



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:03 PM GMT

PDB ID : 4BDO  
Title : Crystal structure of the GluK2 K531A-T779G LBD dimer in complex with kainate  
Authors : Nayeem, N.; Mayans, O.; Green, T.  
Deposited on : 2012-10-05  
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

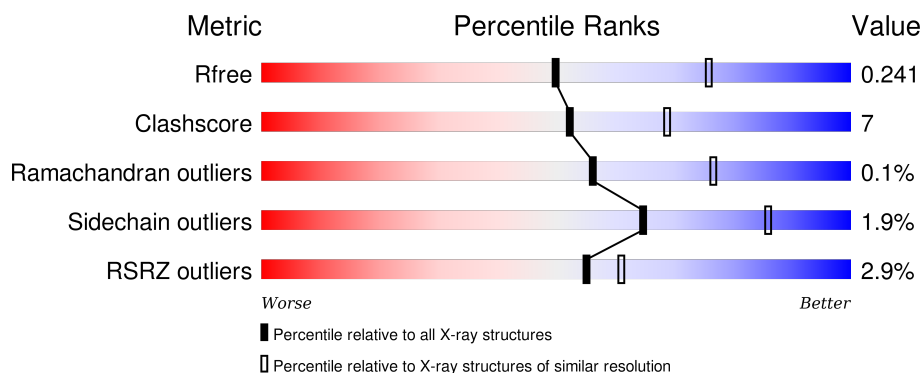
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	 4% 77% 15% 7%
1	B	261	 % 77% 16% • 6%
1	C	261	 4% 80% 14% 6%
1	D	261	 2% 74% 18% 8%

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
2	KAI	D	900[A]	-	-	-	X
3	NA	A	902	-	-	-	X
3	NA	B	902	-	-	-	X
3	NA	C	902	-	-	-	X
3	NA	D	902	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7977 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, IONOTROPIC KAINATE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1934	1241	318	364	11			
1	B	245	Total	C	N	O	S	0	0	0
			1947	1247	318	370	12			
1	C	246	Total	C	N	O	S	0	0	0
			1956	1253	320	372	11			
1	D	240	Total	C	N	O	S	0	0	0
			1912	1228	312	360	12			

There are 28 discrepancies between the modelled and reference sequences:

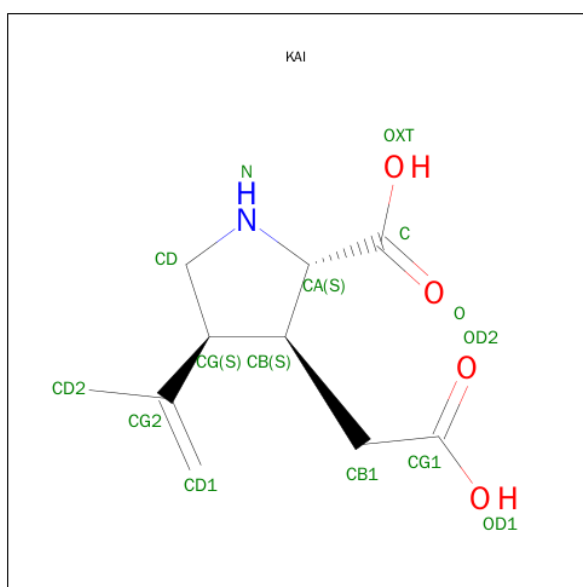
Chain	Residue	Modelled	Actual	Comment	Reference
A	428	GLY	-	EXPRESSION TAG	UNP P42260
A	531	ALA	LYS	ENGINEERED MUTATION	UNP P42260
A	555	GLY	-	LINKER	UNP P42260
A	566	THR	-	LINKER	UNP P42260
A	779	GLY	THR	ENGINEERED MUTATION	UNP P42260
A	807	PRO	-	EXPRESSION TAG	UNP P42260
A	808	ARG	-	EXPRESSION TAG	UNP P42260
B	428	GLY	-	EXPRESSION TAG	UNP P42260
B	531	ALA	LYS	ENGINEERED MUTATION	UNP P42260
B	555	GLY	-	LINKER	UNP P42260
B	566	THR	-	LINKER	UNP P42260
B	779	GLY	THR	ENGINEERED MUTATION	UNP P42260
B	807	PRO	-	EXPRESSION TAG	UNP P42260
B	808	ARG	-	EXPRESSION TAG	UNP P42260
C	428	GLY	-	EXPRESSION TAG	UNP P42260
C	531	ALA	LYS	ENGINEERED MUTATION	UNP P42260
C	555	GLY	-	LINKER	UNP P42260
C	566	THR	-	LINKER	UNP P42260
C	779	GLY	THR	ENGINEERED MUTATION	UNP P42260
C	807	PRO	-	EXPRESSION TAG	UNP P42260
C	808	ARG	-	EXPRESSION TAG	UNP P42260

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Chain	Residue	Modelled	Actual	Comment	Reference
D	428	GLY	-	EXPRESSION TAG	UNP P42260
D	531	ALA	LYS	ENGINEERED MUTATION	UNP P42260
D	555	GLY	-	LINKER	UNP P42260
D	566	THR	-	LINKER	UNP P42260
D	779	GLY	THR	ENGINEERED MUTATION	UNP P42260
D	807	PRO	-	EXPRESSION TAG	UNP P42260
D	808	ARG	-	EXPRESSION TAG	UNP P42260

- 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	1
			15	10	1	4		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

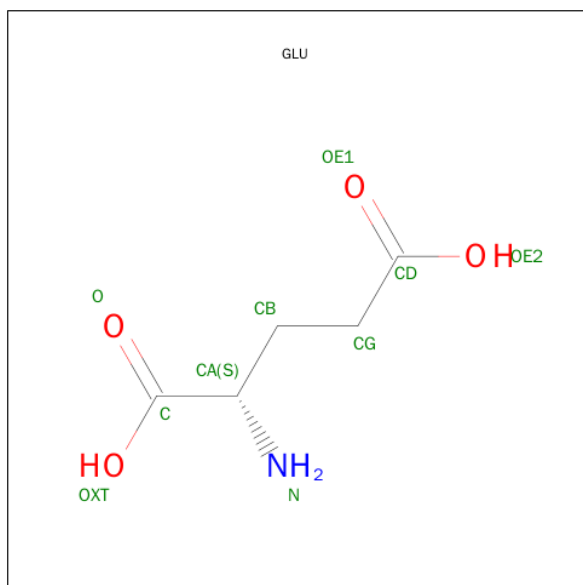
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	1
			10	5	1	4		

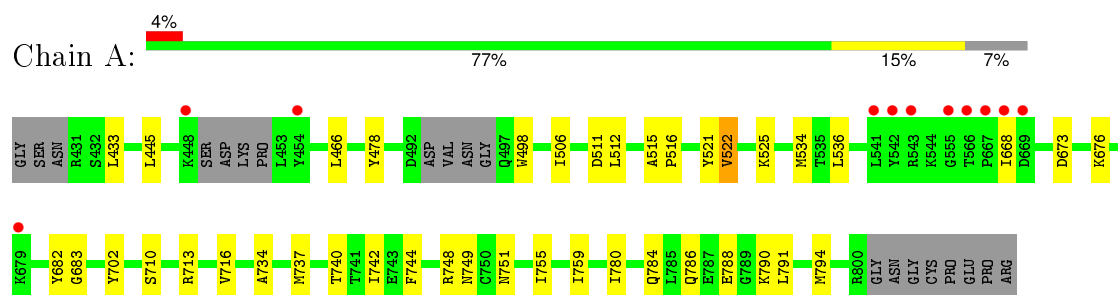
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	39	Total	O	0	0
			39	39		
5	C	40	Total	O	0	0
			40	40		
5	D	25	Total	O	0	0
			25	25		

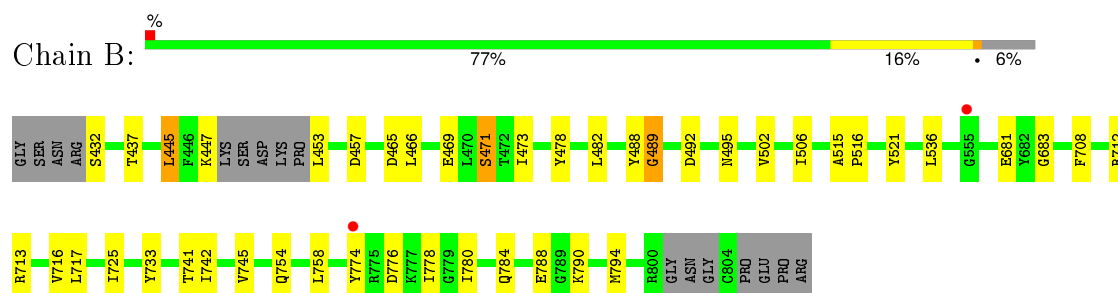
### 3 Residue-property plots

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.

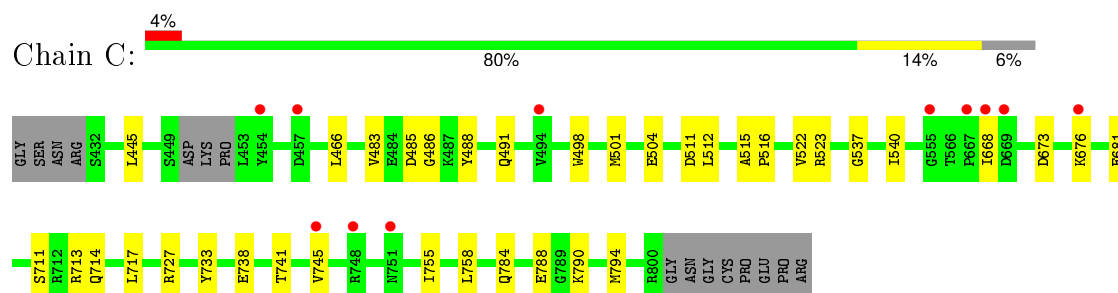
#### • Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 2



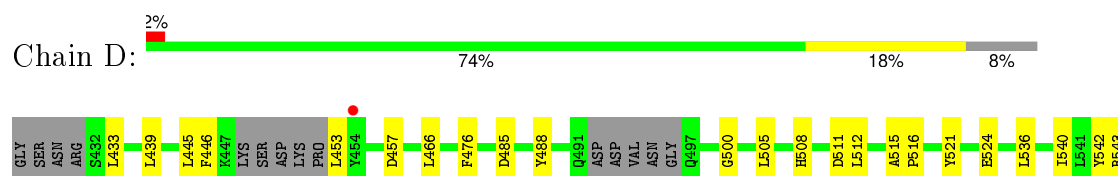
#### • Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 2

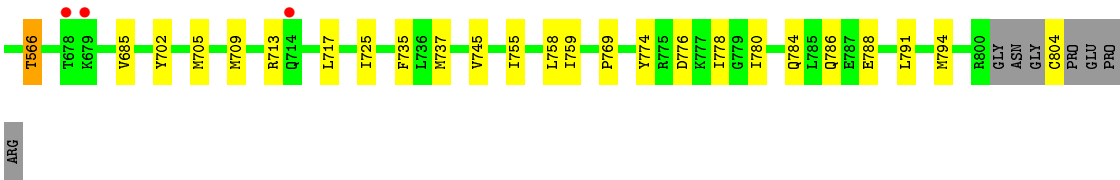


#### • Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 2



#### • Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 2





ARG

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.84Å 99.82Å 124.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.78 – 2.55 40.78 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.78-2.55) 99.6 (40.78-2.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.191 , 0.241 0.191 , 0.241	Depositor DCC
$R_{free}$ test set	1777 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 35532 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, KAI

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	0.29	0/1969	0.55	0/2651
1	B	0.25	0/1982	0.45	0/2671
1	C	0.25	0/1992	0.43	0/2685
1	D	0.26	0/1946	0.44	0/2620
All	All	0.26	0/7889	0.47	0/10627

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	1934	0	1944	26	0
1	B	1947	0	1943	32	0
1	C	1956	0	1959	22	0
1	D	1912	0	1916	27	0
2	A	15	0	13	0	0
2	B	15	0	13	2	0
2	C	15	0	13	3	0
2	D	15	0	13	3	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	10	0	5	0	0
5	A	50	0	0	1	0
5	B	39	0	0	1	0
5	C	40	0	0	0	0
5	D	25	0	0	1	0
All	All	7977	0	7819	104	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.

All (104) 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:788:GLU:HG3	1:C:790:LYS:HG2	1.46	0.98
1:C:681:GLU:O	1:C:733:TYR:HA	1.83	0.79
1:D:784:GLN:O	1:D:788:GLU:HG2	1.88	0.72
1:D:713:ARG:HG3	1:D:717:LEU:HD12	1.73	0.70
1:A:737:MET:HG2	1:A:742:ILE:HG13	1.73	0.69
1:D:786:GLN:HG3	1:D:791:LEU:HD12	1.75	0.68
1:B:713:ARG:HG3	1:B:717:LEU:HD12	1.75	0.68
1:A:498:TRP:HH2	1:A:522:VAL:HG13	1.59	0.68
1:B:788:GLU:HG3	1:B:790:LYS:HG2	1.77	0.67
1:C:727:ARG:HG3	1:C:733:TYR:CD1	2.33	0.64
1:C:488:TYR:CE1	2:C:900:KAI:HD22	2.33	0.63
1:D:466:LEU:HB2	1:D:794:MET:HE1	1.83	0.60
1:A:668:ILE:HG22	1:A:755:ILE:HG21	1.84	0.59
1:D:735:PHE:CE2	1:D:737:MET:HG3	2.37	0.59
1:D:488:TYR:CE1	2:D:900[A]:KAI:HD22	2.37	0.59
1:C:466:LEU:HB2	1:C:794:MET:HE1	1.84	0.59
1:A:784:GLN:O	1:A:788:GLU:HG2	2.04	0.57
1:C:537:GLY:HA3	1:C:758:LEU:HG	1.87	0.57
1:A:466:LEU:HB2	1:A:794:MET:HE1	1.88	0.56
1:D:488:TYR:CE1	2:D:900[A]:KAI:HG	2.40	0.56
1:C:668:ILE:HG22	1:C:755:ILE:HG21	1.89	0.54
1:D:515:ALA:HB1	1:D:516:PRO:HD2	1.89	0.54
1:B:488:TYR:CE2	2:B:900:KAI:HD1	2.43	0.54
1:D:453:LEU:HD22	1:D:457:ASP:HB3	1.88	0.54
1:D:725:ILE:HD11	1:D:745:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:HB2	1:B:794:MET:HE1	1.91	0.53
1:D:543:ARG:HD2	5:D:2015:HOH:O	2.08	0.53
1:A:788:GLU:HG3	1:A:790:LYS:HG2	1.89	0.53
1:C:515:ALA:HB1	1:C:516:PRO:HD2	1.91	0.52
1:B:784:GLN:O	1:B:788:GLU:HG2	2.10	0.52
1:C:673:ASP:HA	1:C:676:LYS:HE2	1.93	0.51
1:A:521:TYR:CZ	1:A:525:LYS:HD2	2.45	0.50
1:A:498:TRP:CH2	1:A:522:VAL:HG13	2.42	0.50
1:D:505:LEU:HD22	1:D:769:PRO:HD3	1.93	0.50
1:B:515:ALA:HB1	1:B:516:PRO:HD2	1.92	0.50
1:D:705:MET:O	1:D:709:MET:HE2	2.12	0.50
1:B:453:LEU:HD12	1:B:453:LEU:N	2.25	0.50
1:D:433:LEU:HD12	1:D:476:PHE:CD1	2.46	0.50
1:C:738:GLU:OE2	2:C:900:KAI:HA	2.12	0.50
1:B:469:GLU:O	1:B:473:ILE:HG13	2.12	0.50
1:D:485:ASP:OD1	1:D:500:GLY:HA2	2.12	0.50
1:A:506:ILE:HA	5:A:2011:HOH:O	2.11	0.49
1:B:489:GLY:HA3	1:B:502:VAL:CG2	2.43	0.49
1:B:488:TYR:CE1	2:B:900:KAI:HD22	2.47	0.49
1:B:774:TYR:O	1:B:778:ILE:HG13	2.13	0.48
1:D:439:LEU:HD11	1:D:446:PHE:CE2	2.48	0.48
1:A:683:GLY:HA3	1:A:716:VAL:O	2.13	0.48
1:C:741:THR:O	1:C:745:VAL:HG23	2.13	0.48
1:B:453:LEU:HD22	1:B:457:ASP:HB3	1.94	0.48
1:B:683:GLY:HA3	1:B:716:VAL:O	2.14	0.48
1:D:540:ILE:HB	1:D:755:ILE:HB	1.97	0.47
1:D:508:HIS:CE1	1:D:769:PRO:HB3	2.50	0.47
1:C:727:ARG:HG3	1:C:733:TYR:CG	2.49	0.46
1:C:713:ARG:HB2	1:C:717:LEU:HD12	1.98	0.46
1:B:492:ASP:O	1:B:495:ASN:O	2.34	0.46
1:D:774:TYR:O	1:D:778:ILE:HB	2.15	0.46
1:A:749:ASN:OD1	1:A:751:ASN:OD1	2.34	0.46
1:A:788:GLU:HG3	1:A:790:LYS:CG	2.45	0.46
1:D:524:GLU:HG3	1:D:524:GLU:O	2.16	0.46
1:A:534:MET:SD	1:A:740:THR:HG21	2.57	0.45
1:B:471:SER:HB2	1:B:478:TYR:CE1	2.52	0.45
1:B:465:ASP:O	1:B:469:GLU:HG2	2.16	0.45
1:B:437:THR:HG23	1:B:482:LEU:HD23	1.99	0.45
1:A:511:ASP:O	1:A:512:LEU:HD23	2.17	0.45
1:A:748:ARG:HG3	1:A:748:ARG:HH11	1.81	0.45
1:B:725:ILE:HD11	1:B:745:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:ASP:O	1:C:512:LEU:HD23	2.16	0.45
1:D:488:TYR:CZ	2:D:900[A]:KAI:HG	2.51	0.45
1:B:708:PHE:CZ	1:B:712:ARG:HD2	2.51	0.45
1:C:491:GLN:HB2	1:C:498:TRP:CE2	2.52	0.45
1:A:744:PHE:CE1	1:A:748:ARG:CZ	3.00	0.44
1:A:710:SER:HA	1:A:713:ARG:HG3	1.98	0.44
1:B:712:ARG:O	1:B:716:VAL:HG22	2.17	0.44
1:C:483:VAL:HG13	1:C:486:GLY:HA2	2.00	0.44
1:A:515:ALA:HB1	1:A:516:PRO:HD2	1.98	0.44
1:D:542:TYR:CE2	1:D:566:THR:HG21	2.53	0.44
1:B:489:GLY:HA3	1:B:502:VAL:HG23	1.99	0.44
1:D:685:VAL:HG23	1:D:735:PHE:HZ	1.83	0.43
1:B:681:GLU:O	1:B:733:TYR:HA	2.18	0.43
1:A:521:TYR:CE1	1:B:780:ILE:HG22	2.53	0.43
1:D:776:ASP:O	1:D:780:ILE:HG13	2.17	0.43
1:B:506:ILE:HA	5:B:2010:HOH:O	2.18	0.43
1:C:485:ASP:C	1:C:485:ASP:OD1	2.57	0.43
1:B:713:ARG:HG3	1:B:717:LEU:CD1	2.46	0.43
1:B:741:THR:O	1:B:745:VAL:HG23	2.19	0.43
1:A:673:ASP:HA	1:A:676:LYS:HE2	2.01	0.43
1:A:682:TYR:HA	1:A:734:ALA:O	2.19	0.43
1:B:445:LEU:N	1:B:445:LEU:HD23	2.34	0.42
1:A:521:TYR:CE2	1:A:525:LYS:HD2	2.54	0.42
1:A:786:GLN:HB2	1:A:791:LEU:HD12	2.01	0.42
1:C:784:GLN:HB2	1:D:521:TYR:CD1	2.54	0.42
1:B:776:ASP:O	1:B:780:ILE:HG13	2.20	0.42
1:C:488:TYR:CE2	2:C:900:KAI:HD1	2.54	0.42
1:C:540:ILE:HB	1:C:755:ILE:HB	2.02	0.41
1:D:702:TYR:CZ	1:D:759:ILE:HG23	2.55	0.41
1:C:501:MET:O	1:C:504:GLU:HB2	2.20	0.41
1:A:702:TYR:CZ	1:A:759:ILE:HG23	2.55	0.41
1:C:522:VAL:HG23	1:C:523:ARG:N	2.35	0.41
1:B:471:SER:HB2	1:B:478:TYR:HE1	1.86	0.41
1:A:433:LEU:O	1:A:478:TYR:HA	2.21	0.41
1:A:780:ILE:HG23	1:B:521:TYR:CD1	2.55	0.41
1:D:511:ASP:O	1:D:512:LEU:HD23	2.20	0.41
1:B:447:LYS:HE3	1:B:457:ASP:O	2.20	0.41
1:B:742:ILE:HG21	1:B:754:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	236/261 (90%)	231 (98%)	5 (2%)	0	100	100
1	B	240/261 (92%)	233 (97%)	6 (2%)	1 (0%)	39	60
1	C	242/261 (93%)	234 (97%)	8 (3%)	0	100	100
1	D	233/261 (89%)	221 (95%)	12 (5%)	0	100	100
All	All	951/1044 (91%)	919 (97%)	31 (3%)	1 (0%)	56	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	489	GLY

### 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	209/225 (93%)	206 (99%)	3 (1%)	74	90
1	B	211/225 (94%)	206 (98%)	5 (2%)	57	81
1	C	212/225 (94%)	209 (99%)	3 (1%)	74	90
1	D	207/225 (92%)	202 (98%)	5 (2%)	57	81
All	All	839/900 (93%)	823 (98%)	16 (2%)	65	86

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	LEU
1	A	522	VAL
1	A	536	LEU
1	B	432	SER
1	B	445	LEU
1	B	471	SER
1	B	536	LEU
1	B	758	LEU
1	C	445	LEU
1	C	711	SER
1	C	714	GLN
1	D	445	LEU
1	D	536	LEU
1	D	566	THR
1	D	758	LEU
1	D	804	CYS

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

Mol	Chain	Res	Type
1	B	786	GLN
1	D	508	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	KAI	A	900	-	8,15,15	1.73	1 (12%)	7,21,21	3.17	5 (71%)
2	KAI	B	900	-	8,15,15	1.73	1 (12%)	7,21,21	3.10	4 (57%)
2	KAI	C	900	-	8,15,15	1.72	1 (12%)	7,21,21	3.14	4 (57%)
2	KAI	D	900[A]	-	8,15,15	1.71	1 (12%)	7,21,21	3.17	4 (57%)
4	GLU	D	901[B]	-	3,9,9	0.38	0	2,11,11	0.10	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	900	-	-	0/6/25/25	0/1/1/1
2	KAI	B	900	-	-	0/6/25/25	0/1/1/1
2	KAI	C	900	-	-	0/6/25/25	0/1/1/1
2	KAI	D	900[A]	-	-	0/6/25/25	0/1/1/1
4	GLU	D	901[B]	-	-	0/3/9/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	KAI	CD1-CG2	4.10	1.52	1.34
2	A	900	KAI	CD1-CG2	4.12	1.52	1.34
2	D	900[A]	KAI	CD1-CG2	4.15	1.52	1.34
2	B	900	KAI	CD1-CG2	4.18	1.52	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900[A]	KAI	CD2-CG2-CD1	-5.73	111.22	121.39
2	B	900	KAI	CD2-CG2-CD1	-5.56	111.52	121.39
2	A	900	KAI	CD2-CG2-CD1	-5.44	111.74	121.39
2	C	900	KAI	CD2-CG2-CD1	-5.17	112.21	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	KAI	CG-CG2-CD1	-4.61	110.63	120.88
2	D	900[A]	KAI	CG-CG2-CD1	-4.27	111.37	120.88
2	A	900	KAI	CG-CG2-CD1	-4.18	111.58	120.88
2	B	900	KAI	CG-CG2-CD1	-4.14	111.67	120.88
2	A	900	KAI	CD2-CG2-CG	-3.44	110.36	117.63
2	C	900	KAI	CD2-CG2-CG	-3.15	110.98	117.63
2	B	900	KAI	CD2-CG2-CG	-3.07	111.15	117.63
2	D	900[A]	KAI	CD2-CG2-CG	-2.96	111.38	117.63
2	C	900	KAI	CB-CG-CG2	-2.68	110.34	116.00
2	A	900	KAI	CB-CG-CG2	-2.38	110.99	116.00
2	A	900	KAI	CG1-CB1-CB	-2.30	111.68	115.89
2	D	900[A]	KAI	CG1-CB1-CB	-2.15	111.94	115.89
2	B	900	KAI	CG1-CB1-CB	-2.12	112.00	115.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	KAI	2	0
2	C	900	KAI	3	0
2	D	900[A]	KAI	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	242/261 (92%)	0.05	11 (4%) 37 43	26, 47, 78, 94	0
1	B	245/261 (93%)	-0.26	2 (0%) 87 89	27, 46, 70, 97	0
1	C	246/261 (94%)	0.04	11 (4%) 37 43	22, 47, 91, 105	0
1	D	240/261 (91%)	-0.08	4 (1%) 73 77	29, 48, 74, 110	0
All	All	973/1044 (93%)	-0.06	28 (2%) 55 61	22, 47, 81, 110	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	668	ILE	4.7
1	D	454	TYR	4.1
1	A	679	LYS	4.0
1	A	667	PRO	3.9
1	A	555	GLY	3.4
1	C	454	TYR	3.4
1	A	454	TYR	3.3
1	C	667	PRO	3.3
1	C	751	ASN	3.1
1	D	678	THR	3.0
1	A	566	THR	2.9
1	C	669	ASP	2.7
1	C	457	ASP	2.7
1	D	714	GLN	2.7
1	C	748	ARG	2.6
1	A	543	ARG	2.5
1	C	676	LYS	2.5
1	A	669	ASP	2.4
1	A	448	LYS	2.4
1	B	555	GLY	2.4
1	C	494	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	774	TYR	2.2
1	A	541	LEU	2.1
1	C	745	VAL	2.1
1	A	668	ILE	2.1
1	C	555	GLY	2.1
1	A	542	TYR	2.1
1	D	679	LYS	2.1

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	D	902	1/1	0.94	0.31	10.87	26,26,26,26	0
3	NA	A	902	1/1	0.88	0.19	4.66	29,29,29,29	0
3	NA	B	902	1/1	0.90	0.20	4.43	27,27,27,27	0
2	KAI	D	900[A]	15/15	0.96	0.19	3.47	46,55,58,58	15
3	NA	C	902	1/1	0.95	0.18	3.29	19,19,19,19	0
2	KAI	B	900	15/15	0.96	0.15	1.85	36,40,46,47	0
4	GLU	D	901[B]	10/10	0.97	0.15	1.46	46,55,57,58	10
2	KAI	C	900	15/15	0.97	0.14	0.51	33,40,54,55	0
2	KAI	A	900	15/15	0.98	0.15	0.36	34,40,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.