



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:42 pm BST

PDB ID : 2WJX  
Title : Crystal structure of the human ionotropic glutamate receptor GluR2 ATD region at 4.1 Å resolution  
Authors : Clayton, A.; Siebold, C.; Gilbert, R.J.C.; Sutton, G.C.; Harlos, K.; McIlhinney, R.A.J.; Jones, E.Y.; Aricescu, A.R.  
Deposited on : 2009-06-01  
Resolution : 4.10 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

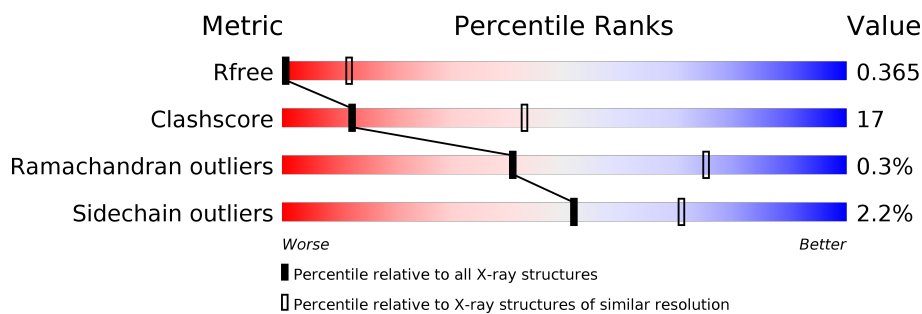
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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))
$R_{free}$	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)

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 respectively. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	388	67% 23% •• 6%
1	B	388	70% 22% • 6%
1	C	388	72% 19% •• 6%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8706 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.

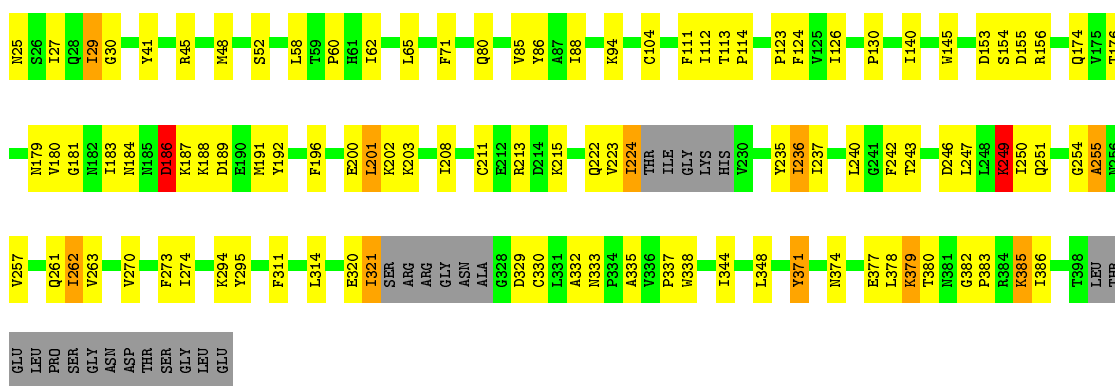
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	Total 2902	C 1852	N 489	O 551	S 10	0	0	0
1	B	363	Total 2902	C 1852	N 489	O 551	S 10	0	0	0
1	C	363	Total 2902	C 1852	N 489	O 551	S 10	0	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

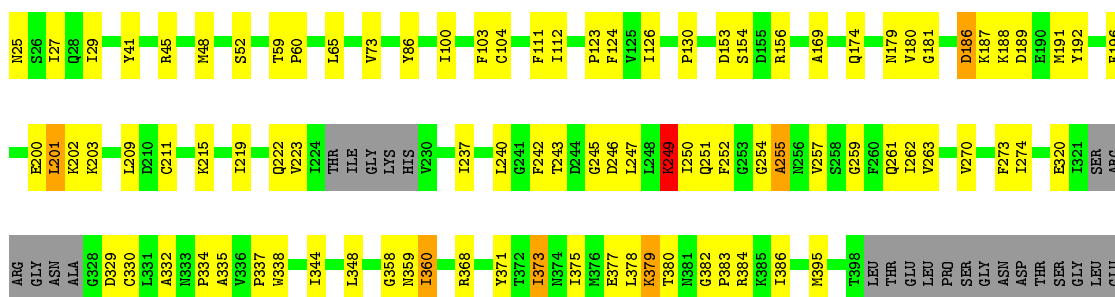
- Molecule 1: GLUTAMATE RECEPTOR 2

Chain A: 



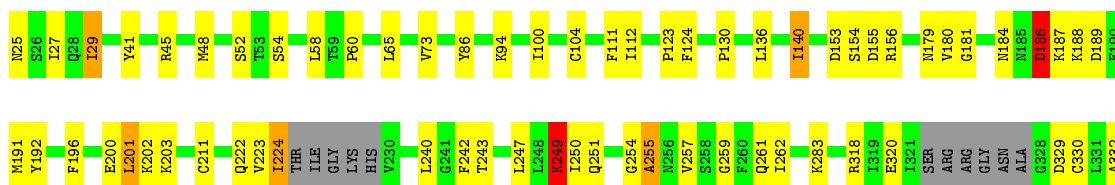
- Molecule 1: GLUTAMATE RECEPTOR 2

Chain B: 



- Molecule 1: GLUTAMATE RECEPTOR 2

Chain C: 



A335	V336	P337	W338	I344	G358	N359	I360	N370	Y371	N374	E377	L378	K379	T380	N381	G382	P383	R384	K385	I386	E391	T398	LEU	THR	GLU	LEU	LEU	PRO	SER	GLY	ASN	ASP	THR	SER	SER	GLY	LEU	GLU
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.25Å 224.25Å 76.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 4.10 48.38 – 4.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.38-4.10) 100.0 (48.38-4.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.82 (at 4.14Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.290 , 0.354 0.311 , 0.365	Depositor DCC
$R_{free}$ test set	802 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	152.3	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 195.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	215.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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

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	0.47	3/2961 (0.1%)	0.82	12/4003 (0.3%)
1	B	0.54	4/2961 (0.1%)	0.81	12/4003 (0.3%)
1	C	0.50	3/2961 (0.1%)	0.92	13/4003 (0.3%)
All	All	0.51	10/8883 (0.1%)	0.85	37/12009 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
All	All	0	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	ILE	C-N	12.84	1.63	1.34
1	C	249	LYS	C-N	-11.81	1.06	1.34
1	A	249	LYS	C-N	-11.79	1.06	1.34
1	B	249	LYS	C-N	-11.78	1.06	1.34
1	C	371	TYR	C-N	10.70	1.58	1.34
1	C	130	PRO	C-N	10.26	1.57	1.34
1	B	371	TYR	C-N	-9.08	1.13	1.34
1	A	385	LYS	C-N	7.43	1.51	1.34
1	B	263	VAL	C-N	-7.06	1.17	1.34
1	A	130	PRO	C-N	6.84	1.49	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ASP	CB-CG-OD2	-27.18	93.83	118.30
1	C	186	ASP	CB-CG-OD2	-27.09	93.92	118.30
1	A	186	ASP	CB-CG-OD2	-27.08	93.93	118.30
1	C	130	PRO	O-C-N	21.62	157.30	122.70
1	C	130	PRO	CA-C-N	-16.23	81.49	117.20
1	A	186	ASP	OD1-CG-OD2	-15.66	93.55	123.30
1	C	186	ASP	OD1-CG-OD2	-15.62	93.62	123.30
1	B	186	ASP	OD1-CG-OD2	-15.62	93.62	123.30
1	C	130	PRO	C-N-CA	-13.99	86.72	121.70
1	A	130	PRO	O-C-N	13.61	144.47	122.70
1	C	261	GLN	O-C-N	10.99	140.29	122.70
1	B	261	GLN	O-C-N	10.97	140.25	122.70
1	A	130	PRO	CA-C-N	-10.22	94.72	117.20
1	A	130	PRO	C-N-CA	-9.52	97.90	121.70
1	C	261	GLN	CA-C-N	-9.04	97.32	117.20
1	B	261	GLN	CA-C-N	-9.03	97.34	117.20
1	B	261	GLN	C-N-CA	-8.90	99.45	121.70
1	C	261	GLN	C-N-CA	-8.90	99.46	121.70
1	A	249	LYS	O-C-N	-8.51	109.09	122.70
1	C	249	LYS	O-C-N	-8.50	109.11	122.70
1	B	249	LYS	O-C-N	-8.48	109.12	122.70
1	A	261	GLN	O-C-N	7.36	134.48	122.70
1	B	384	ARG	O-C-N	-6.95	111.58	122.70
1	B	130	PRO	O-C-N	6.61	133.27	122.70
1	A	371	TYR	O-C-N	-6.30	112.62	122.70
1	C	379	LYS	CA-CB-CG	-5.91	100.39	113.40
1	A	379	LYS	CA-CB-CG	-5.91	100.40	113.40
1	B	379	LYS	CA-CB-CG	-5.91	100.40	113.40
1	A	249	LYS	CA-C-N	5.78	129.92	117.20
1	C	249	LYS	CA-C-N	5.78	129.91	117.20
1	B	249	LYS	CA-C-N	5.76	129.88	117.20
1	A	261	GLN	CA-C-N	-5.60	104.89	117.20
1	C	371	TYR	C-N-CA	-5.57	107.77	121.70
1	C	371	TYR	CA-C-N	-5.56	104.97	117.20
1	B	130	PRO	C-N-CA	-5.25	108.57	121.70
1	A	261	GLN	C-N-CA	-5.08	109.00	121.70
1	B	384	ARG	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	A	249	LYS	Peptide
1	A	371	TYR	Mainchain
1	B	186	ASP	Sidechain
1	B	249	LYS	Peptide
1	C	186	ASP	Sidechain
1	C	249	LYS	Peptide
1	C	371	TYR	Mainchain

## 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	2902	0	2852	134	1
1	B	2902	0	2849	89	8
1	C	2902	0	2852	81	9
All	All	8706	0	8553	292	11

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 17.

All (292) 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:A:249:LYS:O	1:A:250:ILE:HG12	1.22	1.34
1:B:249:LYS:O	1:B:250:ILE:HG13	1.16	1.28
1:C:249:LYS:O	1:C:250:ILE:HG13	1.16	1.25
1:A:224:ILE:HG13	1:C:224:ILE:CG1	1.69	1.22
1:A:224:ILE:CG1	1:C:224:ILE:HG13	1.69	1.21
1:A:208:ILE:HD13	1:A:236:ILE:HB	1.37	1.06
1:A:249:LYS:O	1:A:250:ILE:CG1	2.03	1.06
1:C:249:LYS:O	1:C:250:ILE:CG1	2.03	1.06
1:B:249:LYS:O	1:B:250:ILE:CG1	2.03	1.05
1:B:360:ILE:HD12	1:B:368:ARG:NH2	1.73	1.03
1:B:262:ILE:HG22	1:B:373:ILE:HD12	1.39	1.02
1:A:262:ILE:HD11	1:A:295:TYR:HB2	1.50	0.94
1:A:85:VAL:HG21	1:A:88:ILE:HD11	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:O	1:A:274:ILE:HD13	1.71	0.90
1:B:270:VAL:O	1:B:274:ILE:HD13	1.71	0.89
1:A:94:LYS:NZ	1:A:155:ASP:HA	1.88	0.88
1:A:94:LYS:CE	1:A:155:ASP:HA	2.06	0.86
1:A:314:LEU:CD1	1:A:344:ILE:HD13	2.06	0.85
1:A:208:ILE:CD1	1:A:236:ILE:HB	2.06	0.85
1:A:314:LEU:HD11	1:A:344:ILE:HD13	1.59	0.84
1:A:224:ILE:HG13	1:C:224:ILE:HG13	0.88	0.83
1:A:273:PHE:HD2	1:A:274:ILE:HD12	1.46	0.81
1:A:237:ILE:HD11	1:A:257:VAL:CG1	2.11	0.81
1:B:273:PHE:HD2	1:B:274:ILE:HD12	1.46	0.81
1:A:154:SER:HB3	1:A:179:ASN:HD21	1.46	0.80
1:B:154:SER:HB3	1:B:179:ASN:HD21	1.46	0.80
1:C:240:LEU:HD22	1:C:262:ILE:CG2	2.11	0.79
1:C:154:SER:HB3	1:C:179:ASN:HD21	1.46	0.79
1:A:254:GLY:O	1:A:255:ALA:CB	2.32	0.78
1:C:254:GLY:O	1:C:255:ALA:CB	2.32	0.77
1:B:254:GLY:O	1:B:255:ALA:CB	2.32	0.77
1:A:27:ILE:HG23	1:A:86:TYR:HD2	1.51	0.75
1:A:262:ILE:H	1:A:262:ILE:HD12	1.50	0.75
1:A:154:SER:HB3	1:A:179:ASN:ND2	2.02	0.74
1:B:27:ILE:HG23	1:B:86:TYR:HD2	1.52	0.74
1:A:262:ILE:HD13	1:A:263:VAL:N	2.02	0.74
1:C:27:ILE:HG23	1:C:86:TYR:HD2	1.52	0.74
1:A:224:ILE:CG1	1:C:224:ILE:CG1	2.46	0.73
1:B:154:SER:HB3	1:B:179:ASN:ND2	2.02	0.73
1:C:154:SER:HB3	1:C:179:ASN:ND2	2.02	0.73
1:B:262:ILE:HG22	1:B:373:ILE:CD1	2.18	0.72
1:B:73:VAL:HG11	1:B:100:ILE:HD11	1.69	0.72
1:C:73:VAL:HG11	1:C:100:ILE:HD11	1.69	0.72
1:A:262:ILE:HD11	1:A:295:TYR:CB	2.19	0.71
1:A:321:ILE:H	1:A:321:ILE:HD13	1.55	0.71
1:A:237:ILE:HD11	1:A:257:VAL:HG13	1.73	0.71
1:B:112:ILE:HD13	1:B:126:ILE:HB	1.72	0.70
1:B:358:GLY:O	1:B:360:ILE:HD13	1.90	0.70
1:A:112:ILE:HD13	1:A:126:ILE:CB	2.23	0.69
1:A:94:LYS:HE3	1:A:154:SER:O	1.93	0.69
1:C:377:GLU:HG3	1:C:386:ILE:HD13	1.73	0.69
1:A:311:PHE:CE1	1:A:344:ILE:HD12	2.27	0.69
1:A:112:ILE:HD13	1:A:126:ILE:HB	1.72	0.69
1:B:112:ILE:HD13	1:B:126:ILE:CB	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:NE2	1:B:174:GLN:NE2	2.40	0.68
1:C:240:LEU:HD22	1:C:262:ILE:HG23	1.74	0.67
1:A:176:THR:HG23	1:B:169:ALA:HB2	1.75	0.67
1:A:254:GLY:O	1:A:255:ALA:HB2	1.96	0.65
1:A:140:ILE:HD11	1:A:208:ILE:HD11	1.79	0.65
1:A:112:ILE:HD11	1:A:348:LEU:HD22	1.79	0.65
1:B:112:ILE:HD11	1:B:348:LEU:HD22	1.79	0.65
1:A:240:LEU:O	1:A:262:ILE:HD12	1.96	0.64
1:B:254:GLY:O	1:B:255:ALA:HB2	1.96	0.64
1:C:254:GLY:O	1:C:255:ALA:HB2	1.96	0.64
1:A:377:GLU:HG3	1:A:386:ILE:HD13	1.79	0.64
1:B:29:ILE:HD11	1:B:60:PRO:HB3	1.78	0.64
1:B:360:ILE:HD12	1:B:368:ARG:CZ	2.28	0.63
1:C:94:LYS:CE	1:C:155:ASP:HA	2.29	0.63
1:A:379:LYS:HG2	1:A:380:THR:N	2.14	0.63
1:B:379:LYS:HG2	1:B:380:THR:N	2.14	0.63
1:A:85:VAL:HG21	1:A:88:ILE:CD1	2.28	0.62
1:A:94:LYS:HE3	1:A:155:ASP:HA	1.80	0.62
1:C:180:VAL:O	1:C:180:VAL:HG12	2.00	0.62
1:B:180:VAL:O	1:B:180:VAL:HG12	2.00	0.61
1:A:237:ILE:N	1:A:237:ILE:HD12	2.14	0.61
1:C:379:LYS:HG2	1:C:380:THR:N	2.14	0.61
1:A:262:ILE:H	1:A:262:ILE:CD1	2.14	0.61
1:B:262:ILE:CG2	1:B:373:ILE:HD12	2.24	0.61
1:A:180:VAL:HG12	1:A:180:VAL:O	2.00	0.61
1:B:249:LYS:HG2	1:B:249:LYS:O	2.01	0.61
1:C:370:ASN:N	1:C:391:GLU:OE2	2.22	0.60
1:B:257:VAL:HG23	1:B:378:LEU:HD22	1.83	0.60
1:C:257:VAL:HG23	1:C:378:LEU:HD22	1.83	0.60
1:A:94:LYS:CD	1:A:154:SER:O	2.50	0.60
1:A:48:MET:SD	1:A:60:PRO:HG3	2.42	0.59
1:A:249:LYS:HG2	1:A:249:LYS:O	2.01	0.59
1:A:251:GLN:NE2	1:A:382:GLY:HA2	2.17	0.59
1:A:257:VAL:HG23	1:A:378:LEU:HD22	1.83	0.59
1:B:48:MET:SD	1:B:60:PRO:HG3	2.42	0.59
1:C:48:MET:SD	1:C:60:PRO:HG3	2.42	0.59
1:A:377:GLU:CG	1:A:386:ILE:HG21	2.32	0.59
1:B:251:GLN:NE2	1:B:382:GLY:HA2	2.17	0.59
1:C:249:LYS:O	1:C:249:LYS:HG2	2.01	0.59
1:C:251:GLN:NE2	1:C:382:GLY:HA2	2.17	0.59
1:B:240:LEU:HD22	1:B:262:ILE:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ILE:CD1	1:B:368:ARG:NH2	2.60	0.58
1:A:240:LEU:HD22	1:A:262:ILE:HG23	1.85	0.58
1:A:240:LEU:HD22	1:A:262:ILE:CG2	2.33	0.57
1:A:374:ASN:CG	1:A:385:LYS:HD2	2.25	0.57
1:C:240:LEU:HB3	1:C:262:ILE:HG23	1.87	0.57
1:C:377:GLU:CG	1:C:386:ILE:HG21	2.35	0.57
1:C:94:LYS:HE3	1:C:155:ASP:HA	1.87	0.57
1:B:377:GLU:HG3	1:B:386:ILE:HD13	1.87	0.56
1:A:174:GLN:NE2	1:B:174:GLN:HE21	2.02	0.56
1:A:377:GLU:HG3	1:A:386:ILE:HG21	1.88	0.56
1:C:224:ILE:C	1:C:224:ILE:HD13	2.27	0.55
1:A:224:ILE:C	1:A:224:ILE:HD13	2.27	0.55
1:A:29:ILE:HD13	1:A:29:ILE:H	1.71	0.55
1:C:29:ILE:H	1:C:29:ILE:HD13	1.71	0.55
1:A:262:ILE:HD13	1:A:263:VAL:H	1.71	0.55
1:A:213:ARG:HH22	1:A:294:LYS:NZ	2.04	0.55
1:A:154:SER:H	1:A:181:GLY:HA3	1.72	0.55
1:C:136:LEU:O	1:C:140:ILE:HD13	2.07	0.55
1:A:126:ILE:HD12	1:A:126:ILE:N	2.23	0.54
1:B:375:ILE:HD13	1:B:395:MET:CE	2.37	0.54
1:C:154:SER:H	1:C:181:GLY:HA3	1.73	0.54
1:B:154:SER:H	1:B:181:GLY:HA3	1.73	0.54
1:A:201:LEU:C	1:A:203:LYS:H	2.11	0.54
1:A:243:THR:HG22	1:A:383:PRO:HG3	1.90	0.53
1:C:243:THR:HG22	1:C:383:PRO:HG3	1.91	0.53
1:A:145:TRP:CH2	1:A:236:ILE:HD13	2.44	0.53
1:B:243:THR:HG22	1:B:383:PRO:HG3	1.91	0.53
1:C:192:TYR:HB3	1:C:222:GLN:HG2	1.91	0.53
1:A:174:GLN:HE22	1:B:174:GLN:NE2	2.06	0.53
1:A:62:ILE:HD12	1:A:62:ILE:N	2.24	0.53
1:A:192:TYR:HB3	1:A:222:GLN:HG2	1.91	0.53
1:A:94:LYS:CE	1:A:154:SER:O	2.57	0.53
1:B:192:TYR:HB3	1:B:222:GLN:HG2	1.91	0.53
1:A:180:VAL:CG1	1:A:183:ILE:HD11	2.39	0.52
1:C:377:GLU:HG3	1:C:386:ILE:HG21	1.90	0.52
1:B:187:LYS:H	1:B:187:LYS:HD2	1.74	0.52
1:A:174:GLN:HE22	1:B:174:GLN:HE21	1.57	0.52
1:C:201:LEU:C	1:C:203:LYS:H	2.11	0.52
1:B:377:GLU:HG3	1:B:386:ILE:HG21	1.92	0.52
1:C:187:LYS:H	1:C:187:LYS:HD2	1.74	0.52
1:A:187:LYS:H	1:A:187:LYS:HD2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:C	1:B:203:LYS:H	2.11	0.51
1:A:262:ILE:N	1:A:262:ILE:CD1	2.72	0.51
1:A:262:ILE:HD13	1:A:263:VAL:HG23	1.91	0.51
1:A:377:GLU:CG	1:A:386:ILE:HD13	2.41	0.51
1:C:112:ILE:N	1:C:112:ILE:HD12	2.26	0.51
1:C:257:VAL:CG2	1:C:378:LEU:HD22	2.41	0.51
1:A:257:VAL:CG2	1:A:378:LEU:HD22	2.41	0.51
1:C:196:PHE:O	1:C:200:GLU:HB2	2.11	0.51
1:B:196:PHE:O	1:B:200:GLU:HB2	2.12	0.50
1:A:314:LEU:CD1	1:A:344:ILE:CD1	2.86	0.50
1:A:196:PHE:O	1:A:200:GLU:HB2	2.11	0.50
1:A:201:LEU:HD12	1:A:201:LEU:C	2.32	0.50
1:C:377:GLU:CG	1:C:386:ILE:HD13	2.39	0.50
1:B:201:LEU:C	1:B:201:LEU:HD12	2.32	0.50
1:B:257:VAL:CG2	1:B:378:LEU:HD22	2.41	0.50
1:B:273:PHE:CD2	1:B:274:ILE:HD12	2.36	0.50
1:A:273:PHE:CD2	1:A:274:ILE:HD12	2.36	0.50
1:A:27:ILE:N	1:A:27:ILE:HD12	2.27	0.50
1:A:321:ILE:HD13	1:A:321:ILE:N	2.24	0.49
1:A:224:ILE:O	1:A:224:ILE:HD13	2.12	0.49
1:C:29:ILE:HD12	1:C:58:LEU:HB3	1.94	0.49
1:A:29:ILE:HD12	1:A:58:LEU:HB3	1.94	0.49
1:C:201:LEU:HD12	1:C:201:LEU:C	2.32	0.49
1:A:140:ILE:CD1	1:A:208:ILE:HD11	2.42	0.49
1:B:359:ASN:C	1:B:360:ILE:HD13	2.32	0.49
1:C:224:ILE:O	1:C:224:ILE:HD13	2.12	0.49
1:A:80:GLN:HB3	1:A:88:ILE:HD11	1.95	0.49
1:A:94:LYS:HZ2	1:A:155:ASP:HA	1.76	0.49
1:A:154:SER:OG	1:A:181:GLY:HA3	2.12	0.49
1:A:65:LEU:HD23	1:A:65:LEU:N	2.28	0.48
1:C:154:SER:OG	1:C:181:GLY:HA3	2.12	0.48
1:B:65:LEU:HD23	1:B:65:LEU:N	2.28	0.48
1:A:237:ILE:H	1:A:237:ILE:HD12	1.78	0.48
1:B:196:PHE:CE1	1:B:223:VAL:HG22	2.49	0.48
1:B:192:TYR:CE1	1:B:219:ILE:HD13	2.49	0.48
1:B:240:LEU:HD22	1:B:262:ILE:HG23	1.94	0.48
1:C:27:ILE:HG23	1:C:86:TYR:CD2	2.41	0.48
1:B:154:SER:OG	1:B:181:GLY:HA3	2.13	0.48
1:A:237:ILE:HD13	1:A:242:PHE:HE1	1.77	0.48
1:C:196:PHE:CE1	1:C:223:VAL:HG22	2.49	0.47
1:C:254:GLY:O	1:C:255:ALA:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LEU:N	1:C:65:LEU:HD23	2.28	0.47
1:A:30:GLY:HA3	1:A:88:ILE:CD1	2.44	0.47
1:A:86:TYR:HD1	1:A:338:TRP:CH2	2.32	0.47
1:B:180:VAL:HG11	1:B:219:ILE:HD11	1.96	0.47
1:B:254:GLY:O	1:B:255:ALA:HB3	2.13	0.47
1:C:86:TYR:HD1	1:C:338:TRP:CH2	2.32	0.47
1:A:183:ILE:HD12	1:A:215:LYS:HD2	1.96	0.47
1:B:86:TYR:HD1	1:B:338:TRP:CH2	2.33	0.47
1:A:187:LYS:O	1:A:191:MET:HG3	2.15	0.47
1:B:154:SER:HB3	1:B:179:ASN:CG	2.35	0.47
1:A:154:SER:HB3	1:A:179:ASN:CG	2.35	0.47
1:B:41:TYR:CE2	1:B:45:ARG:HD2	2.50	0.47
1:B:240:LEU:HB3	1:B:262:ILE:HG23	1.97	0.47
1:C:188:LYS:HD3	1:C:189:ASP:N	2.31	0.47
1:A:377:GLU:OE2	1:A:386:ILE:HD13	2.14	0.46
1:C:187:LYS:O	1:C:191:MET:HG3	2.15	0.46
1:A:196:PHE:CE1	1:A:223:VAL:HG22	2.49	0.46
1:C:154:SER:HB3	1:C:179:ASN:CG	2.35	0.46
1:C:374:ASN:CG	1:C:385:LYS:HD2	2.35	0.46
1:A:41:TYR:CE2	1:A:45:ARG:HD2	2.50	0.46
1:B:188:LYS:HG2	1:B:192:TYR:CE2	2.51	0.46
1:B:73:VAL:HG11	1:B:100:ILE:CD1	2.43	0.46
1:A:188:LYS:HD3	1:A:189:ASP:N	2.30	0.46
1:B:188:LYS:HD3	1:B:189:ASP:N	2.30	0.46
1:B:377:GLU:CG	1:B:386:ILE:HG21	2.46	0.46
1:C:188:LYS:HG2	1:C:192:TYR:CE2	2.51	0.46
1:A:188:LYS:HG2	1:A:192:TYR:CE2	2.51	0.46
1:C:41:TYR:CE2	1:C:45:ARG:HD2	2.50	0.46
1:B:209:LEU:HD12	1:B:237:ILE:CD1	2.45	0.45
1:B:187:LYS:O	1:B:191:MET:HG3	2.15	0.45
1:C:73:VAL:HG11	1:C:100:ILE:CD1	2.43	0.45
1:B:187:LYS:N	1:B:187:LYS:HD2	2.32	0.45
1:C:187:LYS:N	1:C:187:LYS:HD2	2.32	0.45
1:A:140:ILE:HD11	1:A:208:ILE:CD1	2.46	0.45
1:A:187:LYS:N	1:A:187:LYS:HD2	2.32	0.44
1:A:180:VAL:HG12	1:A:183:ILE:HD11	1.98	0.44
1:C:335:ALA:O	1:C:337:PRO:HD3	2.18	0.44
1:A:176:THR:HG23	1:B:169:ALA:CB	2.43	0.44
1:A:237:ILE:CD1	1:A:257:VAL:CG1	2.90	0.44
1:A:335:ALA:O	1:A:337:PRO:HD3	2.18	0.44
1:B:100:ILE:N	1:B:100:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LYS:CG	1:A:380:THR:N	2.81	0.44
1:C:379:LYS:CG	1:C:380:THR:N	2.81	0.44
1:A:236:ILE:N	1:A:236:ILE:CD1	2.81	0.44
1:B:335:ALA:O	1:B:337:PRO:HD3	2.17	0.43
1:A:246:ASP:O	1:A:247:LEU:C	2.56	0.43
1:A:311:PHE:CE1	1:A:344:ILE:CD1	2.98	0.43
1:A:48:MET:O	1:A:52:SER:HB3	2.18	0.43
1:B:153:ASP:HB3	1:B:156:ARG:HB2	2.00	0.43
1:B:360:ILE:N	1:B:360:ILE:HD13	2.33	0.43
1:B:48:MET:O	1:B:52:SER:HB3	2.18	0.43
1:C:153:ASP:HB3	1:C:156:ARG:HB2	2.00	0.43
1:B:123:PRO:O	1:B:124:PHE:HB2	2.18	0.43
1:B:246:ASP:O	1:B:247:LEU:C	2.56	0.43
1:A:224:ILE:CG1	1:C:224:ILE:HG12	2.45	0.43
1:A:254:GLY:O	1:A:255:ALA:HB3	2.13	0.43
1:C:100:ILE:HD12	1:C:100:ILE:N	2.33	0.43
1:C:48:MET:O	1:C:52:SER:HB3	2.18	0.43
1:B:249:LYS:O	1:B:250:ILE:CB	2.55	0.43
1:A:377:GLU:HG3	1:A:386:ILE:CG2	2.48	0.43
1:A:153:ASP:HB3	1:A:156:ARG:HB2	2.00	0.43
1:B:27:ILE:HG23	1:B:86:TYR:CD2	2.41	0.43
1:C:123:PRO:O	1:C:124:PHE:HB2	2.18	0.43
1:B:379:LYS:CG	1:B:380:THR:N	2.81	0.43
1:A:123:PRO:O	1:A:124:PHE:HB2	2.18	0.42
1:B:104:CYS:SG	1:B:111:PHE:HB2	2.59	0.42
1:B:154:SER:HB3	1:B:179:ASN:OD1	2.19	0.42
1:A:235:TYR:O	1:A:236:ILE:HD12	2.19	0.42
1:B:338:TRP:CH2	1:B:344:ILE:HD12	2.54	0.42
1:C:140:ILE:N	1:C:140:ILE:CD1	2.82	0.42
1:C:242:PHE:CD1	1:C:259:GLY:HA3	2.54	0.42
1:A:104:CYS:SG	1:A:111:PHE:HB2	2.59	0.42
1:A:213:ARG:HH22	1:A:294:LYS:HZ2	1.65	0.42
1:A:329:ASP:HB3	1:A:332:ALA:HB2	2.02	0.42
1:A:29:ILE:HD13	1:A:29:ILE:N	2.34	0.42
1:C:154:SER:HB3	1:C:179:ASN:OD1	2.19	0.42
1:B:65:LEU:HD23	1:B:65:LEU:H	1.85	0.42
1:C:104:CYS:SG	1:C:111:PHE:HB2	2.59	0.42
1:A:270:VAL:O	1:A:274:ILE:CD1	2.56	0.42
1:B:215:LYS:HB2	1:B:215:LYS:HE2	1.86	0.42
1:B:329:ASP:HB3	1:B:332:ALA:HB2	2.02	0.42
1:C:184:ASN:C	1:C:186:ASP:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:N	1:C:29:ILE:HD13	2.34	0.42
1:A:154:SER:HB3	1:A:179:ASN:OD1	2.19	0.42
1:B:242:PHE:CD1	1:B:259:GLY:HA3	2.54	0.42
1:A:62:ILE:HD12	1:A:62:ILE:H	1.84	0.42
1:A:94:LYS:HZ1	1:A:155:ASP:HA	1.77	0.42
1:B:180:VAL:O	1:B:180:VAL:CG1	2.68	0.42
1:A:184:ASN:C	1:A:186:ASP:N	2.73	0.41
1:A:27:ILE:HG23	1:A:86:TYR:CD2	2.41	0.41
1:A:71:PHE:HD1	1:B:103:PHE:CD2	2.38	0.41
1:B:112:ILE:HD13	1:B:126:ILE:HG13	2.02	0.41
1:C:398:THR:O	1:C:398:THR:HG22	2.19	0.41
1:A:113:THR:HA	1:A:114:PRO:HD3	1.88	0.41
1:A:202:LYS:HG2	1:A:202:LYS:O	2.20	0.41
1:A:153:ASP:HB2	1:A:211:CYS:HA	2.03	0.41
1:C:338:TRP:CH2	1:C:344:ILE:HD12	2.55	0.41
1:A:237:ILE:CD1	1:A:257:VAL:HG12	2.50	0.41
1:C:153:ASP:HB2	1:C:211:CYS:HA	2.03	0.41
1:C:65:LEU:H	1:C:65:LEU:HD23	1.84	0.41
1:C:180:VAL:O	1:C:180:VAL:CG1	2.68	0.41
1:C:202:LYS:O	1:C:202:LYS:HG2	2.20	0.41
1:C:329:ASP:HB3	1:C:332:ALA:HB2	2.02	0.41
1:A:112:ILE:HD13	1:A:126:ILE:CG1	2.51	0.41
1:A:30:GLY:HA3	1:A:88:ILE:HD13	2.02	0.41
1:C:100:ILE:HD12	1:C:100:ILE:H	1.86	0.41
1:B:153:ASP:HB2	1:B:211:CYS:HA	2.03	0.41
1:B:202:LYS:O	1:B:202:LYS:HG2	2.20	0.41
1:B:29:ILE:C	1:B:29:ILE:HD12	2.42	0.40
1:C:201:LEU:C	1:C:203:LYS:N	2.75	0.40
1:A:201:LEU:C	1:A:203:LYS:N	2.75	0.40
1:C:242:PHE:O	1:C:247:LEU:HD23	2.21	0.40
1:C:358:GLY:O	1:C:360:ILE:HD12	2.21	0.40
1:C:377:GLU:HB2	1:C:386:ILE:CG2	2.51	0.40
1:B:112:ILE:HD13	1:B:126:ILE:CG1	2.51	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:SER:CB	1:C:318:ARG:NH2[8_554]	1.28	0.92
1:B:245:GLY:CA	1:C:283:LYS:NZ[3_444]	1.37	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLY:C	1:C:283:LYS:NZ[3_444]	1.48	0.72
1:C:54:SER:OG	1:C:318:ARG:NH2[8_554]	1.73	0.47
1:B:245:GLY:O	1:C:283:LYS:CE[3_444]	1.74	0.46
1:B:245:GLY:C	1:C:283:LYS:CE[3_444]	1.84	0.36
1:B:59:THR:CG2	1:B:334:PRO:CG[3_444]	1.87	0.33
1:B:252:PHE:CZ	1:C:48:MET:CE[3_444]	2.00	0.20
1:B:252:PHE:CE2	1:C:48:MET:CE[3_444]	2.05	0.15
1:B:246:ASP:N	1:C:283:LYS:NZ[3_444]	2.08	0.12
1:A:60:PRO:O	1:A:333:ASN:O[4_545]	2.13	0.07

### 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	357/388 (92%)	336 (94%)	20 (6%)	1 (0%)	41 75
1	B	357/388 (92%)	336 (94%)	20 (6%)	1 (0%)	41 75
1	C	357/388 (92%)	335 (94%)	21 (6%)	1 (0%)	41 75
All	All	1071/1164 (92%)	1007 (94%)	61 (6%)	3 (0%)	41 75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ALA
1	B	255	ALA
1	C	255	ALA

#### 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	316/336 (94%)	307 (97%)	9 (3%)	43	65
1	B	316/336 (94%)	311 (98%)	5 (2%)	62	78
1	C	316/336 (94%)	309 (98%)	7 (2%)	52	71
All	All	948/1008 (94%)	927 (98%)	21 (2%)	52	71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	29	ILE
1	A	201	LEU
1	A	224	ILE
1	A	236	ILE
1	A	262	ILE
1	A	320	GLU
1	A	321	ILE
1	A	330	CYS
1	B	25	ASN
1	B	201	LEU
1	B	320	GLU
1	B	330	CYS
1	B	360	ILE
1	C	25	ASN
1	C	29	ILE
1	C	140	ILE
1	C	201	LEU
1	C	224	ILE
1	C	320	GLU
1	C	330	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	251	GLN
1	B	174	GLN
1	B	251	GLN
1	C	25	ASN

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Mol	Chain	Res	Type
1	C	251	GLN

### 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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	373:ILE	C	374:ASN	N	1.63
1	B	263:VAL	C	264:ASP	N	1.17
1	B	371:TYR	C	372:THR	N	1.13
1	B	249:LYS	C	250:ILE	N	1.07

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	249:LYS	C	250:ILE	N	1.06
1	C	249:LYS	C	250:ILE	N	1.06

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.