



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:08 PM GMT

PDB ID : 5CGD
Title : Structure of the human class C GPCR metabotropic glutamate receptor 5 transmembrane domain in complex with the negative allosteric modulator 3-chloro-5-[6-(5-fluoropyridin-2-yl)pyrimidin-4-yl]benzonitrile - (HTL14242)
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Deposited on : 2015-07-09
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

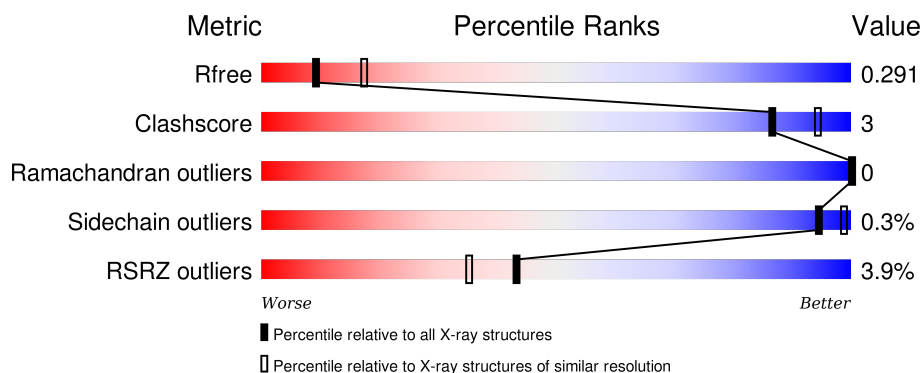
1 Overall quality at a glance

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 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	444	

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
2	OLA	A	4001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLA	A	4002	-	-	-	X
2	OLA	A	4003	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3345 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.

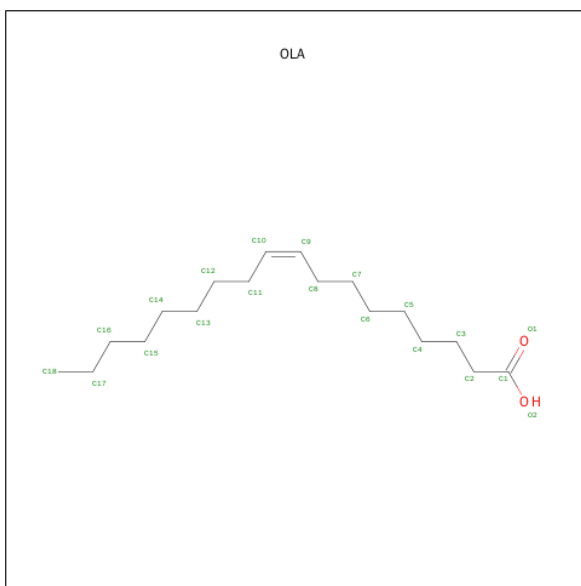
- Molecule 1 is a protein called Metabotropic glutamate receptor 5,Endolysin,Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3196	2088	530	554	24			

There are 26 discrepancies between the modelled and reference sequences:

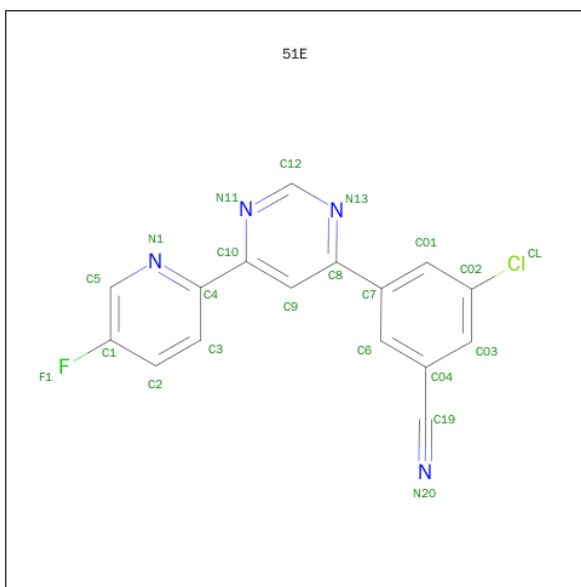
Chain	Residue	Modelled	Actual	Comment	Reference
A	566	ALA	-	expression tag	UNP P41594
A	567	ALA	-	expression tag	UNP P41594
A	568	SER	-	expression tag	UNP P41594
A	579	ALA	GLU	engineered mutation	UNP P41594
A	667	TYR	ASN	engineered mutation	UNP P41594
A	669	ALA	ILE	engineered mutation	UNP P41594
A	675	MET	GLY	engineered mutation	UNP P41594
A	1012	GLY	ARG	engineered mutation	UNP P00720
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	1137	ARG	ILE	engineered mutation	UNP P00720
A	742	ALA	THR	engineered mutation	UNP P41594
A	753	ALA	SER	engineered mutation	UNP P41594
A	837	ALA	-	expression tag	UNP P41594
A	838	ALA	-	expression tag	UNP P41594
A	839	ALA	-	expression tag	UNP P41594
A	840	HIS	-	expression tag	UNP P41594
A	841	HIS	-	expression tag	UNP P41594
A	842	HIS	-	expression tag	UNP P41594
A	843	HIS	-	expression tag	UNP P41594
A	844	HIS	-	expression tag	UNP P41594
A	845	HIS	-	expression tag	UNP P41594
A	846	HIS	-	expression tag	UNP P41594
A	847	HIS	-	expression tag	UNP P41594
A	848	HIS	-	expression tag	UNP P41594
A	849	HIS	-	expression tag	UNP P41594

- Molecule 2 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C	O	0	0
			15	13	2		
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C	O	0	0
			13	11	2		

- Molecule 3 is 3-chloro-5-[6-(5-fluoropyridin-2-yl)pyrimidin-4-yl]benzonitrile (three-letter code: 51E) (formula: $C_{16}H_8ClFN_4$).



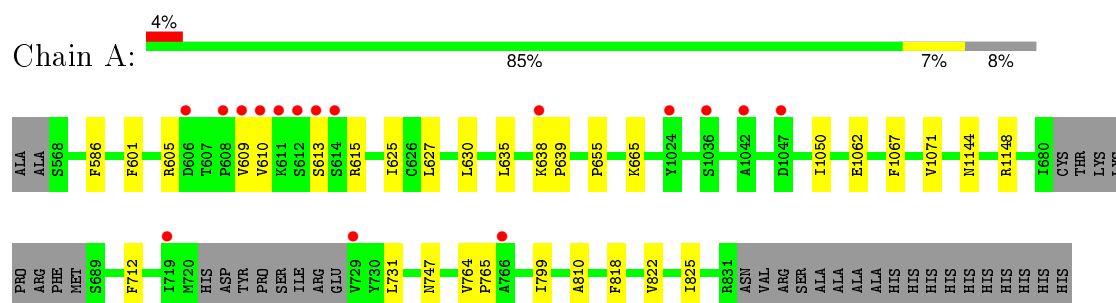
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	0	0
			22	16	1	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		

i

- Molecule 1: Metabotropic glutamate receptor 5,Endolysin,Metabotropic glutamate receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.57Å 43.73Å 81.86Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	29.75 – 2.60 34.51 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.75-2.60) 94.6 (34.51-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.242 , 0.285 0.245 , 0.291	Depositor DCC
R_{free} test set	702 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14891 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3345	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OLA, 51E

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	0.22	0/3261	0.38	0/4424

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	3196	0	3331	17	0
2	A	62	0	87	2	0
3	A	22	0	8	1	0
4	A	65	0	0	2	0
All	All	3345	0	3426	18	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 3.

All (18) 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:613:SER:OG	1:A:665:LYS:NZ	2.37	0.58
1:A:639:PRO:HA	1:A:731:LEU:HD13	1.87	0.55
1:A:627:LEU:HD23	1:A:630:LEU:HD12	1.90	0.52
1:A:638:LYS:NZ	4:A:4108:HOH:O	2.43	0.51
1:A:1144:ASN:OD1	1:A:1148:ARG:NH1	2.38	0.47
1:A:655:PRO:HG3	3:A:4005:51E:C9	2.44	0.47
1:A:625:ILE:HG23	1:A:810:ALA:HB1	1.96	0.47
2:A:4001:OLA:H182	2:A:4001:OLA:H151	1.84	0.45
1:A:747:ASN:ND2	4:A:4110:HOH:O	2.48	0.45
1:A:635:LEU:HB3	1:A:799:ILE:HG23	1.99	0.44
1:A:1050:ILE:HD12	1:A:1062:GLU:HB3	1.99	0.44
1:A:764:VAL:HA	1:A:765:PRO:HD3	1.84	0.44
1:A:605:ARG:HD3	1:A:615:ARG:NH1	2.35	0.42
1:A:822:VAL:O	1:A:825:ILE:HG22	2.20	0.41
1:A:1067:PHE:O	1:A:1071:VAL:HG23	2.20	0.41
1:A:601:PHE:HE1	1:A:818:PHE:HD1	1.68	0.41
1:A:609:VAL:HG13	1:A:610:VAL:HG23	2.03	0.41
1:A:712:PHE:HB3	2:A:4003:OLA:H21	2.02	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	402/444 (90%)	394 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	343/373 (92%)	342 (100%)	1 (0%)	94	99

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	586	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

5 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	OLA	A	4001	-	16,19,19	0.12	0	16,19,19	0.67	0
2	OLA	A	4002	-	11,14,19	0.13	0	10,14,19	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLA	A	4003	-	10,13,19	0.22	0	10,13,19	0.65	0
2	OLA	A	4004	-	9,12,19	0.19	0	9,12,19	0.67	0
3	51E	A	4005	-	23,24,24	0.90	1 (4%)	32,33,33	1.12	2 (6%)

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	OLA	A	4001	-	-	0/15/17/17	0/0/0/0
2	OLA	A	4002	-	-	0/10/12/17	0/0/0/0
2	OLA	A	4003	-	-	0/9/11/17	0/0/0/0
2	OLA	A	4004	-	-	0/8/10/17	0/0/0/0
3	51E	A	4005	-	-	0/10/10/10	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4005	51E	C2-C1	2.03	1.41	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4005	51E	C2-C1-C5	-3.92	118.31	123.32
3	A	4005	51E	C7-C01-C02	2.04	121.12	118.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	OLA	1	0
2	A	4003	OLA	1	0
3	A	4005	51E	1	0

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	408/444 (91%)	0.19	16 (3%) 43 35	23, 34, 55, 77	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	612	SER	6.7
1	A	613	SER	6.1
1	A	609	VAL	4.7
1	A	610	VAL	4.4
1	A	606	ASP	3.5
1	A	1036	SER	3.2
1	A	638	LYS	2.9
1	A	614	SER	2.5
1	A	729	VAL	2.4
1	A	611	LYS	2.4
1	A	1024	TYR	2.4
1	A	1042	ALA	2.3
1	A	766	ALA	2.2
1	A	719	ILE	2.2
1	A	608	PRO	2.1
1	A	1047	ASP	2.0

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](#)

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(Å ²)	Q<0.9
2	OLA	A	4002	15/20	0.76	0.36	7.25	48,56,59,63	0
2	OLA	A	4001	20/20	0.88	0.29	4.20	29,38,49,52	0
2	OLA	A	4003	14/20	0.79	0.36	2.14	37,48,58,61	0
2	OLA	A	4004	13/20	0.75	0.40	1.52	49,58,65,65	0
3	51E	A	4005	22/22	0.95	0.20	0.52	19,24,26,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.