Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 10:08 AM EST

PDB ID	:	2RL0
Title	:	Crystal structure of the fourth and fifth fibronectin F1 modules in complex with a fragment of staphylococcus aureus fnbpa-5
Authors	:	Bingham, R.J.
Deposited on	:	2007-10-18
Resolution	:	2.00 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 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:

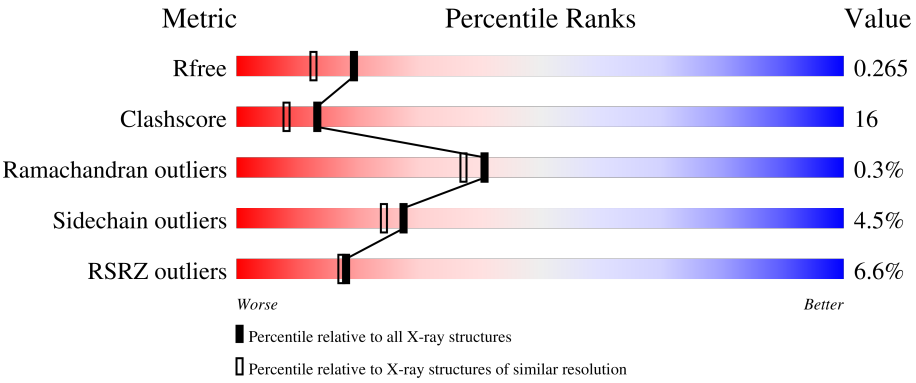
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	89	89% 10%
1	B	89	81% 18%
1	D	89	12% 63% 35%
1	F	89	4% 74% 22%
1	I	89	12% 60% 26% 11%

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Mol	Chain	Length	Quality of chain
1	K	89	4% 82% 15%
2	C	18	83% 11% 6%
2	E	18	22% 61% 17% 11% 11%
2	G	18	6% 78% 17% 6%
2	H	18	6% 56% 39% 6%
2	J	18	6% 56% 17% 28%
2	L	18	11% 67% 17% 11% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5338 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 Fibronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	1	0
			709	427	134	138	10			
1	B	89	Total	C	N	O	S	0	0	0
			702	422	132	138	10			
1	D	89	Total	C	N	O	S	0	0	0
			696	419	129	138	10			
1	F	88	Total	C	N	O	S	0	0	0
			690	417	127	136	10			
1	I	79	Total	C	N	O	S	0	0	0
			618	372	112	124	10			
1	K	89	Total	C	N	O	S	0	0	0
			702	422	132	138	10			

- Molecule 2 is a protein called Fibronectin-binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	17	Total	C	N	O	0	0	0
			131	78	19	34			
2	C	17	Total	C	N	O	0	0	0
			132	79	19	34			
2	E	16	Total	C	N	O	0	0	0
			127	76	18	33			
2	H	17	Total	C	N	O	0	0	0
			132	79	19	34			
2	J	13	Total	C	N	O	0	0	0
			105	64	14	27			
2	L	17	Total	C	N	O	0	0	0
			132	79	19	34			

- Molecule 3 is water.

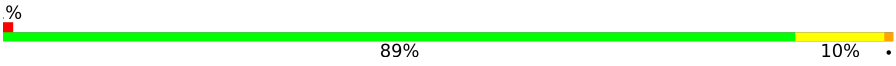
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	G	14	Total O 14 14	0	0
3	B	95	Total O 95 95	0	0
3	C	14	Total O 14 14	0	0
3	D	51	Total O 51 51	0	0
3	E	8	Total O 8 8	0	0
3	F	61	Total O 61 61	0	0
3	H	8	Total O 8 8	0	0
3	I	37	Total O 37 37	0	0
3	J	6	Total O 6 6	0	0
3	K	59	Total O 59 59	0	0
3	L	10	Total O 10 10	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: Fibronectin

Chain A:



• Molecule 1: Fibronectin

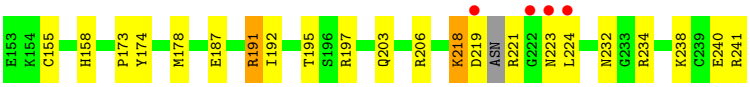
Chain B:

• Molecule 1: Fibronectin

Chain D:

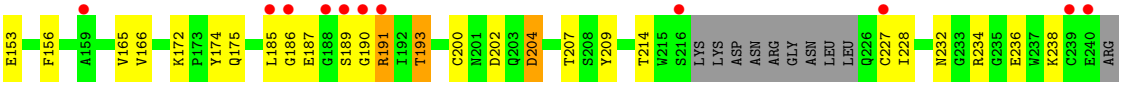
• Molecule 1: Fibronectin

Chain F:



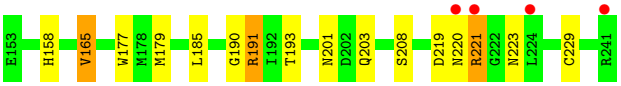
• Molecule 1: Fibronectin

Chain I:



• Molecule 1: Fibronectin

Chain K:

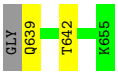


• Molecule 2: Fibronectin-binding protein

Chain G:

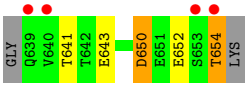
• Molecule 2: Fibronectin-binding protein

Chain C:



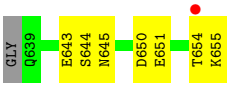
• Molecule 2: Fibronectin-binding protein

Chain E:



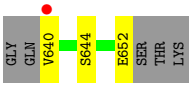
• Molecule 2: Fibronectin-binding protein

Chain H:



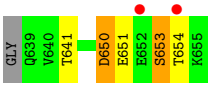
• Molecule 2: Fibronectin-binding protein

Chain J:



• Molecule 2: Fibronectin-binding protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.58Å 85.58Å 230.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.16 – 2.00 28.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.16-2.00) 99.1 (28.16-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.266 0.216 , 0.265	Depositor DCC
R_{free} test set	2954 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5338	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.86	0/726	0.82	1/976 (0.1%)
1	B	0.86	0/715	0.83	1/961 (0.1%)
1	D	0.70	0/709	0.71	0/954
1	F	0.78	0/702	0.77	0/942
1	I	0.73	1/630 (0.2%)	0.73	0/848
1	K	0.73	0/715	0.77	0/961
2	C	0.92	0/132	0.85	0/179
2	E	0.80	0/127	0.84	0/172
2	G	1.00	0/131	0.83	0/177
2	H	0.84	0/132	0.81	0/179
2	J	0.84	0/105	0.81	0/142
2	L	0.91	0/132	0.76	0/179
All	All	0.80	1/4956 (0.0%)	0.78	2/6670 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	200	CYS	CB-SG	-5.21	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	199	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	709	0	653	12	0
1	B	702	0	646	17	0
1	D	696	0	635	36	0
1	F	690	0	632	31	0
1	I	618	0	552	31	0
1	K	702	0	646	23	0
2	C	132	0	112	5	0
2	E	127	0	110	5	0
2	G	131	0	113	6	0
2	H	132	0	112	7	0
2	J	105	0	90	1	0
2	L	132	0	112	10	0
3	A	99	0	0	0	0
3	B	95	0	0	4	0
3	C	14	0	0	0	0
3	D	51	0	0	3	0
3	E	8	0	0	1	0
3	F	61	0	0	6	0
3	G	14	0	0	1	0
3	H	8	0	0	1	0
3	I	37	0	0	6	0
3	J	6	0	0	1	0
3	K	59	0	0	3	0
3	L	10	0	0	2	0
All	All	5338	0	4413	150	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 (150) 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)
1:F:206:ARG:HD2	3:F:274:HOH:O	1.41	1.19
1:F:173:PRO:HG3	1:K:179:MET:CE	1.79	1.13
1:I:214:THR:HG22	1:I:228:ILE:HD12	1.11	1.11
1:D:205:THR:HG22	1:D:217:LYS:HG3	1.33	1.10
2:G:649:PHE:HB3	2:C:639:GLN:HG3	1.37	1.06
1:I:214:THR:HG22	1:I:228:ILE:CD1	1.84	1.06
1:A:191:ARG:HG3	1:A:191:ARG:HH11	0.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:HG3	1:A:191:ARG:NH1	1.57	1.03
1:F:219:ASP:OD1	1:F:223:ASN:HB2	1.53	1.03
1:F:173:PRO:HG3	1:K:179:MET:HE1	1.39	1.01
2:G:647:VAL:HG13	3:G:675:HOH:O	1.57	1.01
1:F:224:LEU:HD23	1:F:241:ARG:HH21	1.23	1.01
1:I:156:PHE:HB3	3:I:269:HOH:O	1.63	0.99
1:A:191:ARG:HH11	1:A:191:ARG:CG	1.76	0.98
1:K:190:GLY:O	2:L:653:SER:HB2	1.67	0.95
1:D:205:THR:CG2	1:D:217:LYS:HG3	1.96	0.94
1:K:158:HIS:CE1	2:L:654:THR:O	2.24	0.90
1:F:206:ARG:CD	3:F:268:HOH:O	2.19	0.90
1:F:219:ASP:OD2	1:F:223:ASN:N	2.04	0.89
1:A:185:LEU:HD12	1:A:191:ARG:HD3	1.54	0.89
1:B:187:GLU:OE1	1:B:191:ARG:HD2	1.73	0.89
1:F:224:LEU:HD23	1:F:241:ARG:NH2	1.87	0.88
1:I:189:SER:HB2	2:J:652:GLU:HB3	1.54	0.85
1:I:227:CYS:HA	1:I:238:LYS:O	1.78	0.83
1:I:214:THR:CG2	1:I:228:ILE:HD12	2.03	0.82
1:B:191:ARG:HG3	1:B:191:ARG:NH1	1.96	0.81
1:F:158:HIS:NE2	2:H:654:THR:O	2.14	0.80
1:B:154:LYS:HE3	1:D:210:ARG:NH1	1.97	0.79
1:F:206:ARG:HD3	3:F:268:HOH:O	1.80	0.79
1:I:187:GLU:OE1	1:I:191:ARG:NH1	2.16	0.78
1:B:191:ARG:HG3	1:B:191:ARG:HH11	1.48	0.78
1:F:158:HIS:CE1	2:H:654:THR:O	2.36	0.78
2:G:649:PHE:CB	2:C:639:GLN:HG3	2.12	0.77
1:F:195:THR:HG21	1:F:197:ARG:NH1	2.01	0.75
1:I:234:ARG:NH2	1:I:236:GLU:OE2	2.19	0.75
1:F:224:LEU:CD2	1:F:241:ARG:NH2	2.48	0.75
1:A:158[A]:HIS:CE1	2:G:654:THR:O	2.40	0.74
1:D:210:ARG:HD3	3:D:288:HOH:O	1.88	0.74
1:I:193:THR:CG2	3:I:260:HOH:O	2.36	0.73
1:I:202:ASP:OD1	1:I:204:ASP:HB2	1.89	0.72
1:I:234:ARG:HH21	1:I:236:GLU:CD	1.93	0.72
1:B:238:LYS:NZ	2:C:642:THR:OG1	2.24	0.70
1:I:214:THR:CG2	1:I:228:ILE:CD1	2.68	0.69
1:I:193:THR:HG22	3:I:260:HOH:O	1.90	0.69
1:F:219:ASP:C	1:F:221:ARG:HB2	2.12	0.69
1:F:219:ASP:CG	1:F:223:ASN:HB2	2.12	0.68
1:F:173:PRO:HG3	1:K:179:MET:HE2	1.73	0.68
1:D:216:SER:O	1:D:217:LYS:HG2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158[A]:HIS:HE1	2:G:654:THR:O	1.76	0.68
1:A:197:ARG:NH1	1:A:198:ASN:OD1	2.27	0.68
1:F:232:ASN:O	1:F:234:ARG:HG3	1.95	0.66
1:K:158:HIS:NE2	2:L:654:THR:O	2.30	0.65
1:K:193:THR:HG22	2:L:650:ASP:CB	2.27	0.65
1:B:191:ARG:HH11	1:B:191:ARG:CG	2.11	0.64
2:G:649:PHE:HB3	2:C:639:GLN:CG	2.22	0.64
1:A:191:ARG:NH1	1:A:191:ARG:CG	2.42	0.63
1:F:173:PRO:CG	1:K:179:MET:CE	2.67	0.63
1:K:177:TRP:CZ2	1:K:203:GLN:HG2	2.33	0.63
1:I:234:ARG:NH2	1:I:236:GLU:CD	2.52	0.63
1:D:225:LEU:HD23	1:D:241:ARG:HA	1.82	0.62
1:F:240:GLU:O	1:F:241:ARG:HB2	2.01	0.61
2:L:641:THR:CG2	3:L:663:HOH:O	2.47	0.61
1:K:158:HIS:HE1	2:L:654:THR:O	1.81	0.60
1:D:193:THR:HG23	3:D:280:HOH:O	2.01	0.60
1:F:234:ARG:HD3	3:F:288:HOH:O	2.00	0.60
1:K:193:THR:HG22	2:L:650:ASP:HB2	1.84	0.60
3:F:287:HOH:O	1:K:179:MET:HE3	2.02	0.59
1:D:216:SER:O	1:D:217:LYS:CG	2.50	0.59
1:K:177:TRP:CH2	1:K:203:GLN:HG2	2.38	0.59
1:F:174:TYR:O	1:F:178:MET:HB2	2.03	0.58
1:D:225:LEU:CD2	1:D:241:ARG:HA	2.35	0.57
1:A:185:LEU:CD1	1:A:191:ARG:HD3	2.33	0.57
1:D:225:LEU:HA	1:D:240:GLU:O	2.05	0.56
1:I:207:THR:HG21	1:I:209:TYR:CZ	2.39	0.56
1:K:193:THR:HG22	2:L:650:ASP:HB3	1.88	0.56
1:B:221:ARG:HD2	3:B:307:HOH:O	2.06	0.56
1:I:234:ARG:NH2	1:I:236:GLU:OE1	2.33	0.56
1:I:227:CYS:CA	1:I:238:LYS:O	2.51	0.55
2:E:650:ASP:OD1	2:E:650:ASP:C	2.45	0.55
1:D:169:THR:HG23	1:D:182:CYS:O	2.06	0.55
1:K:165:VAL:HG22	3:K:248:HOH:O	2.08	0.54
1:F:224:LEU:CD2	1:F:241:ARG:HH21	2.04	0.54
1:I:207:THR:CG2	1:I:209:TYR:CZ	2.91	0.54
1:F:206:ARG:HD2	3:F:268:HOH:O	1.94	0.53
1:I:193:THR:HG22	1:I:193:THR:O	2.08	0.53
1:D:216:SER:O	1:D:217:LYS:HD3	2.09	0.53
1:F:173:PRO:CG	1:K:179:MET:HE2	2.35	0.53
1:D:232:ASN:HD22	1:D:236:GLU:HB3	1.73	0.53
1:D:179:MET:H	1:D:201:ASN:HD21	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:TYR:O	1:D:175:GLN:C	2.48	0.52
1:D:156:PHE:HB2	2:E:654:THR:HA	1.92	0.51
1:D:174:TYR:CZ	1:D:175:GLN:HG2	2.45	0.51
1:D:216:SER:HB3	1:D:224:LEU:HD11	1.92	0.51
1:D:205:THR:CG2	1:D:217:LYS:CG	2.81	0.51
1:F:158:HIS:HE1	2:H:655:LYS:CB	2.24	0.50
1:B:197:ARG:HG3	3:B:257:HOH:O	2.11	0.50
1:I:165:VAL:HG22	1:I:166:VAL:N	2.27	0.50
1:I:232:ASN:ND2	1:I:236:GLU:OE2	2.45	0.49
2:E:641:THR:HG21	3:E:660:HOH:O	2.11	0.49
2:L:641:THR:HG21	3:L:663:HOH:O	2.10	0.49
1:B:153:GLU:N	3:B:325:HOH:O	2.46	0.49
1:D:219:ASP:OD1	1:D:219:ASP:C	2.51	0.49
1:B:241:ARG:NH2	2:C:639:GLN:NE2	2.61	0.48
1:I:193:THR:HG23	3:I:274:HOH:O	2.13	0.48
1:B:154:LYS:HE3	1:D:210:ARG:HH12	1.72	0.48
1:I:165:VAL:HG22	1:I:166:VAL:H	1.79	0.48
1:A:169:THR:HG23	1:A:182:CYS:O	2.13	0.48
1:I:185:LEU:HD12	1:I:185:LEU:N	2.28	0.47
1:D:216:SER:O	1:D:217:LYS:CD	2.62	0.47
1:F:155:CYS:HB3	1:F:192:ILE:HD11	1.97	0.47
1:K:219:ASP:OD2	1:K:223:ASN:HB2	2.14	0.47
1:D:174:TYR:CE2	1:D:175:GLN:HG2	2.50	0.46
1:B:187:GLU:OE2	1:F:238:LYS:HE3	2.15	0.46
1:K:185:LEU:HD12	1:K:191:ARG:HD3	1.98	0.46
1:D:179:MET:H	1:D:201:ASN:ND2	2.14	0.45
1:K:190:GLY:O	2:L:653:SER:CB	2.53	0.45
2:H:645:ASN:ND2	3:H:661:HOH:O	2.49	0.45
1:D:227:CYS:HA	1:D:238:LYS:O	2.16	0.45
1:D:189:SER:HB2	2:E:652:GLU:HB3	1.98	0.45
1:D:228:ILE:HG12	1:D:229:CYS:N	2.32	0.45
1:B:169:THR:HG23	1:B:182:CYS:O	2.16	0.44
1:F:203:GLN:HB2	1:I:175:GLN:NE2	2.32	0.44
2:H:643:GLU:OE2	1:I:174:TYR:OH	2.28	0.44
1:I:193:THR:HG21	3:I:260:HOH:O	2.09	0.44
1:D:178:MET:HG2	1:D:201:ASN:HB3	2.00	0.44
1:I:187:GLU:CD	1:I:191:ARG:NH1	2.70	0.44
1:F:218:LYS:HE2	1:F:218:LYS:HB3	1.77	0.44
1:D:219:ASP:OD1	1:D:220:ASN:N	2.50	0.43
1:D:177:TRP:CH2	1:D:203:GLN:HA	2.53	0.43
1:A:220:ASN:HB3	1:B:175:GLN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ARG:NH1	2:H:650:ASP:OD2	2.52	0.43
1:K:191:ARG:CZ	3:K:284:HOH:O	2.65	0.43
1:D:187:GLU:OE1	1:D:191:ARG:HD2	2.19	0.43
1:I:156:PHE:HD1	3:I:269:HOH:O	2.02	0.43
1:B:187:GLU:OE1	1:B:191:ARG:CD	2.57	0.42
1:I:172:LYS:HE2	3:J:660:HOH:O	2.20	0.42
1:B:185:LEU:HD12	1:B:191:ARG:HD3	2.00	0.42
1:K:220:ASN:OD1	1:K:221:ARG:HD3	2.19	0.42
1:B:179:MET:H	1:B:201:ASN:HD21	1.66	0.42
2:H:644:SER:O	2:H:645:ASN:OD1	2.38	0.41
1:D:169:THR:HA	1:D:182:CYS:O	2.20	0.41
1:I:186:GLY:HA2	1:I:190:GLY:HA2	2.03	0.41
1:F:218:LYS:HA	1:F:223:ASN:O	2.20	0.41
1:K:201:ASN:ND2	1:K:208:SER:HB2	2.36	0.41
1:A:193:THR:O	1:A:193:THR:HG23	2.21	0.41
1:D:154:LYS:HE2	3:D:246:HOH:O	2.21	0.41
3:B:323:HOH:O	1:D:154:LYS:HD2	2.20	0.40
1:D:169:THR:CG2	1:D:182:CYS:O	2.69	0.40
1:K:229:CYS:O	3:K:282:HOH:O	2.22	0.40
1:D:239:CYS:HB2	2:E:641:THR:CG2	2.52	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	88/89 (99%)	84 (96%)	4 (4%)	0	100 100
1	B	87/89 (98%)	84 (97%)	3 (3%)	0	100 100
1	D	87/89 (98%)	83 (95%)	4 (5%)	0	100 100
1	F	84/89 (94%)	79 (94%)	4 (5%)	1 (1%)	13 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	75/89 (84%)	71 (95%)	3 (4%)	1 (1%)	12 6
1	K	87/89 (98%)	82 (94%)	5 (6%)	0	100 100
2	C	15/18 (83%)	15 (100%)	0	0	100 100
2	E	14/18 (78%)	14 (100%)	0	0	100 100
2	G	15/18 (83%)	15 (100%)	0	0	100 100
2	H	15/18 (83%)	15 (100%)	0	0	100 100
2	J	11/18 (61%)	11 (100%)	0	0	100 100
2	L	15/18 (83%)	15 (100%)	0	0	100 100
All	All	593/642 (92%)	568 (96%)	23 (4%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	204	ASP
1	F	187	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	77/76 (101%)	76 (99%)	1 (1%)	69 74
1	B	76/76 (100%)	73 (96%)	3 (4%)	32 30
1	D	75/76 (99%)	72 (96%)	3 (4%)	31 29
1	F	74/76 (97%)	72 (97%)	2 (3%)	44 46
1	I	67/76 (88%)	64 (96%)	3 (4%)	27 24
1	K	76/76 (100%)	73 (96%)	3 (4%)	32 30
2	C	16/17 (94%)	16 (100%)	0	100 100
2	E	16/17 (94%)	13 (81%)	3 (19%)	1 0
2	G	16/17 (94%)	16 (100%)	0	100 100
2	H	16/17 (94%)	15 (94%)	1 (6%)	18 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	13/17 (76%)	11 (85%)	2 (15%)	2 1
2	L	16/17 (94%)	13 (81%)	3 (19%)	1 0
All	All	538/558 (96%)	514 (96%)	24 (4%)	27 24

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	ARG
1	B	172	LYS
1	B	191	ARG
1	B	192	ILE
1	D	158	HIS
1	D	189	SER
1	D	228	ILE
2	E	643	GLU
2	E	650	ASP
2	E	654	THR
1	F	191	ARG
1	F	218	LYS
2	H	651	GLU
1	I	153	GLU
1	I	191	ARG
1	I	193	THR
2	J	640	VAL
2	J	644	SER
1	K	165	VAL
1	K	191	ARG
1	K	221	ARG
2	L	650	ASP
2	L	651	GLU
2	L	653	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	232	ASN
1	B	201	ASN
1	B	203	GLN
2	C	639	GLN

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Mol	Chain	Res	Type
1	D	158	HIS
1	D	201	ASN
1	D	226	GLN
1	D	232	ASN
1	F	175	GLN
1	F	201	ASN
2	H	645	ASN
1	I	201	ASN
1	I	232	ASN
1	K	201	ASN

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

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, 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	89/89 (100%)	-0.13	1 (1%) 80 79	16, 25, 40, 43	0
1	B	89/89 (100%)	-0.06	1 (1%) 80 79	16, 25, 45, 49	0
1	D	89/89 (100%)	0.77	11 (12%) 4 3	29, 44, 61, 64	0
1	F	88/89 (98%)	0.09	4 (4%) 33 32	21, 33, 51, 59	0
1	I	79/89 (88%)	0.64	11 (13%) 2 2	26, 43, 58, 60	0
1	K	89/89 (100%)	0.21	4 (4%) 33 32	24, 37, 50, 58	0
2	C	17/18 (94%)	0.18	0 100 100	18, 28, 53, 54	0
2	E	16/18 (88%)	1.34	4 (25%) 0 0	35, 44, 62, 63	0
2	G	17/18 (94%)	0.05	1 (5%) 22 21	18, 27, 47, 47	0
2	H	17/18 (94%)	0.85	1 (5%) 22 21	34, 39, 48, 53	0
2	J	13/18 (72%)	1.20	1 (7%) 13 12	31, 40, 53, 55	0
2	L	17/18 (94%)	0.79	2 (11%) 4 4	30, 36, 56, 56	0
All	All	620/642 (96%)	0.32	41 (6%) 18 17	16, 36, 56, 64	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	224	LEU	5.6
2	E	654	THR	4.9
1	D	223	ASN	4.6
1	D	221	ARG	4.6
1	F	223	ASN	4.3
1	D	218	LYS	4.1
2	H	654	THR	4.1
1	D	222	GLY	4.0
2	J	640	VAL	3.6
1	K	221	ARG	3.6
2	E	653	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	225	LEU	3.4
1	I	190	GLY	3.4
1	I	191	ARG	3.3
1	I	189	SER	3.2
1	I	227	CYS	2.9
1	F	222	GLY	2.8
1	B	158	HIS	2.7
2	L	654	THR	2.7
1	D	217	LYS	2.7
1	I	239	CYS	2.6
1	I	216	SER	2.6
1	I	159	ALA	2.6
1	I	186	GLY	2.5
1	K	224	LEU	2.5
1	D	158	HIS	2.4
1	A	158[A]	HIS	2.4
1	F	224	LEU	2.4
1	D	188	GLY	2.3
2	E	639	GLN	2.3
1	D	220	ASN	2.3
2	E	640	VAL	2.2
2	G	638	GLY	2.1
1	D	219	ASP	2.1
1	K	241	ARG	2.1
1	I	188	GLY	2.1
1	I	185	LEU	2.0
2	L	652	GLU	2.0
1	K	220	ASN	2.0
1	I	240	GLU	2.0
1	F	219	ASP	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.