



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 04:44 PM EST

PDB ID : 4U1W
Title : Full length GluA2-kainate-(R,R)-2b complex crystal form A
Authors : Chen, L.; Gouaux, E.
Deposited on : unknown
Resolution : 3.25 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

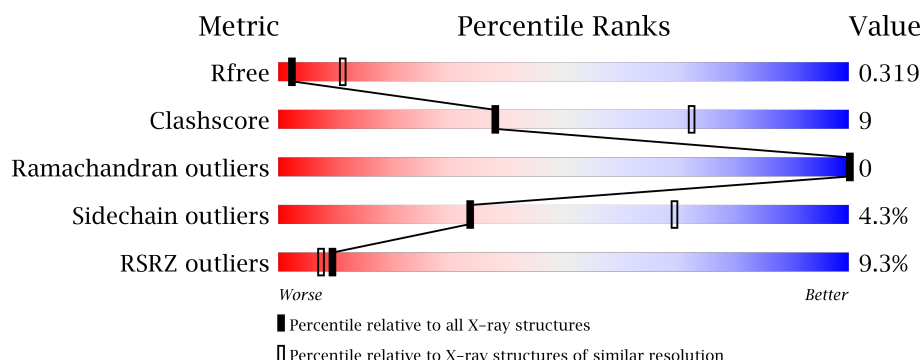
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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 $\leq 5\%$. 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	824	<div> <div>9%</div> <div>71%</div> <div>16%</div> <div>11%</div> </div>
1	B	824	<div> <div>7%</div> <div>71%</div> <div>19%</div> <div>9%</div> </div>
1	C	824	<div> <div>8%</div> <div>67%</div> <div>22%</div> <div>11%</div> </div>
1	D	824	<div> <div>10%</div> <div>68%</div> <div>21%</div> <div>9%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KAI	D	901	-	-	-	X
4	FWF	A	903	-	-	-	X
4	FWF	C	903	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23011 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	731	Total	C	N	O	S	0	0	0
			5571	3582	908	1055	26			
1	B	751	Total	C	N	O	S	0	0	0
			5767	3707	952	1083	25			
1	C	736	Total	C	N	O	S	0	0	0
			5713	3668	945	1075	25			
1	D	750	Total	C	N	O	S	0	0	0
			5780	3715	951	1088	26			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLU	ASN	engineered mutation	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	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	528	ALA	CYS	engineered mutation	UNP P19491
A	585	PHE	MET	engineered mutation	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	598	ALA	GLY	engineered mutation	UNP P19491
A	602	ALA	GLY	engineered mutation	UNP P19491
A	815	ALA	CYS	engineered mutation	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	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491

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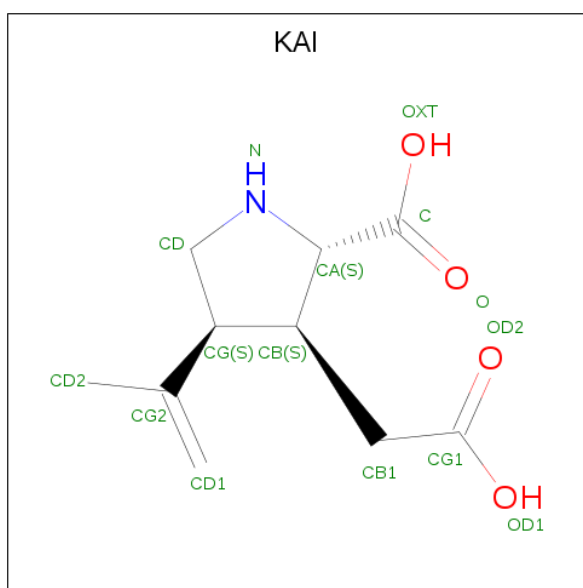
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	528	ALA	CYS	engineered mutation	UNP P19491
B	585	PHE	MET	engineered mutation	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	598	ALA	GLY	engineered mutation	UNP P19491
B	602	ALA	GLY	engineered mutation	UNP P19491
B	815	ALA	CYS	engineered mutation	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
C	239	GLU	ASN	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	?	-	GLY	deletion	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	528	ALA	CYS	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	815	ALA	CYS	engineered mutation	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	engineered mutation	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	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	528	ALA	CYS	engineered mutation	UNP P19491
D	585	PHE	MET	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
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	815	ALA	CYS	engineered mutation	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: $C_{10}H_{15}NO_4$).



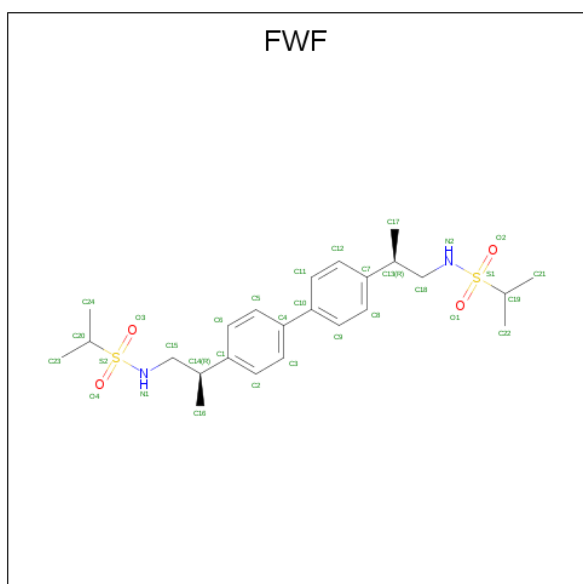
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

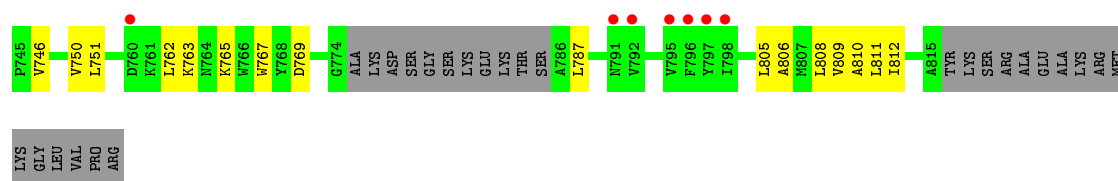


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

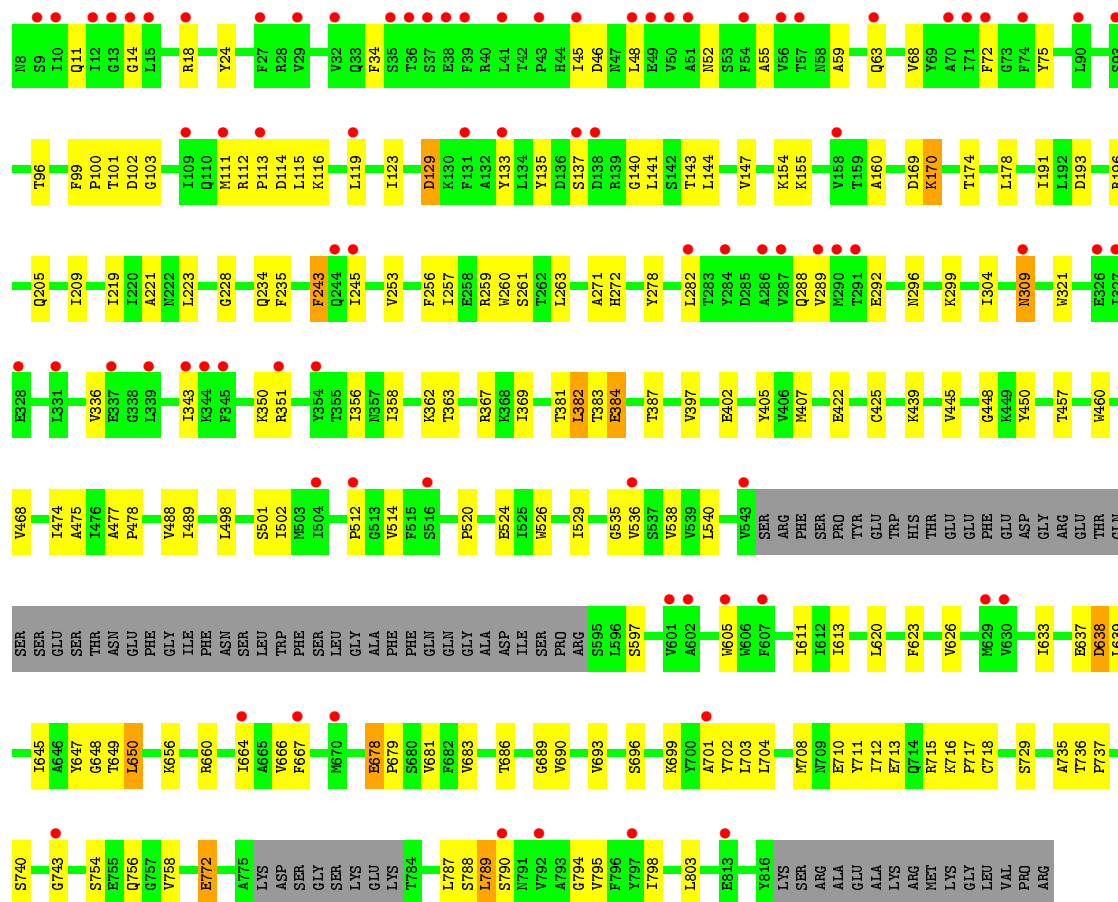
- Molecule 4 is N,N'-[biphenyl-4,4'-diyl-di(2R)propane-2,1-diyl]dipropylsulfonamide (three-letter code: FWF) (formula: C₂₄H₃₆N₂O₄S₂).



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



• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.50Å 151.11Å 332.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 3.25 83.21 – 3.25	Depositor EDS
% Data completeness (in resolution range)	79.8 (29.91-3.25) 79.7 (83.21-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.26Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.270 , 0.316 0.270 , 0.319	Depositor DCC
R_{free} test set	3359 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	23011	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/5685	0.44	0/7719
1	B	0.25	0/5884	0.45	0/7974
1	C	0.25	0/5826	0.44	0/7888
1	D	0.25	0/5900	0.46	0/8002
All	All	0.25	0/23295	0.45	0/31583

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5571	0	5425	90	0
1	B	5767	0	5672	97	0
1	C	5713	0	5643	115	0
1	D	5780	0	5656	113	0
2	A	15	0	13	1	0
2	B	15	0	13	3	0
2	C	15	0	13	2	0
2	D	15	0	13	1	0
3	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	2	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	32	0	36	4	0
4	C	32	0	36	5	0
All	All	23011	0	22572	395	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 9.

The worst 5 of 395 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:D:112:ARG:HG3	1:D:223:LEU:HD11	1.61	0.81
1:D:75:TYR:HE1	1:D:96:THR:HG21	1.51	0.74
1:B:292:GLU:O	1:B:296:ASN:ND2	2.20	0.73
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.72	0.72
1:B:475:ALA:HB3	1:B:735:ALA:HB3	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	723/824 (88%)	703 (97%)	20 (3%)	0	100	100
1	B	743/824 (90%)	727 (98%)	16 (2%)	0	100	100
1	C	726/824 (88%)	710 (98%)	16 (2%)	0	100	100
1	D	744/824 (90%)	725 (97%)	19 (3%)	0	100	100
All	All	2936/3296 (89%)	2865 (98%)	71 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	580/701 (83%)	562 (97%)	18 (3%)	45	77
1	B	605/701 (86%)	572 (94%)	33 (6%)	25	63
1	C	605/701 (86%)	580 (96%)	25 (4%)	35	71
1	D	604/701 (86%)	577 (96%)	27 (4%)	32	68
All	All	2394/2804 (85%)	2291 (96%)	103 (4%)	33	69

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	638	ASP
1	C	376	ASP
1	D	597	SER
1	B	708	MET
1	C	172	ASP

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

Mol	Chain	Res	Type
1	C	300	GLN
1	D	180	GLN

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](#)

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
2	KAI	A	901	-	7,15,15	0.78	0	6,21,21	0.83	0
3	NAG	A	902	1	14,14,15	1.18	1 (7%)	15,19,21	0.78	1 (6%)
4	FWF	A	903	-	29,33,33	0.48	0	36,48,48	1.37	5 (13%)
2	KAI	B	901	-	7,15,15	0.92	0	6,21,21	1.39	1 (16%)
3	NAG	B	902	1	14,14,15	0.51	0	15,19,21	0.58	0
2	KAI	C	901	-	7,15,15	0.99	0	6,21,21	1.22	1 (16%)
3	NAG	C	902	1	14,14,15	0.45	0	15,19,21	0.72	0
4	FWF	C	903	-	29,33,33	0.48	0	36,48,48	1.18	1 (2%)
2	KAI	D	901	-	7,15,15	0.81	0	6,21,21	1.19	0
3	NAG	D	902	1	14,14,15	0.83	1 (7%)	15,19,21	0.34	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	KAI	A	901	-	-	0/6/25/25	0/1/1/1
3	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	FWF	A	903	-	-	0/32/36/36	0/2/2/2
2	KAI	B	901	-	-	0/6/25/25	0/1/1/1
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
2	KAI	C	901	-	-	0/6/25/25	0/1/1/1
3	NAG	C	902	1	-	0/6/23/26	0/1/1/1
4	FWF	C	903	-	-	0/32/36/36	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAI	D	901	-	-	0/6/25/25	0/1/1/1
3	NAG	D	902	1	-	0/6/23/26	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	-4.19	1.36	1.43
3	D	902	NAG	O5-C1	-2.76	1.39	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	KAI	CG1-CB1-CB	-2.71	110.36	115.68
4	A	903	FWF	C3-C4-C10	-2.23	117.44	121.38
2	C	901	KAI	CG1-CB1-CB	-2.20	111.36	115.68
4	A	903	FWF	C9-C8-C7	-2.10	119.07	121.20
4	A	903	FWF	O4-S2-C20	2.03	110.66	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	KAI	1	0
4	A	903	FWF	4	0
2	B	901	KAI	3	0
3	B	902	NAG	2	0
2	C	901	KAI	2	0
4	C	903	FWF	5	0
2	D	901	KAI	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	731/824 (88%)	0.55	72 (9%) 8 6	84, 150, 201, 227	0
1	B	751/824 (91%)	0.49	56 (7%) 15 11	59, 127, 207, 262	0
1	C	736/824 (89%)	0.56	66 (8%) 10 8	70, 145, 221, 257	0
1	D	750/824 (91%)	0.63	82 (10%) 6 5	65, 161, 238, 284	0
All	All	2968/3296 (90%)	0.56	276 (9%) 9 7	59, 146, 220, 284	0

The worst 5 of 276 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	GLY	14.2
1	C	13	GLY	12.1
1	C	12	ILE	9.0
1	C	15	LEU	8.9
1	B	779	GLY	7.7

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(\AA^2)	Q<0.9
2	KAI	D	901	15/15	0.93	0.46	2.53	96,118,158,169	0
4	FWF	A	903	32/32	0.94	0.53	1.79	84,109,162,172	0
4	FWF	C	903	32/32	0.94	0.43	1.54	43,87,148,165	0
3	NAG	A	902	14/15	0.89	0.32	0.68	95,132,174,174	0
2	KAI	C	901	15/15	0.96	0.36	0.34	91,103,128,132	0
2	KAI	A	901	15/15	0.91	0.33	-0.01	106,122,133,135	0
3	NAG	C	902	14/15	0.88	0.24	-0.29	99,124,138,140	0
2	KAI	B	901	15/15	0.96	0.30	-0.31	66,81,99,101	0
3	NAG	D	902	14/15	0.90	0.21	-0.45	136,157,168,172	0
3	NAG	B	902	14/15	0.65	0.37	-	140,155,166,170	0

6.5 Other polymers [i](#)

There are no such residues in this entry.