



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2019 – 08:37 AM EST

PDB ID : 6B0T  
Title : Structural Insights into the Induced-fit Inhibition of Fascin by a Small Molecule  
Authors : Dey, R.; Huang, X.Y.  
Deposited on : 2017-09-15  
Resolution : 2.80 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

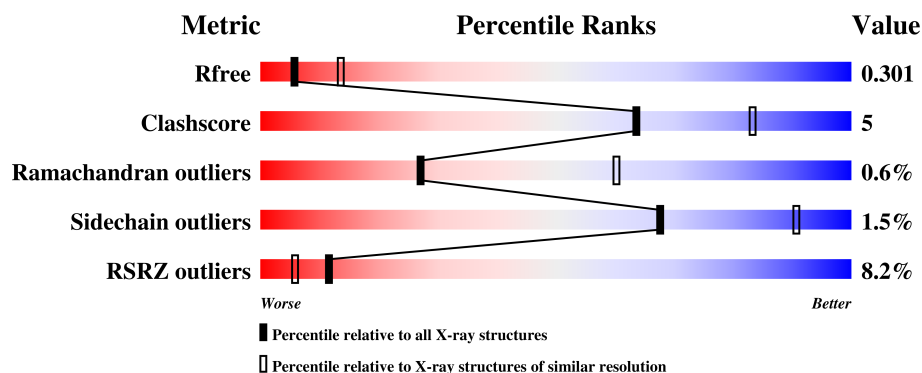
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	487	
1	B	487	
1	C	487	
1	D	487	
1	E	487	

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Mol	Chain	Length	Quality of chain
1	F	487	<div><div></div><div>10%</div><div>89%</div><div>11%</div></div>

## 2 Entry composition [i](#)

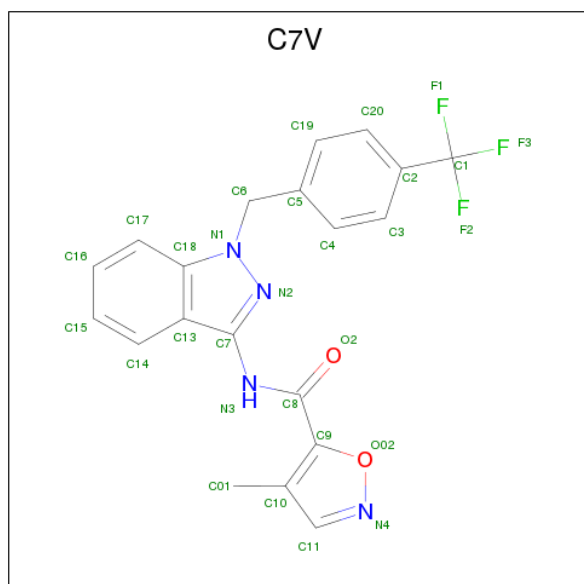
There are 3 unique types of molecules in this entry. The entry contains 45507 atoms, of which 22171 are hydrogens and 0 are deuteriums.

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 Fascin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	B	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	C	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	D	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	E	487	Total	C	H	N	O	S	0	0	0
			7474	2376	3671	680	733	14			
1	F	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			

- Molecule 2 is 4-methyl-N-(1-{[4-(trifluoromethyl)phenyl]methyl}-1H-indazol-3-yl)-1,2-oxazole-5-carboxamide (three-letter code: C7V) (formula: C<sub>20</sub>H<sub>15</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 44	C 20	F 3	H 15	N 4	O 2	0	0
2	B	1	Total 44	C 20	F 3	H 15	N 4	O 2	0	0
2	C	1	Total 44	C 20	F 3	H 15	N 4	O 2	0	0
2	D	1	Total 44	C 20	F 3	H 15	N 4	O 2	0	0
2	E	1	Total 44	C 20	F 3	H 15	N 4	O 2	0	0
2	F	1	Total 44	C 20	F 3	H 15	N 4	O 2	0	0

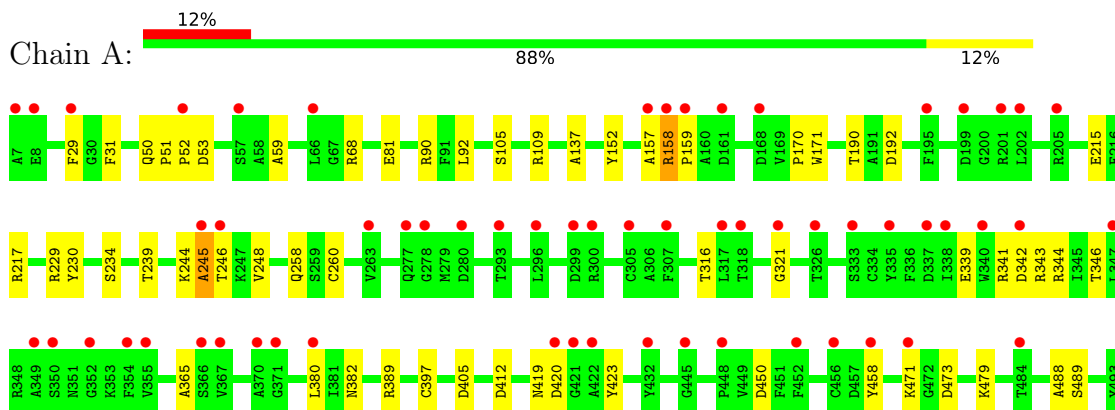
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	B	78	Total 78	O 78	0	0
3	C	89	Total 89	O 89	0	0
3	D	40	Total 40	O 40	0	0
3	E	58	Total 58	O 58	0	0
3	F	47	Total 47	O 47	0	0

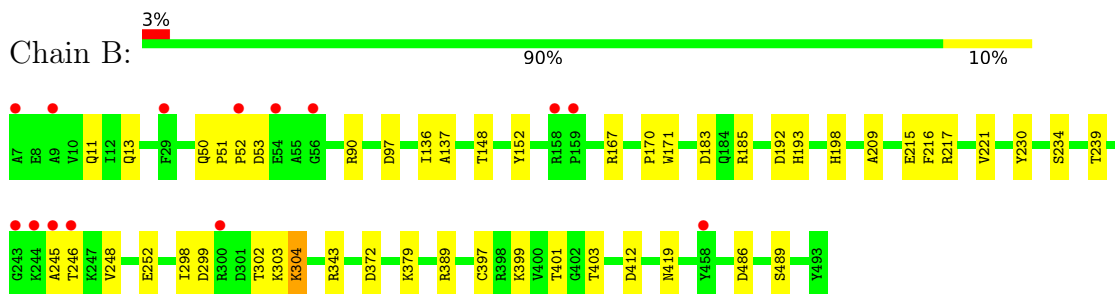
### 3 Residue-property plots [i](#)

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.

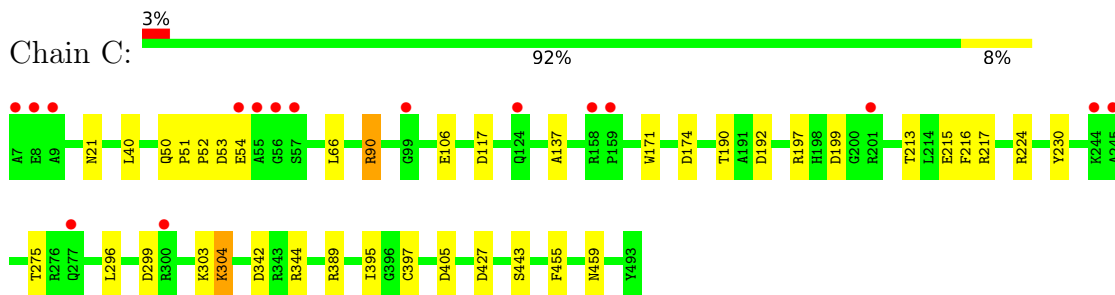
- Molecule 1: Fascin



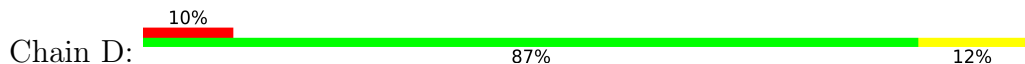
- Molecule 1: Fascin

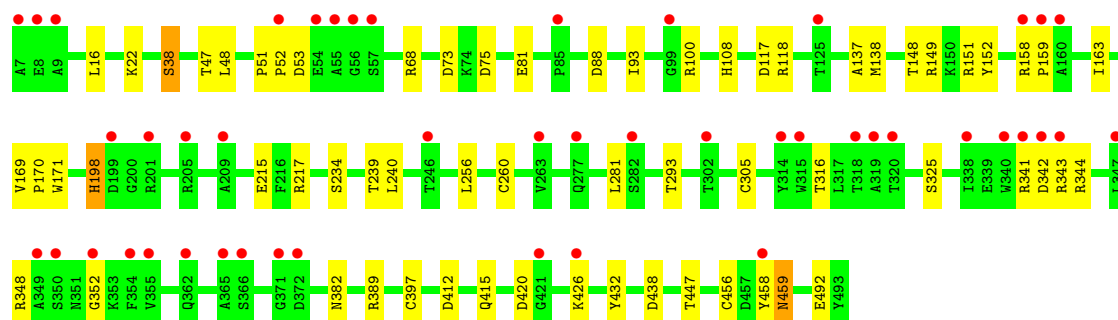


- Molecule 1: Fascin

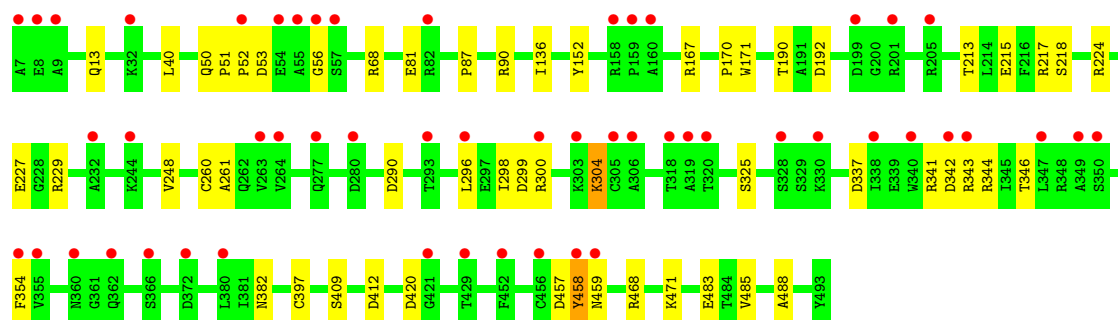
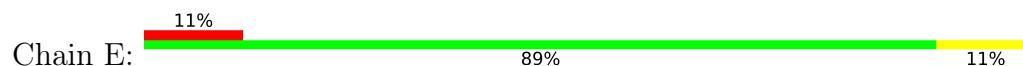


- Molecule 1: Fascin

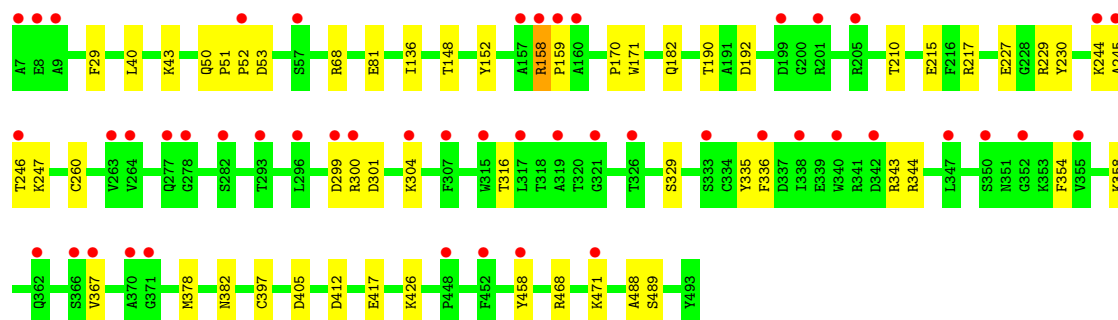
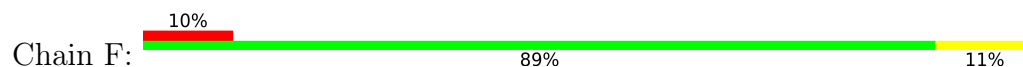




• Molecule 1: Fascin



• Molecule 1: Fascin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.58Å 59.26Å 293.65Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	45.44 – 2.80 46.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.44-2.80) 88.6 (46.11-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.265 , 0.303 0.266 , 0.301	Depositor DCC
$R_{free}$ test set	10489 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	45507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	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 71.33 % 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 2.6790e-06. 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, 0.333 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: C7V

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	0.27	0/3884	0.47	0/5252
1	B	0.26	0/3884	0.46	0/5252
1	C	0.28	0/3884	0.47	0/5252
1	D	0.28	0/3884	0.47	0/5252
1	E	0.26	0/3884	0.46	0/5252
1	F	0.27	0/3884	0.48	0/5252
All	All	0.27	0/23304	0.47	0/31512

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	3803	3682	3682	40	0
1	B	3803	3682	3682	34	0
1	C	3803	3682	3682	22	0
1	D	3803	3682	3682	38	0
1	E	3803	3671	3682	34	0
1	F	3803	3682	3682	37	0
2	A	29	15	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	15	0	4	0
2	C	29	15	0	3	0
2	D	29	15	0	2	0
2	E	29	15	0	5	0
2	F	29	15	0	2	0
3	A	32	0	0	2	0
3	B	78	0	0	4	0
3	C	89	0	0	2	0
3	D	40	0	0	4	0
3	E	58	0	0	3	0
3	F	47	0	0	10	0
All	All	23336	22171	22092	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 207 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:50:GLN:HG2	2:A:501:C7V:N4	1.74	1.02
1:A:157:ALA:O	1:A:158:ARG:O	1.85	0.93
1:F:152:TYR:CE2	1:F:170:PRO:HD3	2.03	0.92
1:D:215:GLU:OE2	1:D:217:ARG:NH2	2.02	0.92
1:F:215:GLU:OE2	1:F:217:ARG:NH2	2.02	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	485/487 (100%)	439 (90%)	41 (8%)	5 (1%)	17 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	485/487 (100%)	443 (91%)	39 (8%)	3 (1%)	27	60
1	C	485/487 (100%)	445 (92%)	38 (8%)	2 (0%)	36	70
1	D	485/487 (100%)	440 (91%)	44 (9%)	1 (0%)	49	81
1	E	485/487 (100%)	447 (92%)	35 (7%)	3 (1%)	27	60
1	F	485/487 (100%)	442 (91%)	40 (8%)	3 (1%)	27	60
All	All	2910/2922 (100%)	2656 (91%)	237 (8%)	17 (1%)	27	60

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	159	PRO
1	A	458	TYR
1	B	304	LYS
1	E	458	TYR

### 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	400/400 (100%)	396 (99%)	4 (1%)	78	94
1	B	400/400 (100%)	396 (99%)	4 (1%)	78	94
1	C	400/400 (100%)	392 (98%)	8 (2%)	58	86
1	D	400/400 (100%)	390 (98%)	10 (2%)	50	82
1	E	400/400 (100%)	396 (99%)	4 (1%)	78	94
1	F	400/400 (100%)	393 (98%)	7 (2%)	62	88
All	All	2400/2400 (100%)	2363 (98%)	37 (2%)	67	91

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	38	SER

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Mol	Chain	Res	Type
1	D	198	HIS
1	F	316	THR
1	D	47	THR
1	D	169	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	193	HIS

### 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](#)

6 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$
2	C7V	A	501	-	26,32,32	1.19	4 (15%)	30,47,47	2.01	9 (30%)
2	C7V	B	501	-	26,32,32	1.19	4 (15%)	30,47,47	2.01	9 (30%)
2	C7V	C	501	-	26,32,32	1.19	3 (11%)	30,47,47	2.01	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	C7V	D	501	-	26,32,32	1.19	4 (15%)	30,47,47	2.01	8 (26%)
2	C7V	E	501	-	26,32,32	1.19	4 (15%)	30,47,47	2.01	9 (30%)
2	C7V	F	501	-	26,32,32	1.19	4 (15%)	30,47,47	2.01	9 (30%)

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
2	C7V	A	501	-	-	0/12/18/18	0/4/4/4
2	C7V	B	501	-	-	0/12/18/18	0/4/4/4
2	C7V	C	501	-	-	0/12/18/18	0/4/4/4
2	C7V	D	501	-	-	0/12/18/18	0/4/4/4
2	C7V	E	501	-	-	0/12/18/18	0/4/4/4
2	C7V	F	501	-	-	0/12/18/18	0/4/4/4

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	C7V	C01-C10	-2.22	1.46	1.51
2	B	501	C7V	C01-C10	-2.21	1.46	1.51
2	F	501	C7V	C01-C10	-2.21	1.46	1.51
2	A	501	C7V	C01-C10	-2.20	1.46	1.51
2	E	501	C7V	C01-C10	-2.20	1.46	1.51

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	C7V	C5-C6-N1	-7.03	102.19	112.48
2	E	501	C7V	C5-C6-N1	-7.02	102.20	112.48
2	A	501	C7V	C5-C6-N1	-7.01	102.22	112.48
2	B	501	C7V	C5-C6-N1	-7.01	102.22	112.48
2	F	501	C7V	C5-C6-N1	-7.00	102.24	112.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	C7V	3	0
2	B	501	C7V	4	0
2	C	501	C7V	3	0
2	D	501	C7V	2	0
2	E	501	C7V	5	0
2	F	501	C7V	2	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	487/487 (100%)	0.54	60 (12%) 4 2	29, 78, 128, 196	2 (0%)
1	B	487/487 (100%)	-0.31	14 (2%) 51 41	24, 44, 82, 195	2 (0%)
1	C	487/487 (100%)	-0.24	16 (3%) 46 36	21, 43, 91, 197	2 (0%)
1	D	487/487 (100%)	0.53	47 (9%) 8 4	30, 75, 129, 207	2 (0%)
1	E	487/487 (100%)	0.49	53 (10%) 5 3	27, 73, 126, 233	2 (0%)
1	F	487/487 (100%)	0.44	49 (10%) 7 3	30, 74, 128, 169	2 (0%)
All	All	2922/2922 (100%)	0.24	239 (8%) 11 6	21, 64, 122, 233	12 (0%)

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	15.5
1	F	350	SER	11.4
1	E	350	SER	11.2
1	D	350	SER	10.9
1	E	458	TYR	9.9

### 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 [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. 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
2	C7V	A	501	29/29	0.67	0.27	60,73,105,192	0
2	C7V	E	501	29/29	0.67	0.28	58,70,105,192	0
2	C7V	D	501	29/29	0.68	0.29	59,71,105,192	0
2	C7V	B	501	29/29	0.70	0.28	51,66,105,192	0
2	C7V	F	501	29/29	0.74	0.23	57,69,105,192	0
2	C7V	C	501	29/29	0.77	0.29	58,71,105,192	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.