



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 4KK5 / pdb_00004kk5
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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

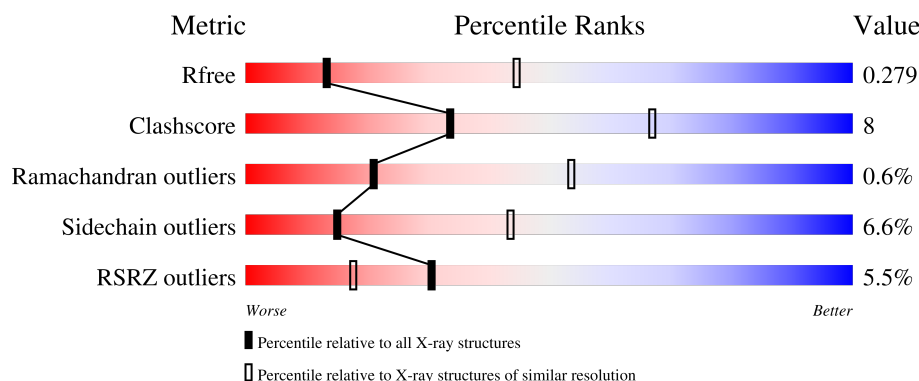
1 Overall quality at a glance

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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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 $\leq 5\%$. 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	6% 76% 21% .
1	B	446	4% 76% 20% ..
2	C	222	4% 76% 22% .
2	E	222	7% 76% 23%
3	D	211	10% 74% 23% .

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Mol	Chain	Length	Quality of chain
3	F	211	3% 79% 19%

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			

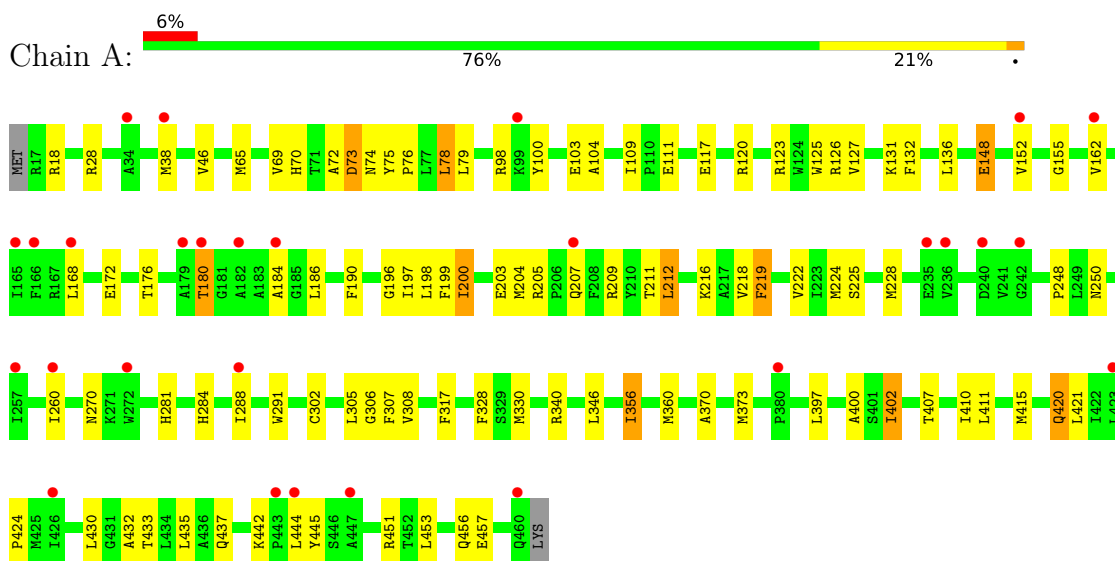
- Molecule 3 is a protein called Fab, light chain.

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			

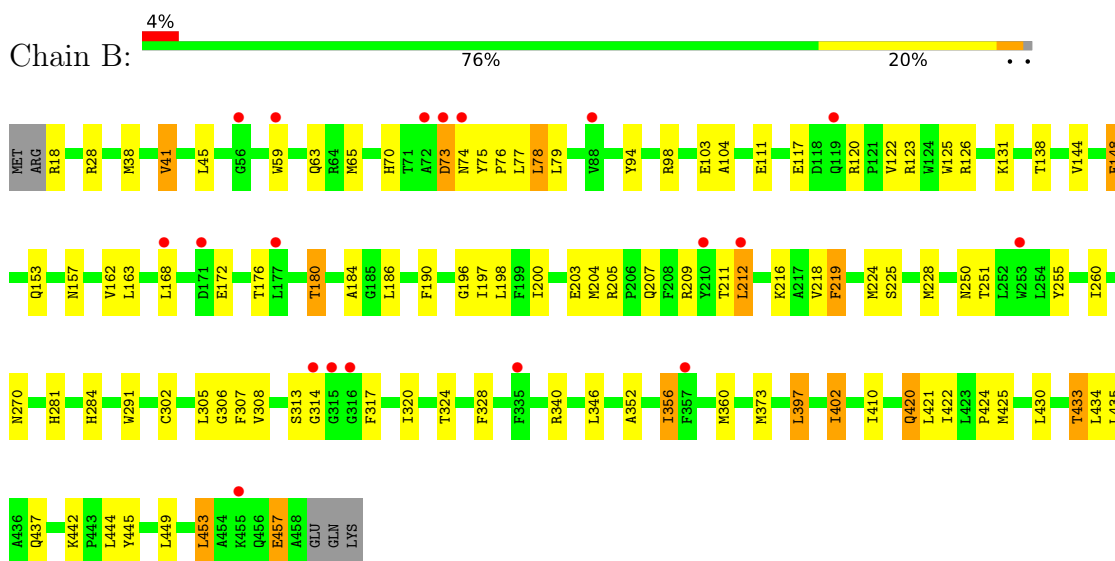
3 Residue-property plots

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.

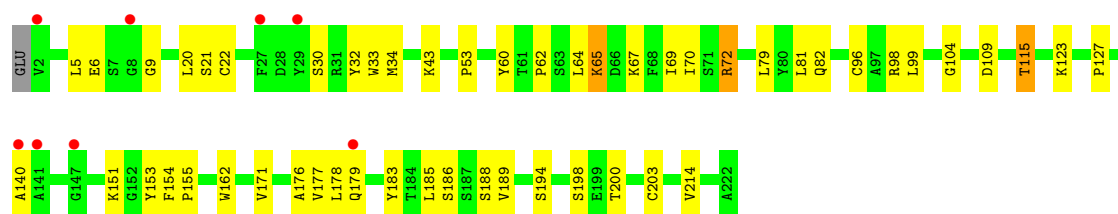
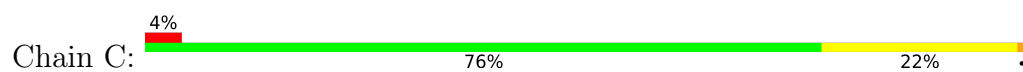
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



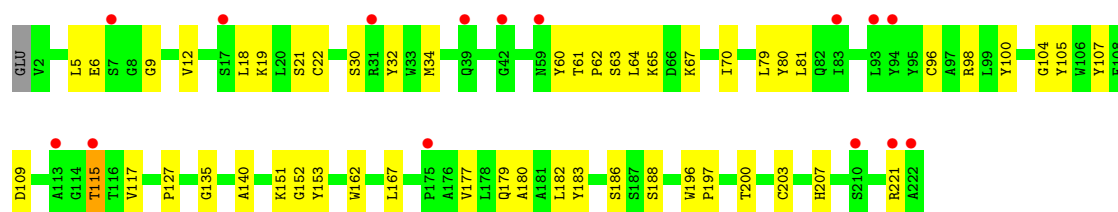
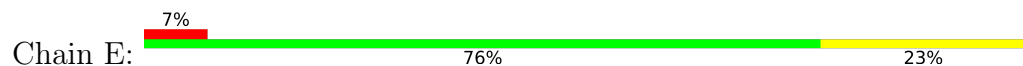
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



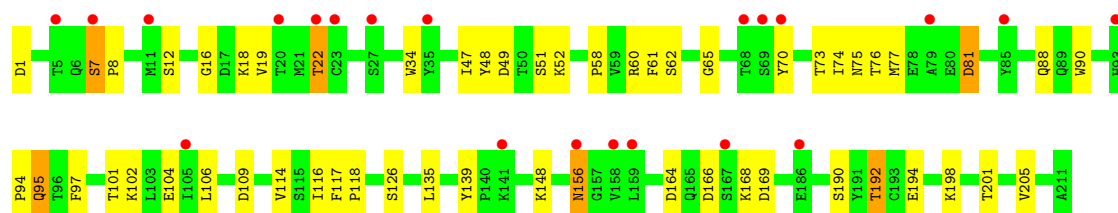
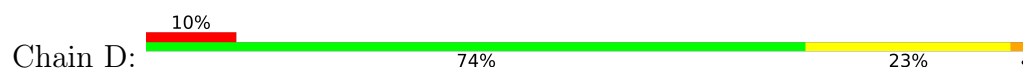
- Molecule 2: Fab, heavy chain



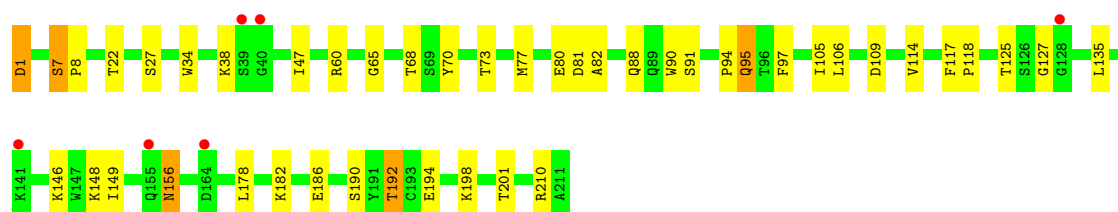
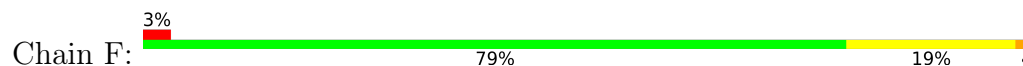
• Molecule 2: Fab, heavy chain



• 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, 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) 98.2 (39.78-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.271 0.237 , 0.279	Depositor DCC
R_{free} test set	2390 reflections (4.99%)	wwPDB-VP
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 , 6.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for h,-k,-h-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.45	0/3405	0.76	1/4621 (0.0%)
1	B	0.44	0/3376	0.77	1/4583 (0.0%)
2	C	0.42	0/1721	0.74	0/2355
2	E	0.43	0/1721	0.76	2/2355 (0.1%)
3	D	0.41	0/1660	0.80	2/2257 (0.1%)
3	F	0.42	0/1660	0.78	2/2257 (0.1%)
All	All	0.43	0/13543	0.77	8/18428 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	SER	CA-C-N	-7.88	110.55	120.79
3	D	7	SER	C-N-CA	-7.88	110.55	120.79
3	F	7	SER	CA-C-N	-7.29	111.31	120.79
3	F	7	SER	C-N-CA	-7.29	111.31	120.79
1	A	356	ILE	N-CA-C	-6.30	106.86	112.90
1	B	356	ILE	N-CA-C	-5.47	107.47	113.43
2	E	207	HIS	CA-C-N	5.39	125.03	119.05
2	E	207	HIS	C-N-CA	5.39	125.03	119.05

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	3333	0	3484	62	0
1	B	3304	0	3457	60	0
2	C	1672	0	1654	23	0
2	E	1672	0	1654	25	0
3	D	1621	0	1546	30	0
3	F	1621	0	1546	22	0
All	All	13223	0	13341	205	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 (205) 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:B:148:GLU:H	1:B:148:GLU:CD	2.08	0.61
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.81	0.61
1:A:402:ILE:HD11	1:A:445:TYR:CE1	2.36	0.61
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.34	0.61
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.34	0.61
1:B:73:ASP:N	1:B:73:ASP:OD1	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
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.86	0.58
3:D:166:ASP:OD1	3:D:168:LYS:N	2.35	0.58
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:104:ALA:O	1:A:131:LYS:NZ	2.37	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:148:GLU:H	1:A:148:GLU:CD	2.13	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:D:65:GLY:HA3	3:D:70:TYR:HA	1.90	0.54
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.88	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: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:198:LEU:HG	1:B:410:ILE:HD12	1.90	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:B:38:MET:HG3	1:B:168:LEU:HD11	1.91	0.50
2:E:6:GLU:HA	2:E:22:CYS:HA	1.92	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:125:TRP:CD1	1:B:126:ARG:HG3	2.46	0.50
1:B:172:GLU:HG3	1:B:212:LEU:O	2.11	0.50
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.92	0.49
1:B:176:THR:O	1:B:180:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:30:SER:C	2:C:32:TYR:H	2.20	0.49
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
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
3:F:156:ASN:OD1	3:F:156:ASN:N	2.46	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
2:E:30:SER:C	2:E:32:TYR:H	2.21	0.48
3:D:156:ASN:N	3:D:156:ASN:OD1	2.46	0.48
3:F:127:GLY:O	3:F:182:LYS:N	2.44	0.48
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.46	0.48
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.96	0.48
1:A:172:GLU:HG3	1:A:212:LEU:O	2.13	0.48
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.48	0.48
2:C:20:LEU:HD12	2:C:81:LEU:HD23	1.96	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:A:219:PHE:HB3	1:B:430:LEU:HD21	1.95	0.48
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.95	0.48
3:D:95:GLN:N	3:D:95:GLN:CD	2.72	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
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:B:397:LEU:HA	1:B:397:LEU:HD23	1.80	0.47
2:C:6:GLU:HA	2:C:22:CYS:HA	1.95	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
3:F:95:GLN:N	3:F:95:GLN:CD	2.73	0.47
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.96	0.46
1:B:104:ALA:O	1:B:131:LYS:NZ	2.31	0.46
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.50	0.46
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:GLY:HA2	2:E:182:LEU:CD2	2.28	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
2:E:182:LEU:HG	2:E:183:TYR:H	1.81	0.46
1:A:132:PHE:O	1:A:136:LEU:HB2	2.17	0.46
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.97	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
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:75:TYR:HB3	1:A:76:PRO:HD3	2.00	0.44
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
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
1:A:328:PHE:O	1:A:373:MET:HE1	2.17	0.44
3:D:7:SER:HB3	3:D:22:THR:HB	1.99	0.44
1:A:411:LEU:HG	1:A:415:MET:HE2	1.99	0.44
2:C:33:TRP:HB2	2:C:99:LEU:HB2	2.00	0.44
3:F:186:GLU:HA	3:F:210:ARG:CZ	2.48	0.44
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.53	0.44
1:A:270:ASN:ND2	1:A:442:LYS:O	2.51	0.44
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.53	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
1:B:75:TYR:HA	1:B:78:LEU:HD12	2.00	0.43
1:B:260:ILE:HG23	1:B:435:LEU:HG	2.00	0.43
2:C:9:GLY:H	2:C:115:THR:HG21	1.84	0.43
2:C:69:ILE:HB	2:C:82:GLN:HB2	2.00	0.43
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.53	0.43
3:D:90:TRP:CD2	3:D:95:GLN:HB3	2.54	0.43
1:A:197:ILE:HG12	1:A:222:VAL:HG21	2.01	0.43
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:VAL:O	3:D:73:THR:HA	2.19	0.42
1:B:420:GLN:H	1:B:420:GLN:HG3	1.55	0.42
1:A:180:THR:HG22	1:A:218:VAL:HA	2.02	0.42
1:A:330:MET:HE1	1:A:370:ALA:HB1	2.02	0.42
1:B:197:ILE:H	1:B:197:ILE:HG13	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:A:250:ASN:OD1	2:C:104:GLY:HA3	2.20	0.42
1:B:138:THR:HG21	1:B:352:ALA:HB1	2.02	0.42
2:E:19:LYS:HE3	2:E:80:TYR:CD2	2.55	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
1:B:422:ILE:HD12	1:B:425:MET:HE3	2.02	0.41
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
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.55	0.41
2:E:70:ILE:HG12	2:E:81:LEU:HD13	2.01	0.41
1:A:199:PHE:CD1	1:A:407:THR:HG21	2.56	0.41
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.21	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:184:ALA:HB1	1:B:225:SER:HB2	2.02	0.41
1:B:313:SER:OG	1:B:314:GLY:N	2.52	0.41
1:B:328:PHE:O	1:B:373:MET:HE1	2.20	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
1:A:400:ALA:HB2	1:A:432:ALA:HB1	2.02	0.41
1:A:421:LEU:C	1:A:424:PRO:HD2	2.46	0.41
3:D:12:SER:HA	3:D:104:GLU:O	2.20	0.41
3:D:60:ARG:HB2	3:D:75:ASN:O	2.20	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:H	1:A:420:GLN:HG3	1.58	0.41
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.57	0.40
3:F:114:VAL:HG22	3:F:135:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:421:LEU:C	1:B:424:PRO:HD2	2.45	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
1:A:402:ILE:HD11	1:A:445:TYR:CZ	2.57	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
3:D:1:ASP:HB3	3:D:94:PRO:HD2	2.04	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%)	43	72
1	B	439/446 (98%)	418 (95%)	20 (5%)	1 (0%)	43	72
2	C	219/222 (99%)	200 (91%)	16 (7%)	3 (1%)	9	36
2	E	219/222 (99%)	201 (92%)	15 (7%)	3 (1%)	9	36
3	D	209/211 (99%)	189 (90%)	18 (9%)	2 (1%)	12	43
3	F	209/211 (99%)	188 (90%)	21 (10%)	0	100	100
All	All	1737/1758 (99%)	1617 (93%)	110 (6%)	10 (1%)	21	53

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 ⓘ

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%)	312 (93%)	23 (7%)	14	42
1	B	332/337 (98%)	307 (92%)	25 (8%)	12	39
2	C	181/182 (100%)	166 (92%)	15 (8%)	10	35
2	E	181/182 (100%)	171 (94%)	10 (6%)	19	49
3	D	185/185 (100%)	176 (95%)	9 (5%)	22	52
3	F	185/185 (100%)	174 (94%)	11 (6%)	18	47
All	All	1399/1408 (99%)	1306 (93%)	93 (7%)	15	43

All (93) 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	79	LEU
1	A	103	GLU
1	A	148	GLU
1	A	162	VAL
1	A	180	THR

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Mol	Chain	Res	Type
1	A	200	ILE
1	A	205	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
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
1	B	41	VAL
1	B	65	MET
1	B	70	HIS
1	B	73	ASP
1	B	78	LEU
1	B	79	LEU
1	B	103	GLU
1	B	122	VAL
1	B	148	GLU
1	B	162	VAL
1	B	180	THR
1	B	205	ARG
1	B	211	THR
1	B	212	LEU
1	B	219	PHE
1	B	251	THR
1	B	340	ARG
1	B	346	LEU
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
1	B	444	LEU
1	B	453	LEU
1	B	457	GLU
2	C	5	LEU
2	C	21	SER
2	C	43	LYS

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Mol	Chain	Res	Type
2	C	65	LYS
2	C	72	ARG
2	C	96	CYS
2	C	115	THR
2	C	123	LYS
2	C	151	LYS
2	C	177	VAL
2	C	179	GLN
2	C	186	SER
2	C	188	SER
2	C	200	THR
2	C	214	VAL
3	D	22	THR
3	D	77	MET
3	D	81	ASP
3	D	95	GLN
3	D	116	ILE
3	D	156	ASN
3	D	190	SER
3	D	192	THR
3	D	201	THR
2	E	5	LEU
2	E	21	SER
2	E	96	CYS
2	E	115	THR
2	E	151	LYS
2	E	167	LEU
2	E	177	VAL
2	E	186	SER
2	E	188	SER
2	E	200	THR
3	F	1	ASP
3	F	22	THR
3	F	73	THR
3	F	77	MET
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	GLN
1	A	61	GLN
1	A	175	HIS
1	A	420	GLN
1	B	61	GLN
1	B	63	GLN
1	B	175	HIS
1	B	420	GLN
2	C	163	ASN
2	C	172	HIS
3	D	37	GLN
3	D	209	ASN
2	E	39	GLN
2	E	172	HIS
2	E	179	GLN
3	F	123	GLN
3	F	137	ASN

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 ⓘ

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, 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	444/446 (99%)	0.34	28 (6%)	26 15	46, 65, 89, 123	0
1	B	441/446 (98%)	0.16	19 (4%)	40 23	49, 68, 101, 134	0
2	C	221/222 (99%)	0.22	8 (3%)	46 27	39, 65, 101, 127	0
2	E	221/222 (99%)	0.40	15 (6%)	23 13	40, 68, 96, 128	0
3	D	211/211 (100%)	0.52	21 (9%)	12 7	48, 72, 97, 114	0
3	F	211/211 (100%)	0.12	6 (2%)	55 34	41, 61, 103, 117	0
All	All	1749/1758 (99%)	0.28	97 (5%)	30 18	39, 67, 99, 134	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	7	SER	8.2
1	A	168	LEU	7.5
3	D	22	THR	6.4
3	D	20	THR	6.0
3	F	39	SER	5.7
1	A	166	PHE	5.5
1	A	235	GLU	5.3
1	B	210	TYR	5.0
2	E	115	THR	4.8
1	A	288	ILE	4.7
2	E	221	ARG	4.5
1	B	315	GLY	4.3
1	A	460	GLN	4.2
2	E	42	GLY	4.2
1	A	240	ASP	4.1
3	D	167	SER	4.1
2	E	93	LEU	4.1
2	C	8	GLY	4.1
1	A	182	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	39	GLN	4.0
1	A	99	LYS	3.9
1	B	73	ASP	3.8
2	C	29	TYR	3.7
1	A	236	VAL	3.7
3	F	164	ASP	3.7
1	A	207	GLN	3.7
3	D	69	SER	3.7
1	A	447	ALA	3.6
2	C	27	PHE	3.6
2	E	222	ALA	3.5
1	A	38	MET	3.3
3	D	23	CYS	3.3
2	E	210	SER	3.3
1	B	119	GLN	3.3
3	D	93	HIS	3.3
2	C	2	VAL	3.2
1	B	168	LEU	3.2
3	F	155	GLN	3.2
1	A	34	ALA	3.1
2	E	94	TYR	3.1
1	B	59	TRP	3.1
1	A	444	LEU	3.0
1	B	171	ASP	3.0
1	A	179	ALA	3.0
1	B	88	VAL	3.0
3	D	5	THR	3.0
1	B	177	LEU	2.9
1	A	162	VAL	2.9
1	A	242	GLY	2.9
2	E	7	SER	2.8
1	A	380	PRO	2.7
1	A	423	LEU	2.7
2	C	179	GLN	2.7
1	A	165	ILE	2.7
2	E	17	SER	2.7
1	B	72	ALA	2.7
3	F	40	GLY	2.6
1	A	184	ALA	2.5
2	E	31	ARG	2.5
3	D	156	ASN	2.5
3	D	11	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	180	THR	2.4
3	F	128	GLY	2.4
1	B	357	PHE	2.4
3	D	70	TYR	2.4
3	D	105	ILE	2.3
2	C	141	ALA	2.3
3	D	79	ALA	2.3
2	E	59	ASN	2.3
3	D	186	GLU	2.3
2	E	175	PRO	2.2
3	D	159	LEU	2.2
3	D	27	SER	2.2
3	D	85	TYR	2.2
1	A	426	ILE	2.2
3	D	158	VAL	2.2
2	C	140	ALA	2.2
3	F	141	LYS	2.2
3	D	35	TYR	2.2
1	A	152	VAL	2.2
1	B	74	ASN	2.2
1	B	212	LEU	2.2
1	A	443	PRO	2.2
3	D	141	LYS	2.2
1	A	272	TRP	2.2
1	A	257	ILE	2.2
1	B	56	GLY	2.2
1	B	335	PHE	2.2
1	B	314	GLY	2.1
1	B	316	GLY	2.1
3	D	68	THR	2.1
2	E	113	ALA	2.1
2	E	83	ILE	2.0
1	B	455	LYS	2.0
1	A	260	ILE	2.0
1	B	253	TRP	2.0
2	C	147	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.