wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:52 PM GMT

PDB ID	:	4U5F
Title	:	Crystal structure of GluA2, con-ikot-ikot snail toxin, partial agonist KA and postitive modulator (R,R)-2b complex, GluA2cryst2 construct
Authors	:	Chen, L.; Gouaux, E.
Deposited on	:	2014-07-25
Resolution	:	3.70 Å(reported)

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

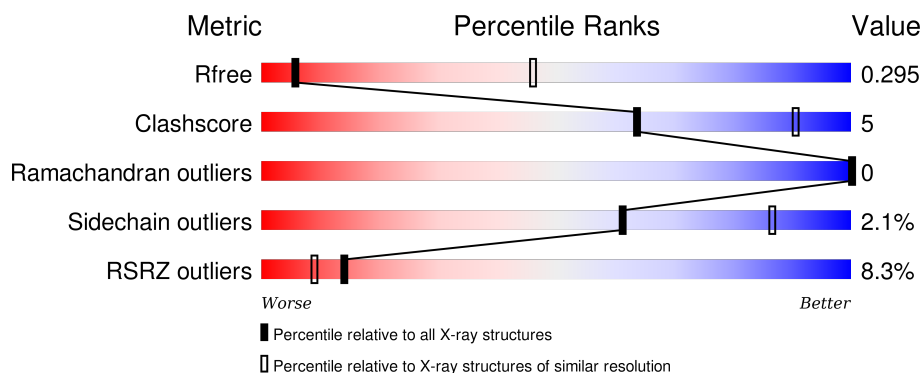|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.70 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	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	
1	B	814	
1	C	814	
1	D	814	
2	E	90	

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Mol	Chain	Length	Quality of chain
2	F	90	2% ▇ (red) 78% (green) 17% (yellow) 6% (grey)

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	KAI	B	902	-	-	-	X
5	FWF	B	901	-	-	-	X
5	FWF	D	901	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23700 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	735	Total 5535	C 3562	N 903	O 1043	S 27	0	0	0
1	B	738	Total 5618	C 3610	N 926	O 1055	S 27	0	0	0
1	C	747	Total 5507	C 3531	N 908	O 1041	S 27	0	0	0
1	D	742	Total 5578	C 3591	N 911	O 1049	S 27	0	0	0

There are 92 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	?	-	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	589	ALA	CYS	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
A	?	-	MET	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P19491
A	?	-	VAL	deletion	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	?	-	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	589	ALA	CYS	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
B	?	-	MET	deletion	UNP P19491
B	?	-	LYS	deletion	UNP P19491
B	?	-	VAL	deletion	UNP P19491
C	184	GLY	LYS	engineered mutation	UNP P19491
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	?	-	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	589	ALA	CYS	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	821	LEU	GLU	engineered mutation	UNP P19491
C	822	VAL	ALA	engineered mutation	UNP P19491
C	823	PRO	LYS	engineered mutation	UNP P19491
C	?	-	MET	deletion	UNP P19491
C	?	-	LYS	deletion	UNP P19491
C	?	-	VAL	deletion	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	?	-	ARG	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLN	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	565	GLU	SER	engineered mutation	UNP P19491
D	589	ALA	CYS	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
D	?	-	MET	deletion	UNP P19491
D	?	-	LYS	deletion	UNP P19491
D	?	-	VAL	deletion	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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: $C_{10}H_{15}NO_4$).
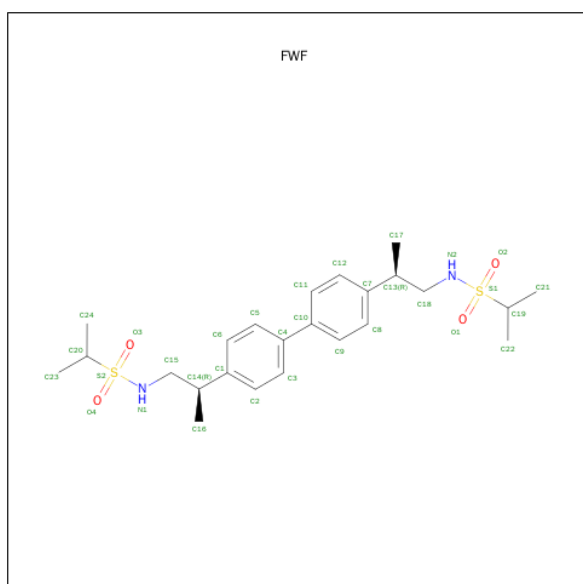

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	1	4		
3	B	1	Total	C	N	O	0	0
			15	10	1	4		
3	C	1	Total	C	N	O	0	0
			15	10	1	4		
3	D	1	Total	C	N	O	0	0
			15	10	1	4		

- 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 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0
4	D	1	Total 14	C 8	N 1	O 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: $C_{24}H_{36}N_2O_4S_2$).
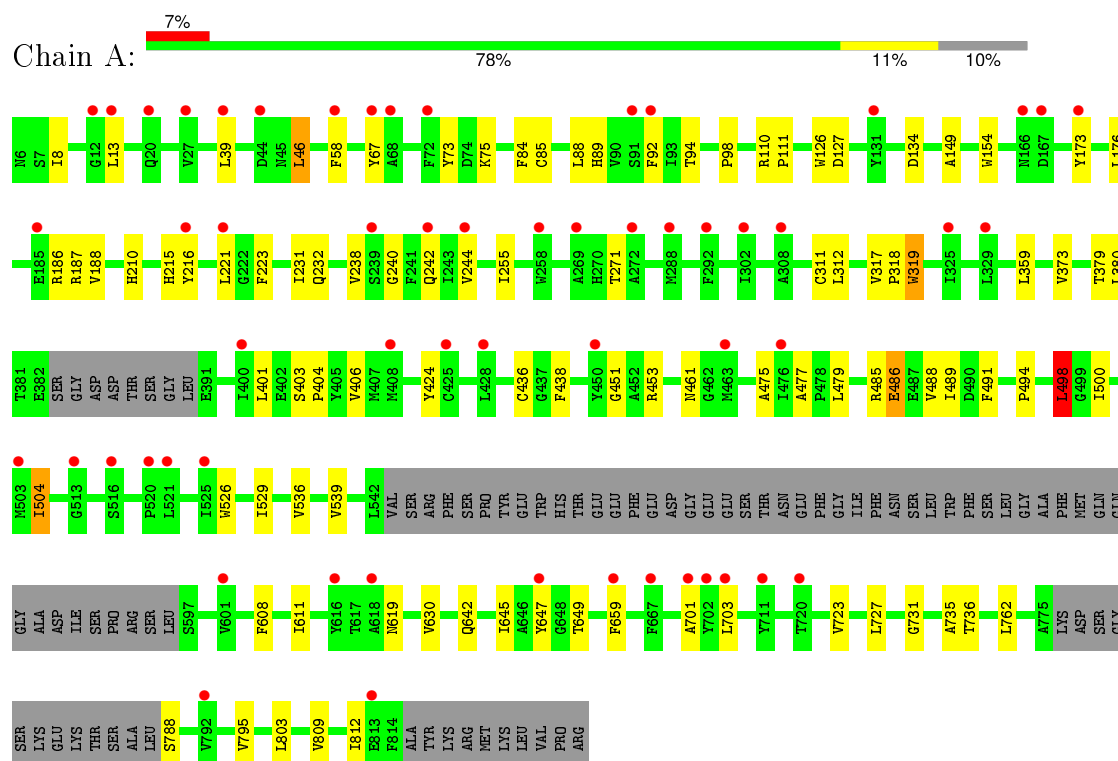
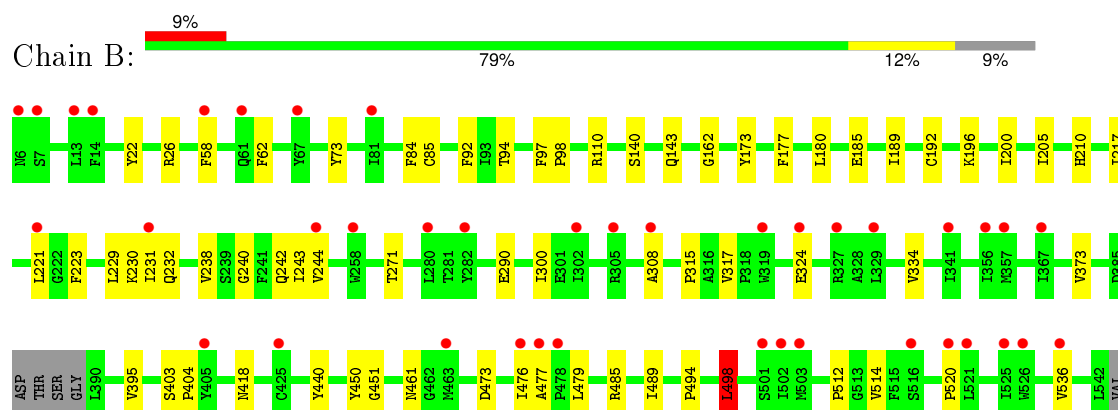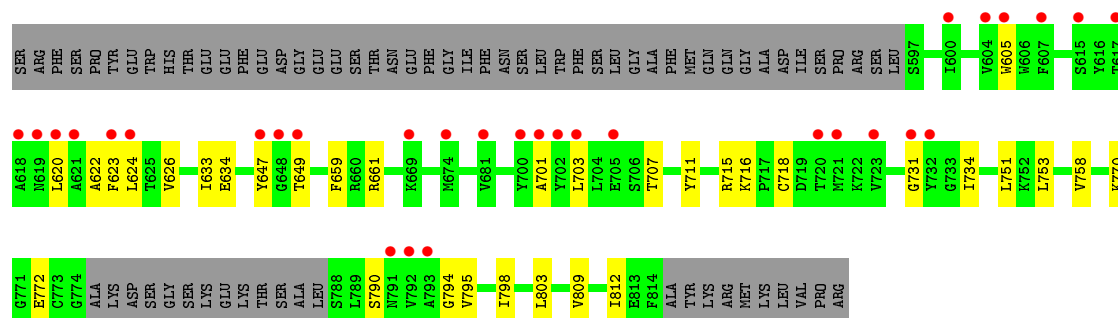| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 32	C 24	N 2	O 4	S 2	0	0
5	D	1	Total 32	C 24	N 2	O 4	S 2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.
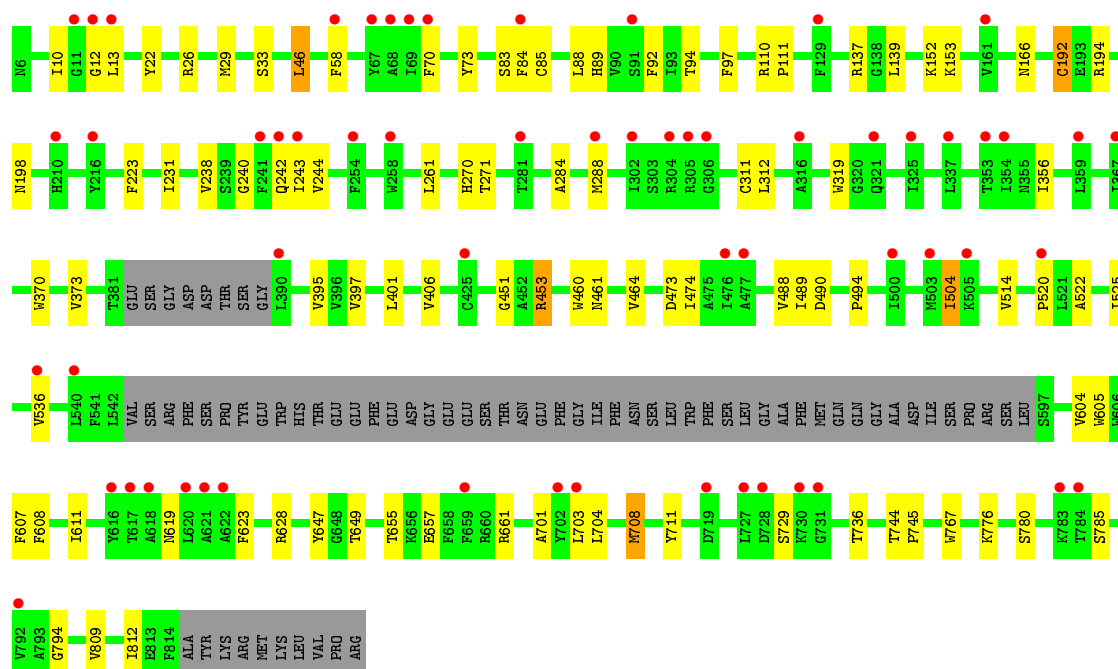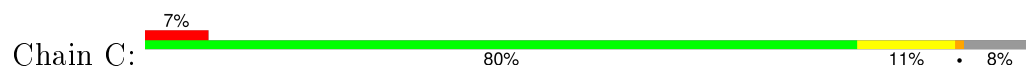
- Molecule 1: Glutamate receptor 2

- Molecule 1: Glutamate receptor 2

• Molecule 1: Glutamate receptor 2

Chain C:

• Molecule 1: Glutamate receptor 2

Chain D:

ARG SER LEU S597 G598 R599 I600 V601 V604 F608 I611 L620 A621 A622 F623 S635 A636 Q642 I645 A646 Y647 G648 T649 L650 E657 F658 F659 R660 R661 W671 M674 Y700 A701 Y702 L703 T707 M708 M721 G731 I734 A735 T736 V746

G774 ALA LYS ASP SER GLY SER LYS GLU K783 T784 S785 A786 N791 V792 V795 L799 V809 I812 E813 F814 ALA TYR LYS ARG MET LYS LEU VAL PRO ARG

● Molecule 2: Con-ikot-ikot

Chain E:

%

71% 23% 6%

GLY PRO GLY SER SER G2 D5 R8 C13 L21 Q22 R23 G26 R27 E28 V32 S33 F34 C35 Y36 Q37 E38 N47 C52 Q57 M58 R62 N67 S80 N83 P84 C85 A86

● Molecule 2: Con-ikot-ikot

Chain F:

2%

78% 17% 6%

GLY PRO GLY SER SER G2 P3 A4 D5 C6 C7 N18 F34 C35 Y36 Q37 E38 F46 N47 E48 I49 V50 Q57 H73 C85 A86

4   Data and refinement statistics $\;$ (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	160.29Å 365.42Å 108.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.70 146.79 – 3.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.99-3.70) 93.4 (146.79-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.250 , 0.286 0.266 , 0.295	Depositor DCC
R_{free} test set	3247 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	122.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 85.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Outliers	0 of 64593 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	23700	wwPDB-VP
Average B, all atoms (Å^2)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.23	0/5651	0.42	1/7684 (0.0%)
1	B	0.24	0/5734	0.42	1/7782 (0.0%)
1	C	0.23	0/5620	0.41	0/7653
1	D	0.24	0/5694	0.42	1/7746 (0.0%)
2	E	0.25	0/651	0.44	0/873
2	F	0.25	0/651	0.43	0/873
All	All	0.24	0/24001	0.42	3/32611 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	498	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	498	LEU	CA-CB-CG	5.13	127.11	115.30
1	D	498	LEU	CA-CB-CG	5.12	127.09	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	5535	0	5296	57	0
1	B	5618	0	5428	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5507	0	5175	59	0
1	D	5578	0	5336	66	0
2	E	641	0	593	14	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	2	0
3	D	15	0	13	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	1	0
5	B	32	0	36	4	0
5	D	32	0	36	1	0
All	All	23700	0	22597	240	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 5.

The worst 5 of 240 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:611:ILE:HG21	1:D:795:VAL:HG21	1.69	0.74
1:A:232:GLN:HA	1:A:359:LEU:HD21	1.72	0.71
1:B:661:ARG:HG2	1:B:661:ARG:HH11	1.56	0.70
1:A:187:ARG:NH2	2:E:67:ASN:OD1	2.23	0.70
1:C:464:VAL:HG13	1:C:489:ILE:HD11	1.72	0.70

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	727/814 (89%)	705 (97%)	22 (3%)	0	100	100
1	B	730/814 (90%)	712 (98%)	18 (2%)	0	100	100
1	C	741/814 (91%)	720 (97%)	21 (3%)	0	100	100
1	D	734/814 (90%)	711 (97%)	23 (3%)	0	100	100
2	E	83/90 (92%)	79 (95%)	4 (5%)	0	100	100
2	F	83/90 (92%)	80 (96%)	3 (4%)	0	100	100
All	All	3098/3436 (90%)	3007 (97%)	91 (3%)	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%)	546 (97%)	15 (3%)	52	83
1	B	576/693 (83%)	567 (98%)	9 (2%)	70	90
1	C	541/693 (78%)	529 (98%)	12 (2%)	60	86
1	D	564/693 (81%)	553 (98%)	11 (2%)	63	87
2	E	73/76 (96%)	72 (99%)	1 (1%)	74	91
2	F	73/76 (96%)	72 (99%)	1 (1%)	74	91
All	All	2388/2924 (82%)	2339 (98%)	49 (2%)	61	86

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	634	GLU
1	C	166	ASN
1	D	504	ILE
1	C	10	ILE
1	C	192	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	619	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 ⓘ

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	1.05	0	7,21,21	1.16	0
4	NAG	A	902	1	14,14,15	0.44	0	15,19,21	0.46	0
5	FWF	B	901	-	31,33,33	0.54	0	28,48,48	1.73	2 (7%)
3	KAI	B	902	-	8,15,15	0.97	0	7,21,21	1.23	1 (14%)
4	NAG	B	903	1	14,14,15	0.28	0	15,19,21	0.26	0
3	KAI	C	901	-	8,15,15	1.06	0	7,21,21	1.24	1 (14%)
4	NAG	C	902	1	14,14,15	0.23	0	15,19,21	0.41	0
5	FWF	D	901	-	31,33,33	0.54	0	28,48,48	1.90	2 (7%)
3	KAI	D	902	-	8,15,15	1.25	1 (12%)	7,21,21	1.38	1 (14%)
4	NAG	D	903	1	14,14,15	0.36	0	15,19,21	0.50	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	B	901	-	-	0/32/36/36	0/2/2/2
3	KAI	B	902	-	-	0/6/25/25	0/1/1/1
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
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
5	FWF	D	901	-	-	0/32/36/36	0/2/2/2
3	KAI	D	902	-	-	0/6/25/25	0/1/1/1
4	NAG	D	903	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	902	KAI	CA-N	-2.28	1.44	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	901	FWF	O2-S1-O1	-6.26	109.05	119.34
5	D	901	FWF	O3-S2-O4	-6.09	109.34	119.34
5	B	901	FWF	O3-S2-O4	-5.84	109.75	119.34
5	B	901	FWF	O2-S1-O1	-5.17	110.85	119.34
3	D	902	KAI	CG1-CB1-CB	-2.36	111.55	115.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	KAI	1	0
5	B	901	FWF	4	0
3	B	902	KAI	2	0
3	C	901	KAI	2	0
5	D	901	FWF	1	0
3	D	902	KAI	1	0
4	D	903	NAG	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 (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	735/814 (90%)	0.48	57 (7%)	16	9	90, 162, 261, 344	0
1	B	738/814 (90%)	0.54	71 (9%)	10	6	100, 169, 267, 342	0
1	C	747/814 (91%)	0.44	60 (8%)	15	9	110, 186, 277, 329	0
1	D	742/814 (91%)	0.54	68 (9%)	11	7	85, 164, 256, 325	0
2	E	85/90 (94%)	0.33	1 (1%)	81	68	110, 141, 185, 254	0
2	F	85/90 (94%)	0.44	2 (2%)	62	46	127, 159, 209, 246	0
All	All	3132/3436 (91%)	0.49	259 (8%)	14	9	85, 169, 264, 344	0

The worst 5 of 259 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	68	ALA	8.0
1	B	791	ASN	7.0
1	D	12	GLY	6.8
1	C	390	LEU	6.2
1	A	167	ASP	6.1

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, 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	LLDF	B-factors($Å^2$)	Q<0.9
3	KAI	B	902	15/15	0.91	0.63	1.21	115,136,171,184	0
5	FWF	D	901	32/32	0.95	0.46	0.91	62,116,163,189	0
4	NAG	A	902	14/15	0.85	0.39	0.81	94,128,159,163	0
5	FWF	B	901	32/32	0.95	0.52	0.59	95,136,149,159	0
4	NAG	C	902	14/15	0.88	0.33	0.25	74,144,189,208	0
3	KAI	C	901	15/15	0.94	0.33	-0.43	108,133,171,178	0
3	KAI	D	902	15/15	0.94	0.38	-0.44	74,99,152,153	0
3	KAI	A	901	15/15	0.95	0.29	-0.97	79,113,128,134	0
4	NAG	D	903	14/15	0.84	0.23	-	177,232,493,493	0
4	NAG	B	903	14/15	0.88	0.20	-	127,191,223,243	0

6.5   Other polymers (i)

There are no such residues in this entry.