



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:46 AM UTC

PDB ID : 1ISS / pdb_00001iss
Title : Crystal Structure of Metabotropic Glutamate Receptor Subtype 1 Complexed with an antagonist
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Deposited on : 2001-12-21
Resolution : 3.30 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

<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
Mogul : 2022.3.0, CSD as543be (2022)
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

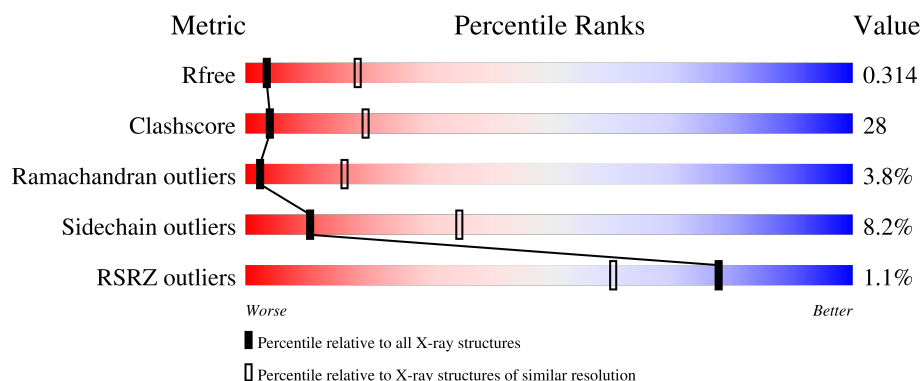
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	490	
1	B	490	

2 Entry composition [i](#)

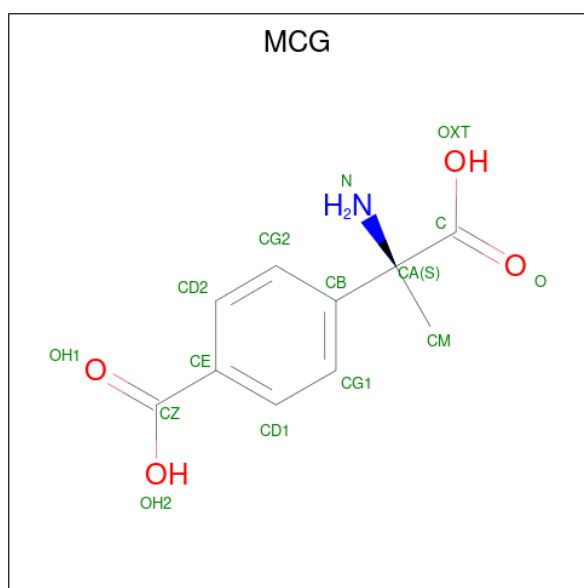
There are 2 unique types of molecules in this entry. The entry contains 7124 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Metabotropic Glutamate Receptor subtype 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3547	2250	613	664	20			
1	B	452	Total	C	N	O	S	0	0	0
			3547	2250	613	664	20			

- Molecule 2 is (S)--(ALPHA)-METHYL-4-CARBOXYPHENYLGLYCINE (CCD ID: MCG) (formula: $C_{10}H_{11}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		

ASN	K443	S449	S263	I190
LYS	P444	F350	N264	D191
SER	I445		A265	L192
GLY	D446	R358		S193
MET	G447	L359	F270	D194
VAL	R448	D360	L273	K195
ARG	K449	T361		T196
SER	L450	N362	L277	L197
	L451	T363	R278	Y200
	F453	R364	E279	F201
	L454	N365	R280	L202
	I455	P366	L281	R203
	K456	V367	P282	V204
	S457	F368	K283	V205
	S458	P369	A284	P206
	F459	E370	R285	S207
	V460	F371	V286	D208
	G461	V372	V287	T209
	V462	Q373	V288	L210
	S463	H374	C289	Q211
	G464	R375	F290	
	E465	F376		M215
	E466	Q377	R304	L216
	V467	C378	K305	D217
			L306	I218
	D470	H383	G307	V219
	E471	L384	V308	
	K472	E386	E311	N223
	G473	N387		V224
	D474	P388	G316	T225
	A475	H389	S317	Y226
	P476	F390	D318	V227
	G477		G319	S228
	R478	Y404	W320	A229
	Y479		A321	V230
	D480	M410	D322	H231
	I481	G411	R323	T232
	M482	F412	D324	
		V413		G240
		I414	I327	M241
	E488		E328	D242
	A489	I417	G329	A243
	N490	Y418	Y330	F244
	R491	A419	E331	K245
	Y492	M420	V332	E246
	D493		E333	L247
	Y494	G423	A334	A248
		L424	H335	
		Q425	T339	E251
	V497	M426	I340	C254
	G498	N427	K341	T255
	T499		L342	A256
	W500		Q343	H257
	H501	L431		S258
	E502	V436		D259
				K260
	L505			T261
				Y262
	I512			
	GLN			
	MET			

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.14Å 112.14Å 289.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	91.1 (20.00-3.30) 96.8 (20.00-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.29Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.257 , 0.314 0.266 , 0.314	Depositor DCC
R_{free} test set	2224 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7124	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: MCG

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	0.57	0/3627	1.04	23/4913 (0.5%)
1	B	0.59	0/3627	1.02	16/4913 (0.3%)
All	All	0.58	0/7254	1.03	39/9826 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	THR	N-CA-C	-7.24	102.19	111.02
1	A	96	LEU	CA-C-N	7.09	128.70	119.84
1	A	96	LEU	C-N-CA	7.09	128.70	119.84
1	A	340	ILE	CB-CA-C	-6.37	102.18	110.84
1	B	321	ALA	CB-CA-C	-6.33	109.25	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	TYR	Sidechain

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	3547	0	3421	199	0
1	B	3547	0	3421	199	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
All	All	7124	0	6860	392	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 28.

The worst 5 of 392 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:39:ALA:HB3	1:B:105:ILE:HB	1.44	0.97
1:A:41:MET:HE1	1:A:364:ARG:HH11	1.35	0.92
1:A:41:MET:HE1	1:A:364:ARG:NH1	1.86	0.91
1:A:123:ILE:HD12	1:A:178:PHE:CE1	2.09	0.88
1:B:368:PHE:HB3	1:B:369:PRO:HD3	1.57	0.86

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	448/490 (91%)	352 (79%)	79 (18%)	17 (4%)	2	16
1	B	448/490 (91%)	353 (79%)	78 (17%)	17 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	896/980 (91%)	705 (79%)	157 (18%)	34 (4%)	2 16

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	B	223	ASN
1	B	256	ALA
1	B	331	GLU
1	B	489	ALA

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	376/422 (89%)	349 (93%)	27 (7%)	13 40
1	B	376/422 (89%)	341 (91%)	35 (9%)	8 30
All	All	752/844 (89%)	690 (92%)	62 (8%)	10 35

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	B	436	VAL
1	B	197	LEU
1	B	410	MET
1	B	488	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	ASN
1	B	231	HIS
1	B	483	ASN

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Mol	Chain	Res	Type
1	B	211	GLN
1	B	250	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MCG	A	1001	-	14,15,15	1.45	1 (7%)	16,22,22	0.82	0
2	MCG	B	2001	-	14,15,15	1.52	2 (14%)	16,22,22	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MCG	A	1001	-	-	6/15/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MCG	B	2001	-	-	7/15/16/16	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	MCG	CA-CB	-3.11	1.50	1.53
2	A	1001	MCG	CE-CZ	-2.44	1.44	1.49
2	B	2001	MCG	CE-CZ	-2.14	1.44	1.49

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MCG	CD2-CE-CZ-OH1
2	B	2001	MCG	CD2-CE-CZ-OH1
2	A	1001	MCG	CD1-CE-CZ-OH1
2	B	2001	MCG	CD1-CE-CZ-OH1
2	B	2001	MCG	CD1-CE-CZ-OH2

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 [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	452/490 (92%)	-0.15	4 (0%)	81 65	10, 65, 119, 164	0
1	B	452/490 (92%)	-0.09	6 (1%)	75 56	14, 67, 123, 162	0
All	All	904/980 (92%)	-0.12	10 (1%)	78 60	10, 66, 120, 164	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	ASN	4.3
1	B	224	TRP	2.8
1	B	385	LEU	2.6
1	A	381	PRO	2.5
1	B	389	ASN	2.4

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](#)

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
2	MCG	B	2001	15/15	0.90	0.09	56,70,75,76	0
2	MCG	A	1001	15/15	0.95	0.08	50,59,67,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.