



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 09:03 PM EDT

PDB ID : 3TDJ
Title : Crystal structure of the GluA2 ligand-binding domain (S1S2J-L483Y-N754S) in complex with glutamate and BPAM-97 at 1.95 Å resolution
Authors : Krintel, C.; Frydenvang, K.; Gajhede, M.; Kastrop, J.S.
Deposited on : 2011-08-11
Resolution : 1.95 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

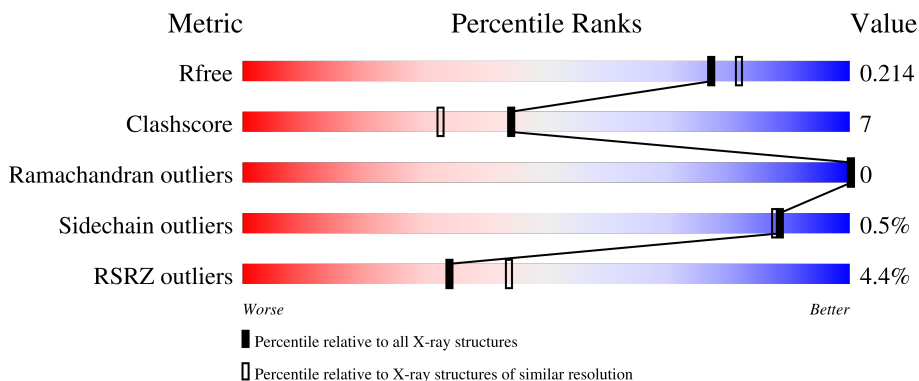
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


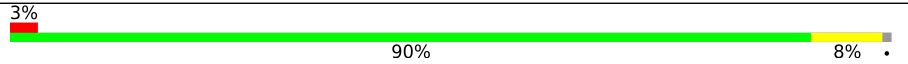
The reported resolution of this entry is 1.95 Å.

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	263	
1	B	263	

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
5	GOL	A	268	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4782 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.

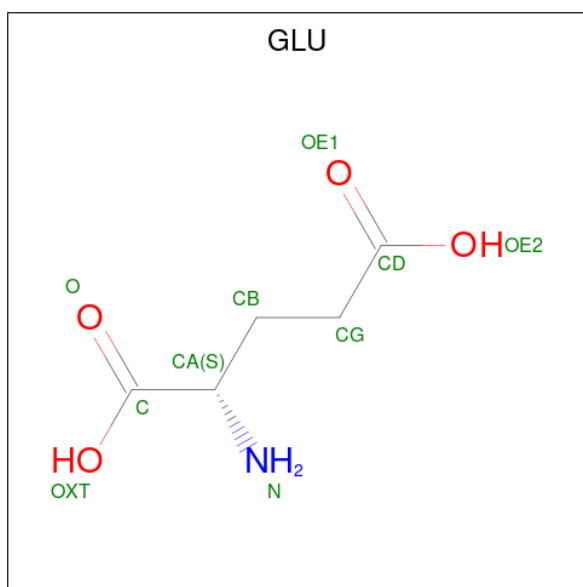
- Molecule 1 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2062	1320	339	388	15	0	7	0
1	B	260	2066	1323	340	388	15	0	7	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P19491
A	2	ALA	-	expression tag	UNP P19491
A	94	TYR	LEU	engineered mutation	UNP P19491
A	118	GLY	-	linker	UNP P19491
A	119	THR	-	linker	UNP P19491
A	242	SER	ASN	engineered mutation	UNP P19491
B	1	GLY	-	expression tag	UNP P19491
B	2	ALA	-	expression tag	UNP P19491
B	94	TYR	LEU	engineered mutation	UNP P19491
B	118	GLY	-	linker	UNP P19491
B	119	THR	-	linker	UNP P19491
B	242	SER	ASN	engineered mutation	UNP P19491

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O S		
3	A	1	5	4 1	0	0
3	B	1	5	4 1	0	0

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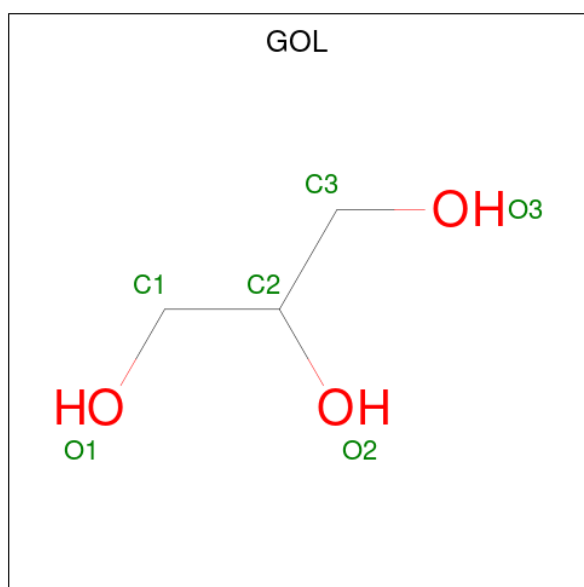
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



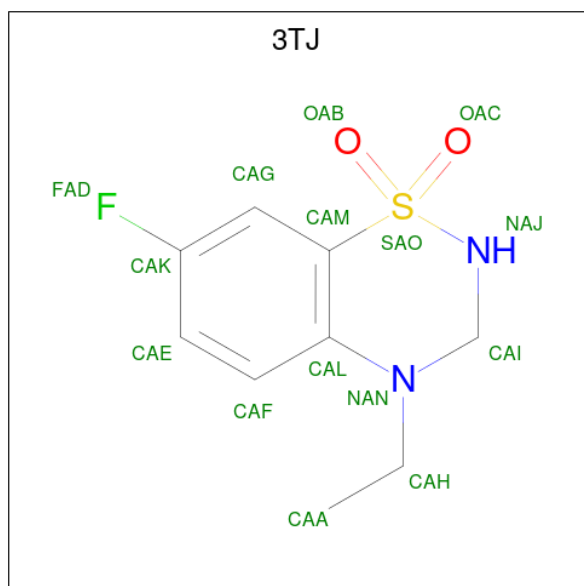
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 4-ethyl-7-fluoro-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (three-letter code: 3TJ) (formula: C₉H₁₁FN₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	B	1	Total	C	F	N	O	S	0	0
			15	9	1	2	2	1		
6	B	1	Total	C	F	N	O	S	0	0
			15	9	1	2	2	1		

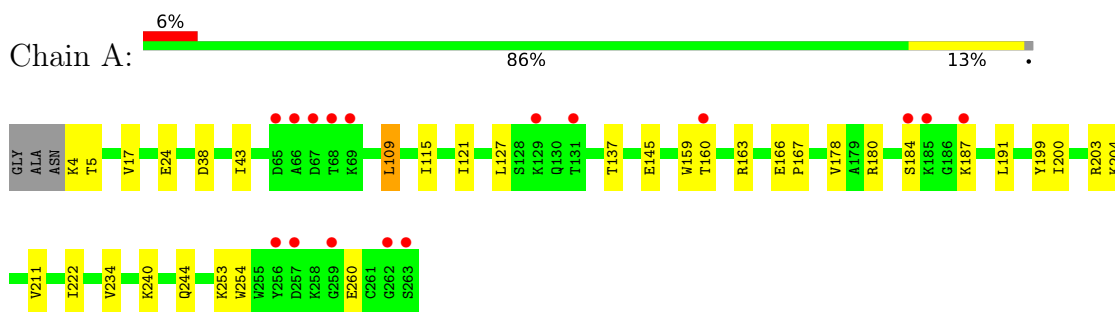
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	237	Total	O	0	0
			237	237		
7	B	281	Total	O	0	0
			281	281		

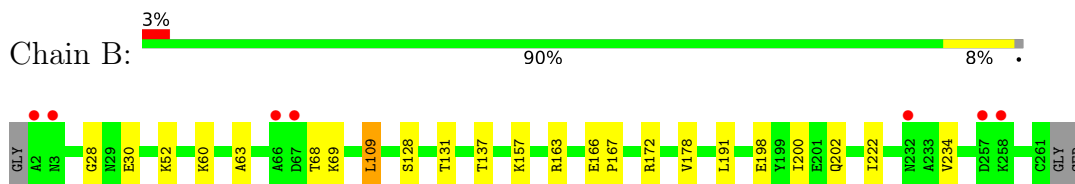
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.86Å 121.30Å 47.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.22 – 1.95 24.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.22-1.95) 99.9 (24.26-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.170 , 0.215 0.165 , 0.214	Depositor DCC
R_{free} test set	2137 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtrriage
Anisotropy	0.236	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4782	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5737e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, 3TJ, SO4

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	0.35	0/2122	0.51	0/2851
1	B	0.36	0/2124	0.52	0/2854
All	All	0.36	0/4246	0.51	0/5705

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 [i](#)

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	2062	0	2106	36	0
1	B	2066	0	2125	19	0
2	A	10	0	5	0	0
2	B	10	0	5	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
5	A	30	0	40	6	0
5	B	36	0	48	3	0
6	B	30	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	237	0	0	5	0
7	B	281	0	0	4	0
All	All	4782	0	4351	57	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 (57) 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)
5:A:268:GOL:H31	5:A:269:GOL:H32	1.65	0.79
1:A:121:ILE:HD13	1:A:127:LEU:HD23	1.63	0.79
1:A:184:SER:O	1:A:187:LYS:HG2	1.92	0.69
1:B:60[A]:LYS:HZ1	1:B:172:ARG:NH1	1.90	0.69
1:A:180:ARG:O	1:A:184:SER:HB2	1.93	0.68
1:B:30:GLU:HG2	7:B:509:HOH:O	1.92	0.68
1:A:121:ILE:HD13	1:A:127:LEU:CD2	2.24	0.66
1:A:43[B]:ILE:HD13	1:A:222:ILE:HD13	1.78	0.65
1:B:68:THR:O	1:B:69:LYS:HG2	1.97	0.65
1:A:178:VAL:HG21	1:A:200[B]:ILE:HD13	1.81	0.63
1:A:115:ILE:HD11	1:A:211:VAL:HG11	1.80	0.62
1:B:163:ARG:HH21	5:B:267:GOL:H31	1.66	0.61
1:B:198:GLU:OE1	7:B:410:HOH:O	2.16	0.61
1:B:222:ILE:HG21	1:B:234:VAL:HG11	1.84	0.59
1:A:244:GLN:HE21	5:A:268:GOL:H32	1.66	0.59
1:A:4[A]:LYS:HG2	1:A:5:THR:H	1.68	0.59
1:B:60[A]:LYS:HZ1	1:B:172:ARG:HH11	1.51	0.58
1:B:63:ALA:HA	5:B:268:GOL:H12	1.84	0.57
1:A:4[B]:LYS:HD2	1:A:5:THR:N	2.19	0.57
1:A:145:GLU:HG2	7:A:333:HOH:O	2.03	0.57
1:B:178:VAL:CG2	1:B:200[B]:ILE:HD13	2.35	0.56
1:A:43[B]:ILE:HD11	1:A:222:ILE:HD11	1.87	0.56
1:B:60[A]:LYS:NZ	1:B:172:ARG:HH11	2.04	0.56
1:A:159:TRP:HZ2	5:A:270:GOL:H11	1.72	0.55
1:A:204:LYS:HG3	1:A:260:GLU:HB3	1.88	0.55
1:A:43[B]:ILE:HD13	1:A:222:ILE:CD1	2.36	0.54
1:A:43[B]:ILE:CD1	1:A:222:ILE:CD1	2.87	0.53
1:B:131:THR:HG22	7:B:388:HOH:O	2.08	0.53
1:A:184:SER:HB3	7:A:338:HOH:O	2.08	0.53
1:A:199:TYR:CZ	1:A:203:ARG:HD2	2.44	0.52
1:A:43[B]:ILE:CD1	1:A:222:ILE:HD11	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HG21	7:A:415:HOH:O	2.10	0.50
1:A:178:VAL:CG2	1:A:200[B]:ILE:HD13	2.40	0.50
1:B:178:VAL:HG22	1:B:200[B]:ILE:HD13	1.94	0.50
1:A:24:GLU:HG3	7:A:528:HOH:O	2.12	0.49
1:A:109:LEU:C	1:A:109:LEU:HD22	2.32	0.49
1:A:115:ILE:CD1	1:A:211:VAL:HG11	2.44	0.48
1:A:159:TRP:O	1:A:163:ARG:HG2	2.14	0.47
1:A:166:GLU:HA	1:A:167:PRO:C	2.35	0.47
5:A:268:GOL:C3	5:A:269:GOL:H32	2.42	0.47
1:B:137:THR:HG22	1:B:191:LEU:HB2	1.97	0.47
1:B:128:SER:O	1:B:157:LYS:HE3	2.15	0.46
1:A:184:SER:OG	1:A:187:LYS:HG2	2.17	0.45
1:B:109:LEU:C	1:B:109:LEU:HD22	2.38	0.44
1:B:28:GLY:HA2	1:B:52:LYS:HZ2	1.83	0.43
1:B:202:GLN:NE2	7:B:478:HOH:O	2.50	0.43
1:A:163:ARG:HH21	5:A:270:GOL:H31	1.83	0.43
1:A:137:THR:HG22	1:A:191:LEU:HB2	2.00	0.43
1:A:240:LYS:NZ	5:A:268:GOL:H11	2.33	0.43
1:A:17:VAL:HG23	7:A:298:HOH:O	2.20	0.42
1:A:121:ILE:CD1	1:A:127:LEU:HD23	2.42	0.42
1:A:222:ILE:HG21	1:A:234:VAL:HG11	2.02	0.41
1:B:166:GLU:HA	1:B:167:PRO:C	2.41	0.41
1:A:4[A]:LYS:HG2	1:A:5:THR:N	2.32	0.41
1:A:38:ASP:OD2	1:A:253:LYS:HE2	2.20	0.41
1:A:253:LYS:HE2	1:A:254:TRP:NE1	2.36	0.41
1:B:198:GLU:OE2	5:B:269:GOL:H11	2.22	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	264/263 (100%)	259 (98%)	5 (2%)	0	100	100
1	B	265/263 (101%)	262 (99%)	3 (1%)	0	100	100
All	All	529/526 (101%)	521 (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	225/219 (103%)	224 (100%)	1 (0%)	91	90
1	B	225/219 (103%)	224 (100%)	1 (0%)	91	90
All	All	450/438 (103%)	448 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LEU
1	B	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	244	GLN
1	B	202	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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
5	GOL	B	267	-	5,5,5	0.95	0	5,5,5	1.12	0
3	SO4	B	273	-	4,4,4	0.17	0	6,6,6	0.11	0
2	GLU	B	399	-	8,9,9	1.03	1 (12%)	10,11,11	1.34	2 (20%)
3	SO4	A	265	-	4,4,4	0.12	0	6,6,6	0.26	0
5	GOL	A	268	-	5,5,5	0.92	0	5,5,5	1.23	0
5	GOL	A	269	-	5,5,5	0.78	0	5,5,5	1.27	0
3	SO4	B	266	-	4,4,4	0.12	0	6,6,6	0.37	0
5	GOL	A	270	-	5,5,5	1.03	0	5,5,5	1.07	0
5	GOL	A	272	-	5,5,5	1.02	0	5,5,5	1.02	0
2	GLU	A	401	-	8,9,9	1.14	1 (12%)	10,11,11	1.15	1 (10%)
5	GOL	B	269	-	5,5,5	0.85	0	5,5,5	1.25	0
5	GOL	B	268	-	5,5,5	0.91	0	5,5,5	1.17	0
5	GOL	B	270	-	5,5,5	0.97	0	5,5,5	1.13	0
5	GOL	B	272	-	5,5,5	0.96	0	5,5,5	1.09	0
5	GOL	B	271	-	5,5,5	0.89	0	5,5,5	1.27	0
6	3TJ	B	265	-	15,16,16	7.20	7 (46%)	21,24,24	3.20	8 (38%)
5	GOL	A	271	-	5,5,5	0.94	0	5,5,5	1.19	0
6	3TJ	B	400	-	15,16,16	7.26	7 (46%)	21,24,24	3.22	6 (28%)

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
5	GOL	B	267	-	-	2/4/4/4	-
2	GLU	B	399	-	-	0/9/9/9	-
5	GOL	A	269	-	-	2/4/4/4	-
5	GOL	A	268	-	-	1/4/4/4	-
5	GOL	A	270	-	-	2/4/4/4	-
5	GOL	B	269	-	-	3/4/4/4	-
5	GOL	A	272	-	-	2/4/4/4	-
2	GLU	A	401	-	-	1/9/9/9	-
5	GOL	B	268	-	-	1/4/4/4	-
5	GOL	B	270	-	-	0/4/4/4	-
5	GOL	B	272	-	-	1/4/4/4	-
5	GOL	B	271	-	-	1/4/4/4	-
6	3TJ	B	265	-	-	0/2/18/18	0/2/2/2
5	GOL	A	271	-	-	0/4/4/4	-
6	3TJ	B	400	-	-	2/2/18/18	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	400	3TJ	OAB-SAO	18.33	1.64	1.43
6	B	265	3TJ	OAB-SAO	17.65	1.63	1.43
6	B	400	3TJ	OAC-SAO	17.29	1.63	1.43
6	B	265	3TJ	OAC-SAO	16.95	1.62	1.43
6	B	265	3TJ	CAL-CAM	7.11	1.48	1.40
6	B	400	3TJ	CAE-CAK	7.10	1.51	1.37
6	B	400	3TJ	CAL-CAM	6.87	1.47	1.40
6	B	265	3TJ	CAE-CAK	6.81	1.50	1.37
6	B	265	3TJ	SAO-NAJ	-5.65	1.55	1.63
6	B	400	3TJ	SAO-NAJ	-5.20	1.56	1.63
6	B	265	3TJ	CAM-SAO	5.01	1.80	1.75
6	B	265	3TJ	CAL-NAN	4.54	1.55	1.43
6	B	400	3TJ	CAL-NAN	4.38	1.55	1.43
6	B	400	3TJ	CAM-SAO	3.06	1.78	1.75
2	A	401	GLU	OXT-C	-2.16	1.23	1.30
2	B	399	GLU	OXT-C	-2.04	1.23	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	265	3TJ	CAI-NAN-CAL	10.00	121.74	110.68
6	B	400	3TJ	CAI-NAN-CAL	9.74	121.45	110.68
6	B	400	3TJ	CAM-SAO-NAJ	8.27	108.91	102.37
6	B	265	3TJ	CAM-SAO-NAJ	7.34	108.18	102.37
6	B	400	3TJ	OAC-SAO-OAB	-4.52	113.85	118.46
6	B	265	3TJ	OAC-SAO-OAB	-3.60	114.78	118.46
6	B	265	3TJ	CAG-CAM-SAO	3.13	122.39	119.82
6	B	265	3TJ	CAK-CAG-CAM	2.83	118.79	116.86
6	B	265	3TJ	OAB-SAO-CAM	-2.65	106.02	109.29
2	B	399	GLU	OXT-C-CA	2.62	122.31	113.38
2	B	399	GLU	OXT-C-O	-2.42	118.60	124.09
6	B	265	3TJ	CAE-CAK-CAG	-2.38	120.20	123.29
2	A	401	GLU	OXT-C-O	-2.21	119.06	124.09
6	B	400	3TJ	OAB-SAO-NAJ	2.13	109.91	107.92
6	B	265	3TJ	CAF-CAE-CAK	2.13	120.57	118.36
6	B	400	3TJ	CAE-CAK-CAG	-2.13	120.53	123.29
6	B	400	3TJ	CAK-CAG-CAM	2.12	118.30	116.86

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	268	GOL	C1-C2-C3-O3
5	A	269	GOL	C1-C2-C3-O3
5	A	272	GOL	O1-C1-C2-O2
5	A	272	GOL	O1-C1-C2-C3
5	B	267	GOL	C1-C2-C3-O3
6	B	400	3TJ	CAA-CAH-NAN-CAI
5	B	267	GOL	O2-C2-C3-O3
5	B	269	GOL	C1-C2-C3-O3
5	A	269	GOL	O2-C2-C3-O3
5	A	270	GOL	O2-C2-C3-O3
5	B	269	GOL	O1-C1-C2-O2
5	A	270	GOL	C1-C2-C3-O3
5	B	268	GOL	O1-C1-C2-O2
5	B	271	GOL	O2-C2-C3-O3
5	B	272	GOL	O2-C2-C3-O3
5	B	269	GOL	O1-C1-C2-C3
6	B	400	3TJ	CAA-CAH-NAN-CAL
2	A	401	GLU	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	267	GOL	1	0
5	A	268	GOL	4	0
5	A	269	GOL	2	0
5	A	270	GOL	2	0
5	B	269	GOL	1	0
5	B	268	GOL	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	260/263 (98%)	0.21	16 (6%) 20 29	9, 20, 47, 66	0
1	B	260/263 (98%)	-0.03	7 (2%) 54 63	8, 15, 36, 58	0
All	All	520/526 (98%)	0.09	23 (4%) 34 44	8, 17, 42, 66	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	ASP	5.4
1	A	67	ASP	5.1
1	B	2	ALA	5.0
1	A	66	ALA	4.8
1	B	3	ASN	4.7
1	A	256	TYR	4.0
1	B	66	ALA	4.0
1	A	262	GLY	3.9
1	A	68	THR	3.4
1	A	259	GLY	3.3
1	A	263	SER	3.1
1	A	257	ASP	3.0
1	A	69	LYS	2.8
1	A	65	ASP	2.7
1	A	160	THR	2.7
1	A	187	LYS	2.6
1	B	258	LYS	2.6
1	B	232	ASN	2.3
1	A	129	LYS	2.2
1	A	185	LYS	2.2
1	A	184	SER	2.1
1	A	131	THR	2.1
1	B	257	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 monosaccharides 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
4	CL	A	273	1/1	0.80	0.16	53,53,53,53	0
5	GOL	A	271	6/6	0.80	0.25	33,44,49,51	0
5	GOL	A	269	6/6	0.81	0.26	26,38,45,46	0
4	CL	B	274	1/1	0.82	0.12	62,62,62,62	0
5	GOL	B	270	6/6	0.82	0.17	37,47,50,54	0
5	GOL	B	267	6/6	0.84	0.16	26,38,44,48	0
5	GOL	B	271	6/6	0.85	0.32	36,46,51,53	0
3	SO4	B	273	5/5	0.86	0.42	53,60,84,87	0
5	GOL	B	272	6/6	0.86	0.26	28,41,51,55	0
5	GOL	B	269	6/6	0.88	0.21	29,41,46,47	0
5	GOL	A	268	6/6	0.88	0.21	39,47,50,54	0
5	GOL	A	270	6/6	0.89	0.16	30,39,44,53	0
5	GOL	A	272	6/6	0.91	0.21	20,24,46,58	0
4	CL	A	266	1/1	0.91	0.08	49,49,49,49	0
4	CL	A	267	1/1	0.93	0.09	57,57,57,57	0
3	SO4	A	265	5/5	0.95	0.20	30,33,39,42	0
5	GOL	B	268	6/6	0.95	0.13	16,28,36,44	0
4	CL	A	274	1/1	0.96	0.12	42,42,42,42	0
2	GLU	A	401	10/10	0.97	0.13	8,11,14,15	0
3	SO4	B	266	5/5	0.98	0.09	22,23,25,27	0
6	3TJ	B	400	15/15	0.98	0.09	10,13,15,16	0
6	3TJ	B	265	15/15	0.98	0.10	8,13,18,20	0
2	GLU	B	399	10/10	0.99	0.12	6,8,10,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.