



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:33 PM GMT

PDB ID : 4LZ8  
Title : Crystal structures of GLuR2 ligand-binding-domain in complex with glutamate and positive allosteric modulators  
Authors : Pandit, J.  
Deposited on : 2013-07-31  
Resolution : 1.85 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

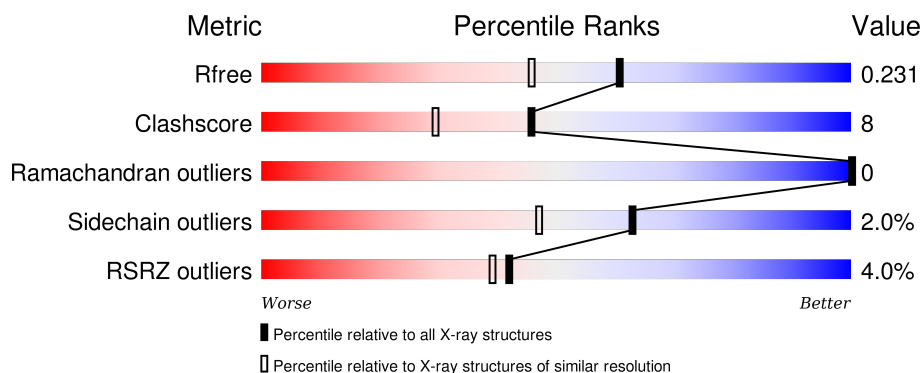
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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  $\geq 3$ , 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	275	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	275	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	C	275	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1YX	A	802[A]	-	-	X	-
3	1YX	B	805	-	-	X	-
4	ZN	B	801	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6503 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	258	Total	C	N	O	S	0	0	0
			2018	1286	336	382	14			
1	B	257	Total	C	N	O	S	0	0	0
			2009	1280	334	381	14			
1	C	257	Total	C	N	O	S	0	0	0
			2008	1279	334	381	14			

There are 30 discrepancies between the modelled and reference sequences:

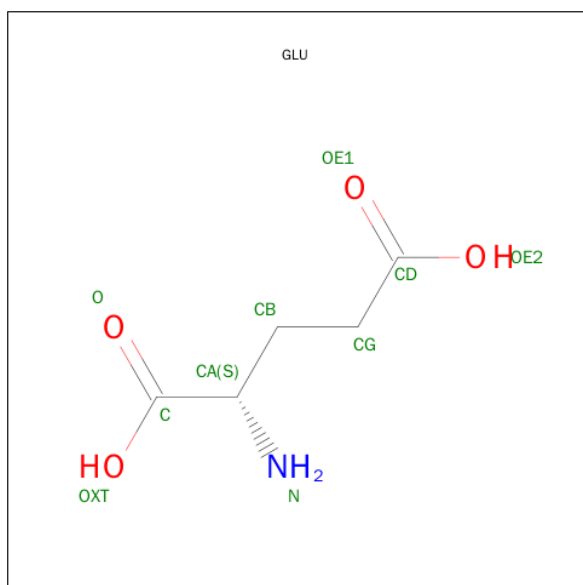
Chain	Residue	Modelled	Actual	Comment	Reference
A	378	GLY	-	EXPRESSION TAG	UNP P19491
A	379	SER	-	EXPRESSION TAG	UNP P19491
A	380	ALA	-	EXPRESSION TAG	UNP P19491
A	381	MET	-	EXPRESSION TAG	UNP P19491
A	382	GLY	-	EXPRESSION TAG	UNP P19491
A	389	ARG	GLY	ENGINEERED MUTATION	UNP P19491
A	390	GLY	LEU	ENGINEERED MUTATION	UNP P19491
A	391	ALA	GLU	ENGINEERED MUTATION	UNP P19491
A	507	GLY	-	LINKER	UNP P19491
A	508	THR	-	LINKER	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	507	GLY	-	LINKER	UNP P19491
B	508	THR	-	LINKER	UNP P19491
C	378	GLY	-	EXPRESSION TAG	UNP P19491
C	379	SER	-	EXPRESSION TAG	UNP P19491
C	380	ALA	-	EXPRESSION TAG	UNP P19491

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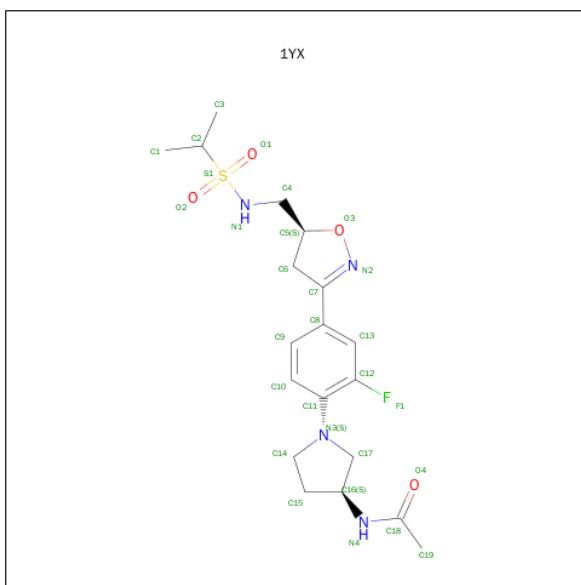
Chain	Residue	Modelled	Actual	Comment	Reference
C	381	MET	-	EXPRESSION TAG	UNP P19491
C	382	GLY	-	EXPRESSION TAG	UNP P19491
C	389	ARG	GLY	ENGINEERED MUTATION	UNP P19491
C	390	GLY	LEU	ENGINEERED MUTATION	UNP P19491
C	391	ALA	GLU	ENGINEERED MUTATION	UNP P19491
C	507	GLY	-	LINKER	UNP P19491
C	508	THR	-	LINKER	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
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is N-[(3S)-1-{2-FLUORO-4-[(5S)-5-{[(PROPAN-2-YLSULFONYL)AMINO]METHYL}-4,5-DIHYDRO-1,2-OXAZOL-3-YL]PHENYL}PYRROLIDIN-3-YL]ACETAMIDE (three-letter code: 1YX) (formula: C<sub>19</sub>H<sub>27</sub>FN<sub>4</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	
			58	38	2	8	8	2	1
3	B	1	Total	C	F	N	O	S	
			29	19	1	4	4	1	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

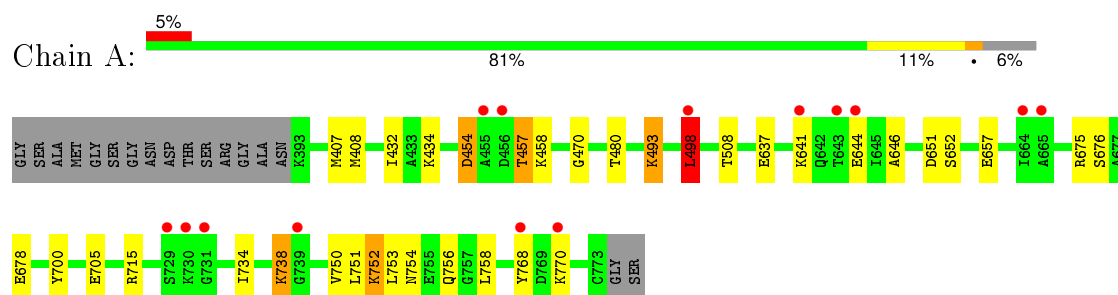
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O		
			105	105	0	0
5	B	142	Total	O		
			142	142	0	0
5	C	99	Total	O		
			99	99	0	0

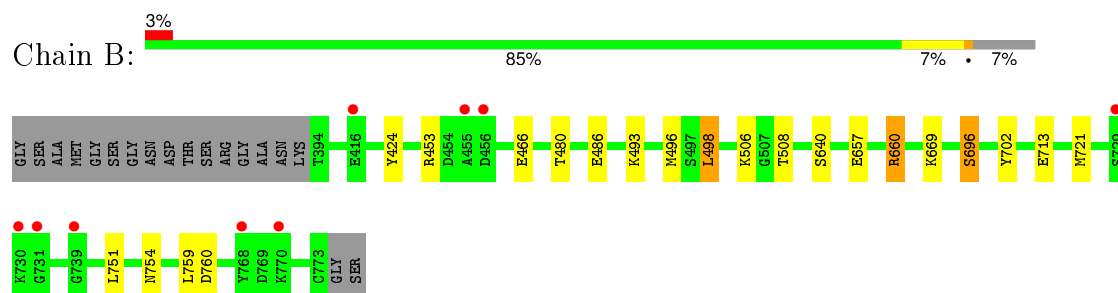
### 3 Residue-property plots [i](#)

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.

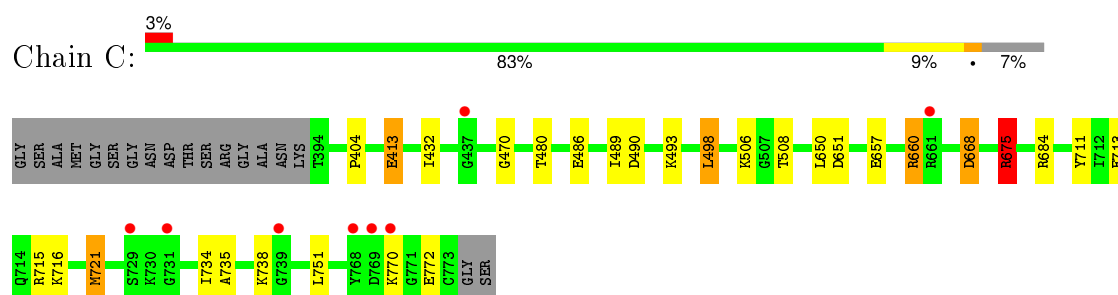
#### • Molecule 1: Glutamate receptor 2



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#### • 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, $\alpha$ , $\beta$ , $\gamma$	113.68Å 164.95Å 47.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.66 – 1.85 36.45 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (93.66-1.85) 96.9 (36.45-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.196 , 0.232 0.204 , 0.231	Depositor DCC
$R_{free}$ test set	3834 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 74877 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.07% 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, 0.375 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: ZN, 1YX

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	0.96	4/2054 (0.2%)	0.96	5/2762 (0.2%)
1	B	1.02	4/2045 (0.2%)	0.98	4/2751 (0.1%)
1	C	0.93	2/2044 (0.1%)	0.97	6/2749 (0.2%)
All	All	0.97	10/6143 (0.2%)	0.97	15/8262 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	508	THR	C-N	9.21	1.51	1.34
1	C	713	GLU	CD-OE1	-8.04	1.16	1.25
1	B	696	SER	CB-OG	7.44	1.51	1.42
1	B	508	THR	C-N	6.76	1.47	1.34
1	B	713	GLU	CD-OE1	-6.07	1.19	1.25
1	A	676	SER	CB-OG	5.76	1.49	1.42
1	B	702	TYR	CE1-CZ	-5.73	1.31	1.38
1	A	678	GLU	CD-OE2	5.45	1.31	1.25
1	A	644	GLU	CD-OE1	5.36	1.31	1.25
1	A	508	THR	C-N	5.01	1.43	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	660	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	738	LYS	CD-CE-NZ	6.36	126.33	111.70
1	A	498	LEU	CB-CG-CD2	6.30	121.71	111.00
1	B	498	LEU	CA-CB-CG	6.23	129.62	115.30
1	C	660	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	407	MET	CG-SD-CE	-5.97	90.64	100.20
1	C	684	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	721	MET	CG-SD-CE	-5.88	90.80	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	LEU	CA-CB-CG	5.64	128.27	115.30
1	C	675	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	760	ASP	CB-CG-OD1	5.12	122.90	118.30
1	C	490	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	768	TYR	CB-CA-C	5.04	120.49	110.40
1	A	454	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	B	660	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2018	0	2050	35	0
1	B	2009	0	2037	21	0
1	C	2008	0	2033	34	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
2	C	10	0	5	1	0
3	A	58	0	54	24	0
3	B	29	0	27	12	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
5	A	105	0	0	10	0
5	B	142	0	0	4	0
5	C	99	0	0	11	0
All	All	6503	0	6216	95	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 8.

All (95) 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:493:LYS:HB3	3:A:802[A]:1YX:H5	1.46	0.95
1:B:493:LYS:HB3	3:B:805:1YX:H5	1.49	0.94
3:A:802[B]:1YX:H22	3:A:802[B]:1YX:O4	1.74	0.85
1:A:657:GLU:HG2	5:A:1036:HOH:O	1.75	0.84
1:B:493:LYS:CB	3:B:805:1YX:H5	2.12	0.80
1:A:652:SER:HB3	5:A:1053:HOH:O	1.82	0.79
1:B:486:GLU:OE2	5:B:957:HOH:O	2.07	0.73
5:A:1062:HOH:O	1:C:657:GLU:HG2	1.92	0.70
1:C:651:ASP:HA	5:C:964:HOH:O	1.91	0.69
1:A:715:ARG:HB2	5:A:1101:HOH:O	1.93	0.68
1:A:752:LYS:O	1:A:756:GLN:HG3	1.94	0.68
1:A:493:LYS:CB	3:A:802[A]:1YX:H5	2.23	0.68
1:B:754:ASN:CB	3:B:805:1YX:H1	2.22	0.67
1:C:738:LYS:HE2	5:C:938:HOH:O	1.94	0.66
1:A:454:ASP:HB3	1:A:457:THR:HG22	1.76	0.66
1:C:716:LYS:HG3	1:C:772:GLU:HG3	1.78	0.66
1:B:453:ARG:HD2	5:B:993:HOH:O	1.96	0.64
3:A:802[A]:1YX:O4	3:A:802[A]:1YX:H22	1.97	0.64
1:A:652:SER:OG	1:A:652:SER:O	2.18	0.62
1:A:751:LEU:HD23	3:A:802[A]:1YX:H6	1.83	0.61
1:C:651:ASP:CA	5:C:964:HOH:O	2.48	0.61
1:A:493:LYS:HB3	3:A:802[A]:1YX:C3	2.28	0.60
1:C:675:ARG:HH11	1:C:675:ARG:CG	2.14	0.60
1:C:470:GLY:HA2	5:C:995:HOH:O	2.01	0.59
1:C:668:ASP:OD1	5:C:965:HOH:O	2.17	0.59
1:A:754:ASN:CB	3:A:802[A]:1YX:H1	2.33	0.58
1:C:721:MET:CE	5:C:939:HOH:O	2.51	0.57
1:A:432:ILE:CD1	1:A:734:ILE:CD1	2.83	0.57
1:B:466:GLU:OE1	5:B:1033:HOH:O	2.17	0.57
1:A:756:GLN:NE2	5:A:1072:HOH:O	2.38	0.55
1:A:751:LEU:CD2	3:A:802[A]:1YX:H6	2.36	0.55
3:B:805:1YX:O4	3:B:805:1YX:H22	2.07	0.54
1:B:751:LEU:CD2	3:B:805:1YX:H6	2.37	0.54
1:B:751:LEU:HD23	3:B:805:1YX:H6	1.90	0.53
1:C:675:ARG:HH11	1:C:675:ARG:HG2	1.72	0.53
1:B:657:GLU:OE1	1:B:660:ARG:NH1	2.40	0.53
1:B:754:ASN:HB2	3:B:805:1YX:H1	1.91	0.52
1:A:750:VAL:HG12	3:A:802[A]:1YX:H7	1.92	0.52
1:C:480:THR:HG1	2:C:803:GLU:N	2.07	0.52
1:A:651:ASP:OD1	1:A:651:ASP:O	2.28	0.52
1:A:754:ASN:HB2	3:A:802[A]:1YX:H1	1.92	0.51
3:A:802[B]:1YX:H7	1:C:751:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:MET:HE3	5:C:939:HOH:O	2.11	0.50
3:A:802[B]:1YX:H2	1:C:751:LEU:HA	1.94	0.50
1:B:493:LYS:CB	3:B:805:1YX:C3	2.86	0.49
1:C:413:GLU:CG	5:C:934:HOH:O	2.61	0.49
1:A:637:GLU:CG	1:A:641:LYS:HE2	2.43	0.49
1:A:493:LYS:CB	3:A:802[A]:1YX:C3	2.88	0.49
1:A:480:THR:HG1	2:A:801:GLU:N	2.10	0.48
1:B:754:ASN:HB2	1:B:759:LEU:HD12	1.95	0.48
1:A:432:ILE:HD11	1:A:734:ILE:CD1	2.43	0.48
1:B:696:SER:HB2	5:B:916:HOH:O	2.14	0.47
1:B:506:LYS:HG2	1:B:721:MET:HE3	1.95	0.47
3:A:802[B]:1YX:H5	1:C:493:LYS:HB3	1.97	0.47
1:A:470:GLY:HA2	5:A:1067:HOH:O	2.13	0.47
1:C:657:GLU:OE1	1:C:660:ARG:NH1	2.43	0.47
1:B:480:THR:HG1	2:B:804:GLU:N	2.14	0.46
1:C:651:ASP:CB	5:C:964:HOH:O	2.64	0.46
1:A:753:LEU:HD22	1:A:758:LEU:HD22	1.96	0.46
1:A:637:GLU:HG3	1:A:641:LYS:HE2	1.98	0.46
1:C:651:ASP:HB2	5:C:989:HOH:O	2.15	0.46
1:A:434:LYS:NZ	5:A:1088:HOH:O	2.41	0.46
1:A:493:LYS:NZ	1:C:486:GLU:OE2	2.43	0.45
1:A:652:SER:N	5:A:1053:HOH:O	2.50	0.45
1:C:404:PRO:HB3	1:C:711:TYR:CE1	2.52	0.45
1:B:493:LYS:HB2	3:B:805:1YX:C3	2.46	0.45
3:A:802[A]:1YX:H3	5:A:1099:HOH:O	2.17	0.45
1:C:432:ILE:CD1	1:C:734:ILE:CD1	2.95	0.44
1:B:424:TYR:CZ	1:B:496:MET:HE3	2.53	0.44
3:A:802[B]:1YX:C3	1:C:751:LEU:CD2	2.96	0.44
1:C:650:LEU:HG	1:C:651:ASP:O	2.18	0.44
1:B:640:SER:O	1:B:669:LYS:HE2	2.17	0.43
1:A:754:ASN:HB2	3:A:802[A]:1YX:C1	2.47	0.43
3:A:802[B]:1YX:H7	1:C:751:LEU:HD21	2.01	0.43
1:C:432:ILE:HD13	1:C:734:ILE:CD1	2.49	0.43
1:C:721:MET:HE1	5:C:939:HOH:O	2.14	0.43
3:A:802[B]:1YX:C3	1:C:493:LYS:HB3	2.49	0.43
1:C:432:ILE:CD1	1:C:734:ILE:HD11	2.49	0.43
1:B:754:ASN:HB3	3:B:805:1YX:C1	2.49	0.43
1:C:432:ILE:HD11	1:C:734:ILE:HD11	2.01	0.43
1:A:498:LEU:HD23	1:A:705:GLU:HG2	2.01	0.43
1:B:754:ASN:CB	3:B:805:1YX:C1	2.94	0.42
1:A:432:ILE:CD1	1:A:734:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:ASN:HB3	3:B:805:1YX:H1	2.01	0.42
1:A:432:ILE:HD13	1:A:734:ILE:HD13	2.01	0.42
1:A:646:ALA:O	1:A:700:TYR:HA	2.20	0.42
3:A:802[B]:1YX:C3	1:C:751:LEU:HD23	2.50	0.41
1:A:751:LEU:HD23	3:A:802[A]:1YX:H3	2.01	0.41
3:A:802[A]:1YX:C14	3:A:802[A]:1YX:F1	2.59	0.41
1:C:715:ARG:NH1	1:C:770:LYS:O	2.53	0.41
3:A:802[A]:1YX:O4	3:A:802[A]:1YX:C17	2.68	0.41
1:A:754:ASN:CB	3:A:802[A]:1YX:C1	2.99	0.40
1:C:489:ILE:HD12	1:C:735:ALA:HB1	2.02	0.40
1:A:408:MET:HG2	5:A:1104:HOH:O	2.21	0.40
1:C:506:LYS:HG2	1:C:721:MET:HE3	2.03	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	256/275 (93%)	250 (98%)	6 (2%)	0	100	100
1	B	255/275 (93%)	251 (98%)	4 (2%)	0	100	100
1	C	255/275 (93%)	251 (98%)	4 (2%)	0	100	100
All	All	766/825 (93%)	752 (98%)	14 (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	217/227 (96%)	209 (96%)	8 (4%)	41	20
1	B	216/227 (95%)	215 (100%)	1 (0%)	92	90
1	C	216/227 (95%)	212 (98%)	4 (2%)	65	49
All	All	649/681 (95%)	636 (98%)	13 (2%)	63	47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	457	THR
1	A	458	LYS
1	A	493	LYS
1	A	498	LEU
1	A	675	ARG
1	A	738	LYS
1	A	752	LYS
1	A	770	LYS
1	B	498	LEU
1	C	413	GLU
1	C	498	LEU
1	C	668	ASP
1	C	675	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	411	ASN
1	B	744	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	A	801	-	3,9,9	0.61	0	2,11,11	0.71	0
3	1YX	A	802[A]	-	30,31,31	0.66	0	31,45,45	1.31	3 (9%)
3	1YX	A	802[B]	-	30,31,31	0.68	1 (3%)	31,45,45	1.00	3 (9%)
2	GLU	B	804	-	3,9,9	0.39	0	2,11,11	0.58	0
3	1YX	B	805	-	30,31,31	1.22	3 (10%)	31,45,45	1.49	3 (9%)
2	GLU	C	803	-	3,9,9	0.61	0	2,11,11	1.34	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	GLU	A	801	-	-	0/3/9/9	0/0/0/0
3	1YX	A	802[A]	-	-	0/22/42/42	0/3/3/3
3	1YX	A	802[B]	-	-	0/22/42/42	0/3/3/3
2	GLU	B	804	-	-	0/3/9/9	0/0/0/0
3	1YX	B	805	-	-	0/22/42/42	0/3/3/3
2	GLU	C	803	-	-	0/3/9/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	805	1YX	O3-C5	-4.23	1.41	1.46
3	B	805	1YX	C4-N1	-3.25	1.41	1.47
3	A	802[B]	1YX	O3-C5	-2.59	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	805	1YX	S1-N1	3.08	1.68	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802[A]	1YX	C4-C5-C6	-3.27	105.70	113.48
3	B	805	1YX	C4-C5-C6	-2.20	108.25	113.48
3	A	802[B]	1YX	C14-N3-C11	2.06	127.43	121.49
3	A	802[B]	1YX	O1-S1-O2	2.70	123.78	119.34
3	A	802[B]	1YX	O3-C5-C6	3.39	106.20	104.29
3	A	802[A]	1YX	O3-C5-C6	3.58	106.31	104.29
3	A	802[A]	1YX	O1-S1-O2	4.81	127.25	119.34
3	B	805	1YX	O1-S1-O2	4.89	127.37	119.34
3	B	805	1YX	O3-C5-C6	5.16	107.20	104.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GLU	1	0
3	A	802[A]	1YX	16	0
3	A	802[B]	1YX	8	0
2	B	804	GLU	1	0
3	B	805	1YX	12	0
2	C	803	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	258/275 (93%)	0.10	14 (5%) 29 28	4, 20, 53, 63	0
1	B	257/275 (93%)	-0.11	9 (3%) 48 45	2, 14, 42, 59	0
1	C	257/275 (93%)	-0.02	8 (3%) 52 49	4, 20, 47, 63	0
All	All	772/825 (93%)	-0.01	31 (4%) 42 39	2, 18, 47, 63	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	ALA	4.5
1	A	456	ASP	4.5
1	C	770	LYS	4.1
1	A	731	GLY	3.8
1	B	731	GLY	3.8
1	A	665	ALA	3.8
1	A	768	TYR	3.7
1	B	768	TYR	3.7
1	A	664	ILE	3.6
1	B	456	ASP	3.6
1	B	455	ALA	3.5
1	C	731	GLY	3.5
1	C	768	TYR	3.4
1	C	739	GLY	3.3
1	A	729	SER	3.1
1	C	661	ARG	3.0
1	A	643	THR	2.6
1	B	770	LYS	2.6
1	B	739	GLY	2.6
1	A	498	LEU	2.4
1	C	729	SER	2.3
1	A	644	GLU	2.3
1	B	416	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	729	SER	2.2
1	A	730	LYS	2.1
1	A	739	GLY	2.1
1	C	769	ASP	2.1
1	A	770	LYS	2.0
1	B	730	LYS	2.0
1	C	437	GLY	2.0
1	A	641	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
4	ZN	B	801	1/1	0.97	0.13	2.47	39,39,39,39	0
2	GLU	A	801	10/10	0.95	0.15	1.54	7,10,14,14	0
3	1YX	B	805	29/29	0.95	0.27	1.45	20,25,42,45	29
3	1YX	A	802[B]	29/29	0.95	0.24	1.18	24,28,42,46	29
3	1YX	A	802[A]	29/29	0.95	0.24	1.16	27,30,45,46	29
2	GLU	C	803	10/10	0.97	0.13	0.75	4,6,9,10	0
2	GLU	B	804	10/10	0.98	0.11	0.18	3,5,6,7	0
4	ZN	B	802	1/1	0.97	0.13	0.11	43,43,43,43	0
4	ZN	C	801	1/1	0.99	0.13	0.03	37,37,37,37	0
4	ZN	B	803	1/1	0.96	0.07	-2.35	47,47,47,47	0
4	ZN	C	802	1/1	0.74	0.08	-	104,104,104,104	0

## 6.5 Other polymers

There are no such residues in this entry.