WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2014 – 01:37 PM GMT

PDB ID : 2H2P
Title : Crystal structure of CLC-ec1 in complex with Fab fragment in SeCN-
Authors : Nguitragool, W.; Miller, C.
Deposited on : 2006-05-19
Resolution : 3.10 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	FAILED
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.285
Clashscore		42
Ramachandran outliers		5.0%
Sidechain outliers		5.4%
RSRZ outliers		0.1%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	465	
1	B	465	
2	C	221	
2	E	221	
3	D	211	
3	F	211	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13231 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CLC Cl transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total 3333	C 2190	N 560	O 563	S 20	0	0	0
1	B	441	Total 3304	C 2174	N 553	O 557	S 20	0	0	0

- Molecule 2 is a protein called FAB fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total 1672	C 1077	N 274	O 315	S 6	0	0	0
2	E	221	Total 1672	C 1077	N 274	O 315	S 6	0	0	0

- Molecule 3 is a protein called FAB fragment, light chain.

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

- Molecule 4 is SELENOCYANATE ION (three-letter code: SEK) (formula: CNSe).

Se⁻————————N

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Se 1	0	0
4	B	1	Total 1	Se 1	0	0
4	A	1	Total 1	Se 1	1	0
4	B	1	Total 1	Se 1	1	0
4	A	1	Total 1	Se 1	1	0
4	B	1	Total 1	Se 1	1	0
4	A	1	Total 1	Se 1	1	0
4	B	1	Total 1	Se 1	1	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.
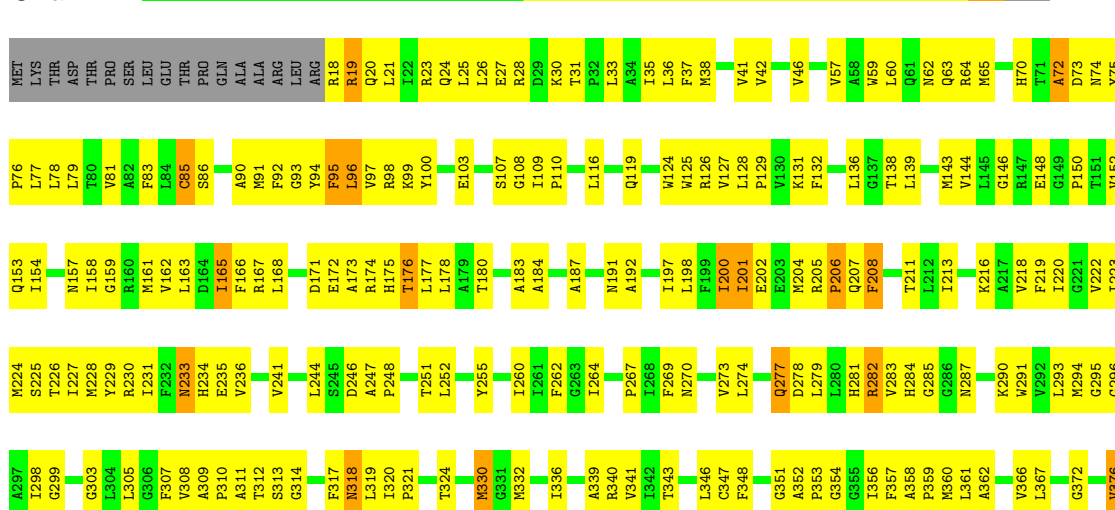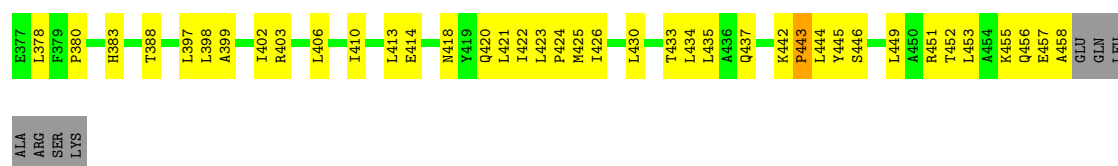
- Molecule 1: CLC Cl transporter
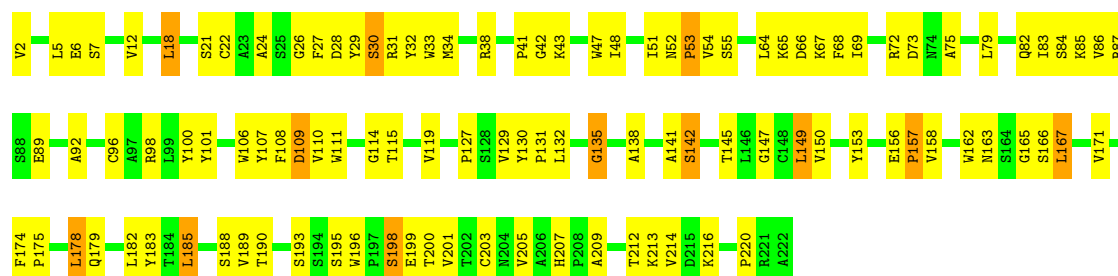
Chain A:

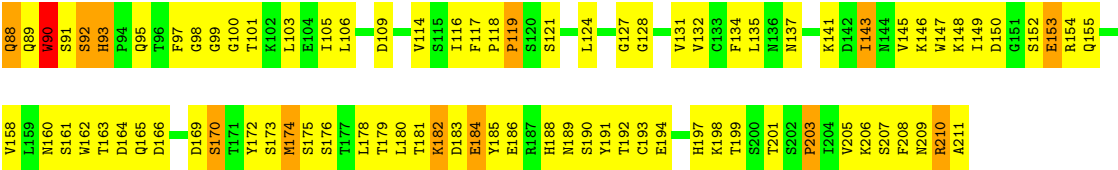- Molecule 1: CLC Cl transporter

Chain B:

E377 L378 F379 P380 H383 T388 L397 L398 A399 I402 R403 L406 I410 L413 E414 N418 Y419 Q420 L421 I422 L423 P424 M425 I426 L430 T433 L434 L435 Q437 K442 P443 L444 Y445 S446 L449 A450 R451 T452 L453 A454 K455 Q456 E457 A458 GLU GLN LEU

ALA ARG SER LYS

● Molecule 2: FAB fragment, heavy chain

Chain C:

V2 L5 E6 S7 V12 L18 S21 C22 A23 A24 S25 G26 F27 D28 Y29 S30 R31 Y32 W33 M34 R38 P41 G42 K43 W47 I48 I51 N52 P53 V54 S55 L64 K65 D66 K67 F68 I69 R72 D73 N74 A75 L79 Q82 I83 S84 K85 V86 R87

S88 E89 A92 C96 A97 R98 L99 Y100 Y101 W106 Y107 F108 D109 V110 W111 G114 T115 V119 P127 S128 Y129 Y130 P131 L132 G135 A138 A141 S142 T145 L146 G147 C148 L149 V150 Y153 E156 P157 V158 W162 N163 S164 G165 S166 L167 V171

F174 P175 L178 Q179 L182 Y183 T184 L185 S188 V189 T190 S193 S194 S195 W196 P197 S198 E199 T200 V201 T202 C203 N204 V205 A206 H207 P208 A209 T212 K213 V214 D215 K216 P220 R221 A222

● Molecule 2: FAB fragment, heavy chain

Chain E:

V2 V12 G16 S17 L18 K19 L20 S21 C22 F27 D28 Y29 S30 R31 Y32 W33 M34 S35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 W47 I48 G49 E50 I51 N52 P53 V54 I58 N59 Y60 T61 P62 S63 L64 K65 D66 K67 F68 I69 D73 K76 D77 T78 L79 Y80

L81 Q82 I83 S84 K85 V86 R87 S88 E89 D90 T91 A92 L93 Y94 R98 L99 Y100 V105 W106 Y107 F108 D109 V110 W111 T115 T116 V117 T118 V119 S120 S121 A122 P127 L132 A133 P134 G135 A138 A139 A140 M143 V144 T145 L146 G147 V150 K151 G152 Y153 P157

W162 N163 S166 L167 F174 L178 Q179 A180 A181 L182 Y183 T184 L185 S188 V189 T190 V191 S195 E199 T200 V201 T202 C203 N204 V205 D215 I218 R221 A222

● Molecule 3: FAB fragment, light chain

Chain D:

D1 I2 V3 L4 T5 Q6 S7 P8 A9 I10 M11 S12 A13 A14 P15 G16 D17 K18 V19 T22 C23 S27 S28 V29 S30 Y31 Y35 K38 T41 S42 P43 R45 W46 I47 Y48 D49 T50 S51 K52 L53 T54 V57 P58 V59 R60 F61 S64 G65 S66 G67 Y70

S71 L72 T73 I74 N75 T76 M77 E78 A79 E80 D81 A82 A83 T84 Y85 Y86 C87 Q88 Q89 W90 S91 S92 H93 P94 Q95 T96 F97 G100 T101 K102 L103 E104 I105 L106 R107 A108 D109 A110 A111 P112 T113 V114 S115 I116 F117 P118 P119 Q123 L124 T125 S126 G127 G128 A129 S130 V131 F134

L135 N136 N137 F138 Y139 P140 K141 K146 W147 K148 I149 D150 G151 S152 E153 R154 V158 L159 N160 S161 W162 T163 D164 Q165 D166 S167 K168 D169 S170 T171 Y172 S173 M174 L178 T179 L180 T181 K182 D183 E184 Y185 E186 R187 H188 N189 S190 Y191 T192 C193 E194 H197 K198 T199 S200 T201 S202

P203 I204 V205 K206 S207 F208 N209 R210 A211

● Molecule 3: FAB fragment, light chain

Chain F:

D1 I2 V3 L4 T5 Q6 S7 P8 S12 A13 A14 P15 M21 T22 C23 S24 S27 Y31 I32 H33 Q37 K38 S39 G40 T41 D49 T50 L53 T54 S55 F61 G65 S66 G67 T68 S69 Y70 S71 L72 T73 I74 N75 T76 M77 E78 A83 T84 Y85 Y86 C87

Q88 Q89 W90 S91 S92 H93 P94 Q95 T96 F97 G98 G99 G100 T101 K102 L103 E104 I105 L106 D109 V114 S115 I116 F117 P118 P119 S120 S121 L124 G127 G128 V131 V132 C133 F134 L135 N136 N137 K141 D142 I143 N144 V145 K146 W147 K148 I149 D150 G151 S152 E153 R154 Q155

V158 L159 N160 S161 W162 T163 D164 Q165 D166 D169 S170 T171 Y172 S173 M174 S175 S176 T177 L178 T179 L180 T181 K182 D183 E184 Y185 E186 R187 H188 N189 S190 Y191 T192 C193 E194 H197 K198 T199 S200 T201 S202 P203 I204 V205 K206 S207 F208 N209 R210 A211

4 Data and refinement statistics ⓘ

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	220.58Å 121.58Å 151.24Å 90.00° 128.25° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 37.67 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.10) 98.0 (37.67-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.278 , 0.280 0.281 , 0.285	Depositor DCC
R_{free} test set	3070 reflections (5.27%)	DCC
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13231	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

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: SEK

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	0.48	0/3405	0.64	0/4621
1	B	0.48	0/3376	0.63	0/4583
2	C	0.52	0/1721	0.76	0/2355
2	E	0.52	0/1721	0.78	0/2355
3	D	0.48	0/1660	0.73	1/2257 (0.0%)
3	F	0.52	0/1660	0.77	0/2257
All	All	0.49	0/13543	0.70	1/18428 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	16	GLY	N-CA-C	-6.80	96.11	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3482	267	0
1	B	3304	0	3456	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1672	0	1654	122	0
2	E	1672	0	1654	125	0
3	D	1621	0	1544	230	0
3	F	1621	0	1546	172	0
4	A	4	0	0	2	0
4	B	4	0	0	2	0
All	All	13231	0	13336	1109	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

The worst 5 of 1109 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:107:TYR:CE1	3:D:45:ARG:NH1	1.70	1.56
1:A:274:LEU:CD2	1:A:451:ARG:NH1	1.71	1.53
3:D:186:GLU:HA	3:D:210:ARG:NH2	1.27	1.45
2:E:163:ASN:HD22	2:E:167:LEU:CD1	1.35	1.39
1:A:18:ARG:NH1	1:B:456:GLN:OE1	1.62	1.30

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	442/465 (95%)	344 (78%)	80 (18%)	18 (4%)	4	27
1	B	439/465 (94%)	336 (76%)	85 (19%)	18 (4%)	4	27
2	C	219/221 (99%)	187 (85%)	22 (10%)	10 (5%)	4	24
2	E	219/221 (99%)	184 (84%)	24 (11%)	11 (5%)	3	22
3	D	209/211 (99%)	153 (73%)	40 (19%)	16 (8%)	1	11
3	F	209/211 (99%)	168 (80%)	28 (13%)	13 (6%)	2	16
All	All	1737/1794 (97%)	1372 (79%)	279 (16%)	86 (5%)	3	22

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	283	VAL
1	B	201	ILE
1	B	283	VAL
2	C	53	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	335/353 (95%)	328 (98%)	7 (2%)	66	92
1	B	332/353 (94%)	323 (97%)	9 (3%)	57	89
2	C	181/181 (100%)	172 (95%)	9 (5%)	34	75
2	E	181/181 (100%)	165 (91%)	16 (9%)	14	49
3	D	185/185 (100%)	168 (91%)	17 (9%)	13	45
3	F	185/185 (100%)	168 (91%)	17 (9%)	13	45
All	All	1399/1438 (97%)	1324 (95%)	75 (5%)	31	72

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	96	THR
3	D	208	PHE
3	F	161	SER
3	D	106	LEU
3	D	169	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	ASN
1	B	284	HIS
2	E	163	ASN
1	B	207	GLN

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Mol	Chain	Res	Type
1	B	287	ASN

5.3.3   RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 8 are modelled with single atom - 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.

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	444/465 (95%)	-0.17	1 (0%)	93	61	77, 77, 77, 77	0
1	B	441/465 (94%)	-0.12	0	100	100	77, 77, 77, 77	0
2	C	221/221 (100%)	-0.16	0	100	100	77, 77, 77, 77	0
2	E	221/221 (100%)	-0.15	0	100	100	77, 77, 77, 77	0
3	D	211/211 (100%)	-0.17	0	100	100	77, 77, 77, 77	0
3	F	211/211 (100%)	-0.13	0	100	100	77, 77, 77, 77	0
All	All	1749/1794 (97%)	-0.15	1 (0%)	93	70	77, 77, 77, 77	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	2.2

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SEK	A	468	1/3	-	-	76,76,76,76	1
4	SEK	B	466	1/3	0.46	-	76,76,76,76	0
4	SEK	A	466	1/3	0.36	-	76,76,76,76	0
4	SEK	B	468	1/3	-	-	76,76,76,76	1
4	SEK	B	467	1/3	-	-	76,76,76,76	1
4	SEK	A	467	1/3	-	-	76,76,76,76	1
4	SEK	A	469	1/3	-	-	76,76,76,76	1
4	SEK	B	469	1/3	-	-	76,76,76,76	1

6.5 Other polymers ⓘ

There are no such residues in this entry.