



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 05:47 PM BST

PDB ID : 4N07
Title : Crystal structure of the GluA2 ligand-binding domain (S1S2J-L483Y-N754S)
in complex with glutamate and BPAM-344 at 1.87 Å resolution
Authors : Noerholm, A.B.; Frydenvang, K.; Kastrup, J.S.
Deposited on : 2013-10-01
Resolution : 1.87 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 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 : 2.14.4.dev1
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) : 2.14.4.dev1

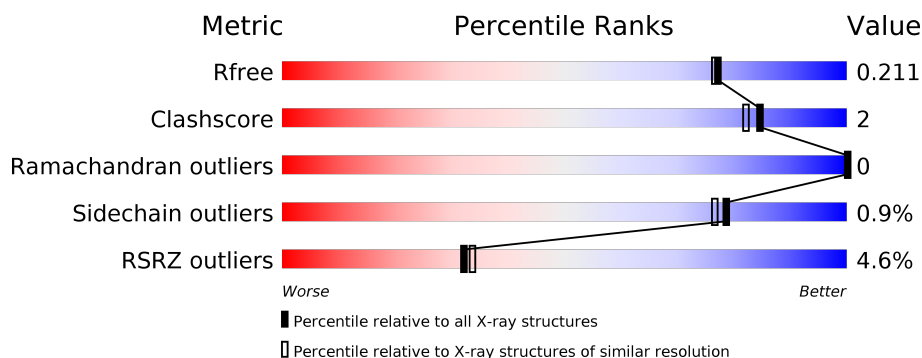
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
1	B	263	<div> <div>6%</div> <div>94%</div> <div>5%</div> </div>
1	C	263	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7058 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.

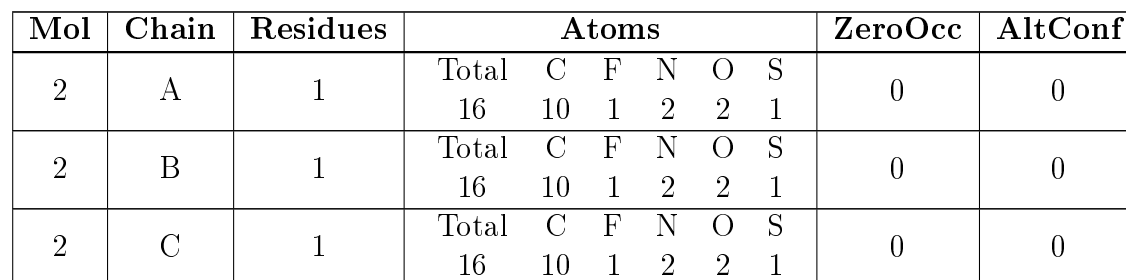
- Molecule 1 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	8	0
			2079	1327	342	395	15			
1	B	260	Total	C	N	O	S	0	3	0
			2046	1306	338	387	15			
1	C	262	Total	C	N	O	S	0	5	0
			2065	1317	340	393	15			

There are 18 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
C	1	GLY	-	EXPRESSION TAG	UNP P19491
C	2	ALA	-	EXPRESSION TAG	UNP P19491
C	94	TYR	LEU	ENGINEERED MUTATION	UNP P19491
C	118	GLY	-	LINKER	UNP P19491
C	119	THR	-	LINKER	UNP P19491
C	242	SER	ASN	ENGINEERED MUTATION	UNP P19491

- Molecule 2 is 4-cyclopropyl-7-fluoro-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (three-letter code: 2J9) (formula: C₁₀H₁₁FN₂O₂S).



- GLU
-
- The diagram shows the chemical structure of Glutamate (GLU). The central carbon atom is labeled 'C' and is bonded to a hydrogen atom (H), an amino group (NH₂), a carboxyl group (COOH), and a side chain. The side chain consists of a methylene group (CH₂) and another carboxyl group (COOH). The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), nitrogen (blue), and sulfur (yellow). The labels for the atoms are: C (grey), O (red), H (white), N (blue), and S (yellow). The labels for the groups are: HO (red), OXT (green), CA(S) (green), CB (green), CG (green), CD (green), OE1 (green), and OE2 (green). The labels for the bonds are: C=O (red), C-N (blue), C-H (grey), C-C (grey), C=O (red), and O-H (red).

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



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

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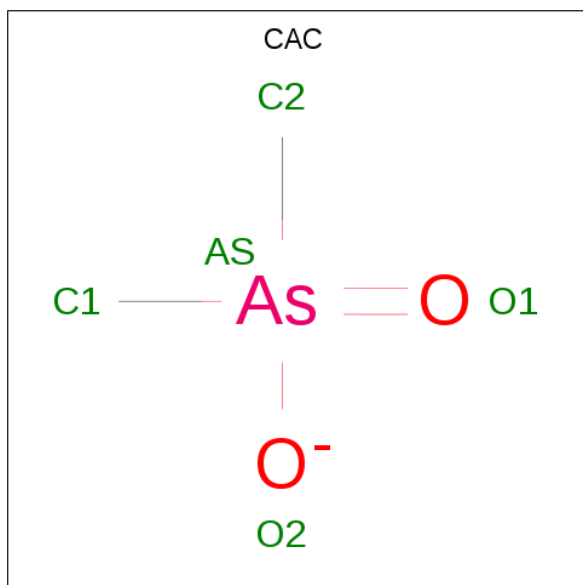
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Zn	0	0
			3	3		
5	A	4	Total	Zn	0	0
			4	4		
5	C	3	Total	Zn	0	0
			3	3		

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

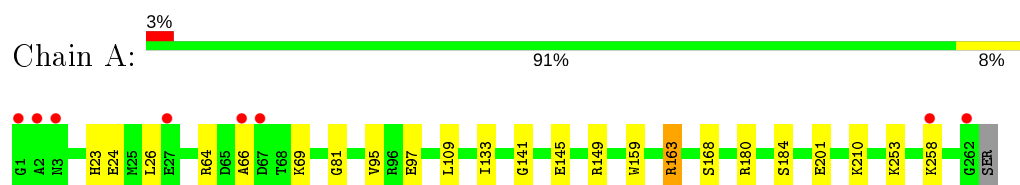
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	270	Total	O	0	0
			270	270		
8	B	210	Total	O	0	0
			210	210		
8	C	207	Total	O	0	0
			207	207		

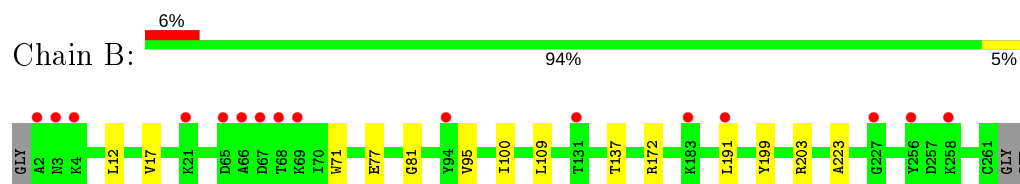
3 Residue-property plots [i](#)

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.

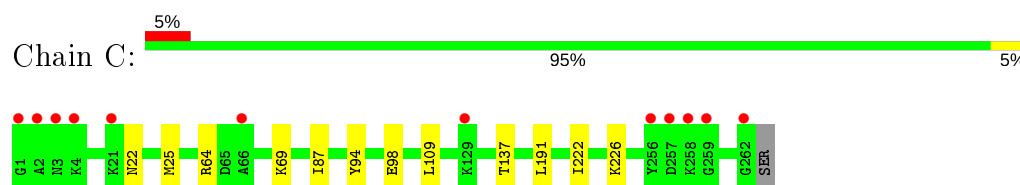
- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2



- 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	113.90 Å 164.03 Å 47.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.48 – 1.87 28.48 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.48-1.87) 99.7 (28.48-1.87)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.87 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.175 , 0.211 0.175 , 0.211	Depositor DCC
R_{free} test set	3737 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7058	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, GOL, ZN, 2J9, ACT

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	0.39	0/2140	0.54	0/2874
1	B	0.37	0/2092	0.52	0/2813
1	C	0.36	0/2117	0.50	0/2846
All	All	0.37	0/6349	0.52	0/8533

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	2079	0	2129	15	0
1	B	2046	0	2083	7	0
1	C	2065	0	2102	8	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
2	C	16	0	11	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	24	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	8	0	6	0	0
4	C	20	0	15	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
6	A	5	0	0	1	0
7	A	24	0	32	4	0
7	B	12	0	16	0	0
8	A	270	0	0	2	0
8	B	210	0	0	2	0
8	C	207	0	0	1	0
All	All	7058	0	6449	30	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 2.

All (30) 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:C:64:ARG:NH2	8:C:566:HOH:O	2.21	0.73
1:C:22:ASN:HB2	1:C:25:MET:HE2	1.71	0.70
1:A:66:ALA:O	1:A:69:LYS:NZ	2.30	0.65
1:A:24:GLU:OE2	8:A:600:HOH:O	2.17	0.57
1:C:137:THR:HG22	1:C:191:LEU:HB2	1.86	0.56
1:A:253:LYS:O	1:A:258:LYS:HG3	2.06	0.56
1:A:201:GLU:OE2	7:A:316:GOL:O3	2.28	0.52
1:B:100:ILE:HD12	1:B:223:ALA:HB1	1.93	0.50
1:C:64:ARG:NH1	1:C:69:LYS:HD2	2.26	0.49
1:A:133:ILE:HD11	7:A:315:GOL:H11	1.95	0.49
1:A:210:LYS:HB3	7:A:316:GOL:H11	1.93	0.49
1:A:141:GLY:O	1:A:145[B]:GLU:HG2	2.13	0.48
1:B:12:LEU:HD23	1:B:17:VAL:HG12	1.98	0.46
1:A:64:ARG:NH2	1:A:69:LYS:HD3	2.31	0.46
1:A:23:HIS:HA	1:A:26:LEU:HD13	1.98	0.45
1:B:77:GLU:OE2	8:B:436:HOH:O	2.20	0.45
1:A:159:TRP:HE1	1:A:163:ARG:CZ	2.31	0.44
1:C:87:ILE:HG12	1:C:222[A]:ILE:HD12	2.00	0.44
1:C:94:TYR:O	1:C:98:GLU:HG3	2.18	0.43
1:C:226:LYS:HD3	1:C:226:LYS:HA	1.75	0.43
1:A:81:GLY:HA2	8:A:472:HOH:O	2.19	0.43
1:B:137:THR:HG22	1:B:191:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG13	1:A:149:ARG:NH1	2.36	0.41
1:A:168:SER:HB2	6:A:313:CAC:O1	2.21	0.41
1:B:199:TYR:O	1:B:203:ARG:HG2	2.20	0.41
1:A:180:ARG:O	1:A:184[A]:SER:HB3	2.21	0.41
1:A:210:LYS:HE3	7:A:316:GOL:H12	2.02	0.41
1:B:81:GLY:HA2	8:B:476:HOH:O	2.20	0.41
1:B:71:TRP:HH2	1:B:95:VAL:HG12	1.85	0.41
1:C:22:ASN:CB	1:C:25:MET:HE2	2.45	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	268/263 (102%)	265 (99%)	3 (1%)	0	100	100
1	B	261/263 (99%)	256 (98%)	5 (2%)	0	100	100
1	C	265/263 (101%)	260 (98%)	5 (2%)	0	100	100
All	All	794/789 (101%)	781 (98%)	13 (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	226/219 (103%)	223 (99%)	3 (1%)	69	64
1	B	221/219 (101%)	219 (99%)	2 (1%)	78	76
1	C	223/219 (102%)	222 (100%)	1 (0%)	91	90
All	All	670/657 (102%)	664 (99%)	6 (1%)	78	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	109	LEU
1	A	163	ARG
1	B	109	LEU
1	B	172	ARG
1	C	109	LEU

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 10 are monoatomic - leaving 26 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	$\# Z > 2$
4	ACT	C	305	5	1,3,3	0.68	0	0,3,3	0.00	-
7	GOL	B	309	-	5,5,5	0.36	0	5,5,5	0.34	0
4	ACT	C	307	5	1,3,3	1.61	0	0,3,3	0.00	-
4	ACT	C	304	-	1,3,3	1.04	0	0,3,3	0.00	-
2	2J9	C	301	-	17,18,18	3.22	7 (41%)	23,28,28	5.37	7 (30%)
2	2J9	B	301	-	17,18,18	3.11	8 (47%)	23,28,28	5.75	6 (26%)
7	GOL	A	316	-	5,5,5	0.42	0	5,5,5	0.24	0
4	ACT	C	306	-	1,3,3	1.51	0	0,3,3	0.00	-
3	GLU	A	302	-	2,9,9	0.44	0	2,11,11	0.27	0
4	ACT	A	307	-	1,3,3	1.15	0	0,3,3	0.00	-
7	GOL	A	314	-	5,5,5	0.38	0	5,5,5	0.31	0
4	ACT	A	303	-	1,3,3	1.13	0	0,3,3	0.00	-
2	2J9	A	301	-	17,18,18	3.15	7 (41%)	23,28,28	5.67	5 (21%)
4	ACT	A	305	5	1,3,3	1.26	0	0,3,3	0.00	-
4	ACT	A	306	5	1,3,3	2.13	1 (100%)	0,3,3	0.00	-
4	ACT	C	303	-	1,3,3	1.21	0	0,3,3	0.00	-
7	GOL	A	317	-	5,5,5	0.36	0	5,5,5	0.30	0
4	ACT	A	304	-	1,3,3	1.43	0	0,3,3	0.00	-
7	GOL	A	315	-	5,5,5	0.43	0	5,5,5	0.52	0
4	ACT	B	304	-	1,3,3	1.58	0	0,3,3	0.00	-
6	CAC	A	313	5	0,4,4	0.00	-	0,6,6	0.00	-
3	GLU	C	302	-	2,9,9	0.29	0	2,11,11	0.63	0
4	ACT	A	308	-	1,3,3	1.43	0	0,3,3	0.00	-
3	GLU	B	302	-	2,9,9	0.38	0	2,11,11	0.23	0
7	GOL	B	308	-	5,5,5	0.37	0	5,5,5	0.37	0
4	ACT	B	303	5	1,3,3	1.27	0	0,3,3	0.00	-

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
7	GOL	A	316	-	-	2/4/4/4	-
7	GOL	A	315	-	-	4/4/4/4	-
7	GOL	B	309	-	-	2/4/4/4	-
3	GLU	C	302	-	-	0/3/9/9	-
3	GLU	A	302	-	-	0/3/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	B	302	-	-	0/3/9/9	-
7	GOL	A	314	-	-	2/4/4/4	-
7	GOL	A	317	-	-	4/4/4/4	-
7	GOL	B	308	-	-	2/4/4/4	-
2	2J9	C	301	-	-	0/4/22/22	0/3/3/3
2	2J9	A	301	-	-	0/4/22/22	0/3/3/3
2	2J9	B	301	-	-	0/4/22/22	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	2J9	OAA-SAP	8.38	1.53	1.43
2	C	301	2J9	OAA-SAP	8.23	1.52	1.43
2	C	301	2J9	OAB-SAP	7.93	1.52	1.43
2	B	301	2J9	OAA-SAP	7.91	1.52	1.43
2	A	301	2J9	OAB-SAP	7.55	1.52	1.43
2	B	301	2J9	OAB-SAP	7.22	1.51	1.43
2	C	301	2J9	CAF-CAK	2.73	1.42	1.37
2	C	301	2J9	CAH-CAN	2.70	1.54	1.48
2	B	301	2J9	CAL-CAM	2.69	1.43	1.40
2	B	301	2J9	CAH-CAN	2.65	1.54	1.48
2	A	301	2J9	CAH-CAN	2.61	1.54	1.48
2	A	301	2J9	CAL-CAM	2.55	1.43	1.40
2	C	301	2J9	CAL-CAM	2.41	1.43	1.40
2	C	301	2J9	CAN-NAO	2.40	1.51	1.47
2	B	301	2J9	CAF-CAK	2.33	1.41	1.37
2	B	301	2J9	CAN-NAO	2.32	1.51	1.47
2	A	301	2J9	CAF-CAK	2.27	1.41	1.37
2	C	301	2J9	CAG-CAN	2.27	1.53	1.48
2	B	301	2J9	CAG-CAN	2.24	1.53	1.48
2	B	301	2J9	CAD-CAK	2.13	1.41	1.37
4	A	306	ACT	CH3-C	2.13	1.51	1.48
2	A	301	2J9	CAG-CAN	2.12	1.53	1.48
2	A	301	2J9	CAN-NAO	2.11	1.51	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	2J9	CAI-NAO-CAL	25.54	121.68	110.25
2	B	301	2J9	CAI-NAO-CAL	25.19	121.52	110.25
2	C	301	2J9	CAI-NAO-CAL	23.83	120.91	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	2J9	OAB-SAP-OAA	-6.84	111.48	118.46
2	A	301	2J9	OAB-SAP-OAA	-6.61	111.72	118.46
2	C	301	2J9	OAB-SAP-OAA	-6.24	112.09	118.46
2	B	301	2J9	CAM-SAP-NAJ	5.32	106.58	102.37
2	B	301	2J9	OAA-SAP-NAJ	4.54	112.15	107.92
2	C	301	2J9	CAM-SAP-NAJ	4.48	105.91	102.37
2	A	301	2J9	CAM-SAP-NAJ	4.26	105.74	102.37
2	C	301	2J9	OAA-SAP-NAJ	3.35	111.04	107.92
2	B	301	2J9	CAI-NAJ-SAP	-2.70	105.28	112.84
2	B	301	2J9	CAM-CAL-NAO	-2.59	119.44	121.57
2	A	301	2J9	OAA-SAP-NAJ	2.37	110.13	107.92
2	C	301	2J9	OAB-SAP-NAJ	2.31	110.07	107.92
2	A	301	2J9	OAB-SAP-NAJ	2.09	109.88	107.92
2	C	301	2J9	CAM-CAL-NAO	-2.06	119.87	121.57
2	C	301	2J9	CAI-NAJ-SAP	-2.03	107.15	112.84

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	314	GOL	O1-C1-C2-C3
7	A	317	GOL	O1-C1-C2-C3
7	A	315	GOL	C1-C2-C3-O3
7	A	315	GOL	O2-C2-C3-O3
7	A	314	GOL	O1-C1-C2-O2
7	B	309	GOL	O1-C1-C2-C3
7	A	316	GOL	O1-C1-C2-C3
7	A	316	GOL	C1-C2-C3-O3
7	A	317	GOL	C1-C2-C3-O3
7	A	315	GOL	O1-C1-C2-C3
7	A	317	GOL	O1-C1-C2-O2
7	A	315	GOL	O1-C1-C2-O2
7	B	309	GOL	O1-C1-C2-O2
7	B	308	GOL	O2-C2-C3-O3
7	A	317	GOL	O2-C2-C3-O3
7	B	308	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	316	GOL	3	0
7	A	315	GOL	1	0
6	A	313	CAC	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	262/263 (99%)	0.08	8 (3%) 49 50	11, 19, 37, 51	0
1	B	260/263 (98%)	0.27	16 (6%) 20 22	13, 25, 43, 60	0
1	C	262/263 (99%)	0.17	12 (4%) 32 34	13, 24, 42, 51	0
All	All	784/789 (99%)	0.18	36 (4%) 32 34	11, 22, 41, 60	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	5.5
1	B	67	ASP	5.3
1	B	66	ALA	5.0
1	B	3	ASN	4.9
1	B	2	ALA	4.6
1	C	262	GLY	3.7
1	A	66	ALA	3.6
1	A	67	ASP	3.5
1	C	3	ASN	3.4
1	B	258	LYS	3.1
1	C	1	GLY	3.0
1	B	21	LYS	3.0
1	C	259	GLY	2.9
1	C	258	LYS	2.9
1	C	256	TYR	2.8
1	A	3	ASN	2.7
1	B	68	THR	2.6
1	B	227	GLY	2.6
1	A	262	GLY	2.6
1	C	66	ALA	2.6
1	B	131	THR	2.5
1	A	258	LYS	2.5
1	B	183	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	129	LYS	2.3
1	A	1	GLY	2.3
1	B	94	TYR	2.3
1	A	27	GLU	2.3
1	B	65	ASP	2.2
1	C	21	LYS	2.2
1	B	69	LYS	2.1
1	C	4	LYS	2.1
1	B	256	TYR	2.1
1	C	257	ASP	2.1
1	B	4	LYS	2.1
1	B	191	LEU	2.0
1	A	2	ALA	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	ACT	C	305	4/4	0.71	0.16	38,43,47,50	0
7	GOL	A	316	6/6	0.78	0.17	26,30,41,43	0
4	ACT	C	304	4/4	0.81	0.17	42,44,45,48	0
4	ACT	C	307	4/4	0.82	0.21	34,35,40,47	0
7	GOL	B	309	6/6	0.83	0.18	30,36,43,44	0
4	ACT	A	308	4/4	0.83	0.20	37,43,43,44	0
4	ACT	A	307	4/4	0.84	0.25	42,48,48,50	0
7	GOL	B	308	6/6	0.84	0.28	32,39,45,45	0
7	GOL	A	317	6/6	0.84	0.27	40,41,44,50	0
7	GOL	A	314	6/6	0.84	0.21	28,36,40,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	A	315	6/6	0.85	0.41	28,32,38,46	0
4	ACT	B	304	4/4	0.86	0.34	37,41,43,43	0
4	ACT	A	303	4/4	0.88	0.15	27,27,30,37	0
4	ACT	C	306	4/4	0.90	0.14	34,40,41,46	0
4	ACT	B	303	4/4	0.91	0.21	37,37,37,43	0
4	ACT	A	304	4/4	0.92	0.20	32,32,33,40	0
4	ACT	C	303	4/4	0.93	0.16	21,24,25,29	0
5	ZN	C	309	1/1	0.93	0.11	67,67,67,67	0
4	ACT	A	305	4/4	0.94	0.12	31,31,33,36	0
5	ZN	C	310	1/1	0.94	0.10	35,35,35,35	1
5	ZN	B	307	1/1	0.95	0.14	78,78,78,78	0
5	ZN	A	310	1/1	0.95	0.11	62,62,62,62	0
4	ACT	A	306	4/4	0.96	0.17	29,32,36,38	0
3	GLU	B	302	10/10	0.97	0.16	16,19,22,24	0
5	ZN	B	306	1/1	0.97	0.05	31,31,31,31	0
5	ZN	C	308	1/1	0.97	0.04	47,47,47,47	0
3	GLU	C	302	10/10	0.98	0.17	12,14,20,20	0
2	2J9	A	301	16/16	0.98	0.12	11,12,13,14	0
2	2J9	C	301	16/16	0.98	0.09	11,13,16,17	0
2	2J9	B	301	16/16	0.98	0.12	13,16,18,18	0
3	GLU	A	302	10/10	0.98	0.15	10,13,14,15	0
5	ZN	A	312	1/1	0.99	0.03	29,29,29,29	0
5	ZN	A	311	1/1	0.99	0.05	23,23,23,23	1
5	ZN	A	309	1/1	0.99	0.02	25,25,25,25	0
5	ZN	B	305	1/1	0.99	0.05	17,17,17,17	0
6	CAC	A	313	5/5	0.99	0.09	18,18,24,28	5

6.5 Other polymers ⓘ

There are no such residues in this entry.