



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:12 AM UTC

PDB ID : 4KK6 / pdb_00004kk6
Title : Structure of CLC-ec1 deltaNC construct in 20mM Bromide
Authors : Lim, H.-H.; Miller, C.
Deposited on : 2013-05-05
Resolution : 3.18 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

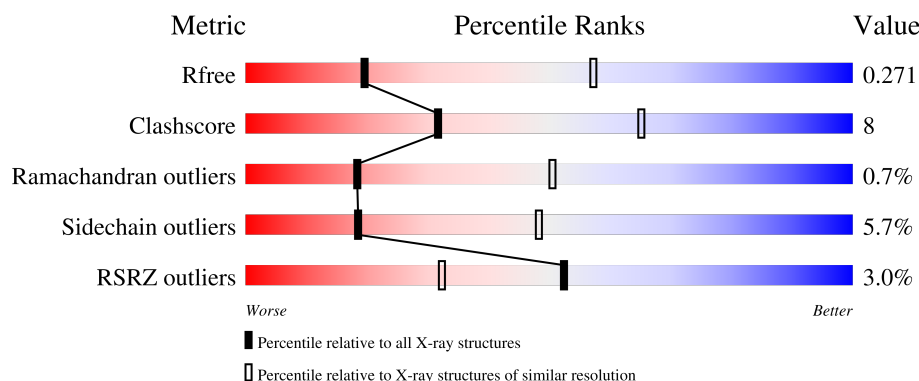
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	 2% 77% 20% ..
1	B	446	 5% 69% 28% ..
2	C	222	 3% 80% 18% .
2	E	222	 3% 84% 13% .
3	D	211	 2% 75% 22% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	A	501	-	-	X	-
4	BR	A	502	-	-	X	-
4	BR	B	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13218 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	443	Total	C	N	O	S	0	0	0
			3324	2185	558	561	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			

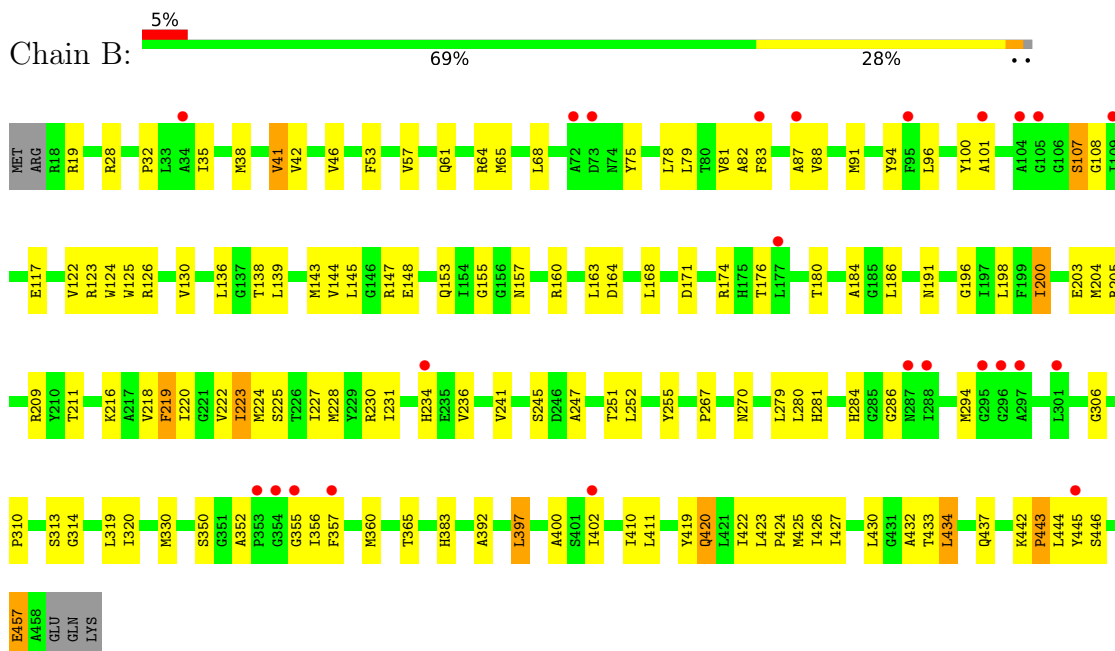
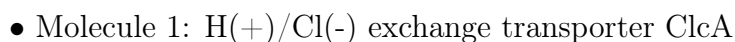
- Molecule 3 is a protein called Fab, light chain.

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			

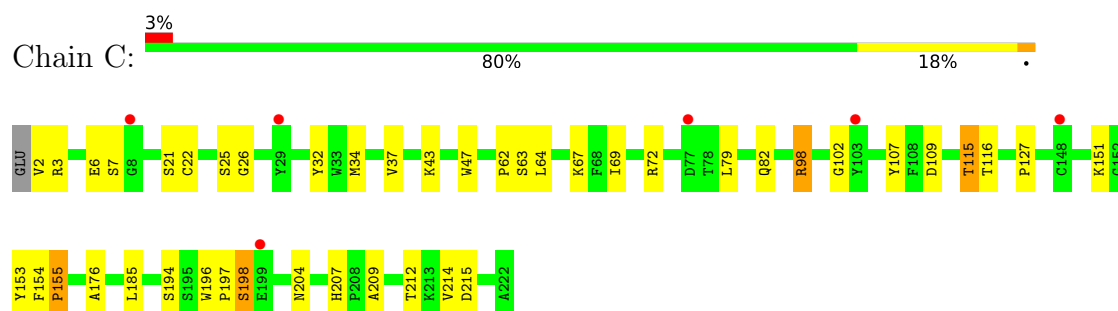
- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Br 2	0	0
4	B	2	Total 2	Br 2	0	0

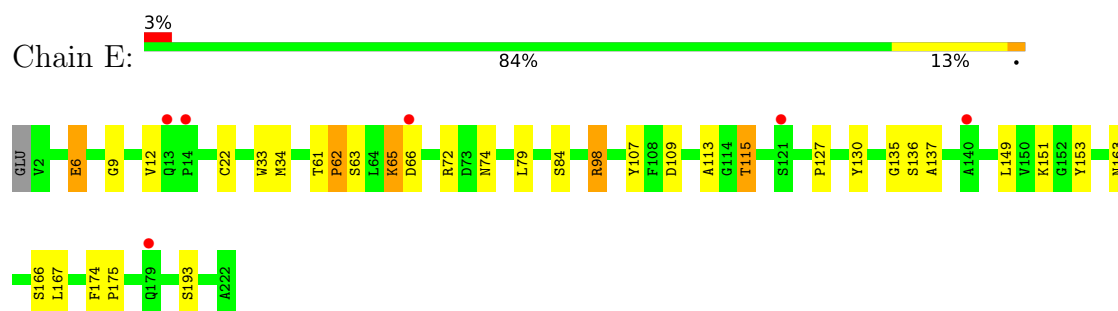
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



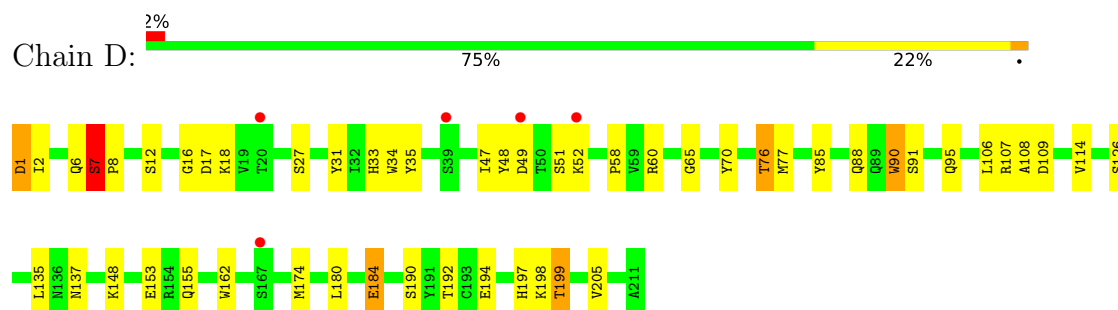
- Molecule 2: Fab, heavy chain



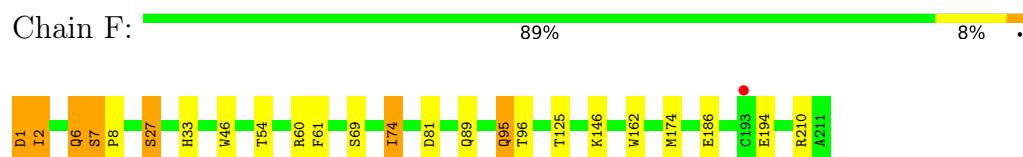
- Molecule 2: Fab, heavy chain



- 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	231.36Å 100.92Å 171.72Å 90.00° 132.12° 90.00°	Depositor
Resolution (Å)	24.88 – 3.18 24.88 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.88-3.18) 98.9 (24.88-3.18)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.235 , 0.269 0.237 , 0.271	Depositor DCC
R_{free} test set	2462 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	101.9	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 8.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13218	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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](#)

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

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	0/3396	0.78	0/4609
1	B	0.44	0/3376	0.80	4/4583 (0.1%)
2	C	0.40	0/1721	0.73	0/2355
2	E	0.42	0/1721	0.73	0/2355
3	D	0.38	0/1660	0.78	3/2257 (0.1%)
3	F	0.41	0/1660	0.80	2/2257 (0.1%)
All	All	0.43	0/13534	0.77	9/18416 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	SER	CA-C-N	-10.57	106.63	119.84
3	F	7	SER	C-N-CA	-10.57	106.63	119.84
3	D	7	SER	CA-C-N	-8.66	109.02	119.84
3	D	7	SER	C-N-CA	-8.66	109.02	119.84
1	B	223	ILE	CB-CA-C	-5.31	105.18	111.81
1	B	108	GLY	N-CA-C	-5.18	108.31	114.48
1	B	247	ALA	CA-C-N	5.17	125.17	119.89
1	B	247	ALA	C-N-CA	5.17	125.17	119.89
3	D	90	TRP	N-CA-C	-5.14	106.02	113.21

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	3324	0	3476	62	0
1	B	3304	0	3457	89	0
2	C	1672	0	1654	22	0
2	E	1672	0	1654	17	0
3	D	1621	0	1546	28	0
3	F	1621	0	1546	13	0
4	A	2	0	0	6	0
4	B	2	0	0	9	0
All	All	13218	0	13333	215	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 (215) 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:356:ILE:N	4:B:501:BR:BR	2.16	1.32
1:A:107:SER:N	4:A:502:BR:BR	2.66	0.83
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.62	0.81
1:B:355:GLY:CA	4:B:501:BR:BR	2.89	0.75
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.20	0.74
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.67	0.74
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.72	0.71
1:A:356:ILE:N	4:A:501:BR:BR	2.79	0.70
1:A:355:GLY:CA	4:A:501:BR:BR	2.95	0.70
1:A:216:LYS:NZ	1:B:437:GLN:OE1	2.24	0.70
1:B:355:GLY:C	4:B:501:BR:BR	2.91	0.69
3:D:153:GLU:OE1	3:D:155:GLN:NE2	2.24	0.69
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.26	0.68
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.76	0.67
1:A:437:GLN:OE1	1:B:216:LYS:NZ	2.25	0.67
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.59	0.67
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.27	0.67
1:A:200:ILE:HA	1:A:204:MET:HB2	1.75	0.66
1:B:445:TYR:OH	4:B:501:BR:BR	2.67	0.66
3:F:1:ASP:OD2	3:F:1:ASP:N	2.28	0.65
3:D:6:GLN:NE2	3:D:85:TYR:O	2.27	0.65
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.78	0.65
1:A:73:ASP:N	1:A:73:ASP:OD1	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLN:O	1:B:157:ASN:ND2	2.23	0.64
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.29	0.64
2:C:194:SER:O	2:C:198:SER:OG	2.15	0.64
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.62	0.64
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.81	0.62
2:C:204:ASN:ND2	2:C:215:ASP:OD1	2.31	0.62
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.34	0.61
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.81	0.61
1:A:355:GLY:HA2	4:A:501:BR:BR	2.56	0.60
1:A:216:LYS:HE2	1:B:433:THR:HG22	1.84	0.59
1:A:148:GLU:CD	1:A:148:GLU:H	2.10	0.59
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.84	0.59
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.28	0.58
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.84	0.58
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.84	0.58
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.86	0.58
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.85	0.58
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.86	0.58
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.37	0.58
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.85	0.58
3:D:17:ASP:H	3:D:77:MET:H	1.50	0.58
1:A:314:GLY:O	1:A:340:ARG:NH2	2.38	0.57
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.86	0.57
1:B:357:PHE:N	4:B:501:BR:BR	2.93	0.57
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.40	0.57
1:A:313:SER:OG	1:A:314:GLY:N	2.37	0.56
3:D:197:HIS:ND1	3:D:199:THR:OG1	2.31	0.56
1:A:435:LEU:O	1:A:439:THR:OG1	2.18	0.55
2:E:61:THR:O	2:E:63:SER:N	2.39	0.55
1:B:148:GLU:CD	1:B:148:GLU:H	2.13	0.55
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.89	0.54
1:B:355:GLY:HA2	4:B:501:BR:BR	2.63	0.54
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.89	0.54
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.43	0.54
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.90	0.54
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.72	0.54
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.90	0.53
1:B:107:SER:HB3	4:B:502:BR:BR	2.63	0.53
1:B:148:GLU:HG2	1:B:357:PHE:HB3	1.90	0.53
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.89	0.53
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:NH1	1:A:86:SER:OG	2.41	0.53
1:B:61:GLN:HA	1:B:64:ARG:HE	1.73	0.53
1:A:355:GLY:HA3	4:A:501:BR:BR	2.64	0.52
1:B:88:VAL:HA	1:B:91:MET:HE2	1.91	0.52
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.91	0.52
1:B:100:TYR:O	1:B:126:ARG:NH1	2.41	0.52
1:B:200:ILE:HA	1:B:204:MET:HB2	1.92	0.51
1:B:68:LEU:HD21	1:B:82:ALA:HB2	1.93	0.51
1:A:414:GLU:OE1	1:B:419:TYR:OH	2.20	0.50
3:D:107:ARG:NE	3:D:108:ALA:O	2.35	0.50
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.92	0.50
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.92	0.50
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.47	0.50
1:B:124:TRP:NE1	1:B:164:ASP:OD1	2.42	0.50
1:A:106:GLY:HA3	4:A:502:BR:BR	2.66	0.50
1:A:72:ALA:HA	1:A:78:LEU:HD12	1.94	0.49
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.94	0.49
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.94	0.49
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.48	0.49
1:B:32:PRO:HD2	1:B:35:ILE:HD12	1.95	0.49
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.76	0.49
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.45	0.49
3:D:95:GLN:OE1	3:D:95:GLN:N	2.34	0.49
2:C:32:TYR:O	2:C:72:ARG:NH2	2.36	0.49
1:A:227:ILE:O	1:A:231:ILE:HG12	2.13	0.48
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.95	0.48
1:B:160:ARG:NE	1:B:163:LEU:HD23	2.28	0.48
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.96	0.48
1:B:176:THR:O	1:B:180:THR:HG23	2.14	0.48
2:C:6:GLU:HA	2:C:22:CYS:HA	1.95	0.48
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.96	0.48
2:E:9:GLY:H	2:E:115:THR:HG21	1.78	0.48
1:A:132:PHE:O	1:A:136:LEU:HB2	2.14	0.47
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.97	0.47
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.96	0.47
1:B:306:GLY:HA2	1:B:310:PRO:HA	1.97	0.47
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.97	0.47
1:B:356:ILE:HG22	4:B:501:BR:BR	2.69	0.47
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.49	0.47
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.96	0.47
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ALA:HA	1:B:425:MET:HG2	1.96	0.47
1:B:422:ILE:O	1:B:426:ILE:HG13	2.15	0.46
1:B:355:GLY:HA3	4:B:501:BR:BR	2.68	0.46
1:A:28:ARG:NH2	1:B:203:GLU:OE1	2.46	0.46
1:B:38:MET:O	1:B:42:VAL:HG23	2.15	0.46
1:B:280:LEU:HD13	1:B:350:SER:HB3	1.97	0.46
2:C:107:TYR:HB3	3:D:33:HIS:CE1	2.50	0.46
1:B:160:ARG:HA	1:B:160:ARG:HD2	1.75	0.46
1:A:360:MET:HE1	1:A:402:ILE:HG13	1.97	0.46
1:B:171:ASP:OD2	1:B:174:ARG:NH1	2.42	0.46
1:B:46:VAL:HG22	1:B:155:GLY:HA2	1.98	0.46
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.49	0.46
1:B:270:ASN:ND2	1:B:442:LYS:O	2.49	0.46
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.51	0.46
1:B:420:GLN:H	1:B:420:GLN:HG3	1.47	0.45
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.98	0.45
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.97	0.45
3:F:2:ILE:HD13	3:F:27:SER:HB2	1.99	0.45
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.82	0.45
1:B:252:LEU:HD22	1:B:427:ILE:HD12	1.99	0.45
3:D:35:TYR:HE1	3:D:88:GLN:HB3	1.81	0.45
1:A:154:ILE:O	1:A:158:ILE:HG12	2.17	0.45
1:A:211:THR:HB	1:A:213:ILE:HG13	1.99	0.45
3:D:180:LEU:HD22	3:D:184:GLU:HG2	1.97	0.45
1:A:430:LEU:HD23	1:B:220:ILE:HG12	1.99	0.45
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.99	0.44
1:A:224:MET:O	1:A:228:MET:HG2	2.18	0.44
1:A:442:LYS:HB3	1:A:442:LYS:HE2	1.82	0.44
1:B:83:PHE:O	1:B:87:ALA:N	2.50	0.44
1:B:284:HIS:C	1:B:286:GLY:H	2.26	0.44
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.73	0.44
1:A:269:PHE:O	1:A:273:VAL:HG12	2.18	0.44
2:C:3:ARG:N	2:C:25:SER:O	2.49	0.44
2:E:6:GLU:HA	2:E:22:CYS:HA	1.99	0.44
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.99	0.44
3:D:197:HIS:CD2	3:D:198:LYS:H	2.36	0.44
3:F:46:TRP:O	3:F:54:THR:OG1	2.36	0.44
1:A:455:LYS:O	1:A:459:GLU:HG2	2.18	0.43
2:C:154:PHE:HA	2:C:155:PRO:HA	1.78	0.43
3:D:17:ASP:OD1	3:D:18:LYS:N	2.51	0.43
2:C:127:PRO:HD2	2:C:212:THR:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MET:O	1:B:145:LEU:N	2.51	0.43
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.27	0.43
1:B:230:ARG:O	1:B:234:HIS:ND1	2.51	0.43
1:B:320:ILE:HG23	1:B:365:THR:HG21	2.00	0.43
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.54	0.43
1:A:176:THR:O	1:A:180:THR:HG23	2.19	0.43
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.99	0.43
1:B:245:SER:O	1:B:420:GLN:NE2	2.52	0.43
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.53	0.43
1:B:224:MET:O	1:B:228:MET:HG2	2.18	0.43
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.54	0.43
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.18	0.43
2:C:34:MET:HB3	2:C:79:LEU:HD22	2.01	0.43
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.54	0.43
3:D:49:ASP:O	3:D:51:SER:N	2.46	0.43
1:B:227:ILE:O	1:B:231:ILE:HG13	2.19	0.43
3:D:114:VAL:HG22	3:D:135:LEU:HD22	2.01	0.43
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.81	0.42
2:E:135:GLY:C	2:E:137:ALA:H	2.26	0.42
2:E:61:THR:OG1	2:E:62:PRO:HD2	2.20	0.42
2:E:6:GLU:OE1	2:E:113:ALA:N	2.52	0.42
2:E:163:ASN:O	2:E:166:SER:OG	2.26	0.42
1:A:176:THR:O	1:A:179:ALA:N	2.51	0.42
1:A:216:LYS:O	1:A:220:ILE:HG13	2.19	0.42
1:A:410:ILE:O	1:A:414:GLU:HG3	2.20	0.42
1:B:218:VAL:O	1:B:222:VAL:HG23	2.19	0.42
2:E:130:TYR:HD2	2:E:149:LEU:HD23	1.84	0.42
3:F:6:GLN:HE21	3:F:6:GLN:HB3	1.60	0.42
1:A:186:LEU:HD23	1:A:196:GLY:HA2	2.00	0.42
2:C:2:VAL:HA	2:C:26:GLY:HA3	2.02	0.42
3:F:186:GLU:HA	3:F:210:ARG:CZ	2.50	0.42
1:B:255:TYR:CG	1:B:424:PRO:HB3	2.55	0.41
1:B:313:SER:OG	1:B:314:GLY:N	2.53	0.41
1:B:75:TYR:O	1:B:79:LEU:HG	2.20	0.41
3:D:34:TRP:HB2	3:D:47:ILE:HB	2.03	0.41
1:A:186:LEU:HD22	1:A:199:PHE:CD2	2.56	0.41
2:E:174:PHE:HA	2:E:175:PRO:HD3	1.96	0.41
3:F:61:PHE:CE2	3:F:74:ILE:HD13	2.55	0.41
3:F:89:GLN:O	3:F:95:GLN:HB2	2.21	0.41
1:B:184:ALA:HB1	1:B:225:SER:HB2	2.02	0.41
2:C:32:TYR:CD2	2:C:98:ARG:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.55	0.41
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.20	0.41
3:D:1:ASP:OD2	3:D:1:ASP:N	2.28	0.41
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.55	0.41
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.55	0.41
3:D:2:ILE:HD12	3:D:27:SER:HB2	2.02	0.41
2:E:34:MET:HB3	2:E:79:LEU:HD22	2.03	0.41
1:A:109:ILE:HG12	1:A:152:VAL:HG11	2.01	0.41
1:A:241:VAL:HG11	1:A:391:ILE:HD11	2.02	0.41
1:B:420:GLN:HE21	1:B:420:GLN:HB2	1.65	0.41
1:A:260:ILE:HG23	1:A:435:LEU:HG	2.02	0.41
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.56	0.41
3:D:58:PRO:HB2	3:D:60:ARG:HG2	2.03	0.40
1:B:19:ARG:HA	1:B:19:ARG:HD2	1.87	0.40
1:B:180:THR:HG22	1:B:218:VAL:HA	2.03	0.40
1:B:267:PRO:HA	1:B:270:ASN:HB2	2.02	0.40
2:C:7:SER:HA	2:C:115:THR:HG21	2.02	0.40
1:B:38:MET:HA	1:B:41:VAL:HG13	2.04	0.40
1:B:294:MET:HE2	1:B:294:MET:HB3	2.00	0.40
2:E:65:LYS:HB2	2:E:66:ASP:H	1.69	0.40
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.87	0.40
1:A:100:TYR:O	1:A:126:ARG:NH1	2.52	0.40
1:A:144:VAL:HG21	1:A:343:THR:HB	2.02	0.40
1:A:409:ILE:HD13	1:A:426:ILE:HG12	2.02	0.40
1:B:53:PHE:HE2	1:B:147:ARG:HG2	1.86	0.40
1:B:53:PHE:O	1:B:57:VAL:HG23	2.22	0.40
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.40	0.40
2:C:196:TRP:CG	2:C:197:PRO:HA	2.56	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	441/446 (99%)	423 (96%)	18 (4%)	0	100	100
1	B	439/446 (98%)	407 (93%)	29 (7%)	3 (1%)	18	50
2	C	219/222 (99%)	203 (93%)	13 (6%)	3 (1%)	9	36
2	E	219/222 (99%)	195 (89%)	21 (10%)	3 (1%)	9	36
3	D	209/211 (99%)	187 (90%)	18 (9%)	4 (2%)	6	30
3	F	209/211 (99%)	187 (90%)	22 (10%)	0	100	100
All	All	1736/1758 (99%)	1602 (92%)	121 (7%)	13 (1%)	18	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	62	PRO
2	E	65	LYS
1	B	107	SER
2	C	62	PRO
3	D	126	SER
1	B	144	VAL
3	D	76	THR
1	B	443	PRO
3	D	137	ASN
2	E	136	SER
3	D	7	SER
2	C	102	GLY
2	C	155	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/337 (99%)	309 (92%)	25 (8%)	12	39
1	B	332/337 (98%)	309 (93%)	23 (7%)	14	42
2	C	181/182 (100%)	172 (95%)	9 (5%)	22	52
2	E	181/182 (100%)	173 (96%)	8 (4%)	25	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	185/185 (100%)	180 (97%)	5 (3%)	39 65
3	F	185/185 (100%)	176 (95%)	9 (5%)	22 52
All	All	1398/1408 (99%)	1319 (94%)	79 (6%)	18 48

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	41	VAL
1	A	73	ASP
1	A	81	VAL
1	A	96	LEU
1	A	162	VAL
1	A	180	THR
1	A	200	ILE
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	223	ILE
1	A	241	VAL
1	A	264	ILE
1	A	273	VAL
1	A	346	LEU
1	A	391	ILE
1	A	397	LEU
1	A	420	GLN
1	A	433	THR
1	A	435	LEU
1	A	444	LEU
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	41	VAL
1	B	65	MET
1	B	96	LEU
1	B	122	VAL
1	B	136	LEU
1	B	139	LEU
1	B	200	ILE
1	B	205	ARG
1	B	211	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	219	PHE
1	B	236	VAL
1	B	241	VAL
1	B	251	THR
1	B	279	LEU
1	B	319	LEU
1	B	330	MET
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	423	LEU
1	B	434	LEU
1	B	444	LEU
1	B	457	GLU
2	C	21	SER
2	C	43	LYS
2	C	63	SER
2	C	98	ARG
2	C	115	THR
2	C	116	THR
2	C	151	LYS
2	C	198	SER
2	C	214	VAL
3	D	1	ASP
3	D	91	SER
3	D	184	GLU
3	D	190	SER
3	D	199	THR
2	E	6	GLU
2	E	12	VAL
2	E	84	SER
2	E	98	ARG
2	E	115	THR
2	E	151	LYS
2	E	167	LEU
2	E	193	SER
3	F	1	ASP
3	F	2	ILE
3	F	6	GLN
3	F	27	SER
3	F	69	SER
3	F	74	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	95	GLN
3	F	96	THR
3	F	125	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	234	HIS
1	B	281	HIS
1	B	284	HIS
1	B	420	GLN
3	D	37	GLN
3	D	75	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](#)

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 [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, 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	443/446 (99%)	0.01	11 (2%) 58 37	45, 67, 94, 130	0
1	B	441/446 (98%)	0.24	24 (5%) 31 18	49, 77, 111, 138	0
2	C	221/222 (99%)	-0.04	6 (2%) 56 35	35, 65, 99, 133	0
2	E	221/222 (99%)	-0.09	6 (2%) 56 35	45, 65, 93, 132	0
3	D	211/211 (100%)	0.18	5 (2%) 59 39	49, 77, 98, 106	0
3	F	211/211 (100%)	-0.18	1 (0%) 87 75	40, 58, 106, 120	0
All	All	1748/1758 (99%)	0.05	53 (3%) 52 32	35, 69, 102, 138	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ALA	7.4
1	B	73	ASP	6.1
1	B	72	ALA	5.0
1	A	168	LEU	4.9
1	B	95	PHE	4.8
1	A	447	ALA	4.0
3	D	52	LYS	3.7
1	B	296	GLY	3.6
1	B	445	TYR	3.5
1	A	171	ASP	3.5
1	A	234	HIS	3.4
1	A	235	GLU	3.3
1	B	83	PHE	3.2
1	B	177	LEU	3.1
2	E	14	PRO	3.0
1	B	357	PHE	2.9
1	B	301	LEU	2.9
2	E	121	SER	2.8
2	C	29	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	353	PRO	2.7
1	B	288	ILE	2.7
1	B	287	ASN	2.7
1	A	255	TYR	2.7
1	B	354	GLY	2.7
3	D	49	ASP	2.6
3	D	20	THR	2.6
1	B	109	ILE	2.5
1	B	295	GLY	2.5
2	C	8	GLY	2.4
1	B	297	ALA	2.4
3	D	39	SER	2.4
1	A	348	PHE	2.3
1	B	105	GLY	2.3
2	C	148	CYS	2.3
1	B	234	HIS	2.3
2	C	77	ASP	2.3
2	E	66	ASP	2.3
2	E	179	GLN	2.3
1	B	87	ALA	2.3
2	C	199	GLU	2.2
1	B	402	ILE	2.2
1	A	445	TYR	2.2
1	B	34	ALA	2.2
1	A	174	ARG	2.2
3	D	167	SER	2.2
3	F	193	CYS	2.2
2	E	140	ALA	2.1
1	B	355	GLY	2.1
1	A	455	LYS	2.1
1	A	258	LEU	2.1
1	B	101	ALA	2.0
2	C	103	TYR	2.0
2	E	13	GLN	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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	BR	B	502	1/1	0.77	0.18	126,126,126,126	0
4	BR	A	502	1/1	0.84	0.21	121,121,121,121	0
4	BR	A	501	1/1	0.91	0.16	98,98,98,98	0
4	BR	B	501	1/1	0.92	0.24	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.