wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 11:43 AM EST

PDB ID	:	4U2Q
Title	:	Full-length AMPA subtype ionotropic glutamate receptor GluA2 in complex with partial agonist kainate
Authors	:	Duerr, K.L.; Chen, L.; Gouaux, E.
Deposited on	:	2014-07-17
Resolution	:	3.52 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

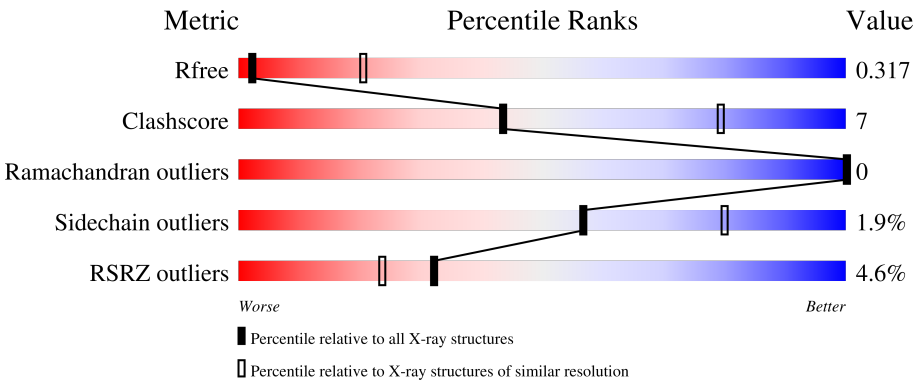
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 >=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 <=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	824	5% 73% 14% 12%
1	B	824	3% 76% 14% 9%
1	C	824	3% 75% 14% 10%
1	D	824	6% 75% 16% 9%

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	NAG	B	902	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22448 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	721	5410	3480	890	1017	23	0	0	0
1	B	746	5674	3649	937	1063	25	0	0	0
1	C	744	5631	3615	933	1057	26	0	0	0
1	D	749	5631	3616	932	1058	25	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLU	ASN	conflict	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	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	528	ALA	CYS	conflict	UNP P19491
A	585	PHE	MET	conflict	UNP P19491
A	589	ALA	CYS	conflict	UNP P19491
A	598	ALA	GLY	conflict	UNP P19491
A	602	ALA	GLY	conflict	UNP P19491
A	815	ALA	CYS	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	239	GLU	ASN	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	528	ALA	CYS	conflict	UNP P19491
B	585	PHE	MET	conflict	UNP P19491
B	589	ALA	CYS	conflict	UNP P19491
B	598	ALA	GLY	conflict	UNP P19491
B	602	ALA	GLY	conflict	UNP P19491
B	815	ALA	CYS	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
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C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
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C	528	ALA	CYS	conflict	UNP P19491
C	585	PHE	MET	conflict	UNP P19491
C	589	ALA	CYS	conflict	UNP P19491
C	598	ALA	GLY	conflict	UNP P19491
C	602	ALA	GLY	conflict	UNP P19491
C	815	ALA	CYS	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	239	GLU	ASN	conflict	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	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	528	ALA	CYS	conflict	UNP P19491
D	585	PHE	MET	conflict	UNP P19491

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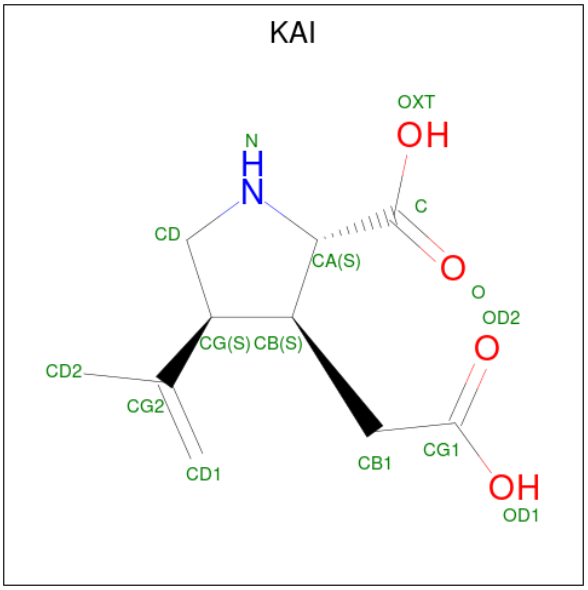
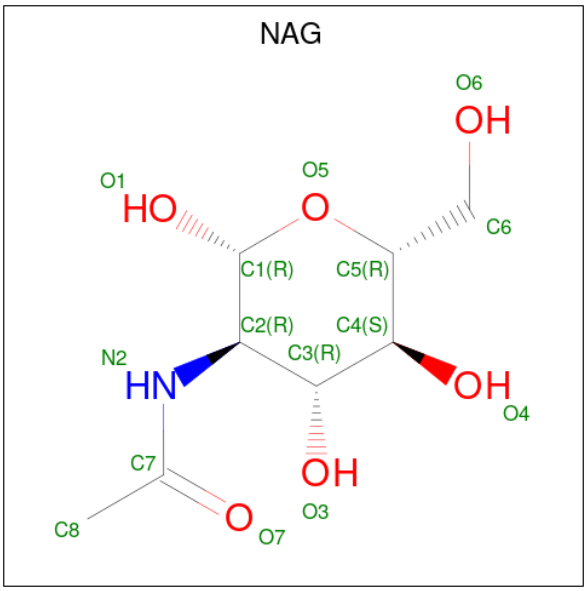
Chain	Residue	Modelled	Actual	Comment	Reference
D	589	ALA	CYS	conflict	UNP P19491
D	598	ALA	GLY	conflict	UNP P19491
D	602	ALA	GLY	conflict	UNP P19491
D	815	ALA	CYS	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is 3-(CARBOXYMETHYL)-4-ISOPROPENYLPROLINE (three-letter code: KAI) (formula: $C_{10}H_{15}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



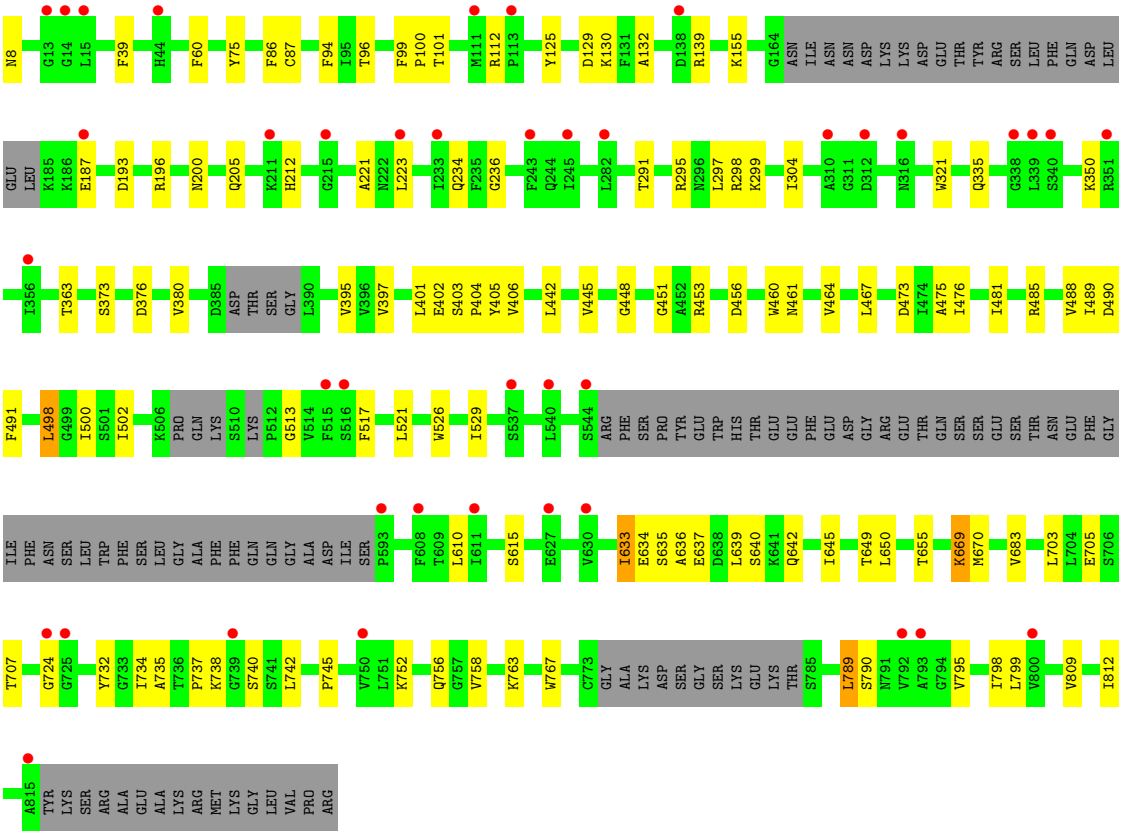
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	B	1	14	8	1	5	0	0
			Total	C	N	O		
3	C	1	14	8	1	5	0	0

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.

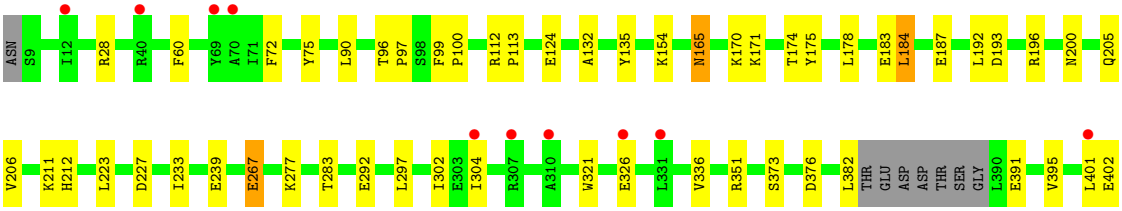
• Molecule 1: Glutamate receptor 2

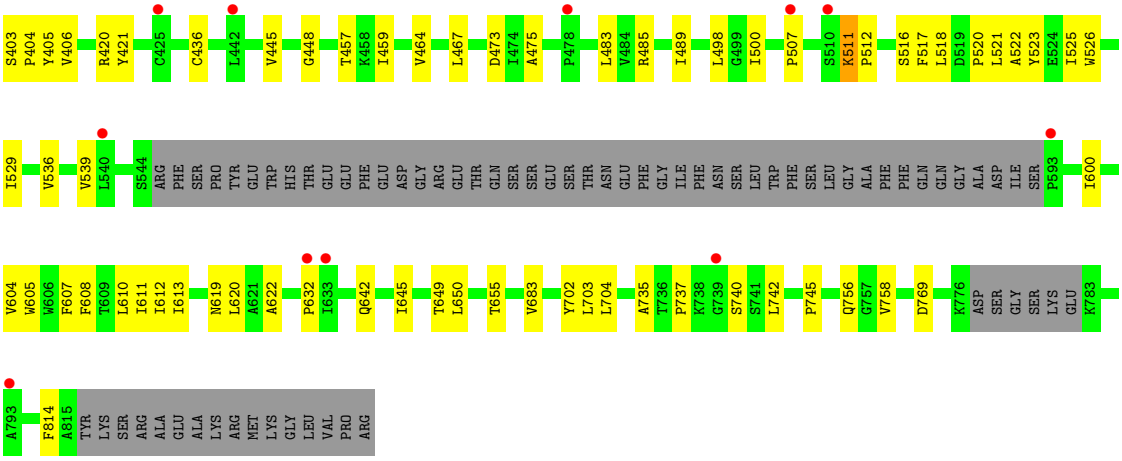
Chain A: 5% 73% 14% 12%



• Molecule 1: Glutamate receptor 2

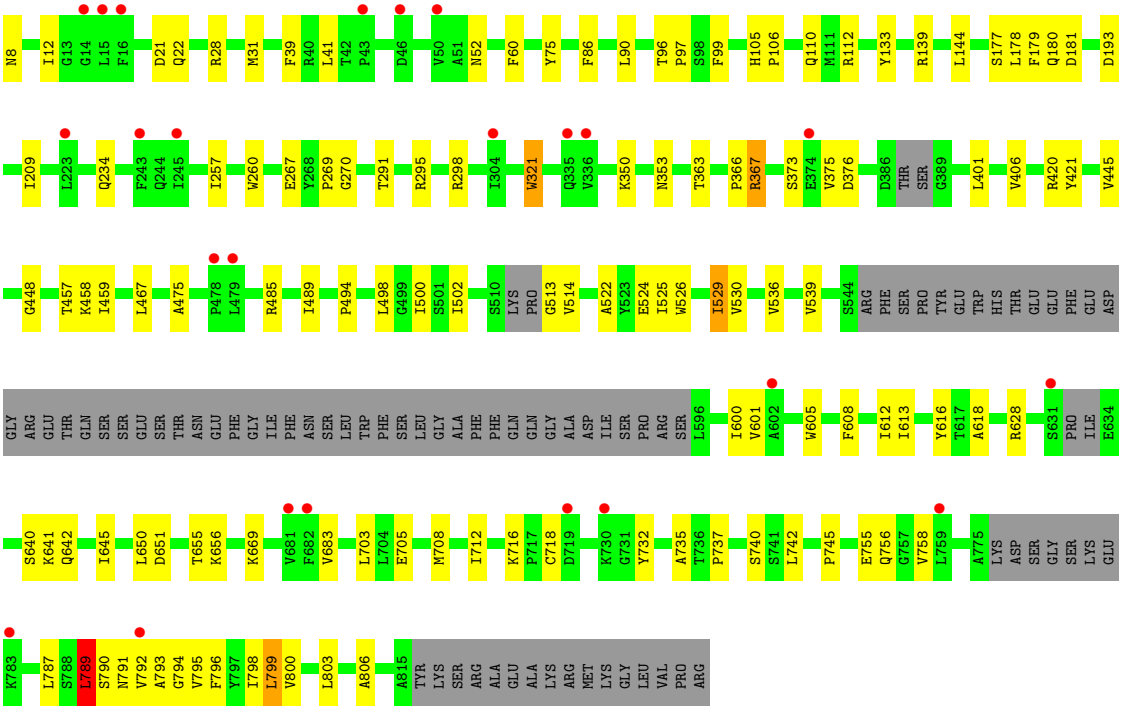
Chain B: 3% 76% 14% 9%





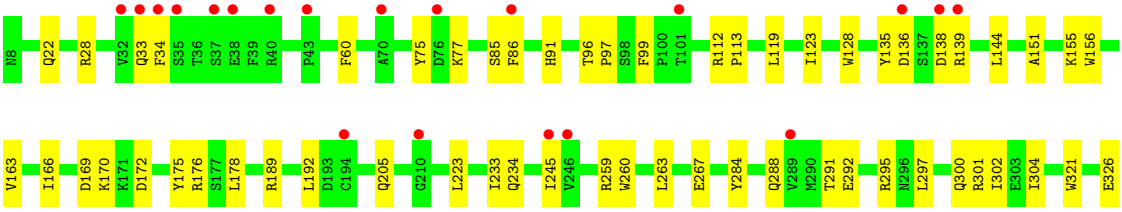
- Molecule 1: Glutamate receptor 2

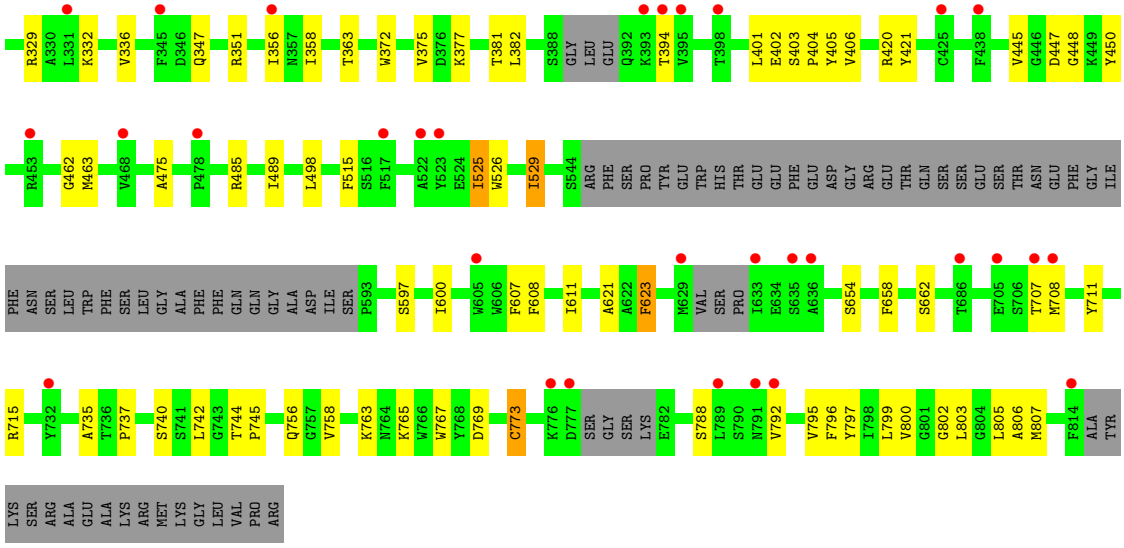
Chain C:



- Molecule 1: Glutamate receptor 2

Chain D:




R329 A330 L331 K332 V336 F345 D346 Q347 R351 I356 N357 I358 T363 W372 V375 D376 K377 T381 L382 S388 GLY LEU GLU Q392 K393 T394 V395 T398 L401 E402 S403 P404 Y405 V406 R420 Y421 C425 F438 V445 G446 D447 G448 K449 Y450
R453 G462 M463 V468 A475 P478 R485 I489 L498 F515 S516 F517 A522 Y523 E524 I525 W526 I529 S544 ARG PHE SER PRO TYR GLU TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER THR ASN GLU PHE GLY ILE
PHE ASN SER LEU TRP PHE SER LEU GLY ALA PHE PHE GLN GLN GLY ALA ASP ILE SER P593 S597 I600 W605 W606 F607 F608 I611 A621 A622 F623 M629 VAL SER PRO I633 E634 S635 A636 S654 F658 S662 T686 E705 S706 T707 M708 Y711
R715 Y732 A735 T736 P737 S740 S741 L742 G743 T744 P745 Q756 G757 V758 K763 N764 K765 W766 W767 Y768 D769 C773 K776 D777 SER GLY SER LYS E782 S788 L789 S790 N791 V792 V795 F796 Y797 I798 L799 V800 G801 G802 L803 G804 L805 A806 M807 F814 ALA TYR
LYS SER ARG ALA GLU ALA LYS ARG MET LYS GLY LEU VAL PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.94Å 148.65Å 337.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.08 – 3.52 83.08 – 3.52	Depositor EDS
% Data completeness (in resolution range)	60.6 (83.08-3.52) 60.6 (83.08-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.269 , 0.318 0.269 , 0.317	Depositor DCC
R_{free} test set	2005 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	126.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 108.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	22448	wwPDB-VP
Average B, all atoms (Å^2)	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: KAI, 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	0.25	0/5521	0.46	0/7493
1	B	0.24	0/5792	0.45	0/7847
1	C	0.25	0/5745	0.46	1/7785 (0.0%)
1	D	0.25	0/5748	0.47	0/7800
All	All	0.25	0/22806	0.46	1/30925 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	789	LEU	CA-CB-CG	5.08	126.98	115.30

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	5410	0	5189	74	0
1	B	5674	0	5525	80	0
1	C	5631	0	5419	87	0
1	D	5631	0	5392	78	0
2	A	15	0	13	1	0
2	B	15	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	13	2	0
2	D	15	0	13	2	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	2	0
All	All	22448	0	21616	295	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 7.

The worst 5 of 295 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:183:GLU:OE1	1:B:211:LYS:NZ	2.00	0.94
1:B:522:ALA:HB3	1:B:525:ILE:HG13	1.66	0.78
1:B:520:PRO:HA	1:B:619:ASN:HD22	1.48	0.78
1:A:521:LEU:HB3	1:A:526:TRP:HE1	1.48	0.78
1:D:302:ILE:HG21	1:D:326:GLU:HG2	1.69	0.74

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	708/824 (86%)	694 (98%)	14 (2%)	0	100	100
1	B	738/824 (90%)	731 (99%)	7 (1%)	0	100	100
1	C	732/824 (89%)	719 (98%)	13 (2%)	0	100	100
1	D	739/824 (90%)	725 (98%)	14 (2%)	0	100	100
All	All	2917/3296 (88%)	2869 (98%)	48 (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	549/701 (78%)	541 (98%)	8 (2%)	65	84
1	B	586/701 (84%)	573 (98%)	13 (2%)	52	77
1	C	573/701 (82%)	565 (99%)	8 (1%)	67	85
1	D	571/701 (82%)	557 (98%)	14 (2%)	47	75
All	All	2279/2804 (81%)	2236 (98%)	43 (2%)	57	80

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	799	LEU
1	D	498	LEU
1	D	91	HIS
1	D	233	ILE
1	D	529	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	342	ASN
1	B	412	HIS
1	D	205	GLN
1	B	200	ASN
1	A	205	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	NAG	A	902	1	14,14,15	1.26	2 (14%)	17,19,21	2.51	6 (35%)
3	NAG	B	902	1	14,14,15	0.50	0	17,19,21	1.02	1 (5%)
2	KAI	D	901	-	13,15,15	1.03	0	14,21,21	0.89	0
3	NAG	C	902	1	14,14,15	0.29	0	17,19,21	1.46	2 (11%)
2	KAI	C	901	-	13,15,15	0.98	0	14,21,21	0.87	0
2	KAI	A	901	-	13,15,15	1.01	0	14,21,21	0.85	0
2	KAI	B	901	-	13,15,15	1.02	0	14,21,21	0.86	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
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
2	KAI	D	901	-	-	0/12/25/25	0/1/1/1
3	NAG	C	902	1	-	3/6/23/26	0/1/1/1
2	KAI	C	901	-	-	0/12/25/25	0/1/1/1
2	KAI	A	901	-	-	4/12/25/25	0/1/1/1
2	KAI	B	901	-	-	1/12/25/25	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	NAG	O5-C1	-2.52	1.39	1.43
3	A	902	NAG	O4-C4	2.29	1.48	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	NAG	C1-O5-C5	5.67	119.87	112.19
3	A	902	NAG	O5-C1-C2	4.98	119.16	111.29
3	C	902	NAG	C2-N2-C7	-4.00	117.21	122.90
3	A	902	NAG	O5-C5-C4	3.40	119.10	110.83
3	A	902	NAG	C6-C5-C4	-2.93	106.15	113.00

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	NAG	C8-C7-N2-C2
3	C	902	NAG	O7-C7-N2-C2
3	A	902	NAG	C8-C7-N2-C2
3	A	902	NAG	O7-C7-N2-C2
3	C	902	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	KAI	2	0
3	C	902	NAG	2	0
2	C	901	KAI	2	0
2	A	901	KAI	1	0
2	B	901	KAI	2	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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	721/824 (87%)	0.13	41 (5%)	23	17	152, 223, 280, 321	0
1	B	746/824 (90%)	0.09	21 (2%)	53	40	144, 216, 276, 314	0
1	C	744/824 (90%)	0.02	24 (3%)	47	36	150, 223, 283, 349	0
1	D	749/824 (90%)	0.18	51 (6%)	17	14	154, 223, 283, 329	0
All	All	2960/3296 (89%)	0.11	137 (4%)	32	24	144, 221, 281, 349	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	777	ASP	10.4
1	A	593	PRO	8.1
1	C	792	VAL	7.1
1	A	339	LEU	6.1
1	D	395	VAL	5.5

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	902	14/15	0.76	0.40	310,368,455,556	0
2	KAI	C	901	15/15	0.93	0.56	167,209,275,295	0
2	KAI	A	901	15/15	0.94	0.73	171,255,312,320	0
3	NAG	C	902	14/15	0.94	0.30	113,199,304,331	0
2	KAI	B	901	15/15	0.95	0.30	116,167,282,304	0
3	NAG	A	902	14/15	0.96	0.29	143,200,293,296	0
2	KAI	D	901	15/15	0.97	0.54	137,198,325,346	0

6.5 Other polymers (i)

There are no such residues in this entry.