



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2016 – 05:28 PM EDT

PDB ID : 5L1B  
Title : AMPA subtype ionotropic glutamate receptor GluA2 in Apo state  
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.  
Deposited on : 2016-07-28  
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

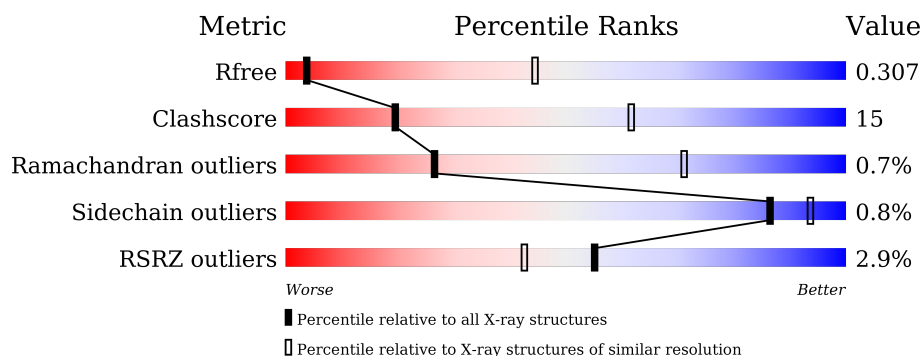
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	803	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>..</div> </div> </div>
1	B	803	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>..</div> </div> </div>
1	C	803	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>
1	D	803	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24156 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	780	Total	C	N	O	S	0	0	0
			6017	3865	995	1128	29			
1	B	780	Total	C	N	O	S	0	0	0
			6022	3868	995	1130	29			
1	C	780	Total	C	N	O	S	0	0	0
			6023	3868	995	1131	29			
1	D	783	Total	C	N	O	S	0	0	0
			6038	3875	998	1136	29			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	?	-	VAL	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	?	-	GLY	deletion	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	564	ASP	-	linker	UNP P19491
A	565	THR	-	linker	UNP P19491
A	566	ASP	-	linker	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	827	GLY	-	cloning artifact	UNP P19491
A	828	LEU	-	cloning artifact	UNP P19491
A	829	VAL	-	cloning artifact	UNP P19491
A	830	PRO	-	cloning artifact	UNP P19491
A	831	ARG	-	cloning artifact	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	-	VAL	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

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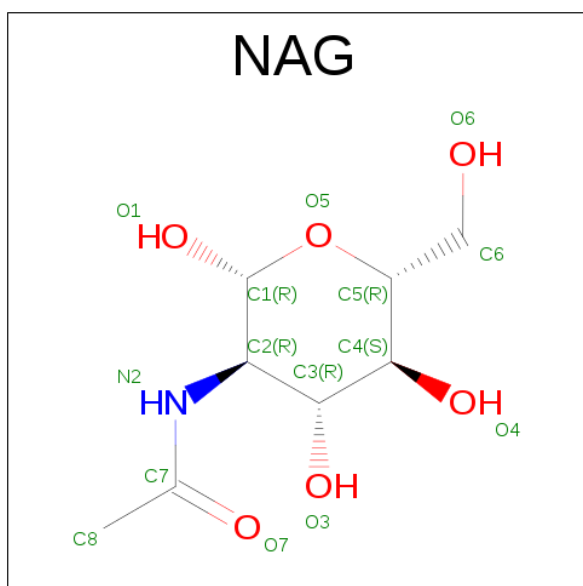
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
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B	829	VAL	-	cloning artifact	UNP P19491
B	830	PRO	-	cloning artifact	UNP P19491
B	831	ARG	-	cloning artifact	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	-	VAL	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
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C	829	VAL	-	cloning artifact	UNP P19491
C	830	PRO	-	cloning artifact	UNP P19491
C	831	ARG	-	cloning artifact	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	-	VAL	deletioin	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	?	-	GLY	deletion	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	545	ASP	-	linker	UNP P19491
D	546	THR	-	linker	UNP P19491
D	547	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491
D	830	PRO	-	cloning artifact	UNP P19491
D	831	ARG	-	cloning artifact	UNP P19491

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

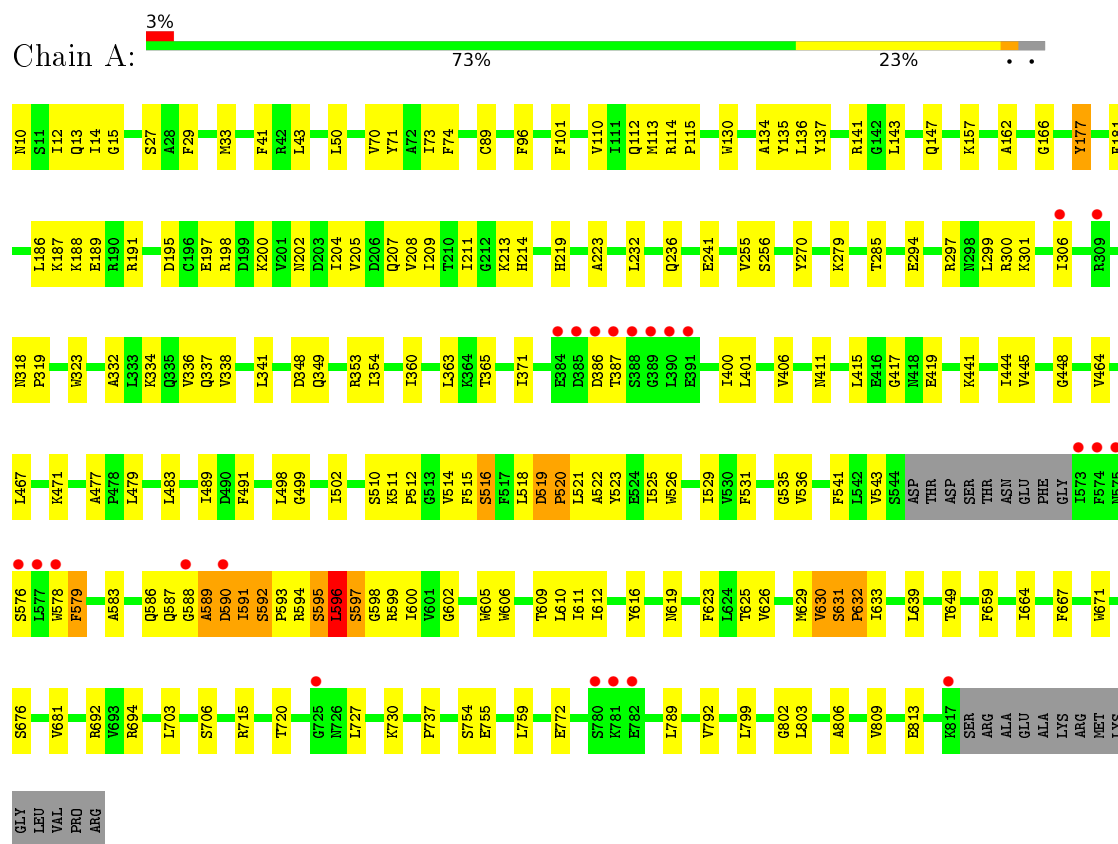


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

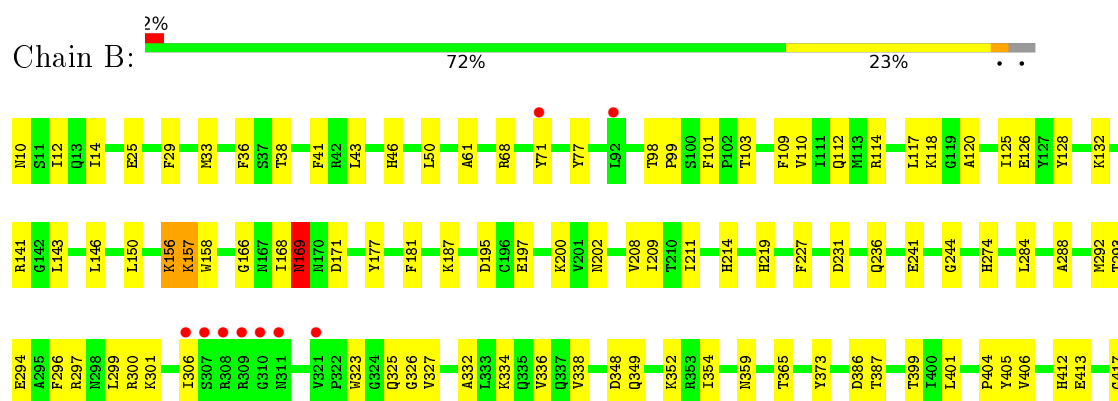
### 3 Residue-property plots

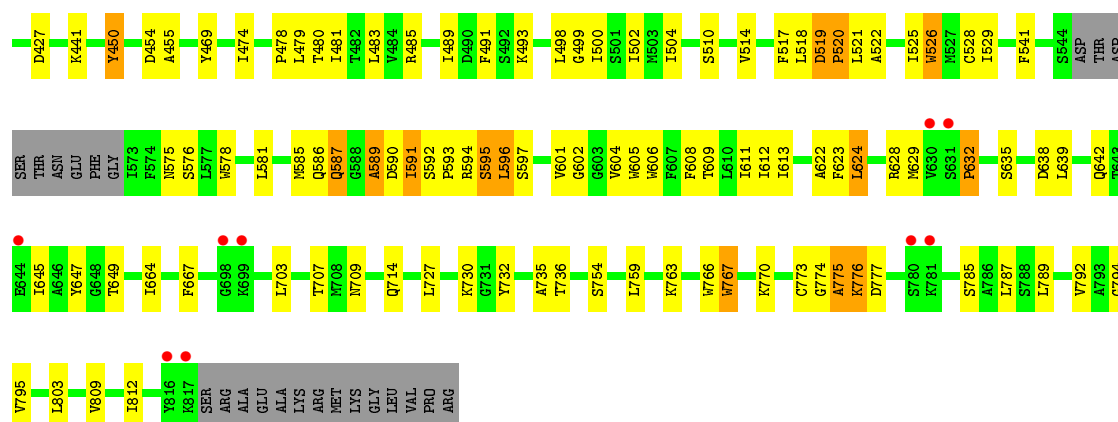
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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

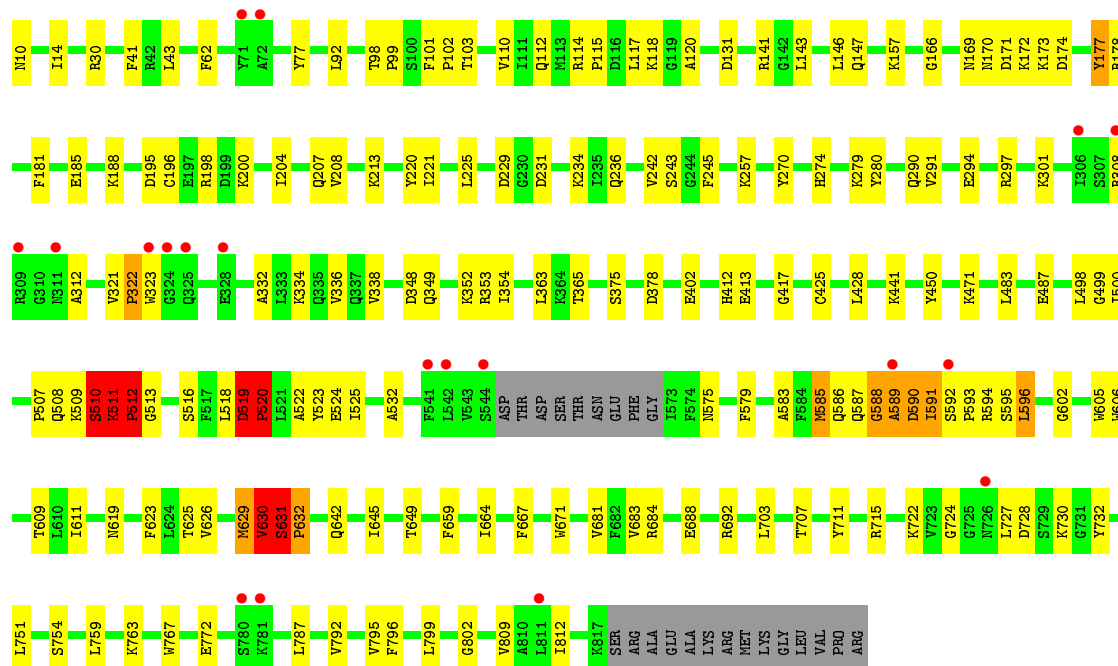
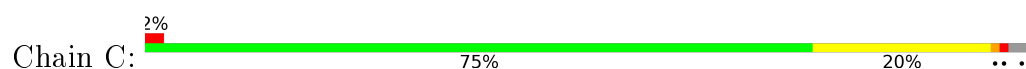


#### • Molecule 1: Glutamate receptor 2

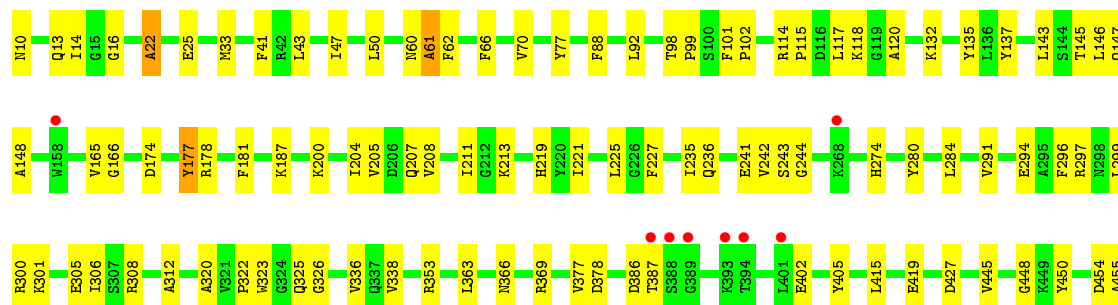
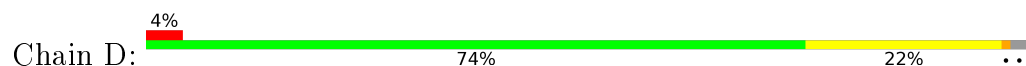




• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.05Å 309.39Å 110.02Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	48.55 – 4.00 48.55 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.55-4.00) 97.7 (48.55-4.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.265 , 0.292 0.283 , 0.307	Depositor DCC
$R_{free}$ test set	2520 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	175.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 94.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	24156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG

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	2/6143 (0.0%)	0.62	14/8319 (0.2%)
1	B	0.35	3/6148 (0.0%)	0.74	22/8326 (0.3%)
1	C	0.50	4/6149 (0.1%)	0.69	26/8327 (0.3%)
1	D	0.41	4/6164 (0.1%)	0.62	14/8349 (0.2%)
All	All	0.41	13/24604 (0.1%)	0.67	76/33321 (0.2%)

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	B	0	1
1	D	0	3
All	All	0	4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	PRO	N-CD	22.80	1.79	1.47
1	D	632	PRO	N-CD	22.49	1.79	1.47
1	A	632	PRO	N-CD	18.31	1.73	1.47
1	C	322	PRO	N-CD	-17.32	1.23	1.47
1	B	520	PRO	N-CD	15.40	1.69	1.47

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	589	ALA	CB-CA-C	-20.51	79.33	110.10
1	C	589	ALA	CB-CA-C	-20.01	80.09	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	ALA	CB-CA-C	-18.58	82.23	110.10
1	B	775	ALA	N-CA-C	18.00	159.61	111.00
1	B	775	ALA	CB-CA-C	-16.71	85.03	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	450	TYR	Peptide
1	D	587	GLN	Mainchain
1	D	595	SER	Peptide
1	D	772	GLU	Peptide

## 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	6017	0	5899	210	1
1	B	6022	0	5906	212	1
1	C	6023	0	5907	180	0
1	D	6038	0	5906	218	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
All	All	24156	0	23670	718	1

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 15.

The worst 5 of 718 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:B:587:GLN:HE22	1:C:586:GLN:CB	1.01	1.55
1:D:711:TYR:HB2	1:D:767:TRP:CZ3	1.49	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:GLN:HE22	1:D:586:GLN:CB	1.29	1.43
1:A:632:PRO:N	1:A:632:PRO:CD	1.73	1.41
1:B:587:GLN:NE2	1:C:586:GLN:CB	1.74	1.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:OG	1:B:469:TYR:OH[1_556]	2.19	0.01

## 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	776/803 (97%)	721 (93%)	51 (7%)	4 (0%)	34	76
1	B	776/803 (97%)	716 (92%)	56 (7%)	4 (0%)	34	76
1	C	776/803 (97%)	722 (93%)	43 (6%)	11 (1%)	14	59
1	D	779/803 (97%)	724 (93%)	52 (7%)	3 (0%)	39	79
All	All	3107/3212 (97%)	2883 (93%)	202 (6%)	22 (1%)	26	71

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	SER
1	C	511	LYS
1	C	585	MET
1	C	629	MET
1	C	631	SER

### 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	631/683 (92%)	626 (99%)	5 (1%)	86	93
1	B	632/683 (92%)	626 (99%)	6 (1%)	84	93
1	C	633/683 (93%)	629 (99%)	4 (1%)	90	95
1	D	633/683 (93%)	628 (99%)	5 (1%)	86	93
All	All	2529/2732 (93%)	2509 (99%)	20 (1%)	86	93

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	517	PHE
1	B	526	TRP
1	D	593	PRO
1	B	177	TYR
1	B	197	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	587	GLN
1	D	219	HIS
1	C	587	GLN
1	B	359	ASN
1	B	714	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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	$\# Z  > 2$
2	NAG	A	901	1	14,14,15	0.17	0	15,19,21	0.39	0
2	NAG	B	901	1	14,14,15	0.24	0	15,19,21	0.30	0
2	NAG	C	901	1	14,14,15	0.19	0	15,19,21	0.36	0
2	NAG	D	901	1	14,14,15	0.21	0	15,19,21	0.35	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	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	587:GLN	C	588:GLY	N	1.20

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	780/803 (97%)	-0.27	23 (2%) 55 42	93, 169, 256, 282	0
1	B	780/803 (97%)	-0.24	18 (2%) 64 52	92, 148, 268, 287	0
1	C	780/803 (97%)	-0.13	19 (2%) 62 51	93, 180, 264, 285	0
1	D	783/803 (97%)	-0.04	31 (3%) 42 31	94, 205, 257, 278	0
All	All	3123/3212 (97%)	-0.17	91 (2%) 55 42	92, 170, 260, 287	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	781	LYS	6.8
1	B	309	ARG	6.0
1	A	781	LYS	5.9
1	A	576	SER	5.5
1	D	779	GLY	4.5

### 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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	901	14/15	0.89	0.18	-	259,259,259,259	0
2	NAG	B	901	14/15	0.91	0.20	-	239,239,239,239	0
2	NAG	D	901	14/15	0.90	0.21	-	216,216,216,216	0
2	NAG	A	901	14/15	0.87	0.24	-	217,217,217,217	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.