



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:56 AM UTC

PDB ID : 5CNI / pdb_00005cni
Title : mGlu2 with Glutamate
Authors : Clawson, D.K.; Atwell, S.; Monn, J.A.
Deposited on : 2015-07-17
Resolution : 2.69 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
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

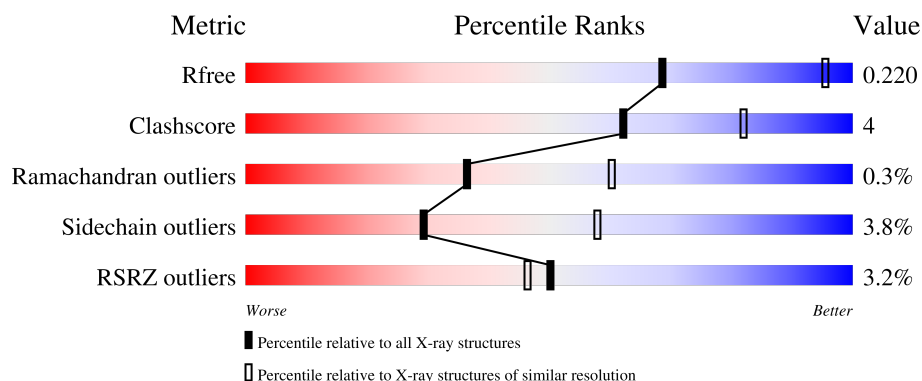
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	2% 74% 10% • 13%
1	B	503	4% 77% 9% • 13%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7131 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	438	Total	C	N	O	S	0	0	0
			3410	2171	600	626	13			
1	B	438	Total	C	N	O	S	0	0	0
			3402	2165	598	626	13			

There are 26 discrepancies between the modelled and reference sequences:

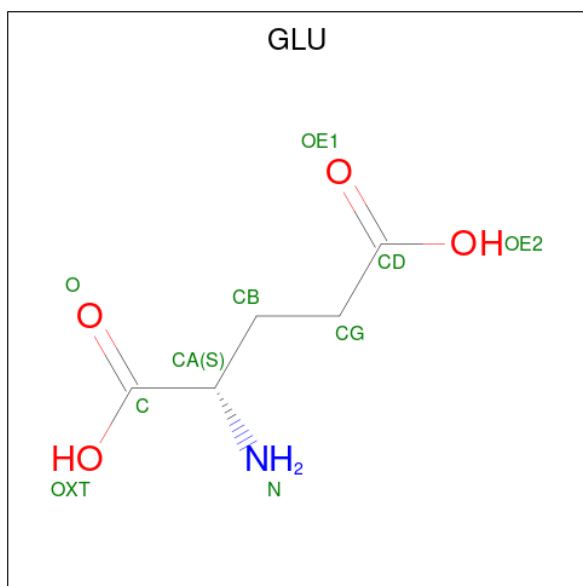
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q14416
A	0	ALA	-	expression tag	UNP Q14416
A	1	LEU	-	expression tag	UNP Q14416
A	234	SER	CYS	conflict	UNP Q14416
A	302	GLU	SER	conflict	UNP Q14416
A	494	GLU	-	expression tag	UNP Q14416
A	495	GLY	-	expression tag	UNP Q14416
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	302	GLU	SER	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	501	HIS	-	expression tag	UNP Q14416

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



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

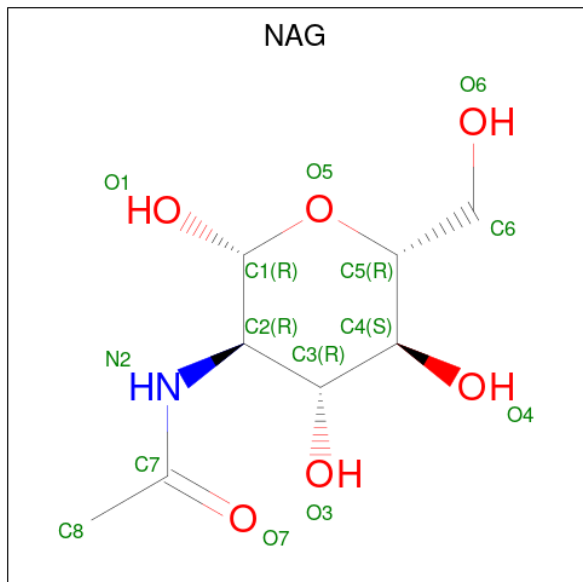
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	119	Total	O	0	0
			119	119		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.08Å 79.33Å 93.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.66 – 2.69 35.66 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.66-2.69) 99.8 (35.66-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.69Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5	Depositor
R, R_{free}	0.168 , 0.222 (Not available) , 0.220	Depositor DCC
R_{free} test set	1038 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7131	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: CL, NAG, NA

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	1.00	7/3492 (0.2%)	1.33	18/4737 (0.4%)
1	B	0.92	2/3483 (0.1%)	1.32	8/4725 (0.2%)
All	All	0.96	9/6975 (0.1%)	1.33	26/9462 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	VAL	C-N	6.26	1.40	1.33
1	A	186	PRO	C-N	5.80	1.40	1.33
1	A	335	ASP	C-N	5.74	1.40	1.34
1	A	183	ARG	C-O	-5.20	1.17	1.23
1	B	388	MET	C-O	-5.10	1.18	1.24
1	A	336	PRO	N-CD	5.08	1.54	1.47
1	B	336	PRO	N-CD	5.07	1.54	1.47
1	A	455	ILE	C-O	-5.06	1.18	1.24
1	A	160	ILE	CA-CB	5.00	1.59	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	GLU	CB-CG-CD	7.34	125.08	112.60
1	A	186	PRO	N-CA-C	7.06	119.31	110.70
1	A	185	VAL	CA-C-N	-6.85	113.32	120.38
1	A	185	VAL	C-N-CA	-6.85	113.32	120.38
1	B	485	ILE	N-CA-CB	6.42	116.05	110.08
1	A	335	ASP	CA-C-N	-6.20	113.34	120.04
1	A	335	ASP	C-N-CA	-6.20	113.34	120.04
1	A	450	ILE	N-CA-C	6.19	117.50	108.58
1	A	186	PRO	CA-C-N	-6.01	114.08	120.03
1	A	186	PRO	C-N-CA	-6.01	114.08	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	179	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	204	TRP	CA-C-N	5.74	128.44	120.29
1	B	204	TRP	C-N-CA	5.74	128.44	120.29
1	A	90	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	318	GLU	CB-CG-CD	5.58	122.09	112.60
1	A	95	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	444	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	297	TRP	N-CA-C	-5.21	104.52	111.24
1	A	324	ILE	CA-C-N	5.19	127.55	120.54
1	A	324	ILE	C-N-CA	5.19	127.55	120.54
1	B	146	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	48	GLU	N-CA-C	5.09	117.43	110.55
1	A	294	SER	CA-C-N	5.03	127.52	120.28
1	A	294	SER	C-N-CA	5.03	127.52	120.28
1	A	269	PHE	N-CA-C	-5.02	101.47	108.54

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	3410	0	3266	35	0
1	B	3402	0	3250	20	0
2	A	10	0	5	0	0
2	B	10	0	5	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
6	A	120	0	0	1	0
6	B	119	0	0	2	0
All	All	7131	0	6578	55	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 (55) 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:186:PRO:HG3	1:A:451:GLY:HA2	1.63	0.80
1:A:221:ILE:HG12	1:A:269:PHE:HB2	1.70	0.73
1:A:450:ILE:N	1:A:450:ILE:HD12	2.04	0.73
1:A:450:ILE:HD12	1:A:450:ILE:H	1.59	0.67
1:A:319:LEU:CD2	1:A:319:LEU:N	2.61	0.62
1:B:221:ILE:HD13	1:B:269:PHE:HB2	1.83	0.60
1:A:319:LEU:H	1:A:319:LEU:HD23	1.68	0.59
1:B:335:ASP:HB3	1:B:338:ASN:CG	2.28	0.58
1:A:191:GLN:HG3	1:A:453:TYR:CE1	2.39	0.58
1:A:95:ASP:HB2	1:A:150:GLN:HG3	1.85	0.58
1:B:83:ARG:NH2	6:B:701:HOH:O	2.37	0.58
1:B:207:VAL:HG12	1:B:265:VAL:HB	1.85	0.56
1:A:105:PHE:HA	1:A:136:ILE:HG13	1.88	0.56
1:A:319:LEU:CD2	1:A:319:LEU:H	2.18	0.56
1:B:95:ASP:HB2	1:B:150:GLN:HG3	1.88	0.55
1:A:186:PRO:HD2	1:A:319:LEU:HD12	1.87	0.55
1:A:210:VAL:HB	1:A:268:LEU:HD22	1.88	0.54
1:A:319:LEU:N	1:A:319:LEU:HD22	2.23	0.53
1:A:155:LEU:HB3	1:A:160:ILE:HB	1.91	0.53
1:A:337:TRP:HE1	1:A:363:ALA:CB	2.22	0.53
1:B:168:THR:HG1	2:B:601:GLU:N	2.07	0.52
1:B:472:GLY:HA3	1:B:480:LEU:HA	1.92	0.52
1:A:241:VAL:HG13	1:A:245:MET:HE2	1.92	0.51
1:A:438:HIS:O	1:A:438:HIS:ND1	2.43	0.51
1:B:146:ASP:O	1:B:150:GLN:HG2	2.11	0.51
1:B:336:PRO:HB2	1:B:337:TRP:CE3	2.45	0.51
1:A:42:GLN:HB2	1:A:52:PRO:HD2	1.92	0.51
1:A:186:PRO:HD2	1:A:319:LEU:CD1	2.41	0.51
1:B:87:HIS:HB3	1:B:136:ILE:HD11	1.93	0.51
1:A:337:TRP:HE1	1:A:363:ALA:HB2	1.75	0.50
1:B:62:LEU:CD1	1:B:88:ILE:HG21	2.41	0.50
1:B:443:PHE:HB3	1:B:447:GLY:HA2	1.94	0.49
1:B:26:LEU:HD11	1:B:66:LEU:HD11	1.95	0.49
1:B:210:VAL:HB	1:B:268:LEU:HD22	1.96	0.48
1:A:434:PRO:HD2	1:A:437:THR:OG1	2.14	0.48
1:A:228:ALA:HB1	1:A:233:ILE:HB	1.98	0.46
1:A:144:TYR:HB3	1:A:146:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD13	1:A:88:ILE:HG21	1.99	0.45
1:B:312:GLU:HG3	1:B:466:TYR:HE1	1.81	0.45
1:A:34:LEU:O	1:A:86:ALA:HA	2.16	0.45
1:A:314:ALA:O	1:A:457:THR:HA	2.17	0.45
1:A:205:THR:HG23	1:A:232:ASN:O	2.17	0.44
1:A:297:TRP:CD1	1:A:297:TRP:C	2.95	0.44
1:A:26:LEU:HB3	1:A:88:ILE:HB	2.00	0.44
1:B:150:GLN:NE2	6:B:702:HOH:O	2.51	0.44
1:B:293:ALA:HB3	1:B:316:THR:HG22	2.00	0.44
1:A:26:LEU:HD22	1:A:88:ILE:HD12	1.99	0.43
1:A:26:LEU:HD13	1:A:62:LEU:HD11	2.00	0.43
1:A:24:LYS:HD2	1:A:343:PRO:HB2	2.00	0.43
1:B:31:ASP:HB2	1:B:82:VAL:HG13	2.01	0.42
1:B:201:PHE:CE2	1:B:480:LEU:HD11	2.55	0.41
1:A:315:ILE:HD11	1:A:487:TRP:HH2	1.86	0.41
1:A:161:PRO:HG2	1:A:418:LEU:HD23	2.02	0.40
1:A:429:ASP:HB3	6:A:769:HOH:O	2.21	0.40
1:B:159:GLN:HB3	1:B:180:TYR:CZ	2.57	0.40

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	430/503 (86%)	414 (96%)	15 (4%)	1 (0%)	43	68
1	B	430/503 (86%)	406 (94%)	22 (5%)	2 (0%)	24	48
All	All	860/1006 (86%)	820 (95%)	37 (4%)	3 (0%)	36	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	GLY
1	B	437	THR
1	B	451	GLY

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	344/402 (86%)	330 (96%)	14 (4%)	27	56
1	B	342/402 (85%)	330 (96%)	12 (4%)	32	61
All	All	686/804 (85%)	660 (96%)	26 (4%)	29	58

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	62	LEU
1	A	96	THR
1	A	104	ASP
1	A	107	ARG
1	A	159	GLN
1	A	191	GLN
1	A	221	ILE
1	A	245	MET
1	A	269	PHE
1	A	279	LEU
1	A	318	GLU
1	A	319	LEU
1	A	379	MET
1	B	25	VAL
1	B	60	GLN
1	B	159	GLN
1	B	221	ILE
1	B	237	THR
1	B	269	PHE
1	B	302	GLU

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Mol	Chain	Res	Type
1	B	356	SER
1	B	410	MET
1	B	455	ILE
1	B	457	THR
1	B	485	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	153	ASN
1	B	383	ASN
1	B	438	HIS
1	B	439	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
2	GLU	B	601	-	8,9,9	2.47	4 (50%)	8,11,11	2.51	3 (37%)
5	NAG	A	604	1	14,14,15	0.33	0	17,19,21	0.62	0
2	GLU	A	601	-	8,9,9	0.75	0	8,11,11	1.65	1 (12%)
5	NAG	B	605	1	14,14,15	0.30	0	17,19,21	0.95	2 (11%)
5	NAG	A	605	1	14,14,15	0.33	0	17,19,21	1.07	3 (17%)
5	NAG	B	604	1	14,14,15	0.29	0	17,19,21	0.57	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	GLU	B	601	-	-	2/9/9/9	-
5	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	GLU	A	601	-	-	3/9/9/9	-
5	NAG	B	605	1	-	0/6/23/26	0/1/1/1
5	NAG	A	605	1	-	0/6/23/26	0/1/1/1
5	NAG	B	604	1	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GLU	O-C	4.32	1.34	1.22
2	B	601	GLU	OE1-CD	4.08	1.35	1.22
2	B	601	GLU	OXT-C	-2.56	1.22	1.30
2	B	601	GLU	OE2-CD	-2.52	1.22	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GLU	OE2-CD-CG	4.50	128.21	114.00
2	A	601	GLU	OXT-C-O	-3.44	116.27	124.08
2	B	601	GLU	OXT-C-O	-3.44	116.27	124.08
2	B	601	GLU	OE1-CD-CG	-3.38	112.37	123.09
5	A	605	NAG	C1-O5-C5	2.91	116.09	112.19
5	B	605	NAG	O5-C1-C2	-2.27	107.78	111.29
5	B	605	NAG	C1-C2-N2	2.25	113.98	110.43
5	A	605	NAG	C1-C2-N2	2.23	113.94	110.43
5	A	605	NAG	O5-C1-C2	-2.08	108.08	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GLU	CA-CB-CG-CD
2	A	601	GLU	OE1-CD-CG-CB
5	B	604	NAG	C4-C5-C6-O6
2	A	601	GLU	OE2-CD-CG-CB
2	B	601	GLU	OE2-CD-CG-CB
2	B	601	GLU	OE1-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GLU	1	0

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	438/503 (87%)	-0.18	10 (2%) 61 58	17, 38, 73, 116	0
1	B	438/503 (87%)	-0.01	18 (4%) 41 37	16, 43, 81, 115	0
All	All	876/1006 (87%)	-0.09	28 (3%) 50 46	16, 40, 77, 116	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	435	ALA	4.7
1	B	462	GLY	4.6
1	B	464	GLY	3.5
1	B	465	ARG	3.5
1	B	461	ALA	3.2
1	A	337	TRP	3.1
1	B	487	TRP	3.0
1	B	482	THR	2.8
1	A	485	ILE	2.6
1	A	487	TRP	2.5
1	A	134	THR	2.4
1	B	474	TRP	2.4
1	B	459	LEU	2.3
1	A	407	CYS	2.3
1	B	50	CYS	2.2
1	B	485	ILE	2.2
1	A	438	HIS	2.2
1	B	205	THR	2.2
1	A	476	GLU	2.2
1	A	109	SER	2.2
1	B	207	VAL	2.2
1	A	480	LEU	2.2
1	A	362	CYS	2.2
1	B	134	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	109	SER	2.2
1	B	484	LEU	2.2
1	B	263	ALA	2.1
1	B	260	LYS	2.1

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
5	NAG	B	605	14/15	0.50	0.16	111,116,117,117	0
5	NAG	A	605	14/15	0.59	0.16	76,82,85,85	0
5	NAG	B	604	14/15	0.70	0.13	110,111,112,112	0
5	NAG	A	604	14/15	0.73	0.12	61,70,75,76	0
4	NA	A	603	1/1	0.93	0.10	63,63,63,63	0
2	GLU	B	601	10/10	0.96	0.07	29,34,36,39	0
2	GLU	A	601	10/10	0.96	0.07	21,30,33,34	0
4	NA	B	603	1/1	0.98	0.03	46,46,46,46	0
3	CL	A	602	1/1	0.99	0.05	36,36,36,36	0
3	CL	B	602	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.