Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 06:27 PM EDT

PDB ID	:	4KJW
Title	:	Structure of the CLC-ec1 deltaNC construct in 100mM fluoride and 20mM bromide
Authors	:	Lim, H.-H.; Miller, C.
Deposited on	:	2013-05-03
Resolution	:	3.03 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:

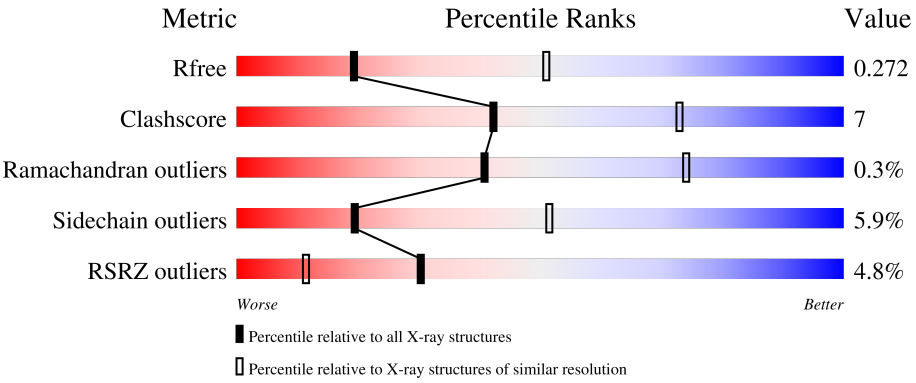
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	446	6% 76% 21%
1	B	446	4% 75% 22%
2	C	222	5% 85% 13%
2	E	222	2% 86% 14%
3	D	211	8% 81% 16%

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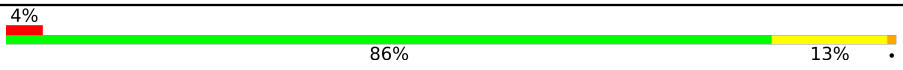
Mol	Chain	Length	Quality of chain
3	F	211	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13223 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P37019
A	461	LYS	-	expression tag	UNP P37019
B	16	MET	-	expression tag	UNP P37019
B	461	LYS	-	expression tag	UNP P37019

- Molecule 2 is a protein called Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab, light chain.

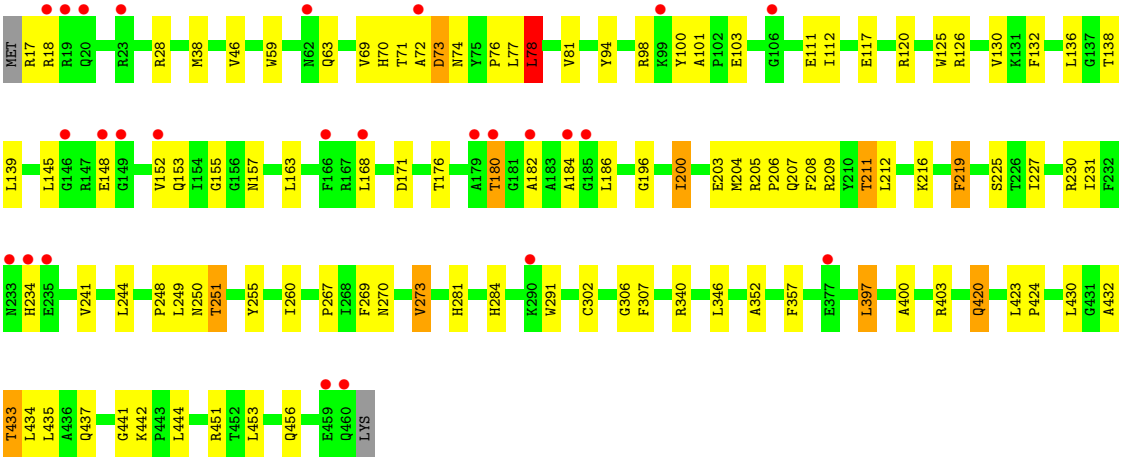
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

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.

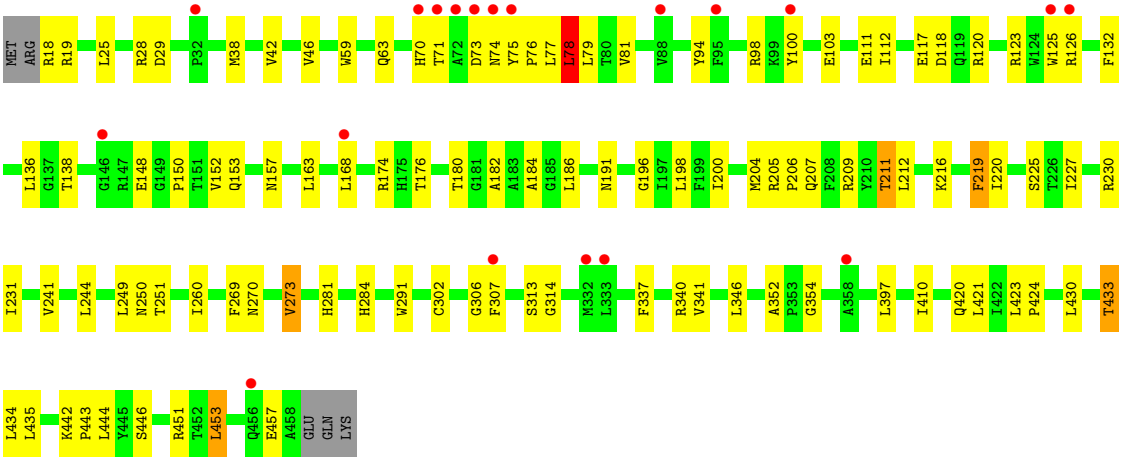
• Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



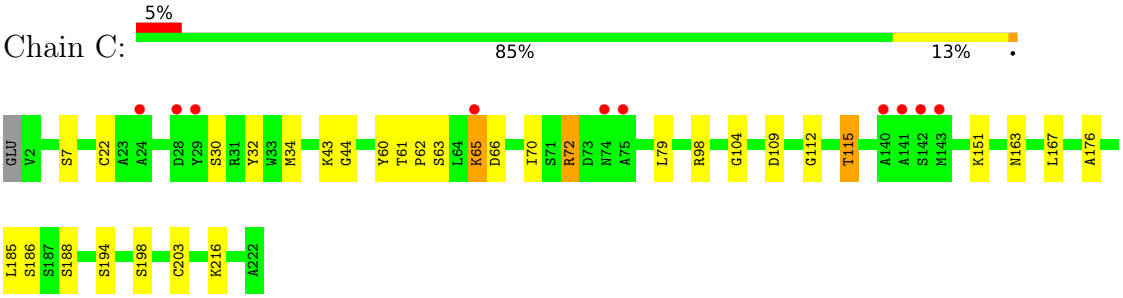
• Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:



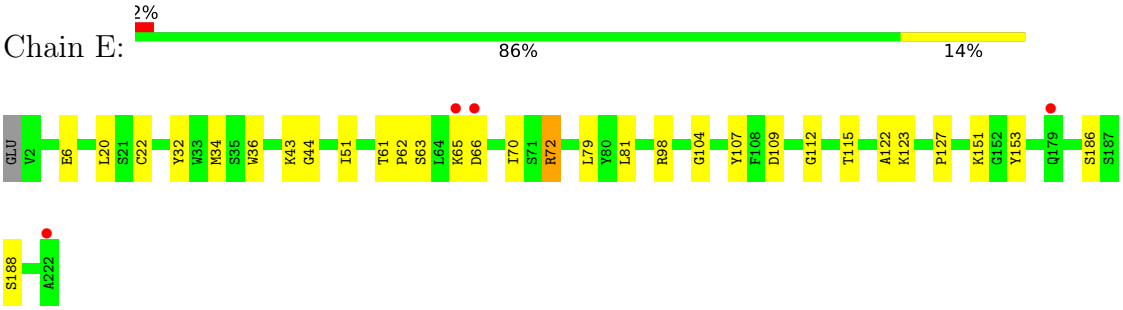
• Molecule 2: Fab, heavy chain

Chain C:



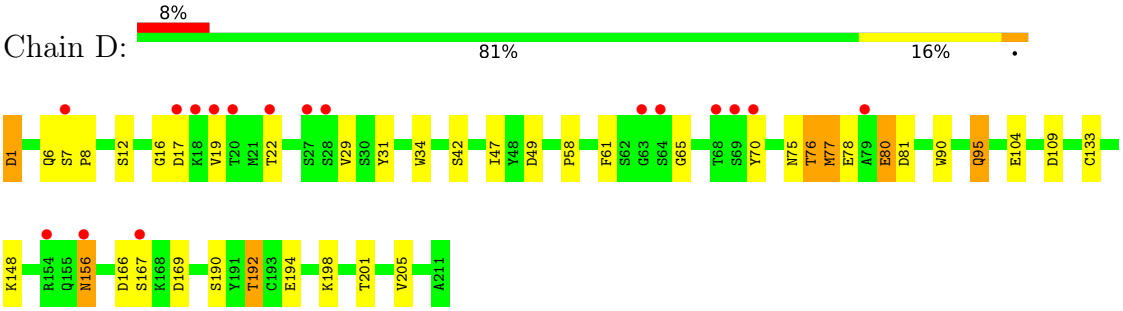
• Molecule 2: Fab, heavy chain

Chain E:



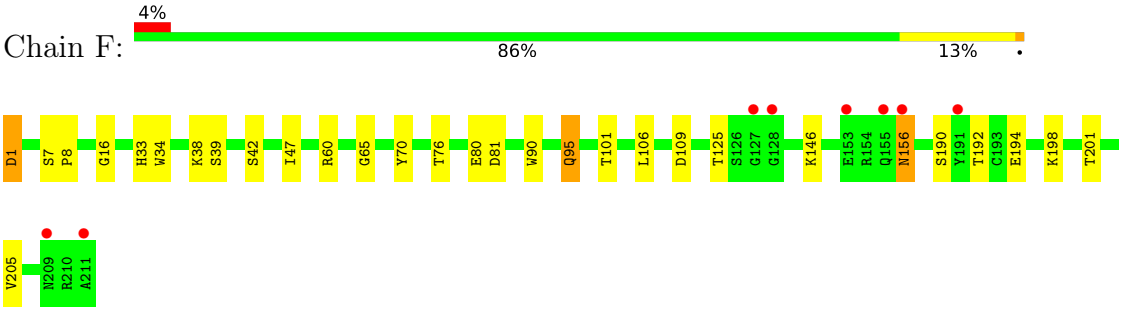
• Molecule 3: Fab, light chain

Chain D:



• Molecule 3: Fab, light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.68Å 98.89Å 172.91Å 90.00° 132.90° 90.00°	Depositor
Resolution (Å)	39.48 – 3.03 39.48 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.48-3.03) 98.9 (39.48-3.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.230 , 0.269 0.235 , 0.272	Depositor DCC
R_{free} test set	2819 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	90.3	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 35.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.30	0/3405	0.43	1/4621 (0.0%)
1	B	0.29	0/3376	0.43	1/4583 (0.0%)
2	C	0.33	0/1721	0.44	0/2355
2	E	0.33	0/1721	0.44	0/2355
3	D	0.35	0/1660	0.51	0/2257
3	F	0.33	0/1660	0.46	0/2257
All	All	0.32	0/13543	0.45	2/18428 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	LEU	CA-CB-CG	5.78	128.58	115.30
1	B	78	LEU	CA-CB-CG	5.64	128.26	115.30

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	3333	0	3484	68	0
1	B	3304	0	3457	69	0
2	C	1672	0	1654	16	0
2	E	1672	0	1654	14	0
3	D	1621	0	1546	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1621	0	1546	18	0
All	All	13223	0	13341	184	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 7.

All (184) 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:A:430:LEU:HD21	1:B:219:PHE:HB3	1.60	0.83
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.61	0.81
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.67	0.76
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.20	0.75
3:D:1:ASP:OD2	3:D:1:ASP:N	2.19	0.72
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.55	0.72
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.55	0.71
3:F:1:ASP:OD2	3:F:1:ASP:N	2.23	0.70
3:F:38:LYS:NZ	3:F:80:GLU:O	2.25	0.70
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.72	0.69
2:C:112:GLY:O	3:D:42:SER:OG	2.12	0.67
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.27	0.67
1:A:73:ASP:OD1	1:A:73:ASP:N	2.26	0.65
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.28	0.65
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.80	0.63
3:D:75:ASN:O	3:D:76:THR:OG1	2.12	0.61
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.82	0.61
1:B:73:ASP:N	1:B:73:ASP:OD1	2.34	0.60
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.84	0.60
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.34	0.60
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.83	0.60
2:C:163:ASN:HD22	2:C:167:LEU:HD13	1.66	0.59
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.84	0.58
3:D:95:GLN:OE1	3:D:95:GLN:N	2.37	0.58
1:B:200:ILE:HA	1:B:204:MET:HB2	1.84	0.58
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.86	0.57
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.87	0.57
1:B:153:GLN:O	1:B:157:ASN:ND2	2.35	0.57
1:A:200:ILE:HA	1:A:204:MET:HB2	1.85	0.56
1:B:111:GLU:OE2	1:B:120:ARG:NE	2.38	0.56
3:F:95:GLN:N	3:F:95:GLN:OE1	2.39	0.56
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.38	0.55
1:A:437:GLN:OE1	1:B:216:LYS:NZ	2.33	0.55
1:A:148:GLU:H	1:A:148:GLU:CD	2.09	0.54
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.90	0.54
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.90	0.54
1:B:148:GLU:H	1:B:148:GLU:CD	2.11	0.53
1:A:132:PHE:O	1:A:136:LEU:HB2	2.09	0.53
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.41	0.53
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.43	0.53
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.90	0.53
2:E:61:THR:O	2:E:63:SER:N	2.42	0.53
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.12	0.52
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.44	0.52
3:F:156:ASN:OD1	3:F:156:ASN:N	2.43	0.52
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.43	0.51
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.45	0.51
1:B:227:ILE:O	1:B:231:ILE:HG12	2.11	0.51
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.25	0.51
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.43	0.51
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.42	0.51
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.93	0.51
2:C:32:TYR:O	2:C:72:ARG:NH2	2.42	0.50
1:A:302:CYS:O	1:A:306:GLY:N	2.42	0.50
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.94	0.50
2:C:7:SER:HA	2:C:115:THR:HG21	1.93	0.50
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.94	0.50
3:F:34:TRP:HB2	3:F:47:ILE:HB	1.93	0.50
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.93	0.50
1:A:227:ILE:O	1:A:231:ILE:HG12	2.12	0.49
1:A:270:ASN:ND2	1:A:442:LYS:O	2.45	0.49
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.93	0.49
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.47	0.49
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.48	0.49
3:D:156:ASN:N	3:D:156:ASN:OD1	2.45	0.49
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.47	0.48
3:F:34:TRP:N	3:F:47:ILE:O	2.44	0.48
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.96	0.48
2:E:32:TYR:O	2:E:72:ARG:NH2	2.46	0.48
3:D:29:VAL:O	3:D:70:TYR:OH	2.22	0.48
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.78	0.47
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.97	0.47
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.96	0.47
1:B:270:ASN:ND2	1:B:442:LYS:O	2.47	0.47
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.49	0.47
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.97	0.47
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.97	0.46
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.97	0.46
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.49	0.46
2:C:61:THR:O	2:C:63:SER:N	2.48	0.46
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.97	0.46
1:A:71:THR:O	1:A:78:LEU:HB2	2.16	0.46
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.97	0.46
1:A:234:HIS:HD1	1:A:234:HIS:H	1.63	0.46
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.98	0.46
1:A:112:ILE:HG13	1:A:153:GLN:HA	1.97	0.45
3:D:95:GLN:CD	3:D:95:GLN:H	2.20	0.45
2:E:36:TRP:HD1	2:E:70:ILE:HD13	1.81	0.45
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.97	0.45
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.98	0.45
1:B:176:THR:O	1:B:180:THR:HG23	2.16	0.45
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.98	0.45
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.98	0.45
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.98	0.45
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.51	0.45
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.81	0.45
1:A:216:LYS:HE2	1:B:433:THR:HB	1.99	0.45
1:B:337:PHE:O	1:B:341:VAL:HG23	2.17	0.45
1:B:269:PHE:O	1:B:273:VAL:HG12	2.18	0.44
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.98	0.44
1:A:208:PHE:HE1	1:B:25:LEU:HD23	1.83	0.44
1:A:249:LEU:HD13	1:B:231:ILE:HD13	1.98	0.44
1:B:59:TRP:O	1:B:63:GLN:HG2	2.17	0.44
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.99	0.44
3:D:65:GLY:HA3	3:D:70:TYR:HA	2.00	0.44
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.52	0.44
1:A:433:THR:HB	1:B:216:LYS:HE2	2.00	0.44
3:D:77:MET:HG3	3:D:81:ASP:HB3	1.99	0.43
1:B:421:LEU:C	1:B:424:PRO:HD2	2.39	0.43
1:B:132:PHE:O	1:B:136:LEU:HB2	2.18	0.43
1:B:198:LEU:HG	1:B:410:ILE:HD12	2.01	0.43
1:A:100:TYR:O	1:A:126:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ALA:HB1	1:A:225:SER:CB	2.48	0.43
1:A:267:PRO:HG3	1:A:441:GLY:HA3	1.99	0.43
1:B:112:ILE:HG13	1:B:153:GLN:HA	2.01	0.43
2:C:65:LYS:H	2:C:65:LYS:HG3	1.42	0.43
1:B:216:LYS:O	1:B:220:ILE:HG13	2.19	0.43
2:C:203:CYS:SG	2:C:216:LYS:HB3	2.59	0.43
1:A:46:VAL:HG22	1:A:155:GLY:HA2	2.01	0.42
1:A:434:LEU:HD21	1:B:220:ILE:HD11	2.00	0.42
1:B:75:TYR:HB3	1:B:76:PRO:HD3	2.01	0.42
3:D:31:TYR:HB3	3:D:49:ASP:HA	2.01	0.42
1:A:139:LEU:CD2	1:A:145:LEU:HB2	2.48	0.42
1:B:150:PRO:HD3	1:B:354:GLY:HA2	2.00	0.42
1:A:138:THR:HG21	1:A:352:ALA:HB1	2.02	0.42
1:B:42:VAL:O	1:B:46:VAL:HG23	2.20	0.42
3:D:12:SER:HA	3:D:104:GLU:O	2.19	0.42
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.84	0.42
1:B:302:CYS:O	1:B:306:GLY:N	2.45	0.42
1:A:69:VAL:HA	1:A:72:ALA:HB2	2.02	0.42
1:B:313:SER:OG	1:B:314:GLY:N	2.52	0.42
1:A:152:VAL:HG13	1:A:182:ALA:HB1	2.02	0.42
3:D:78:GLU:HB2	3:D:80:GLU:HG3	2.02	0.42
3:F:109:ASP:OD2	3:F:198:LYS:NZ	2.52	0.42
2:C:43:LYS:HB3	2:C:44:GLY:H	1.70	0.42
3:F:16:GLY:HA2	3:F:76:THR:HG23	2.02	0.42
1:A:269:PHE:O	1:A:273:VAL:HG12	2.20	0.42
1:B:71:THR:O	1:B:78:LEU:HB2	2.20	0.42
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.23	0.42
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.85	0.42
2:E:112:GLY:O	3:F:42:SER:OG	2.23	0.42
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.55	0.41
1:A:74:ASN:OD1	1:A:76:PRO:HD2	2.21	0.41
1:B:78:LEU:HD13	1:B:79:LEU:HD23	2.02	0.41
1:A:148:GLU:OE1	1:A:357:PHE:HB3	2.20	0.41
1:A:420:GLN:H	1:A:420:GLN:HG3	1.57	0.41
1:B:184:ALA:HB1	1:B:225:SER:HB2	2.03	0.41
1:A:250:ASN:OD1	2:C:104:GLY:HA3	2.19	0.41
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.56	0.41
3:F:8:PRO:O	3:F:101:THR:HG23	2.20	0.41
1:A:403:ARG:NH2	1:A:437:GLN:HB2	2.35	0.41
3:D:6:GLN:HA	3:D:22:THR:O	2.20	0.41
3:D:19:VAL:HG21	3:D:77:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:GLU:HG2	3:F:205:VAL:HG12	2.02	0.41
1:A:248:PRO:O	1:A:251:THR:HG22	2.21	0.41
1:B:138:THR:HG21	1:B:352:ALA:HB1	2.03	0.41
1:B:100:TYR:O	1:B:126:ARG:NH1	2.49	0.41
2:E:6:GLU:HA	2:E:22:CYS:HA	2.03	0.41
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.78	0.41
1:A:403:ARG:NH2	1:B:29:ASP:OD1	2.52	0.41
1:B:136:LEU:HD12	1:B:136:LEU:HA	1.79	0.41
2:C:194:SER:O	2:C:198:SER:OG	2.38	0.41
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.55	0.41
3:D:77:MET:HE2	3:D:77:MET:HB2	1.81	0.41
3:D:166:ASP:OD1	3:D:167:SER:N	2.54	0.41
2:E:51:ILE:HD13	2:E:72:ARG:HG2	2.03	0.41
1:A:139:LEU:HD21	1:A:145:LEU:HB2	2.03	0.40
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.21	0.40
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.57	0.40
1:B:184:ALA:HB1	1:B:225:SER:CB	2.52	0.40
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.90	0.40
2:C:30:SER:C	2:C:32:TYR:H	2.25	0.40
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.57	0.40
2:E:43:LYS:HB3	2:E:44:GLY:H	1.74	0.40
1:A:59:TRP:O	1:A:63:GLN:HG2	2.21	0.40
1:A:176:THR:O	1:A:180:THR:HG23	2.21	0.40
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.29	0.40
1:B:19:ARG:HD2	1:B:19:ARG:HA	1.91	0.40
1:B:125:TRP:HD1	1:B:126:ARG:HG3	1.85	0.40
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.21	0.40
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.57	0.40
1:A:153:GLN:O	1:A:157:ASN:ND2	2.53	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	442/446 (99%)	427 (97%)	15 (3%)	0	100	100
1	B	439/446 (98%)	423 (96%)	16 (4%)	0	100	100
2	C	219/222 (99%)	201 (92%)	17 (8%)	1 (0%)	29	65
2	E	219/222 (99%)	204 (93%)	13 (6%)	2 (1%)	17	52
3	D	209/211 (99%)	191 (91%)	15 (7%)	3 (1%)	11	40
3	F	209/211 (99%)	196 (94%)	13 (6%)	0	100	100
All	All	1737/1758 (99%)	1642 (94%)	89 (5%)	6 (0%)	41	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	76	THR
2	C	62	PRO
2	E	62	PRO
3	D	169	ASP
3	D	16	GLY
2	E	122	ALA

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	335/337 (99%)	308 (92%)	27 (8%)	11	37
1	B	332/337 (98%)	311 (94%)	21 (6%)	18	49
2	C	181/182 (100%)	174 (96%)	7 (4%)	32	66
2	E	181/182 (100%)	173 (96%)	8 (4%)	28	63
3	D	185/185 (100%)	175 (95%)	10 (5%)	22	55
3	F	185/185 (100%)	176 (95%)	9 (5%)	25	59
All	All	1399/1408 (99%)	1317 (94%)	82 (6%)	19	51

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	70	HIS
1	A	73	ASP
1	A	78	LEU
1	A	81	VAL
1	A	103	GLU
1	A	171	ASP
1	A	180	THR
1	A	200	ILE
1	A	205	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	230	ARG
1	A	241	VAL
1	A	244	LEU
1	A	251	THR
1	A	273	VAL
1	A	340	ARG
1	A	346	LEU
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU
1	A	433	THR
1	A	444	LEU
1	A	451	ARG
1	A	453	LEU
1	B	70	HIS
1	B	78	LEU
1	B	81	VAL
1	B	103	GLU
1	B	205	ARG
1	B	211	THR
1	B	212	LEU
1	B	219	PHE
1	B	241	VAL
1	B	244	LEU
1	B	251	THR
1	B	273	VAL
1	B	340	ARG
1	B	346	LEU
1	B	397	LEU
1	B	420	GLN

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Mol	Chain	Res	Type
1	B	423	LEU
1	B	433	THR
1	B	444	LEU
1	B	451	ARG
1	B	453	LEU
2	C	65	LYS
2	C	66	ASP
2	C	72	ARG
2	C	115	THR
2	C	151	LYS
2	C	186	SER
2	C	188	SER
3	D	1	ASP
3	D	17	ASP
3	D	77	MET
3	D	80	GLU
3	D	95	GLN
3	D	133	CYS
3	D	156	ASN
3	D	190	SER
3	D	192	THR
3	D	201	THR
2	E	65	LYS
2	E	66	ASP
2	E	72	ARG
2	E	115	THR
2	E	123	LYS
2	E	151	LYS
2	E	186	SER
2	E	188	SER
3	F	1	ASP
3	F	39	SER
3	F	95	GLN
3	F	106	LEU
3	F	125	THR
3	F	156	ASN
3	F	190	SER
3	F	192	THR
3	F	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	163	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	444/446 (99%)	0.15	26 (5%) 22 7	42, 63, 88, 123	0
1	B	441/446 (98%)	-0.01	19 (4%) 35 14	45, 66, 101, 133	0
2	C	221/222 (99%)	-0.05	10 (4%) 33 12	29, 60, 96, 126	0
2	E	221/222 (99%)	-0.33	4 (1%) 68 40	37, 62, 90, 125	0
3	D	211/211 (100%)	0.07	17 (8%) 12 3	43, 69, 97, 115	0
3	F	211/211 (100%)	0.03	8 (3%) 40 17	38, 55, 101, 119	0
All	All	1749/1758 (99%)	0.00	84 (4%) 30 11	29, 63, 97, 133	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	GLU	7.7
3	F	155	GLN	6.0
3	D	167	SER	5.8
1	A	460	GLN	5.6
3	D	79	ALA	5.1
3	D	18	LYS	5.1
1	B	72	ALA	4.9
1	A	234	HIS	4.8
1	B	74	ASN	4.4
3	F	156	ASN	4.3
3	D	20	THR	4.2
1	A	168	LEU	4.2
2	C	29	TYR	4.1
1	B	73	ASP	4.1
3	D	64	SER	4.0
3	D	70	TYR	4.0
3	F	211	ALA	3.8
3	D	7	SER	3.8
1	A	23	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
3	D	156	ASN	3.7
1	B	71	THR	3.6
3	D	22	THR	3.6
1	A	459	GLU	3.6
1	A	18	ARG	3.5
1	B	95	PHE	3.4
1	B	70	HIS	3.4
2	E	65	LYS	3.4
3	F	127	GLY	3.3
3	D	69	SER	3.3
3	D	68	THR	3.2
1	B	168	LEU	3.1
2	C	141	ALA	3.1
3	D	17	ASP	3.0
3	F	128	GLY	3.0
1	B	307	PHE	3.0
3	D	27	SER	2.9
2	E	222	ALA	2.9
2	C	140	ALA	2.9
1	A	20	GLN	2.9
1	A	166	PHE	2.8
3	F	153	GLU	2.8
1	B	125	TRP	2.7
1	B	32	PRO	2.7
1	A	290	LYS	2.7
1	A	182	ALA	2.7
1	A	148	GLU	2.5
1	B	100	TYR	2.5
1	B	332	MET	2.5
1	B	75	TYR	2.5
2	C	142	SER	2.5
1	B	333	LEU	2.5
1	A	72	ALA	2.4
1	A	99	LYS	2.4
2	C	74	ASN	2.4
1	A	185	GLY	2.3
2	E	66	ASP	2.3
1	B	146	GLY	2.3
2	C	75	ALA	2.3
1	A	146	GLY	2.3
1	A	179	ALA	2.3
2	E	179	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	191	TYR	2.2
1	A	377	GLU	2.2
3	D	19	VAL	2.2
2	C	24	ALA	2.2
1	B	126	ARG	2.1
1	A	19	ARG	2.1
2	C	65	LYS	2.1
1	A	149	GLY	2.1
2	C	28	ASP	2.1
1	A	152	VAL	2.1
2	C	143	MET	2.1
3	D	63	GLY	2.1
1	A	184	ALA	2.1
3	F	209	ASN	2.1
1	B	88	VAL	2.1
1	A	106	GLY	2.1
1	A	62	ASN	2.0
1	A	233	ASN	2.0
3	D	28	SER	2.0
3	D	154	ARG	2.0
1	B	358	ALA	2.0
1	A	180	THR	2.0
1	B	456	GLN	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.