Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:06 PM GMT

PDB ID	:	4KK5
Title	:	Structure of the CLC-ec1 deltaNC construct in 20mM fluoride and 20mM bromide
Authors	:	Lim, H.-H.; Miller, C.
Deposited on	:	2013-05-05
Resolution	:	3.17 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

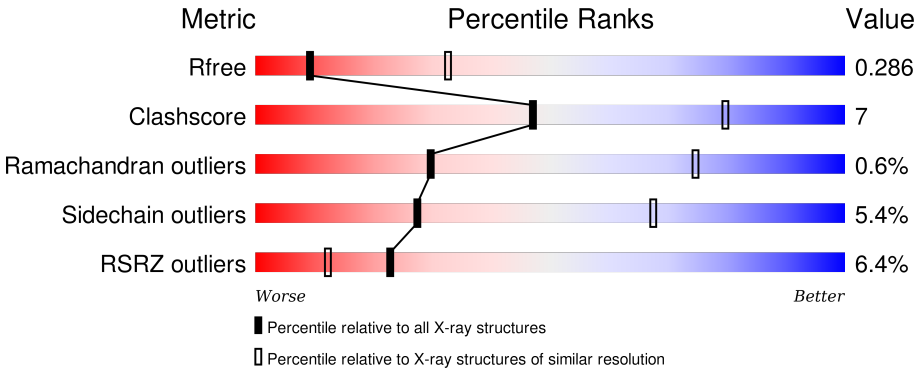
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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}	91344	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 78% 20%
1	B	446	5% 78% 18%
2	C	222	8% 78% 21%
2	E	222	2% 78% 21%
3	D	211	10% 73% 25%

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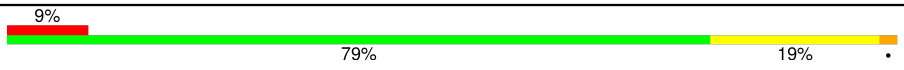
Mol	Chain	Length	Quality of chain
3	F	211	

2 Entry composition

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.

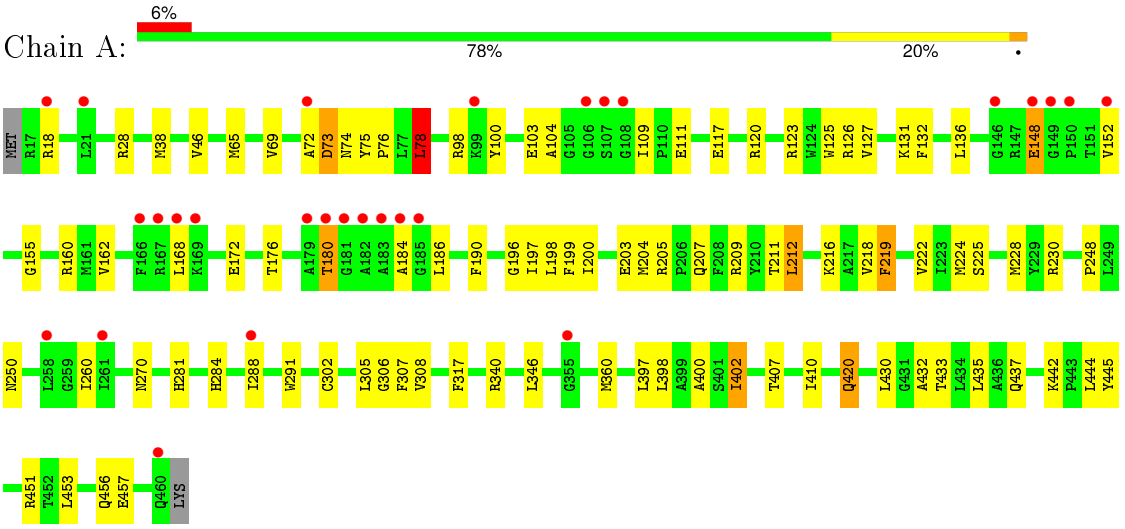
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

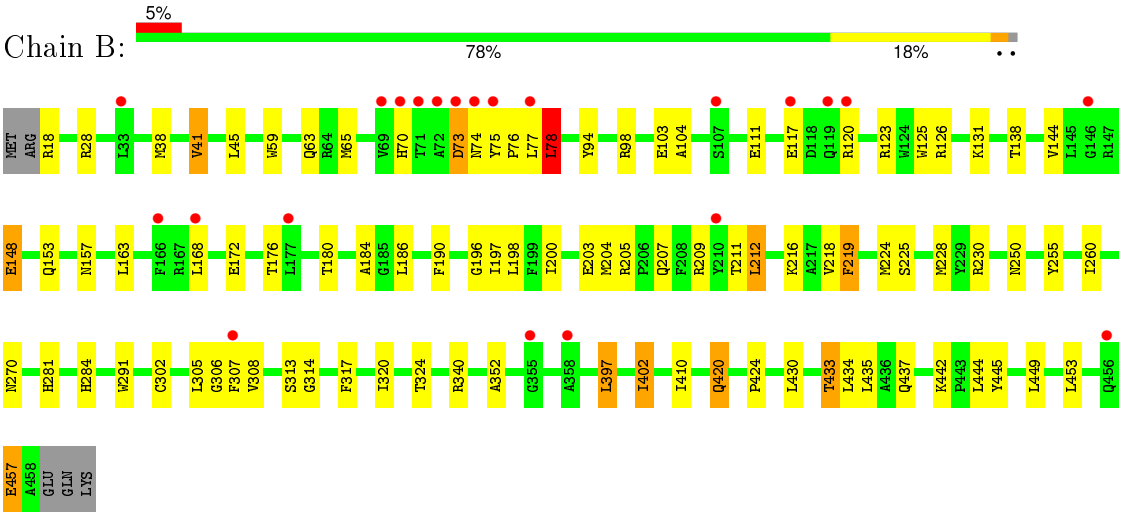
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



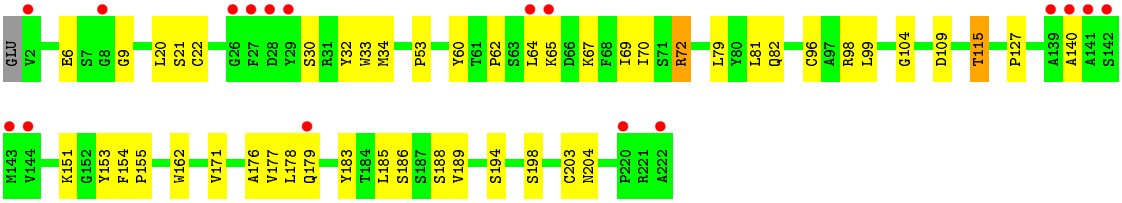
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:

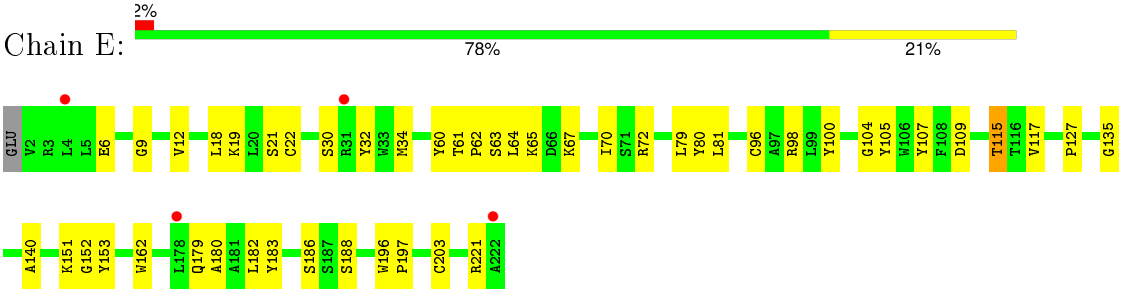


- Molecule 2: Fab, heavy chain

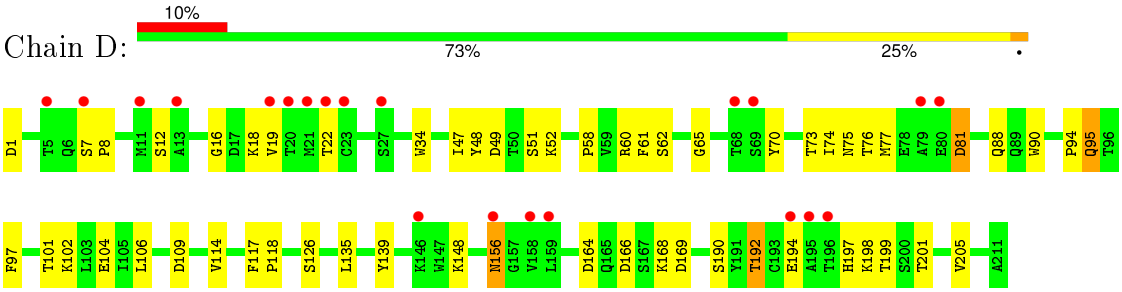
Chain C:



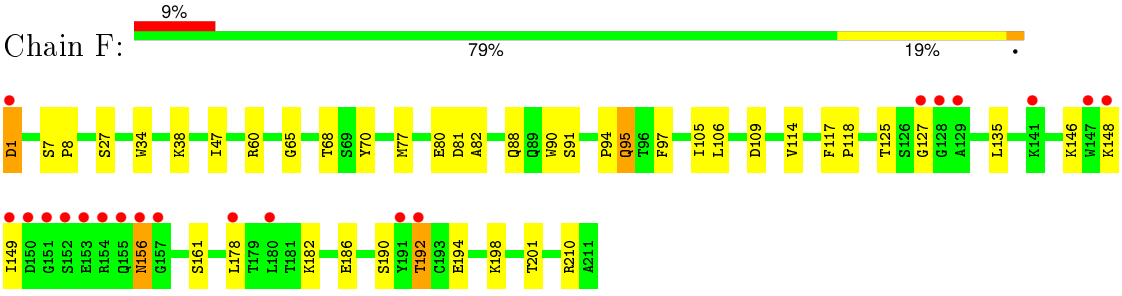
• Molecule 2: Fab, heavy chain



• Molecule 3: Fab, light chain



• Molecule 3: Fab, light chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	229.13Å 98.17Å 169.76Å 90.00° 131.73° 90.00°	Depositor
Resolution (Å)	39.78 – 3.17 39.78 – 3.17	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.78-3.17) 98.3 (39.78-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.271 0.251 , 0.286	Depositor DCC
R_{free} test set	2390 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	87.8	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 14.9	EDS
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 47064 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	13223	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 3.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/3405	0.44	1/4621 (0.0%)
1	B	0.30	0/3376	0.44	1/4583 (0.0%)
2	C	0.35	0/1721	0.47	0/2355
2	E	0.35	0/1721	0.47	0/2355
3	D	0.32	0/1660	0.49	0/2257
3	F	0.34	0/1660	0.47	0/2257
All	All	0.33	0/13543	0.46	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	B	78	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	78	LEU	CA-CB-CG	5.53	128.02	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	58	0
1	B	3304	0	3457	56	0
2	C	1672	0	1654	23	0
2	E	1672	0	1654	25	0
3	D	1621	0	1546	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1621	0	1546	22	0
All	All	13223	0	13341	199	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 (199) 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:152:GLY:HA2	2:E:182:LEU:HD21	1.40	1.04
1:B:153:GLN:O	1:B:157:ASN:ND2	2.10	0.84
3:F:38:LYS:NZ	3:F:80:GLU:O	2.23	0.72
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.23	0.71
1:A:437:GLN:OE1	1:B:216:LYS:NZ	2.25	0.70
1:A:73:ASP:OD1	1:A:73:ASP:N	2.25	0.69
1:A:216:LYS:NZ	1:B:437:GLN:OE1	2.26	0.69
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.74	0.69
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.73	0.68
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.77	0.65
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.62	0.65
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.30	0.64
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.79	0.64
1:A:200:ILE:HA	1:A:204:MET:HB2	1.78	0.64
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.33	0.62
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.82	0.61
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.81	0.61
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.34	0.61
1:A:402:ILE:HD11	1:A:445:TYR:CE1	2.36	0.61
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.34	0.61
1:B:73:ASP:OD1	1:B:73:ASP:N	2.34	0.60
1:B:402:ILE:HD11	1:B:445:TYR:CE1	2.36	0.60
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.85	0.59
2:E:9:GLY:H	2:E:115:THR:HG21	1.66	0.59
3:D:166:ASP:OD1	3:D:168:LYS:N	2.35	0.58
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.86	0.58
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.85	0.58
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.86	0.58
1:B:104:ALA:O	1:B:131:LYS:NZ	2.31	0.57
1:B:148:GLU:CD	1:B:148:GLU:H	2.08	0.57
1:A:104:ALA:HB2	1:A:127:VAL:HG13	1.87	0.56
1:A:457:GLU:HG3	1:B:18:ARG:HH11	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:HA	1:B:204:MET:HB2	1.88	0.56
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.70	0.56
2:E:152:GLY:CA	2:E:182:LEU:HD21	2.27	0.56
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.89	0.55
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.72	0.55
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.88	0.54
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.88	0.54
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.90	0.54
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.89	0.54
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.28	0.54
3:F:149:ILE:HD11	3:F:178:LEU:HD21	1.90	0.54
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.44	0.53
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.90	0.53
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.73	0.53
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.44	0.53
1:B:111:GLU:OE2	1:B:120:ARG:NE	2.41	0.53
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.42	0.52
3:D:102:LYS:NZ	3:D:164:ASP:OD2	2.42	0.52
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.92	0.52
2:E:105:TYR:CD2	3:F:91:SER:HA	2.44	0.52
2:E:179:GLN:O	2:E:180:ALA:HB3	2.10	0.51
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.91	0.51
3:D:74:ILE:HG21	3:D:81:ASP:OD1	2.10	0.51
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.92	0.51
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.92	0.51
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.74	0.51
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.46	0.51
1:A:148:GLU:H	1:A:148:GLU:CD	2.13	0.51
2:E:6:GLU:HA	2:E:22:CYS:HA	1.92	0.50
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.91	0.50
3:F:109:ASP:OD2	3:F:198:LYS:NZ	2.45	0.50
2:E:64:LEU:HB2	2:E:67:LYS:HB2	1.93	0.50
1:B:172:GLU:HG3	1:B:212:LEU:O	2.11	0.50
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.46	0.50
1:B:176:THR:O	1:B:180:THR:HG23	2.12	0.49
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.92	0.49
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.43	0.49
3:D:58:PRO:HB2	3:D:60:ARG:HG2	1.94	0.49
1:A:190:PHE:HE2	1:A:317:PHE:HZ	1.60	0.49
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.94	0.49
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:18:LYS:HA	3:D:74:ILE:O	2.13	0.49
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.78	0.49
3:F:156:ASN:OD1	3:F:156:ASN:N	2.46	0.48
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.48	0.48
3:F:34:TRP:HB2	3:F:47:ILE:HB	1.94	0.48
1:A:28:ARG:NH2	1:B:203:GLU:OE1	2.28	0.48
1:A:176:THR:O	1:A:180:THR:HG23	2.13	0.48
3:F:127:GLY:O	3:F:182:LYS:N	2.44	0.48
3:D:156:ASN:N	3:D:156:ASN:OD1	2.46	0.48
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.96	0.48
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.46	0.48
1:A:172:GLU:HG3	1:A:212:LEU:O	2.13	0.48
2:C:20:LEU:HD12	2:C:81:LEU:HD23	1.96	0.48
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.48	0.48
1:B:180:THR:HG22	1:B:218:VAL:HA	1.95	0.48
1:A:100:TYR:O	1:A:126:ARG:NH1	2.43	0.48
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.78	0.48
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.95	0.48
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.95	0.48
1:A:302:CYS:O	1:A:306:GLY:N	2.44	0.47
3:D:8:PRO:O	3:D:101:THR:HG23	2.14	0.47
2:C:6:GLU:HA	2:C:22:CYS:HA	1.95	0.47
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.80	0.47
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.95	0.47
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.63	0.47
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.50	0.47
2:C:162:TRP:CH2	2:C:203:CYS:HB3	2.50	0.47
2:C:194:SER:O	2:C:198:SER:OG	2.33	0.47
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.50	0.46
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.96	0.46
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.98	0.46
2:E:152:GLY:HA2	2:E:182:LEU:CD2	2.28	0.46
2:E:182:LEU:HG	2:E:183:TYR:H	1.81	0.46
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.51	0.46
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.97	0.46
3:D:197:HIS:ND1	3:D:199:THR:OG1	2.42	0.46
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.98	0.46
1:A:132:PHE:O	1:A:136:LEU:HB2	2.17	0.46
1:B:59:TRP:O	1:B:63:GLN:HG2	2.16	0.45
1:A:109:ILE:HG12	1:A:152:VAL:HG11	1.97	0.45
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:TYR:HE2	2:E:70:ILE:HG13	1.82	0.45
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.51	0.45
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.52	0.45
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.99	0.45
3:F:82:ALA:HB2	3:F:105:ILE:HG12	1.98	0.45
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.99	0.44
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.99	0.44
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.00	0.44
2:C:30:SER:C	2:C:32:TYR:H	2.20	0.44
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.18	0.44
1:A:69:VAL:HA	1:A:72:ALA:HB2	1.99	0.44
3:D:62:SER:O	3:D:73:THR:N	2.49	0.44
3:D:7:SER:HB3	3:D:22:THR:HB	1.99	0.44
3:F:186:GLU:HA	3:F:210:ARG:CZ	2.48	0.44
2:C:33:TRP:HB2	2:C:99:LEU:HB2	2.00	0.44
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.53	0.44
2:E:30:SER:C	2:E:32:TYR:H	2.21	0.44
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.53	0.44
1:A:270:ASN:ND2	1:A:442:LYS:O	2.51	0.44
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.81	0.43
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.99	0.43
3:D:95:GLN:N	3:D:95:GLN:CD	2.72	0.43
1:B:260:ILE:HG23	1:B:435:LEU:HG	2.00	0.43
1:B:75:TYR:HA	1:B:78:LEU:HD12	2.00	0.43
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.53	0.43
2:C:69:ILE:HB	2:C:82:GLN:HB2	2.00	0.43
2:C:9:GLY:H	2:C:115:THR:HG21	1.84	0.43
3:D:90:TRP:CD2	3:D:95:GLN:HB3	2.54	0.43
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.54	0.43
1:A:197:ILE:HG12	1:A:222:VAL:HG21	2.01	0.43
1:B:270:ASN:ND2	1:B:442:LYS:O	2.51	0.42
3:F:7:SER:HB3	3:F:8:PRO:HD3	2.01	0.42
1:B:302:CYS:O	1:B:306:GLY:N	2.47	0.42
3:D:19:VAL:O	3:D:73:THR:HA	2.19	0.42
1:B:420:GLN:HG3	1:B:420:GLN:H	1.55	0.42
1:A:180:THR:HG22	1:A:218:VAL:HA	2.02	0.42
1:B:197:ILE:HG13	1:B:197:ILE:H	1.66	0.42
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.20	0.42
1:A:212:LEU:HD12	1:A:212:LEU:H	1.84	0.42
1:B:138:THR:HG21	1:B:352:ALA:HB1	2.02	0.42
3:F:95:GLN:N	3:F:95:GLN:CD	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:LYS:HE3	2:E:80:TYR:CD2	2.55	0.42
1:A:250:ASN:OD1	2:C:104:GLY:HA3	2.20	0.42
2:E:61:THR:O	2:E:63:SER:N	2.53	0.42
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.85	0.42
2:E:18:LEU:HD11	2:E:117:VAL:HG22	2.01	0.42
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.50	0.41
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.55	0.41
3:F:27:SER:O	3:F:68:THR:HG22	2.20	0.41
1:A:216:LYS:HD3	1:B:434:LEU:HD23	2.02	0.41
2:E:70:ILE:HG12	2:E:81:LEU:HD13	2.01	0.41
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.55	0.41
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.21	0.41
1:A:199:PHE:CD1	1:A:407:THR:HG21	2.56	0.41
1:A:216:LYS:HE2	1:B:433:THR:HG22	2.01	0.41
1:B:449:LEU:O	1:B:453:LEU:HB2	2.21	0.41
3:D:106:LEU:HA	3:D:139:TYR:OH	2.21	0.41
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.81	0.41
1:B:41:VAL:O	1:B:45:LEU:HG	2.21	0.41
1:B:313:SER:OG	1:B:314:GLY:N	2.52	0.41
1:B:184:ALA:HB1	1:B:225:SER:HB2	2.02	0.41
3:D:1:ASP:N	3:D:1:ASP:OD2	2.53	0.41
1:B:224:MET:O	1:B:228:MET:HG2	2.21	0.41
1:A:98:ARG:HB3	1:A:288:ILE:HG13	2.03	0.41
3:D:60:ARG:HB2	3:D:75:ASN:O	2.20	0.41
3:D:12:SER:HA	3:D:104:GLU:O	2.20	0.41
1:A:400:ALA:HB2	1:A:432:ALA:HB1	2.02	0.41
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.56	0.41
2:E:196:TRP:CG	2:E:197:PRO:HA	2.56	0.41
1:A:420:GLN:HG3	1:A:420:GLN:H	1.58	0.41
3:F:114:VAL:HG22	3:F:135:LEU:HD22	2.03	0.40
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.57	0.40
1:A:104:ALA:O	1:A:131:LYS:NZ	2.37	0.40
1:A:224:MET:O	1:A:228:MET:HG2	2.21	0.40
1:B:305:LEU:HA	1:B:308:VAL:HG22	2.02	0.40
1:B:320:ILE:O	1:B:324:THR:OG1	2.29	0.40
3:D:49:ASP:O	3:D:51:SER:N	2.47	0.40
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.89	0.40
1:B:75:TYR:HB3	1:B:76:PRO:HD3	2.02	0.40
1:A:402:ILE:HD11	1:A:445:TYR:CZ	2.57	0.40
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.87	0.40
1:A:248:PRO:HB3	2:C:104:GLY:CA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1:ASP:HB3	3:D:94:PRO:HD2	2.04	0.40
2:C:154:PHE:HA	2:C:155:PRO:HA	1.82	0.40
2:C:171:VAL:HG22	2:C:189:VAL:HG23	2.03	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%)	421 (95%)	20 (4%)	1 (0%)	52 88
1	B	439/446 (98%)	418 (95%)	20 (5%)	1 (0%)	52 88
2	C	219/222 (99%)	200 (91%)	16 (7%)	3 (1%)	14 56
2	E	219/222 (99%)	201 (92%)	15 (7%)	3 (1%)	14 56
3	D	209/211 (99%)	189 (90%)	18 (9%)	2 (1%)	19 64
3	F	209/211 (99%)	188 (90%)	21 (10%)	0	100 100
All	All	1737/1758 (99%)	1617 (93%)	110 (6%)	10 (1%)	30 74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	65	LYS
2	E	65	LYS
2	E	140	ALA
2	C	140	ALA
2	E	62	PRO
2	C	62	PRO
3	D	126	SER
1	A	74	ASN
3	D	169	ASP
1	B	144	VAL

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%)	313 (93%)	22 (7%)	21	60
1	B	332/337 (98%)	313 (94%)	19 (6%)	25	66
2	C	181/182 (100%)	171 (94%)	10 (6%)	27	67
2	E	181/182 (100%)	174 (96%)	7 (4%)	39	77
3	D	185/185 (100%)	178 (96%)	7 (4%)	40	78
3	F	185/185 (100%)	175 (95%)	10 (5%)	27	67
All	All	1399/1408 (99%)	1324 (95%)	75 (5%)	27	67

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	73	ASP
1	A	78	LEU
1	A	103	GLU
1	A	148	GLU
1	A	160	ARG
1	A	162	VAL
1	A	180	THR
1	A	205	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	230	ARG
1	A	340	ARG
1	A	346	LEU
1	A	397	LEU
1	A	402	ILE
1	A	420	GLN
1	A	433	THR
1	A	444	LEU
1	A	451	ARG
1	A	453	LEU

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Mol	Chain	Res	Type
1	B	41	VAL
1	B	65	MET
1	B	70	HIS
1	B	73	ASP
1	B	78	LEU
1	B	103	GLU
1	B	148	GLU
1	B	205	ARG
1	B	211	THR
1	B	212	LEU
1	B	219	PHE
1	B	230	ARG
1	B	340	ARG
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
1	B	444	LEU
1	B	457	GLU
2	C	21	SER
2	C	72	ARG
2	C	96	CYS
2	C	115	THR
2	C	151	LYS
2	C	177	VAL
2	C	179	GLN
2	C	186	SER
2	C	188	SER
2	C	204	ASN
3	D	77	MET
3	D	81	ASP
3	D	95	GLN
3	D	156	ASN
3	D	190	SER
3	D	192	THR
3	D	201	THR
2	E	21	SER
2	E	72	ARG
2	E	96	CYS
2	E	115	THR
2	E	151	LYS
2	E	186	SER

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Mol	Chain	Res	Type
2	E	188	SER
3	F	1	ASP
3	F	77	MET
3	F	95	GLN
3	F	106	LEU
3	F	125	THR
3	F	156	ASN
3	F	161	SER
3	F	190	SER
3	F	192	THR
3	F	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	420	GLN
1	B	420	GLN
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 carbohydrates 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%)	0.12	28 (6%) 23 12	46, 65, 89, 123	0
1	B	441/446 (98%)	0.11	22 (4%) 32 18	49, 68, 101, 134	0
2	C	221/222 (99%)	0.25	17 (7%) 16 9	39, 65, 101, 127	0
2	E	221/222 (99%)	-0.17	4 (1%) 71 58	40, 68, 96, 128	0
3	D	211/211 (100%)	0.21	21 (9%) 9 5	48, 72, 97, 114	0
3	F	211/211 (100%)	0.10	20 (9%) 10 6	41, 61, 103, 117	0
All	All	1749/1758 (99%)	0.11	112 (6%) 23 12	39, 67, 99, 134	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LEU	6.2
3	D	20	THR	5.9
2	C	2	VAL	5.7
3	D	22	THR	5.6
2	C	141	ALA	5.5
1	B	119	GLN	5.5
2	C	29	TYR	5.1
2	C	65	LYS	5.0
3	D	7	SER	5.0
1	B	73	ASP	5.0
3	F	154	ARG	4.6
1	A	460	GLN	4.3
3	D	79	ALA	4.3
1	B	72	ALA	4.3
2	C	27	PHE	4.2
3	F	155	GLN	4.2
3	F	149	ILE	4.1
2	E	31	ARG	4.1
2	C	143	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	74	ASN	3.9
3	F	156	ASN	3.7
1	B	307	PHE	3.7
3	F	151	GLY	3.7
1	A	108	GLY	3.6
3	D	27	SER	3.6
1	A	107	SER	3.5
2	C	142	SER	3.5
2	C	28	ASP	3.4
1	B	168	LEU	3.3
3	D	68	THR	3.3
3	F	153	GLU	3.3
1	B	70	HIS	3.2
1	A	182	ALA	3.2
3	D	21	MET	3.2
3	D	80	GLU	3.2
1	A	166	PHE	3.2
2	E	178	LEU	3.2
3	F	147	TRP	3.1
2	C	222	ALA	3.1
1	B	71	THR	3.1
1	B	107	SER	3.0
3	D	5	THR	3.0
1	A	72	ALA	2.9
2	C	179	GLN	2.9
1	A	149	GLY	2.9
3	F	178	LEU	2.9
3	F	180	LEU	2.9
3	D	19	VAL	2.8
3	F	192	THR	2.7
2	E	222	ALA	2.7
1	A	355	GLY	2.7
3	D	159	LEU	2.7
3	F	152	SER	2.7
3	F	150	ASP	2.7
2	C	140	ALA	2.7
1	A	146	GLY	2.6
2	C	64	LEU	2.6
1	B	210	TYR	2.6
3	F	157	GLY	2.6
3	F	191	TYR	2.6
3	D	23	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	152	VAL	2.5
1	A	167	ARG	2.5
3	D	158	VAL	2.5
1	A	184	ALA	2.5
1	B	177	LEU	2.5
1	A	21	LEU	2.5
1	A	169	LYS	2.5
1	A	180	THR	2.5
1	A	258	LEU	2.5
1	B	355	GLY	2.4
3	F	129	ALA	2.4
1	A	18	ARG	2.4
3	F	127	GLY	2.4
1	A	148	GLU	2.4
2	C	26	GLY	2.4
2	C	8	GLY	2.4
2	C	144	VAL	2.4
1	B	120	ARG	2.4
3	F	141	LYS	2.3
3	D	13	ALA	2.3
1	B	146	GLY	2.3
3	D	195	ALA	2.3
3	F	148	LYS	2.3
1	A	288	ILE	2.3
1	B	456	GLN	2.3
3	D	69	SER	2.3
3	D	156	ASN	2.3
3	D	11	MET	2.2
1	A	183	ALA	2.2
3	F	128	GLY	2.2
1	B	358	ALA	2.2
3	F	1	ASP	2.2
1	B	75	TYR	2.2
1	B	33	LEU	2.2
2	E	4	LEU	2.2
1	B	117	GLU	2.1
3	D	196	THR	2.1
1	B	77	LEU	2.1
2	C	139	ALA	2.1
1	A	179	ALA	2.1
1	A	99	LYS	2.1
1	A	181	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	261	ILE	2.1
1	A	106	GLY	2.1
1	B	166	PHE	2.1
1	A	150	PRO	2.1
2	C	220	PRO	2.1
3	D	146	LYS	2.1
1	A	185	GLY	2.0
3	D	194	GLU	2.0
1	B	69	VAL	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 carbohydrates 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.