



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:59 AM UTC

PDB ID : 5CNJ / pdb_00005cnj
Title : mGlur2 with glutamate analog
Authors : Monn, J.A.; Clawson, D.K.
Deposited on : 2015-07-17
Resolution : 2.65 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

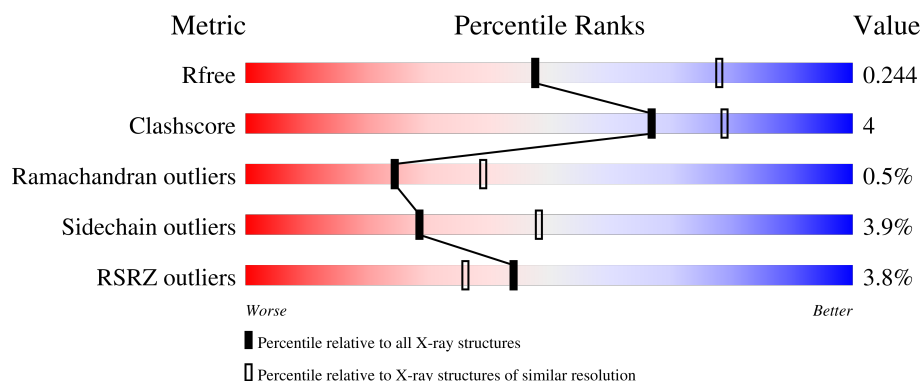
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	503	
1	B	503	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7184 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3496	2220	625	638	13			
1	B	445	Total	C	N	O	S	0	0	0
			3489	2217	621	638	13			

There are 24 discrepancies between the modelled and reference sequences:

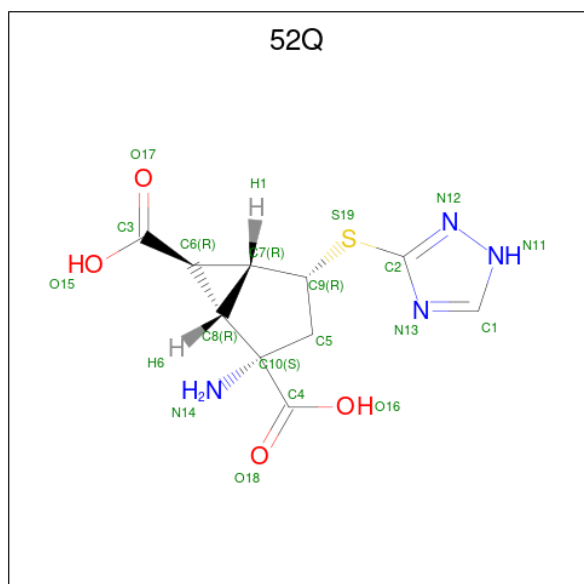
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q14416
A	0	ALA	-	expression tag	UNP Q14416
A	1	LEU	-	expression tag	UNP Q14416
A	234	SER	CYS	conflict	UNP Q14416
A	494	GLU	-	expression tag	UNP Q14416
A	495	GLY	-	expression tag	UNP Q14416
A	496	HIS	-	expression tag	UNP Q14416
A	497	HIS	-	expression tag	UNP Q14416
A	498	HIS	-	expression tag	UNP Q14416
A	499	HIS	-	expression tag	UNP Q14416
A	500	HIS	-	expression tag	UNP Q14416
A	501	HIS	-	expression tag	UNP Q14416
B	-1	MET	-	expression tag	UNP Q14416
B	0	ALA	-	expression tag	UNP Q14416
B	1	LEU	-	expression tag	UNP Q14416
B	234	SER	CYS	conflict	UNP Q14416
B	494	GLU	-	expression tag	UNP Q14416
B	495	GLY	-	expression tag	UNP Q14416
B	496	HIS	-	expression tag	UNP Q14416
B	497	HIS	-	expression tag	UNP Q14416
B	498	HIS	-	expression tag	UNP Q14416
B	499	HIS	-	expression tag	UNP Q14416
B	500	HIS	-	expression tag	UNP Q14416
B	501	HIS	-	expression tag	UNP Q14416

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (1R,2S,4R,5R,6R)-2-amino-4-(1H-1,2,4-triazol-3-ylsulfanyl)bicyclo[3.1.0]hexane-2,6-dicarboxylic acid (CCD ID: 52Q) (formula: $C_{10}H_{12}N_4O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	10	4	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			19	10	4	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	66	Total	O	0	0
			66	66		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.39Å 155.09Å 92.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.04 – 2.65 28.04 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.9 (28.04-2.65) 97.8 (28.04-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.193 , 0.241 0.202 , 0.244	Depositor DCC
R_{free} test set	1005 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: NAG, 52Q

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	0.91	2/3580 (0.1%)	1.36	15/4852 (0.3%)
1	B	0.89	1/3574 (0.0%)	1.37	11/4846 (0.2%)
All	All	0.90	3/7154 (0.0%)	1.36	26/9698 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	370	VAL	CA-C	5.56	1.57	1.52
1	A	445	ARG	CA-C	5.41	1.60	1.52
1	A	143	SER	CA-C	5.34	1.57	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLY	N-CA-C	8.76	121.38	110.96
1	A	361	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	444	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	58	GLY	CA-C-N	6.51	128.77	120.56
1	A	58	GLY	C-N-CA	6.51	128.77	120.56
1	B	444	ASP	CA-C-N	6.14	128.50	120.28
1	B	444	ASP	C-N-CA	6.14	128.50	120.28
1	A	235	VAL	CA-C-N	6.00	128.24	120.44
1	A	235	VAL	C-N-CA	6.00	128.24	120.44
1	A	90	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	450	ILE	N-CA-C	5.69	116.14	108.17
1	B	192	ALA	CA-C-N	5.62	127.81	120.28
1	B	192	ALA	C-N-CA	5.62	127.81	120.28
1	A	362	CYS	N-CA-C	5.57	117.15	111.14
1	B	141	GLY	N-CA-C	5.55	118.67	110.63
1	B	90	ASP	CA-CB-CG	5.42	118.02	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	PRO	CA-C-N	5.40	127.73	120.50
1	B	52	PRO	C-N-CA	5.40	127.73	120.50
1	A	199	LEU	CA-C-N	5.39	127.82	120.54
1	A	199	LEU	C-N-CA	5.39	127.82	120.54
1	B	294	SER	CA-C-N	5.34	128.18	120.38
1	B	294	SER	C-N-CA	5.34	128.18	120.38
1	A	422	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	160	ILE	N-CA-C	5.08	112.18	107.56
1	A	228	ALA	CA-C-N	5.03	127.33	120.54
1	A	228	ALA	C-N-CA	5.03	127.33	120.54

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	3496	0	3406	21	0
1	B	3489	0	3387	30	0
2	A	14	0	13	0	0
3	A	19	0	9	0	0
3	B	19	0	9	0	0
4	A	81	0	0	0	0
4	B	66	0	0	2	0
All	All	7184	0	6824	51	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 4.

All (51) 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:195:MET:HE1	1:A:294:SER:HB3	1.64	0.79
1:B:99:LEU:HD22	1:B:150:GLN:CG	2.23	0.69
1:B:99:LEU:HD22	1:B:150:GLN:HG3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:HA	1:A:485:ILE:HD12	1.78	0.65
1:A:24:LYS:HD3	1:A:343:PRO:HB2	1.79	0.64
1:A:355:CYS:HB2	1:A:361:ASP:HB3	1.78	0.63
1:B:279:LEU:HD21	1:B:311:ALA:HB2	1.81	0.61
1:B:210:VAL:HG12	1:B:211:ALA:N	2.17	0.60
1:B:195:MET:HE2	1:B:267:VAL:HG13	1.85	0.58
1:A:95:ASP:HB2	1:A:150:GLN:HG3	1.86	0.57
1:B:209:THR:OG1	1:B:238:SER:HA	2.06	0.56
1:B:210:VAL:HG12	1:B:211:ALA:H	1.71	0.55
1:A:142:GLY:HA3	1:A:148:SER:OG	2.09	0.52
1:A:187:PRO:HD3	1:A:448:ASP:HB3	1.92	0.52
1:B:219:THR:HA	1:B:222:GLU:HG2	1.91	0.52
1:B:142:GLY:HA3	1:B:148:SER:OG	2.10	0.51
1:B:273:GLU:H	1:B:273:GLU:CD	2.18	0.51
1:B:206:TYR:C	1:B:207:VAL:HG13	2.35	0.51
1:A:210:VAL:HG11	1:A:278:LEU:HD11	1.92	0.51
1:B:25:VAL:HG21	1:B:87:HIS:CE1	2.46	0.51
1:A:141:GLY:HA2	1:A:165:TYR:CE2	2.47	0.50
1:B:482:THR:HG22	1:B:485:ILE:HD12	1.94	0.49
1:A:221:ILE:HG12	1:A:269:PHE:HB2	1.94	0.49
1:B:163:ILE:HA	1:B:182:ALA:O	2.14	0.48
1:A:26:LEU:HD13	1:A:62:LEU:HD11	1.95	0.47
1:B:304:VAL:HG11	1:B:458:TYR:CE2	2.49	0.47
1:B:212:SER:HA	1:B:241:VAL:O	2.14	0.47
1:A:199:LEU:HD13	1:A:207:VAL:HG11	1.96	0.47
1:A:273:GLU:CD	1:A:273:GLU:H	2.23	0.47
1:B:265:VAL:HG22	1:B:290:THR:HB	1.97	0.47
1:B:177:ARG:NH1	4:B:701:HOH:O	2.38	0.46
1:A:207:VAL:HG12	1:A:265:VAL:HB	1.98	0.46
1:B:297:TRP:C	1:B:297:TRP:CD1	2.94	0.45
1:A:225:GLU:HG2	1:A:235:VAL:HG21	1.99	0.45
1:B:159:GLN:O	1:B:415:GLY:HA3	2.16	0.45
1:B:31:ASP:HB2	1:B:82:VAL:HG13	1.99	0.45
1:A:191:GLN:HG2	1:A:195:MET:HE3	1.98	0.45
1:B:207:VAL:HG12	1:B:265:VAL:HB	2.00	0.44
1:A:193:LYS:HE3	1:A:231:ARG:HH22	1.84	0.43
1:A:324:ILE:HD12	1:A:379:MET:HA	2.01	0.43
1:A:36:GLY:HA3	1:A:88:ILE:HG12	2.00	0.43
1:B:304:VAL:HG11	1:B:458:TYR:CZ	2.55	0.42
1:A:298:GLY:HA2	1:A:317:ILE:O	2.19	0.42
1:B:26:LEU:HD11	1:B:66:LEU:HD11	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLY:H	1:A:245:MET:HE3	1.85	0.41
1:B:26:LEU:HB3	1:B:88:ILE:HB	2.01	0.41
1:B:89:LEU:HD13	1:B:101:GLN:HB3	2.02	0.41
1:B:405:ARG:NH1	4:B:702:HOH:O	2.50	0.41
1:B:141:GLY:HA2	1:B:165:TYR:CE2	2.56	0.41
1:B:210:VAL:CG1	1:B:211:ALA:N	2.85	0.40
1:B:295:ASP:HA	1:B:317:ILE:O	2.21	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	441/503 (88%)	423 (96%)	14 (3%)	4 (1%)	14	24
1	B	441/503 (88%)	416 (94%)	25 (6%)	0	100	100
All	All	882/1006 (88%)	839 (95%)	39 (4%)	4 (0%)	24	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	A	325	SER
1	A	360	ARG
1	A	451	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	359/402 (89%)	348 (97%)	11 (3%)	35	56
1	B	358/402 (89%)	341 (95%)	17 (5%)	23	40
All	All	717/804 (89%)	689 (96%)	28 (4%)	28	48

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

Mol	Chain	Res	Type
1	A	24	LYS
1	A	25	VAL
1	A	62	LEU
1	A	93	SER
1	A	179	ASP
1	A	245	MET
1	A	268	LEU
1	A	269	PHE
1	A	273	GLU
1	A	324	ILE
1	A	361	ASP
1	B	60	GLN
1	B	107	ARG
1	B	137	THR
1	B	143	SER
1	B	176	SER
1	B	208	SER
1	B	212	SER
1	B	215	ASP
1	B	257	LEU
1	B	269	PHE
1	B	273	GLU
1	B	285	LEU
1	B	297	TRP
1	B	303	VAL
1	B	335	ASP
1	B	358	ARG
1	B	450	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	B	383	ASN

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 ⓘ

3 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$
3	52Q	A	602	-	17,21,21	2.44	7 (41%)	20,33,33	2.05	7 (35%)
3	52Q	B	601	-	17,21,21	2.63	9 (52%)	20,33,33	1.93	5 (25%)
2	NAG	A	601	1	14,14,15	0.36	0	17,19,21	0.94	2 (11%)

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	52Q	A	602	-	-	5/12/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	52Q	B	601	-	-	4/12/38/38	0/3/3/3
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	52Q	C6-C3	-4.63	1.40	1.51
3	A	602	52Q	C6-C3	-4.59	1.40	1.51
3	A	602	52Q	C9-S19	-4.46	1.77	1.83
3	B	601	52Q	O18-C4	4.15	1.35	1.22
3	B	601	52Q	C2-S19	-4.08	1.70	1.75
3	A	602	52Q	C7-C9	-3.57	1.46	1.54
3	B	601	52Q	C9-S19	-3.55	1.79	1.83
3	B	601	52Q	C7-C9	-3.22	1.46	1.54
3	A	602	52Q	C2-S19	-3.18	1.71	1.75
3	A	602	52Q	C6-C8	-3.09	1.47	1.51
3	B	601	52Q	C6-C8	-3.00	1.47	1.51
3	B	601	52Q	C6-C7	-2.79	1.48	1.52
3	A	602	52Q	C5-C10	-2.77	1.49	1.54
3	B	601	52Q	C5-C10	-2.71	1.49	1.54
3	A	602	52Q	C6-C7	-2.61	1.48	1.52
3	B	601	52Q	C2-N12	-2.11	1.29	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	52Q	C5-C10-C4	-4.57	99.00	111.49
3	A	602	52Q	C5-C10-C4	-4.54	99.10	111.49
3	A	602	52Q	N12-C2-N13	-4.21	109.72	114.87
3	B	601	52Q	N12-C2-N13	-4.00	109.98	114.87
3	A	602	52Q	O18-C4-C10	-3.06	114.65	122.53
2	A	601	NAG	C1-O5-C5	2.82	115.96	112.19
3	A	602	52Q	S19-C2-N12	2.70	129.50	123.38
3	B	601	52Q	O18-C4-C10	-2.55	115.95	122.53
3	B	601	52Q	C8-C6-C7	2.25	60.16	58.67
3	B	601	52Q	O17-C3-C6	-2.23	117.15	122.84
3	A	602	52Q	O17-C3-C6	-2.17	117.29	122.84
3	A	602	52Q	C6-C7-C9	2.16	121.07	117.07
2	A	601	NAG	C1-C2-N2	2.13	113.80	110.43
3	A	602	52Q	C8-C6-C7	2.08	60.04	58.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

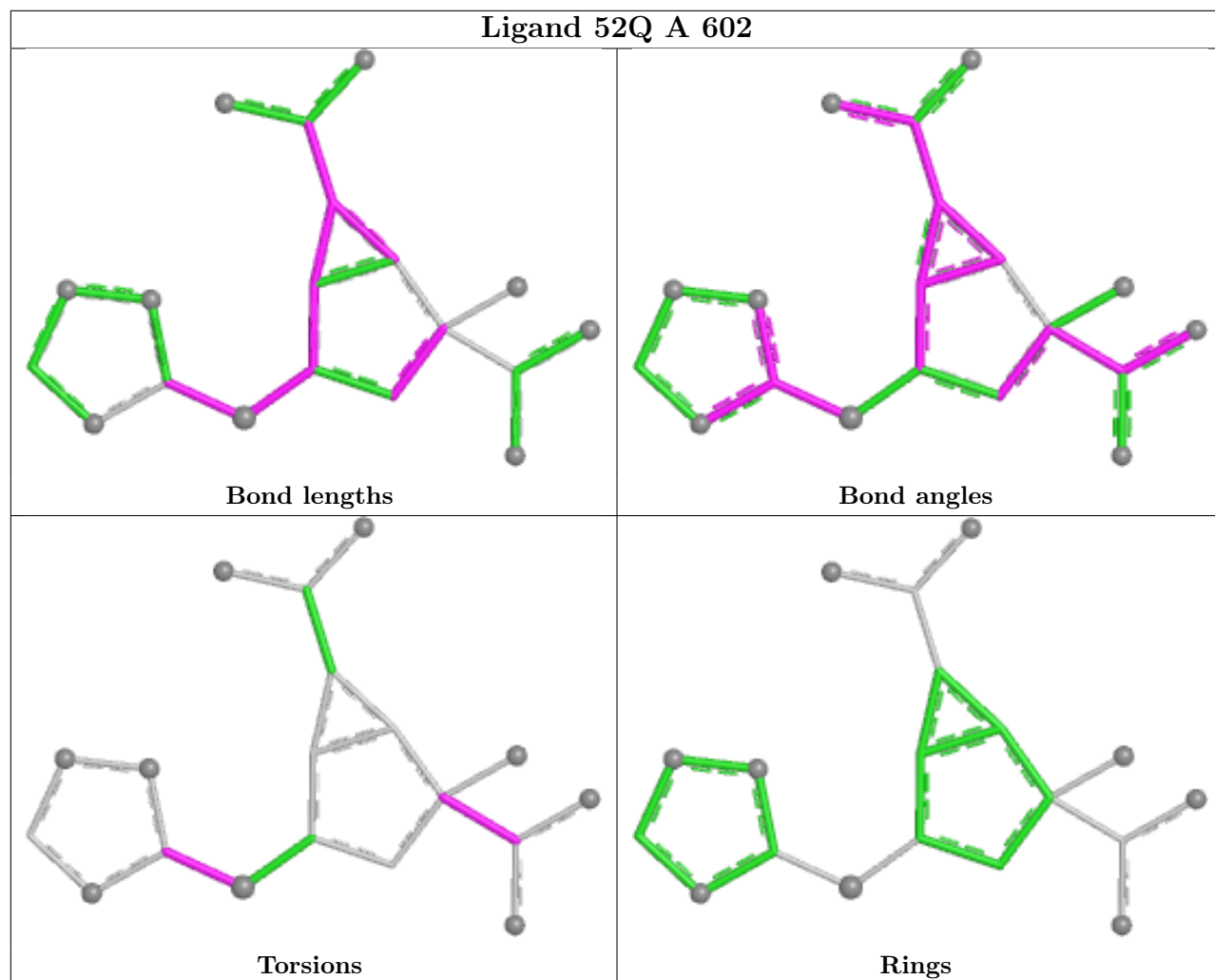
Mol	Chain	Res	Type	Atoms
3	A	602	52Q	N12-C2-S19-C9
3	B	601	52Q	N12-C2-S19-C9
3	A	602	52Q	C8-C10-C4-O16
3	A	602	52Q	C5-C10-C4-O16
3	A	602	52Q	C5-C10-C4-O18
3	B	601	52Q	O15-C3-C6-C7
3	A	602	52Q	C8-C10-C4-O18
3	B	601	52Q	C8-C10-C4-O18
3	B	601	52Q	N13-C2-S19-C9

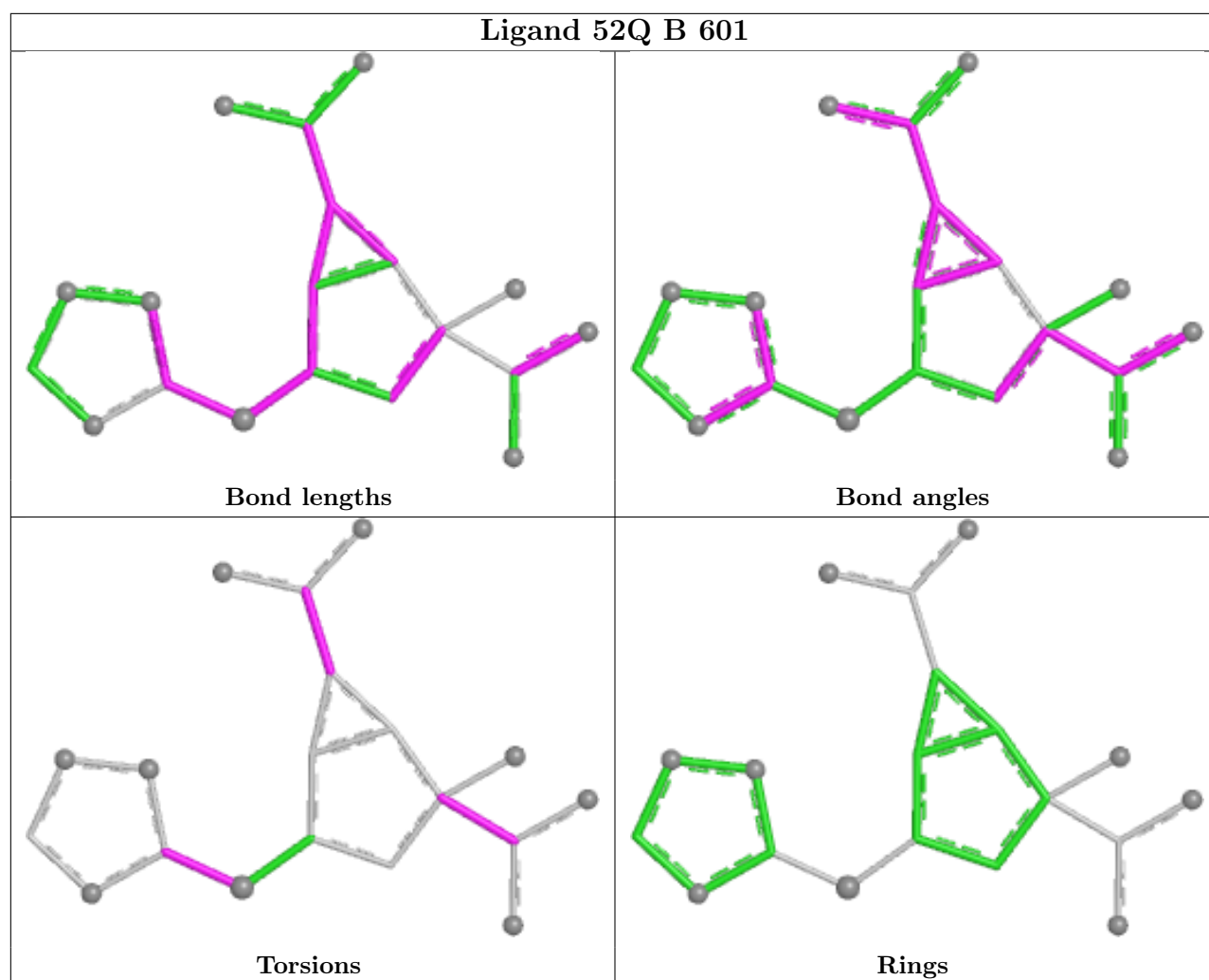
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 52Q A 602





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

6.1 Protein, DNA and RNA chains

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	445/503 (88%)	0.04	11 (2%) 58 52	33, 50, 79, 106	0
1	B	445/503 (88%)	0.35	23 (5%) 33 25	32, 58, 90, 110	0
All	All	890/1006 (88%)	0.19	34 (3%) 44 36	32, 54, 87, 110	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	LEU	4.0
1	B	49	ASP	3.8
1	B	233	ILE	3.6
1	B	476	GLU	3.3
1	A	49	ASP	3.3
1	B	50	CYS	3.2
1	B	242	GLY	3.1
1	B	244	ALA	2.8
1	B	266	ALA	2.8
1	B	436	ASP	2.7
1	A	359	GLN	2.6
1	B	403	THR	2.5
1	B	435	ALA	2.4
1	A	473	TYR	2.3
1	B	23	LYS	2.3
1	A	292	VAL	2.3
1	B	268	LEU	2.3
1	B	437	THR	2.3
1	B	111	SER	2.3
1	A	357	PHE	2.3
1	B	461	ALA	2.3
1	B	257	LEU	2.2
1	B	198	ILE	2.2
1	B	263	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	302	SER	2.2
1	A	22	ALA	2.2
1	B	466	TYR	2.2
1	B	477	GLY	2.1
1	B	337	TRP	2.1
1	B	304	VAL	2.1
1	B	138	GLY	2.1
1	A	362	CYS	2.1
1	A	461	ALA	2.0
1	A	436	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

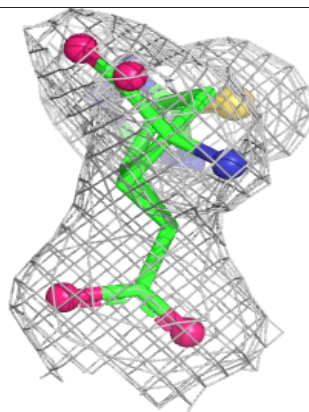
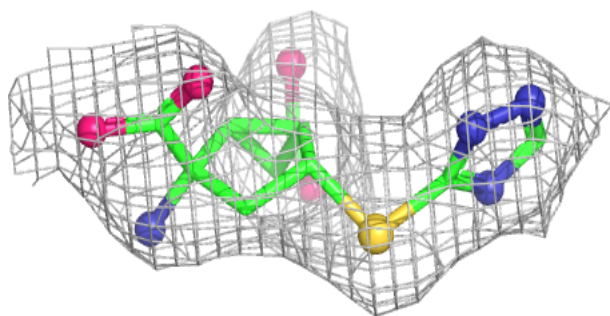
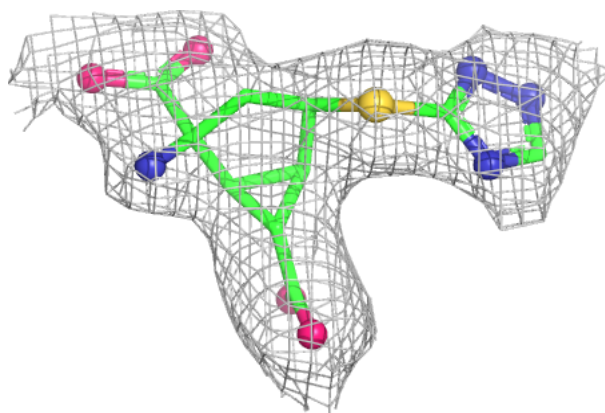
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	601	14/15	0.69	0.12	71,85,90,91	0
3	52Q	A	602	19/19	0.96	0.07	35,46,59,60	0
3	52Q	B	601	19/19	0.97	0.06	29,43,61,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

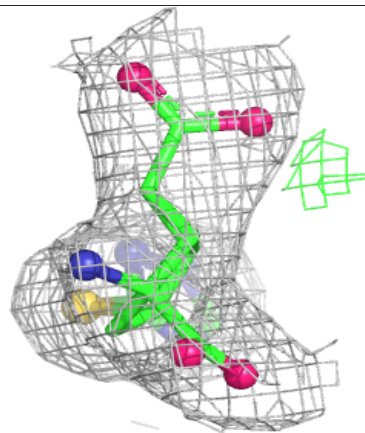
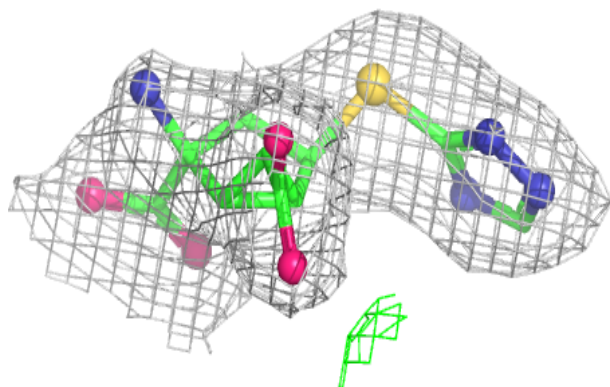
Electron density around 52Q A 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 52Q B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.