W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2014 – 02:58 PM EDT

PDB ID	:	4U4G
Title	:	Structure of GluA2* in complex with competitive antagonist ZK 200775
Authors	:	Yelshanskaya, M.V.; Li, M.; Sobolevsky, A.I.
Deposited on	:	2014-07-23
Resolution	:	4.49 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 4.49 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		7
Ramachandran outliers		1.2%
Sidechain outliers		3.7%
RSRZ outliers		6.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	77520	1000 (5.46-3.52)
Clashscore	88313	1006 (5.30-3.60)
Ramachandran outliers	86584	1043 (5.46-3.52)
Cα geometry	86677	1000 (5.30-3.58)
Sidechain outliers	86556	1023 (5.46-3.52)
RSRZ outliers	77580	1335 (5.50-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	827	
1	B	827	
1	C	827	
1	D	827	

2   Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23812 atoms, of which 0 are hydrogen and 0 are deuterium.

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	773	Total 5966	C 3823	F 3	N 976	O 1135	P 1	S 28	0	0	0
1	B	773	Total 5946	C 3809	F 3	N 966	O 1139	P 1	S 28	0	0	0
1	C	773	Total 5940	C 3805	F 3	N 968	O 1135	P 1	S 28	0	0	0
1	D	773	Total 5960	C 3818	F 3	N 971	O 1139	P 1	S 28	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	828	GLY	-	expression tag	UNP P19491
A	829	LEU	-	expression tag	UNP P19491
A	830	VAL	-	expression tag	UNP P19491
A	831	PRO	-	expression tag	UNP P19491
A	832	ARG	-	expression tag	UNP P19491
A	833	ZK1	-	expression tag	UNP P19491
A	834	NAG	-	expression tag	UNP P19491
A	835	NAG	-	expression tag	UNP P19491
A	836	BMA	-	expression tag	UNP P19491
A	837	BMA	-	expression tag	UNP P19491

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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	828	GLY	-	expression tag	UNP P19491
B	829	LEU	-	expression tag	UNP P19491
B	830	VAL	-	expression tag	UNP P19491
B	831	PRO	-	expression tag	UNP P19491
B	832	ARG	-	expression tag	UNP P19491
B	833	ZK1	-	expression tag	UNP P19491
B	834	NAG	-	expression tag	UNP P19491
B	835	NAG	-	expression tag	UNP P19491
B	836	BMA	-	expression tag	UNP P19491
B	837	BMA	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	828	GLY	-	expression tag	UNP P19491
C	829	LEU	-	expression tag	UNP P19491
C	830	VAL	-	expression tag	UNP P19491
C	831	PRO	-	expression tag	UNP P19491
C	832	ARG	-	expression tag	UNP P19491
C	833	ZK1	-	expression tag	UNP P19491
C	834	NAG	-	expression tag	UNP P19491
C	835	NAG	-	expression tag	UNP P19491
C	836	BMA	-	expression tag	UNP P19491
C	837	BMA	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	828	GLY	-	expression tag	UNP P19491
D	829	LEU	-	expression tag	UNP P19491
D	830	VAL	-	expression tag	UNP P19491
D	831	PRO	-	expression tag	UNP P19491
D	832	ARG	-	expression tag	UNP P19491
D	833	ZK1	-	expression tag	UNP P19491
D	834	NAG	-	expression tag	UNP P19491
D	835	NAG	-	expression tag	UNP P19491
D	836	BMA	-	expression tag	UNP P19491
D	837	BMA	-	expression tag	UNP P19491

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:

- Molecule 1: Glutamate receptor 2

Chain B:

W526 M527 C528 I529 V530 F531 A532 Y533 I534 G535 V536 S537 V538 V539 V543 S544 ARG PHE SER PRO TYR GLU TRP HIS THR GLU GLU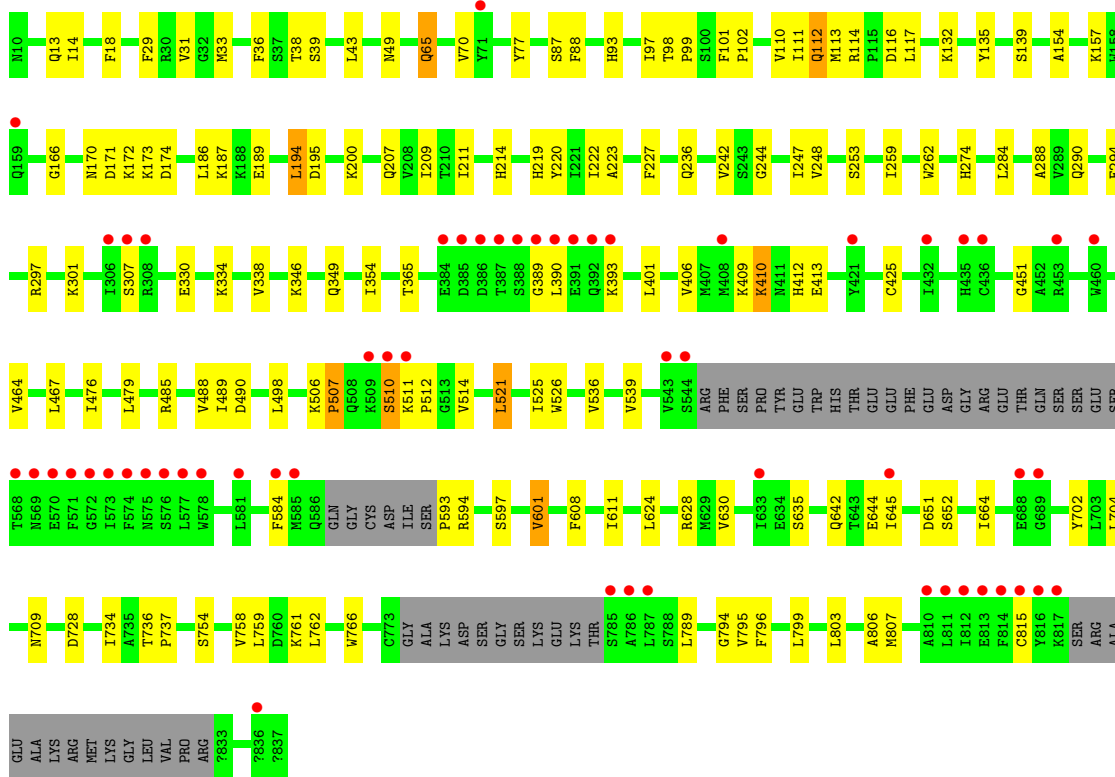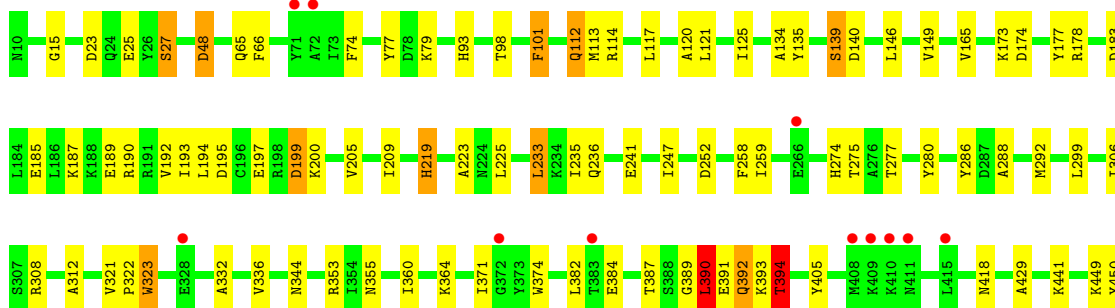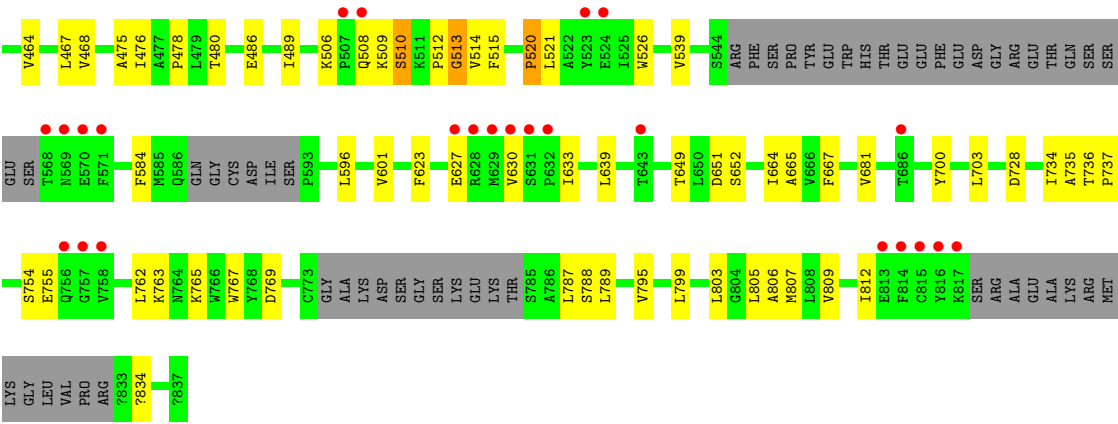 PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER T568 N569 E570 F584 M585 Q586 GLN GLY CYS ASP ILE SER P593 S597 V601 W605

F608 I611 I612 I613 T617 A618 N619 V626 E627 R628 I633 A636 Y647 G648 T649 L650 D651 S652 F659 S662 K663 I664 A665 V666 F667 W671 R684 T685 T686 A687 A701 Y702 L703 T707 M708 N709 E710 Y711 Q714 R715 D719 D728 Y732

A735 G743 D760 K761 L762 K763 W767 C773 GLY ALA LYS ASP SER GLY SER LYS GLU LYS THR S785 L789 S790 N791 V792 A793 G794 L803 V809 A810 L811 F814 C815 Y816 K817 SER ARG GLU ALA LYS ARG MET LYS GLY LEU VAL PRO ARG ?833 ?837

● Molecule 1: Glutamate receptor 2

Chain C:

M10 Q13 I14 F18 F29 R30 V31 G32 M33 F36 S37 T38 S39 L43 N49 Q65 V70 Y71 Y77 S87 F88 H93 I97 T98 P99 S100 F101 P102 V110 I111 Q112 M113 R114 P115 D116 L117 K132 Y135 S139 A154 K157 W158

Q159 G166 N170 D171 K172 K173 D174 L186 K187 K188 E189 L194 D195 K200 Q207 V208 I209 T210 I211 H214 H219 Y220 I221 I222 A223 F227 Q236 V242 S243 G244 I247 V248 S253 I259 W262 H274 L284 A288 V289 Q290 E294

R297 K301 I306 S307 R308 E330 K334 V338 K346 Q349 I354 T365 E384 D385 D386 T387 S388 G389 L390 E391 Q392 K393 L401 V406 M407 M408 K409 K410 N411 H412 E413 Y421 C425 I432 H435 C436 G451 A452 R453 W460

V464 L467 I476 L479 R485 V488 I489 D490 L498 K506 P507 Q508 K509 S510 K511 P512 G513 V514 L521 I525 W526 V536 V539 V543 S544 ARG PHE SER PRO TYR GLU TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER

T568 N569 E570 F571 G572 I573 F574 N575 S576 L577 W578 L581 F584 M585 Q586 GLN GLY CYS ASP ILE SER P593 R594 S597 V601 F608 I611 L624 R628 M629 V630 I633 E634 S635 Q642 T643 E644 I645 D651 S652 I664 E688 G689 Y702 L703 L704

N709 D728 I734 A735 T736 P737 S754 V758 L759 D760 K761 L762 W766 C773 GLY ALA LYS ASP SER GLY SER LYS GLU LYS THR S785 A786 L787 S788 L789 G794 V795 F796 L799 L803 A806 M807 A810 L811 I812 E813 F814 C815 Y816 K817 SER ARG ALA

GLU ALA LYS ARG MET LYS GLY LEU VAL PRO ARG ?833 ?836 ?837

● Molecule 1: Glutamate receptor 2

Chain D:

N10 G15 D23 Q24 E25 Y26 S27 D48 Q65 F66 Y71 A72 I73 F74 Y77 D78 K79 H93 T98 F101 Q112 M113 R114 L117 A120 L121 I125 A134 Y135 S139 D140 L146 V149 V165 K173 D174 Y177 R178 D183

L184 E185 L186 K187 K188 E189 R190 R191 V192 I193 L194 D195 C196 E197 R198 D199 K200 V205 I209 H219 A223 N224 L225 L233 K234 I235 Q236 E241 I247 D252 F258 I259 E266 H274 T275 A276 T277 Y280 Y286 D287 A288 M292 L299 I306

S307 R308 A312 V321 P322 W323 E328 A332 V336 N344 R353 I354 N355 I360 K364 I371 G372 Y373 W374 L382 T383 E384 T387 S388 G389 L390 E391 Q392 K393 I394 Y405 M408 K409 K410 N411 L415 N418 A429 K441 K449 Y450

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.00Å 310.36Å 109.50Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	50.00 – 4.49 48.72 – 4.49	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-4.49) 98.7 (48.72-4.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 4.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.217 , 0.248 0.218 , 0.249	Depositor DCC
R_{free} test set	1796 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	206.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 65.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Outliers	0 of 36039 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23812	wwPDB-VP
Average B, all atoms (Å^2)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, ZK1

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	0.23	0/6010	0.39	0/8148
1	B	0.23	0/5990	0.39	0/8128
1	C	0.23	0/5984	0.40	0/8121
1	D	0.23	0/6004	0.40	0/8143
All	All	0.23	0/23988	0.40	0/32540

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0
1	B	2	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	834	NAG	C1
1	A	836	BMA	C1
1	B	834	NAG	C1
1	B	835	NAG	C1

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5966	0	5794	87	0
1	B	5946	0	5736	85	0
1	C	5940	0	5728	85	0
1	D	5960	0	5769	84	0
All	All	23812	0	23027	307	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 307 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:510:SER:H	1:D:512:PRO:HD3	1.48	0.79
1:B:102:PRO:HD3	1:B:114:ARG:HD2	1.63	0.78
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.72	0.71
1:A:736:THR:HG21	1:A:743:GLY:HA2	1.72	0.71
1:B:255:VAL:HG13	1:B:341:LEU:HD22	1.73	0.70

There are no symmetry-related clashes.

5.3 Torsion angles

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	760/827 (92%)	694 (91%)	57 (8%)	9 (1%)	18	70
1	B	760/827 (92%)	701 (92%)	52 (7%)	7 (1%)	23	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	760/827 (92%)	683 (90%)	70 (9%)	7 (1%)	23	74
1	D	760/827 (92%)	689 (91%)	58 (8%)	13 (2%)	13	64
All	All	3040/3308 (92%)	2767 (91%)	237 (8%)	36 (1%)	18	70

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ASP
1	A	410	LYS
1	A	512	PRO
1	A	597	SER
1	D	514	VAL

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	615/702 (88%)	602 (98%)	13 (2%)	64	89
1	B	611/702 (87%)	584 (96%)	27 (4%)	37	77
1	C	609/702 (87%)	587 (96%)	22 (4%)	45	82
1	D	614/702 (88%)	585 (95%)	29 (5%)	35	76
All	All	2449/2808 (87%)	2358 (96%)	91 (4%)	44	81

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	87	SER
1	C	248	VAL
1	D	508	GLN
1	C	88	PHE
1	C	194	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	B	619	ASN
1	C	13	GLN
1	C	65	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

16 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	NAG	A	834	1	14,14,15	0.53	0	19,19,21	1.25	1 (5%)
1	NAG	A	835	1	14,14,15	0.47	0	19,19,21	0.86	0
1	BMA	A	836	1	11,11,12	0.60	0	15,15,17	0.81	0
1	BMA	A	837	1	11,11,12	0.61	0	15,15,17	0.87	0
1	NAG	B	834	1	14,14,15	0.53	0	19,19,21	1.07	1 (5%)
1	NAG	B	835	1	14,14,15	0.43	0	19,19,21	1.08	2 (10%)
1	BMA	B	836	1	11,11,12	0.60	0	15,15,17	0.87	0
1	BMA	B	837	1	11,11,12	0.58	0	15,15,17	0.89	0
1	NAG	C	834	1	14,14,15	0.55	0	19,19,21	0.99	2 (10%)
1	NAG	C	835	1	14,14,15	0.50	0	19,19,21	0.90	1 (5%)
1	BMA	C	836	1	11,11,12	0.59	0	15,15,17	0.86	0
1	BMA	C	837	1	11,11,12	0.65	0	15,15,17	0.84	0
1	NAG	D	834	1	14,14,15	0.65	0	19,19,21	1.80	4 (21%)
1	NAG	D	835	1	14,14,15	0.49	0	19,19,21	0.84	0
1	BMA	D	836	1	11,11,12	0.56	0	15,15,17	0.82	0
1	BMA	D	837	1	11,11,12	0.64	0	15,15,17	0.85	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
1	NAG	A	834	1	1/1/5/7	0/6/23/26	0/1/1/1
1	NAG	A	835	1	-	0/6/23/26	0/1/1/1
1	BMA	A	836	1	1/1/4/5	0/2/19/22	0/1/1/1
1	BMA	A	837	1	-	0/2/19/22	0/1/1/1
1	NAG	B	834	1	1/1/5/7	0/6/23/26	0/1/1/1
1	NAG	B	835	1	1/1/5/7	2/6/23/26	0/1/1/1
1	BMA	B	836	1	-	0/2/19/22	0/1/1/1
1	BMA	B	837	1	-	0/2/19/22	0/1/1/1
1	NAG	C	834	1	-	0/6/23/26	0/1/1/1
1	NAG	C	835	1	-	0/6/23/26	0/1/1/1
1	BMA	C	836	1	-	0/2/19/22	0/1/1/1
1	BMA	C	837	1	-	0/2/19/22	0/1/1/1
1	NAG	D	834	1	-	0/6/23/26	0/1/1/1
1	NAG	D	835	1	-	0/6/23/26	0/1/1/1
1	BMA	D	836	1	-	0/2/19/22	0/1/1/1
1	BMA	D	837	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	834	NAG	C2-N2-C7	-5.28	116.65	123.42
1	A	834	NAG	C1-C2-C3	3.57	114.80	109.15
1	D	834	NAG	C1-C2-C3	3.16	114.14	109.15
1	B	834	NAG	C1-C2-C3	3.04	113.96	109.15
1	B	835	NAG	C1-O5-C5	2.78	115.71	112.13

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	834	NAG	C1
1	A	834	NAG	C1
1	B	835	NAG	C1
1	A	836	BMA	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	835	NAG	O7-C7-N2-C2
1	B	835	NAG	C8-C7-N2-C2

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	772/827 (93%)	0.29	42 (5%)	24	23	58, 156, 267, 497	0
1	B	772/827 (93%)	0.42	61 (7%)	12	16	41, 167, 300, 506	0
1	C	772/827 (93%)	0.42	57 (7%)	14	17	45, 148, 265, 547	0
1	D	772/827 (93%)	0.32	35 (4%)	31	29	27, 135, 292, 515	0
All	All	3088/3308 (93%)	0.36	195 (6%)	19	21	27, 151, 277, 547	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	571	PHE	11.3
1	C	572	GLY	10.6
1	C	570	GLU	10.5
1	A	309	ARG	9.6
1	A	837	BMA	9.1

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å²)	Q<0.9
1	NAG	A	834	14/15	0.64	16.67	227,227,227,227	0
1	BMA	B	837	11/12	0.44	4.50	231,231,231,231	0
1	NAG	D	835	14/15	0.26	3.44	294,294,294,294	0
1	NAG	B	834	14/15	0.52	2.65	167,167,167,167	0
1	NAG	C	834	14/15	0.53	2.47	211,211,211,211	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
1	NAG	D	834	14/15	0.30	1.52	336,336,336,336	0
1	BMA	B	836	11/12	0.40	-	232,232,232,232	0
1	BMA	D	836	11/12	0.22	-	233,233,233,233	0
1	BMA	D	837	11/12	0.24	-	264,264,264,264	0
1	BMA	A	837	11/12	1.82	-	269,269,269,269	0
1	BMA	C	837	11/12	0.54	-	287,287,287,287	0
1	NAG	A	835	14/15	0.68	-	269,269,269,269	0
1	BMA	C	836	11/12	0.70	-	254,254,254,254	0
1	NAG	C	835	14/15	0.43	-	225,225,225,225	0
1	NAG	B	835	14/15	0.26	-	180,180,180,180	0
1	BMA	A	836	11/12	0.79	-	280,280,280,280	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.