Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:52 PM GMT

PDB ID	:	4U5E
Title	:	Crystal structure of GluA2 T625G, con-ikot-ikot snail toxin, partial agonist KA and postitive modulator (R,R)-2b complex
Authors	:	Chen, L.; Gouaux, E.
Deposited on	:	2014-07-25
Resolution	:	3.51 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

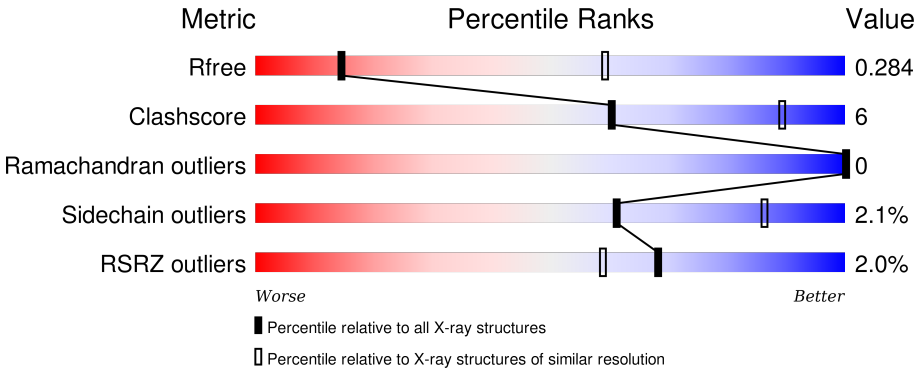
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.51 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	814	2% 77% 13% 9%
1	B	814	3% 77% 14% 9%
1	C	814	2% 80% 11% • 8%
1	D	814	% 77% 13% • 9%
2	E	90	82% 11% • 6%

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Mol	Chain	Length	Quality of chain
2	F	90	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23731 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	738	Total	C	N	O	S	0	0	0
			5553	3575	905	1047	26			
1	B	743	Total	C	N	O	S	0	0	0
			5645	3629	930	1060	26			
1	C	746	Total	C	N	O	S	0	0	0
			5498	3528	902	1042	26			
1	D	738	Total	C	N	O	S	0	0	0
			5573	3591	906	1050	26			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLY	LYS	engineered mutation	UNP P19491
A	237	GLU	ASN	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	461	ASP	ASN	engineered mutation	UNP P19491
A	528	ALA	CYS	engineered mutation	UNP P19491
A	535	LEU	GLY	engineered mutation	UNP P19491
A	?	-	ARG	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLN	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	565	GLU	SER	engineered mutation	UNP P19491
A	577	PHE	LEU	engineered mutation	UNP P19491
A	580	ALA	SER	engineered mutation	UNP P19491
A	582	LYS	GLY	engineered mutation	UNP P19491
A	583	LEU	ALA	engineered mutation	UNP P19491
A	585	PHE	MET	engineered mutation	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	GLY	engineered mutation	UNP P19491
A	602	ALA	GLY	engineered mutation	UNP P19491
A	625	GLY	THR	engineered mutation	UNP P19491
A	815	ALA	CYS	engineered mutation	UNP P19491
A	818	ARG	SER	engineered mutation	UNP P19491
A	819	MET	ARG	engineered mutation	UNP P19491
A	820	LYS	ALA	engineered mutation	UNP P19491
A	821	LEU	GLU	engineered mutation	UNP P19491
A	822	VAL	ALA	engineered mutation	UNP P19491
A	823	PRO	LYS	engineered mutation	UNP P19491
B	184	GLY	LYS	engineered mutation	UNP P19491
B	237	GLU	ASN	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	461	ASP	ASN	engineered mutation	UNP P19491
B	528	ALA	CYS	engineered mutation	UNP P19491
B	535	LEU	GLY	engineered mutation	UNP P19491
B	?	-	ARG	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLN	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	565	GLU	SER	engineered mutation	UNP P19491
B	577	PHE	LEU	engineered mutation	UNP P19491
B	580	ALA	SER	engineered mutation	UNP P19491
B	582	LYS	GLY	engineered mutation	UNP P19491
B	583	LEU	ALA	engineered mutation	UNP P19491
B	585	PHE	MET	engineered mutation	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	598	ALA	GLY	engineered mutation	UNP P19491
B	602	ALA	GLY	engineered mutation	UNP P19491
B	625	GLY	THR	engineered mutation	UNP P19491
B	815	ALA	CYS	engineered mutation	UNP P19491
B	818	ARG	SER	engineered mutation	UNP P19491
B	819	MET	ARG	engineered mutation	UNP P19491
B	820	LYS	ALA	engineered mutation	UNP P19491
B	821	LEU	GLU	engineered mutation	UNP P19491
B	822	VAL	ALA	engineered mutation	UNP P19491
B	823	PRO	LYS	engineered mutation	UNP P19491
C	184	GLY	LYS	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	237	GLU	ASN	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	461	ASP	ASN	engineered mutation	UNP P19491
C	528	ALA	CYS	engineered mutation	UNP P19491
C	535	LEU	GLY	engineered mutation	UNP P19491
C	?	-	ARG	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLN	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	565	GLU	SER	engineered mutation	UNP P19491
C	577	PHE	LEU	engineered mutation	UNP P19491
C	580	ALA	SER	engineered mutation	UNP P19491
C	582	LYS	GLY	engineered mutation	UNP P19491
C	583	LEU	ALA	engineered mutation	UNP P19491
C	585	PHE	MET	engineered mutation	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	598	ALA	GLY	engineered mutation	UNP P19491
C	602	ALA	GLY	engineered mutation	UNP P19491
C	625	GLY	THR	engineered mutation	UNP P19491
C	815	ALA	CYS	engineered mutation	UNP P19491
C	818	ARG	SER	engineered mutation	UNP P19491
C	819	MET	ARG	engineered mutation	UNP P19491
C	820	LYS	ALA	engineered mutation	UNP P19491
C	821	LEU	GLU	engineered mutation	UNP P19491
C	822	VAL	ALA	engineered mutation	UNP P19491
C	823	PRO	LYS	engineered mutation	UNP P19491
D	184	GLY	LYS	engineered mutation	UNP P19491
D	237	GLU	ASN	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	461	ASP	ASN	engineered mutation	UNP P19491
D	528	ALA	CYS	engineered mutation	UNP P19491
D	535	LEU	GLY	engineered mutation	UNP P19491
D	?	-	ARG	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLN	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	565	GLU	SER	engineered mutation	UNP P19491
D	577	PHE	LEU	engineered mutation	UNP P19491
D	580	ALA	SER	engineered mutation	UNP P19491
D	582	LYS	GLY	engineered mutation	UNP P19491
D	583	LEU	ALA	engineered mutation	UNP P19491
D	585	PHE	MET	engineered mutation	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	598	ALA	GLY	engineered mutation	UNP P19491
D	602	ALA	GLY	engineered mutation	UNP P19491
D	625	GLY	THR	engineered mutation	UNP P19491
D	815	ALA	CYS	engineered mutation	UNP P19491
D	818	ARG	SER	engineered mutation	UNP P19491
D	819	MET	ARG	engineered mutation	UNP P19491
D	820	LYS	ALA	engineered mutation	UNP P19491
D	821	LEU	GLU	engineered mutation	UNP P19491
D	822	VAL	ALA	engineered mutation	UNP P19491
D	823	PRO	LYS	engineered mutation	UNP P19491

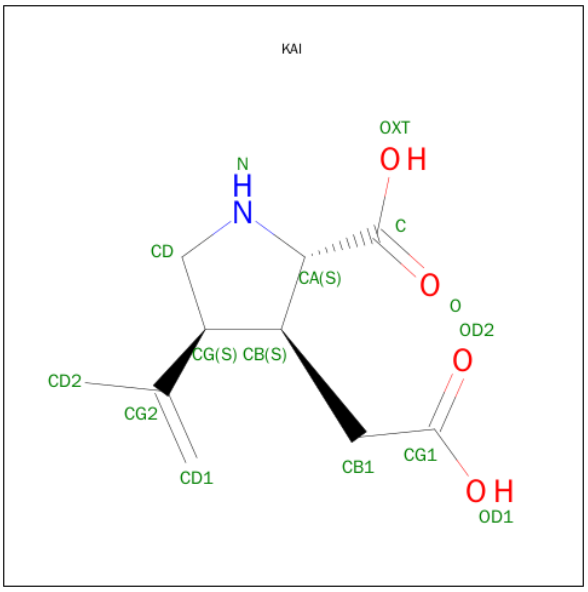
- Molecule 2 is a protein called Con-ikot-ikot.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	85	Total	C	N	O	S	0	0	0
			641	387	113	125	16			
2	F	85	Total	C	N	O	S	0	0	0
			641	387	113	125	16			

There are 8 discrepancies between the modelled and reference sequences:

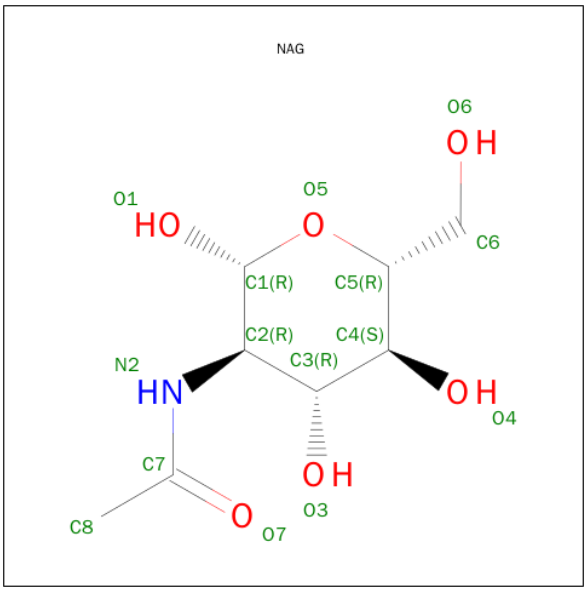
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P0CB20
E	-2	PRO	-	expression tag	UNP P0CB20
E	-1	GLY	-	expression tag	UNP P0CB20
E	0	SER	-	expression tag	UNP P0CB20
F	-3	GLY	-	expression tag	UNP P0CB20
F	-2	PRO	-	expression tag	UNP P0CB20
F	-1	GLY	-	expression tag	UNP P0CB20
F	0	SER	-	expression tag	UNP P0CB20

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



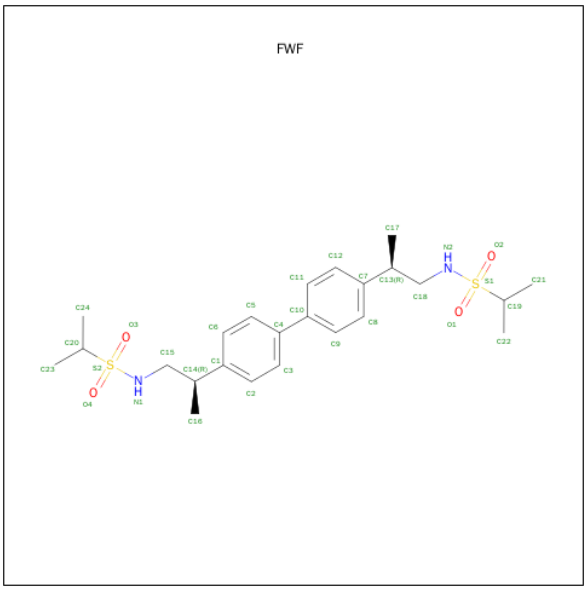
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	1	4		
3	B	1	Total	C	N	O	0	0
			15	10	1	4		
3	C	1	Total	C	N	O	0	0
			15	10	1	4		
3	D	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is N,N'-[biphenyl-4,4'-diyldi(2R)propane-2,1-diyl]dipropane-2-sulfonamide (three-letter code: FWF) (formula: $C_{24}H_{36}N_2O_4S_2$).



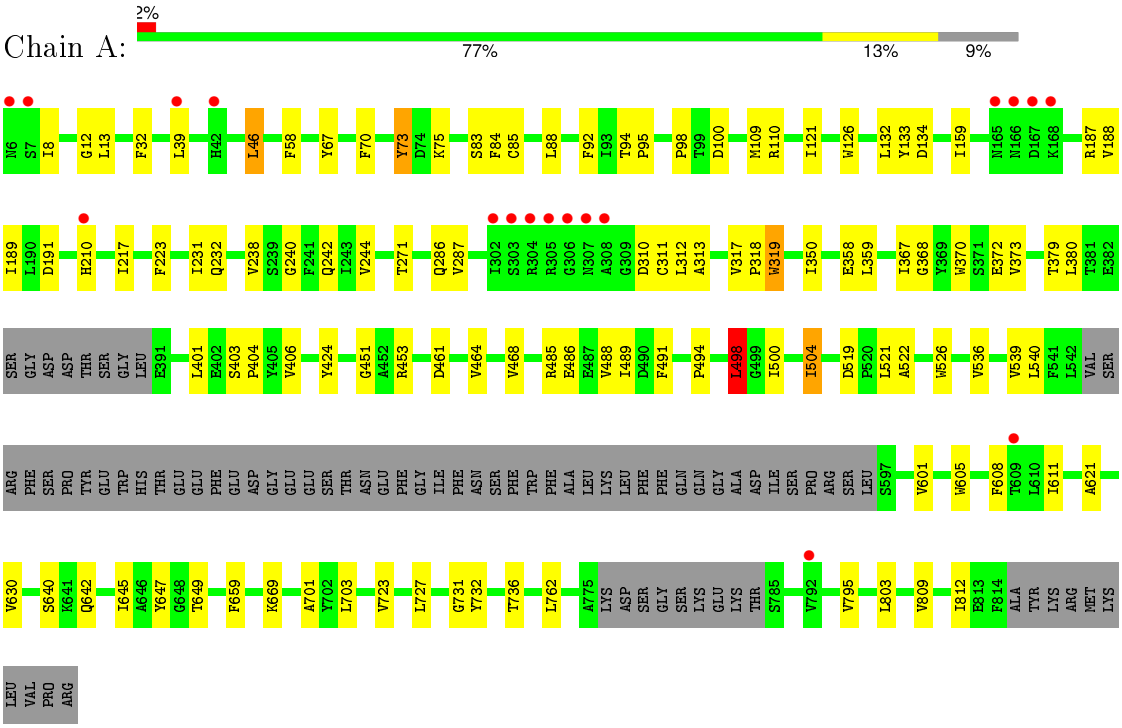
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 32 24 2 4 2	0	0
5	B	1	Total C N O S 32 24 2 4 2	0	0

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.

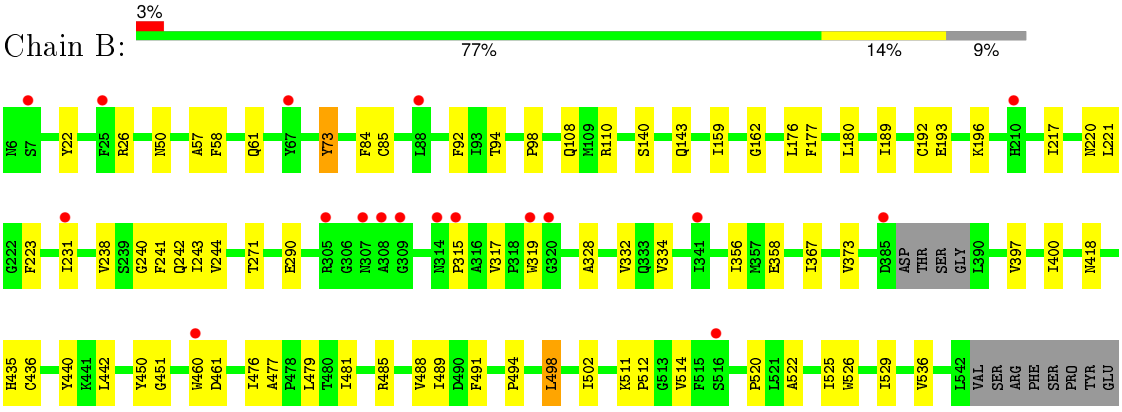
- Molecule 1: Glutamate receptor 2

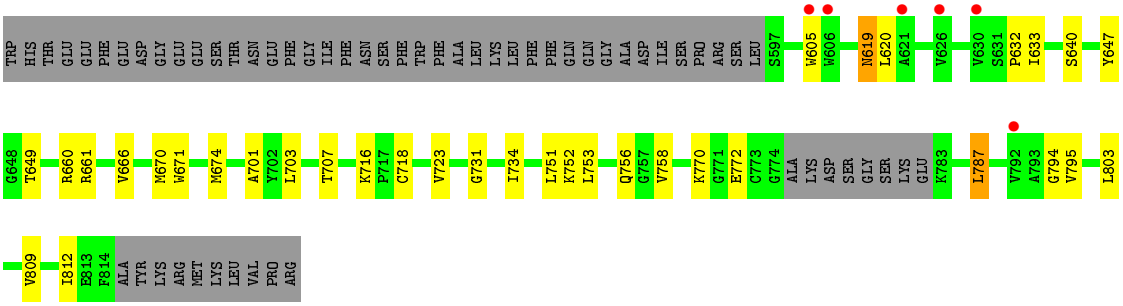
Chain A:



- Molecule 1: Glutamate receptor 2

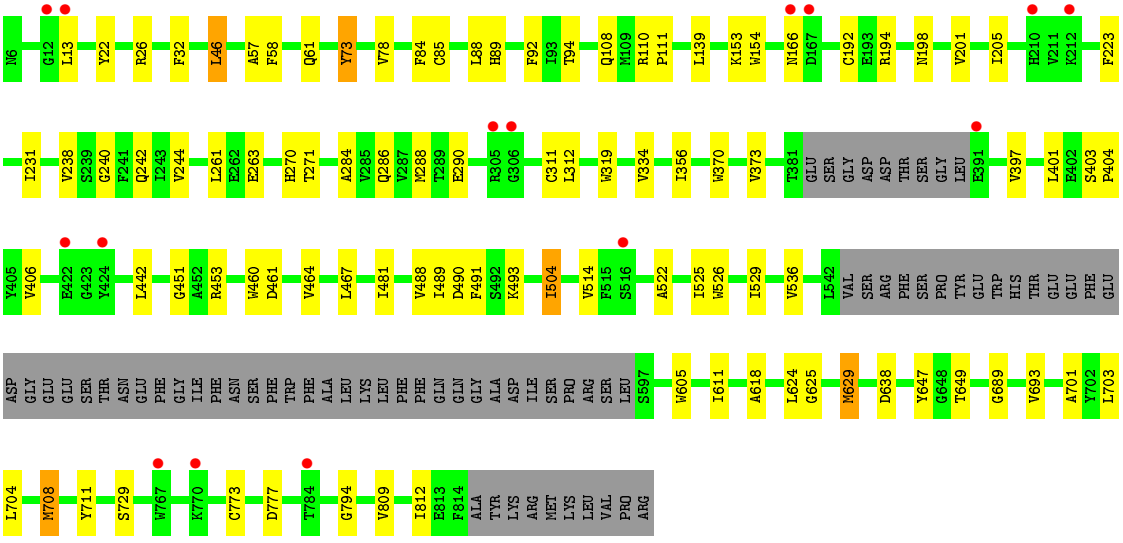
Chain B:





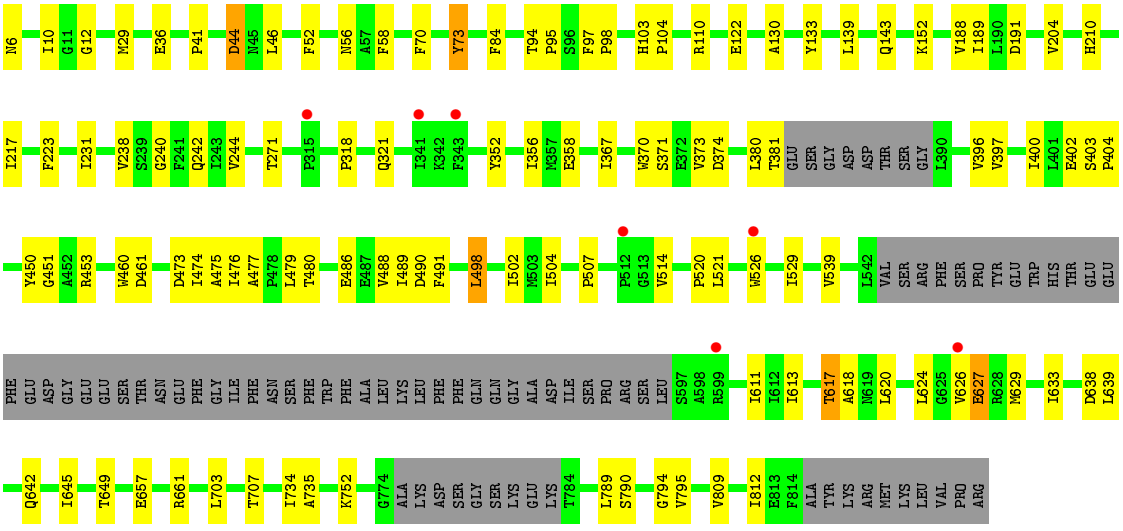
• Molecule 1: Glutamate receptor 2

Chain C:



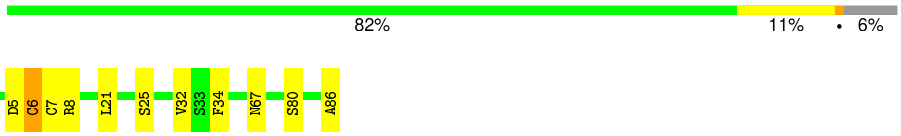
• Molecule 1: Glutamate receptor 2

Chain D:



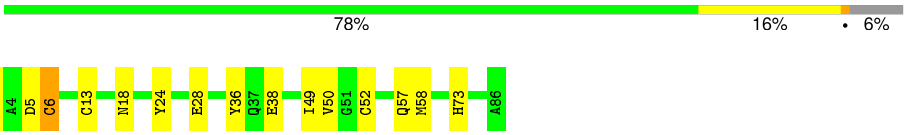
• Molecule 2: Con-ikot-ikot

Chain E:



- Molecule 2: Con-ikot-ikot

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	161.27Å 366.69Å 109.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.51 97.41 – 3.51	Depositor EDS
% Data completeness (in resolution range)	79.6 (19.99-3.51) 79.7 (97.41-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.240 , 0.276 0.253 , 0.284	Depositor DCC
R_{free} test set	3256 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	110.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 98.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 65270 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	23731	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 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: FWF, 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	0.24	0/5669	0.43	1/7710 (0.0%)
1	B	0.25	0/5761	0.43	0/7821
1	C	0.24	0/5611	0.42	0/7644
1	D	0.25	0/5689	0.43	0/7739
2	E	0.30	0/651	0.46	0/873
2	F	0.26	0/651	0.43	0/873
All	All	0.25	0/24032	0.43	1/32660 (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	A	498	LEU	CA-CB-CG	5.06	126.95	115.30

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	5553	0	5314	70	0
1	B	5645	0	5447	70	0
1	C	5498	0	5161	56	0
1	D	5573	0	5347	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	641	0	593	11	0
2	F	641	0	593	11	0
3	A	15	0	13	1	0
3	B	15	0	13	2	0
3	C	15	0	13	0	0
3	D	15	0	13	0	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	32	0	36	1	0
5	B	32	0	36	4	0
All	All	23731	0	22631	258	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 6.

All (258) 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:C:464:VAL:HG13	1:C:489:ILE:HD11	1.63	0.79
1:D:657:GLU:OE1	1:D:661:ARG:NH1	2.19	0.75
1:A:494:PRO:O	5:A:903:FWF:N1	2.24	0.71
1:D:633:ILE:HG23	1:D:638:ASP:HB2	1.74	0.70
1:C:356:ILE:HD11	1:C:370:TRP:HB2	1.77	0.67
1:A:379:THR:HG22	1:A:380:LEU:H	1.61	0.65
1:A:350:ILE:HG23	4:A:902:NAG:H61	1.80	0.64
1:D:476:ILE:HG12	1:D:734:ILE:HD12	1.79	0.64
1:A:187:ARG:NH2	2:E:67:ASN:OD1	2.31	0.64
1:D:789:LEU:HD12	1:D:790:SER:N	2.14	0.63
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.80	0.62
1:D:488:VAL:HG23	1:D:489:ILE:HG12	1.81	0.62
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.82	0.61
1:D:44:ASP:N	1:D:44:ASP:OD1	2.31	0.61
1:D:356:ILE:HD11	1:D:370:TRP:HB2	1.82	0.61
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.83	0.61
2:F:5:ASP:OD1	2:F:6:CYS:N	2.29	0.60
1:A:88:LEU:HD11	1:A:311:CYS:HB2	1.83	0.60
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.83	0.60
1:D:380:LEU:HG	1:D:381:THR:HG23	1.82	0.60
1:A:231:ILE:HD12	1:A:238:VAL:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ILE:HD12	1:D:238:VAL:HG21	1.85	0.59
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.85	0.59
1:A:539:VAL:HG21	1:B:803:LEU:HB3	1.85	0.59
1:C:242:GLN:HE21	1:C:244:VAL:H	1.51	0.58
1:A:232:GLN:HA	1:A:359:LEU:HD21	1.86	0.58
1:D:752:LYS:NZ	2:E:86:ALA:O	2.37	0.57
1:D:98:PRO:HD3	1:D:110:ARG:HD2	1.86	0.57
1:D:633:ILE:HD13	1:D:639:LEU:HG	1.87	0.56
1:D:396:VAL:HG23	1:D:473:ASP:H	1.70	0.56
1:A:519:ASP:O	1:B:787:LEU:HD12	2.05	0.56
2:E:6:CYS:SG	2:E:7:CYS:N	2.78	0.56
1:A:640:SER:OG	1:A:669:LYS:HD2	2.05	0.55
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.87	0.55
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.89	0.55
1:C:489:ILE:HG22	1:C:490:ASP:H	1.71	0.55
1:B:162:GLY:HA2	1:B:196:LYS:HE2	1.88	0.55
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.88	0.55
1:A:13:LEU:HD23	1:A:46:LEU:HD21	1.89	0.55
1:B:514:VAL:HG13	1:B:794:GLY:HA3	1.89	0.54
2:E:5:ASP:HB3	2:E:8:ARG:HB3	1.89	0.54
1:D:520:PRO:HG2	1:D:620:LEU:HD23	1.88	0.54
1:D:122:GLU:OE1	1:D:152:LYS:NZ	2.40	0.54
1:B:494:PRO:O	5:B:903:FWF:N1	2.27	0.53
2:E:21:LEU:HD21	2:E:32:VAL:HA	1.89	0.53
2:E:5:ASP:OD1	2:E:6:CYS:N	2.29	0.53
1:D:486:GLU:HG2	1:D:491:PHE:HD2	1.73	0.53
1:C:522:ALA:HB3	1:C:525:ILE:HG13	1.90	0.53
1:C:453:ARG:NH2	2:F:38:GLU:OE1	2.42	0.53
1:B:520:PRO:HG2	1:B:620:LEU:HD23	1.90	0.52
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.91	0.52
1:C:460:TRP:NE1	1:C:488:VAL:HG11	2.25	0.52
1:C:488:VAL:HG23	1:C:489:ILE:HG13	1.91	0.52
1:D:489:ILE:HG22	1:D:490:ASP:H	1.74	0.52
1:D:613:ILE:O	1:D:617:THR:OG1	2.26	0.52
1:C:13:LEU:HD23	1:C:46:LEU:HD21	1.92	0.52
1:D:451:GLY:HA2	1:D:461:ASP:O	2.08	0.52
1:B:315:PRO:C	1:B:317:VAL:H	2.14	0.52
1:A:504:ILE:HD11	1:A:723:VAL:HG21	1.92	0.51
1:B:753:LEU:HD22	1:B:758:VAL:HG11	1.92	0.51
1:B:242:GLN:HE21	1:B:244:VAL:H	1.57	0.51
1:C:194:ARG:O	1:C:198:ASN:ND2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:VAL:HA	1:B:812:ILE:HG12	1.93	0.50
1:C:88:LEU:HD11	1:C:311:CYS:HB2	1.93	0.50
1:C:231:ILE:HD12	1:C:238:VAL:HG21	1.94	0.50
1:B:451:GLY:HA2	1:B:461:ASP:O	2.10	0.50
1:C:58:PHE:CE2	1:C:84:PHE:HB3	2.47	0.50
1:D:58:PHE:CE2	1:D:84:PHE:HB3	2.47	0.50
1:B:159:ILE:HG21	1:B:176:LEU:HD13	1.92	0.50
1:A:803:LEU:HB3	1:D:539:VAL:HG21	1.94	0.50
1:D:498:LEU:HB3	1:D:707:THR:HG23	1.93	0.50
1:C:139:LEU:HD12	1:D:139:LEU:HD12	1.94	0.50
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.77	0.49
1:D:626:VAL:O	1:D:627:GLU:HG3	2.11	0.49
1:A:73:TYR:CE2	1:A:94:THR:HG21	2.47	0.49
1:B:315:PRO:HB2	1:B:317:VAL:O	2.13	0.49
1:C:73:TYR:CE2	1:C:94:THR:HG21	2.47	0.49
1:A:58:PHE:CE2	1:A:84:PHE:HB3	2.48	0.49
1:A:109:MET:HE1	1:A:287:VAL:HG21	1.93	0.49
1:D:6:ASN:ND2	1:D:36:GLU:O	2.33	0.49
1:B:647:TYR:HB3	1:B:701:ALA:HB3	1.95	0.49
1:A:126:TRP:CG	1:A:187:ARG:HD3	2.48	0.48
1:B:177:PHE:HA	1:B:180:LEU:HB2	1.95	0.48
1:A:521:LEU:O	1:A:526:TRP:NE1	2.46	0.48
1:C:451:GLY:HA2	1:C:461:ASP:O	2.12	0.48
1:A:98:PRO:HD3	1:A:110:ARG:HD2	1.96	0.48
1:B:140:SER:HA	1:B:143:GLN:HE21	1.78	0.48
1:B:290:GLU:HG3	1:B:334:VAL:HG11	1.95	0.48
1:C:263:GLU:HG2	1:C:270:HIS:HB2	1.95	0.48
1:A:424:TYR:CE2	1:A:762:LEU:HB3	2.49	0.48
1:B:223:PHE:CD1	1:B:240:GLY:HA3	2.48	0.48
1:A:451:GLY:HA2	1:A:461:ASP:O	2.13	0.48
1:D:352:TYR:HE1	1:D:370:TRP:HZ3	1.61	0.48
2:E:80:SER:HB2	2:F:3:PRO:HG2	1.95	0.48
1:B:460:TRP:NE1	1:B:488:VAL:HG11	2.29	0.47
1:C:223:PHE:CD1	1:C:240:GLY:HA3	2.49	0.47
1:A:621:ALA:HA	1:D:618:ALA:HB1	1.96	0.47
1:D:97:PHE:HA	1:D:110:ARG:HD2	1.96	0.47
1:B:221:LEU:HB3	1:B:243:ILE:HB	1.96	0.47
1:C:284:ALA:O	1:C:288:MET:HG3	2.14	0.47
1:B:58:PHE:CE2	1:B:84:PHE:HB3	2.49	0.47
1:D:189:ILE:HG12	1:D:217:ILE:HB	1.95	0.47
1:B:73:TYR:CE2	1:B:94:THR:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:TYR:CE2	1:D:94:THR:HG21	2.49	0.47
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.96	0.47
1:A:486:GLU:HG2	1:A:491:PHE:HD2	1.80	0.47
1:B:640:SER:HB3	1:B:666:VAL:HG13	1.97	0.47
1:A:608:PHE:O	1:A:611:ILE:HG13	2.14	0.47
1:A:611:ILE:HG12	1:B:795:VAL:HG11	1.95	0.47
1:D:809:VAL:HA	1:D:812:ILE:HG12	1.97	0.47
1:B:619:ASN:C	1:B:619:ASN:HD22	2.17	0.47
1:B:231:ILE:HD12	1:B:238:VAL:HG21	1.96	0.47
1:A:488:VAL:HG12	2:E:34:PHE:HD2	1.80	0.47
1:D:502:ILE:HD13	1:D:639:LEU:HD11	1.97	0.47
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.97	0.47
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.50	0.47
1:B:418:ASN:ND2	1:B:440:TYR:O	2.46	0.46
1:D:507:PRO:HG2	1:D:629:MET:HB2	1.97	0.46
1:A:522:ALA:HB2	1:B:787:LEU:HD13	1.98	0.46
1:B:502:ILE:HB	1:B:723:VAL:HG23	1.98	0.46
1:A:32:PHE:CZ	1:A:286:GLN:HB2	2.50	0.46
1:A:485:ARG:O	1:A:489:ILE:HG13	2.15	0.46
2:F:24:TYR:O	2:F:28:GLU:HG3	2.16	0.46
1:B:85:CYS:SG	1:B:92:PHE:HB2	2.55	0.46
1:A:540:LEU:HG	1:A:601:VAL:HG11	1.97	0.46
1:A:464:VAL:O	1:A:468:VAL:HG23	2.15	0.46
1:A:809:VAL:HA	1:A:812:ILE:HG12	1.97	0.46
1:B:498:LEU:HD13	1:B:731:GLY:HA2	1.98	0.46
1:D:460:TRP:NE1	1:D:488:VAL:HG11	2.31	0.45
1:A:94:THR:HA	1:A:95:PRO:HD3	1.83	0.45
1:B:498:LEU:HB3	1:B:707:THR:HG23	1.99	0.45
1:B:522:ALA:HB3	1:B:525:ILE:HG13	1.97	0.45
1:C:514:VAL:HG13	1:C:794:GLY:HA3	1.99	0.45
1:B:632:PRO:HB2	1:B:633:ILE:HD12	1.98	0.45
1:C:22:TYR:CE2	1:C:26:ARG:HD2	2.50	0.45
1:B:751:LEU:HA	5:B:903:FWF:H34	1.97	0.45
1:B:477:ALA:O	1:B:479:LEU:N	2.49	0.45
1:B:400:ILE:HG21	1:B:450:TYR:CZ	2.52	0.45
1:C:625:GLY:O	1:C:629:MET:HB2	2.17	0.45
1:B:328:ALA:O	1:B:332:VAL:HG23	2.17	0.45
1:B:397:VAL:HB	1:B:442:LEU:HD23	1.98	0.45
1:C:84:PHE:CE1	1:D:52:PHE:HA	2.52	0.45
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.52	0.45
1:D:103:HIS:HA	1:D:104:PRO:HD2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:VAL:HG13	1:C:442:LEU:HA	1.99	0.44
1:C:201:VAL:O	1:C:205:ILE:HG13	2.17	0.44
1:B:481:ILE:HA	1:B:491:PHE:CE2	2.52	0.44
1:D:29:MET:SD	1:D:41:PRO:HG3	2.57	0.44
1:A:134:ASP:OD1	1:A:134:ASP:N	2.51	0.44
1:C:85:CYS:SG	1:C:92:PHE:HB2	2.58	0.44
1:A:500:ILE:HB	1:A:727:LEU:HB2	1.98	0.44
1:A:132:LEU:HD23	1:A:188:VAL:HG13	2.00	0.44
1:C:32:PHE:CZ	1:C:286:GLN:HB2	2.52	0.44
2:E:80:SER:HA	2:F:5:ASP:OD2	2.18	0.43
1:B:666:VAL:O	1:B:670:MET:HG3	2.18	0.43
1:A:100:ASP:N	1:A:100:ASP:OD1	2.49	0.43
1:D:204:VAL:HG12	1:D:210:HIS:HB3	2.00	0.43
1:A:121:ILE:HG23	1:A:126:TRP:HB2	2.00	0.43
1:A:187:ARG:HH12	2:E:25:SER:HB2	1.83	0.43
1:B:98:PRO:HD3	1:B:110:ARG:HD2	2.00	0.43
1:D:400:ILE:HG21	1:D:450:TYR:CZ	2.53	0.43
1:A:126:TRP:CD2	1:A:187:ARG:HD3	2.53	0.43
1:C:139:LEU:HD11	1:D:143:GLN:OE1	2.19	0.43
1:D:242:GLN:HE21	1:D:244:VAL:H	1.65	0.43
1:C:773:CYS:O	1:C:777:ASP:N	2.39	0.43
1:D:402:GLU:HG3	1:D:450:TYR:OH	2.19	0.43
1:A:403:SER:HA	1:A:404:PRO:HA	1.75	0.43
1:B:193:GLU:HG2	1:B:193:GLU:H	1.65	0.43
1:A:310:ASP:HB3	1:A:313:ALA:HB2	2.01	0.43
1:B:716:LYS:HA	1:B:718:CYS:H	1.83	0.43
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.82	0.43
1:C:467:LEU:HD23	1:C:489:ILE:HG21	2.01	0.43
2:F:18:ASN:HB2	2:F:73:HIS:CE1	2.54	0.43
1:D:97:PHE:HA	1:D:98:PRO:HD3	1.89	0.42
1:D:371:SER:HB3	1:D:374:ASP:HB2	2.00	0.42
1:A:223:PHE:CD1	1:A:240:GLY:HA3	2.54	0.42
1:D:223:PHE:CD1	1:D:240:GLY:HA3	2.54	0.42
1:B:752:LYS:HZ1	2:F:50:VAL:HG22	1.85	0.42
1:C:290:GLU:HG3	1:C:334:VAL:HG11	2.00	0.42
1:C:647:TYR:HB3	1:C:701:ALA:HB3	2.01	0.42
1:B:511:LYS:HA	1:B:512:PRO:HD2	1.87	0.42
1:A:659:PHE:CE2	1:A:703:LEU:HD13	2.54	0.42
1:B:485:ARG:O	1:B:489:ILE:HG13	2.19	0.42
1:C:110:ARG:HA	1:C:111:PRO:HD3	1.89	0.42
5:B:903:FWF:H8	1:C:729:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:OG	1:B:50:ASN:OD1	2.37	0.42
3:A:901:KAI:HD12	3:A:901:KAI:HD2	1.71	0.42
1:C:57:ALA:O	1:C:61:GLN:HG2	2.19	0.42
1:B:436:CYS:HA	2:F:58:MET:HE3	2.01	0.42
1:B:22:TYR:CE2	1:B:26:ARG:HD2	2.54	0.42
1:D:397:VAL:HG13	1:D:474:ILE:HG23	2.01	0.42
1:A:12:GLY:HA2	1:A:70:PHE:O	2.19	0.42
1:A:132:LEU:HD13	1:A:159:ILE:HB	2.00	0.42
1:B:716:LYS:HA	1:B:718:CYS:N	2.34	0.42
1:D:514:VAL:HG13	1:D:794:GLY:HA3	2.01	0.42
1:C:312:LEU:O	1:D:56:ASN:ND2	2.46	0.42
1:A:647:TYR:HB3	1:A:701:ALA:HB3	2.02	0.42
1:A:242:GLN:HE21	1:A:244:VAL:H	1.68	0.42
1:A:368:GLY:HA2	1:A:379:THR:OG1	2.20	0.42
1:D:94:THR:HA	1:D:95:PRO:HD3	1.86	0.42
1:A:189:ILE:HG12	1:A:217:ILE:HB	2.02	0.42
1:B:476:ILE:HG12	1:B:734:ILE:HG23	2.02	0.42
1:D:489:ILE:HG22	1:D:490:ASP:N	2.35	0.42
3:B:901:KAI:HD2	3:B:901:KAI:HD12	1.67	0.42
1:A:85:CYS:SG	1:A:92:PHE:HB2	2.60	0.42
1:D:358:GLU:OE2	1:D:367:ILE:HD13	2.20	0.42
1:C:403:SER:HA	1:C:404:PRO:HA	1.75	0.42
1:D:453:ARG:NH2	1:D:460:TRP:HE1	2.18	0.42
1:B:770:LYS:HB3	1:B:770:LYS:HE2	1.90	0.42
1:D:10:ILE:O	1:D:41:PRO:HA	2.20	0.41
1:A:67:TYR:HD1	1:A:319:TRP:HH2	1.67	0.41
1:A:232:GLN:HG3	1:A:359:LEU:HD21	2.02	0.41
1:C:261:LEU:O	1:C:270:HIS:ND1	2.47	0.41
1:A:358:GLU:OE2	1:A:367:ILE:HD13	2.20	0.41
1:A:133:TYR:HA	1:A:191:ASP:O	2.20	0.41
1:C:481:ILE:HA	1:C:491:PHE:CE2	2.55	0.41
1:A:488:VAL:HG12	2:E:34:PHE:CD2	2.55	0.41
1:B:450:TYR:CE2	3:B:901:KAI:HD1	2.55	0.41
1:D:130:ALA:HB3	1:D:188:VAL:HG22	2.02	0.41
1:B:671:TRP:HA	1:B:674:MET:HE2	2.02	0.41
1:B:619:ASN:HA	1:C:624:LEU:HD13	2.02	0.41
2:F:36:TYR:CG	2:F:57:GLN:HG3	2.56	0.41
1:B:660:ARG:HD2	1:B:661:ARG:NH1	2.35	0.41
5:B:903:FWF:H30	1:C:493:LYS:HB3	2.03	0.41
1:C:153:LYS:O	1:C:154:TRP:HD1	2.03	0.41
1:C:704:LEU:HD12	1:C:708:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:VAL:HG21	1:A:605:TRP:CE3	2.56	0.41
1:C:522:ALA:H	1:C:525:ILE:HD12	1.86	0.41
1:B:526:TRP:O	1:B:529:ILE:HG22	2.20	0.41
2:F:13:CYS:HB2	2:F:52:CYS:HB2	1.80	0.41
1:D:526:TRP:O	1:D:529:ILE:HG22	2.21	0.41
1:B:220:ASN:O	1:B:241:PHE:HB2	2.20	0.41
1:D:318:PRO:HG2	1:D:321:GLN:HG2	2.03	0.41
1:A:8:ILE:HB	1:A:39:LEU:HD23	2.01	0.41
1:C:504:ILE:HD13	1:C:504:ILE:H	1.85	0.41
1:C:689:GLY:O	1:C:693:VAL:HG23	2.21	0.41
1:C:526:TRP:O	1:C:529:ILE:HG22	2.21	0.41
1:B:356:ILE:HG13	1:B:356:ILE:O	2.20	0.41
1:A:494:PRO:HA	1:A:732:TYR:O	2.21	0.41
1:D:133:TYR:HA	1:D:191:ASP:O	2.21	0.41
1:A:370:TRP:CH2	1:A:372:GLU:HA	2.57	0.41
1:B:189:ILE:HG12	1:B:217:ILE:HB	2.03	0.41
1:D:12:GLY:HA2	1:D:70:PHE:O	2.21	0.41
1:B:57:ALA:O	1:B:61:GLN:HG2	2.21	0.41
1:D:477:ALA:O	1:D:479:LEU:N	2.51	0.41
1:A:642:GLN:NE2	1:A:645:ILE:HB	2.36	0.40
1:A:498:LEU:HD13	1:A:731:GLY:HA2	2.02	0.40
1:C:489:ILE:HG22	1:C:490:ASP:N	2.35	0.40
1:C:73:TYR:CD2	1:C:78:VAL:HG23	2.56	0.40
1:B:358:GLU:OE1	1:B:367:ILE:HD13	2.20	0.40
1:A:317:VAL:HA	1:A:318:PRO:HD3	1.86	0.40
1:A:521:LEU:CA	1:B:787:LEU:HD11	2.52	0.40
1:C:618:ALA:HB3	1:D:620:LEU:HD12	2.03	0.40
1:B:435:HIS:NE2	1:B:752:LYS:HD3	2.36	0.40
1:B:243:ILE:HG23	1:B:244:VAL:HG23	2.03	0.40
1:C:404:PRO:HD3	1:C:711:TYR:CG	2.57	0.40
1:B:756:GLN:HG2	2:F:49:ILE:HD13	2.03	0.40
1:D:403:SER:HA	1:D:404:PRO:HA	1.76	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	730/814 (90%)	714 (98%)	16 (2%)	0	100	100
1	B	735/814 (90%)	717 (98%)	18 (2%)	0	100	100
1	C	740/814 (91%)	726 (98%)	14 (2%)	0	100	100
1	D	730/814 (90%)	712 (98%)	18 (2%)	0	100	100
2	E	83/90 (92%)	78 (94%)	5 (6%)	0	100	100
2	F	83/90 (92%)	79 (95%)	4 (5%)	0	100	100
All	All	3101/3436 (90%)	3026 (98%)	75 (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	561/693 (81%)	548 (98%)	13 (2%)	58	85
1	B	575/693 (83%)	565 (98%)	10 (2%)	68	89
1	C	539/693 (78%)	526 (98%)	13 (2%)	57	85
1	D	566/693 (82%)	554 (98%)	12 (2%)	61	86
2	E	73/76 (96%)	72 (99%)	1 (1%)	74	91
2	F	73/76 (96%)	72 (99%)	1 (1%)	74	91
All	All	2387/2924 (82%)	2337 (98%)	50 (2%)	61	86

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	73	TYR
1	A	75	LYS

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Mol	Chain	Res	Type
1	A	210	HIS
1	A	271	THR
1	A	312	LEU
1	A	319	TRP
1	A	373	VAL
1	A	453	ARG
1	A	498	LEU
1	A	504	ILE
1	A	630	VAL
1	A	736	THR
1	B	73	TYR
1	B	108	GLN
1	B	192	CYS
1	B	271	THR
1	B	319	TRP
1	B	373	VAL
1	B	498	LEU
1	B	619	ASN
1	B	772	GLU
1	B	787	LEU
1	C	46	LEU
1	C	73	TYR
1	C	89	HIS
1	C	108	GLN
1	C	166	ASN
1	C	192	CYS
1	C	271	THR
1	C	319	TRP
1	C	373	VAL
1	C	504	ILE
1	C	629	MET
1	C	638	ASP
1	C	708	MET
1	D	44	ASP
1	D	46	LEU
1	D	73	TYR
1	D	271	THR
1	D	373	VAL
1	D	480	THR
1	D	498	LEU
1	D	504	ILE
1	D	521	LEU

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Mol	Chain	Res	Type
1	D	617	THR
1	D	624	LEU
1	D	627	GLU
2	E	6	CYS
2	F	6	CYS

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

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	KAI	A	901	-	8,15,15	1.02	0	7,21,21	1.07	0
4	NAG	A	902	1	14,14,15	0.27	0	15,19,21	0.58	0
5	FWF	A	903	-	31,33,33	0.57	0	28,48,48	1.94	2 (7%)
3	KAI	B	901	-	8,15,15	0.95	0	7,21,21	1.19	0
4	NAG	B	902	1	14,14,15	0.54	0	15,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FWF	B	903	-	31,33,33	0.56	0	28,48,48	1.91	2 (7%)
3	KAI	C	901	-	8,15,15	1.05	0	7,21,21	1.18	0
4	NAG	C	902	1	14,14,15	0.37	0	15,19,21	0.57	0
3	KAI	D	901	-	8,15,15	1.17	1 (12%)	7,21,21	1.04	0
4	NAG	D	902	1	14,14,15	0.39	0	15,19,21	0.26	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	KAI	A	901	-	-	0/6/25/25	0/1/1/1
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
5	FWF	A	903	-	-	0/32/36/36	0/2/2/2
3	KAI	B	901	-	-	0/6/25/25	0/1/1/1
4	NAG	B	902	1	-	0/6/23/26	0/1/1/1
5	FWF	B	903	-	-	0/32/36/36	0/2/2/2
3	KAI	C	901	-	-	0/6/25/25	0/1/1/1
4	NAG	C	902	1	-	0/6/23/26	0/1/1/1
3	KAI	D	901	-	-	0/6/25/25	0/1/1/1
4	NAG	D	902	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	KAI	CA-N	-2.25	1.44	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	903	FWF	O3-S2-O4	-6.34	108.93	119.34
5	A	903	FWF	O2-S1-O1	-6.24	109.09	119.34
5	A	903	FWF	O3-S2-O4	-6.06	109.39	119.34
5	B	903	FWF	O2-S1-O1	-5.70	109.98	119.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	KAI	1	0
4	A	902	NAG	1	0
5	A	903	FWF	1	0
3	B	901	KAI	2	0
5	B	903	FWF	4	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^{th} 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	738/814 (90%)	-0.13	18 (2%) 62 52	97, 159, 239, 315	0
1	B	743/814 (91%)	-0.04	24 (3%) 51 42	105, 163, 236, 294	0
1	C	746/814 (91%)	-0.13	15 (2%) 68 59	115, 176, 264, 342	0
1	D	738/814 (90%)	-0.13	7 (0%) 85 78	95, 162, 242, 328	0
2	E	85/90 (94%)	-0.06	0 100 100	109, 137, 176, 250	0
2	F	85/90 (94%)	-0.11	0 100 100	118, 152, 200, 245	0
All	All	3135/3436 (91%)	-0.11	64 (2%) 68 59	95, 164, 246, 342	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	ASP	9.6
1	A	305	ARG	7.3
1	B	308	ALA	6.5
1	B	314	ASN	5.8
1	A	166	ASN	4.8
1	C	167	ASP	4.3
1	B	319	TRP	4.3
1	B	305	ARG	4.2
1	C	391	GLU	4.1
1	A	210	HIS	4.1
1	A	306	GLY	4.1
1	B	309	GLY	3.9
1	A	6	ASN	3.9
1	B	307	ASN	3.6
1	B	320	GLY	3.6
1	B	315	PRO	3.6
1	C	12	GLY	3.5
1	A	307	ASN	3.5
1	D	343	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	7	SER	3.2
1	A	165	ASN	3.1
1	C	305	ARG	3.1
1	B	460	TRP	3.0
1	B	385	ASP	3.0
1	B	7	SER	2.8
1	C	306	GLY	2.8
1	B	630	VAL	2.8
1	D	512	PRO	2.8
1	A	609	THR	2.7
1	B	67	TYR	2.7
1	C	166	ASN	2.6
1	C	784	THR	2.6
1	A	792	VAL	2.6
1	A	302	ILE	2.6
1	C	212	LYS	2.5
1	B	626	VAL	2.5
1	A	304	ARG	2.4
1	A	42	HIS	2.4
1	D	599	ARG	2.4
1	C	210	HIS	2.4
1	C	424	TYR	2.4
1	A	303	SER	2.3
1	B	792	VAL	2.3
1	B	25	PHE	2.3
1	A	168	LYS	2.3
1	B	516	SER	2.3
1	D	341	ILE	2.2
1	D	315	PRO	2.2
1	B	88	LEU	2.2
1	C	13	LEU	2.2
1	A	39	LEU	2.1
1	B	210	HIS	2.1
1	B	606	TRP	2.1
1	C	767	TRP	2.1
1	B	341	ILE	2.1
1	A	308	ALA	2.1
1	B	621	ALA	2.1
1	B	231	ILE	2.1
1	B	605	TRP	2.1
1	D	626	VAL	2.1
1	C	422	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	526	TRP	2.0
1	C	516	SER	2.0
1	C	770	LYS	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 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^{th} 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^2)	Q<0.9
5	FWF	B	903	32/32	0.93	0.38	1.33	91,127,150,167	0
3	KAI	D	901	15/15	0.92	0.31	0.84	90,114,141,141	0
4	NAG	A	902	14/15	0.88	0.30	0.57	102,145,164,167	0
5	FWF	A	903	32/32	0.93	0.31	0.55	86,120,139,277	0
3	KAI	A	901	15/15	0.94	0.31	0.13	88,121,143,149	0
3	KAI	B	901	15/15	0.91	0.22	-0.32	120,138,156,161	0
4	NAG	C	902	14/15	0.92	0.23	-0.50	102,147,177,178	0
3	KAI	C	901	15/15	0.93	0.20	-0.87	117,132,159,171	0
4	NAG	D	902	14/15	0.79	0.36	-	199,233,243,267	0
4	NAG	B	902	14/15	0.77	0.24	-	194,219,229,244	0

6.5 Other polymers (i)

There are no such residues in this entry.