



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 08:13 am GMT

PDB ID : 5FTH  
Title : Crystal structure of the GluA2 K738M-T744K LBD in complex with glutamate (zinc form)  
Authors : Nayeem, N.; Green, T.  
Deposited on : 2016-01-13  
Resolution : 2.90 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](mailto: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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

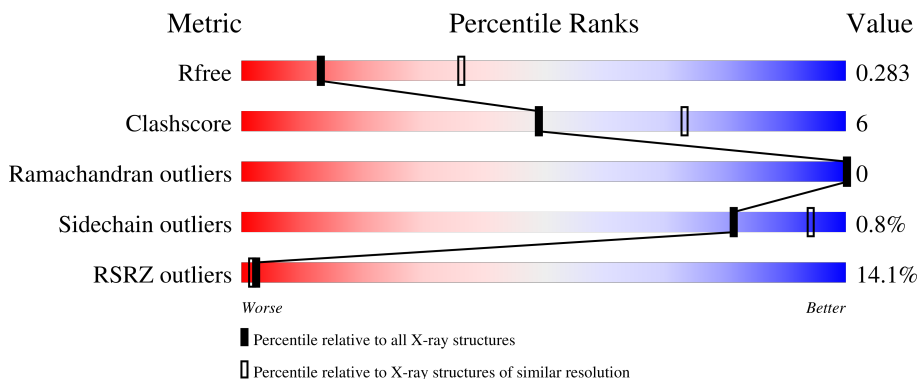
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	291	
1	B	291	
1	C	291	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5908 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	248	1944	1247	320	362	15	0	0	0
1	B	249	1947	1244	320	368	15	0	0	0
1	C	254	1982	1267	327	374	14	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	MET	-	expression tag	UNP P19491
A	363	HIS	-	expression tag	UNP P19491
A	364	HIS	-	expression tag	UNP P19491
A	365	HIS	-	expression tag	UNP P19491
A	366	HIS	-	expression tag	UNP P19491
A	367	HIS	-	expression tag	UNP P19491
A	368	HIS	-	expression tag	UNP P19491
A	369	HIS	-	expression tag	UNP P19491
A	370	HIS	-	expression tag	UNP P19491
A	371	SER	-	expression tag	UNP P19491
A	372	SER	-	expression tag	UNP P19491
A	373	GLY	-	expression tag	UNP P19491
A	374	LEU	-	expression tag	UNP P19491
A	375	VAL	-	expression tag	UNP P19491
A	376	PRO	-	expression tag	UNP P19491
A	377	ARG	-	expression tag	UNP P19491
A	378	GLY	-	expression tag	UNP P19491
A	379	SER	-	expression tag	UNP P19491
A	380	ALA	-	expression tag	UNP P19491
A	381	MET	-	expression tag	UNP P19491
A	382	GLY	-	expression tag	UNP P19491
A	389	ARG	GLY	engineered mutation	UNP P19491
A	390	GLY	LEU	engineered mutation	UNP P19491

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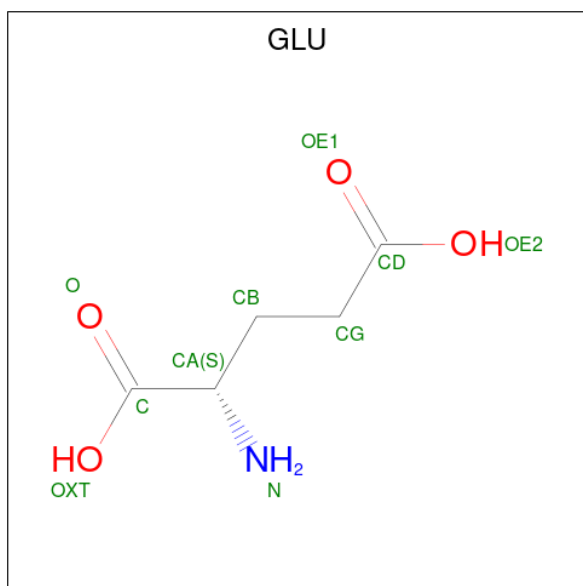
Chain	Residue	Modelled	Actual	Comment	Reference
A	391	ALA	GLU	engineered mutation	UNP P19491
A	555	GLY	-	linker	UNP P19491
A	566	THR	-	linker	UNP P19491
A	738	MET	LYS	engineered mutation	UNP P19491
A	744	LYS	THR	engineered mutation	UNP P19491
B	362	MET	-	expression tag	UNP P19491
B	363	HIS	-	expression tag	UNP P19491
B	364	HIS	-	expression tag	UNP P19491
B	365	HIS	-	expression tag	UNP P19491
B	366	HIS	-	expression tag	UNP P19491
B	367	HIS	-	expression tag	UNP P19491
B	368	HIS	-	expression tag	UNP P19491
B	369	HIS	-	expression tag	UNP P19491
B	370	HIS	-	expression tag	UNP P19491
B	371	SER	-	expression tag	UNP P19491
B	372	SER	-	expression tag	UNP P19491
B	373	GLY	-	expression tag	UNP P19491
B	374	LEU	-	expression tag	UNP P19491
B	375	VAL	-	expression tag	UNP P19491
B	376	PRO	-	expression tag	UNP P19491
B	377	ARG	-	expression tag	UNP P19491
B	378	GLY	-	expression tag	UNP P19491
B	379	SER	-	expression tag	UNP P19491
B	380	ALA	-	expression tag	UNP P19491
B	381	MET	-	expression tag	UNP P19491
B	382	GLY	-	expression tag	UNP P19491
B	389	ARG	GLY	engineered mutation	UNP P19491
B	390	GLY	LEU	engineered mutation	UNP P19491
B	391	ALA	GLU	engineered mutation	UNP P19491
B	555	GLY	-	linker	UNP P19491
B	566	THR	-	linker	UNP P19491
B	738	MET	LYS	engineered mutation	UNP P19491
B	744	LYS	THR	engineered mutation	UNP P19491
C	362	MET	-	expression tag	UNP P19491
C	363	HIS	-	expression tag	UNP P19491
C	364	HIS	-	expression tag	UNP P19491
C	365	HIS	-	expression tag	UNP P19491
C	366	HIS	-	expression tag	UNP P19491
C	367	HIS	-	expression tag	UNP P19491
C	368	HIS	-	expression tag	UNP P19491
C	369	HIS	-	expression tag	UNP P19491
C	370	HIS	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	371	SER	-	expression tag	UNP P19491
C	372	SER	-	expression tag	UNP P19491
C	373	GLY	-	expression tag	UNP P19491
C	374	LEU	-	expression tag	UNP P19491
C	375	VAL	-	expression tag	UNP P19491
C	376	PRO	-	expression tag	UNP P19491
C	377	ARG	-	expression tag	UNP P19491
C	378	GLY	-	expression tag	UNP P19491
C	379	SER	-	expression tag	UNP P19491
C	380	ALA	-	expression tag	UNP P19491
C	381	MET	-	expression tag	UNP P19491
C	382	GLY	-	expression tag	UNP P19491
C	389	ARG	GLY	engineered mutation	UNP P19491
C	390	GLY	LEU	engineered mutation	UNP P19491
C	391	ALA	GLU	engineered mutation	UNP P19491
C	555	GLY	-	linker	UNP P19491
C	566	THR	-	linker	UNP P19491
C	738	MET	LYS	engineered mutation	UNP P19491
C	744	LYS	THR	engineered mutation	UNP P19491

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



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

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

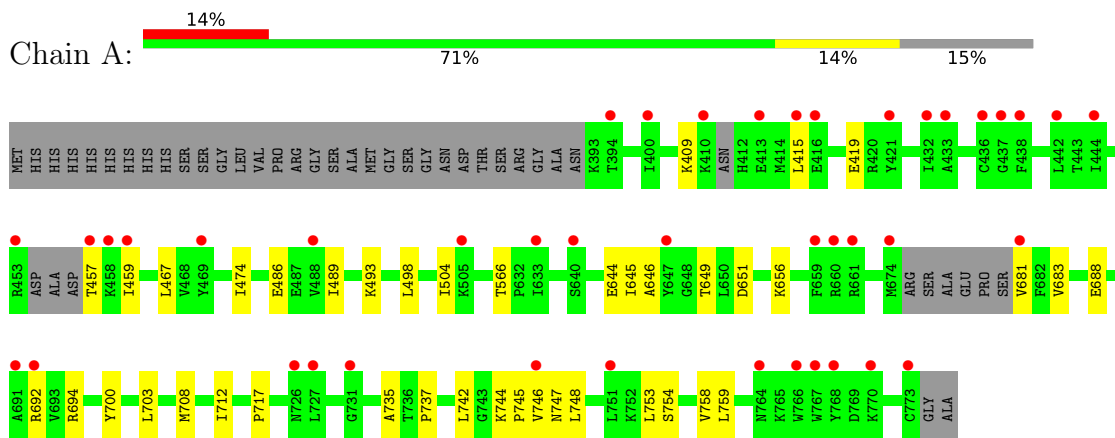
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	1	1	1	0	0

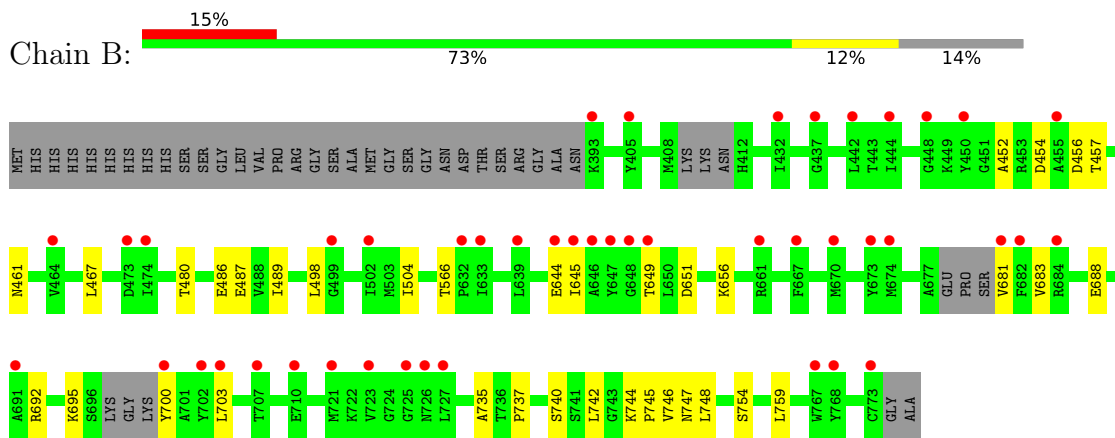
### 3 Residue-property plots [i](#)

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.

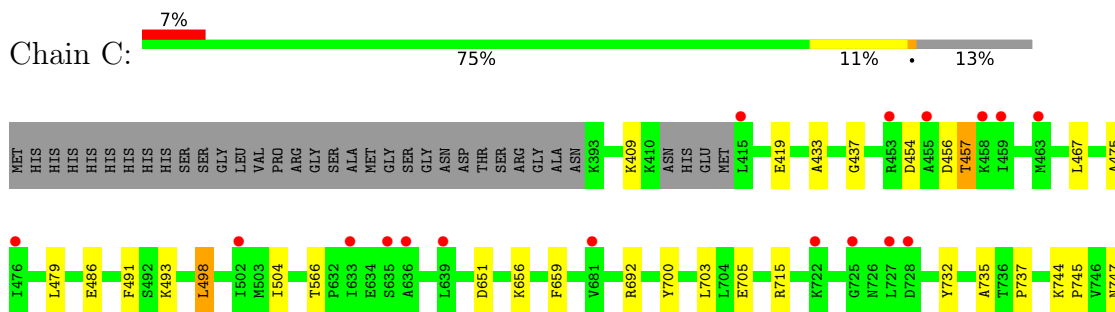
- Molecule 1: GLUTAMATE RECEPTOR 2

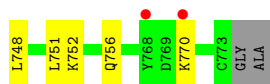


- Molecule 1: GLUTAMATE RECEPTOR 2



- Molecule 1: GLUTAMATE RECEPTOR 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.38Å 110.52Å 167.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.21 – 2.90 92.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (92.21-2.90) 99.6 (92.21-2.90)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.91Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.243 , 0.283 0.245 , 0.283	Depositor DCC
$R_{free}$ test set	979 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.4	Xtrriage
Anisotropy	0.752	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 66.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.21% 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:  
ZN

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	0.31	0/1977	0.51	0/2652
1	B	0.30	0/1980	0.50	0/2661
1	C	0.33	0/2017	0.53	0/2711
All	All	0.31	0/5974	0.51	0/8024

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	1944	0	1989	28	0
1	B	1947	0	1970	24	0
1	C	1982	0	2023	21	1
2	A	10	0	5	0	0
2	B	10	0	5	1	0
2	C	10	0	5	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	5908	0	5997	70	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 6.

All (70) 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:486:GLU:OE2	1:B:747:ASN:ND2	2.12	0.81
1:C:409:LYS:NZ	1:C:419:GLU:OE2	2.14	0.79
1:A:747:ASN:ND2	1:B:486:GLU:OE2	2.15	0.78
1:B:454:ASP:HB3	1:B:457:THR:HG22	1.68	0.76
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.71	0.72
1:A:504:ILE:HD12	1:A:566:THR:HB	1.79	0.65
1:C:651:ASP:OD1	1:C:656:LYS:NZ	2.31	0.62
1:C:454:ASP:HB3	1:C:457:THR:HG22	1.81	0.61
1:C:456:ASP:OD1	1:C:457:THR:N	2.33	0.61
1:C:744:LYS:HE3	1:C:748:LEU:HD11	1.82	0.61
1:C:715:ARG:NH2	1:C:770:LYS:O	2.30	0.59
1:B:452:ALA:N	1:B:461:ASN:OD1	2.25	0.59
1:A:651:ASP:OD1	1:A:656:LYS:NZ	2.36	0.59
1:A:644:GLU:HG3	1:A:645:ILE:HG13	1.86	0.58
1:A:708:MET:O	1:A:712:ILE:HG12	2.05	0.56
1:C:744:LYS:HB3	1:C:745:PRO:HD3	1.88	0.54
1:A:493:LYS:NZ	1:A:747:ASN:HD21	2.06	0.53
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.91	0.51
1:A:694:ARG:CZ	1:A:717:PRO:HD2	2.40	0.51
1:B:456:ASP:OD1	1:B:457:THR:N	2.44	0.51
1:A:742:LEU:O	1:A:746:VAL:HG13	2.11	0.51
1:A:415:LEU:HD13	1:A:419:GLU:HG3	1.93	0.50
1:C:493:LYS:HG3	1:C:751:LEU:HD21	1.92	0.50
1:A:409:LYS:NZ	1:A:419:GLU:OE2	2.45	0.50
1:C:692:ARG:HG2	1:C:700:TYR:CD2	2.47	0.49
1:A:744:LYS:HB3	1:A:745:PRO:HD3	1.94	0.49
1:A:467:LEU:HD22	1:A:737:PRO:HD3	1.94	0.49
1:B:744:LYS:HB3	1:B:745:PRO:HD3	1.94	0.48
1:C:493:LYS:NZ	1:C:747:ASN:HD21	2.11	0.48
1:C:651:ASP:O	1:C:656:LYS:HD3	2.13	0.48
1:C:705:GLU:OE1	2:C:900:GLU:N	2.46	0.48
1:A:457:THR:HG23	1:A:459:ILE:H	1.79	0.47
1:A:744:LYS:O	1:A:748:LEU:HD12	2.14	0.47
1:A:744:LYS:HD2	1:A:744:LYS:HA	1.78	0.47
1:B:742:LEU:O	1:B:746:VAL:HG13	2.15	0.46
1:B:692:ARG:HG2	1:B:700:TYR:CD2	2.49	0.46
1:B:504:ILE:HD12	1:B:566:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.97	0.46
1:B:644:GLU:HG3	1:B:645:ILE:HG13	1.97	0.46
1:B:754:SER:HB2	1:B:759:LEU:HD12	1.98	0.45
1:A:651:ASP:O	1:A:656:LYS:HD3	2.16	0.45
1:A:474:ILE:CD1	1:A:746:VAL:HG11	2.47	0.45
1:B:744:LYS:HD2	1:B:744:LYS:HA	1.86	0.45
1:C:498:LEU:HD22	1:C:732:TYR:CE2	2.52	0.44
1:C:752:LYS:O	1:C:756:GLN:HG2	2.18	0.44
1:B:681:VAL:HA	1:B:692:ARG:NH2	2.33	0.44
1:C:504:ILE:HD12	1:C:566:THR:HB	1.99	0.44
1:A:742:LEU:C	1:A:745:PRO:HD2	2.39	0.43
1:A:681:VAL:HA	1:A:692:ARG:HH22	1.83	0.43
1:C:491:PHE:CE1	1:C:735:ALA:HB2	2.53	0.43
1:B:683:VAL:HB	1:B:688:GLU:HB3	2.01	0.43
1:A:493:LYS:HG2	1:A:747:ASN:OD1	2.19	0.43
1:B:467:LEU:HD22	1:B:737:PRO:HD3	2.01	0.43
1:A:753:LEU:HD22	1:A:758:VAL:HG11	2.01	0.42
1:C:659:PHE:CE2	1:C:703:LEU:HD13	2.55	0.42
1:A:748:LEU:HD21	1:B:487:GLU:HA	2.00	0.42
1:B:737:PRO:HG2	1:B:740:SER:HB2	2.02	0.42
1:B:744:LYS:HE3	1:B:748:LEU:HD11	2.01	0.42
1:A:683:VAL:HB	1:A:688:GLU:HB3	2.02	0.41
1:C:479:LEU:HD23	1:C:491:PHE:HE1	1.84	0.41
1:A:754:SER:HB2	1:A:759:LEU:HD12	2.01	0.41
1:B:480:THR:HG1	2:B:900:GLU:N	2.19	0.41
1:B:651:ASP:O	1:B:656:LYS:HD3	2.21	0.41
1:A:489:ILE:HD13	1:A:735:ALA:HB1	2.03	0.41
1:C:433:ALA:O	1:C:437:GLY:N	2.52	0.41
1:A:646:ALA:O	1:A:700:TYR:HA	2.21	0.40
1:B:742:LEU:HA	1:B:742:LEU:HD23	1.82	0.40
1:C:475:ALA:HB3	1:C:735:ALA:HB3	2.03	0.40
1:B:489:ILE:HD13	1:B:735:ALA:HB1	2.03	0.40
1:B:742:LEU:C	1:B:745:PRO:HD2	2.42	0.40

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:C:486:GLU:OE2	1:C:747:ASN:ND2[2_558]	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	240/291 (82%)	238 (99%)	2 (1%)	0	100	100
1	B	241/291 (83%)	239 (99%)	2 (1%)	0	100	100
1	C	250/291 (86%)	248 (99%)	2 (1%)	0	100	100
All	All	731/873 (84%)	725 (99%)	6 (1%)	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	210/242 (87%)	209 (100%)	1 (0%)	88	96
1	B	210/242 (87%)	208 (99%)	2 (1%)	76	92
1	C	214/242 (88%)	212 (99%)	2 (1%)	78	93
All	All	634/726 (87%)	629 (99%)	5 (1%)	81	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	LEU
1	B	498	LEU
1	B	695	LYS
1	C	457	THR
1	C	498	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	C	900	-	8,9,9	1.06	1 (12%)	10,11,11	1.21	2 (20%)
2	GLU	A	900	-	8,9,9	1.02	1 (12%)	10,11,11	1.18	2 (20%)
2	GLU	B	900	-	8,9,9	1.04	1 (12%)	10,11,11	1.28	2 (20%)

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	C	900	-	-	0/9/9/9	-
2	GLU	A	900	-	-	0/9/9/9	-
2	GLU	B	900	-	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	GLU	OXT-C	-2.15	1.23	1.30
2	B	900	GLU	OXT-C	-2.07	1.23	1.30
2	A	900	GLU	OXT-C	-2.01	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	GLU	OXT-C-O	-2.52	118.36	124.09
2	B	900	GLU	OXT-C-CA	2.44	121.70	113.38
2	B	900	GLU	OXT-C-O	-2.43	118.56	124.09
2	A	900	GLU	OXT-C-CA	2.34	121.37	113.38
2	C	900	GLU	OXT-C-CA	2.05	120.35	113.38
2	A	900	GLU	OXT-C-O	-2.04	119.46	124.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	GLU	1	0
2	B	900	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, 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	248/291 (85%)	0.90	42 (16%) <b>1</b> <b>1</b>	66, 90, 126, 141	0
1	B	249/291 (85%)	1.03	45 (18%) <b>1</b> <b>1</b>	65, 103, 142, 166	0
1	C	254/291 (87%)	0.73	19 (7%) <b>14</b> <b>11</b>	70, 88, 113, 142	0
All	All	751/873 (86%)	0.88	106 (14%) <b>2</b> <b>2</b>	65, 92, 132, 166	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	GLU	6.5
1	B	455	ALA	5.9
1	B	726	ASN	5.8
1	B	633	ILE	5.0
1	C	458	LYS	4.9
1	B	649	THR	4.6
1	B	437	GLY	4.6
1	B	700	TYR	4.5
1	C	636	ALA	4.5
1	B	691	ALA	4.4
1	B	702	TYR	4.4
1	A	459	ILE	4.3
1	B	681	VAL	4.0
1	A	453	ARG	3.9
1	B	768	TYR	3.9
1	B	723	VAL	3.8
1	C	633	ILE	3.8
1	A	444	ILE	3.7
1	C	459	ILE	3.6
1	A	410	LYS	3.6
1	A	727	LEU	3.6
1	A	469	TYR	3.6
1	C	453	ARG	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	488	VAL	3.5
1	A	674	MET	3.4
1	B	502	ILE	3.4
1	B	674	MET	3.3
1	B	721	MET	3.3
1	A	681	VAL	3.3
1	C	681	VAL	3.2
1	B	473	ASP	3.2
1	C	727	LEU	3.2
1	B	639	LEU	3.1
1	B	727	LEU	3.1
1	B	499	GLY	3.0
1	C	768	TYR	3.0
1	B	684	ARG	3.0
1	B	464	VAL	3.0
1	B	703	LEU	3.0
1	C	502	ILE	3.0
1	A	400	ILE	2.9
1	A	691	ALA	2.9
1	B	644	GLU	2.9
1	B	773	CYS	2.8
1	A	640	SER	2.8
1	A	433	ALA	2.8
1	B	432	ILE	2.8
1	B	661	ARG	2.8
1	C	415	LEU	2.8
1	A	659	PHE	2.8
1	B	725	GLY	2.7
1	A	432	ILE	2.7
1	C	722	LYS	2.7
1	B	444	ILE	2.7
1	A	773	CYS	2.6
1	A	647	TYR	2.6
1	B	448	GLY	2.6
1	C	728	ASP	2.6
1	B	670	MET	2.6
1	A	421	TYR	2.6
1	A	436	CYS	2.6
1	B	707	THR	2.6
1	A	768	TYR	2.6
1	A	751	LEU	2.5
1	B	645	ILE	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	476	ILE	2.5
1	A	458	LYS	2.5
1	A	415	LEU	2.5
1	A	438	PHE	2.5
1	B	648	GLY	2.5
1	A	457	THR	2.4
1	A	767	TRP	2.4
1	C	725	GLY	2.4
1	A	442	LEU	2.4
1	A	660	ARG	2.4
1	B	673	TYR	2.4
1	A	766	TRP	2.3
1	C	635	SER	2.3
1	A	505	LYS	2.3
1	A	770	LYS	2.3
1	A	692	ARG	2.3
1	A	764	ASN	2.3
1	B	646	ALA	2.3
1	C	463	MET	2.3
1	C	639	LEU	2.2
1	A	633	ILE	2.2
1	B	667	PHE	2.2
1	B	682	PHE	2.2
1	A	726	ASN	2.2
1	A	437	GLY	2.2
1	A	416	GLU	2.2
1	B	632	PRO	2.2
1	B	450	TYR	2.2
1	A	731	GLY	2.1
1	B	767	TRP	2.1
1	B	442	LEU	2.1
1	A	746	VAL	2.1
1	A	394	THR	2.1
1	B	405	TYR	2.1
1	B	393	LYS	2.1
1	B	710	GLU	2.1
1	C	455	ALA	2.1
1	B	474	ILE	2.0
1	C	770	LYS	2.0
1	A	661	ARG	2.0
1	B	647	TYR	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	B	902	1/1	0.82	0.26	141,141,141,141	0
2	GLU	B	900	10/10	0.86	0.23	80,89,92,95	0
3	ZN	C	902	1/1	0.88	0.17	114,114,114,114	0
2	GLU	C	900	10/10	0.89	0.26	74,87,89,90	0
3	ZN	B	901	1/1	0.91	0.19	126,126,126,126	0
2	GLU	A	900	10/10	0.93	0.19	85,88,98,114	0
3	ZN	A	902	1/1	0.97	0.26	93,93,93,93	0
3	ZN	A	901	1/1	0.97	0.21	122,122,122,122	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.