



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 07:18 am GMT

PDB ID : 3IO1
Title : Crystal Structure of Aminobenzoyl-glutamate utilization protein from *Klebsiella pneumoniae*
Authors : Kumaran, D.; Baumann, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-08-13
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

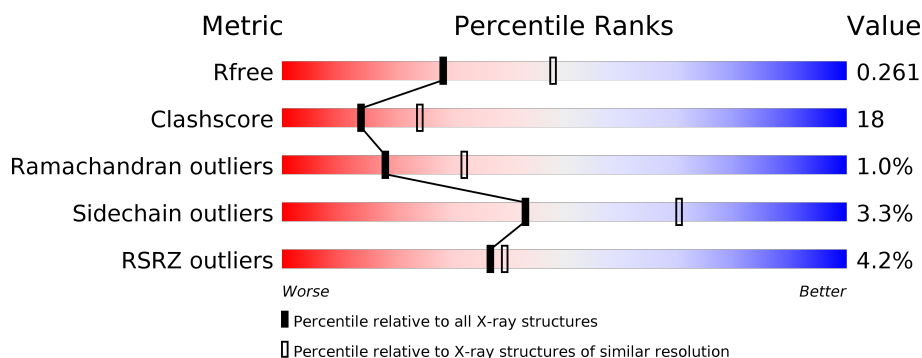
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	445	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	445	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>•</div> <div>12%</div> </div> </div>

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
3	NA	B	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5995 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 Aminobenzoyl-glutamate utilization protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	Se	0	0	0
			2966	1857	537	557	2	13			
1	B	393	Total	C	N	O	S	Se	0	0	0
			2932	1838	531	549	1	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	expression tag	UNP A6T8P4
A	1	SER	-	expression tag	UNP A6T8P4
A	2	LEU	-	expression tag	UNP A6T8P4
A	437	GLU	-	expression tag	UNP A6T8P4
A	438	GLY	-	expression tag	UNP A6T8P4
A	439	HIS	-	expression tag	UNP A6T8P4
A	440	HIS	-	expression tag	UNP A6T8P4
A	441	HIS	-	expression tag	UNP A6T8P4
A	442	HIS	-	expression tag	UNP A6T8P4
A	443	HIS	-	expression tag	UNP A6T8P4
A	444	HIS	-	expression tag	UNP A6T8P4
B	0	MSE	-	expression tag	UNP A6T8P4
B	1	SER	-	expression tag	UNP A6T8P4
B	2	LEU	-	expression tag	UNP A6T8P4
B	437	GLU	-	expression tag	UNP A6T8P4
B	438	GLY	-	expression tag	UNP A6T8P4
B	439	HIS	-	expression tag	UNP A6T8P4
B	440	HIS	-	expression tag	UNP A6T8P4
B	441	HIS	-	expression tag	UNP A6T8P4
B	442	HIS	-	expression tag	UNP A6T8P4
B	443	HIS	-	expression tag	UNP A6T8P4
B	444	HIS	-	expression tag	UNP A6T8P4

- Molecule 2 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Y 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	57	Total O 57 57	0	0

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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 60% 27% 11%
- MSE SER L2 D5 E6 Y7 L8 R9 A12 P13 S14 M15 T16 Q17 W18 R19 R20 D21 F22 H25 A26 E32 F33 R34 S37 A38 L46 G53 M63 E69 T70 R73 E76 R77 A78 R79 E80 Q81 P84 E85 L88 P89 A90 F91 F95 L96 G97 V98 T104 G105 T106 R109 T110 R114 V115 D118 A119 L120 R121 L122 ASN GLU GLN HIS ASP SER HIS ARG PRO HIS ARG ASP HIS PHE ALA SER CYS ASN GLY ALA MSE HIS ALA C148 G149 H150 D151 H162 V163 L164 K165 Q166 M172 G173 A174 I175 L178 F179 Q180 E184 G185 T186 R187 G188 A189 R190 A191 M192 F204 I207 T211 G212 V213 P214 A215 V219 L253 I266 P267 P268 H269 S270 A271 R275 G279 V280 M281 Q282 R287 K297 V298 E299 T300 R301 F312 Q316 R333 M334 M335 G336 S344 P345 V348 D349 Y350 L351 R352 E353 Q354 V358 P359 G360 V361 A364 G365 D366 R367 I368 A369 E375 D376 A377 M380 K381 A391 S392 Y393 M394 I395 F396 G397 T398 E399 L400 SER ALA GLY HIS HIS ASN GLU LYS PHE ASP PHE D412 V415 M416 A417 V418 A419 V420 E421 T422 L423

- Chain B:
-
- | Category | Value |
|----------|-------|
| M381 | 0.005 |
| Y393 | 0.005 |
| M394 | 0.005 |
| F396 | 0.005 |
| GLU | 0.005 |
| LEU | 0.005 |
| SER | 0.005 |
| ALA | 0.005 |
| GLY | 0.005 |
| HIS | 0.005 |
| ASN | 0.005 |
| GLU | 0.005 |
| LYS | 0.005 |
| PHE | 0.005 |
| ASP | 0.005 |
| PHE | 0.005 |
| ASP | 0.005 |
| E413 | 0.005 |
| M416 | 0.005 |
| V420 | 0.005 |
| E421 | 0.005 |
| T422 | 0.005 |
| L423 | 0.005 |
| A424 | 0.005 |
| R425 | 0.005 |
| P431 | 0.005 |
| W432 | 0.005 |
| G433 | 0.005 |
| R434 | 0.005 |
| G435 | 0.005 |
| V436 | 0.005 |
| GLU | 0.005 |
| GLY | 0.005 |
| HIS | 0.005 |
| HIS | 0.005 |
| HIS | 0.005 |
| HIS | 0.005 |
| HIS | 0.005 |
| F235 | 0.005 |
| K245 | 0.005 |
| D248 | 0.005 |
| G249 | 0.005 |
| R250 | 0.005 |
| L253 | 0.005 |
| A257 | 0.005 |
| L261 | 0.005 |
| H269 | 0.005 |
| S270 | 0.005 |
| A271 | 0.005 |
| M281 | 0.005 |
| Q282 | 0.005 |
| A283 | 0.005 |
| G284 | 0.005 |
| A294 | 0.005 |
| L295 | 0.005 |
| L296 | 0.005 |
| K297 | 0.005 |
| V298 | 0.005 |
| E299 | 0.005 |
| T300 | 0.005 |
| N308 | 0.005 |
| R314 | 0.005 |
| L332 | 0.005 |
| R333 | 0.005 |
| M334 | 0.005 |
| M335 | 0.005 |
| S344 | 0.005 |
| V348 | 0.005 |
| D349 | 0.005 |
| E353 | 0.005 |
| P359 | 0.005 |
| G360 | 0.005 |
| V361 | 0.005 |
| Q362 | 0.005 |
| V365 | 0.005 |
| D366 | 0.005 |
| R367 | 0.005 |
| E375 | 0.005 |
| D376 | 0.005 |
| HIS | 0.005 |
| ASP | 0.005 |
| SER | 0.005 |
| L2 | 0.005 |
| Q3 | 0.005 |
| L4 | 0.005 |
| D5 | 0.005 |
| E6 | 0.005 |
| Y7 | 0.005 |
| Q10 | 0.005 |
| L11 | 0.005 |
| A12 | 0.005 |
| P13 | 0.005 |
| S14 | 0.005 |
| M15 | 0.005 |
| R19 | 0.005 |
| R20 | 0.005 |
| G29 | 0.005 |
| W30 | 0.005 |
| S37 | 0.005 |
| L43 | 0.005 |
| L46 | 0.005 |
| S61 | 0.005 |
| E76 | 0.005 |
| R79 | 0.005 |
| E80 | 0.005 |
| P84 | 0.005 |
| L88 | 0.005 |
| P89 | 0.005 |
| V98 | 0.005 |
| T99 | 0.005 |
| A100 | 0.005 |
| T101 | 0.005 |
| L102 | 0.005 |
| R106 | 0.005 |
| R114 | 0.005 |
| V115 | 0.005 |
| D116 | 0.005 |
| M117 | 0.005 |
| D118 | 0.005 |
| A119 | 0.005 |
| L120 | 0.005 |
| D121 | 0.005 |
| L122 | 0.005 |
| ASN | 0.005 |
| GLU | 0.005 |
| D322 | 0.005 |

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	183.39Å 48.52Å 108.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.02 – 2.50 46.53 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.02-2.50) 96.8 (46.53-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.260 0.223 , 0.261	Depositor DCC
R_{free} test set	1667 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5995	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, YT3

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	0.33	0/3010	0.58	0/4063
1	B	0.36	0/2975	0.62	0/4016
All	All	0.35	0/5985	0.60	0/8079

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2966	0	2906	115	0
1	B	2932	0	2882	96	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	37	0	0	1	0
4	B	57	0	0	5	0
All	All	5995	0	5788	206	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 18.

The worst 5 of 206 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:2:LEU:HD22	1:B:6:GLU:CB	1.81	1.11
1:B:2:LEU:HD22	1:B:6:GLU:HB3	1.16	1.10
1:B:2:LEU:CD1	1:B:7:TYR:HA	1.86	1.06
1:B:431:PRO:HB3	1:B:434:ARG:HG3	1.46	0.98
1:B:2:LEU:HD12	1:B:7:TYR:HA	1.43	0.97

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	391/445 (88%)	365 (93%)	22 (6%)	4 (1%)	18	32
1	B	387/445 (87%)	364 (94%)	19 (5%)	4 (1%)	18	32
All	All	778/890 (87%)	729 (94%)	41 (5%)	8 (1%)	18	32

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	B	4	LEU
1	B	359	PRO
1	A	365	VAL
1	B	360	GLY

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	289/313 (92%)	280 (97%)	9 (3%)	45	73
1	B	285/313 (91%)	275 (96%)	10 (4%)	41	68
All	All	574/626 (92%)	555 (97%)	19 (3%)	43	70

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	VAL
1	B	98	VAL
1	B	314	ARG
1	A	412	ASP
1	B	359	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	GLN
1	A	316	GLN
1	B	234	GLN
1	A	308	ASN
1	B	269	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 3 ligands modelled in this entry, 3 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

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	384/445 (86%)	0.53	27 (7%) 17 17	19, 50, 70, 79	0
1	B	380/445 (85%)	-0.04	5 (1%) 77 78	15, 34, 61, 78	0
All	All	764/890 (85%)	0.25	32 (4%) 37 39	15, 41, 69, 79	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	LEU	8.5
1	A	148	CYS	8.1
1	A	120	LEU	5.2
1	A	121	ASP	4.6
1	A	26	ALA	4.5

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	B	502	1/1	0.94	0.21	2.13	49,49,49,49	0
3	NA	A	501	1/1	0.92	0.36	1.70	49,49,49,49	0
2	YT3	A	500	1/1	0.96	0.10	-	84,84,84,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.