



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:52 PM GMT

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

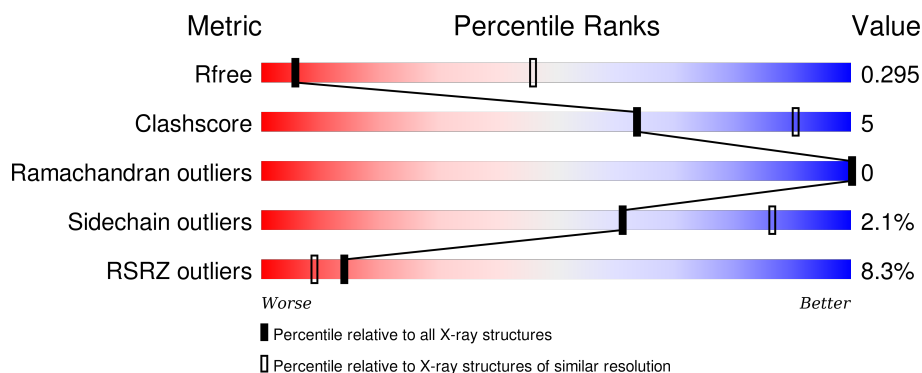
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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  $\geq 3$ , 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	814	<div> <div>7%</div> <div>78% 11% 10%</div> </div>
1	B	814	<div> <div>9%</div> <div>79% 12% 9%</div> </div>
1	C	814	<div> <div>7%</div> <div>80% 11% 8%</div> </div>
1	D	814	<div> <div>8%</div> <div>78% 13% 9%</div> </div>
2	E	90	<div> <div>%</div> <div>71% 23% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	90	

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

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	C	N	O	S	0	0	0
			5535	3562	903	1043	27			
1	B	738	Total	C	N	O	S	0	0	0
			5618	3610	926	1055	27			
1	C	747	Total	C	N	O	S	0	0	0
			5507	3531	908	1041	27			
1	D	742	Total	C	N	O	S	0	0	0
			5578	3591	911	1049	27			

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:

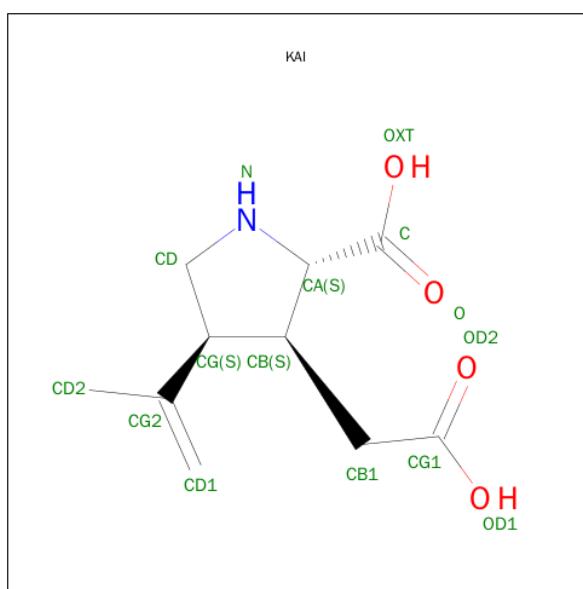
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P0CB20

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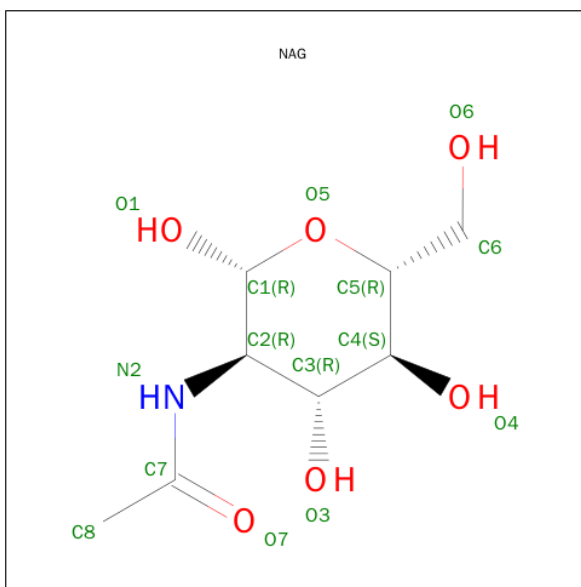
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	PRO	-	expression tag	UNP P0CB20
E	-1	GLY	-	expression tag	UNP P0CB20
E	0	SER	-	expression tag	UNP P0CB20
F	-3	GLY	-	expression tag	UNP P0CB20
F	-2	PRO	-	expression tag	UNP P0CB20
F	-1	GLY	-	expression tag	UNP P0CB20
F	0	SER	-	expression tag	UNP P0CB20

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



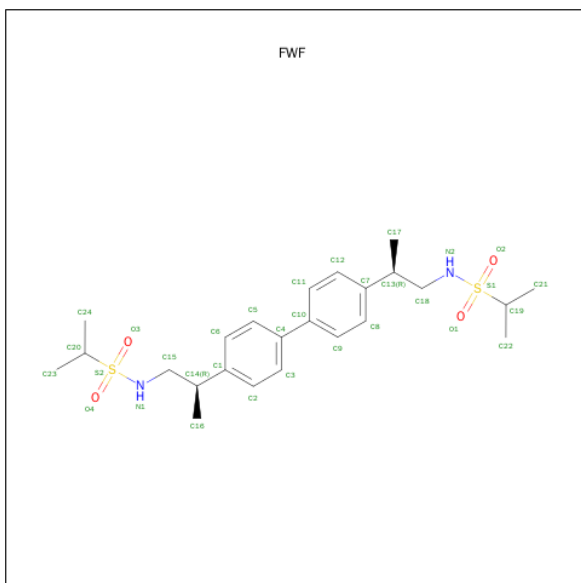
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	1	4		
3	B	1	Total	C	N	O	0	0
			15	10	1	4		
3	C	1	Total	C	N	O	0	0
			15	10	1	4		
3	D	1	Total	C	N	O	0	0
			15	10	1	4		

- 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	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is N,N'-[biphenyl-4,4'-diyl]di(2R)propane-2,1-diyl]dipropyl-2-sulfonamide (three-letter code: FWF) (formula: C<sub>24</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>).

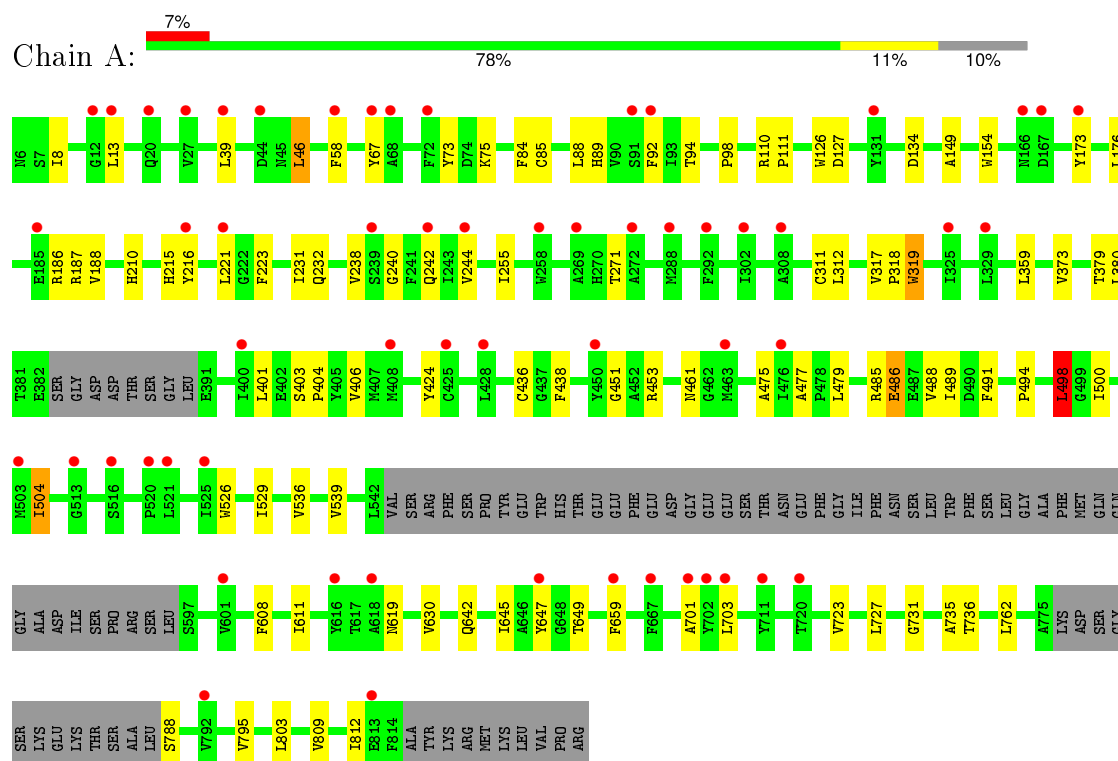


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			32	24	2	4	2		
5	D	1	Total	C	N	O	S	0	0
			32	24	2	4	2		

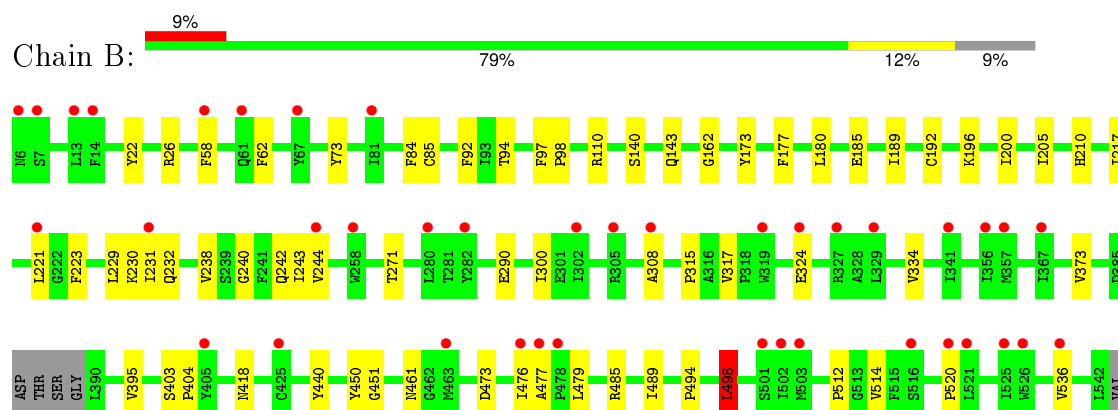
### 3 Residue-property plots [i](#)

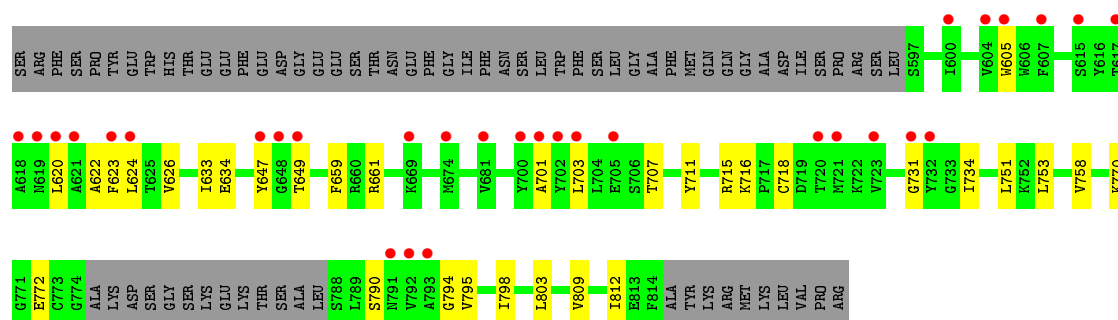
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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

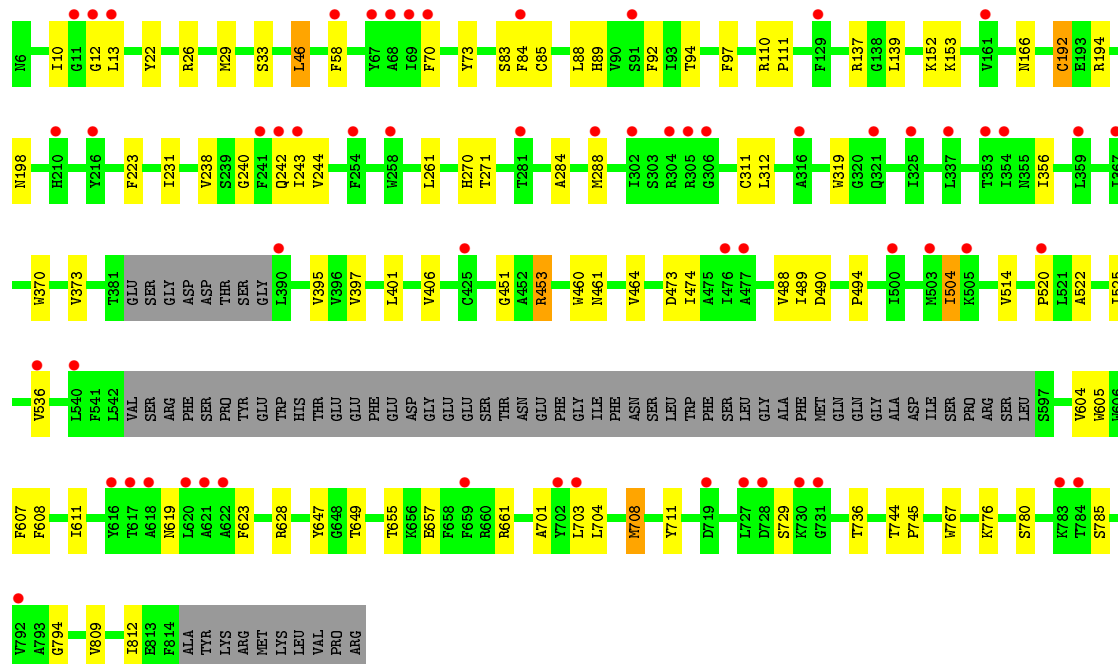
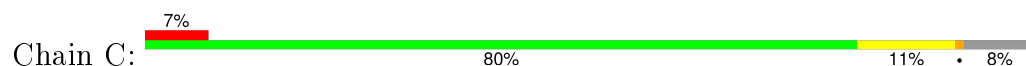


#### • Molecule 1: Glutamate receptor 2

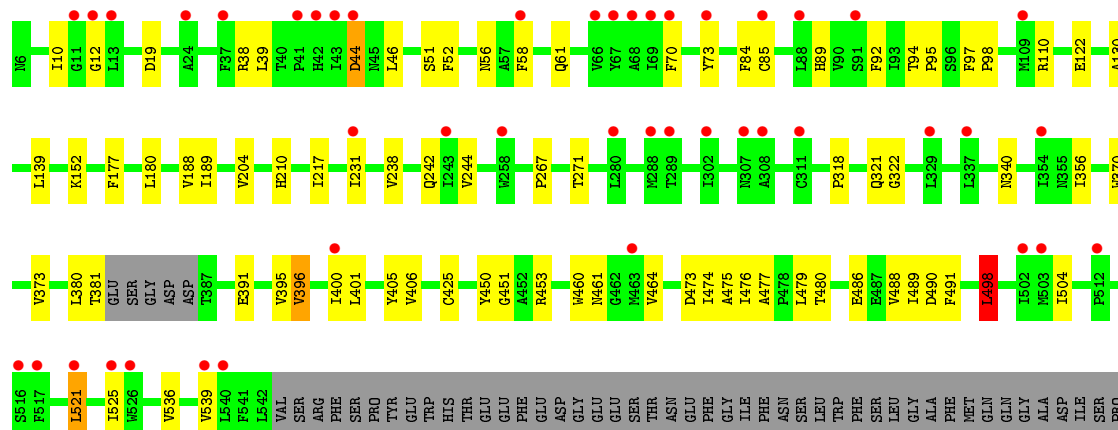
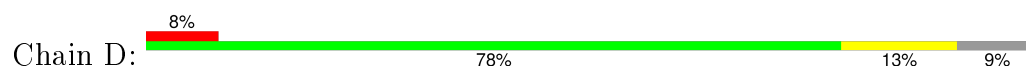


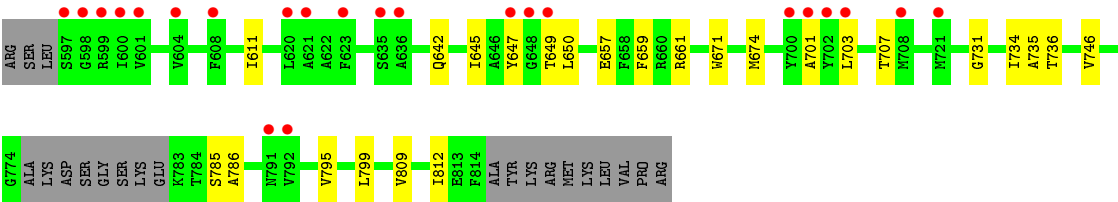


• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2

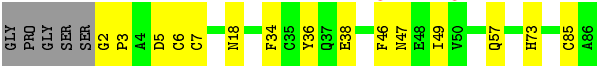
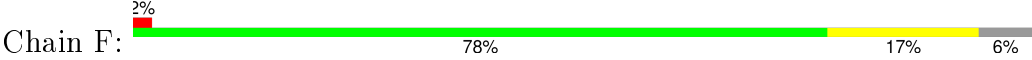




• Molecule 2: Con-ikot-ikot



• Molecule 2: Con-ikot-ikot



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	122.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 85.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	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 <sup>2</sup> )	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.*

<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: 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(°)	Ideal(°)
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.

All (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
1:D:122:GLU:OE1	1:D:152:LYS:NZ	2.26	0.69
1:D:476:ILE:HG12	1:D:734:ILE:HD12	1.76	0.67
1:A:453:ARG:NH1	2:E:38:GLU:OE2	2.27	0.67
1:D:44:ASP:N	1:D:44:ASP:OD1	2.27	0.66
1:C:356:ILE:HD11	1:C:370:TRP:HB2	1.75	0.66
1:D:488:VAL:HG23	1:D:489:ILE:HG12	1.78	0.66
1:D:356:ILE:HD11	1:D:370:TRP:HB2	1.78	0.66
1:A:231:ILE:HD12	1:A:238:VAL:HG21	1.78	0.66
1:A:379:THR:HG22	1:A:380:LEU:H	1.62	0.63
1:C:312:LEU:O	1:D:56:ASN:ND2	2.28	0.63
1:D:231:ILE:HD12	1:D:238:VAL:HG21	1.80	0.63
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.81	0.62
1:D:486:GLU:HG2	1:D:491:PHE:HD2	1.64	0.62
1:B:162:GLY:HA2	1:B:196:LYS:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:901:FWF:N2	1:C:494:PRO:O	2.27	0.60
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.83	0.60
1:C:13:LEU:HD23	1:C:46:LEU:HD21	1.84	0.59
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.85	0.58
1:D:657:GLU:OE1	1:D:661:ARG:NH1	2.37	0.57
1:A:611:ILE:HG12	1:B:795:VAL:HG11	1.86	0.57
1:A:494:PRO:O	5:D:901:FWF:N1	2.31	0.57
1:D:451:GLY:HA2	1:D:461:ASN:O	2.04	0.57
1:C:194:ARG:O	1:C:198:ASN:ND2	2.38	0.57
1:A:242:GLN:HE21	1:A:244:VAL:H	1.53	0.56
1:A:486:GLU:HG2	1:A:491:PHE:HD2	1.71	0.56
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.86	0.56
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.71	0.56
2:E:47:ASN:ND2	2:E:85:CYS:O	2.26	0.56
1:B:395:VAL:HG13	1:B:473:ASP:HB2	1.88	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.88	0.55
2:E:80:SER:HB3	2:F:5:ASP:HB2	1.88	0.55
1:C:488:VAL:HG23	1:C:489:ILE:HG13	1.89	0.55
1:D:453:ARG:NH2	1:D:460:TRP:HE1	2.06	0.54
1:B:514:VAL:HG13	1:B:794:GLY:HA3	1.90	0.54
1:C:73:TYR:CE2	1:C:94:THR:HG21	2.43	0.54
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.90	0.53
1:A:803:LEU:HB3	1:D:539:VAL:HG21	1.90	0.53
1:D:97:PHE:HA	1:D:110:ARG:HD2	1.90	0.53
1:A:803:LEU:HD21	1:D:536:VAL:HG22	1.91	0.53
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.89	0.53
1:A:126:TRP:CG	1:A:187:ARG:HD3	2.43	0.53
5:B:901:FWF:H8	1:C:729:SER:HB2	1.91	0.53
1:B:711:TYR:OH	1:B:715:ARG:NH1	2.42	0.53
1:A:88:LEU:HD11	1:A:311:CYS:HB2	1.90	0.53
1:C:231:ILE:HD12	1:C:238:VAL:HG21	1.91	0.53
1:D:489:ILE:HG22	1:D:490:ASP:H	1.74	0.52
1:B:494:PRO:O	5:B:901:FWF:N1	2.35	0.52
1:D:396:VAL:HG23	1:D:473:ASP:H	1.73	0.52
1:C:453:ARG:NH2	2:F:38:GLU:OE2	2.42	0.52
1:B:58:PHE:CE2	1:B:84:PHE:HB3	2.44	0.52
1:B:97:PHE:HA	1:B:110:ARG:HD2	1.90	0.52
1:B:221:LEU:HB3	1:B:243:ILE:HB	1.92	0.52
1:C:655:THR:OG1	3:C:901:KAI:OD2	2.22	0.51
2:E:5:ASP:HB3	2:E:8:ARG:HB3	1.93	0.51
1:D:204:VAL:HG12	1:D:210:HIS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.91	0.51
1:C:522:ALA:HB3	1:C:525:ILE:HG13	1.92	0.51
2:E:21:LEU:HD21	2:E:32:VAL:HA	1.92	0.51
1:C:489:ILE:HG22	1:C:490:ASP:H	1.75	0.51
1:D:73:TYR:CE2	1:D:94:THR:HG21	2.46	0.51
1:D:58:PHE:CE2	1:D:84:PHE:HB3	2.46	0.51
1:C:704:LEU:HD12	1:C:708:MET:HB2	1.93	0.50
1:A:504:ILE:HD11	1:A:723:VAL:HG21	1.94	0.50
1:A:58:PHE:CE2	1:A:84:PHE:HB3	2.47	0.50
1:A:67:TYR:HD1	1:A:319:TRP:HH2	1.60	0.50
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.94	0.50
1:A:453:ARG:NH2	2:E:37:GLN:OE1	2.41	0.50
1:D:395:VAL:HG13	1:D:473:ASP:HB2	1.93	0.49
1:C:522:ALA:H	1:C:525:ILE:HD12	1.77	0.49
1:A:647:TYR:HB3	1:A:701:ALA:HB3	1.95	0.49
1:D:242:GLN:HE21	1:D:244:VAL:H	1.60	0.49
1:B:809:VAL:HA	1:B:812:ILE:HG12	1.94	0.49
1:B:140:SER:HA	1:B:143:GLN:HE21	1.77	0.49
1:B:477:ALA:O	1:B:479:LEU:N	2.45	0.49
1:B:73:TYR:CE2	1:B:94:THR:HG21	2.48	0.49
1:C:261:LEU:O	1:C:270:HIS:ND1	2.45	0.48
1:C:139:LEU:HD12	1:D:139:LEU:HD12	1.96	0.48
1:C:488:VAL:HG12	2:F:34:PHE:HD2	1.79	0.48
1:B:498:LEU:HD13	1:B:731:GLY:HA2	1.95	0.48
1:A:424:TYR:CE2	1:A:762:LEU:HB3	2.49	0.48
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.95	0.48
1:C:514:VAL:HG13	1:C:794:GLY:HA3	1.95	0.48
1:B:85:CYS:SG	1:B:92:PHE:HB2	2.53	0.48
1:D:659:PHE:CE2	1:D:703:LEU:HD13	2.49	0.48
1:C:88:LEU:HD11	1:C:311:CYS:HB2	1.96	0.48
2:F:36:TYR:CG	2:F:57:GLN:HG3	2.48	0.47
1:C:647:TYR:HB3	1:C:701:ALA:HB3	1.95	0.47
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.79	0.47
1:B:223:PHE:CD1	1:B:240:GLY:HA3	2.48	0.47
1:D:809:VAL:HA	1:D:812:ILE:HG12	1.97	0.47
1:C:152:LYS:HG3	1:C:153:LYS:H	1.79	0.47
1:A:608:PHE:O	1:A:611:ILE:HG13	2.14	0.47
1:B:622:ALA:O	1:B:626:VAL:HG23	2.14	0.47
1:C:619:ASN:HD21	1:D:786:ALA:HB3	1.80	0.47
1:A:13:LEU:HD23	1:A:46:LEU:HD21	1.97	0.47
1:B:315:PRO:HB2	1:B:317:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLY:HA2	1:A:461:ASN:O	2.14	0.47
2:E:36:TYR:CG	2:E:57:GLN:HG3	2.50	0.47
1:D:477:ALA:O	1:D:479:LEU:N	2.45	0.47
1:B:177:PHE:HA	1:B:180:LEU:HB2	1.97	0.47
1:D:189:ILE:HG12	1:D:217:ILE:HB	1.96	0.47
2:F:18:ASN:HB2	2:F:73:HIS:CE1	2.50	0.46
1:A:73:TYR:CE2	1:A:94:THR:HG21	2.50	0.46
1:C:284:ALA:O	1:C:288:MET:HG3	2.15	0.46
2:E:83:ASN:ND2	2:E:85:CYS:SG	2.86	0.46
1:C:223:PHE:CD1	1:C:240:GLY:HA3	2.50	0.46
1:B:315:PRO:C	1:B:317:VAL:H	2.19	0.46
1:D:98:PRO:HD3	1:D:110:ARG:HD2	1.98	0.46
1:B:22:TYR:CE2	1:B:26:ARG:HD2	2.51	0.46
1:A:111:PRO:HD2	1:A:221:LEU:HD11	1.98	0.46
1:D:318:PRO:HG2	1:D:321:GLN:HG2	1.96	0.46
1:D:400:ILE:HG21	1:D:450:TYR:CZ	2.50	0.46
2:F:36:TYR:CE1	2:F:57:GLN:HB2	2.51	0.46
1:C:628:ARG:NH1	1:C:785:SER:O	2.49	0.45
1:A:485:ARG:O	1:A:489:ILE:HG13	2.15	0.45
2:E:58:MET:O	2:E:62:ARG:HG2	2.16	0.45
1:C:657:GLU:O	1:C:661:ARG:HG3	2.15	0.45
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.98	0.45
1:B:716:LYS:HA	1:B:718:CYS:H	1.82	0.45
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.52	0.45
1:B:62:PHE:CZ	1:B:308:ALA:HB1	2.52	0.45
1:D:340:ASN:ND2	4:D:903:NAG:O5	2.50	0.45
1:A:134:ASP:N	1:A:134:ASP:OD1	2.50	0.45
1:A:317:VAL:HA	1:A:318:PRO:HD3	1.81	0.45
1:C:520:PRO:O	1:C:619:ASN:ND2	2.49	0.45
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.97	0.45
1:C:22:TYR:CE2	1:C:26:ARG:HD2	2.51	0.45
1:A:126:TRP:CD2	1:A:187:ARG:HD3	2.52	0.45
1:A:216:TYR:HB2	1:A:238:VAL:HG22	1.99	0.45
1:B:498:LEU:HB3	1:B:707:THR:HG23	1.99	0.45
1:A:539:VAL:HG21	1:B:803:LEU:HB3	1.98	0.45
1:D:130:ALA:HB3	1:D:188:VAL:HG22	1.99	0.44
1:A:488:VAL:HG12	2:E:34:PHE:HD2	1.82	0.44
1:D:177:PHE:HA	1:D:180:LEU:HB2	1.99	0.44
1:D:734:ILE:HG21	1:D:746:VAL:HG11	1.99	0.44
1:D:85:CYS:SG	1:D:92:PHE:HB2	2.58	0.44
1:B:647:TYR:HB3	1:B:701:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ILE:HD13	1:D:39:LEU:HD23	2.00	0.44
1:B:290:GLU:HG3	1:B:334:VAL:HG11	1.99	0.44
1:B:242:GLN:HE21	1:B:244:VAL:H	1.65	0.44
2:F:47:ASN:ND2	2:F:85:CYS:O	2.47	0.44
1:D:498:LEU:HD13	1:D:731:GLY:HA2	1.98	0.44
1:A:500:ILE:HB	1:A:727:LEU:HB2	2.00	0.44
1:C:84:PHE:CE1	1:D:52:PHE:HA	2.53	0.44
1:D:498:LEU:HB3	1:D:707:THR:HG23	2.00	0.44
1:D:89:HIS:HB3	1:D:322:GLY:HA3	1.99	0.44
1:B:173:TYR:HE1	1:B:200:ILE:HG12	1.83	0.44
1:B:451:GLY:HA2	1:B:461:ASN:O	2.18	0.44
1:C:623:PHE:CZ	1:D:785:SER:HA	2.52	0.44
1:C:242:GLN:HE21	1:C:244:VAL:H	1.66	0.44
1:B:300:ILE:HG21	1:B:324:GLU:HG2	1.99	0.44
1:B:520:PRO:HG2	1:B:620:LEU:HD13	2.00	0.43
3:C:901:KAI:HD2	3:C:901:KAI:HD12	1.70	0.43
1:A:223:PHE:CD1	1:A:240:GLY:HA3	2.54	0.43
1:A:611:ILE:HD13	1:B:795:VAL:HG21	2.01	0.43
1:B:485:ARG:O	1:B:489:ILE:HG13	2.18	0.43
1:A:788:SER:O	1:D:525:ILE:HD11	2.18	0.43
1:D:521:LEU:HG	1:D:525:ILE:HD12	2.00	0.43
1:B:418:ASN:ND2	1:B:440:TYR:O	2.50	0.43
1:A:8:ILE:HB	1:A:39:LEU:HD23	2.00	0.43
1:D:19:ASP:HB3	1:D:267:PRO:HB2	2.01	0.43
1:D:650:LEU:HD13	3:D:902:KAI:HD23	1.99	0.43
1:D:405:TYR:HB3	1:D:425:CYS:SG	2.59	0.43
1:A:403:SER:HA	1:A:404:PRO:HA	1.72	0.43
1:B:450:TYR:CE2	3:B:902:KAI:HD1	2.53	0.43
1:C:711:TYR:HB2	1:C:767:TRP:NE1	2.34	0.43
1:B:98:PRO:HD3	1:B:110:ARG:HD2	2.00	0.43
1:B:403:SER:HA	1:B:404:PRO:HA	1.75	0.43
1:B:210:HIS:HE1	1:D:210:HIS:HE1	1.67	0.43
1:A:98:PRO:HD3	1:A:110:ARG:HD2	2.00	0.43
1:C:97:PHE:HA	1:C:110:ARG:HD2	2.00	0.43
1:D:460:TRP:NE1	1:D:488:VAL:HG11	2.34	0.42
1:C:604:VAL:HG12	1:D:799:LEU:HD12	2.00	0.42
1:A:477:ALA:O	1:A:479:LEU:N	2.49	0.42
1:B:661:ARG:NH1	1:B:661:ARG:HG2	2.29	0.42
1:C:83:SER:HB3	1:D:51:SER:HB2	2.00	0.42
1:A:186:ARG:O	1:A:188:VAL:HG23	2.18	0.42
1:D:671:TRP:HA	1:D:674:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:SER:HB2	2:F:3:PRO:HG2	2.01	0.42
1:B:659:PHE:CE2	1:B:703:LEU:HD13	2.54	0.42
1:B:189:ILE:HG12	1:B:217:ILE:HB	2.01	0.42
1:A:149:ALA:HA	1:A:154:TRP:HB2	2.01	0.42
2:F:6:CYS:HB3	2:F:46:PHE:HE2	1.83	0.42
1:C:243:ILE:HG23	1:C:244:VAL:HG23	2.01	0.42
1:C:58:PHE:CE2	1:C:84:PHE:HB3	2.54	0.42
1:C:809:VAL:HA	1:C:812:ILE:HG12	2.00	0.42
1:B:229:LEU:HD23	1:B:232:GLN:OE1	2.20	0.42
1:D:464:VAL:HG13	1:D:489:ILE:HG13	2.02	0.42
1:A:489:ILE:HD13	1:A:735:ALA:HB1	2.01	0.42
2:E:13:CYS:HB2	2:E:52:CYS:HB2	1.90	0.42
1:C:474:ILE:HG13	1:C:736:THR:HG22	2.01	0.42
1:D:647:TYR:HB3	1:D:701:ALA:HB3	2.02	0.42
1:B:753:LEU:HD22	1:B:758:VAL:HG11	2.02	0.42
2:F:2:GLY:HA2	2:F:3:PRO:HD3	1.90	0.42
1:A:436:CYS:HB2	1:A:438:PHE:CE2	2.55	0.42
1:A:809:VAL:HA	1:A:812:ILE:HG12	2.01	0.42
3:A:901:KAI:HD12	3:A:901:KAI:HD2	1.71	0.42
1:C:395:VAL:HG13	1:C:473:ASP:HB2	2.02	0.42
2:E:26:GLY:H	2:E:28:GLU:CD	2.23	0.42
1:C:451:GLY:HA2	1:C:461:ASN:O	2.20	0.42
1:A:173:TYR:HA	1:A:176:LEU:HB3	2.02	0.42
1:A:619:ASN:HA	1:B:624:LEU:HD13	2.01	0.41
1:A:526:TRP:O	1:A:529:ILE:HG22	2.20	0.41
1:B:205:ILE:CD1	1:B:230:LYS:HB3	2.50	0.41
1:B:795:VAL:HA	1:B:798:ILE:HG22	2.02	0.41
3:B:902:KAI:HD12	3:B:902:KAI:HD2	1.69	0.41
1:A:127:ASP:N	1:A:127:ASP:OD1	2.53	0.41
1:A:85:CYS:SG	1:A:92:PHE:HB2	2.61	0.41
1:C:85:CYS:SG	1:C:92:PHE:HB2	2.60	0.41
1:B:751:LEU:HA	5:B:901:FWF:H34	2.01	0.41
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.55	0.41
1:B:476:ILE:HG12	1:B:734:ILE:HG23	2.02	0.41
1:C:137:ARG:HH22	1:C:192:CYS:C	2.24	0.41
1:C:460:TRP:CE2	1:C:488:VAL:HG11	2.56	0.41
1:C:607:PHE:O	1:C:611:ILE:HG12	2.21	0.41
1:D:642:GLN:OE1	1:D:645:ILE:N	2.37	0.41
1:B:716:LYS:HA	1:B:718:CYS:N	2.35	0.41
1:C:110:ARG:HA	1:C:111:PRO:HD3	1.85	0.41
1:C:504:ILE:HD13	1:C:504:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:HD12	1:B:238:VAL:HG21	2.02	0.41
1:A:659:PHE:CE2	1:A:703:LEU:HD13	2.56	0.41
1:C:608:PHE:CD1	1:D:799:LEU:HD22	2.56	0.41
1:D:12:GLY:HA2	1:D:70:PHE:O	2.21	0.41
1:B:770:LYS:HE2	1:B:770:LYS:HB3	1.84	0.41
1:D:380:LEU:HG	1:D:381:THR:HG23	2.03	0.41
1:C:776:LYS:O	1:C:780:SER:N	2.52	0.41
1:D:44:ASP:OD1	1:D:61:GLN:NE2	2.54	0.40
1:D:94:THR:HA	1:D:95:PRO:HD3	1.90	0.40
1:C:744:THR:HB	1:C:745:PRO:HD3	2.03	0.40
1:C:12:GLY:HA2	1:C:70:PHE:O	2.21	0.40
1:B:512:PRO:HB2	1:B:790:SER:HB2	2.03	0.40
1:B:205:ILE:HG23	1:B:210:HIS:CE1	2.56	0.40
1:C:661:ARG:NH2	2:F:49:ILE:HA	2.36	0.40
1:C:29:MET:O	1:C:33:SER:HB3	2.22	0.40
1:A:498:LEU:HD13	1:A:731:GLY:HA2	2.03	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	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 ⓘ

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

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	75	LYS
1	A	89	HIS
1	A	210	HIS
1	A	215	HIS
1	A	255	ILE
1	A	271	THR
1	A	312	LEU
1	A	319	TRP
1	A	373	VAL
1	A	486	GLU
1	A	498	LEU
1	A	504	ILE
1	A	630	VAL
1	A	736	THR
1	B	185	GLU
1	B	192	CYS
1	B	271	THR
1	B	373	VAL

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Mol	Chain	Res	Type
1	B	498	LEU
1	B	623	PHE
1	B	633	ILE
1	B	634	GLU
1	B	772	GLU
1	C	10	ILE
1	C	46	LEU
1	C	89	HIS
1	C	166	ASN
1	C	192	CYS
1	C	271	THR
1	C	319	TRP
1	C	373	VAL
1	C	397	VAL
1	C	453	ARG
1	C	504	ILE
1	C	708	MET
1	D	38	ARG
1	D	44	ASP
1	D	46	LEU
1	D	271	THR
1	D	373	VAL
1	D	391	GLU
1	D	396	VAL
1	D	480	THR
1	D	498	LEU
1	D	504	ILE
1	D	521	LEU
2	E	23	ARG
2	F	7	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	C	901	KAI	CG1-CB1-CB	-2.02	112.18	115.89
3	B	902	KAI	CG1-CB1-CB	-2.02	112.19	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 ⓘ

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 ⓘ

### 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	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

All (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
1	C	67	TYR	5.9
1	C	618	ALA	5.7
1	A	792	VAL	5.2
1	D	68	ALA	5.2
1	B	702	TYR	5.2
1	C	91	SER	5.1
1	D	11	GLY	5.0
1	D	621	ALA	4.9
1	D	516	SER	4.8
1	A	67	TYR	4.8
1	B	792	VAL	4.7
1	D	792	VAL	4.7
1	C	305	ARG	4.7
1	A	520	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	597	SER	4.6
1	D	702	TYR	4.4
1	C	731	GLY	4.3
1	B	305	ARG	4.3
1	D	791	ASN	4.2
1	C	302	ILE	4.1
1	D	620	LEU	4.1
1	B	67	TYR	4.1
1	D	525	ILE	4.1
1	D	601	VAL	4.1
1	B	700	TYR	3.9
1	C	540	LEU	3.9
1	B	647	TYR	3.8
1	D	648	GLY	3.8
1	B	703	LEU	3.8
1	C	13	LEU	3.8
1	A	13	LEU	3.8
1	C	702	TYR	3.7
1	A	302	ILE	3.7
1	C	620	LEU	3.7
1	D	701	ALA	3.7
1	A	166	ASN	3.7
1	D	67	TYR	3.7
1	D	647	TYR	3.7
1	D	649	THR	3.7
1	B	502	ILE	3.7
1	D	600	ILE	3.7
1	B	58	PHE	3.6
1	B	619	ASN	3.6
1	C	477	ALA	3.5
1	B	721	MET	3.5
1	B	701	ALA	3.5
1	A	12	GLY	3.5
1	C	476	ILE	3.5
1	D	517	PHE	3.5
1	A	242	GLN	3.4
1	B	476	ILE	3.4
1	D	302	ILE	3.4
1	A	701	ALA	3.4
1	B	503	MET	3.4
1	C	12	GLY	3.4
1	D	503	MET	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	46	PHE	3.3
1	D	69	ILE	3.3
1	C	11	GLY	3.3
1	C	353	THR	3.3
1	B	620	LEU	3.3
1	C	258	TRP	3.3
1	C	727	LEU	3.2
1	C	354	ILE	3.2
1	B	6	ASN	3.2
1	D	635	SER	3.2
1	A	702	TYR	3.1
1	B	648	GLY	3.1
1	D	700	TYR	3.1
1	A	720	THR	3.1
1	A	329	LEU	3.1
1	D	598	GLY	3.0
1	C	500	ILE	3.0
1	B	732	TYR	3.0
1	B	341	ILE	3.0
1	B	367	ILE	3.0
1	D	311	CYS	3.0
1	D	13	LEU	3.0
1	B	624	LEU	2.9
1	A	325	ILE	2.9
1	D	329	LEU	2.9
1	B	617	THR	2.9
1	C	792	VAL	2.9
1	A	400	ILE	2.9
1	A	813	GLU	2.9
1	B	674	MET	2.9
1	B	425	CYS	2.9
1	B	607	PHE	2.8
1	C	304	ARG	2.8
1	A	292	PHE	2.8
1	D	540	LEU	2.8
1	D	66	VAL	2.8
1	D	521	LEU	2.7
1	D	289	THR	2.7
1	A	703	LEU	2.7
1	C	621	ALA	2.7
1	B	478	PRO	2.7
1	C	321	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	58	PHE	2.7
1	B	604	VAL	2.7
1	D	354	ILE	2.7
1	D	502	ILE	2.7
1	C	337	LEU	2.7
1	D	41	PRO	2.7
1	C	241	PHE	2.6
1	B	302	ILE	2.6
1	C	783	LYS	2.6
2	E	57	GLN	2.6
1	A	408	MET	2.6
1	A	503	MET	2.6
1	D	539	VAL	2.6
1	B	61	GLN	2.6
1	C	325	ILE	2.6
2	F	50	VAL	2.6
1	A	68	ALA	2.6
1	C	520	PRO	2.6
1	B	516	SER	2.6
1	A	244	VAL	2.6
1	B	258	TRP	2.6
1	A	450	TYR	2.6
1	B	615	SER	2.6
1	B	308	ALA	2.6
1	B	731	GLY	2.6
1	D	58	PHE	2.6
1	C	622	ALA	2.6
1	C	242	GLN	2.5
1	B	13	LEU	2.5
1	A	516	SER	2.5
1	A	618	ALA	2.5
1	C	69	ILE	2.5
1	D	70	PHE	2.5
1	A	221	LEU	2.5
1	D	337	LEU	2.5
1	A	269	ALA	2.5
1	C	728	ASP	2.5
1	B	477	ALA	2.5
1	B	282	TYR	2.5
1	B	329	LEU	2.5
1	C	359	LEU	2.5
1	D	623	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	476	ILE	2.5
1	A	288	MET	2.4
1	C	58	PHE	2.4
1	B	356	ILE	2.4
1	D	91	SER	2.4
1	A	463	MET	2.4
1	D	512	PRO	2.4
1	D	703	LEU	2.4
1	C	505	LYS	2.4
1	C	703	LEU	2.4
1	D	288	MET	2.4
1	C	616	TYR	2.4
1	B	357	MET	2.4
1	A	44	ASP	2.4
1	B	649	THR	2.3
1	A	272	ALA	2.3
1	C	216	TYR	2.3
1	C	730	LYS	2.3
1	A	72	PHE	2.3
1	C	161	VAL	2.3
1	D	280	LEU	2.3
1	C	719	ASP	2.3
1	A	27	VAL	2.3
1	B	324	GLU	2.3
1	B	720	THR	2.3
1	C	536	VAL	2.3
1	B	221	LEU	2.3
1	C	316	ALA	2.3
1	C	503	MET	2.3
1	B	521	LEU	2.3
1	D	88	LEU	2.3
1	D	109	MET	2.3
1	A	616	TYR	2.3
1	B	7	SER	2.3
1	C	210	HIS	2.3
1	D	42	HIS	2.3
1	B	231	ILE	2.3
1	C	784	THR	2.3
1	C	288	MET	2.3
1	C	84	PHE	2.3
1	B	526	TRP	2.2
1	D	608	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	513	GLY	2.2
1	C	425	CYS	2.2
1	B	244	VAL	2.2
1	C	306	GLY	2.2
1	D	24	ALA	2.2
1	B	463	MET	2.2
1	B	501	SER	2.2
1	B	705	GLU	2.2
1	B	280	LEU	2.2
1	D	44	ASP	2.2
1	D	85	CYS	2.2
1	D	463	MET	2.2
1	C	367	ILE	2.2
1	D	526	TRP	2.2
1	A	601	VAL	2.2
1	A	258	TRP	2.2
1	D	307	ASN	2.2
1	C	243	ILE	2.2
1	B	618	ALA	2.2
1	B	520	PRO	2.2
1	B	319	TRP	2.2
1	B	14	PHE	2.2
1	C	129	PHE	2.2
1	B	669	LYS	2.2
1	D	43	ILE	2.2
1	A	525	ILE	2.2
1	B	605	TRP	2.1
1	B	81	ILE	2.1
1	A	659	PHE	2.1
1	D	73	TYR	2.1
1	B	621	ALA	2.1
1	A	185	GLU	2.1
1	B	525	ILE	2.1
1	B	536	VAL	2.1
1	D	599	ARG	2.1
1	D	400	ILE	2.1
1	A	667	PHE	2.1
1	C	70	PHE	2.1
1	A	521	LEU	2.1
1	D	721	MET	2.1
1	B	327	ARG	2.1
1	A	425	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	131	TYR	2.1
1	D	308	ALA	2.1
1	D	258	TRP	2.1
1	C	281	THR	2.1
1	A	39	LEU	2.1
1	A	20	GLN	2.1
1	D	231	ILE	2.1
1	A	216	TYR	2.1
1	D	243	ILE	2.1
1	D	604	VAL	2.1
1	A	173	TYR	2.1
1	A	91	SER	2.1
1	A	428	LEU	2.1
1	B	793	ALA	2.1
1	B	405	TYR	2.1
1	B	623	PHE	2.1
1	C	659	PHE	2.1
1	D	37	PHE	2.1
1	A	711	TYR	2.0
1	B	600	ILE	2.0
1	B	681	VAL	2.0
1	D	636	ALA	2.0
1	D	708	MET	2.0
1	A	239	SER	2.0
1	A	647	TYR	2.0
1	A	308	ALA	2.0
1	C	617	THR	2.0
1	C	254	PHE	2.0
1	A	92	PHE	2.0
1	B	723	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	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.