Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:35 AM GMT

PDB ID	:	2R9H
Title	:	Crystal Structure of Q207C Mutant of CLC-ec1 in complex with Fab
Authors	:	Nguitragool, W.; Miller, C.
Deposited on	:	2007-09-12
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 3.10 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.
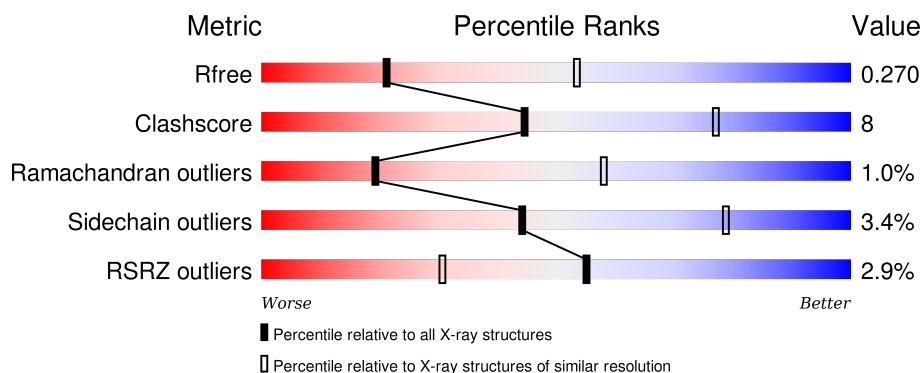
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	444	2% 81% 18% •
1	B	444	5% 75% 23% ••
2	C	221	3% 84% 16%
2	E	221	% 85% 14%
3	D	211	3% 83% 16% •

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Mol	Chain	Length	Quality of chain
3	F	211	4% 82% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13221 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	73	0	0
			3330	2188	559	562	21			
1	B	441	Total	C	N	O	S	73	0	0
			3301	2172	552	556	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	CYS	GLN	ENGINEERED	UNP P37019
B	207	CYS	GLN	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab fragment.

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 fragment.

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			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	2	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	2	0

3 Residue-property plots ⓘ

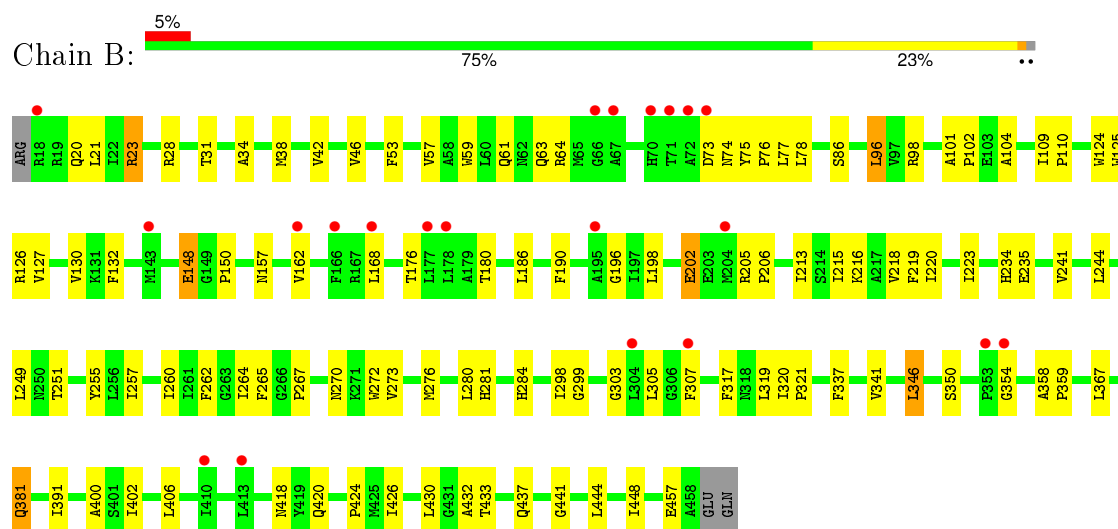These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.
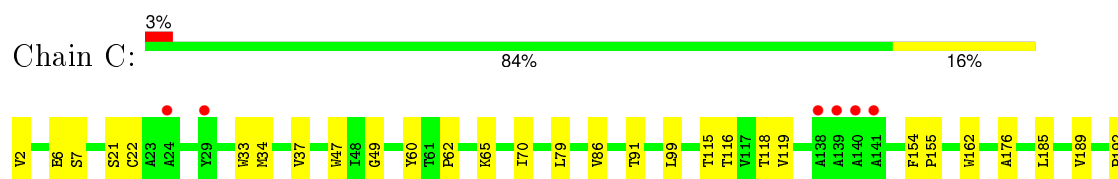
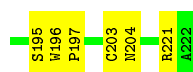- Molecule 1: H(+)/Cl(-) exchange transporter clcA
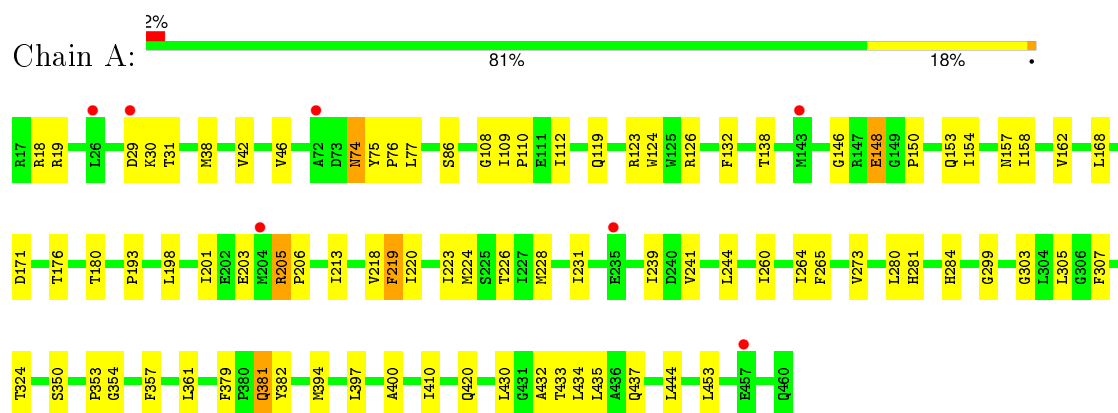
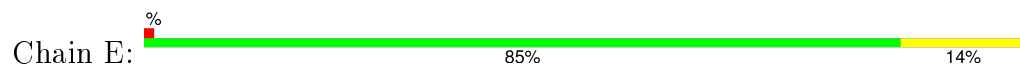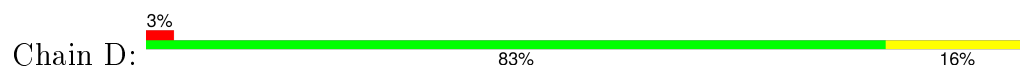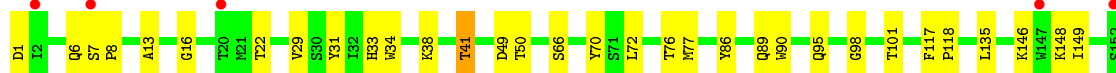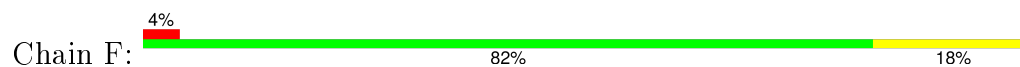- Molecule 1: H(+)/Cl(-) exchange transporter clcA

- Molecule 2: Fab fragment

S195 W196 P197 C203 N204 R221 A222

• Molecule 2: Fab fragment

Chain E:

• Molecule 3: Fab fragment

Chain D:

• Molecule 3: Fab fragment

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	233.10Å 98.36Å 171.92Å 90.00° 131.77° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.18 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-3.10) 99.3 (49.18-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.75 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.280 0.249 , 0.270	Depositor DCC
R_{free} test set	2638 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	105.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.4	EDS
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.51$, $<L^2> = 0.34$	Xtriage
Outliers	0 of 52493 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13221	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.37	0/3402	0.48	0/4617
1	B	0.40	0/3373	0.49	0/4579
2	C	0.35	0/1721	0.53	0/2355
2	E	0.33	0/1721	0.51	0/2355
3	D	0.34	0/1660	0.49	0/2257
3	F	0.33	0/1660	0.50	0/2257
All	All	0.36	0/13537	0.50	0/18420

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	3330	0	3481	69	0
1	B	3301	0	3454	87	0
2	C	1672	0	1654	19	0
2	E	1672	0	1654	12	0
3	D	1621	0	1546	18	0
3	F	1621	0	1546	29	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
All	All	13221	0	13335	206	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 8.

All (206) 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:B:381:GLN:HE21	1:B:381:GLN:H	0.95	0.93
1:A:30:LYS:HA	1:B:437:GLN:NE2	1.84	0.92
1:B:444:LEU:CD2	1:B:448:ILE:HD12	2.04	0.87
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.59	0.85
1:A:381:GLN:HE21	1:A:381:GLN:H	1.20	0.84
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.09	0.83
1:A:31:THR:H	1:B:437:GLN:HE22	1.26	0.81
1:B:244:LEU:H	1:B:418:ASN:HD21	1.29	0.81
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.63	0.81
1:B:381:GLN:N	1:B:381:GLN:HE21	1.77	0.80
1:B:148:GLU:CD	1:B:148:GLU:H	1.88	0.77
1:B:381:GLN:NE2	1:B:381:GLN:H	1.77	0.77
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.67	0.76
1:A:42:VAL:HG22	1:A:162:VAL:HG21	1.69	0.74
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.67	0.74
1:A:30:LYS:HA	1:B:437:GLN:HE21	1.52	0.73
3:F:95:GLN:N	3:F:95:GLN:OE1	2.21	0.73
1:B:444:LEU:CD2	1:B:448:ILE:CD1	2.67	0.72
3:D:95:GLN:N	3:D:95:GLN:OE1	2.16	0.72
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.72	0.71
1:B:180:THR:HG22	1:B:218:VAL:HA	1.72	0.71
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.71	0.70
1:B:444:LEU:HD23	1:B:448:ILE:HD12	1.74	0.70
1:B:234:HIS:HD1	1:B:235:GLU:HG2	1.56	0.69
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.75	0.69
1:B:38:MET:O	1:B:42:VAL:HG23	1.93	0.68
1:B:444:LEU:HD21	1:B:448:ILE:CD1	2.23	0.68
1:A:38:MET:O	1:A:42:VAL:HG23	1.93	0.68
1:B:202:GLU:OE1	1:B:406:LEU:HB3	1.94	0.68
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.57	0.68
1:B:444:LEU:O	1:B:444:LEU:HD23	1.94	0.68
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LEU:HD21	1:B:448:ILE:HD11	1.79	0.65
1:A:146:GLY:HA3	1:A:148:GLU:OE2	1.96	0.65
1:B:109:ILE:N	1:B:110:PRO:HD2	2.12	0.64
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.14	0.62
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.82	0.62
2:C:7:SER:HA	2:C:115:THR:HG21	1.81	0.62
1:B:267:PRO:HB3	1:B:441:GLY:HA3	1.81	0.62
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.82	0.61
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.35	0.61
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.35	0.61
1:B:337:PHE:O	1:B:341:VAL:HG23	2.01	0.60
1:B:273:VAL:HG11	1:B:444:LEU:HD11	1.84	0.58
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.51	0.57
3:D:189:ASN:HD21	3:D:211:ALA:H	1.52	0.57
1:A:86:SER:HB3	1:A:299:GLY:O	2.04	0.57
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.87	0.57
1:A:31:THR:H	1:B:437:GLN:NE2	2.00	0.57
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.25	0.57
1:A:119:GLN:HG3	1:B:21:LEU:HD22	1.86	0.56
1:B:34:ALA:O	1:B:38:MET:HG2	2.06	0.56
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.07	0.55
1:A:42:VAL:O	1:A:46:VAL:HG23	2.07	0.55
1:B:244:LEU:H	1:B:418:ASN:ND2	2.00	0.55
1:A:430:LEU:CD2	1:B:223:ILE:CD1	2.83	0.55
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.41	0.55
1:B:176:THR:O	1:B:180:THR:HG23	2.08	0.54
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.88	0.54
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.90	0.54
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.89	0.54
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.88	0.54
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.73	0.54
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.91	0.53
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.90	0.53
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.91	0.53
1:B:59:TRP:O	1:B:63:GLN:HG2	2.08	0.53
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.74	0.52
2:C:189:VAL:O	2:C:189:VAL:HG13	2.10	0.52
1:A:154:ILE:O	1:A:158:ILE:HG12	2.09	0.52
2:C:192:PRO:HG2	2:C:195:SER:HB2	1.93	0.51
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.93	0.51
1:B:42:VAL:O	1:B:46:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:HA	1:B:28:ARG:HH22	1.75	0.51
1:B:234:HIS:ND1	1:B:235:GLU:HG2	2.25	0.51
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.73	0.51
1:A:29:ASP:O	1:B:437:GLN:NE2	2.38	0.51
2:E:6:GLU:HA	2:E:22:CYS:HA	1.93	0.51
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.46	0.51
2:E:32:TYR:O	2:E:72:ARG:NH2	2.41	0.51
1:A:180:THR:HG22	1:A:218:VAL:HA	1.92	0.51
1:B:23:ARG:HA	1:B:23:ARG:HH11	1.76	0.50
1:B:96:LEU:HD12	1:B:130:VAL:HA	1.94	0.50
3:F:6:GLN:HA	3:F:22:THR:O	2.10	0.50
1:A:176:THR:O	1:A:180:THR:HG23	2.10	0.50
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.46	0.50
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.27	0.50
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.94	0.50
1:B:272:TRP:O	1:B:276:MET:HB2	2.12	0.50
1:B:280:LEU:HD13	1:B:350:SER:HB3	1.94	0.50
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.46	0.50
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.77	0.50
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.94	0.50
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.93	0.50
1:A:193:PRO:HG3	1:A:226:THR:HG21	1.94	0.49
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.94	0.49
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.93	0.49
1:A:239:ILE:HG22	1:A:241:VAL:HG23	1.94	0.49
3:F:34:TRP:CD2	3:F:72:LEU:HD12	2.48	0.49
1:B:264:ILE:HG13	1:B:265:PHE:N	2.28	0.49
3:F:66:SER:HA	3:F:70:TYR:CZ	2.48	0.49
3:D:7:SER:CB	3:D:8:PRO:HD3	2.42	0.49
2:C:91:THR:HG23	2:C:118:THR:HA	1.94	0.49
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.78	0.48
1:A:224:MET:O	1:A:228:MET:HG2	2.14	0.48
1:A:430:LEU:CD2	1:B:223:ILE:HD12	2.38	0.48
1:A:280:LEU:HD13	1:A:350:SER:HB3	1.96	0.48
3:F:90:TRP:CH2	3:F:95:GLN:NE2	2.82	0.48
2:C:221:ARG:HH22	3:D:120:SER:HA	1.80	0.47
1:B:244:LEU:HB2	1:B:418:ASN:ND2	2.29	0.47
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.97	0.47
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.29	0.47
3:F:34:TRP:CE3	3:F:72:LEU:HD12	2.50	0.47
3:F:7:SER:CB	3:F:8:PRO:HD3	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.95	0.47
1:A:305:LEU:C	1:A:307:PHE:H	2.18	0.47
1:A:264:ILE:HG13	1:A:265:PHE:N	2.30	0.47
1:A:203:GLU:HA	1:B:28:ARG:NH2	2.30	0.46
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.97	0.46
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.96	0.46
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.80	0.46
1:B:444:LEU:HD23	1:B:448:ILE:CD1	2.41	0.46
1:A:241:VAL:CG1	1:A:324:THR:HG21	2.45	0.46
2:E:16:GLY:O	2:E:86:VAL:HG23	2.15	0.46
2:C:6:GLU:HA	2:C:21:SER:O	2.15	0.46
2:E:160:VAL:HG22	2:E:205:VAL:HG22	1.97	0.46
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.51	0.46
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.98	0.46
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.81	0.46
2:E:66:ASP:HB3	2:E:69:ILE:HD11	1.98	0.45
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.97	0.45
3:F:29:VAL:HG23	3:F:70:TYR:HE1	1.82	0.45
1:B:305:LEU:C	1:B:307:PHE:H	2.20	0.45
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.17	0.45
1:B:270:ASN:OD1	1:B:444:LEU:HD12	2.16	0.45
1:A:74:ASN:HD22	1:A:77:LEU:H	1.65	0.45
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.98	0.45
2:E:91:THR:HG23	2:E:118:THR:HA	1.98	0.45
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.85	0.45
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.32	0.45
3:F:7:SER:HB3	3:F:8:PRO:CD	2.40	0.44
3:F:89:GLN:O	3:F:95:GLN:HB2	2.17	0.44
3:D:12:SER:HA	3:D:104:GLU:O	2.17	0.44
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.99	0.44
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.99	0.44
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.99	0.44
3:D:19:VAL:HG11	3:D:103:LEU:HD13	2.00	0.44
1:A:437:GLN:NE2	1:B:31:THR:H	2.15	0.44
1:A:260:ILE:HG23	1:A:435:LEU:HG	2.00	0.44
2:C:33:TRP:HB2	2:C:99:LEU:HB2	2.00	0.44
3:F:29:VAL:HG23	3:F:70:TYR:CE1	2.52	0.44
2:E:28:ASP:O	2:E:31:ARG:HB2	2.18	0.44
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.52	0.44
1:A:381:GLN:NE2	1:A:381:GLN:H	2.00	0.43
3:D:79:ALA:C	3:D:81:ASP:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:TYR:CE2	1:B:424:PRO:HB3	2.53	0.43
3:F:149:ILE:HD11	3:F:178:LEU:HD21	2.00	0.43
1:B:257:ILE:HA	1:B:260:ILE:HD12	2.01	0.43
2:C:176:ALA:HB2	2:C:185:LEU:HD23	2.00	0.43
1:A:273:VAL:HG11	1:A:444:LEU:CD1	2.48	0.43
2:C:37:VAL:HG22	2:C:47:TRP:HA	2.00	0.43
1:B:75:TYR:O	1:B:78:LEU:HG	2.18	0.43
1:A:239:ILE:HD13	1:A:394:MET:HE1	2.01	0.43
1:A:241:VAL:HG13	1:A:324:THR:HG21	2.01	0.43
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.54	0.43
1:B:125:TRP:HD1	1:B:126:ARG:HG3	1.84	0.43
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.53	0.42
1:A:220:ILE:HA	1:A:223:ILE:HD12	2.01	0.42
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.54	0.42
1:B:101:ALA:HB3	1:B:130:VAL:HG11	2.02	0.42
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.82	0.42
1:A:379:PHE:HB3	1:A:382:TYR:CD2	2.54	0.42
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.95	0.42
1:A:223:ILE:HD13	1:B:430:LEU:HD22	2.01	0.42
1:A:437:GLN:HE22	1:B:31:THR:H	1.67	0.42
1:A:138:THR:HG21	1:A:353:PRO:HD2	2.02	0.42
1:A:108:GLY:O	1:A:112:ILE:HG12	2.20	0.42
1:A:109:ILE:N	1:A:110:PRO:CD	2.83	0.42
3:D:31:TYR:HA	3:D:50:THR:OG1	2.19	0.42
3:F:13:ALA:HB3	3:F:77:MET:CE	2.49	0.42
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.55	0.42
2:C:154:PHE:HA	2:C:155:PRO:HA	1.83	0.42
1:A:86:SER:OG	1:A:303:GLY:HA3	2.20	0.42
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.01	0.42
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.85	0.42
2:C:6:GLU:HA	2:C:22:CYS:HA	2.01	0.41
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.55	0.41
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.88	0.41
1:B:109:ILE:N	1:B:110:PRO:CD	2.82	0.41
1:B:86:SER:OG	1:B:303:GLY:HA3	2.20	0.41
3:F:154:ARG:HA	3:F:154:ARG:HD2	1.86	0.41
1:B:86:SER:HB3	1:B:299:GLY:O	2.19	0.41
3:D:22:THR:HG22	3:D:23:CYS:N	2.35	0.41
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.88	0.41
2:E:127:PRO:HB3	2:E:153:TYR:HB3	2.03	0.41
1:B:53:PHE:O	1:B:57:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLN:N	1:A:381:GLN:HE21	2.01	0.41
3:F:8:PRO:O	3:F:101:THR:HG23	2.22	0.40
1:A:361:LEU:HD22	1:A:394:MET:HG2	2.03	0.40
3:F:38:LYS:O	3:F:41:THR:HG22	2.21	0.40
3:F:49:ASP:O	3:F:50:THR:HB	2.20	0.40
2:C:7:SER:CA	2:C:115:THR:HG21	2.50	0.40
1:A:239:ILE:CG2	1:A:241:VAL:HG23	2.52	0.40
2:C:86:VAL:HG12	2:C:119:VAL:HG21	2.04	0.40
1:A:201:ILE:HG13	1:A:201:ILE:O	2.21	0.40
1:B:298:ILE:HG12	1:B:346:LEU:HD23	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	442/444 (100%)	416 (94%)	22 (5%)	4 (1%)	21	61
1	B	439/444 (99%)	414 (94%)	21 (5%)	4 (1%)	21	61
2	C	219/221 (99%)	204 (93%)	13 (6%)	2 (1%)	21	61
2	E	219/221 (99%)	202 (92%)	13 (6%)	4 (2%)	11	42
3	D	209/211 (99%)	191 (91%)	15 (7%)	3 (1%)	14	48
3	F	209/211 (99%)	193 (92%)	15 (7%)	1 (0%)	34	72
All	All	1737/1752 (99%)	1620 (93%)	99 (6%)	18 (1%)	19	58

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	PRO
1	B	206	PRO

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Mol	Chain	Res	Type
2	C	65	LYS
2	E	65	LYS
2	E	136	SER
1	A	213	ILE
3	D	55	SER
3	D	80	GLU
2	E	62	PRO
1	A	205	ARG
1	B	132	PHE
1	A	132	PHE
1	B	205	ARG
1	B	213	ILE
2	C	62	PRO
3	D	31	TYR
2	E	64	LEU
3	F	31	TYR

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	335/335 (100%)	323 (96%)	12 (4%)	42	77
1	B	332/335 (99%)	317 (96%)	15 (4%)	34	70
2	C	181/181 (100%)	178 (98%)	3 (2%)	68	89
2	E	181/181 (100%)	174 (96%)	7 (4%)	39	75
3	D	185/185 (100%)	178 (96%)	7 (4%)	40	76
3	F	185/185 (100%)	182 (98%)	3 (2%)	70	89
All	All	1399/1402 (100%)	1352 (97%)	47 (3%)	44	79

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	148	GLU
1	A	171	ASP
1	A	205	ARG
1	A	219	PHE
1	A	244	LEU
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	433	THR
1	A	453	LEU
1	B	20	GLN
1	B	23	ARG
1	B	73	ASP
1	B	96	LEU
1	B	148	GLU
1	B	202	GLU
1	B	215	ILE
1	B	219	PHE
1	B	251	THR
1	B	319	LEU
1	B	346	LEU
1	B	381	GLN
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
2	C	2	VAL
2	C	116	THR
2	C	204	ASN
3	D	1	ASP
3	D	28	SER
3	D	46	TRP
3	D	59	VAL
3	D	68	THR
3	D	81	ASP
3	D	192	THR
2	E	72	ARG
2	E	96	CYS
2	E	115	THR
2	E	151	LYS
2	E	167	LEU
2	E	188	SER
2	E	202	THR

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Mol	Chain	Res	Type
3	F	1	ASP
3	F	41	THR
3	F	135	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	153	GLN
1	A	157	ASN
1	A	270	ASN
1	A	277	GLN
1	A	327	ASN
1	A	381	GLN
1	A	420	GLN
1	A	437	GLN
1	A	460	GLN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	277	GLN
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	418	ASN
1	B	420	GLN
1	B	437	GLN
3	D	6	GLN
3	D	36	GLN
3	D	136	ASN
3	D	137	ASN
3	D	189	ASN
2	E	172	HIS
3	F	6	GLN
3	F	36	GLN
3	F	136	ASN
3	F	137	ASN
3	F	209	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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	436/444 (98%)	0.24	7 (1%)	74	55	81, 104, 132, 150	0
1	B	433/444 (97%)	0.29	21 (4%)	34	15	81, 103, 132, 149	0
2	C	221/221 (100%)	0.12	6 (2%)	58	34	76, 104, 129, 149	0
2	E	221/221 (100%)	-0.01	3 (1%)	78	60	79, 104, 130, 149	0
3	D	211/211 (100%)	0.23	6 (2%)	56	32	83, 113, 132, 140	0
3	F	211/211 (100%)	0.34	8 (3%)	44	21	68, 99, 131, 141	0
All	All	1733/1752 (98%)	0.22	51 (2%)	55	31	68, 105, 132, 150	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	139	ALA	4.6
1	B	18	ARG	4.5
1	B	353	PRO	4.5
2	E	136	SER	4.2
1	B	307	PHE	4.0
1	A	29	ASP	3.8
1	B	73	ASP	3.5
1	B	168	LEU	3.3
3	F	155	GLN	3.2
1	B	67	ALA	3.2
1	B	354	GLY	3.1
1	B	72	ALA	3.0
2	C	29	TYR	2.7
3	F	211	ALA	2.7
1	B	177	LEU	2.7
1	B	71	THR	2.7
1	B	204	MET	2.7
1	B	143	MET	2.6
1	A	72	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	457	GLU	2.6
1	B	70	HIS	2.6
2	E	135	GLY	2.6
1	A	235	GLU	2.5
2	E	221	ARG	2.5
2	C	138	ALA	2.5
3	F	147	TRP	2.4
3	D	72	LEU	2.4
1	B	166	PHE	2.3
3	F	20	THR	2.3
1	A	204	MET	2.3
1	B	195	ALA	2.2
2	C	140	ALA	2.2
3	D	79	ALA	2.2
3	D	154	ARG	2.2
1	B	66	GLY	2.2
1	B	410	ILE	2.2
3	D	153	GLU	2.1
1	B	178	LEU	2.1
1	B	304	LEU	2.1
2	C	141	ALA	2.1
2	C	24	ALA	2.1
3	F	7	SER	2.1
3	F	2	ILE	2.1
1	B	413	LEU	2.1
3	F	152	SER	2.1
3	F	153	GLU	2.1
1	B	162	VAL	2.1
1	A	143	MET	2.1
1	A	26	LEU	2.0
3	D	148	LYS	2.0
3	D	22	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CL	B	4	1/1	-	-	-	22,22,22,22	1
4	CL	B	3	1/1	-	-	-	22,22,22,22	1
4	CL	A	1	1/1	-	-	-	22,22,22,22	1
4	CL	A	2	1/1	-	-	-	22,22,22,22	1

6.5 Other polymers (i)

There are no such residues in this entry.