



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 09:26 PM EDT

PDB ID : 4KKB  
Title : Structure of the E148A mutant of CLC-ec1 deltaNC construct in 20mM fluoride and 20mM Bromide  
Authors : Lim, H.-H.; Miller, C.  
Deposited on : 2013-05-05  
Resolution : 3.02 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

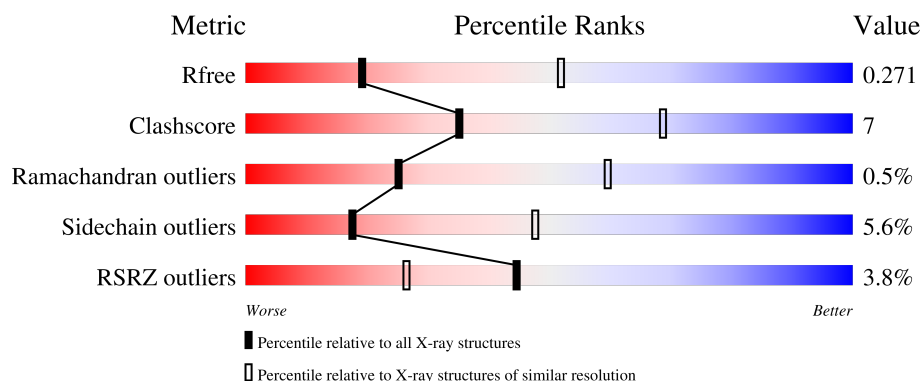
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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))
$R_{free}$	164625	2927 (3.04-3.00)
Clashscore	180529	3300 (3.04-3.00)
Ramachandran outliers	177936	3188 (3.04-3.00)
Sidechain outliers	177891	3191 (3.04-3.00)
RSRZ outliers	164620	2939 (3.04-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	446	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>
2	C	222	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
2	E	222	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
3	D	211	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	211	<div><div><div>%</div><div><div></div></div><div>84%</div><div>14%</div><div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13215 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
			3329	2188	560	561	20			
1	B	441	Total	C	N	O	S	0	0	0
			3300	2172	553	555	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P37019
A	148	ALA	GLU	engineered mutation	UNP P37019
A	461	LYS	-	expression tag	UNP P37019
B	16	MET	-	expression tag	UNP P37019
B	148	ALA	GLU	engineered mutation	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			

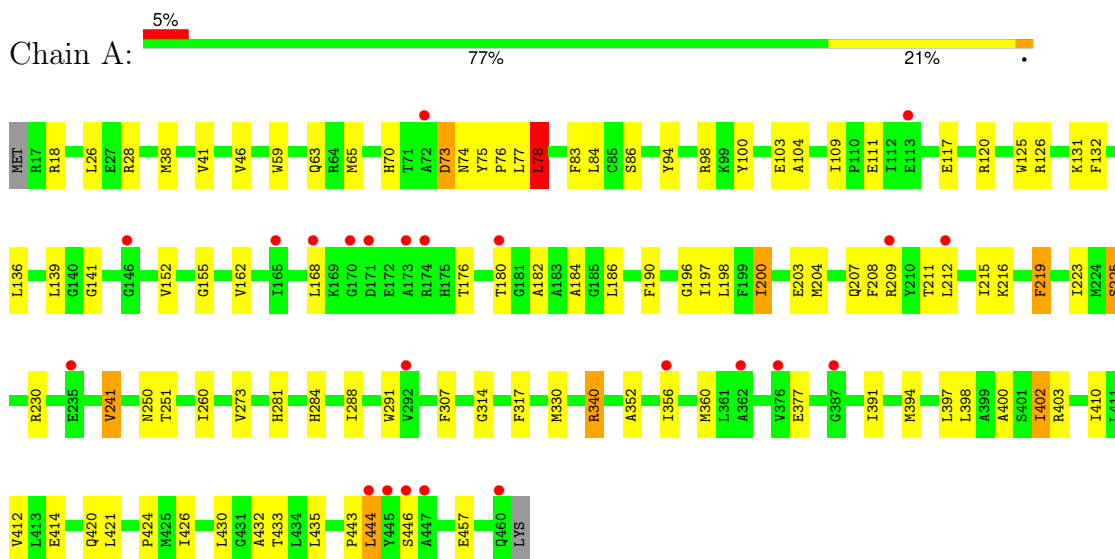
- Molecule 3 is a protein called Fab, light chain.

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			

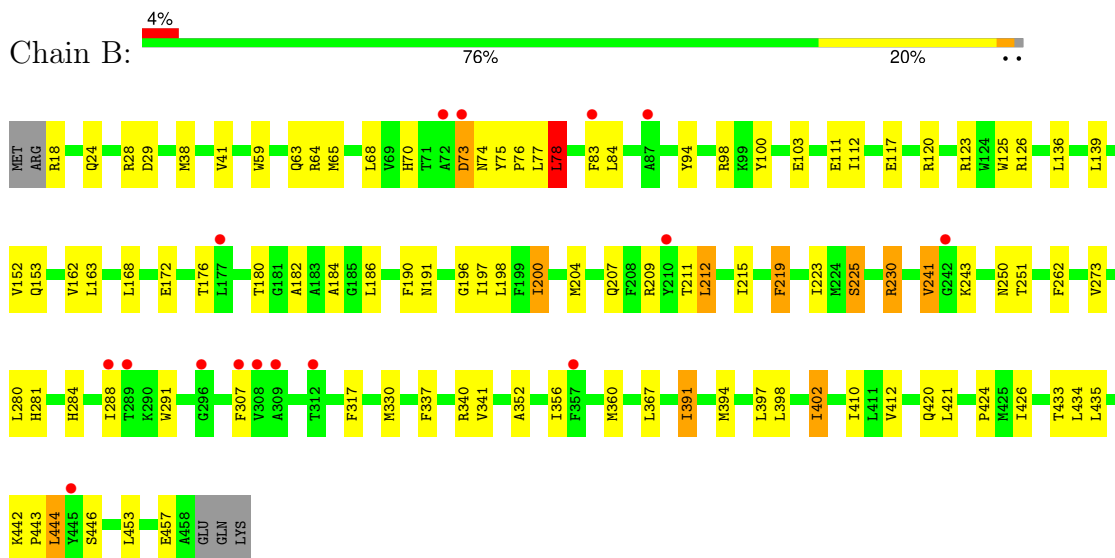
### 3 Residue-property plots [i](#)

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.

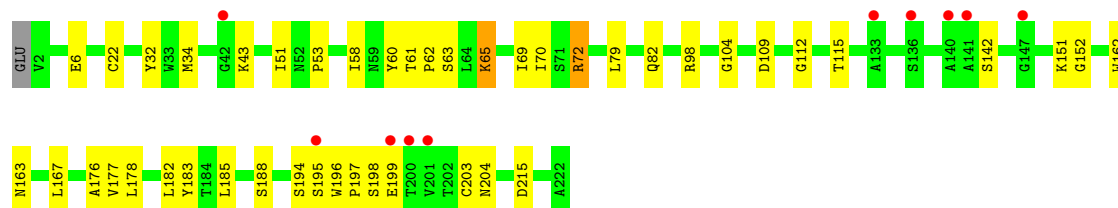
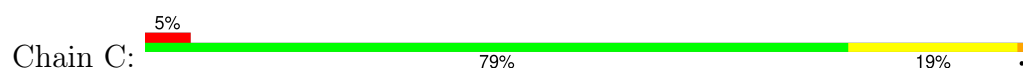
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



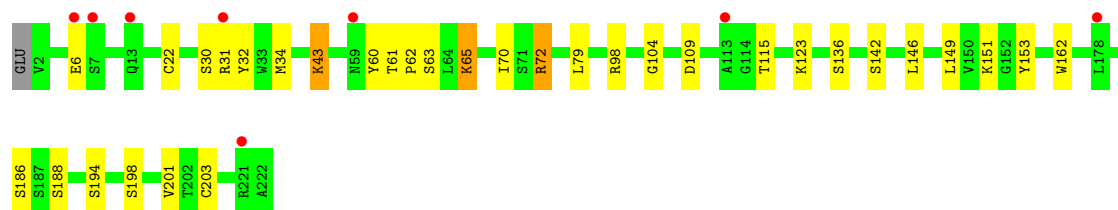
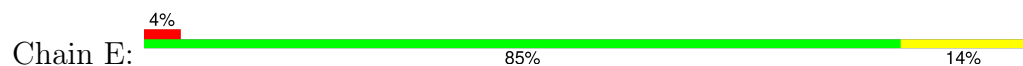
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



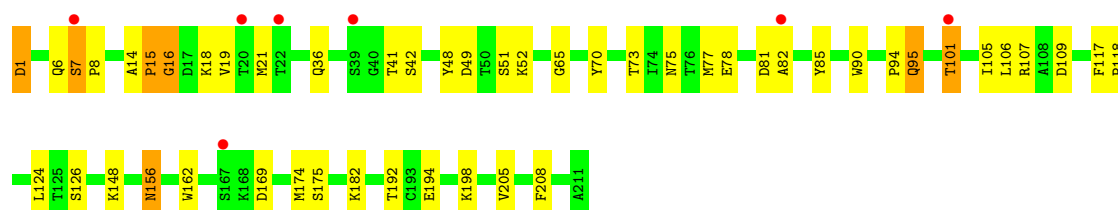
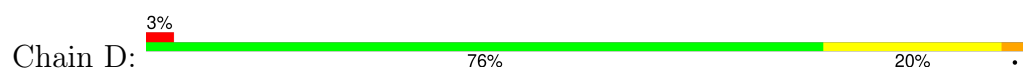
- Molecule 2: Fab, heavy chain



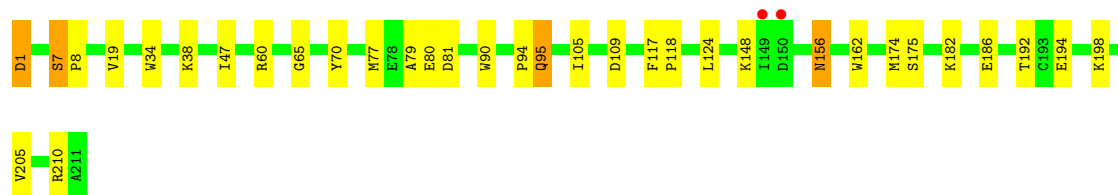
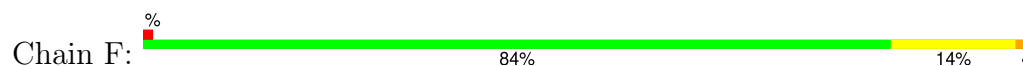
• Molecule 2: Fab, heavy chain



• Molecule 3: Fab, light chain



• Molecule 3: Fab, light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.72Å 97.53Å 170.57Å 90.00° 131.75° 90.00°	Depositor
Resolution (Å)	29.73 – 3.02 29.73 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.73-3.02) 98.6 (29.73-3.02)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.236 , 0.268 0.238 , 0.271	Depositor DCC
$R_{free}$ test set	2787 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 18.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0/3401	0.43	1/4616 (0.0%)
1	B	0.30	0/3372	0.43	1/4578 (0.0%)
2	C	0.32	0/1721	0.45	0/2355
2	E	0.34	0/1721	0.47	0/2355
3	D	0.33	0/1660	0.49	0/2257
3	F	0.33	0/1660	0.47	0/2257
All	All	0.32	0/13535	0.45	2/18418 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	78	LEU	CA-CB-CG	5.37	127.64	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3329	0	3483	60	0
1	B	3300	0	3456	61	0
2	C	1672	0	1654	24	0
2	E	1672	0	1654	18	0
3	D	1621	0	1546	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1621	0	1546	21	0
All	All	13215	0	13339	195	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 (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.63	0.78
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.18	0.76
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.67	0.75
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.68	0.74
3:D:6:GLN:NE2	3:D:101:THR:OG1	2.23	0.72
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.22	0.71
3:F:38:LYS:NZ	3:F:80:GLU:O	2.25	0.70
3:F:1:ASP:OD2	3:F:1:ASP:N	2.25	0.70
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.73	0.69
3:D:85:TYR:O	3:D:101:THR:OG1	2.08	0.69
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.62	0.64
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.80	0.64
3:D:1:ASP:OD2	3:D:1:ASP:N	2.31	0.64
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.30	0.64
1:A:184:ALA:HB1	1:A:225:SER:HB3	1.79	0.63
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.32	0.63
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.80	0.62
1:A:394:MET:HE2	1:A:412:VAL:HG13	1.80	0.62
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.81	0.62
3:D:82:ALA:HB2	3:D:105:ILE:HG13	1.81	0.62
1:A:73:ASP:OD1	1:A:73:ASP:N	2.29	0.62
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.30	0.62
3:D:21:MET:HB2	3:D:101:THR:HG21	1.83	0.60
1:A:457:GLU:HB3	1:B:18:ARG:HH11	1.69	0.58
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.86	0.58
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.86	0.57
3:D:156:ASN:N	3:D:156:ASN:OD1	2.36	0.57
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.86	0.57
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.70	0.57
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.87	0.56
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.87	0.56
3:D:14:ALA:O	3:D:16:GLY:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.86	0.56
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.38	0.56
1:B:184:ALA:HB1	1:B:225:SER:HB3	1.87	0.56
1:A:200:ILE:HA	1:A:204:MET:HB2	1.87	0.55
1:A:100:TYR:O	1:A:126:ARG:NH1	2.36	0.55
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.89	0.55
1:B:111:GLU:OE2	1:B:120:ARG:NE	2.40	0.54
3:F:156:ASN:OD1	3:F:156:ASN:N	2.40	0.54
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.42	0.54
3:F:7:SER:CB	3:F:8:PRO:HD3	2.37	0.54
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.91	0.54
3:D:106:LEU:HD23	3:D:107:ARG:N	2.23	0.54
2:C:112:GLY:O	3:D:42:SER:OG	2.23	0.53
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.27	0.53
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.90	0.53
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.74	0.53
1:B:73:ASP:OD1	1:B:73:ASP:N	2.40	0.53
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.44	0.52
2:C:61:THR:O	2:C:63:SER:N	2.42	0.52
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.45	0.52
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.92	0.52
2:E:61:THR:O	2:E:63:SER:N	2.43	0.52
1:A:132:PHE:O	1:A:136:LEU:HB2	2.10	0.52
3:D:18:LYS:HG3	3:D:75:ASN:HA	1.90	0.52
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.45	0.52
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.92	0.51
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.92	0.51
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.92	0.51
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.45	0.51
1:B:98:ARG:HB3	1:B:288:ILE:HG13	1.92	0.51
1:A:398:LEU:O	1:A:402:ILE:HG22	2.10	0.51
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.42	0.51
3:D:7:SER:CB	3:D:8:PRO:HD3	2.37	0.50
1:B:243:LYS:HB3	2:E:31:ARG:HH21	1.76	0.50
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.47	0.50
1:A:98:ARG:HB3	1:A:288:ILE:HG13	1.93	0.50
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.27	0.50
2:E:32:TYR:O	2:E:72:ARG:NH2	2.44	0.50
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.76	0.49
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.46	0.49
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLY:O	1:A:340:ARG:NH2	2.46	0.49
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.47	0.49
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.47	0.49
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.47	0.49
1:A:86:SER:OG	1:A:141:GLY:O	2.24	0.49
3:F:124:LEU:HD22	3:F:182:LYS:HG3	1.95	0.49
2:C:32:TYR:O	2:C:72:ARG:NH2	2.45	0.49
2:C:204:ASN:ND2	2:C:215:ASP:OD1	2.39	0.49
2:E:149:LEU:HD12	2:E:186:SER:HB3	1.94	0.48
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.94	0.48
1:A:152:VAL:HG13	1:A:182:ALA:HB1	1.96	0.48
1:A:403:ARG:NH2	1:B:29:ASP:OD1	2.44	0.48
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.61	0.48
1:B:398:LEU:O	1:B:402:ILE:HG22	2.13	0.48
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.48	0.48
1:A:190:PHE:HE2	1:A:317:PHE:HZ	1.61	0.47
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.96	0.47
1:B:100:TYR:O	1:B:126:ARG:NH1	2.46	0.47
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.49	0.47
1:A:176:THR:O	1:A:180:THR:HG23	2.15	0.47
1:B:176:THR:O	1:B:180:THR:HG23	2.14	0.47
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.96	0.47
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.95	0.47
1:B:273:VAL:HG11	1:B:444:LEU:HD11	1.96	0.46
2:E:60:TYR:HE2	2:E:70:ILE:HG13	1.80	0.46
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.98	0.46
1:A:26:LEU:HD22	1:B:442:LYS:HZ2	1.80	0.46
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.50	0.46
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.79	0.46
1:B:200:ILE:HA	1:B:204:MET:HB2	1.98	0.46
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.98	0.45
1:A:109:ILE:HG12	1:A:152:VAL:HG11	1.98	0.45
1:B:394:MET:HE2	1:B:412:VAL:HG13	1.99	0.45
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.51	0.45
2:E:153:TYR:HD1	2:E:153:TYR:O	1.99	0.45
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.31	0.45
1:A:104:ALA:O	1:A:131:LYS:NZ	2.37	0.45
3:D:78:GLU:N	3:D:81:ASP:OD1	2.49	0.44
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.53	0.44
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.49	0.44
3:F:19:VAL:HG21	3:F:77:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TRP:O	1:A:63:GLN:HG2	2.18	0.44
2:C:194:SER:O	2:C:198:SER:OG	2.29	0.44
3:F:34:TRP:N	3:F:47:ILE:O	2.47	0.44
3:F:109:ASP:OD2	3:F:198:LYS:NZ	2.51	0.44
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.83	0.44
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.99	0.44
1:A:443:PRO:HB2	1:A:446:SER:HB2	2.00	0.44
1:B:59:TRP:O	1:B:63:GLN:HG2	2.18	0.44
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.99	0.43
3:D:124:LEU:HD22	3:D:182:LYS:HG3	2.00	0.43
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.53	0.43
1:A:74:ASN:OD1	1:A:76:PRO:HD2	2.17	0.43
2:E:6:GLU:HA	2:E:22:CYS:HA	2.00	0.43
1:B:75:TYR:HB3	1:B:76:PRO:HD3	2.00	0.43
3:D:41:THR:OG1	3:D:42:SER:N	2.51	0.43
1:B:38:MET:HA	1:B:41:VAL:HG13	2.01	0.43
1:A:83:PHE:HD1	1:A:84:LEU:HD23	1.84	0.43
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.83	0.43
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.54	0.43
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.54	0.43
1:B:83:PHE:HD1	1:B:84:LEU:HD23	1.84	0.42
2:E:43:LYS:HB3	2:E:43:LYS:HE2	1.66	0.42
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.77	0.42
2:C:65:LYS:H	2:C:65:LYS:HG3	1.57	0.42
1:B:356:ILE:O	1:B:360:MET:HG3	2.19	0.42
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.18	0.42
1:B:241:VAL:HG11	1:B:391:ILE:HD11	2.00	0.42
2:C:195:SER:O	2:C:199:GLU:HB3	2.19	0.42
3:D:15:PRO:HA	3:D:77:MET:O	2.19	0.42
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.55	0.42
3:F:194:GLU:HG2	3:F:205:VAL:HG12	2.01	0.42
1:B:172:GLU:HG3	1:B:212:LEU:O	2.20	0.42
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.19	0.42
1:B:337:PHE:O	1:B:341:VAL:HG23	2.20	0.42
3:D:19:VAL:O	3:D:73:THR:HA	2.19	0.42
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.02	0.42
1:A:273:VAL:HG11	1:A:444:LEU:HD11	2.02	0.42
3:D:49:ASP:O	3:D:51:SER:N	2.50	0.42
2:E:65:LYS:H	2:E:65:LYS:HG3	1.58	0.42
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.55	0.42
1:A:356:ILE:O	1:A:360:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:C	1:A:424:PRO:HD2	2.40	0.42
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.88	0.42
2:E:153:TYR:O	2:E:153:TYR:CD1	2.73	0.42
2:C:6:GLU:HA	2:C:22:CYS:HA	2.01	0.41
2:C:51:ILE:HG13	2:C:58:ILE:HG12	2.01	0.41
1:A:38:MET:HA	1:A:41:VAL:HG13	2.02	0.41
1:A:430:LEU:HD22	1:B:219:PHE:HD2	1.85	0.41
1:B:112:ILE:HG13	1:B:153:GLN:HA	2.00	0.41
3:D:95:GLN:N	3:D:95:GLN:CD	2.74	0.41
1:B:421:LEU:C	1:B:424:PRO:HD2	2.40	0.41
2:C:152:GLY:HA2	2:C:182:LEU:HB3	2.03	0.41
2:E:194:SER:O	2:E:198:SER:OG	2.35	0.41
1:A:260:ILE:HG23	1:A:435:LEU:HG	2.01	0.41
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.55	0.41
3:D:1:ASP:HB3	3:D:94:PRO:HD2	2.03	0.41
1:A:410:ILE:O	1:A:414:GLU:HG3	2.20	0.41
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.56	0.41
2:C:51:ILE:HD13	2:C:72:ARG:HG2	2.02	0.41
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.19	0.41
3:F:65:GLY:HA3	3:F:70:TYR:HA	2.03	0.41
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.56	0.41
2:E:146:LEU:HD12	2:E:201:VAL:HG11	2.02	0.41
1:A:117:GLU:HA	1:A:209:ARG:HH22	1.86	0.41
1:A:250:ASN:OD1	2:C:104:GLY:HA3	2.20	0.41
1:B:74:ASN:OD1	1:B:76:PRO:HD2	2.21	0.41
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.96	0.41
2:C:196:TRP:CG	2:C:197:PRO:HA	2.55	0.41
3:F:186:GLU:HA	3:F:210:ARG:CZ	2.51	0.41
3:D:65:GLY:HA3	3:D:70:TYR:HA	2.02	0.40
2:E:31:ARG:HA	2:E:31:ARG:HD3	1.94	0.40
3:F:34:TRP:HB2	3:F:47:ILE:HB	2.03	0.40
1:B:64:ARG:O	1:B:68:LEU:HG	2.22	0.40
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.96	0.40
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.52	0.40
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.56	0.40
3:D:90:TRP:CD2	3:D:95:GLN:HB3	2.56	0.40
3:F:79:ALA:HA	3:F:105:ILE:HD12	2.04	0.40
1:B:78:LEU:HD11	1:B:307:PHE:CZ	2.57	0.40
2:C:69:ILE:HB	2:C:82:GLN:HB2	2.03	0.40
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	426 (96%)	16 (4%)	0	100	100
1	B	439/446 (98%)	421 (96%)	18 (4%)	0	100	100
2	C	219/222 (99%)	202 (92%)	16 (7%)	1 (0%)	25	59
2	E	219/222 (99%)	202 (92%)	16 (7%)	1 (0%)	25	59
3	D	209/211 (99%)	188 (90%)	16 (8%)	5 (2%)	5	23
3	F	209/211 (99%)	191 (91%)	17 (8%)	1 (0%)	25	59
All	All	1737/1758 (99%)	1630 (94%)	99 (6%)	8 (0%)	25	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	PRO
3	D	7	SER
3	D	16	GLY
3	D	169	ASP
2	E	62	PRO
3	F	7	SER
3	D	126	SER
3	D	15	PRO

### 5.3.2 Protein sidechains

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/336 (99%)	310 (93%)	24 (7%)	12	38
1	B	331/336 (98%)	305 (92%)	26 (8%)	10	34
2	C	181/182 (100%)	173 (96%)	8 (4%)	24	56
2	E	181/182 (100%)	171 (94%)	10 (6%)	18	48
3	D	185/185 (100%)	179 (97%)	6 (3%)	34	66
3	F	185/185 (100%)	181 (98%)	4 (2%)	47	75
All	All	1397/1406 (99%)	1319 (94%)	78 (6%)	17	48

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	70	HIS
1	A	73	ASP
1	A	78	LEU
1	A	103	GLU
1	A	139	LEU
1	A	162	VAL
1	A	200	ILE
1	A	211	THR
1	A	212	LEU
1	A	215	ILE
1	A	219	PHE
1	A	225	SER
1	A	230	ARG
1	A	241	VAL
1	A	251	THR
1	A	330	MET
1	A	340	ARG
1	A	377	GLU
1	A	397	LEU
1	A	402	ILE
1	A	420	GLN
1	A	433	THR
1	A	444	LEU
1	B	65	MET
1	B	70	HIS
1	B	73	ASP

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Mol	Chain	Res	Type
1	B	78	LEU
1	B	103	GLU
1	B	136	LEU
1	B	139	LEU
1	B	162	VAL
1	B	200	ILE
1	B	211	THR
1	B	212	LEU
1	B	215	ILE
1	B	219	PHE
1	B	225	SER
1	B	230	ARG
1	B	241	VAL
1	B	251	THR
1	B	330	MET
1	B	340	ARG
1	B	391	ILE
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
1	B	435	LEU
1	B	444	LEU
2	C	43	LYS
2	C	65	LYS
2	C	72	ARG
2	C	115	THR
2	C	142	SER
2	C	151	LYS
2	C	177	VAL
2	C	188	SER
3	D	1	ASP
3	D	36	GLN
3	D	95	GLN
3	D	101	THR
3	D	156	ASN
3	D	175	SER
2	E	30	SER
2	E	43	LYS
2	E	65	LYS
2	E	72	ARG
2	E	115	THR

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Mol	Chain	Res	Type
2	E	123	LYS
2	E	136	SER
2	E	142	SER
2	E	151	LYS
2	E	188	SER
3	F	1	ASP
3	F	95	GLN
3	F	156	ASN
3	F	175	SER

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

Mol	Chain	Res	Type
3	D	36	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	444/446 (99%)	0.24	23 (5%)	34 19	54, 74, 99, 128	0
1	B	441/446 (98%)	0.14	16 (3%)	46 27	54, 76, 109, 135	0
2	C	221/222 (99%)	0.09	10 (4%)	39 23	43, 70, 101, 137	0
2	E	221/222 (99%)	0.15	8 (3%)	46 27	50, 73, 100, 129	0
3	D	211/211 (100%)	0.25	7 (3%)	49 29	57, 79, 100, 109	0
3	F	211/211 (100%)	-0.07	2 (0%)	81 63	47, 66, 107, 123	0
All	All	1749/1758 (99%)	0.15	66 (3%)	44 26	43, 74, 103, 137	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ALA	5.6
3	D	20	THR	5.0
2	C	199	GLU	4.9
1	A	168	LEU	4.7
3	D	39	SER	4.3
3	D	22	THR	4.2
1	A	444	LEU	4.1
1	B	72	ALA	4.1
1	A	445	TYR	4.0
2	E	59	ASN	3.9
1	B	307	PHE	3.8
3	D	167	SER	3.6
2	E	7	SER	3.5
1	A	171	ASP	3.3
1	B	242	GLY	3.3
2	E	31	ARG	3.2
3	D	82	ALA	3.2
1	A	173	ALA	3.2
1	B	357	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	210	TYR	3.0
1	A	174	ARG	3.0
1	A	209	ARG	3.0
1	B	289	THR	2.9
1	A	362	ALA	2.9
1	A	212	LEU	2.7
2	C	201	VAL	2.7
1	B	83	PHE	2.7
2	C	136	SER	2.6
1	B	308	VAL	2.6
2	E	221	ARG	2.6
2	C	147	GLY	2.6
1	A	180	THR	2.5
1	A	446	SER	2.5
1	A	460	GLN	2.4
1	B	309	ALA	2.4
1	A	292	VAL	2.4
1	B	445	TYR	2.4
2	E	178	LEU	2.4
2	E	6	GLU	2.4
3	D	101	THR	2.3
1	A	387	GLY	2.3
1	B	288	ILE	2.3
3	F	149	ILE	2.3
1	B	87	ALA	2.3
1	A	376	VAL	2.2
1	B	177	LEU	2.2
2	C	200	THR	2.2
1	A	113	GLU	2.2
2	E	13	GLN	2.2
1	A	72	ALA	2.2
2	C	140	ALA	2.2
1	B	73	ASP	2.2
2	C	133	ALA	2.1
2	C	141	ALA	2.1
1	A	146	GLY	2.1
3	D	7	SER	2.1
1	A	235	GLU	2.1
2	C	195	SER	2.1
1	B	296	GLY	2.1
2	E	113	ALA	2.1
1	A	165	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	312	THR	2.1
2	C	42	GLY	2.0
1	A	356	ILE	2.0
3	F	150	ASP	2.0
1	A	170	GLY	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.