



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:06 PM UTC

PDB ID : 1FTJ / pdb_00001ftj
Title : CRYSTAL STRUCTURE OF THE GLUR2 LIGAND BINDING CORE (S1S2J) IN COMPLEX WITH GLUTAMATE AT 1.9 RESOLUTION
Authors : Armstrong, N.; Gouaux, E.
Deposited on : 2000-09-12
Resolution : 1.90 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

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

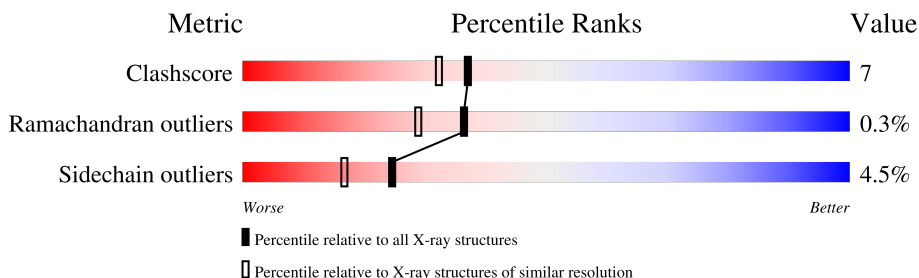
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	263	
1	B	263	
1	C	263	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6190 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 GLUTAMATE RECEPTOR SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1962	1252	326	370	14			
1	B	259	Total	C	N	O	S	0	0	0
			1985	1264	331	376	14			
1	C	258	Total	C	N	O	S	0	0	0
			1941	1239	323	366	13			

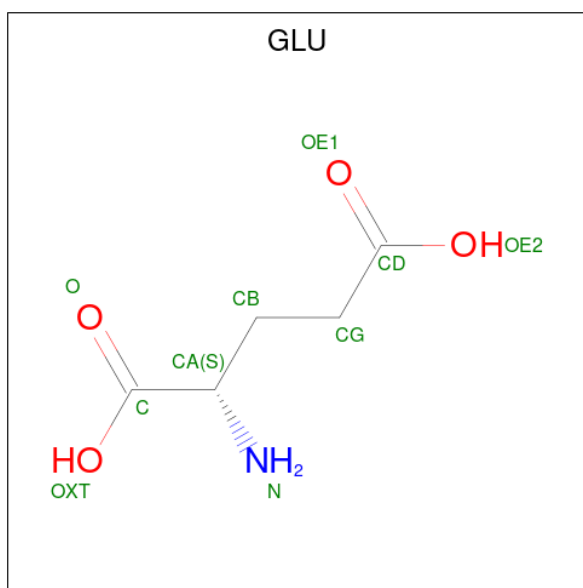
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P19491
A	2	ALA	-	cloning artifact	UNP P19491
B	1	GLY	-	cloning artifact	UNP P19491
B	2	ALA	-	cloning artifact	UNP P19491
C	1	GLY	-	cloning artifact	UNP P19491
C	2	ALA	-	cloning artifact	UNP P19491
A	118	GLY	-	linker	UNP P19491
A	119	THR	-	linker	UNP P19491
B	118	GLY	-	linker	UNP P19491
B	119	THR	-	linker	UNP P19491
C	118	GLY	-	linker	UNP P19491
C	119	THR	-	linker	UNP P19491

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	110	Total	O	0	0
			110	110		
4	C	63	Total	O	0	0
			63	63		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.00Å 163.36Å 47.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.90)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.226 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6190	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.67	0/1998	1.03	7/2689 (0.3%)
1	B	0.64	0/2021	1.02	5/2719 (0.2%)
1	C	0.63	0/1977	1.03	3/2660 (0.1%)
All	All	0.65	0/5996	1.03	15/8068 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	LYS	CA-C-N	-7.28	113.26	123.08
1	C	117	LYS	C-N-CA	-7.28	113.26	123.08
1	A	153	ALA	N-CA-C	6.25	118.61	111.11
1	A	105	PRO	N-CA-C	5.81	120.21	111.14
1	A	88	ALA	N-CA-C	5.81	113.24	108.07
1	B	32	TYR	N-CA-C	5.73	119.40	110.17
1	A	184	SER	N-CA-C	5.68	119.84	113.02
1	B	57	GLY	N-CA-C	5.42	119.45	112.83
1	B	116	LYS	N-CA-C	-5.32	102.41	110.28
1	A	104	LYS	N-CA-C	-5.30	102.33	110.01
1	A	150	SER	N-CA-C	5.17	117.72	109.96
1	A	103	SER	N-CA-C	-5.10	103.95	110.53
1	C	182	ARG	N-CA-C	5.06	116.79	111.28
1	B	120	PRO	CA-N-CD	-5.03	104.96	112.00
1	B	139	ASP	N-CA-C	5.01	117.64	111.82

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	1962	0	1952	26	0
1	B	1985	0	1990	35	0
1	C	1941	0	1925	21	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
3	C	10	0	5	0	0
4	A	94	0	0	2	0
4	B	110	0	0	3	0
4	C	63	0	0	1	0
All	All	6190	0	5882	82	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 (82) 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:65:ASP:HB3	1:A:68:THR:HG22	1.54	0.86
1:A:179:ALA:O	1:A:183:LYS:HD3	1.81	0.81
1:B:100:ILE:HD12	1:B:223:ALA:HB1	1.63	0.80
1:B:118:GLY:O	1:B:120:PRO:HD3	1.86	0.75
1:C:180:ARG:HA	1:C:183:LYS:HE2	1.71	0.73
1:A:160:THR:HA	1:A:163:ARG:NH1	2.04	0.72
1:B:241:LEU:HD22	1:B:246:LEU:HD22	1.72	0.72
1:B:240:LYS:O	1:B:244:GLN:HG2	1.92	0.70
1:B:130:GLN:HG3	4:B:340:HOH:O	1.92	0.69
1:B:179:ALA:O	1:B:183:LYS:HE2	1.92	0.68
1:B:117:LYS:HG2	1:B:209:MET:HE2	1.76	0.67
1:C:241:LEU:HD22	1:C:246:LEU:HD22	1.80	0.63
1:A:66:ALA:O	1:A:69:LYS:HE3	2.01	0.60
1:C:64:ARG:HH11	1:C:64:ARG:HB3	1.67	0.59
1:B:120:PRO:C	1:B:121:ILE:HD12	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:O	1:A:244:GLN:HG2	2.04	0.58
1:C:137:THR:HG22	1:C:191:LEU:HB2	1.85	0.57
1:B:130:GLN:HG2	1:B:131:THR:N	2.19	0.56
1:B:121:ILE:CD1	1:B:133:ILE:HD12	2.36	0.56
1:A:68:THR:CG2	1:A:70:ILE:H	2.18	0.55
1:A:230:LEU:O	1:A:234:VAL:HG13	2.06	0.55
1:A:196:MET:HE1	1:A:220:TYR:OH	2.08	0.54
1:B:100:ILE:HD12	1:B:223:ALA:CB	2.36	0.53
1:A:68:THR:HG23	1:A:70:ILE:H	1.73	0.53
1:C:199:TYR:CZ	1:C:203:ARG:HD2	2.44	0.53
1:A:8:VAL:HG22	1:A:85:ILE:CG2	2.39	0.53
1:C:218:LYS:HE3	4:C:338:HOH:O	2.09	0.53
1:C:100:ILE:HD12	1:C:223:ALA:HB1	1.90	0.52
1:C:116:LYS:O	1:C:117:LYS:C	2.53	0.52
1:B:206:CYS:CB	1:B:261:CYS:SG	2.98	0.51
1:C:39:LEU:O	1:C:43:ILE:HG23	2.11	0.51
1:A:25:MET:HG2	4:A:287:HOH:O	2.12	0.49
1:A:184:SER:HB2	4:A:350:HOH:O	2.12	0.49
1:C:118:GLY:O	1:C:120:PRO:HD3	2.13	0.49
1:A:65:ASP:HB3	1:A:68:THR:CG2	2.36	0.49
1:C:134:ALA:O	1:C:188:TYR:HA	2.13	0.48
1:B:120:PRO:O	1:B:121:ILE:HD12	2.14	0.48
1:B:54:THR:CG2	4:B:311:HOH:O	2.62	0.47
1:B:125:GLU:HG2	1:B:129:LYS:HZ2	1.79	0.47
1:B:125:GLU:O	1:B:129:LYS:HG3	2.14	0.47
1:A:166:GLU:HA	1:A:167:PRO:C	2.40	0.47
1:C:120:PRO:O	1:C:121:ILE:HD13	2.15	0.47
1:B:253:LYS:O	1:B:258:LYS:HG2	2.14	0.47
1:B:119:THR:HG23	1:B:133:ILE:HD13	1.97	0.46
1:B:23:HIS:CD2	1:B:26:LEU:HD13	2.51	0.46
1:B:109:LEU:C	1:B:109:LEU:HD22	2.40	0.46
1:A:91:THR:HG21	1:A:218:LYS:HD2	1.96	0.46
1:A:87:ILE:HG12	1:A:222:ILE:HD12	1.98	0.45
1:A:65:ASP:OD1	1:A:67:ASP:N	2.49	0.45
1:B:8:VAL:O	1:B:54:THR:HG22	2.16	0.45
1:B:117:LYS:HE3	1:B:206:CYS:O	2.16	0.45
1:C:109:LEU:HD22	1:C:109:LEU:C	2.41	0.45
1:B:64:ARG:NH1	1:B:69:LYS:HD2	2.32	0.45
1:C:15:PRO:HB3	1:C:199:TYR:CE1	2.52	0.44
1:C:174:THR:O	1:C:178:VAL:HG23	2.17	0.44
1:B:171:VAL:HG11	1:B:177:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD23	1:A:17:VAL:HG12	1.99	0.44
1:B:54:THR:HG23	4:B:311:HOH:O	2.18	0.44
1:A:194:SER:O	1:A:198:GLU:HG3	2.18	0.43
1:C:12:LEU:HD23	1:C:17:VAL:HG12	2.00	0.43
1:A:109:LEU:HD13	1:A:109:LEU:N	2.33	0.43
1:B:119:THR:HA	1:B:120:PRO:HD2	1.94	0.43
1:B:35:TYR:CZ	1:B:107:MET:HE2	2.54	0.43
1:B:251:LYS:O	1:B:255:TRP:HB2	2.19	0.43
1:C:187:LYS:HA	1:C:187:LYS:HD3	1.83	0.43
1:B:23:HIS:HA	1:B:26:LEU:HD12	2.01	0.42
1:B:109:LEU:HD13	1:B:109:LEU:N	2.35	0.42
1:C:105:PRO:HA	1:C:220:TYR:O	2.19	0.42
1:C:146:PHE:O	1:C:150:SER:HB2	2.20	0.42
1:A:91:THR:CG2	1:A:218:LYS:HD2	2.50	0.42
1:B:105:PRO:HA	1:B:220:TYR:O	2.20	0.42
1:A:160:THR:HA	1:A:163:ARG:HH11	1.82	0.41
1:B:42:GLU:HG3	1:B:246:LEU:HD21	2.03	0.41
1:C:199:TYR:OH	1:C:203:ARG:HD2	2.20	0.41
1:A:15:PRO:HB3	1:A:199:TYR:CE1	2.55	0.41
1:B:121:ILE:HD13	1:B:133:ILE:HD12	2.02	0.41
1:A:109:LEU:HB3	1:A:195:THR:HG23	2.02	0.41
1:B:249:LYS:HB2	1:B:249:LYS:HE3	1.47	0.41
1:C:136:GLY:HA3	1:C:169:VAL:O	2.21	0.41
1:A:209:MET:HE2	1:A:211:VAL:CG1	2.51	0.40
1:A:136:GLY:HA3	1:A:169:VAL:O	2.21	0.40
1:B:97:GLU:HG2	1:B:102:PHE:HD2	1.86	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	256/263 (97%)	252 (98%)	4 (2%)	0	100	100
1	B	257/263 (98%)	249 (97%)	7 (3%)	1 (0%)	30	22
1	C	256/263 (97%)	249 (97%)	6 (2%)	1 (0%)	30	22
All	All	769/789 (98%)	750 (98%)	17 (2%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	120	PRO
1	B	120	PRO

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	204/219 (93%)	194 (95%)	10 (5%)	22	14
1	B	210/219 (96%)	201 (96%)	9 (4%)	26	18
1	C	201/219 (92%)	192 (96%)	9 (4%)	24	17
All	All	615/657 (94%)	587 (95%)	28 (5%)	24	16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	MET
1	A	25	MET
1	A	27	GLU
1	A	68	THR
1	A	78	LEU
1	A	109	LEU
1	A	196	MET
1	A	210	LYS
1	A	234	VAL
1	A	250	LEU
1	B	26	LEU

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Mol	Chain	Res	Type
1	B	30	GLU
1	B	54	THR
1	B	78	LEU
1	B	109	LEU
1	B	121	ILE
1	B	130	GLN
1	B	172	ARG
1	B	209	MET
1	C	43	ILE
1	C	64	ARG
1	C	78	LEU
1	C	109	LEU
1	C	117	LYS
1	C	125	GLU
1	C	185	LYS
1	C	203	ARG
1	C	218	LYS

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

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](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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
3	GLU	A	274	-	8,9,9	1.05	0	8,11,11	0.75	0
3	GLU	B	276	-	8,9,9	1.10	0	8,11,11	1.04	1 (12%)
3	GLU	C	275	-	8,9,9	1.04	0	8,11,11	0.81	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
3	GLU	A	274	-	-	1/9/9/9	-
3	GLU	B	276	-	-	0/9/9/9	-
3	GLU	C	275	-	-	2/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	276	GLU	OE2-CD-CG	2.19	120.90	114.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	274	GLU	O-C-CA-N
3	C	275	GLU	O-C-CA-CB
3	C	275	GLU	OXT-C-CA-CB

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.