



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2016 – 11:14 AM EDT

PDB ID : 5B3J  
Title : Activation of NMDA receptors and the mechanism of inhibition by ifenprodil  
Authors : Tajima, N.; Karakas, E.; Grant, T.; Simorowski, N.; Diaz-Avalos, R.; Grigorieff, N.; Furukawa, H.  
Deposited on : 2016-03-01  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
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) : rb-20027674

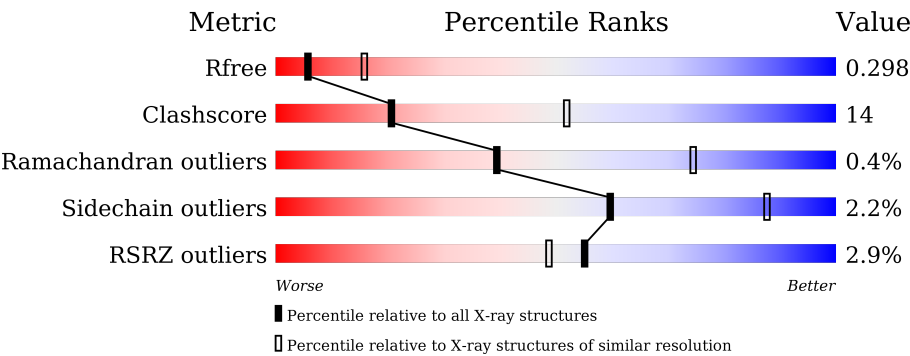
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	383	<div><div>2%</div><div><div></div><div>64%</div><div>25%</div><div>•</div><div>9%</div></div></div>
1	B	383	<div><div>4%</div><div><div></div><div>64%</div><div>23%</div><div>•</div><div>12%</div></div></div>
2	C	364	<div><div>3%</div><div><div></div><div>65%</div><div>26%</div><div>•</div><div>8%</div></div></div>
2	D	364	<div><div>6%</div><div><div></div><div>66%</div><div>23%</div><div>•</div><div>10%</div></div></div>
3	E	224	<div><div>%</div><div><div></div><div>74%</div><div>20%</div><div>•</div><div>•</div></div></div>
3	H	224	<div><div>%</div><div><div></div><div>71%</div><div>23%</div><div>•</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
4	F	213	
4	L	213	

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
5	NA	B	501	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15954 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 NMDA glutamate receptor subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2491	1595	422	464	10			
1	B	338	Total	C	N	O	S	0	0	0
			2370	1516	396	448	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP Q91977
A	371	GLN	ASN	engineered mutation	UNP Q91977
B	61	GLN	ASN	engineered mutation	UNP Q91977
B	371	GLN	ASN	engineered mutation	UNP Q91977

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	335	Total	C	N	O	S	0	2	0
			2390	1536	390	450	14			
2	D	329	Total	C	N	O	S	0	0	0
			2315	1477	386	439	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- Molecule 3 is a protein called Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	215	Total	C	N	O	S	0	0	0
			1536	976	252	300	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1551	983	254	306	8			

- Molecule 4 is a protein called Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	211	Total	C	N	O	S	0	0	0
			1595	1001	269	319	6			
4	L	212	Total	C	N	O	S	0	0	0
			1598	1007	267	318	6			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

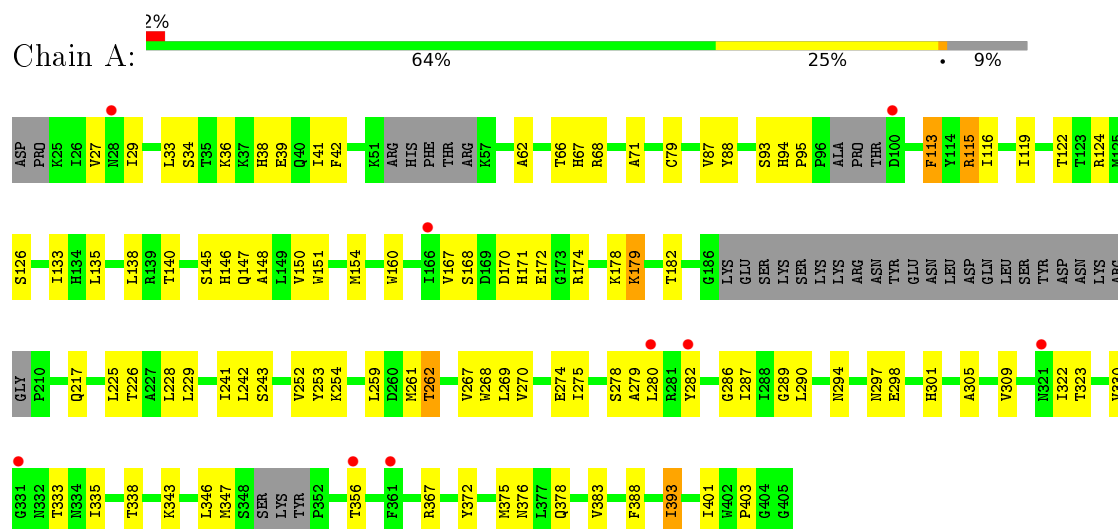
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	8	Total	O	0	0
			8	8		
6	C	11	Total	O	0	0
			11	11		
6	E	10	Total	O	0	0
			10	10		
6	D	10	Total	O	0	0
			10	10		
6	F	16	Total	O	0	0
			16	16		
6	H	21	Total	O	0	0
			21	21		
6	L	18	Total	O	0	0
			18	18		

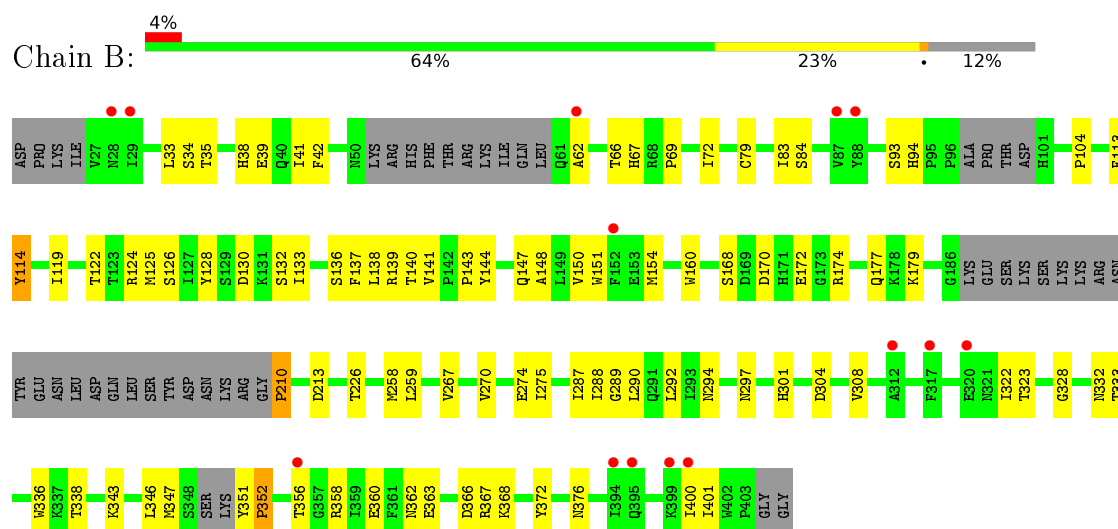
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: NMDA glutamate receptor subunit

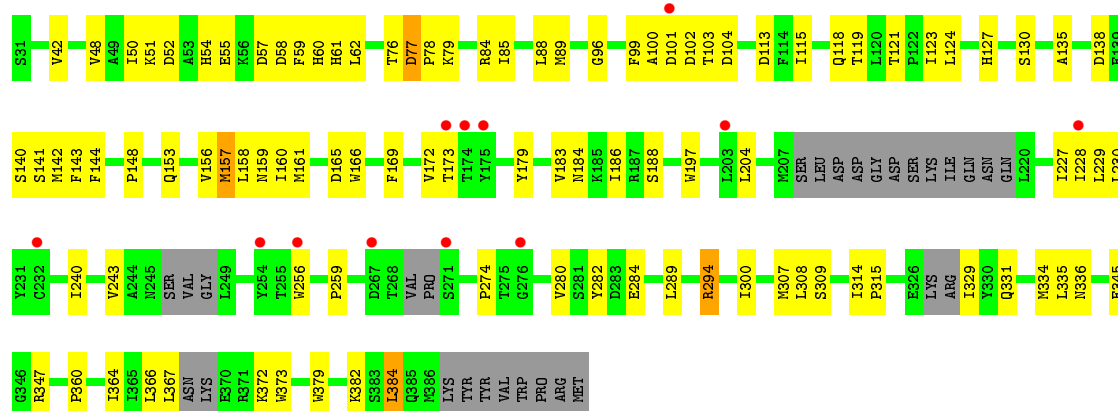


#### • Molecule 1: NMDA glutamate receptor subunit

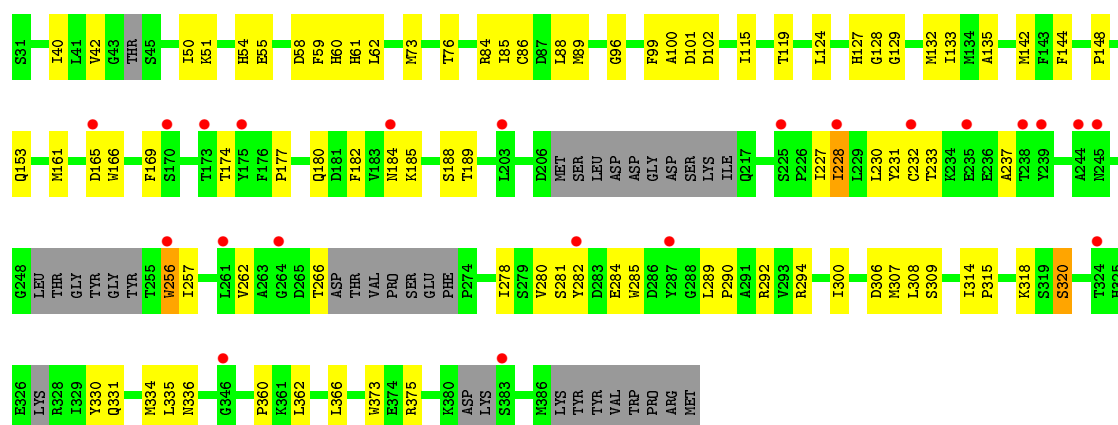


#### • Molecule 2: Glutamate receptor ionotropic, NMDA 2B

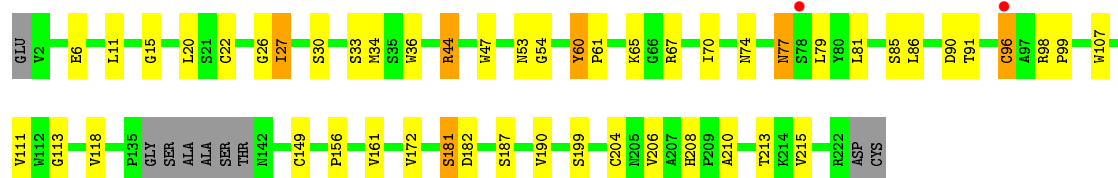
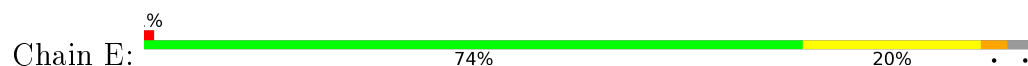




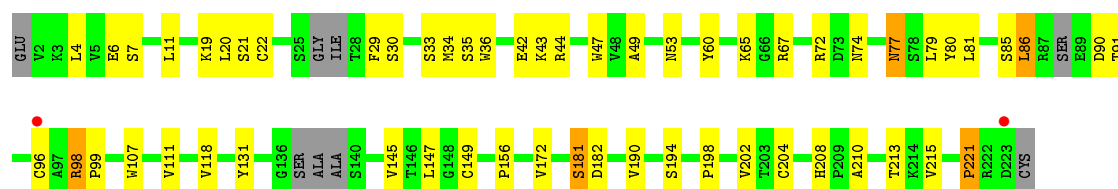
- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



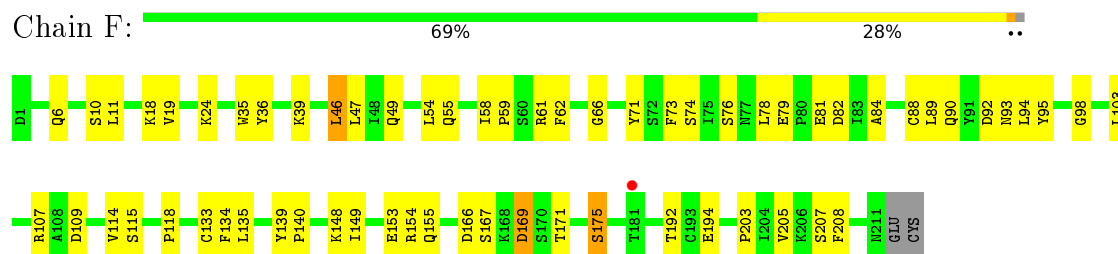
- Molecule 3: Fab, heavy chain



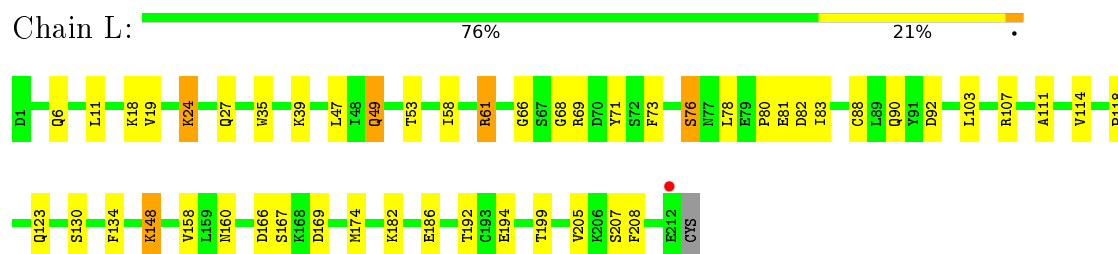
- Molecule 3: Fab, heavy chain



- Molecule 4: Fab, light chain



- Molecule 4: Fab, light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	247.25Å 79.90Å 181.31Å 90.00° 127.09° 90.00°	Depositor
Resolution (Å)	29.93 – 2.90 47.80 – 2.78	Depositor EDS
% Data completeness (in resolution range)	84.1 (29.93-2.90) 77.5 (47.80-2.78)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.273 , 0.302 0.275 , 0.298	Depositor DCC
$R_{free}$ test set	2565 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	15954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.79 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.3533e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.35	0/2539	0.59	2/3470 (0.1%)
1	B	0.43	1/2417 (0.0%)	0.58	0/3317
2	C	0.37	0/2440	0.63	2/3340 (0.1%)
2	D	0.42	2/2361 (0.1%)	0.64	2/3228 (0.1%)
3	E	0.33	0/1580	0.60	1/2175 (0.0%)
3	H	0.39	0/1593	0.67	1/2189 (0.0%)
4	F	0.47	0/1633	0.63	0/2225
4	L	0.36	0/1636	0.62	2/2230 (0.1%)
All	All	0.39	3/16199 (0.0%)	0.62	10/22174 (0.0%)

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
3	E	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	PRO	N-CD	-12.50	1.30	1.47
2	D	256	TRP	CB-CG	6.59	1.62	1.50
2	D	228	ILE	CG1-CD1	-5.60	1.11	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	148	LYS	CD-CE-NZ	-7.57	94.30	111.70
2	C	384	LEU	CB-CG-CD2	-7.38	98.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	228	ILE	CA-CB-CG1	-7.22	97.28	111.00
3	H	149	CYS	CA-CB-SG	6.46	125.62	114.00
3	E	149	CYS	CA-CB-SG	6.33	125.39	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	26	GLY	Peptide
3	E	27	ILE	Peptide

## 5.2 Too-close contacts

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	2491	0	2330	84	0
1	B	2370	0	2148	73	0
2	C	2390	0	2148	74	0
2	D	2315	0	2025	73	0
3	E	1536	0	1399	34	0
3	H	1551	0	1417	41	0
4	F	1595	0	1485	43	0
4	L	1598	0	1499	34	0
5	B	1	0	0	0	0
6	A	13	0	0	1	0
6	B	8	0	0	1	0
6	C	11	0	0	0	0
6	D	10	0	0	1	0
6	E	10	0	0	0	0
6	F	16	0	0	0	0
6	H	21	0	0	0	0
6	L	18	0	0	0	0
All	All	15954	0	14451	438	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 14.

The worst 5 of 438 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)
2:D:228:ILE:HD11	2:D:256:TRP:HA	1.47	0.93
1:B:210:PRO:HA	1:B:213:ASP:OD1	1.74	0.88
1:A:333:THR:HG1	2:C:76:THR:HG1	1.21	0.87
1:A:138:LEU:HD11	1:A:343:LYS:HG3	1.58	0.85
3:E:34:MET:HG2	3:E:98:ARG:HB2	1.59	0.84

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	337/383 (88%)	312 (93%)	25 (7%)	0	100	100
1	B	328/383 (86%)	307 (94%)	18 (6%)	3 (1%)	21	57
2	C	325/364 (89%)	294 (90%)	31 (10%)	0	100	100
2	D	315/364 (86%)	291 (92%)	24 (8%)	0	100	100
3	E	211/224 (94%)	194 (92%)	15 (7%)	2 (1%)	21	57
3	H	208/224 (93%)	192 (92%)	12 (6%)	4 (2%)	10	35
4	F	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
4	L	210/213 (99%)	198 (94%)	12 (6%)	0	100	100
All	All	2143/2368 (90%)	1986 (93%)	148 (7%)	9 (0%)	39	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	TYR
3	H	43	LYS
3	E	181	SER
3	H	181	SER

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Mol	Chain	Res	Type
3	H	221	PRO

### 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	238/329 (72%)	232 (98%)	6 (2%)	55	85
1	B	219/329 (67%)	218 (100%)	1 (0%)	92	98
2	C	227/327 (69%)	224 (99%)	3 (1%)	76	94
2	D	213/327 (65%)	209 (98%)	4 (2%)	65	89
3	E	159/191 (83%)	153 (96%)	6 (4%)	40	76
3	H	163/191 (85%)	160 (98%)	3 (2%)	66	90
4	F	171/190 (90%)	165 (96%)	6 (4%)	43	78
4	L	172/190 (90%)	167 (97%)	5 (3%)	50	83
All	All	1562/2074 (75%)	1528 (98%)	34 (2%)	60	88

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	204	CYS
2	D	330	TYR
4	L	76	SER
2	D	306	ASP
1	B	136	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	90	GLN
4	F	155	GLN
4	L	49	GLN
4	F	6	GLN

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Mol	Chain	Res	Type
4	L	6	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	347/383 (90%)	0.32	9 (2%) 59 54	36, 48, 68, 88	0
1	B	338/383 (88%)	0.35	14 (4%) 41 34	38, 53, 72, 86	0
2	C	335/364 (92%)	0.39	12 (3%) 46 38	27, 48, 79, 123	0
2	D	329/364 (90%)	0.50	22 (6%) 21 15	28, 53, 92, 140	0
3	E	215/224 (95%)	0.13	2 (0%) 85 84	27, 42, 58, 69	0
3	H	216/224 (96%)	0.21	2 (0%) 85 84	28, 40, 52, 66	0
4	F	211/213 (99%)	0.01	1 (0%) 91 90	23, 32, 50, 67	0
4	L	212/213 (99%)	0.09	1 (0%) 91 90	24, 32, 47, 82	0
All	All	2203/2368 (93%)	0.28	63 (2%) 55 49	23, 45, 74, 140	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	239	TYR	7.6
1	B	87	VAL	4.5
2	D	244	ALA	4.0
2	D	245	ASN	3.8
2	D	264	GLY	3.5

### 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	NA	B	501	1/1	0.85	0.49	13.90	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.