



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:07 AM UTC

PDB ID : 2REJ / pdb_00002rej
Title : ABC-transporter choline binding protein in unliganded semi-closed conformation
Authors : Oswald, C.; Smits, S.H.J.; Hoeing, M.; Sohn-Boeser, L.; Le Rudulier, D.; Schmitt, L.; Bremer, E.
Deposited on : 2007-09-26
Resolution : 2.60 Å(reported)

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

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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

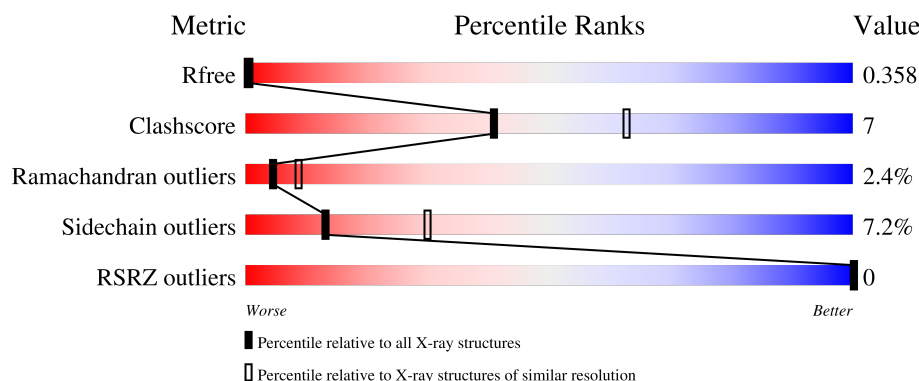
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	298	
1	B	298	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4352 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 PUTATIVE GLYCINE BETAINES ABC TRANSPORTER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2176	1371	357	439	9			
1	B	288	Total	C	N	O	S	0	0	0
			2176	1371	357	439	9			

There are 16 discrepancies between the modelled and reference sequences:

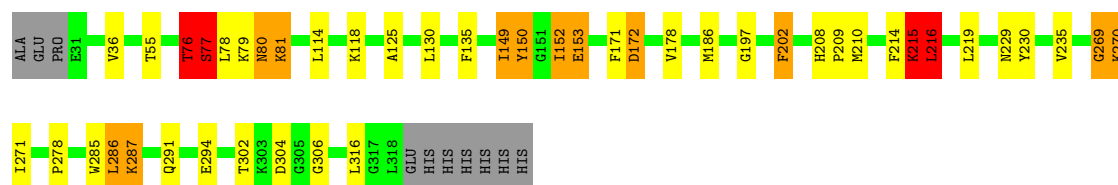
Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ASP	GLY	engineered mutation	UNP Q92N37
A	319	GLU	-	expression tag	UNP Q92N37
A	320	HIS	-	expression tag	UNP Q92N37
A	321	HIS	-	expression tag	UNP Q92N37
A	322	HIS	-	expression tag	UNP Q92N37
A	323	HIS	-	expression tag	UNP Q92N37
A	324	HIS	-	expression tag	UNP Q92N37
A	325	HIS	-	expression tag	UNP Q92N37
B	251	ASP	GLY	engineered mutation	UNP Q92N37
B	319	GLU	-	expression tag	UNP Q92N37
B	320	HIS	-	expression tag	UNP Q92N37
B	321	HIS	-	expression tag	UNP Q92N37
B	322	HIS	-	expression tag	UNP Q92N37
B	323	HIS	-	expression tag	UNP Q92N37
B	324	HIS	-	expression tag	UNP Q92N37
B	325	HIS	-	expression tag	UNP Q92N37

3 Residue-property plots [i](#)

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.

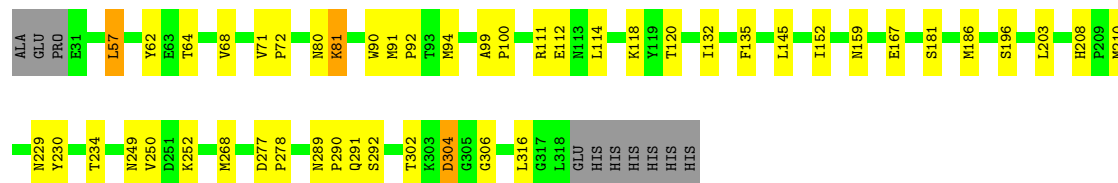
• Molecule 1: PUTATIVE GLYCINE BETAIN E ABC TRANSPORTER PROTEIN

Chain A: 



• Molecule 1: PUTATIVE GLYCINE BETAIN E ABC TRANSPORTER PROTEIN

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	34.10Å 232.50Å 47.30Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.60) 98.2 (20.00-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.296 , 0.359 0.297 , 0.358	Depositor DCC
R_{free} test set	1158 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.318 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4352	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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

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	0.68	1/2217 (0.0%)	1.11	17/3009 (0.6%)
1	B	0.63	0/2217	0.96	1/3009 (0.0%)
All	All	0.66	1/4434 (0.0%)	1.04	18/6018 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	PHE	CA-C	5.16	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	THR	N-CA-C	8.12	121.72	111.24
1	A	286	LEU	N-CA-C	7.83	123.09	112.68
1	A	214	PHE	N-CA-C	7.37	120.64	108.48
1	A	286	LEU	CA-C-N	6.61	133.60	121.70
1	A	286	LEU	C-N-CA	6.61	133.60	121.70
1	A	80	ASN	N-CA-C	6.46	121.36	112.90
1	A	76	THR	CA-C-N	6.36	133.14	121.70
1	A	76	THR	C-N-CA	6.36	133.14	121.70
1	A	149	ILE	N-CA-C	-6.07	100.34	108.35
1	A	215	LYS	CA-C-N	5.92	132.35	121.70
1	A	215	LYS	C-N-CA	5.92	132.35	121.70
1	A	202	PHE	N-CA-C	5.60	115.51	108.45
1	A	149	ILE	CA-C-N	5.57	131.73	121.70
1	A	149	ILE	C-N-CA	5.57	131.73	121.70
1	A	214	PHE	CA-C-N	5.21	131.08	121.70
1	A	214	PHE	C-N-CA	5.21	131.08	121.70
1	A	125	ALA	N-CA-C	5.08	116.50	111.07
1	B	120	THR	N-CA-C	5.02	114.46	107.73

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	2176	0	2122	35	0
1	B	2176	0	2122	21	0
All	All	4352	0	4244	56	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 7.

All (56) 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:A:269:GLY:HA3	1:A:270:LYS:CB	1.75	1.14
1:A:269:GLY:HA3	1:A:270:LYS:HB2	1.17	1.08
1:A:149:ILE:HA	1:A:150:TYR:HB2	1.39	1.02
1:A:208:HIS:HD2	1:A:210:MET:HB2	1.31	0.94
1:A:215:LYS:CB	1:A:216:LEU:HB2	1.99	0.93
1:B:111:ARG:HG2	1:B:112:GLU:H	1.44	0.82
1:A:215:LYS:HB2	1:A:216:LEU:HB2	1.61	0.82
1:A:215:LYS:CA	1:A:216:LEU:HB2	2.14	0.76
1:B:302:THR:HG22	1:B:306:GLY:H	1.54	0.73
1:B:111:ARG:HG2	1:B:112:GLU:N	2.04	0.72
1:A:302:THR:HG22	1:A:306:GLY:H	1.54	0.71
1:A:149:ILE:O	1:A:178:VAL:HA	1.94	0.68
1:B:208:HIS:HD2	1:B:210:MET:HB2	1.58	0.68
1:A:269:GLY:CA	1:A:270:LYS:CB	2.61	0.67
1:A:269:GLY:CA	1:A:270:LYS:HB2	2.10	0.67
1:B:57:LEU:HD23	1:B:62:TYR:HB2	1.78	0.65
1:A:80:ASN:N	1:A:81:LYS:HA	2.10	0.65
1:A:208:HIS:CD2	1:A:210:MET:HB2	2.23	0.63
1:A:171:PHE:N	1:A:172:ASP:HA	2.14	0.63
1:A:229:ASN:O	1:A:230:TYR:HB2	1.97	0.62
1:A:269:GLY:HA3	1:A:270:LYS:HB3	1.77	0.62
1:A:186:MET:HE2	1:A:202:PHE:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:TRP:O	1:B:94:MET:HB2	1.99	0.62
1:A:149:ILE:CA	1:A:150:TYR:HB2	2.23	0.61
1:A:76:THR:CA	1:A:77:SER:HB2	2.30	0.60
1:A:215:LYS:HB2	1:A:216:LEU:CB	2.31	0.60
1:B:291:GLN:HG2	1:B:292:SER:HA	1.83	0.59
1:B:111:ARG:CG	1:B:112:GLU:H	2.15	0.59
1:B:80:ASN:O	1:B:81:LYS:HB2	2.02	0.58
1:B:208:HIS:CD2	1:B:210:MET:HB2	2.39	0.56
1:B:91:MET:HB3	1:B:92:PRO:HA	1.88	0.54
1:A:76:THR:CB	1:A:77:SER:HB2	2.39	0.53
1:A:215:LYS:HA	1:A:216:LEU:HB2	1.90	0.52
1:A:286:LEU:H	1:A:287:LYS:HB3	1.73	0.52
1:A:271:ILE:HD11	1:A:278:PRO:HG3	1.91	0.51
1:A:149:ILE:HA	1:A:150:TYR:CB	2.28	0.51
1:B:71:VAL:HB	1:B:72:PRO:HD3	1.92	0.51
1:A:118:LYS:HE3	1:A:230:TYR:HB3	1.92	0.49
1:A:152:ILE:HG23	1:A:153:GLU:N	2.27	0.49
1:A:152:ILE:HG23	1:A:153:GLU:H	1.78	0.48
1:B:229:ASN:O	1:B:230:TYR:HB2	2.13	0.48
1:B:152:ILE:H	1:B:159:ASN:HD21	1.62	0.47
1:B:289:ASN:C	1:B:291:GLN:H	2.23	0.46
1:A:76:THR:N	1:A:77:SER:HB2	2.30	0.46
1:A:76:THR:O	1:A:79:LYS:HB3	2.17	0.44
1:A:76:THR:H	1:A:77:SER:HB2	1.83	0.44
1:A:76:THR:H	1:A:77:SER:CB	2.31	0.43
1:B:186:MET:HE1	1:B:203:LEU:HB2	2.00	0.43
1:B:99:ALA:HB3	1:B:100:PRO:HD3	2.01	0.43
1:A:208:HIS:CD2	1:A:210:MET:H	2.37	0.43
1:A:76:THR:N	1:A:77:SER:CB	2.82	0.42
1:A:80:ASN:H	1:A:81:LYS:HA	1.79	0.42
1:B:302:THR:HG23	1:B:304:ASP:H	1.85	0.42
1:B:249:ASN:O	1:B:252:LYS:HB3	2.20	0.42
1:B:277:ASP:HA	1:B:278:PRO:HD3	1.96	0.41
1:B:302:THR:HG22	1:B:306:GLY:N	2.31	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	286/298 (96%)	245 (86%)	31 (11%)	10 (4%)	3	4
1	B	286/298 (96%)	263 (92%)	19 (7%)	4 (1%)	9	19
All	All	572/596 (96%)	508 (89%)	50 (9%)	14 (2%)	4	9

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	150	TYR
1	A	216	LEU
1	B	81	LYS
1	A	269	GLY
1	A	270	LYS
1	A	285	TRP
1	A	291	GLN
1	A	287	LYS
1	B	181	SER
1	B	196	SER
1	A	209	PRO
1	A	197	GLY
1	B	290	PRO

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	230/240 (96%)	211 (92%)	19 (8%)	10	23
1	B	230/240 (96%)	216 (94%)	14 (6%)	17	37
All	All	460/480 (96%)	427 (93%)	33 (7%)	13	30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	55	THR
1	A	76	THR
1	A	77	SER
1	A	78	LEU
1	A	81	LYS
1	A	114	LEU
1	A	130	LEU
1	A	135	PHE
1	A	152	ILE
1	A	153	GLU
1	A	172	ASP
1	A	215	LYS
1	A	216	LEU
1	A	219	LEU
1	A	235	VAL
1	A	294	GLU
1	A	304	ASP
1	A	316	LEU
1	B	57	LEU
1	B	64	THR
1	B	68	VAL
1	B	114	LEU
1	B	118	LYS
1	B	132	ILE
1	B	135	PHE
1	B	145	LEU
1	B	167	GLU
1	B	234	THR
1	B	250	VAL
1	B	268	MET
1	B	304	ASP
1	B	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	159	ASN
1	A	208	HIS
1	A	273	ASN
1	B	159	ASN
1	B	184	GLN
1	B	189	GLN
1	B	208	HIS
1	B	238	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 [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	288/298 (96%)	-1.58	0 100 100	21, 30, 40, 43	0
1	B	288/298 (96%)	-1.57	0 100 100	21, 32, 40, 44	0
All	All	576/596 (96%)	-1.58	0 100 100	21, 31, 40, 44	0

There are no RSRZ outliers to report.

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 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.