



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2019 – 08:56 AM EST

PDB ID : 6N4I  
Title : Structural basis of Nav1.7 inhibition by a gating-modifier spider toxin  
Authors : Xu, H.; Koth, C.M.; Payandeh, J.  
Deposited on : 2018-11-19  
Resolution : 3.54 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

<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  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

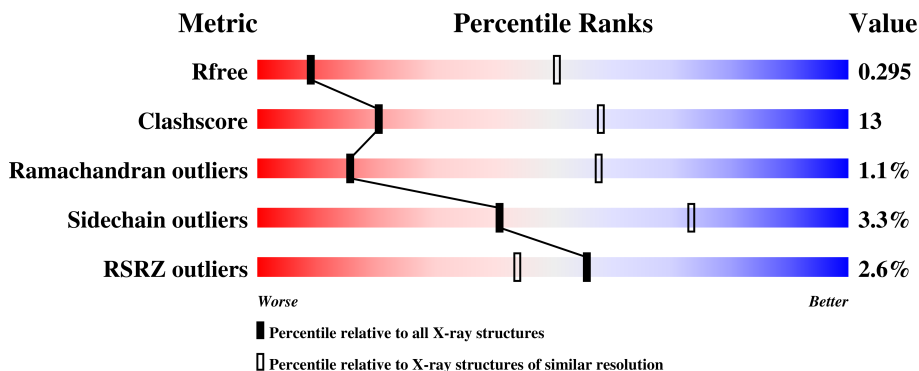
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.54 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))
$R_{free}$	111664	1023 (3.64-3.44)
Clashscore	122126	1049 (3.62-3.46)
Ramachandran outliers	120053	1016 (3.62-3.46)
Sidechain outliers	120020	1017 (3.62-3.46)
RSRZ outliers	108989	1036 (3.66-3.42)

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	288	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>25%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	288	<div> <div></div> <div>52%</div> <div>25%</div> <div>•</div> <div>22%</div> </div>
1	C	288	<div> <div></div> <div>61%</div> <div>16%</div> <div>•</div> <div>22%</div> </div>
1	D	288	<div> <div>%</div> <div>56%</div> <div>20%</div> <div>•</div> <div>22%</div> </div>
2	E	30	<div> <div>13%</div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	30	
2	G	30	
2	H	30	

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	6OU	D	1005	-	-	-	X
3	6OU	E	101	-	-	-	X
3	6OU	G	101	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8629 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.

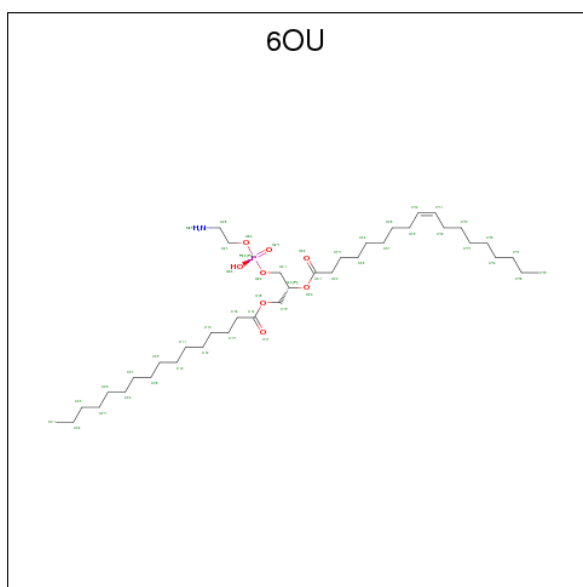
- Molecule 1 is a protein called Nav1.7 VSD2-NavAb channel chimera protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1823	1238	273	299	13			
1	B	225	Total	C	N	O	S	0	0	0
			1819	1235	272	299	13			
1	C	226	Total	C	N	O	S	0	0	0
			1818	1235	270	300	13			
1	D	225	Total	C	N	O	S	0	0	0
			1808	1229	269	297	13			

- Molecule 2 is a protein called Beta/omega-theraphotoxin-Tp2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	30	Total	C	N	O	S	0	0	0
			262	168	46	40	8			
2	F	30	Total	C	N	O	S	0	0	0
			262	168	46	40	8			
2	G	30	Total	C	N	O	S	0	0	0
			258	165	45	40	8			
2	H	30	Total	C	N	O	S	0	0	0
			262	168	46	40	8			

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ( {Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 24	C 15	O 8	P 1	0	0	
3	A	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	A	1	Total 16	C 7	N 1	O 7	P 1	0	0
3	B	1	Total 24	C 15	O 8	P 1	0	0	
3	B	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	B	1	Total 18	C 9	N 1	O 7	P 1	0	0
3	C	1	Total 24	C 15	O 8	P 1	0	0	
3	C	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	D	1	Total 24	C 15	O 8	P 1	0	0	
3	D	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	D	1	Total 14	C 6	N 1	O 6	P 1	0	0
3	D	1	Total 17	C 8	N 1	O 7	P 1	0	0
3	D	1	Total 11	C 5	N 1	O 4	P 1	0	0
3	E	1	Total 13	C 6	O 6	P 1	0	0	

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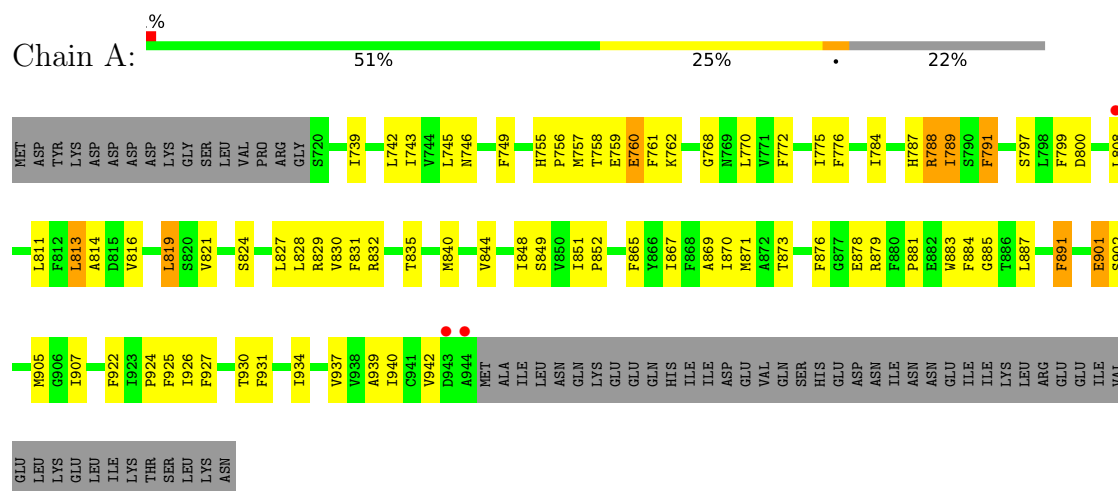
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			9	3	1	4	1		
3	G	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

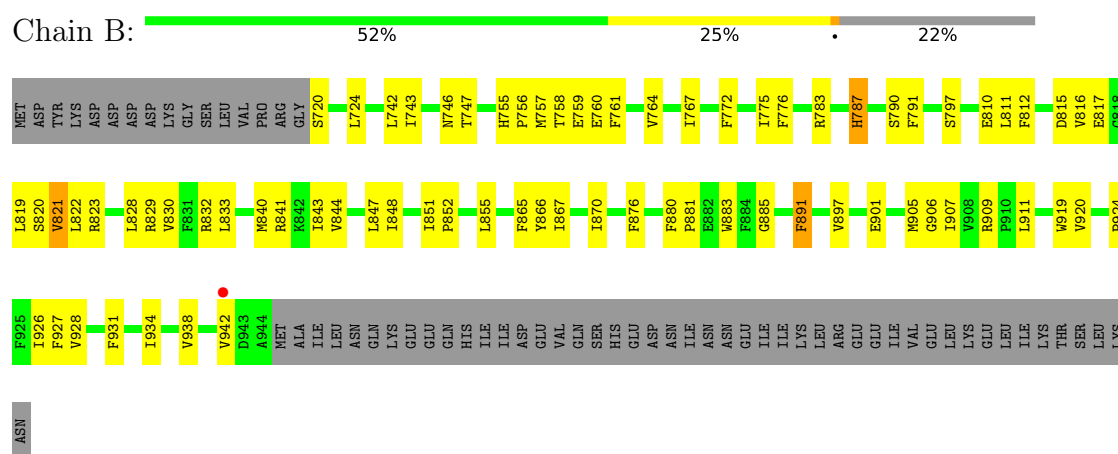
### 3 Residue-property plots

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 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.

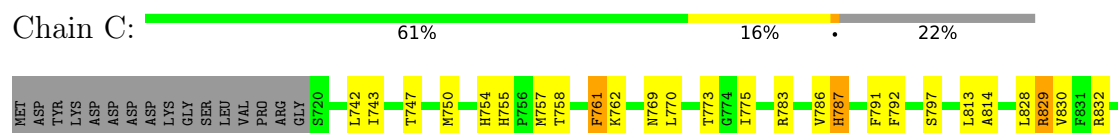
- Molecule 1: Nav1.7 VSD2-NavAb channel chimera protein

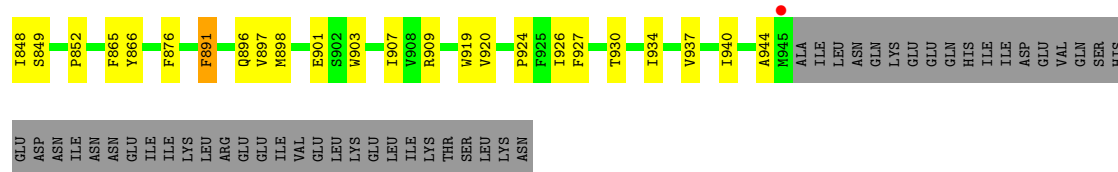


- Molecule 1: Nav1.7 VSD2-NavAb channel chimera protein

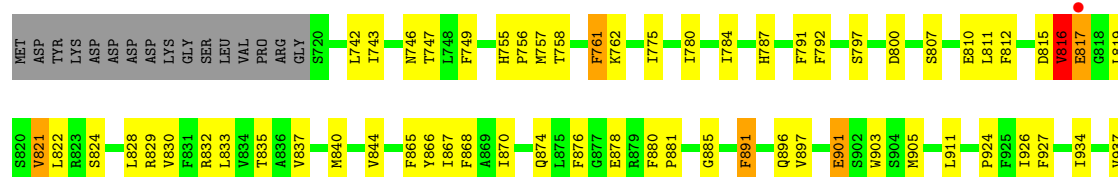


- Molecule 1: Nav1.7 VSD2-NavAb channel chimera protein

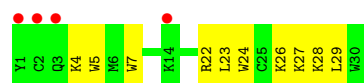




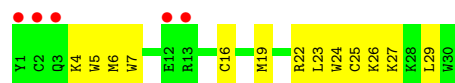
- Molecule 1: Nav1.7 VSD2-NavAb channel chimera protein



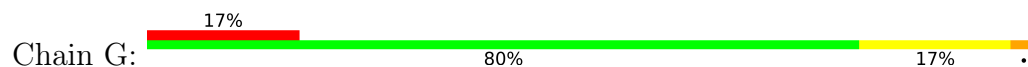
- Molecule 2: Beta/omega-theraphotoxin-Tp2a



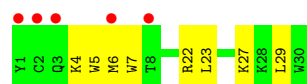
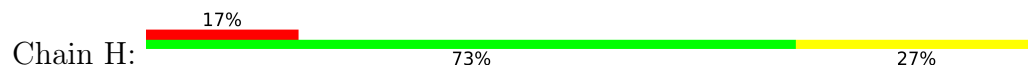
- Molecule 2: Beta/omega-theraphotoxin-Tp2a



- Molecule 2: Beta/omega-theraphotoxin-Tp2a



- Molecule 2: Beta/omega-theraphotoxin-Tp2a



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.22Å 123.53Å 123.99Å 90.00° 124.00° 90.00°	Depositor
Resolution (Å)	36.89 – 3.54 45.85 – 3.54	Depositor EDS
% Data completeness (in resolution range)	81.5 (36.89-3.54) 81.6 (45.85-3.54)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 3.57Å)	Xtriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, $R_{free}$	0.275 , 0.294 0.280 , 0.295	Depositor DCC
$R_{free}$ test set	1376 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.018 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.035 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.035 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.388 for $-h+k-l, -l, -k$ 0.379 for $-h-k-l, l, k$ 0.037 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.022 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.038 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.022 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.397 for $-h-2^*l, -k, l$	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	8629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	wwPDB-VP

<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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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: 6OU

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	0.33	0/1875	0.50	0/2554
1	B	0.32	0/1871	0.51	0/2550
1	C	0.32	0/1870	0.51	0/2550
1	D	0.32	0/1860	0.50	0/2536
2	E	0.32	0/270	0.53	0/360
2	F	0.38	0/270	0.59	0/360
2	G	0.32	0/266	0.58	0/356
2	H	0.32	0/270	0.51	0/360
All	All	0.32	0/8552	0.51	0/11626

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	1823	0	1865	60	0
1	B	1819	0	1854	59	0
1	C	1818	0	1845	43	0
1	D	1808	0	1834	47	0
2	E	262	0	254	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	262	0	254	19	0
2	G	258	0	243	10	0
2	H	262	0	254	10	0
3	A	67	0	0	1	0
3	B	69	0	0	0	0
3	C	51	0	0	1	0
3	D	93	0	0	0	0
3	E	13	0	0	0	0
3	F	9	0	0	0	0
3	G	15	0	0	0	0
All	All	8629	0	8403	226	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 13.

The worst 5 of 226 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:800:ASP:OD1	1:A:835:THR:OG1	1.96	0.82
1:D:800:ASP:OD1	1:D:835:THR:OG1	1.97	0.82
2:H:4:LYS:HG2	2:H:5:TRP:H	1.45	0.82
1:C:769:ASN:OD1	1:C:829:ARG:NH2	2.15	0.77
2:H:4:LYS:HG2	2:H:5:TRP:N	2.01	0.75

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	223/288 (77%)	207 (93%)	12 (5%)	4 (2%)	<b>9</b> 47
1	B	223/288 (77%)	209 (94%)	11 (5%)	3 (1%)	<b>13</b> 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	224/288 (78%)	214 (96%)	9 (4%)	1 (0%)	36	74
1	D	223/288 (77%)	210 (94%)	10 (4%)	3 (1%)	13	54
2	E	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	F	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	G	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
2	H	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
All	All	1005/1272 (79%)	939 (93%)	55 (6%)	11 (1%)	16	58

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	760	GLU
1	A	788	ARG
1	A	789	ILE
1	C	829	ARG
1	A	829	ARG

### 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	201/265 (76%)	190 (94%)	11 (6%)	24	60
1	B	200/265 (76%)	195 (98%)	5 (2%)	50	79
1	C	199/265 (75%)	195 (98%)	4 (2%)	58	82
1	D	197/265 (74%)	188 (95%)	9 (5%)	29	65
2	E	29/29 (100%)	29 (100%)	0	100	100
2	F	29/29 (100%)	29 (100%)	0	100	100
2	G	28/29 (97%)	27 (96%)	1 (4%)	38	71
2	H	29/29 (100%)	29 (100%)	0	100	100
All	All	912/1176 (78%)	882 (97%)	30 (3%)	41	73

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	891	PHE
1	C	761	PHE
1	D	891	PHE
1	B	931	PHE
1	C	787	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

16 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	6OU	A	1001	-	23,23,48	1.55	5 (21%)	27,28,53	1.06	2 (7%)
3	6OU	A	1002	-	26,26,48	1.24	3 (11%)	29,31,53	1.11	2 (6%)
3	6OU	A	1003	-	15,15,48	1.11	0	17,19,53	0.86	0
3	6OU	B	1001	-	23,23,48	1.59	4 (17%)	27,28,53	1.13	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	6OU	B	1002	-	26,26,48	1.24	2 (7%)	29,31,53	1.14	2 (6%)
3	6OU	B	1003	-	17,17,48	1.20	2 (11%)	19,21,53	0.87	1 (5%)
3	6OU	C	1001	-	23,23,48	1.56	4 (17%)	27,28,53	1.17	2 (7%)
3	6OU	C	1002	-	26,26,48	1.23	3 (11%)	29,31,53	1.14	2 (6%)
3	6OU	D	1001	-	23,23,48	1.57	4 (17%)	27,28,53	1.17	2 (7%)
3	6OU	D	1002	-	26,26,48	1.23	2 (7%)	29,31,53	1.07	2 (6%)
3	6OU	D	1003	-	13,13,48	0.91	0	14,16,53	0.51	0
3	6OU	D	1004	-	16,16,48	1.25	1 (6%)	18,20,53	1.16	1 (5%)
3	6OU	D	1005	-	10,10,48	0.99	0	11,12,53	0.46	0
3	6OU	E	101	-	12,12,48	1.58	2 (16%)	13,16,53	1.70	1 (7%)
3	6OU	F	101	-	8,8,48	1.05	0	9,10,53	0.43	0
3	6OU	G	101	-	14,14,48	1.48	2 (14%)	15,18,53	1.49	1 (6%)

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	6OU	A	1001	-	-	0/25/25/52	0/0/0/0
3	6OU	A	1002	-	-	0/30/30/52	0/0/0/0
3	6OU	A	1003	-	-	0/16/16/52	0/0/0/0
3	6OU	B	1001	-	-	0/25/25/52	0/0/0/0
3	6OU	B	1002	-	-	0/30/30/52	0/0/0/0
3	6OU	B	1003	-	-	0/19/19/52	0/0/0/0
3	6OU	C	1001	-	-	0/25/25/52	0/0/0/0
3	6OU	C	1002	-	-	0/30/30/52	0/0/0/0
3	6OU	D	1001	-	-	0/25/25/52	0/0/0/0
3	6OU	D	1002	-	-	0/30/30/52	0/0/0/0
3	6OU	D	1003	-	-	0/14/14/52	0/0/0/0
3	6OU	D	1004	-	-	0/18/18/52	0/0/0/0
3	6OU	D	1005	-	-	0/10/10/52	0/0/0/0
3	6OU	E	101	-	-	0/13/13/52	0/0/0/0
3	6OU	F	101	-	-	0/8/8/52	0/0/0/0
3	6OU	G	101	-	-	0/15/15/52	0/0/0/0

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	101	6OU	O30-C20	-3.29	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	101	6OU	O30-C20	-3.19	1.41	1.47
3	A	1002	6OU	O30-C20	-2.40	1.40	1.46
3	C	1001	6OU	O30-C20	-2.32	1.40	1.46
3	A	1001	6OU	O30-C20	-2.27	1.40	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	6OU	O18-C16-C15	2.46	119.02	111.92
3	B	1002	6OU	O18-C16-C15	2.62	119.49	111.92
3	D	1002	6OU	O18-C16-C15	2.63	119.51	111.92
3	B	1003	6OU	O18-C16-C15	2.69	119.71	111.92
3	A	1001	6OU	O30-C31-C33	2.71	118.57	110.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	6OU	1	0
3	C	1001	6OU	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	225/288 (78%)	-0.43	3 (1%) 77 66	48, 121, 219, 285	0
1	B	225/288 (78%)	-0.51	1 (0%) 92 88	40, 126, 197, 276	0
1	C	226/288 (78%)	-0.49	1 (0%) 92 88	41, 117, 190, 262	0
1	D	225/288 (78%)	-0.41	3 (1%) 77 66	34, 120, 206, 274	0
2	E	30/30 (100%)	0.39	4 (13%) 3 3	86, 208, 268, 293	0
2	F	30/30 (100%)	1.02	5 (16%) 1 2	103, 230, 318, 377	0
2	G	30/30 (100%)	0.52	5 (16%) 1 2	121, 217, 265, 272	0
2	H	30/30 (100%)	0.50	5 (16%) 1 2	109, 221, 266, 284	0
All	All	1021/1272 (80%)	-0.34	27 (2%) 56 44	34, 130, 240, 377	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	TYR	18.0
2	E	1	TYR	11.9
2	G	2	CYS	9.2
2	F	2	CYS	7.9
1	A	943	ASP	5.9

### 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

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	6OU	E	101	13/49	0.64	0.52	134,181,291,318	0
3	6OU	D	1005	11/49	0.66	0.86	129,194,338,351	0
3	6OU	A	1002	27/49	0.72	0.22	62,151,197,230	0
3	6OU	F	101	9/49	0.72	0.24	125,183,312,330	0
3	6OU	C	1002	27/49	0.74	0.25	42,161,191,220	0
3	6OU	G	101	15/49	0.75	0.40	153,203,290,293	0
3	6OU	D	1002	27/49	0.77	0.24	35,150,204,281	0
3	6OU	D	1004	17/49	0.84	0.19	75,105,178,210	0
3	6OU	B	1002	27/49	0.85	0.20	52,100,150,177	0
3	6OU	A	1003	16/49	0.87	0.16	74,109,213,219	0
3	6OU	B	1003	18/49	0.88	0.15	34,142,217,261	0
3	6OU	D	1001	24/49	0.88	0.23	55,93,118,180	0
3	6OU	D	1003	14/49	0.89	0.13	29,127,176,188	0
3	6OU	B	1001	24/49	0.89	0.26	23,77,144,196	0
3	6OU	C	1001	24/49	0.90	0.27	59,87,132,202	0
3	6OU	A	1001	24/49	0.91	0.19	47,77,103,196	0

## 6.5 Other polymers

There are no such residues in this entry.