wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 02:00 am BST

PDB ID	:	2YKS
Title	:	PENTAMERIC LIGAND GATED ION CHANNEL ELIC MUTANT F246A
Authors	:	Zimmermann, I.; Dutzler, R.
Deposited on	:	2011-05-30
Resolution	:	3.30 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

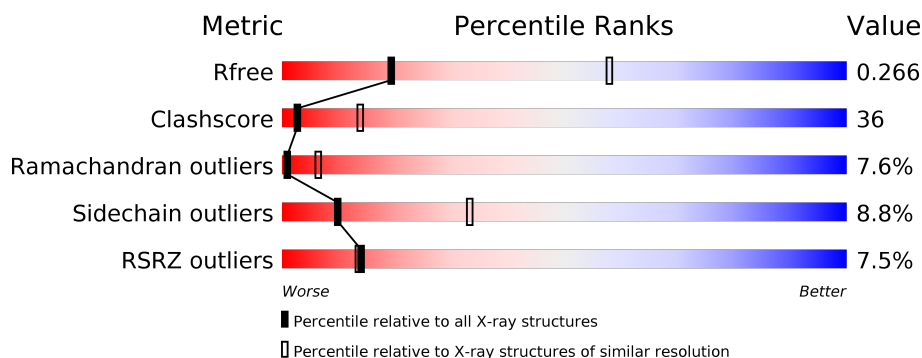|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.30 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		0.266
Clashscore		36
Ramachandran outliers		7.6%
Sidechain outliers		8.8%
RSRZ outliers		7.5%

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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 <=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	321	8% 41% · 45% · 9% · 5%
1	B	321	7% 44% · 42% · 8% · 5%
1	C	321	6% 43% · 42% · 9% · 5%
1	D	321	7% 42% · 44% · 8% · 5%
1	E	321	6% 43% · 44% · 8% · 5%
1	F	321	7% 42% · 44% · 9% · 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	321	6% 45% 42% 8% 5%
1	H	321	9% 42% 44% 8% 5%
1	I	321	6% 42% 44% 8% 5%
1	J	321	10% 42% 43% 9% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 24950 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 CYS-LOOP LIGAND-GATED ION CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	B	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	C	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	D	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	E	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	F	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	G	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	H	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	I	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	J	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	ALA	PHE	engineered mutation	UNP P0C7B7
A	288	ASN	MET	conflict	UNP P0C7B7
B	246	ALA	PHE	engineered mutation	UNP P0C7B7
B	288	ASN	MET	conflict	UNP P0C7B7
C	246	ALA	PHE	engineered mutation	UNP P0C7B7
C	288	ASN	MET	conflict	UNP P0C7B7
D	246	ALA	PHE	engineered mutation	UNP P0C7B7
D	288	ASN	MET	conflict	UNP P0C7B7
E	246	ALA	PHE	engineered mutation	UNP P0C7B7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	288	ASN	MET	conflict	UNP P0C7B7
F	246	ALA	PHE	engineered mutation	UNP P0C7B7
F	288	ASN	MET	conflict	UNP P0C7B7
G	246	ALA	PHE	engineered mutation	UNP P0C7B7
G	288	ASN	MET	conflict	UNP P0C7B7
H	246	ALA	PHE	engineered mutation	UNP P0C7B7
H	288	ASN	MET	conflict	UNP P0C7B7
I	246	ALA	PHE	engineered mutation	UNP P0C7B7
I	288	ASN	MET	conflict	UNP P0C7B7
J	246	ALA	PHE	engineered mutation	UNP P0C7B7
J	288	ASN	MET	conflict	UNP P0C7B7

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 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: CYS-LOOP LIGAND-GATED ION CHANNEL

- Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain C:

• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain D:

• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain E:

• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain F:

7%

42%   44%   9%   5%

• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain G:

6%

45%   42%   8%   5%

S170 D171 I172 R173 Y174 D175 H176 L177 S178 S179 V180 Q181 P182 N183 Q184 N185 E186 F187 R189 I190 R193 V197 R198 N199 P200 S201 Y202 Y203 L204 I208 L209 P210 L211 I214 I215 S218 W219 S220 V221 F222 W223 E225 S226 F227 S228 E229 R230 L231 Q232 T233 S234 F235 T236

L237 M238 L239 T240 A245 A246 Y247 T248 S249 N250 I251 L252 P253 R254 L255 P256 Y257 T258 T259 V260 I261 D262 Q263 I266 A267 I276 I280 R285 Q286 A287 N288 G289 V290 E291 D292 D293 L294 L295 I296 Q297 R298 C299 R300 L301 A302 F303 P304 L305 G306 F307 L308 A309 I310 G311 C312
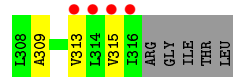
V313 L314 V315 I316 ARG GLY ILE THR LEU

● **Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL**

Chain H:

9%

42% 44% 8% • 5%

ALA PRO ALA ASP ASN ALA ALA ASP ALA ARG P11 V16 F19 I23 N27 T28 L29 T32 I39 V40 W43 T44 P47 R48 K49 T50 P51 G52 D53 K54 P55 L56 I57 V58 E59 N60 T61 Q62 I63 E64 R65 W66 I67 N68 L71 W72 V73 P74 F78 I79

N80 V81 P85 N89 K90 R91 L92 D97 G98 R99 Y102 F110 S111 N112 D113 M114 D115 F116 R117 L118 F119 P120 R123 Q124 Q125 F126 V127 L128 F133 S134 Y135 N136 N137 Q138 Q139 L140 R141 F142 I145 Q146 V147 Y148 T149 E150 N151 I152 D153 N154 E155 E156 I157

W161 I162 R163 K164 A165 S466 T167 H168 I169 S170 D171 I172 R173 Y174 D175 H176 L177 S178 S179 V180 Q181 P182 N183 Q184 N185 E186 F187 S188 R189 I190 T191 V192 R193 V197 R198 N199 P200 S201 Y202 Y203 L204 I208 L209 P210 L211 I214 I215 S218 W219 S220 V221 F222 W223 L224 E225 S226

F227 S228 E229 R230 L231 Q232 F235 T236 L237 M238 L239 T240 Y244 A245 A246 Y247 T248 S249 N250 I251 L252 P253 R254 L255 P256 Y257 T258 T259 D262 Q263 I266 A267 G268 Y269 I276 I280 R285 Q286 A287 N288 G289 V290 E291 D292 D293 L294 L295 I296 Q297 R298 C299 R300 L301
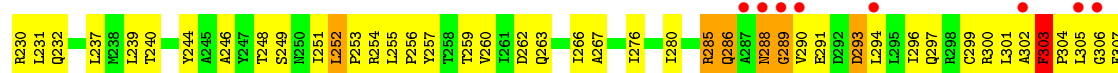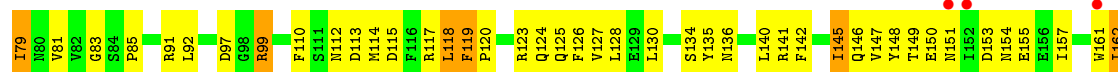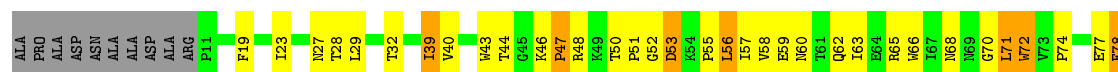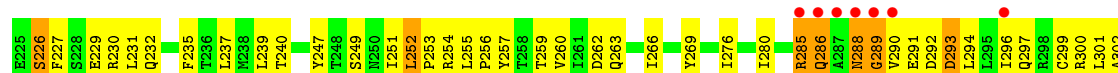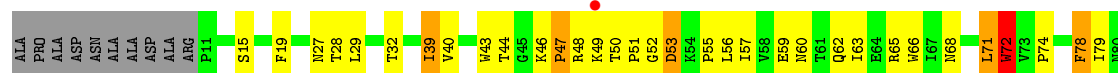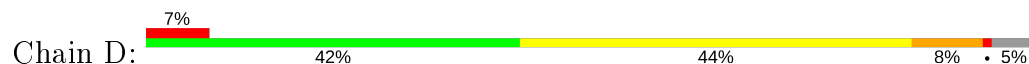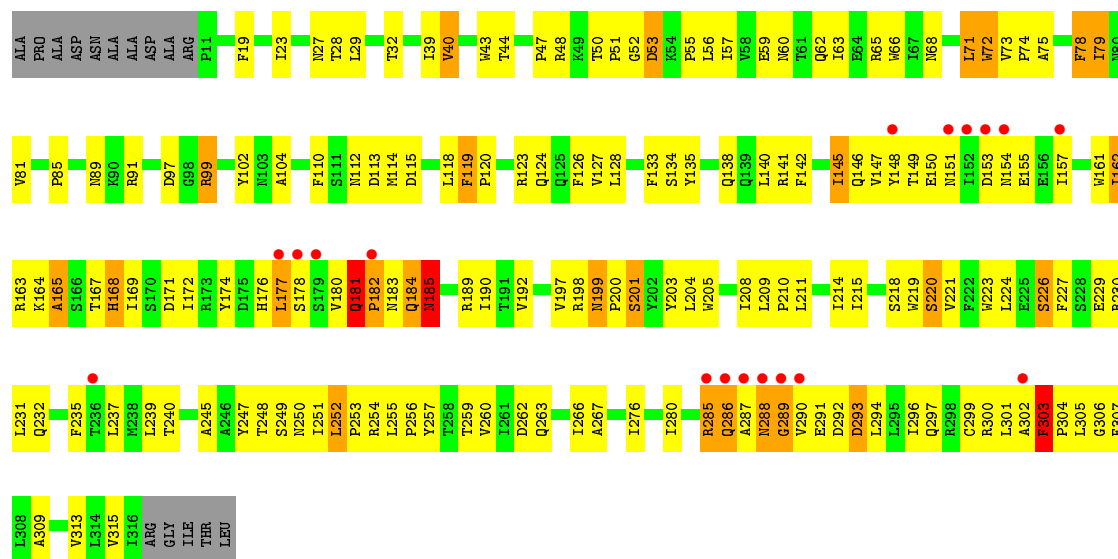
A302 F303 P304 L305 G306 F307 I308 A309 I310 V313 L314 V315 I316 ARG GLY ILE THR LEU

● **Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL**

Chain I:

6%

42% 44% 8% • 5%

ALA PRO ALA ASP ASN ALA ALA ASP ALA ARG P11 V16 S17 I18 F19 I23 N27 T28 L29 T32 I39 V40 W43 T44 G45 K46 P47 R48 K49 T50 P51 G52 D53 K54 P55 L56 I57 V58 E59 N60 T61 Q62 I63 E64 R65 N68 L71 W72 V73 P74 F78

I79 N80 V81 P85 N89 L92 D97 G98 R99 Y102 N103 A104 F110 S111 N112 D113 M114 D115 L118 F119 P120 R123 Q124 Q125 F126 V127 L128 E129 L130 F133 S134 Y135 Q138 Q139 L140 R141 F142 S143 D144 I145 Q146 V147 Y148 T149 E150 N151 I152 D153 N154 E155

E156 I157 W161 I162 R163 K164 A165 S466 T167 H168 I169 S170 D171 I172 R173 Y174 D175 H176 L177 S178 S179 V180 Q181 P182 N183 Q184 N185 E186 F187 S188 R189 I190 T191 V192 V197 R198 M199 P200 S201 Y202 Y203 L204 I208 L209 P210 L211 I214 I215 S218 W219 S220 V221 F222 W223 L224

E225 S226 F227 S228 E229 R230 L231 Q232 F235 T236 L237 M238 L239 T240 Y247 T248 S249 L252 P253 R254 L255 P256 Y257 T258 T259 V260 I261 D262 Q263 M264 I265 I266 A267 I280 H283 H284 R285 Q286 A287 N288 G289 V290 E291 D292 D293 L294 L295 I296 Q297 R298 C299 R300 L301 A302 F303

P304 L305 G306 F307 L308 A309 V313 L314 V315 I316 ARG GLY ILE THR LEU

● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain J:

10%

42%   43%   9% ● 5%

ALA PRO ALA ASP ASN ALA ALA ASP ALA ARG P11 V16 S17 I23 N27 T28 L29 T32 I39 V40 W43 T44 P47 R48 K49 T50 P51 G52 D53 K54 P55 L56 I57 V58 E59 N60 T61 Q62 I63 E64 R65 W66 L71 W72 V73 P74 E77 F78 I79 N80 V81

P85 N89 K90 R91 L92 D97 G98 R99 Y102 N103 A104 L107 F110 S111 N112 D113 M114 D115 L118 F119 P120 R123 Q124 Q125 F126 V127 L128 E129 L130 F133 S134 Y135 L140 F141 F142 S143 D144 I145 Q146 V147 Y148 T149 E150 N151 I152 D153 N154 E155 E156 I157

D158 W161 I162 R163 K164 A165 S166 T167 H168 I169 S170 D171 I172 R173 Y174 D175 H176 L177 S178 S179 V180 Q181 P182 N183 Q184 M185 E186 F187 S188 R189 I190 T191 V192 R193 V197 R198 M199 P200 S201 Y202 Y203 L204 I208 L209 P210 L211 I214 I215 A216 A217 S218 W219 S220 V221 F222 W223

L224 E225 S226 F227 S228 E229 R230 L231 Q232 T236 L237 M238 L239 T240 Y247 T248 S249 N250 I251 L252 P253 R254 L255 P256 Y257 T258 T259 V260 I261 D262 Q263 I266 A267 I276 I280 F281 R285 Q286 A287 N288 G289 V290 E291 D292 D293 L294 L295 I296 Q297 R298 C299 R300 L301 A302

F303 P304 L305 G306 F307 L308 A309 V313 L314 V315 I316 ARG GLY ILE THR LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.50Å 266.15Å 110.85Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	19.97 – 3.30 40.48 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.97-3.30) 96.6 (40.48-3.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.16 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.242 , 0.265 0.246 , 0.266	Depositor DCC
R_{free} test set	4322 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	103.0	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 76.5	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	24950	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.66	0/2562	0.75	1/3493 (0.0%)
1	B	0.73	0/2562	0.78	1/3493 (0.0%)
1	C	0.72	0/2562	0.77	1/3493 (0.0%)
1	D	0.75	2/2562 (0.1%)	0.77	1/3493 (0.0%)
1	E	0.69	0/2562	0.76	0/3493
1	F	0.67	0/2562	0.78	0/3493
1	G	0.75	0/2562	0.79	0/3493
1	H	0.70	0/2562	0.76	0/3493
1	I	0.77	0/2562	0.78	1/3493 (0.0%)
1	J	0.70	0/2562	0.77	1/3493 (0.0%)
All	All	0.71	2/25620 (0.0%)	0.77	6/34930 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	TRP	CD2-CE2	5.75	1.48	1.41
1	D	72	TRP	CZ3-CH2	5.25	1.48	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	ILE	CG1-CB-CG2	-5.91	98.40	111.40
1	I	39	ILE	CG1-CB-CG2	-5.89	98.44	111.40
1	C	39	ILE	CG1-CB-CG2	-5.67	98.92	111.40
1	B	138	GLN	N-CA-C	-5.12	97.17	111.00
1	J	39	ILE	CG1-CB-CG2	-5.07	100.25	111.40

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	2495	0	2471	204	1
1	B	2495	0	2471	204	0
1	C	2495	0	2471	200	0
1	D	2495	0	2471	196	2
1	E	2495	0	2471	196	1
1	F	2495	0	2471	198	1
1	G	2495	0	2471	209	2
1	H	2495	0	2471	193	0
1	I	2495	0	2471	208	0
1	J	2495	0	2471	196	1
All	All	24950	0	24710	1786	4

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 36.

The worst 5 of 1786 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:164:LYS:HG2	1:I:163:ARG:HB3	1.28	1.16
1:I:164:LYS:NZ	1:I:165:ALA:H	1.52	1.06
1:D:164:LYS:NZ	1:D:165:ALA:H	1.54	1.05
1:B:164:LYS:NZ	1:B:165:ALA:H	1.52	1.05
1:G:164:LYS:NZ	1:G:165:ALA:H	1.58	1.01

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ASN:O	1:J:49:LYS:O[1_655]	1.93	0.27
1:D:139:GLN:NE2	1:G:173:ARG:NH2[2_354]	2.01	0.19
1:E:287:ALA:O	1:F:142:PHE:CD2[2_355]	2.12	0.08
1:A:291:GLU:OE1	1:D:49:LYS:NZ[1_556]	2.17	0.03

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	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	B	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6
1	C	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	D	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6
1	E	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	F	304/321 (95%)	236 (78%)	45 (15%)	23 (8%)	1	6
1	G	304/321 (95%)	236 (78%)	45 (15%)	23 (8%)	1	6
1	H	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	I	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6
1	J	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
All	All	3040/3210 (95%)	2371 (78%)	439 (14%)	230 (8%)	1	6

5 of 230 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	119	PHE
1	A	141	ARG
1	A	151	ASN
1	A	168	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/283 (97%)	249 (91%)	25 (9%)	9	31
1	B	274/283 (97%)	249 (91%)	25 (9%)	9	31
1	C	274/283 (97%)	250 (91%)	24 (9%)	10	33
1	D	274/283 (97%)	250 (91%)	24 (9%)	10	33
1	E	274/283 (97%)	250 (91%)	24 (9%)	10	33
1	F	274/283 (97%)	250 (91%)	24 (9%)	10	33
1	G	274/283 (97%)	251 (92%)	23 (8%)	11	35
1	H	274/283 (97%)	250 (91%)	24 (9%)	10	33
1	I	274/283 (97%)	251 (92%)	23 (8%)	11	35
1	J	274/283 (97%)	250 (91%)	24 (9%)	10	33
All	All	2740/2830 (97%)	2500 (91%)	240 (9%)	10	33

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	145	ILE
1	F	171	ASP
1	J	71	LEU
1	E	171	ASP
1	E	303	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	136	ASN
1	F	151	ASN
1	J	124	GLN
1	E	151	ASN
1	E	297	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 carbohydrates 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 (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	306/321 (95%)	0.16	27 (8%)	10	10	64, 105, 278, 412	0
1	B	306/321 (95%)	0.15	22 (7%)	15	15	60, 103, 278, 412	0
1	C	306/321 (95%)	0.19	20 (6%)	18	18	60, 104, 278, 412	0
1	D	306/321 (95%)	0.28	21 (6%)	16	16	59, 103, 277, 401	0
1	E	306/321 (95%)	0.15	18 (5%)	22	22	62, 105, 278, 413	0
1	F	306/321 (95%)	0.09	21 (6%)	16	16	62, 105, 277, 412	0
1	G	306/321 (95%)	0.21	18 (5%)	22	22	59, 104, 277, 412	0
1	H	306/321 (95%)	0.37	29 (9%)	8	8	63, 104, 278, 413	0
1	I	306/321 (95%)	0.20	20 (6%)	18	18	56, 102, 278, 407	0
1	J	306/321 (95%)	0.14	32 (10%)	6	6	62, 105, 278, 412	0
All	All	3060/3210 (95%)	0.20	228 (7%)	14	13	56, 104, 287, 413	0

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	179	SER	18.6
1	E	289	GLY	16.4
1	H	290	VAL	14.6
1	H	289	GLY	11.4
1	C	152	ILE	11.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.