



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 11:43 AM EST

PDB ID : 4U5C  
Title : Crystal structure of GluA2, con-ikot-ikot snail toxin, partial agonist FW and positive modulator (R,R)-2b complex  
Authors : Chen, L.; Gouaux, E.  
Deposited on : unknown  
Resolution : 3.69 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 : 1.7.2 (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

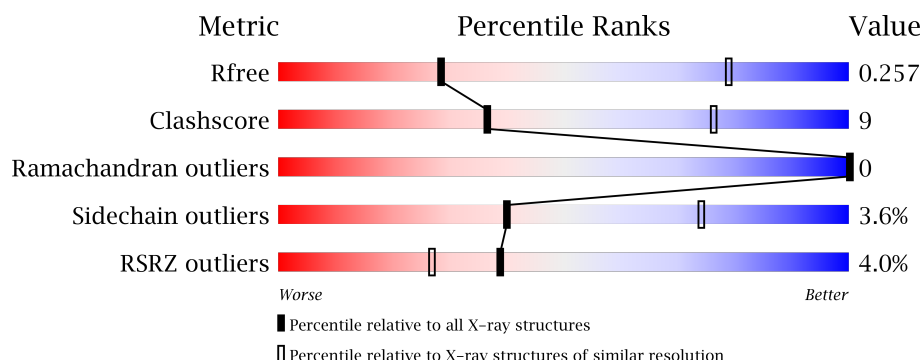
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.69 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	1161 (3.86-3.50)
Clashscore	112137	1295 (3.86-3.50)
Ramachandran outliers	110173	1245 (3.86-3.50)
Sidechain outliers	110143	1242 (3.86-3.50)
RSRZ outliers	101464	1188 (3.86-3.50)

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>3%</div> <div>71%</div> <div>20%</div> <div>8%</div> </div>
1	B	814	<div> <div>4%</div> <div>70%</div> <div>21%</div> <div>8%</div> </div>
1	C	814	<div> <div>5%</div> <div>70%</div> <div>21%</div> <div>8%</div> </div>
1	D	814	<div> <div>3%</div> <div>69%</div> <div>22%</div> <div>7%</div> </div>
2	E	90	<div> <div>72%</div> <div>21%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	90	 87% 8% 6%

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	NAG	C	901	-	-	-	X
5	FWF	B	903	-	-	-	X
5	FWF	D	903	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24451 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	747	Total	C	N	O	S	0	0	0
			5766	3715	941	1084	26			
1	B	746	Total	C	N	O	S	0	0	0
			5706	3665	940	1075	26			
1	C	745	Total	C	N	O	S	0	0	0
			5702	3663	933	1080	26			
1	D	753	Total	C	N	O	S	0	0	0
			5815	3737	961	1091	26			

There are 120 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	GLY	engineered mutation	UNP P19491
A	602	ALA	GLY	engineered mutation	UNP P19491
A	815	ALA	CYS	engineered mutation	UNP P19491
A	818	ARG	SER	engineered mutation	UNP P19491
A	819	MET	ARG	engineered mutation	UNP P19491
A	820	LYS	ALA	engineered mutation	UNP P19491
A	821	LEU	GLU	engineered mutation	UNP P19491
A	822	VAL	ALA	engineered mutation	UNP P19491
A	823	PRO	LYS	engineered mutation	UNP P19491
B	184	GLY	LYS	engineered mutation	UNP P19491
B	237	GLU	ASN	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
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B	535	LEU	GLY	engineered mutation	UNP P19491
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B	?	-	GLU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
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B	583	LEU	ALA	engineered mutation	UNP P19491
B	585	PHE	MET	engineered mutation	UNP P19491
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C	?	-	LEU	deletion	UNP P19491

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

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

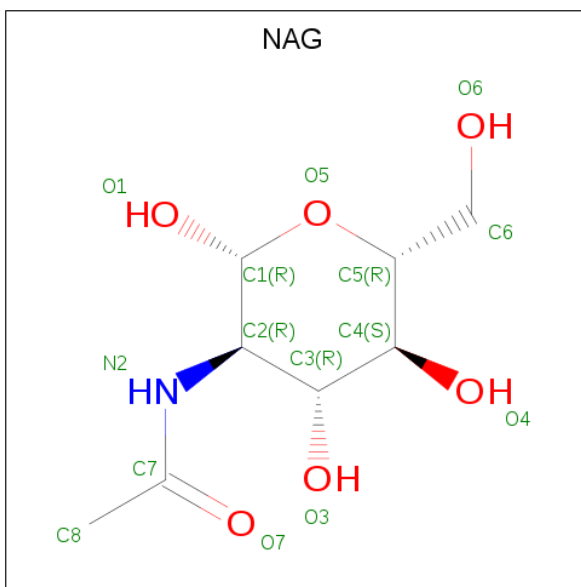
- Molecule 2 is a protein called Con-ikot-ikot.

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

There are 8 discrepancies between the modelled and reference sequences:

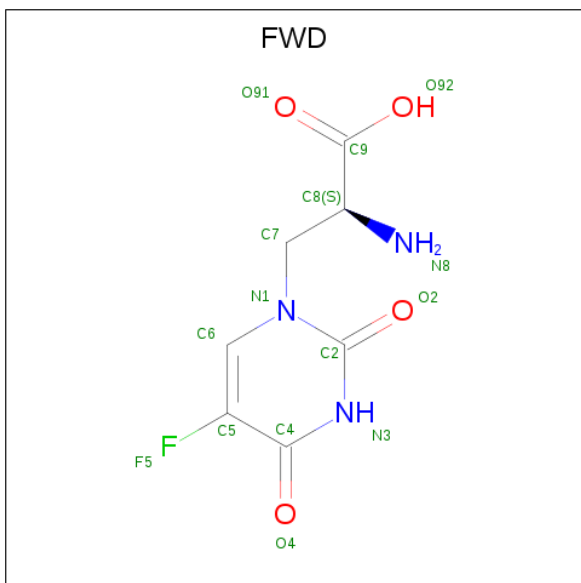
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P0CB20
E	-2	PRO	-	expression tag	UNP P0CB20
E	-1	GLY	-	expression tag	UNP P0CB20
E	0	SER	-	expression tag	UNP P0CB20
F	-3	GLY	-	expression tag	UNP P0CB20
F	-2	PRO	-	expression tag	UNP P0CB20
F	-1	GLY	-	expression tag	UNP P0CB20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

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

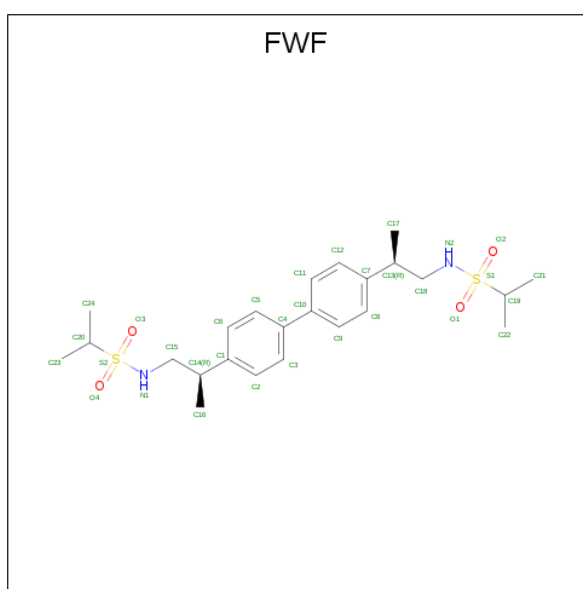
- Molecule 4 is 2-AMINO-3-(5-FLUORO-2,4-DIOXO-3,4-DIHYDRO-2H-PYRIMIDIN-1-YL)-PROPIONIC ACID (three-letter code: FWD) (formula:  $C_7H_8FN_3O_4$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			15	7	1	3	4		
4	B	1	Total	C	F	N	O	0	0
			15	7	1	3	4		
4	C	1	Total	C	F	N	O	0	0
			15	7	1	3	4		
4	D	1	Total	C	F	N	O	0	0
			15	7	1	3	4		

- Molecule 5 is N,N'-[biphenyl-4,4'-diyl-di(2R)propane-2,1-diyl]dipropylsulfonamide (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>).

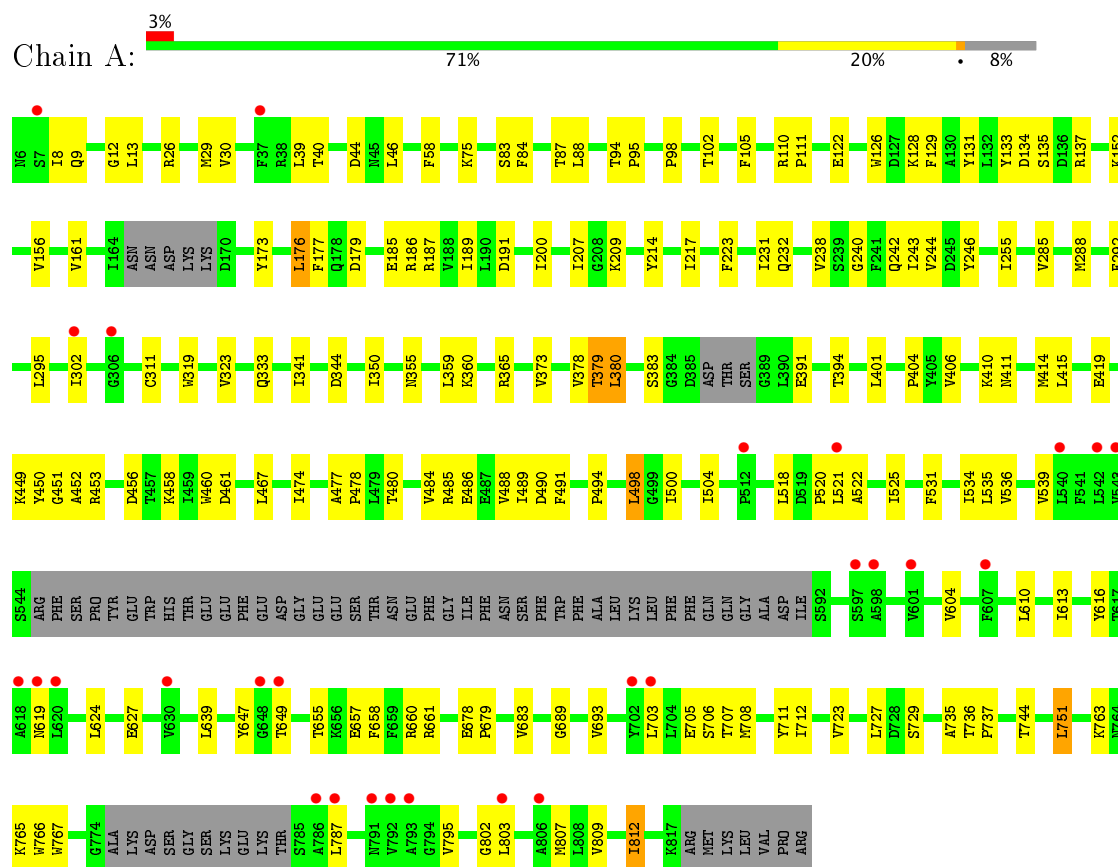


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			32	24	2	4	2		
5	D	1	Total	C	N	O	S	0	0
			32	24	2	4	2		

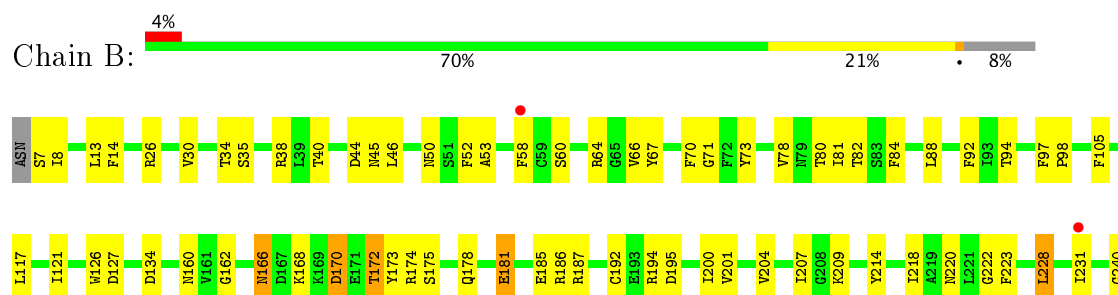
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

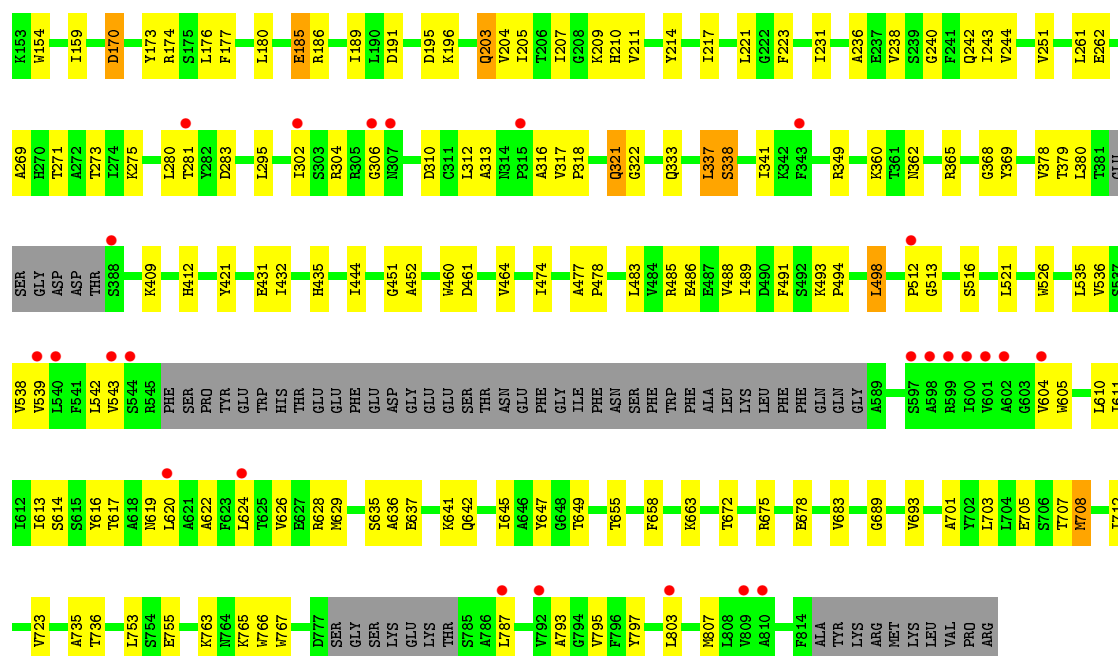
#### • Molecule 1: Glutamate receptor 2



#### • Molecule 1: Glutamate receptor 2







• Molecule 2: Con-ikot-ikot

Chain E: 72% 21% 6%



• Molecule 2: Con-ikot-ikot

Chain F: 87% 8% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.07Å 364.78Å 109.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.69 148.87 – 3.69	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.98-3.69) 97.9 (148.87-3.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.207 , 0.254 0.214 , 0.257	Depositor DCC
$R_{free}$ test set	3553 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	116.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 112.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24451	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, 0.333 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: FWD, FWF, 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	0/5884	0.47	0/7970
1	B	0.26	0/5823	0.47	0/7900
1	C	0.25	0/5819	0.46	0/7897
1	D	0.26	0/5933	0.48	0/8037
2	E	0.29	0/651	0.45	0/873
2	F	0.26	0/651	0.46	0/873
All	All	0.25	0/24761	0.47	0/33550

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	5766	0	5686	108	0
1	B	5706	0	5560	109	0
1	C	5702	0	5556	112	0
1	D	5815	0	5737	122	0
2	E	641	0	593	13	0
2	F	641	0	593	4	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	0	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
4	A	15	0	7	5	0
4	B	15	0	7	2	0
4	C	15	0	7	1	0
4	D	15	0	7	0	0
5	B	32	0	36	0	0
5	D	32	0	36	3	0
All	All	24451	0	23877	434	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.

All (434) 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:159:ILE:HG21	1:D:176:LEU:HD11	1.63	0.79
1:C:633:ILE:HG21	1:C:639:LEU:HD12	1.66	0.76
1:C:657:GLU:HG2	1:C:660:ARG:HH21	1.50	0.76
1:C:98:PRO:HD3	1:C:110:ARG:HD2	1.71	0.73
1:B:476:ILE:HD13	1:B:734:ILE:HD12	1.70	0.72
1:A:360:LYS:HD2	1:A:365:ARG:HD3	1.71	0.72
1:A:624:LEU:HD13	1:D:619:ASN:HD22	1.55	0.71
1:A:137:ARG:NH2	1:A:191:ASP:OD1	2.23	0.71
1:B:510:SER:OG	1:B:511:LYS:N	2.24	0.70
1:B:752:LYS:NZ	1:B:756:GLN:OE1	2.23	0.69
1:A:295:LEU:HD13	1:A:302:ILE:HG21	1.73	0.68
1:A:490:ASP:OD1	1:A:736:THR:OG1	2.11	0.68
1:B:8:ILE:HG23	1:B:67:TYR:HD2	1.58	0.68
1:D:379:THR:HG22	1:D:380:LEU:HG	1.76	0.68
1:A:486:GLU:OE2	1:D:493:LYS:NZ	2.27	0.67
1:B:73:TYR:HB3	1:B:81:ILE:HD12	1.77	0.67
1:C:224:THR:OG1	1:C:242:GLN:NE2	2.28	0.66
1:D:242:GLN:HE21	1:D:244:VAL:H	1.42	0.65
1:B:222:GLY:O	1:B:242:GLN:NE2	2.30	0.65
1:C:451:GLY:HA2	1:C:461:ASP:O	1.96	0.65
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.79	0.65
1:C:137:ARG:NH2	1:C:191:ASP:OD1	2.30	0.64
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.78	0.63
1:D:451:GLY:HA2	1:D:461:ASP:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ILE:HG13	1:B:209:LYS:HG2	1.81	0.63
1:C:110:ARG:NH1	1:C:276:TYR:OH	2.32	0.62
1:B:7:SER:N	1:B:38:ARG:O	2.32	0.62
1:B:340:ASN:O	1:B:349:ARG:NH2	2.32	0.62
1:D:173:TYR:OH	1:D:196:LYS:NZ	2.31	0.62
1:D:186:ARG:NH1	1:D:214:TYR:OH	2.34	0.61
2:F:21:LEU:HD21	2:F:32:VAL:HA	1.82	0.60
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.84	0.60
1:D:137:ARG:NH2	1:D:191:ASP:OD1	2.35	0.60
1:A:494:PRO:O	5:D:903:FWF:N1	2.32	0.60
1:B:181:GLU:OE2	1:B:186:ARG:NH1	2.35	0.60
1:B:755:GLU:OE2	1:C:661:ARG:NH1	2.35	0.60
1:D:318:PRO:HD2	1:D:321:GLN:HG2	1.83	0.59
1:B:134:ASP:O	1:B:160:ASN:ND2	2.36	0.59
1:B:525:ILE:HG12	1:C:792:VAL:HG21	1.84	0.59
1:D:521:LEU:HB2	1:D:526:TRP:NE1	2.17	0.59
1:D:338:SER:HB2	1:D:349:ARG:HH22	1.67	0.59
1:B:126:TRP:CD1	1:B:187:ARG:HD3	2.39	0.58
1:C:450:TYR:O	1:C:463:MET:N	2.36	0.58
1:A:126:TRP:CD1	1:A:187:ARG:HD3	2.39	0.58
1:C:126:TRP:CD1	1:C:187:ARG:HD3	2.38	0.58
1:C:510:SER:O	1:C:511:LYS:HG2	2.04	0.58
1:C:500:ILE:HG12	1:C:655:THR:HG23	1.85	0.57
1:A:380:LEU:HG	1:A:383:SER:H	1.70	0.57
1:B:597:SER:OG	1:C:806:ALA:O	2.20	0.57
1:B:201:VAL:HG13	1:B:231:ILE:HD12	1.86	0.57
1:A:500:ILE:HB	1:A:727:LEU:HB2	1.85	0.57
1:A:451:GLY:HA2	1:A:461:ASP:O	2.04	0.57
1:A:231:ILE:HD12	1:A:238:VAL:HG21	1.87	0.57
1:C:526:TRP:HA	1:C:529:ILE:HG22	1.87	0.57
1:C:67:TYR:HE1	1:C:304:ARG:HB2	1.70	0.57
1:A:705:GLU:HB2	1:A:708:MET:HE2	1.87	0.56
1:C:8:ILE:HG23	1:C:67:TYR:HD2	1.70	0.56
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.86	0.56
1:B:635:SER:OG	1:B:636:ALA:N	2.35	0.56
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.86	0.56
1:B:204:VAL:HG13	1:B:209:LYS:HB2	1.88	0.56
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.88	0.56
1:A:88:LEU:HD11	1:A:311:CYS:HB2	1.88	0.56
1:D:98:PRO:HD3	1:D:110:ARG:HD2	1.88	0.55
1:D:130:ALA:HB2	1:D:185:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ILE:HD11	1:C:370:TRP:HB2	1.88	0.55
1:A:802:GLY:HA3	1:D:604:VAL:HG21	1.88	0.55
1:D:221:LEU:HD13	1:D:243:ILE:HD12	1.89	0.55
1:A:453:ARG:HD3	2:E:41:VAL:HG21	1.88	0.55
1:B:50:ASN:HD22	1:B:53:ALA:HB2	1.71	0.54
1:B:601:VAL:HG22	1:C:806:ALA:HB1	1.88	0.54
1:D:207:ILE:HG13	1:D:209:LYS:HG2	1.89	0.54
1:D:122:GLU:OE2	1:D:152:LYS:NZ	2.27	0.54
1:D:170:ASP:HA	1:D:203:GLN:HE21	1.72	0.54
1:B:488:VAL:HG23	1:B:489:ILE:HG23	1.89	0.54
1:C:88:LEU:HD11	1:C:311:CYS:HB2	1.88	0.54
1:D:223:PHE:CD1	1:D:240:GLY:HA3	2.43	0.54
1:B:451:GLY:HA2	1:B:461:ASP:O	2.08	0.54
1:D:271:THR:HG22	1:D:273:THR:H	1.72	0.54
1:D:464:VAL:HG13	1:D:489:ILE:HD13	1.90	0.54
1:C:73:TYR:HE2	1:C:94:THR:HG21	1.73	0.53
2:E:16:ARG:HD2	2:E:42:THR:HG21	1.90	0.53
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.90	0.53
1:A:131:TYR:CE2	1:A:133:TYR:HB3	2.43	0.53
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.91	0.53
1:D:20:GLN:HE21	1:D:275:LYS:HG3	1.73	0.53
1:A:161:VAL:HG21	1:A:200:ILE:HD11	1.91	0.53
1:C:223:PHE:CD1	1:C:240:GLY:HA3	2.43	0.53
1:A:522:ALA:HB3	1:A:525:ILE:HG13	1.91	0.53
1:B:310:ASP:HB3	1:B:313:ALA:HB3	1.90	0.53
1:B:522:ALA:HB3	1:B:525:ILE:HG13	1.90	0.53
1:A:803:LEU:HD22	1:D:539:VAL:HG21	1.91	0.53
1:A:75:LYS:HD3	1:A:135:SER:O	2.08	0.52
1:C:75:LYS:HB3	1:C:136:ASP:O	2.09	0.52
1:A:683:VAL:HG11	1:A:689:GLY:HA2	1.90	0.52
1:B:326:GLU:OE2	1:B:330:LYS:NZ	2.42	0.52
1:C:32:PHE:CZ	1:C:286:GLN:HB2	2.44	0.52
1:A:624:LEU:HA	1:A:627:GLU:HG2	1.92	0.52
1:B:450:TYR:CZ	4:B:902:FWD:H6	2.45	0.52
1:B:604:VAL:HG12	1:C:799:LEU:HD12	1.92	0.52
1:A:8:ILE:HG23	1:A:39:LEU:HA	1.90	0.52
1:A:467:LEU:HD22	1:A:737:PRO:HD3	1.91	0.52
1:D:75:LYS:HB3	1:D:136:ASP:O	2.10	0.52
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.92	0.52
1:D:70:PHE:CZ	1:D:281:THR:HG23	2.44	0.52
1:A:520:PRO:O	1:A:619:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:539:VAL:O	1:D:543:VAL:HG23	2.10	0.52
1:A:498:LEU:HB2	1:A:706:SER:HB3	1.92	0.52
1:C:595:SER:OG	1:C:596:LEU:N	2.42	0.52
1:B:228:LEU:HD22	1:B:359:LEU:HD22	1.92	0.51
1:D:317:VAL:HG22	1:D:318:PRO:O	2.10	0.51
1:B:134:ASP:OD1	1:B:134:ASP:N	2.42	0.51
1:C:409:LYS:HG2	1:C:422:GLU:HG2	1.92	0.51
1:A:122:GLU:OE2	1:A:152:LYS:HE3	2.10	0.51
1:A:474:ILE:HG13	1:A:736:THR:HG22	1.92	0.51
1:B:70:PHE:CZ	1:B:281:THR:HG23	2.45	0.51
1:C:8:ILE:HB	1:C:39:LEU:HD23	1.93	0.51
1:D:70:PHE:CE2	1:D:281:THR:HG23	2.46	0.51
1:A:379:THR:O	1:A:380:LEU:HB3	2.10	0.51
1:A:657:GLU:OE1	1:A:660:ARG:NH2	2.26	0.51
1:D:170:ASP:O	1:D:174:ARG:HG2	2.10	0.51
1:B:597:SER:O	1:B:601:VAL:HG23	2.11	0.51
1:C:372:GLU:OE1	3:C:901:NAG:O6	2.29	0.50
1:B:753:LEU:HD22	1:B:758:VAL:HG11	1.92	0.50
2:E:5:ASP:OD2	2:F:10:LYS:NZ	2.38	0.50
1:A:177:PHE:HB3	1:A:209:LYS:HE3	1.93	0.50
1:C:485:ARG:O	1:C:489:ILE:HG12	2.10	0.50
1:B:223:PHE:CD1	1:B:240:GLY:HA3	2.46	0.50
1:C:204:VAL:HG13	1:C:209:LYS:HB2	1.94	0.50
1:C:491:PHE:CE1	1:C:735:ALA:HB2	2.46	0.50
1:C:221:LEU:HD13	1:C:243:ILE:HG13	1.93	0.50
1:D:34:THR:OG1	1:D:35:SER:N	2.44	0.50
1:D:494:PRO:O	5:D:903:FWF:N2	2.36	0.50
1:A:531:PHE:O	1:A:534:ILE:HG13	2.12	0.49
1:D:498:LEU:HD23	1:D:705:GLU:HB3	1.93	0.49
1:C:8:ILE:O	1:C:40:THR:N	2.45	0.49
1:D:708:MET:O	1:D:712:ILE:HG12	2.12	0.49
1:B:474:ILE:HG13	1:B:736:THR:HG22	1.95	0.49
1:C:803:LEU:O	1:C:807:MET:N	2.42	0.49
1:A:173:TYR:HA	1:A:176:LEU:HD23	1.94	0.49
1:A:207:ILE:HG13	1:A:209:LYS:HG2	1.95	0.49
1:D:12:GLY:HA2	1:D:70:PHE:O	2.12	0.49
1:C:706:SER:OG	1:C:707:THR:N	2.46	0.49
1:C:391:GLU:HG3	1:C:392:GLN:H	1.77	0.49
1:C:614:SER:HG	1:D:616:TYR:HD1	1.61	0.49
1:B:629:MET:HG2	1:B:630:VAL:H	1.78	0.49
2:E:17:VAL:HG22	2:E:36:TYR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:ILE:HD13	1:C:750:VAL:HG21	1.95	0.49
1:B:500:ILE:HG12	1:B:655:THR:HG22	1.95	0.48
1:D:54:VAL:HG11	1:D:77:SER:HB2	1.95	0.48
1:D:763:LYS:O	1:D:767:TRP:HB2	2.12	0.48
1:A:189:ILE:HG12	1:A:217:ILE:HB	1.95	0.48
1:B:301:GLU:OE2	1:B:301:GLU:N	2.46	0.48
1:D:536:VAL:HG21	1:D:605:TRP:HE3	1.78	0.48
1:D:614:SER:O	1:D:617:THR:OG1	2.26	0.48
1:D:622:ALA:O	1:D:626:VAL:HG23	2.13	0.48
1:B:134:ASP:HB2	1:B:162:GLY:HA3	1.95	0.48
1:B:271:THR:HG22	1:B:273:THR:H	1.78	0.48
1:D:513:GLY:O	1:D:516:SER:OG	2.24	0.48
1:A:242:GLN:HB3	1:A:355:ASN:HB2	1.95	0.48
1:A:449:LYS:HD2	1:A:461:ASP:OD2	2.14	0.48
1:A:521:LEU:HD13	1:A:616:TYR:HD2	1.78	0.48
1:B:404:PRO:HD3	1:B:711:TYR:CG	2.49	0.48
1:C:131:TYR:CE2	1:C:133:TYR:HB3	2.48	0.48
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.94	0.48
1:C:488:VAL:HG23	1:C:489:ILE:HG23	1.96	0.48
1:D:316:ALA:O	1:D:317:VAL:HB	2.13	0.48
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.95	0.48
1:C:450:TYR:CD1	4:C:902:FWD:H71	2.49	0.48
1:C:535:LEU:HG	1:D:803:LEU:HD13	1.96	0.48
1:D:803:LEU:O	1:D:807:MET:HG2	2.13	0.48
1:A:9:GLN:HA	1:A:40:THR:HB	1.95	0.47
1:C:122:GLU:OE1	1:C:152:LYS:NZ	2.47	0.47
1:B:659:PHE:CE2	1:B:703:LEU:HD13	2.49	0.47
1:B:708:MET:O	1:B:712:ILE:HG12	2.15	0.47
1:C:711:TYR:HB2	1:C:767:TRP:NE1	2.30	0.47
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.96	0.47
1:C:12:GLY:HA2	1:C:70:PHE:O	2.14	0.47
1:D:204:VAL:HG13	1:D:209:LYS:HB2	1.96	0.47
1:A:610:LEU:O	1:A:613:ILE:HG13	2.14	0.47
1:A:613:ILE:HG22	1:D:610:LEU:HD21	1.97	0.47
1:D:295:LEU:HD13	1:D:302:ILE:HG21	1.97	0.47
1:D:58:PHE:CE2	1:D:84:PHE:HB3	2.50	0.47
1:D:708:MET:SD	1:D:708:MET:N	2.87	0.47
1:B:166:ASN:C	1:B:166:ASN:HD22	2.11	0.47
1:B:500:ILE:HB	1:B:727:LEU:HB2	1.97	0.47
1:D:189:ILE:HG12	1:D:217:ILE:HB	1.96	0.47
1:D:488:VAL:HG23	1:D:489:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASP:OD1	1:A:134:ASP:N	2.48	0.46
1:A:83:SER:OG	1:B:50:ASN:OD1	2.32	0.46
1:C:29:MET:O	1:C:33:SER:HB3	2.16	0.46
1:D:637:GLU:HG2	1:D:641:LYS:HE2	1.97	0.46
1:A:708:MET:O	1:A:712:ILE:HG12	2.15	0.46
1:D:610:LEU:O	1:D:613:ILE:HG13	2.15	0.46
1:A:765:LYS:HD3	1:A:766:TRP:NE1	2.31	0.46
1:C:611:ILE:HD12	1:D:795:VAL:HG13	1.97	0.46
1:D:251:VAL:HG22	1:D:337:LEU:HD13	1.96	0.46
1:B:173:TYR:CE1	1:B:200:ILE:HG12	2.51	0.46
1:D:15:PRO:HA	1:D:46:LEU:O	2.16	0.46
1:A:410:LYS:HG3	1:A:411:ASN:H	1.80	0.46
1:B:322:GLY:HA2	1:B:325:ILE:HD12	1.98	0.46
1:B:58:PHE:HE2	1:B:88:LEU:HD12	1.81	0.46
1:C:418:ASN:HD21	1:C:441:LYS:HA	1.80	0.46
1:C:75:LYS:HE3	1:C:75:LYS:HB2	1.64	0.46
1:D:409:LYS:O	1:D:412:HIS:ND1	2.45	0.46
1:D:302:ILE:HG13	1:D:302:ILE:H	1.63	0.46
1:C:752:LYS:HE3	1:C:752:LYS:HB2	1.69	0.46
1:D:360:LYS:HG3	1:D:365:ARG:HE	1.81	0.46
1:D:655:THR:O	1:D:658:PHE:HB3	2.16	0.46
1:B:498:LEU:HB3	1:B:707:THR:HG23	1.98	0.45
2:E:60:MET:HA	2:E:63:VAL:HG12	1.97	0.45
1:A:133:TYR:HA	1:A:191:ASP:O	2.16	0.45
1:B:105:PHE:HZ	1:B:323:VAL:HG22	1.81	0.45
1:B:697:LYS:HD2	1:B:697:LYS:HA	1.78	0.45
1:C:499:GLY:H	1:C:706:SER:HB3	1.81	0.45
1:A:787:LEU:HD13	1:D:619:ASN:ND2	2.31	0.45
1:D:647:TYR:HB3	1:D:701:ALA:HB3	1.97	0.45
1:D:672:THR:HG23	1:D:675:ARG:NH2	2.31	0.45
1:D:683:VAL:HG11	1:D:689:GLY:HA2	1.97	0.45
1:D:94:THR:HA	1:D:95:PRO:HD3	1.70	0.45
1:A:176:LEU:HA	1:A:179:ASP:OD2	2.17	0.45
1:B:751:LEU:HD13	1:C:486:GLU:HG2	1.99	0.45
1:C:21:GLU:OE1	1:C:21:GLU:N	2.50	0.45
1:C:737:PRO:HG2	1:C:740:SER:HB2	1.97	0.45
1:D:117:LEU:O	1:D:121:ILE:HG13	2.16	0.45
1:D:231:ILE:HD12	1:D:238:VAL:HG21	1.98	0.45
1:D:536:VAL:HG21	1:D:605:TRP:CE3	2.50	0.45
1:C:70:PHE:CE1	1:C:95:PRO:HD3	2.52	0.45
1:C:481:ILE:HD11	1:C:733:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.99	0.45
1:A:29:MET:HE1	1:A:39:LEU:HB2	1.99	0.45
1:C:126:TRP:HA	1:C:187:ARG:HH11	1.81	0.45
1:C:319:TRP:HD1	1:C:319:TRP:H	1.65	0.45
1:D:131:TYR:CE2	1:D:133:TYR:HB3	2.52	0.45
1:D:486:GLU:OE1	1:D:491:PHE:HB2	2.16	0.45
2:E:33:SER:HB3	2:E:61:ILE:HD11	1.99	0.45
1:A:411:ASN:N	1:A:411:ASN:OD1	2.50	0.45
1:A:803:LEU:O	1:A:807:MET:HG2	2.17	0.45
1:A:485:ARG:NH1	4:A:902:FWD:O92	2.40	0.45
1:B:26:ARG:O	1:B:30:VAL:HG23	2.17	0.45
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.57	0.45
1:C:73:TYR:CE2	1:C:94:THR:HG21	2.52	0.45
1:D:321:GLN:HB3	1:D:322:GLY:H	1.37	0.45
1:B:60:SER:O	1:B:64:ARG:HG3	2.16	0.45
1:B:683:VAL:HG11	1:B:689:GLY:HA2	1.99	0.45
1:C:486:GLU:OE1	1:C:491:PHE:HB2	2.17	0.45
1:D:642:GLN:OE1	1:D:645:ILE:N	2.35	0.45
1:A:128:LYS:HE2	1:A:185:GLU:CD	2.37	0.44
1:B:14:PHE:O	1:B:45:ASN:HA	2.17	0.44
1:B:209:LYS:HD2	1:B:214:TYR:CE2	2.52	0.44
1:C:109:MET:HE1	1:C:287:VAL:HG21	1.98	0.44
1:D:109:MET:HB3	1:D:280:LEU:HD22	1.98	0.44
1:D:637:GLU:O	1:D:641:LYS:HG3	2.17	0.44
1:D:70:PHE:CE1	1:D:95:PRO:HD3	2.52	0.44
1:A:763:LYS:O	1:A:767:TRP:HB2	2.17	0.44
1:C:400:ILE:O	1:C:406:VAL:HB	2.16	0.44
1:D:620:LEU:O	1:D:624:LEU:HB2	2.16	0.44
1:A:232:GLN:HA	1:A:359:LEU:HD11	1.99	0.44
1:A:415:LEU:HD23	1:A:419:GLU:HB3	2.00	0.44
1:B:526:TRP:HA	1:B:529:ILE:HG22	1.99	0.44
1:C:217:ILE:HG12	1:C:239:SER:OG	2.17	0.44
1:C:597:SER:O	1:C:601:VAL:HG23	2.18	0.44
1:D:512:PRO:HB2	1:D:516:SER:OG	2.18	0.44
1:D:628:ARG:HG2	1:D:629:MET:H	1.82	0.44
1:B:689:GLY:O	1:B:693:VAL:HG23	2.18	0.44
1:B:73:TYR:HE2	1:B:94:THR:HG21	1.82	0.44
1:A:689:GLY:O	1:A:693:VAL:HG23	2.18	0.44
1:B:13:LEU:O	1:B:71:GLY:HA2	2.17	0.44
1:B:333:GLN:HA	1:B:341:ILE:O	2.17	0.44
1:C:70:PHE:HE1	1:C:95:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:TYR:HB2	1:B:767:TRP:NE1	2.33	0.44
1:B:789:LEU:HA	1:B:789:LEU:HD12	1.85	0.44
1:C:795:VAL:O	1:C:798:ILE:HG22	2.18	0.44
1:B:499:GLY:H	1:B:706:SER:HB3	1.83	0.44
1:B:795:VAL:O	1:B:798:ILE:HG22	2.18	0.44
1:B:81:ILE:HD13	1:B:92:PHE:CZ	2.53	0.44
1:D:205:ILE:HG23	1:D:210:HIS:CE1	2.53	0.44
1:A:411:ASN:ND2	1:A:414:MET:SD	2.82	0.43
1:B:450:TYR:CD1	4:B:902:FWD:H71	2.53	0.43
1:C:134:ASP:N	1:C:134:ASP:OD1	2.49	0.43
1:C:455:ALA:O	1:C:458:LYS:NZ	2.49	0.43
1:C:689:GLY:O	1:C:693:VAL:HG23	2.18	0.43
1:B:127:ASP:OD1	1:B:127:ASP:N	2.50	0.43
1:B:170:ASP:O	1:B:174:ARG:HG3	2.18	0.43
1:B:452:ALA:O	1:B:460:TRP:HA	2.18	0.43
1:D:689:GLY:O	1:D:693:VAL:HG23	2.18	0.43
1:A:488:VAL:HG23	1:A:489:ILE:HG23	2.00	0.43
1:B:397:VAL:HB	1:B:442:LEU:HD23	2.01	0.43
1:D:368:GLY:HA2	1:D:379:THR:HB	1.99	0.43
1:A:678:GLU:HA	1:A:679:PRO:C	2.39	0.43
1:C:498:LEU:HB3	1:C:707:THR:HG23	2.01	0.43
1:A:246:TYR:CD1	1:A:255:ILE:HD11	2.53	0.43
1:C:683:VAL:HG11	1:C:689:GLY:HA2	2.00	0.43
1:D:421:TYR:CE1	1:D:444:ILE:HD11	2.53	0.43
1:D:707:THR:OG1	1:D:708:MET:SD	2.75	0.43
1:D:793:ALA:O	1:D:797:TYR:HD1	2.02	0.43
1:B:78:VAL:O	1:B:82:THR:HG23	2.19	0.43
1:B:751:LEU:HD22	1:C:483:LEU:HA	2.00	0.43
1:A:729:SER:HB2	5:D:903:FWF:H19	2.00	0.43
1:A:661:ARG:HH21	2:E:49:ILE:HA	1.84	0.43
2:E:47:ASN:ND2	2:E:85:CYS:O	2.52	0.43
1:A:333:GLN:HA	1:A:341:ILE:O	2.19	0.43
1:A:450:TYR:CZ	4:A:902:FWD:H6	2.53	0.43
1:B:243:ILE:HG23	1:B:244:VAL:HG23	2.00	0.43
1:C:26:ARG:NH2	1:C:266:TYR:HD1	2.17	0.43
1:D:134:ASP:N	1:D:134:ASP:OD1	2.50	0.43
1:D:209:LYS:HD2	1:D:214:TYR:CE2	2.54	0.43
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.89	0.43
1:A:604:VAL:HG21	1:B:802:GLY:HA3	2.01	0.43
1:C:637:GLU:O	1:C:640:SER:OG	2.29	0.43
1:B:637:GLU:O	1:B:641:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TRP:CG	1:C:187:ARG:HD3	2.54	0.43
1:A:98:PRO:HD3	1:A:110:ARG:HD2	2.01	0.42
1:B:181:GLU:HG2	1:B:209:LYS:HE2	2.00	0.42
1:C:177:PHE:HA	1:C:180:LEU:HD12	2.00	0.42
1:C:536:VAL:HG21	1:C:605:TRP:HE3	1.84	0.42
1:A:26:ARG:O	1:A:30:VAL:HG23	2.19	0.42
1:A:809:VAL:HA	1:A:812:ILE:HG23	2.01	0.42
1:B:34:THR:OG1	1:B:35:SER:N	2.53	0.42
1:B:657:GLU:OE2	1:B:661:ARG:NH1	2.52	0.42
1:B:8:ILE:O	1:B:40:THR:N	2.45	0.42
1:C:193:GLU:O	1:C:197:VAL:HG23	2.19	0.42
1:D:177:PHE:HA	1:D:180:LEU:HD12	2.01	0.42
1:A:186:ARG:HB3	1:A:214:TYR:HA	2.02	0.42
1:B:373:VAL:HG23	1:B:374:ASP:H	1.85	0.42
1:B:625:THR:HG22	1:B:626:VAL:HG13	2.01	0.42
1:B:97:PHE:HA	1:B:98:PRO:HD3	1.86	0.42
1:C:406:VAL:HG13	1:C:421:TYR:HB3	2.00	0.42
1:D:485:ARG:O	1:D:489:ILE:HG12	2.19	0.42
1:A:452:ALA:O	1:A:460:TRP:HA	2.18	0.42
1:D:261:LEU:HD12	1:D:269:ALA:HB1	2.00	0.42
1:D:310:ASP:HB3	1:D:313:ALA:CB	2.50	0.42
1:D:111:PRO:HG3	1:D:349:ARG:HD3	2.01	0.42
1:C:172:THR:O	1:C:176:LEU:HG	2.19	0.42
2:E:21:LEU:HD21	2:E:32:VAL:HA	2.02	0.42
1:A:450:TYR:CE1	4:A:902:FWD:H6	2.54	0.42
1:B:425:CYS:SG	1:B:477:ALA:HA	2.60	0.42
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.54	0.42
1:A:498:LEU:HB3	1:A:707:THR:HG23	2.00	0.42
1:B:242:GLN:HB3	1:B:355:ASN:HB2	2.02	0.42
1:C:117:LEU:O	1:C:121:ILE:HG13	2.19	0.42
1:C:159:ILE:HD11	1:C:176:LEU:HD13	2.01	0.42
1:C:535:LEU:O	1:C:539:VAL:HG23	2.20	0.42
1:C:498:LEU:HD23	1:C:705:GLU:HB3	2.01	0.42
1:C:763:LYS:O	1:C:767:TRP:HB2	2.18	0.42
1:D:283:ASP:OD2	1:D:338:SER:OG	2.38	0.42
1:A:94:THR:HA	1:A:95:PRO:HD3	1.69	0.42
1:C:641:LYS:HE2	1:C:641:LYS:HB3	1.84	0.42
1:D:663:LYS:HB3	1:D:663:LYS:HE2	1.89	0.42
1:A:458:LYS:HD2	2:E:41:VAL:HG22	2.02	0.42
1:A:223:PHE:CD1	1:A:240:GLY:HA3	2.54	0.42
1:A:485:ARG:HH12	4:A:902:FWD:C9	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:PHE:CE2	1:A:84:PHE:HB3	2.55	0.42
1:B:321:GLN:O	1:B:325:ILE:HG13	2.20	0.42
2:F:36:TYR:CD1	2:F:57:GLN:HB2	2.54	0.42
1:B:168:LYS:O	1:B:172:THR:HG22	2.20	0.42
1:C:522:ALA:HB3	1:C:525:ILE:HG13	2.00	0.42
2:E:18:ASN:O	2:E:22:GLN:HG3	2.20	0.42
1:A:12:GLY:C	1:A:13:LEU:HD12	2.40	0.41
1:A:292:PHE:CD1	1:A:295:LEU:HD12	2.55	0.41
1:A:450:TYR:CD1	4:A:902:FWD:H71	2.55	0.41
1:C:405:TYR:HB3	1:C:425:CYS:SG	2.60	0.41
1:C:58:PHE:CE2	1:C:84:PHE:HB3	2.55	0.41
1:C:476:ILE:HD13	1:C:734:ILE:HG12	2.01	0.41
1:D:304:ARG:HG2	1:D:306:GLY:O	2.20	0.41
1:D:73:TYR:HE2	1:D:94:THR:HG21	1.84	0.41
1:B:175:SER:O	1:B:178:GLN:HB3	2.21	0.41
1:B:477:ALA:HB1	1:B:478:PRO:HD2	2.02	0.41
1:B:763:LYS:O	1:B:767:TRP:HB2	2.20	0.41
1:D:211:VAL:O	1:D:236:ALA:HB2	2.20	0.41
1:D:538:VAL:O	1:D:542:LEU:HG	2.20	0.41
1:D:765:LYS:HD3	1:D:766:TRP:NE1	2.35	0.41
1:A:111:PRO:HG2	1:A:243:ILE:HD11	2.00	0.41
1:A:491:PHE:CE1	1:A:735:ALA:HB2	2.55	0.41
1:B:218:ILE:HG22	1:B:220:ASN:H	1.84	0.41
1:A:84:PHE:CE1	1:B:52:PHE:HA	2.56	0.41
1:C:635:SER:HB2	1:C:638:ASP:OD2	2.20	0.41
1:A:105:PHE:HZ	1:A:323:VAL:HG22	1.84	0.41
1:C:521:LEU:HA	1:D:787:LEU:HB2	2.01	0.41
1:D:333:GLN:HA	1:D:341:ILE:O	2.21	0.41
1:A:129:PHE:CZ	1:A:156:VAL:HG12	2.55	0.41
1:A:404:PRO:HD3	1:A:711:TYR:CG	2.54	0.41
1:C:373:VAL:HG23	1:C:374:ASP:H	1.85	0.41
1:D:221:LEU:HB3	1:D:243:ILE:HB	2.03	0.41
1:A:661:ARG:NH1	1:D:755:GLU:OE2	2.54	0.41
1:A:344:ASP:HB3	1:A:350:ILE:HG13	2.01	0.41
1:B:638:ASP:O	1:B:642:GLN:HG3	2.21	0.41
1:C:539:VAL:O	1:C:543:VAL:HG23	2.21	0.41
1:C:78:VAL:O	1:C:82:THR:HG23	2.19	0.41
2:E:32:VAL:HB	2:E:61:ILE:HG13	2.02	0.41
1:A:133:TYR:O	1:A:161:VAL:HG22	2.21	0.41
1:B:711:TYR:CZ	1:B:715:ARG:HD3	2.55	0.41
1:C:452:ALA:O	1:C:460:TRP:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:O	1:B:121:ILE:HG13	2.21	0.41
1:D:127:ASP:O	1:D:154:TRP:HA	2.20	0.41
1:D:435:HIS:NE2	1:D:753:LEU:HD21	2.36	0.41
1:A:639:LEU:HD21	1:A:647:TYR:CG	2.56	0.41
1:A:480:THR:OG1	1:A:705:GLU:OE2	2.32	0.41
1:B:702:TYR:CE2	1:B:704:LEU:HB3	2.56	0.41
1:C:651:ASP:N	1:C:683:VAL:O	2.54	0.41
2:E:83:ASN:HA	2:E:84:PRO:HD2	1.89	0.41
1:A:477:ALA:HB1	1:A:478:PRO:HD2	2.03	0.41
1:A:58:PHE:HE2	1:A:88:LEU:HD12	1.86	0.41
1:C:97:PHE:HA	1:C:98:PRO:HD3	1.92	0.41
1:D:14:PHE:O	1:D:45:ASN:HA	2.20	0.41
1:A:535:LEU:O	1:A:539:VAL:HG23	2.21	0.41
1:A:787:LEU:HD23	1:D:521:LEU:HD22	2.03	0.41
1:B:58:PHE:CE2	1:B:84:PHE:HB3	2.55	0.41
1:C:109:MET:HB3	1:C:280:LEU:HD22	2.02	0.41
1:C:607:PHE:O	1:C:611:ILE:HG13	2.21	0.41
1:C:670:MET:HB3	1:C:674:MET:HE3	2.02	0.41
1:D:20:GLN:NE2	1:D:275:LYS:HG3	2.35	0.41
1:A:751:LEU:HD13	1:D:486:GLU:HG2	2.03	0.41
1:C:26:ARG:HH22	1:C:267:PRO:HD2	1.85	0.40
1:B:619:ASN:HA	1:C:624:LEU:HD13	2.03	0.40
1:D:421:TYR:HE1	1:D:444:ILE:HD11	1.86	0.40
1:D:635:SER:OG	1:D:636:ALA:N	2.45	0.40
1:A:87:THR:HG21	1:B:52:PHE:CE1	2.56	0.40
1:B:485:ARG:O	1:B:489:ILE:HG12	2.20	0.40
1:B:734:ILE:HG21	1:B:746:VAL:HG11	2.03	0.40
1:C:197:VAL:O	1:C:201:VAL:HG23	2.21	0.40
1:D:295:LEU:HA	1:D:295:LEU:HD23	1.96	0.40
2:F:17:VAL:HG22	2:F:36:TYR:HA	2.02	0.40
1:A:285:VAL:HA	1:A:288:MET:HE2	2.03	0.40
1:A:655:THR:O	1:A:658:PHE:HB3	2.22	0.40
1:C:181:GLU:CG	1:C:209:LYS:HE3	2.51	0.40
1:D:535:LEU:O	1:D:538:VAL:HG12	2.22	0.40
1:B:209:LYS:HD2	1:B:214:TYR:CZ	2.56	0.40
1:B:321:GLN:O	1:B:324:GLU:HB3	2.22	0.40
1:C:221:LEU:HD22	1:C:243:ILE:HG12	2.03	0.40
1:D:452:ALA:O	1:D:460:TRP:HA	2.21	0.40
1:D:477:ALA:HB1	1:D:478:PRO:HD2	2.04	0.40
1:B:498:LEU:HD23	1:B:705:GLU:HB3	2.03	0.40
1:D:431:GLU:O	1:D:435:HIS:HD2	2.04	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	737/814 (90%)	714 (97%)	23 (3%)	0	100	100
1	B	738/814 (91%)	709 (96%)	29 (4%)	0	100	100
1	C	737/814 (90%)	710 (96%)	27 (4%)	0	100	100
1	D	745/814 (92%)	714 (96%)	31 (4%)	0	100	100
2	E	83/90 (92%)	79 (95%)	4 (5%)	0	100	100
2	F	83/90 (92%)	78 (94%)	5 (6%)	0	100	100
All	All	3123/3436 (91%)	3004 (96%)	119 (4%)	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	607/694 (88%)	586 (96%)	21 (4%)	41	75
1	B	592/694 (85%)	568 (96%)	24 (4%)	35	72
1	C	595/694 (86%)	575 (97%)	20 (3%)	42	76
1	D	612/694 (88%)	588 (96%)	24 (4%)	37	73
2	E	73/76 (96%)	71 (97%)	2 (3%)	50	80
2	F	73/76 (96%)	72 (99%)	1 (1%)	71	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2552/2928 (87%)	2460 (96%)	92 (4%)	40	74

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	46	LEU
1	A	102	THR
1	A	176	LEU
1	A	244	VAL
1	A	319	TRP
1	A	373	VAL
1	A	378	VAL
1	A	379	THR
1	A	380	LEU
1	A	391	GLU
1	A	394	THR
1	A	456	ASP
1	A	484	VAL
1	A	498	LEU
1	A	504	ILE
1	A	518	LEU
1	A	723	VAL
1	A	744	THR
1	A	751	LEU
1	A	812	ILE
1	B	44	ASP
1	B	46	LEU
1	B	66	VAL
1	B	80	THR
1	B	166	ASN
1	B	170	ASP
1	B	172	THR
1	B	181	GLU
1	B	185	GLU
1	B	192	CYS
1	B	194	ARG
1	B	195	ASP
1	B	228	LEU
1	B	295	LEU
1	B	302	ILE
1	B	319	TRP

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Mol	Chain	Res	Type
1	B	340	ASN
1	B	345	GLN
1	B	365	ARG
1	B	378	VAL
1	B	445	VAL
1	B	498	LEU
1	B	723	VAL
1	B	751	LEU
1	C	46	LEU
1	C	52	PHE
1	C	100	ASP
1	C	157	THR
1	C	193	GLU
1	C	195	ASP
1	C	210	HIS
1	C	319	TRP
1	C	334	VAL
1	C	350	ILE
1	C	353	THR
1	C	387	THR
1	C	400	ILE
1	C	422	GLU
1	C	498	LEU
1	C	627	GLU
1	C	723	VAL
1	C	751	LEU
1	C	772	GLU
1	C	807	MET
1	D	9	GLN
1	D	20	GLN
1	D	44	ASP
1	D	46	LEU
1	D	99	THR
1	D	109	MET
1	D	170	ASP
1	D	185	GLU
1	D	195	ASP
1	D	203	GLN
1	D	262	GLU
1	D	312	LEU
1	D	321	GLN
1	D	337	LEU

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Mol	Chain	Res	Type
1	D	338	SER
1	D	362	ASN
1	D	369	TYR
1	D	378	VAL
1	D	432	ILE
1	D	483	LEU
1	D	498	LEU
1	D	678	GLU
1	D	708	MET
1	D	723	VAL
2	E	61	ILE
2	E	80	SER
2	F	27	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	709	ASN
1	B	411	ASN
1	C	242	GLN
1	C	709	ASN
1	D	20	GLN
1	D	435	HIS
1	D	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	NAG	A	901	1	14,14,15	0.66	1 (7%)	15,19,21	0.82	0
4	FWD	A	902	-	8,15,15	3.06	1 (12%)	6,21,21	2.83	2 (33%)
3	NAG	B	901	1	14,14,15	0.27	0	15,19,21	0.47	0
4	FWD	B	902	-	8,15,15	3.02	1 (12%)	6,21,21	2.89	2 (33%)
5	FWF	B	903	-	29,33,33	0.49	0	36,48,48	1.15	3 (8%)
3	NAG	C	901	1	14,14,15	0.56	0	15,19,21	0.95	1 (6%)
4	FWD	C	902	-	8,15,15	3.01	1 (12%)	6,21,21	2.82	2 (33%)
3	NAG	D	901	1	14,14,15	1.02	1 (7%)	15,19,21	0.57	0
4	FWD	D	902	-	8,15,15	2.99	1 (12%)	6,21,21	2.93	2 (33%)
5	FWF	D	903	-	29,33,33	0.46	0	36,48,48	1.37	3 (8%)

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	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	FWD	A	902	-	-	0/3/8/8	0/1/1/1
3	NAG	B	901	1	-	0/6/23/26	0/1/1/1
4	FWD	B	902	-	-	0/3/8/8	0/1/1/1
5	FWF	B	903	-	-	0/32/36/36	0/2/2/2
3	NAG	C	901	1	-	0/6/23/26	0/1/1/1
4	FWD	C	902	-	-	0/3/8/8	0/1/1/1
3	NAG	D	901	1	-	0/6/23/26	0/1/1/1
4	FWD	D	902	-	-	0/3/8/8	0/1/1/1
5	FWF	D	903	-	-	0/32/36/36	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAG	O5-C1	-2.28	1.40	1.43
3	D	901	NAG	O5-C1	3.21	1.49	1.43
4	D	902	FWD	C4-C5	8.15	1.48	1.38
4	C	902	FWD	C4-C5	8.19	1.48	1.38
4	B	902	FWD	C4-C5	8.22	1.48	1.38
4	A	902	FWD	C4-C5	8.31	1.48	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	902	FWD	C5-C4-N3	-3.50	118.69	122.39
4	B	902	FWD	C5-C4-N3	-3.39	118.82	122.39
4	C	902	FWD	C5-C4-N3	-3.30	118.90	122.39
4	A	902	FWD	C5-C4-N3	-3.27	118.94	122.39
5	B	903	FWF	C3-C4-C10	-2.47	117.02	121.38
5	D	903	FWF	C9-C10-C4	-2.42	117.10	121.38
3	C	901	NAG	C1-O5-C5	2.41	115.49	112.17
5	D	903	FWF	O4-S2-N1	2.61	110.91	107.76
5	B	903	FWF	O4-S2-N1	2.65	110.96	107.76
5	B	903	FWF	O1-S1-N2	2.88	111.24	107.76
5	D	903	FWF	O1-S1-N2	4.00	112.58	107.76
4	C	902	FWD	C4-N3-C2	5.95	120.37	115.16
4	A	902	FWD	C4-N3-C2	5.98	120.39	115.16
4	B	902	FWD	C4-N3-C2	6.10	120.50	115.16
4	D	902	FWD	C4-N3-C2	6.16	120.55	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	FWD	5	0
4	B	902	FWD	2	0
3	C	901	NAG	1	0
4	C	902	FWD	1	0
5	D	903	FWF	3	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	747/814 (91%)	0.32	28 (3%)	42	30	52, 121, 243, 357	0
1	B	746/814 (91%)	0.30	29 (3%)	40	28	66, 123, 255, 349	0
1	C	745/814 (91%)	0.35	43 (5%)	24	16	72, 148, 258, 374	0
1	D	753/814 (92%)	0.32	27 (3%)	43	31	53, 122, 245, 354	0
2	E	85/90 (94%)	0.09	0	100	100	59, 90, 127, 184	0
2	F	85/90 (94%)	0.08	0	100	100	82, 113, 166, 227	0
All	All	3161/3436 (91%)	0.31	127 (4%)	39	27	52, 126, 249, 374	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	618	ALA	7.5
1	D	601	VAL	5.9
1	A	792	VAL	4.7
1	D	388	SER	4.6
1	C	649	THR	4.6
1	A	598	ALA	4.3
1	C	388	SER	4.3
1	C	67	TYR	4.0
1	B	619	ASN	4.0
1	A	793	ALA	4.0
1	D	598	ALA	4.0
1	D	604	VAL	3.9
1	D	597	SER	3.9
1	D	599	ARG	3.8
1	C	792	VAL	3.8
1	B	792	VAL	3.7
1	C	648	GLY	3.7
1	B	604	VAL	3.6
1	A	630	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	536	VAL	3.6
1	A	302	ILE	3.5
1	D	540	LEU	3.5
1	D	600	ILE	3.5
1	D	602	ALA	3.5
1	C	600	ILE	3.5
1	A	540	LEU	3.5
1	B	381	THR	3.4
1	C	702	TYR	3.4
1	B	617	THR	3.4
1	A	620	LEU	3.3
1	C	421	TYR	3.3
1	B	536	VAL	3.3
1	B	703	LEU	3.3
1	A	806	ALA	3.3
1	B	605	TRP	3.2
1	D	810	ALA	3.2
1	D	809	VAL	3.1
1	C	598	ALA	3.1
1	C	540	LEU	3.0
1	D	307	ASN	3.0
1	B	308	ALA	2.9
1	A	648	GLY	2.9
1	C	305	ARG	2.9
1	B	315	PRO	2.9
1	C	221	LEU	2.9
1	A	512	PRO	2.8
1	A	803	LEU	2.8
1	C	68	ALA	2.8
1	A	601	VAL	2.8
1	B	791	ASN	2.8
1	A	542	LEU	2.8
1	B	648	GLY	2.8
1	C	701	ALA	2.8
1	C	601	VAL	2.8
1	D	302	ILE	2.8
1	C	505	LYS	2.7
1	C	91	SER	2.7
1	D	539	VAL	2.7
1	C	633	ILE	2.7
1	C	84	PHE	2.7
1	D	306	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	700	TYR	2.6
1	C	803	LEU	2.6
1	D	543	VAL	2.6
1	A	543	VAL	2.6
1	C	618	ALA	2.6
1	B	601	VAL	2.6
1	D	315	PRO	2.6
1	C	58	PHE	2.6
1	A	521	LEU	2.6
1	A	791	ASN	2.5
1	A	597	SER	2.5
1	C	621	ALA	2.5
1	A	702	TYR	2.5
1	A	7	SER	2.5
1	B	368	GLY	2.5
1	B	620	LEU	2.5
1	C	6	ASN	2.5
1	D	620	LEU	2.5
1	C	793	ALA	2.5
1	A	649	THR	2.4
1	B	702	TYR	2.4
1	C	504	ILE	2.4
1	C	337	LEU	2.4
1	D	69	ILE	2.4
1	B	602	ALA	2.4
1	C	476	ILE	2.3
1	B	649	THR	2.3
1	C	359	LEU	2.3
1	D	624	LEU	2.3
1	B	231	ILE	2.3
1	C	474	ILE	2.3
1	C	389	GLY	2.3
1	C	292	PHE	2.3
1	A	787	LEU	2.3
1	B	442	LEU	2.3
1	D	787	LEU	2.3
1	C	304	ARG	2.3
1	D	343	PHE	2.3
1	D	512	PRO	2.2
1	D	281	THR	2.2
1	B	295	LEU	2.2
1	A	786	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	306	GLY	2.2
1	A	703	LEU	2.2
1	A	37	PHE	2.2
1	A	619	ASN	2.2
1	C	231	ILE	2.2
1	C	432	ILE	2.2
1	C	69	ILE	2.2
1	A	607	PHE	2.1
1	C	241	PHE	2.1
1	B	621	ALA	2.1
1	B	618	ALA	2.1
1	B	799	LEU	2.1
1	D	792	VAL	2.1
1	C	652	SER	2.1
1	B	539	VAL	2.1
1	B	700	TYR	2.1
1	B	600	ILE	2.0
1	C	599	ARG	2.0
1	B	58	PHE	2.0
1	C	111	PRO	2.0
1	C	398	THR	2.0
1	B	367	ILE	2.0
1	D	803	LEU	2.0
1	D	544	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
5	FWF	B	903	32/32	0.95	0.50	1.45	51,110,130,159	0
3	NAG	C	901	14/15	0.82	0.45	1.35	120,137,162,180	0
5	FWF	D	903	32/32	0.96	0.42	0.90	11,61,114,151	0
3	NAG	D	901	14/15	0.76	0.33	0.61	137,181,523,523	0
3	NAG	A	901	14/15	0.94	0.31	0.16	77,91,112,129	0
4	FWD	B	902	15/15	0.98	0.38	-0.13	84,107,141,176	0
4	FWD	A	902	15/15	0.96	0.31	-0.57	69,102,169,175	0
4	FWD	C	902	15/15	0.97	0.31	-0.65	74,106,162,180	0
4	FWD	D	902	15/15	0.96	0.26	-1.37	40,76,109,148	0
3	NAG	B	901	14/15	0.78	0.37	-	117,222,245,247	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.