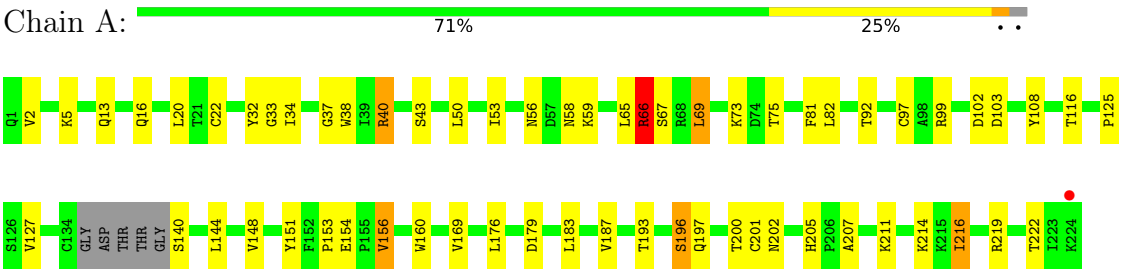
Chain	Residue	Modelled	Actual	Comment	Reference
E	524	ASP	GLY	conflict	UNP Q15303
F	524	ASP	GLY	conflict	UNP Q15303

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.

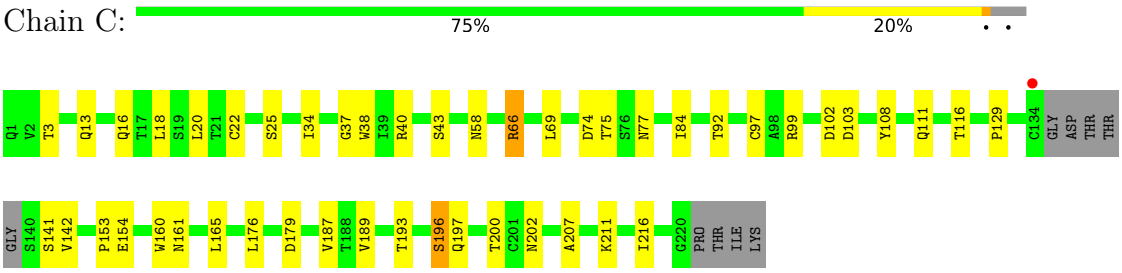
• Molecule 1: Fab Heavy Chain

Chain A:



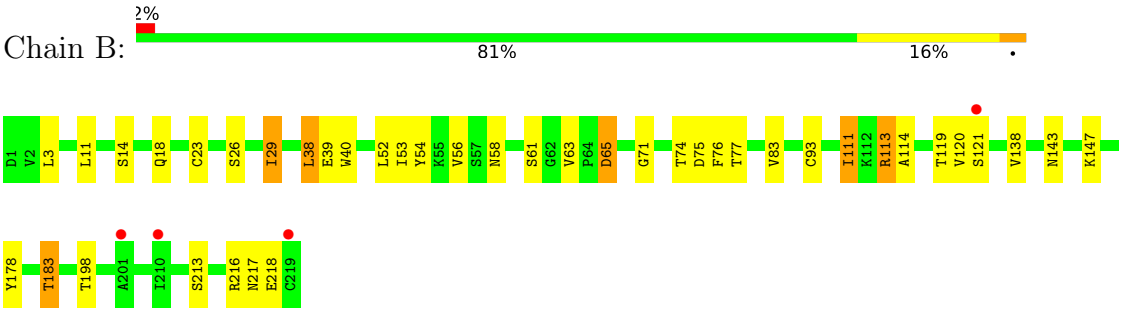
• Molecule 1: Fab Heavy Chain

Chain C:



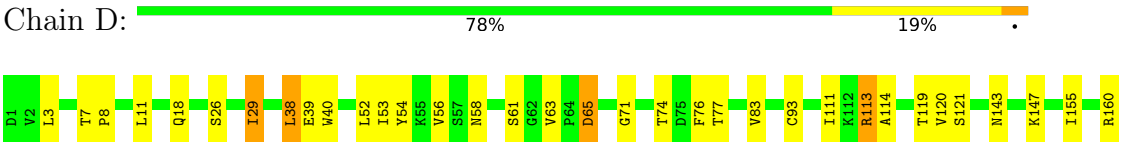
• Molecule 2: Fab Light Chain

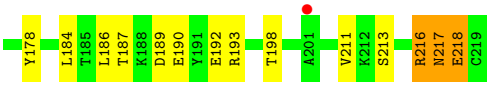
Chain B:



• Molecule 2: Fab Light Chain

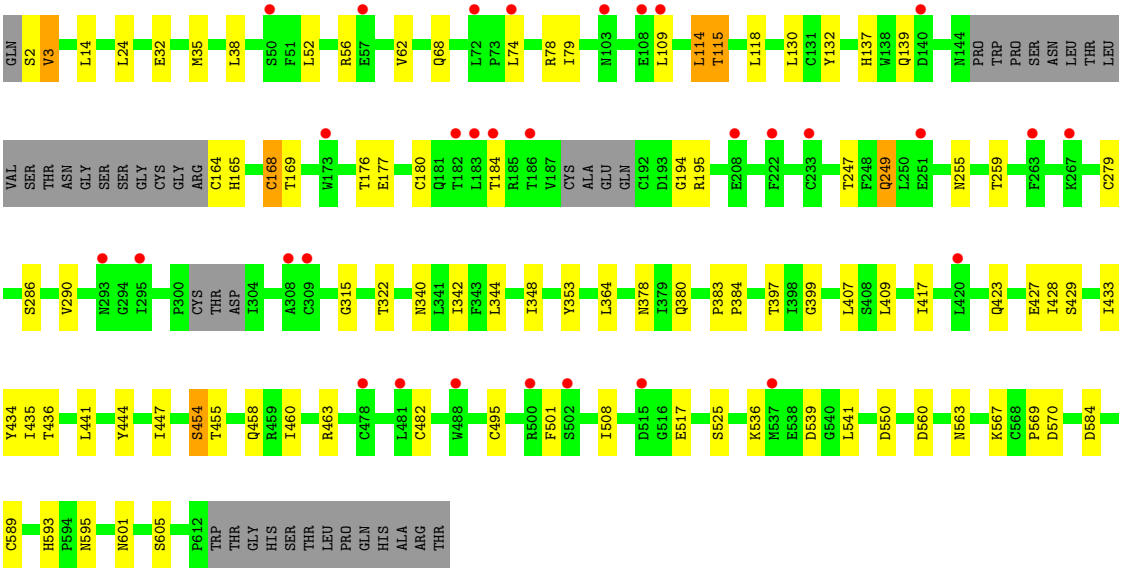
Chain D:





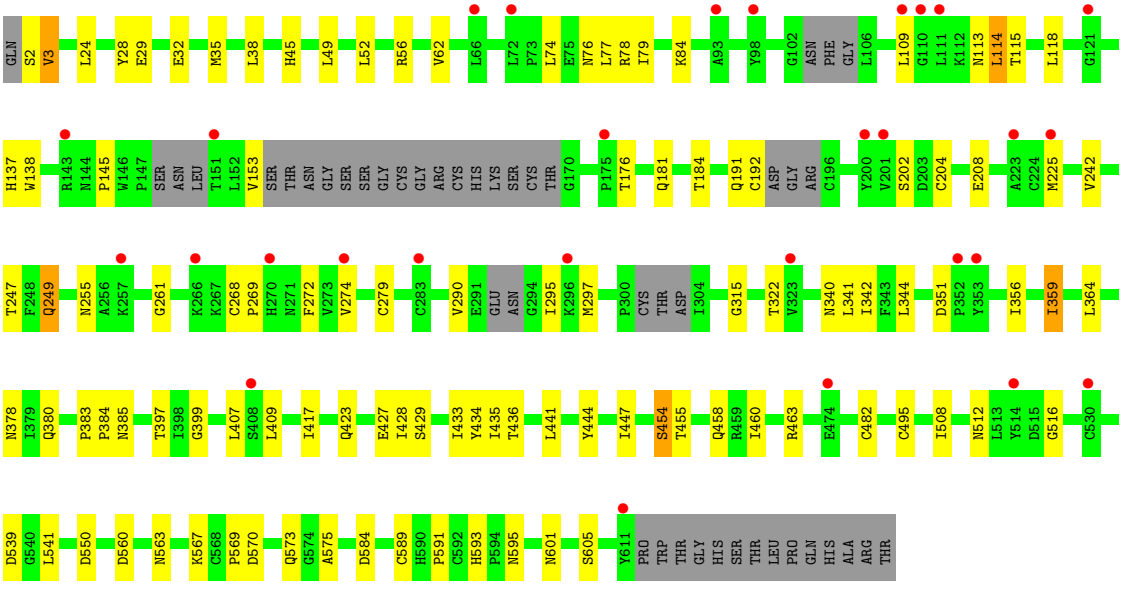
• Molecule 3: Receptor tyrosine-protein kinase erbB-4

Chain E:



• Molecule 3: Receptor tyrosine-protein kinase erbB-4

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.12Å 110.91Å 362.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.26 – 3.42 45.26 – 3.42	Depositor EDS
% Data completeness (in resolution range)	95.3 (45.26-3.42) 95.2 (45.26-3.42)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.40Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.234 , 0.272 0.250 , 0.291	Depositor DCC
R_{free} test set	2236 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	81.0	Xtriage
Anisotropy	1.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15819	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/1721	0.75	0/2357
1	C	0.49	0/1689	0.76	0/2313
2	B	0.45	0/1741	0.69	0/2363
2	D	0.44	0/1741	0.69	0/2363
3	E	0.42	0/4659	0.69	0/6307
3	F	0.42	0/4630	0.69	0/6269
All	All	0.44	0/16181	0.70	0/21972

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

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	1675	0	1645	24	0
1	C	1644	0	1607	16	0
2	B	1701	0	1637	19	0
2	D	1701	0	1637	25	0
3	E	4563	0	4325	36	0
3	F	4535	0	4307	57	0
All	All	15819	0	15158	171	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 6.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:208:GLU:HA	3:F:225:MET:CE	1.36	1.52
3:F:208:GLU:CA	3:F:225:MET:HE2	1.77	1.12
3:F:208:GLU:CA	3:F:225:MET:CE	2.28	1.10
2:D:218:GLU:H	2:D:218:GLU:CD	1.51	1.08
3:F:208:GLU:HA	3:F:225:MET:HE2	1.12	1.07
2:D:217:ASN:HB2	2:D:218:GLU:OE2	1.52	1.07
3:F:208:GLU:HA	3:F:225:MET:HE1	1.33	1.03
2:B:218:GLU:H	2:B:218:GLU:CD	1.57	1.02
3:F:208:GLU:CD	3:F:225:MET:CE	2.33	0.97
2:B:217:ASN:HB2	2:B:218:GLU:OE2	1.64	0.96
3:F:208:GLU:CD	3:F:225:MET:HE2	1.89	0.92
2:D:218:GLU:CD	2:D:218:GLU:N	2.29	0.86
3:F:208:GLU:CB	3:F:225:MET:HE2	2.07	0.84
2:D:190:GLU:OE1	3:E:353:TYR:CB	2.27	0.83
2:D:189:ASP:O	2:D:193:ARG:HG3	1.81	0.81
3:F:208:GLU:CG	3:F:225:MET:HE2	2.11	0.81
3:F:208:GLU:CD	3:F:225:MET:HE3	2.01	0.79
2:B:218:GLU:CD	2:B:218:GLU:N	2.29	0.78
2:D:217:ASN:CB	2:D:218:GLU:OE2	2.30	0.78
2:D:217:ASN:HB2	2:D:218:GLU:CD	2.05	0.77
3:F:208:GLU:OE2	3:F:225:MET:HE3	1.91	0.70
2:D:160:ARG:NH2	2:D:190:GLU:OE2	2.23	0.69
3:F:208:GLU:HA	3:F:225:MET:SD	2.32	0.68
1:A:66:ARG:HD2	1:A:67:SER:H	1.59	0.68
3:E:322:THR:HB	3:E:344:LEU:HD12	1.76	0.68
3:F:269:PRO:O	3:F:272:PHE:HB2	1.94	0.67
3:F:208:GLU:CG	3:F:225:MET:CE	2.71	0.67
3:F:322:THR:HB	3:F:344:LEU:HD12	1.77	0.65
3:F:137:HIS:H	3:F:181:GLN:HE22	1.43	0.65
2:B:217:ASN:HB2	2:B:218:GLU:CD	2.16	0.64
2:D:190:GLU:CD	3:E:353:TYR:CB	2.67	0.63
2:B:217:ASN:CB	2:B:218:GLU:OE2	2.45	0.61
2:D:190:GLU:OE2	3:E:353:TYR:CB	2.48	0.61
2:D:218:GLU:N	2:D:218:GLU:OE1	2.29	0.61
3:F:138:TRP:HE1	3:F:153:VAL:HG11	1.66	0.60
1:A:40:ARG:HG2	1:A:50:LEU:HD21	1.84	0.59
1:A:156:VAL:HG23	1:A:205:HIS:CD2	2.38	0.58
1:C:189:VAL:HG12	3:F:191:GLN:HE22	1.69	0.57
3:F:56:ARG:HA	3:F:77:LEU:HA	1.86	0.57
2:D:71:GLY:HA3	2:D:76:PHE:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:192:CYS:HG	3:F:204:CYS:HG	1.49	0.57
1:A:53:ILE:HD12	1:A:59:LYS:HG2	1.87	0.56
2:B:71:GLY:HA3	2:B:76:PHE:HA	1.87	0.56
1:C:74:ASP:OD2	1:C:77:ASN:HB2	2.05	0.56
1:A:22:CYS:HB2	1:A:38:TRP:CZ2	2.40	0.56
1:A:169:VAL:HG22	1:A:187:VAL:HG23	1.87	0.55
3:F:208:GLU:CA	3:F:225:MET:HE1	2.13	0.55
2:D:192:GLU:HA	2:D:216:ARG:HE	1.71	0.55
3:F:52:LEU:HB3	3:F:74:LEU:HD23	1.89	0.54
3:E:593:HIS:HD2	3:E:595:ASN:H	1.54	0.54
2:B:113:ARG:HD3	2:B:114:ALA:O	2.08	0.54
2:D:198:THR:HG23	2:D:213:SER:HB3	1.89	0.54
3:F:593:HIS:HD2	3:F:595:ASN:H	1.55	0.54
2:D:113:ARG:HD3	2:D:114:ALA:O	2.08	0.54
3:E:436:THR:HG23	3:E:463:ARG:HB3	1.91	0.53
3:E:52:LEU:HB3	3:E:74:LEU:HD23	1.90	0.53
2:B:29:ILE:HD11	2:B:38:LEU:HD23	1.90	0.52
3:F:428:ILE:HD13	3:F:433:ILE:HD11	1.91	0.52
1:C:22:CYS:HB2	1:C:38:TRP:CZ2	2.45	0.52
1:C:37:GLY:O	1:C:97:CYS:HA	2.10	0.51
3:F:208:GLU:OE1	3:F:225:MET:HE2	2.10	0.51
1:C:161:ASN:HD22	1:C:165:LEU:HD13	1.74	0.51
3:F:407:LEU:HD22	3:F:434:TYR:HB2	1.93	0.51
1:C:165:LEU:HD23	1:C:187:VAL:HG21	1.91	0.51
3:E:428:ILE:HD13	3:E:433:ILE:HD11	1.92	0.51
3:F:454:SER:H	3:F:458:GLN:NE2	2.09	0.51
3:F:593:HIS:CE1	3:F:605:SER:HB3	2.46	0.51
1:A:13:GLN:HB2	1:A:16:GLN:NE2	2.26	0.51
3:F:436:THR:HG23	3:F:463:ARG:HB3	1.91	0.50
3:E:454:SER:H	3:E:458:GLN:NE2	2.10	0.50
3:F:76:ASN:HA	3:F:113:ASN:HD22	1.76	0.50
3:F:560:ASP:HA	3:F:589:CYS:HB2	1.92	0.50
1:C:13:GLN:HB2	1:C:16:GLN:NE2	2.25	0.50
3:E:593:HIS:CE1	3:E:605:SER:HB3	2.47	0.50
3:E:348:ILE:HD12	3:E:383:PRO:HD3	1.94	0.49
3:F:417:ILE:HD12	3:F:441:LEU:HD13	1.94	0.49
3:E:407:LEU:HD22	3:E:434:TYR:HB2	1.94	0.49
3:E:560:ASP:HA	3:E:589:CYS:HB2	1.93	0.49
3:F:79:ILE:HD11	3:F:118:LEU:HG	1.94	0.49
3:F:247:THR:HB	3:F:249:GLN:HE21	1.78	0.48
2:B:198:THR:HG23	2:B:213:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:LEU:HA	2:D:63:VAL:HG21	1.96	0.48
3:E:417:ILE:HD12	3:E:441:LEU:HD13	1.94	0.48
3:E:247:THR:HB	3:E:249:GLN:HE21	1.79	0.48
3:F:3:VAL:HG13	3:F:35:MET:HG3	1.96	0.47
2:D:39:GLU:HG3	2:D:54:TYR:HA	1.97	0.47
3:E:3:VAL:HG13	3:E:35:MET:HG3	1.95	0.47
3:F:274:VAL:HG13	3:F:297:MET:HB3	1.96	0.47
1:A:222:THR:HG23	1:A:222:THR:O	2.15	0.47
2:B:138:VAL:HG22	2:B:183:THR:HG23	1.95	0.47
3:E:2:SER:HB3	3:E:32:GLU:H	1.80	0.47
2:B:39:GLU:HG3	2:B:54:TYR:HA	1.97	0.46
3:F:38:LEU:HD23	3:F:62:VAL:HG13	1.98	0.46
2:B:52:LEU:HA	2:B:63:VAL:HG21	1.97	0.46
3:F:2:SER:HB3	3:F:32:GLU:H	1.80	0.46
1:A:37:GLY:O	1:A:97:CYS:HA	2.16	0.46
3:F:397:THR:HG22	3:F:427:GLU:HB2	1.97	0.46
2:B:218:GLU:N	2:B:218:GLU:OE1	2.30	0.46
3:E:79:ILE:HD11	3:E:118:LEU:HG	1.97	0.46
1:A:144:LEU:HD22	1:A:216:ILE:HD11	1.97	0.45
3:E:132:TYR:HH	3:E:164:CYS:N	2.13	0.45
3:E:397:THR:HG22	3:E:427:GLU:HB2	1.98	0.45
2:D:65:ASP:N	2:D:65:ASP:OD1	2.50	0.45
3:F:378:ASN:HD21	3:F:380:GLN:HE21	1.65	0.45
1:A:66:ARG:HD2	1:A:67:SER:N	2.30	0.45
3:E:409:LEU:HB3	3:E:433:ILE:HG13	1.99	0.45
3:E:378:ASN:HD21	3:E:380:GLN:HE21	1.64	0.45
3:E:399:GLY:O	3:E:429:SER:HB2	2.17	0.44
3:F:399:GLY:O	3:F:429:SER:HB2	2.17	0.44
3:E:109:LEU:HG	3:E:130:LEU:HD11	1.99	0.44
1:A:153:PRO:HD2	1:A:207:ALA:CB	2.47	0.44
1:A:160:TRP:CZ3	1:A:201:CYS:HB2	2.53	0.44
2:D:29:ILE:HD11	2:D:38:LEU:HD23	2.00	0.44
1:A:65:LEU:HB2	1:A:69:LEU:CD1	2.48	0.44
1:A:127:VAL:HB	1:A:214:LYS:HD3	1.98	0.44
3:F:138:TRP:NE1	3:F:153:VAL:HG11	2.32	0.44
2:B:3:LEU:HB3	2:B:26:SER:HB3	1.99	0.44
1:C:92:THR:HG23	1:C:116:THR:HA	2.00	0.44
1:C:141:SER:HB2	3:F:202:SER:HA	1.99	0.44
2:D:53:ILE:HA	2:D:58:ASN:O	2.18	0.44
3:E:115:THR:HB	3:E:195:ARG:HH12	1.83	0.44
2:B:65:ASP:OD1	2:B:65:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:383:PRO:HA	3:F:384:PRO:HD3	1.88	0.43
3:F:359:ILE:H	3:F:359:ILE:HG13	1.72	0.43
2:D:40:TRP:CH2	2:D:93:CYS:HB3	2.53	0.43
1:A:156:VAL:HG12	1:A:183:LEU:HD21	2.00	0.43
3:E:165:HIS:CE1	3:E:177:GLU:HG3	2.53	0.43
1:A:69:LEU:HD23	1:A:82:LEU:HD11	2.00	0.43
1:A:92:THR:HG23	1:A:116:THR:HA	1.99	0.43
1:C:99:ARG:NH1	1:C:108:TYR:HD2	2.17	0.43
3:E:454:SER:H	3:E:458:GLN:HE22	1.66	0.43
1:A:56:ASN:HB2	3:F:591:PRO:HG2	2.00	0.43
2:D:3:LEU:HB3	2:D:26:SER:HB3	2.00	0.43
3:F:192:CYS:SG	3:F:204:CYS:SG	3.06	0.43
3:F:433:ILE:HG23	3:F:435:ILE:HD12	2.01	0.43
2:D:147:LYS:HB3	2:D:178:TYR:CE2	2.54	0.43
3:E:38:LEU:HD23	3:E:62:VAL:HG13	2.01	0.43
3:F:409:LEU:HB3	3:F:433:ILE:HG13	2.00	0.43
2:B:147:LYS:HB3	2:B:178:TYR:CE2	2.55	0.42
3:F:444:TYR:HA	3:F:447:ILE:HD12	2.01	0.42
3:E:433:ILE:HG23	3:E:435:ILE:HD12	2.01	0.42
1:C:18:LEU:HD23	1:C:84:ILE:HD12	2.01	0.42
3:F:78:ARG:HA	3:F:114:LEU:HA	2.01	0.42
2:B:40:TRP:CH2	2:B:93:CYS:HB3	2.54	0.42
3:F:454:SER:H	3:F:458:GLN:HE22	1.66	0.42
1:C:129:PRO:HB3	1:C:216:ILE:HG13	2.01	0.42
3:E:444:TYR:HA	3:E:447:ILE:HD12	2.01	0.42
1:A:32:TYR:O	1:A:34:ILE:N	2.51	0.42
3:E:342:ILE:HG22	3:E:344:LEU:HG	2.02	0.42
3:F:351:ASP:H	3:F:356:ILE:HB	1.84	0.42
3:F:512:ASN:HB3	3:F:516:GLY:HA3	2.02	0.42
1:C:69:LEU:HD23	1:C:84:ILE:HG12	2.01	0.41
3:E:501:PHE:CD2	3:E:525:SER:HA	2.56	0.41
2:D:155:ILE:HD11	2:D:184:LEU:HD21	2.02	0.41
3:E:168:CYS:HB3	3:E:180:CYS:HB3	1.96	0.41
3:F:342:ILE:HG22	3:F:344:LEU:HG	2.02	0.41
3:E:78:ARG:HA	3:E:114:LEU:HA	2.01	0.41
1:C:160:TRP:HZ3	1:C:216:ILE:HD13	1.86	0.41
2:D:7:THR:HA	2:D:8:PRO:HA	1.95	0.41
3:E:383:PRO:HA	3:E:384:PRO:HD3	1.88	0.41
1:A:99:ARG:NH1	1:A:108:TYR:HD2	2.18	0.41
1:C:153:PRO:HD2	1:C:207:ALA:CB	2.51	0.41
1:C:193:THR:O	1:C:197:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TYR:OH	1:A:183:LEU:HD23	2.21	0.41
3:E:137:HIS:NE2	3:E:139:GLN:HB2	2.35	0.41
1:A:193:THR:O	1:A:197:GLN:HB2	2.22	0.40
1:A:125:PRO:HB2	1:A:148:VAL:HG13	2.04	0.40
2:B:23:CYS:HB2	2:B:40:TRP:CH2	2.56	0.40
3:F:52:LEU:HB3	3:F:74:LEU:CD2	2.50	0.40
2:B:14:SER:HA	2:B:111:ILE:HD12	2.02	0.40
3:F:341:LEU:HD23	3:F:341:LEU:HA	1.96	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	215/224 (96%)	189 (88%)	20 (9%)	6 (3%)	5 30
1	C	211/224 (94%)	184 (87%)	23 (11%)	4 (2%)	8 37
2	B	217/219 (99%)	201 (93%)	13 (6%)	3 (1%)	11 43
2	D	217/219 (99%)	198 (91%)	15 (7%)	4 (2%)	8 38
3	E	577/625 (92%)	516 (89%)	53 (9%)	8 (1%)	11 43
3	F	566/625 (91%)	500 (88%)	56 (10%)	10 (2%)	8 38
All	All	2003/2136 (94%)	1788 (89%)	180 (9%)	35 (2%)	9 40

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	43	SER
1	A	66	ARG
1	A	103	ASP

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Mol	Chain	Res	Type
1	C	43	SER
1	C	66	ARG
1	C	103	ASP
3	E	423	GLN
3	F	423	GLN
3	F	575	ALA
1	A	33	GLY
1	A	196	SER
1	C	196	SER
3	E	315	GLY
3	E	569	PRO
3	F	45	HIS
3	F	145	PRO
3	F	315	GLY
2	D	217	ASN
3	E	169	THR
3	F	114	LEU
3	F	569	PRO
2	B	143	ASN
2	D	143	ASN
3	E	114	LEU
3	E	194	GLY
3	E	539	ASP
3	F	539	ASP
2	B	83	VAL
2	D	56	VAL
2	D	83	VAL
2	B	56	VAL
3	F	290	VAL
3	E	290	VAL
3	F	261	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/195 (98%)	171 (89%)	21 (11%)	6	28
1	C	188/195 (96%)	170 (90%)	18 (10%)	8	33
2	B	196/196 (100%)	178 (91%)	18 (9%)	9	35
2	D	196/196 (100%)	178 (91%)	18 (9%)	9	35
3	E	518/553 (94%)	487 (94%)	31 (6%)	19	52
3	F	515/553 (93%)	481 (93%)	34 (7%)	16	49
All	All	1805/1888 (96%)	1665 (92%)	140 (8%)	12	42

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	20	LEU
1	A	40	ARG
1	A	58	ASN
1	A	66	ARG
1	A	69	LEU
1	A	73	LYS
1	A	75	THR
1	A	81	PHE
1	A	102	ASP
1	A	140	SER
1	A	154	GLU
1	A	156	VAL
1	A	176	LEU
1	A	179	ASP
1	A	196	SER
1	A	200	THR
1	A	202	ASN
1	A	211	LYS
1	A	216	ILE
1	A	219	ARG
2	B	11	LEU
2	B	18	GLN
2	B	29	ILE
2	B	38	LEU
2	B	53	ILE
2	B	58	ASN

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Mol	Chain	Res	Type
2	B	61	SER
2	B	65	ASP
2	B	74	THR
2	B	75	ASP
2	B	77	THR
2	B	111	ILE
2	B	113	ARG
2	B	119	THR
2	B	120	VAL
2	B	121	SER
2	B	183	THR
2	B	216	ARG
1	C	3	THR
1	C	20	LEU
1	C	25	SER
1	C	34	ILE
1	C	40	ARG
1	C	58	ASN
1	C	66	ARG
1	C	75	THR
1	C	102	ASP
1	C	111	GLN
1	C	142	VAL
1	C	154	GLU
1	C	176	LEU
1	C	179	ASP
1	C	196	SER
1	C	200	THR
1	C	202	ASN
1	C	211	LYS
2	D	11	LEU
2	D	18	GLN
2	D	29	ILE
2	D	38	LEU
2	D	61	SER
2	D	65	ASP
2	D	74	THR
2	D	77	THR
2	D	111	ILE
2	D	113	ARG
2	D	119	THR
2	D	120	VAL

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Mol	Chain	Res	Type
2	D	121	SER
2	D	186	LEU
2	D	187	THR
2	D	211	VAL
2	D	216	ARG
2	D	218	GLU
3	E	3	VAL
3	E	14	LEU
3	E	24	LEU
3	E	56	ARG
3	E	68	GLN
3	E	115	THR
3	E	168	CYS
3	E	176	THR
3	E	184	THR
3	E	249	GLN
3	E	255	ASN
3	E	259	THR
3	E	279	CYS
3	E	286	SER
3	E	340	ASN
3	E	364	LEU
3	E	454	SER
3	E	455	THR
3	E	460	ILE
3	E	482	CYS
3	E	495	CYS
3	E	508	ILE
3	E	517	GLU
3	E	536	LYS
3	E	541	LEU
3	E	550	ASP
3	E	563	ASN
3	E	567	LYS
3	E	570	ASP
3	E	584	ASP
3	E	601	ASN
3	F	3	VAL
3	F	24	LEU
3	F	28	TYR
3	F	29	GLU
3	F	49	LEU

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Mol	Chain	Res	Type
3	F	84	LYS
3	F	109	LEU
3	F	115	THR
3	F	176	THR
3	F	184	THR
3	F	242	VAL
3	F	249	GLN
3	F	255	ASN
3	F	268	CYS
3	F	279	CYS
3	F	295	ILE
3	F	340	ASN
3	F	359	ILE
3	F	364	LEU
3	F	385	ASN
3	F	454	SER
3	F	455	THR
3	F	460	ILE
3	F	482	CYS
3	F	495	CYS
3	F	508	ILE
3	F	541	LEU
3	F	550	ASP
3	F	563	ASN
3	F	567	LYS
3	F	570	ASP
3	F	573	GLN
3	F	584	ASP
3	F	601	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	170	HIS
2	B	35	ASN
2	B	143	ASN
1	C	104	HIS
1	C	161	ASN
1	C	170	HIS
2	D	143	ASN
3	E	45	HIS

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Mol	Chain	Res	Type
3	E	179	HIS
3	E	181	GLN
3	E	249	GLN
3	E	253	ASN
3	E	349	HIS
3	E	365	ASN
3	E	380	GLN
3	E	423	GLN
3	E	458	GLN
3	E	593	HIS
3	F	113	ASN
3	F	119	ASN
3	F	144	ASN
3	F	179	HIS
3	F	181	GLN
3	F	206	HIS
3	F	249	GLN
3	F	253	ASN
3	F	354	ASN
3	F	365	ASN
3	F	380	GLN
3	F	423	GLN
3	F	458	GLN
3	F	593	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 95^{th} 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	219/224 (97%)	0.24	1 (0%)	91	90	66, 91, 122, 153	0
1	C	215/224 (95%)	0.25	1 (0%)	91	90	56, 81, 115, 146	0
2	B	219/219 (100%)	0.28	4 (1%)	68	67	66, 92, 132, 154	1 (0%)
2	D	219/219 (100%)	0.28	1 (0%)	91	90	52, 91, 128, 146	1 (0%)
3	E	585/625 (93%)	0.52	31 (5%)	26	28	55, 123, 203, 247	0
3	F	580/625 (92%)	0.55	29 (5%)	28	29	83, 126, 167, 253	0
All	All	2037/2136 (95%)	0.42	67 (3%)	46	46	52, 107, 172, 253	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	109	LEU	7.5
3	F	352	PRO	6.3
3	F	110	GLY	6.3
3	E	184	THR	5.2
3	F	353	TYR	4.8
3	E	109	LEU	4.3
3	E	183	LEU	4.3
1	C	134	CYS	3.9
3	F	151	THR	3.8
3	F	111	LEU	3.4
3	E	233	CYS	3.4
3	F	121	GLY	3.4
3	E	308	ALA	3.3
3	F	93	ALA	3.1
3	E	309	CYS	3.0
3	E	74	LEU	2.9
3	E	208	GLU	2.9
3	F	72	LEU	2.9
3	E	140	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	173	TRP	2.8
3	E	182	THR	2.7
2	B	201	ALA	2.7
3	F	274	VAL	2.7
2	B	210	ILE	2.7
3	F	408	SER	2.7
3	F	514	TYR	2.6
3	F	98	TYR	2.6
3	F	223	ALA	2.6
3	E	50	SER	2.6
3	E	515	ASP	2.6
3	E	222	PHE	2.5
2	D	201	ALA	2.5
3	E	72	LEU	2.5
3	E	537	MET	2.5
3	E	295	ILE	2.4
3	E	103	ASN	2.4
1	A	224	LYS	2.4
3	E	251	GLU	2.4
3	F	201	VAL	2.4
3	F	257	LYS	2.4
3	F	200	TYR	2.3
3	F	530	CYS	2.3
3	E	420	LEU	2.3
3	E	57	GLU	2.3
3	E	481	LEU	2.3
3	E	488	TRP	2.2
2	B	219	CYS	2.2
3	E	478	CYS	2.2
3	E	500	ARG	2.2
3	F	296	LYS	2.2
3	F	270	HIS	2.2
3	F	283	CYS	2.2
3	E	502	SER	2.2
3	F	474	GLU	2.2
3	E	186	THR	2.2
3	F	143	ARG	2.2
3	E	267	LYS	2.2
3	F	66	LEU	2.1
3	E	108	GLU	2.1
3	F	611	TYR	2.1
2	B	121	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	225	MET	2.0
3	E	293	ASN	2.0
3	F	266	LYS	2.0
3	F	323	VAL	2.0
3	E	263	PHE	2.0
3	F	175	PRO	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.