

# wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 07:20 pm BST

PDB ID : 6GEL

Title: The structure of TWITCH-2B

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Becker, S.

 $Deposited \ on \quad : \quad 2018\text{-}04\text{-}26$ 

Resolution : 2.51 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

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) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

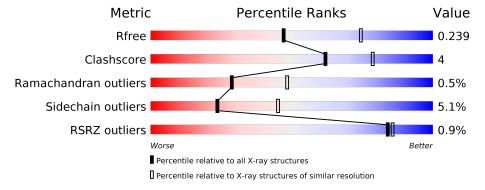
Validation Pipeline (wwPDB-VP) : 2.11

## 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 2.51 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 >=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 <=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	552	86%	9% • •		
1	В	552	82%	11% ••••		



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8685 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 Green fluorescent protein, Optimized Ratiometric Calcium Sensor, Green fluorescent protein, Green fluorescent protein.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	A	532	10001	C 2710	- 1	O 832	S 16	0	3	0
1	В	530	Total 4249	C 2696		O 823	S 17	0	1	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	insertion	UNP P42212
A	65	LEU	PHE	conflict	UNP P42212
A	66	CRF	SER	chromophore	UNP P42212
A	66	CRF	TYR	chromophore	UNP P42212
A	66	CRF	GLY	chromophore	UNP P42212
A	73	ALA	SER	conflict	UNP P42212
A	146	ALA	TYR	conflict	UNP P42212
A	147	ILE	ASN	conflict	UNP P42212
A	148	HIS	SER	conflict	UNP P42212
A	149	GLY	HIS	conflict	UNP P42212
A	154	THR	MET	conflict	UNP P42212
A	164	ALA	VAL	conflict	UNP P42212
A	167	GLY	LYS	conflict	UNP P42212
A	168	LEU	ILE	conflict	UNP P42212
A	169	ASN	ARG	conflict	UNP P42212
A	170	CYS	HIS	conflict	UNP P42212
A	207	LYS	ALA	conflict	UNP P42212
A	229	ARG	-	linker	UNP P42212
A	230	MET	-	linker	UNP P42212
A	231	GLN	-	linker	UNP P42212
A	232	VAL	-	linker	UNP P42212
A	233	ALA	-	linker	UNP P42212
A	234	ASP	-	linker	UNP P42212
A	235	ALA	-	linker	UNP P42212



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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
A	249	PHE	LYS	conflict	UNP W5IDB2
A	300	VAL	MET	conflict	UNP W5IDB2
A	305	PRO	-	linker	UNP W5IDB2
A	306	ILE	_	linker	UNP W5IDB2
A	307	TYR	_	linker	UNP W5IDB2
A	308	PRO	_	linker	UNP W5IDB2
A	309	GLU	_	linker	UNP W5IDB2
A	310	LEU	-	linker	UNP W5IDB2
A	311	MET	_	linker	UNP W5IDB2
A	313	GLY	SER	conflict	UNP P42212
A	341	TYR	THR	conflict	UNP P42212
A	344	LYS	ALA	conflict	UNP P42212
A	369	LEU	HIS	conflict	UNP P42212
A	377	GLY	-	linker	UNP P42212
A	378	GLY	-	linker	UNP P42212
A	379	THR	_	linker	UNP P42212
A	380	GLY	_	linker	UNP P42212
A	381	GLY	_	linker	UNP P42212
A	382	SER	_	linker	UNP P42212
A	384	VAL	-	insertion	UNP P42212
A	413	ARG	SER	conflict	UNP P42212
A	422	ASN	TYR	conflict	UNP P42212
A	429	LEU	PHE	conflict	UNP P42212
A	447	LEU	PHE	conflict	UNP P42212
A	448	CR2	SER	chromophore	UNP P42212
A	448	CR2	TYR	chromophore	UNP P42212
A	448	CR2	GLY	chromophore	UNP P42212
A	451	LEU	VAL	conflict	UNP P42212
A	452	MET	GLN	conflict	UNP P42212
A	455	ALA	SER	conflict	UNP P42212
A	536	THR	MET	conflict	UNP P42212
A	546	ALA	VAL	conflict	UNP P42212
В	2	VAL	_	insertion	UNP P42212
В	65	LEU	PHE	conflict	UNP P42212
В	66	CRF	SER	chromophore	UNP P42212
В	66	CRF	TYR	chromophore	UNP P42212
В	66	CRF	GLY	chromophore	UNP P42212
В	73	ALA	SER	conflict	UNP P42212
В	146	ALA	TYR	conflict	UNP P42212
В	147	ILE	ASN	conflict	UNP P42212
В	148	HIS	SER	conflict	UNP P42212
В	149	GLY	HIS	conflict	UNP P42212



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Chain	Residue	Modelled	Actual	Comment	Reference
В	154	THR	MET	conflict	UNP P42212
В	164	ALA	VAL	conflict	UNP P42212
В	167	GLY	LYS	conflict	UNP P42212
В	168	LEU	ILE	conflict	UNP P42212
В	169	ASN	ARG	conflict	UNP P42212
В	170	CYS	HIS	conflict	UNP P42212
В	207	LYS	ALA	conflict	UNP P42212
В	229	ARG	-	linker	UNP P42212
В	230	MET	_	linker	UNP P42212
В	231	GLN	-	linker	UNP P42212
В	232	VAL	-	linker	UNP P42212
В	233	ALA	-	linker	UNP P42212
В	234	ASP	-	linker	UNP P42212
В	235	ALA	-	linker	UNP P42212
В	249	PHE	LYS	conflict	UNP W5IDB2
В	300	VAL	MET	conflict	UNP W5IDB2
В	305	PRO	-	linker	UNP W5IDB2
В	306	ILE	_	linker	UNP W5IDB2
В	307	TYR	-	linker	UNP W5IDB2
В	308	PRO	-	linker	UNP W5IDB2
В	309	GLU	_	linker	UNP W5IDB2
В	310	LEU	-	linker	UNP W5IDB2
В	311	MET	-	linker	UNP W5IDB2
В	313	GLY	SER	conflict	UNP P42212
В	341	TYR	THR	conflict	UNP P42212
В	344	LYS	ALA	conflict	UNP P42212
В	369	LEU	HIS	conflict	UNP P42212
В	377	GLY	-	linker	UNP P42212
В	378	GLY	-	linker	UNP P42212
В	379	THR	-	linker	UNP P42212
В	380	GLY	-	linker	UNP P42212
В	381	GLY	-	linker	UNP P42212
В	382	SER	-	linker	UNP P42212
В	384	VAL	-	insertion	UNP P42212
В	413	ARG	SER	conflict	UNP P42212
В	422	ASN	TYR	conflict	UNP P42212
В	429	LEU	PHE	conflict	UNP P42212
В	447	LEU	PHE	conflict	UNP P42212
В	448	CR2	SER	chromophore	UNP P42212
В	448	CR2	TYR	chromophore	UNP P42212
В	448	CR2	GLY	chromophore	UNP P42212
В	451	LEU	VAL	conflict	UNP P42212



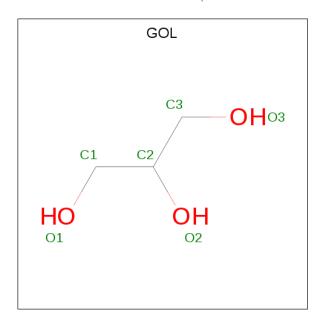
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Chain	Residue	Modelled	Actual	${f Comment}$	Reference
В	452	MET	GLN	$\operatorname{conflict}$	UNP P42212
В	455	ALA	SER	$\operatorname{conflict}$	UNP P42212
В	536	THR	MET	$\operatorname{conflict}$	UNP P42212
В	546	ALA	VAL	$\operatorname{conflict}$	UNP P42212

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Ca 2 2	0	0
2	A	2	Total Ca 2 2	0	0

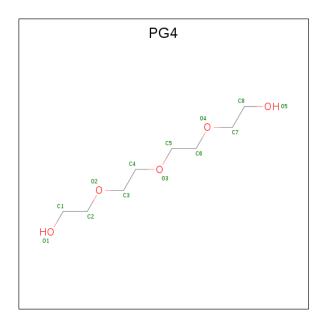
• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0

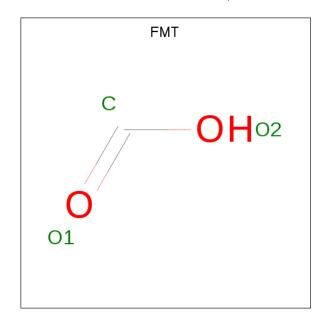
• Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

 $\bullet$  Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula:  $\mathrm{CH_2O_2}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 3 1 2	0	0
5	В	1	Total C O 3 1 2	0	0
5	В	1	Total C O 3 1 2	0	0

### • Molecule 6 is water.

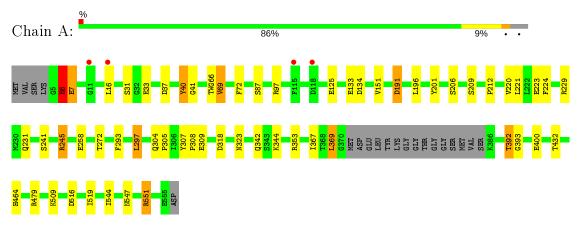
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	66	Total O 66 66	0	0
6	В	47	Total O 47 47	0	0



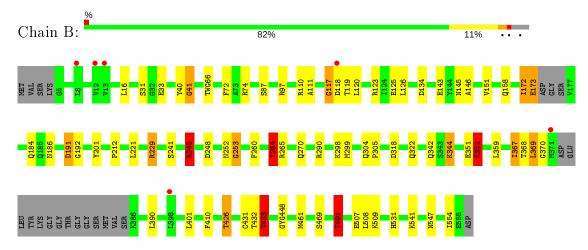
## 3 Residue-property plots (i)

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: Green fluorescent protein, Optimized Ratiometric Calcium Sensor, Green fluorescent protein, Green fluorescent protein



• Molecule 1: Green fluorescent protein, Optimized Ratiometric Calcium Sensor, Green fluorescent protein, Green fluorescent protein





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	58.08Å 156.77Å 169.28Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 - 2.51	Depositor
Resolution (A)	47.89 - 2.51	EDS
% Data completeness	98.7 (47.93-2.51)	Depositor
(in resolution range)	98.7 (47.89-2.51)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
P. P.	0.195 , 0.240	Depositor
$R, R_{free}$	0.199 , 0.239	DCC
$R_{free}$ test set	2656 reflections $(5.00\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.30 , 39.7	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8685	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: CR2, GOL, CA, PG4, CRF, FMT

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		Boı	nd lengths	Bond angles		
MIOI	I Chain	RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.86	4/4323 (0.1%)	0.94	7/5837 (0.1%)	
1	В	0.86	4/4293 (0.1%)	0.97	10/5795~(0.2%)	
All	All	0.86	8/8616 (0.1%)	0.96	17/11632 (0.1%)	

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	5
1	В	0	10
All	All	0	15

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	253	GLY	N-CA	-8.50	1.33	1.46
1	В	173	GLU	N-CA	5.75	1.57	1.46
1	A	400	GLU	CD-OE1	5.63	1.31	1.25
1	A	133	GLU	CD-OE2	5.31	1.31	1.25
1	В	125	GLU	CD-OE1	5.29	1.31	1.25

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	В	97	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	245	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	479	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	В	145	ASN	CB-CA-C	-6.29	97.82	110.40



Mol	Chain	Res	Type	${f Atoms}$	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	353	ARG	NE-CZ-NH2	-6.26	117.17	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	ARG	Sidechain
1	A	369	LEU	Peptide
1	A	392	THR	Peptide
1	A	393	GLY	Peptide
1	A	551	ARG	Sidechain

### 5.2 Too-close contacts (i)

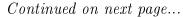
In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4278	0	4117	29	0
1	В	4249	0	4098	46	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
3	A	6	0	8	0	0
3	В	12	0	16	0	0
4	A	8	0	10	1	0
5	A	6	0	2	0	0
5	В	9	0	3	0	0
6	A	66	0	0	1	0
6	В	47	0	0	5	0
All	All	8685	0	8254	74	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 4.

The worst 5 of 74 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:B:241:SER:O	1:B:245[A]:ARG:HG3	1.78	0.82





Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:B:410:PHE:HA	1:B:433:THR:HG21	1.66	0.76
1:A:209:SER:OG	1:A:220:VAL:CG1	2.35	0.74
1:B:184:GLN:HE21	1:B:186:ASN:HD21	1.37	0.72
1:B:352:LYS:H	1:B:352:LYS:CE	2.04	0.70

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	Perce	$_{ m ntiles}$
1	A	525/552~(95%)	508 (97%)	16 (3%)	1 (0%)	47	68
1	В	519/552 (94%)	499 (96%)	16 (3%)	4 (1%)	19	35
All	All	1044/1104 (95%)	1007 (96%)	32 (3%)	5 (0%)	29	48

#### All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	В	41	GLY
1	В	146	ALA
1	В	172	ILE
1	В	117	GLY

#### 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	Percentiles		
1	A	462/476 (97%)	442 (96%)	20 (4%)	29	53
1	В	459/476 (96%)	431 (94%)	28 (6%)	18	36
All	All	921/952 (97%)	873 (95%)	48 (5%)	24	44

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	31	SER
1	В	134	ASP
1	В	469	SER
1	В	33	GLU
1	В	118	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	ASN
1	В	95	GLN
1	В	231	GLN
1	A	488	ASN
1	В	186	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues 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		
	Type		nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CR2	A	448	1	20,20,21	3.71	7 (35%)	25,27,29	4.37	12 (48%)



Mol	Tune	Chain	Res	Link	Bo	Bond lengths			Bond angles		
WIOI	Type		ites		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
1	CRF	A	66	1	25,26,27	3.25	8 (32%)	32,37,39	4.12	13 (40%)	
1	CRF	В	66	1	25,26,27	3.34	9 (36%)	32,37,39	3.84	13 (40%)	
1	CR2	В	448	1	20,20,21	4.16	6 (30%)	25,27,29	3.89	13 (52%)	

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
1	CR2	A	448	1	-	0/6/25/26	0/2/2/2
1	CRF	A	66	1	-	0/10/31/32	0/3/3/3
1	CRF	В	66	1	-	0/10/31/32	0/3/3/3
1	CR2	В	448	1	-	0/6/25/26	0/2/2/2

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	448	CR2	CB2-CA2	16.61	1.49	1.35
1	A	448	CR2	CB2-CA2	14.06	1.46	1.35
1	В	66	CRF	CB2-CA2	13.61	1.46	1.35
1	A	66	CRF	CB2-CA2	13.50	1.46	1.35
1	В	448	CR2	C1-N2	4.34	1.40	1.32

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	448	CR2	CA2-C2-N3	16.21	111.04	103.37
1	A	66	CRF	O2-C2-CA2	-14.31	122.92	130.96
1	В	66	CRF	CA2-C2-N3	14.03	110.00	103.37
1	A	66	CRF	CA2-C2-N3	12.93	109.48	103.37
1	В	448	CR2	O2-C2-CA2	-11.55	124.48	130.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Α	66	CRF	3	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	66	CRF	3	0
1	В	448	CR2	1	0

### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	Tuna	Chain	in Dog	Res Link	В	ond leng	$\operatorname{gths}$	Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
5	FMT	В	607	_	0,2,2	0.00	-	0,1,1	0.00	-
4	PG4	A	605	-	3,3,12	0.80	0	2,2,11	0.24	0
5	FMT	A	607	-	0,2,2	0.00	-	0,1,1	0.00	-
4	PG4	A	604	-	3,3,12	0.65	0	2,2,11	0.87	0
5	FMT	В	606	-	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	В	604	-	5,5,5	0.41	0	5,5,5	0.79	0
3	GOL	В	603	-	5,5,5	0.46	0	5,5,5	0.84	0
3	GOL	A	603	-	5,5,5	0.69	0	5, 5, 5	0.72	0
5	FMT	В	605	-	0,2,2	0.00	=	0,1,1	0.00	=
5	FMT	A	606	-	0,2,2	0.00	-	0,1,1	0.00	-

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
4	PG4	A	605	_	-	1/1/1/10	-
3	GOL	В	603	_	-	2/4/4/4	-
4	PG4	A	604	_	-	1/1/1/10	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	В	604	-	-	2/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	604	GOL	O1-C1-C2-C3
3	В	603	GOL	C1-C2-C3-O3
3	A	603	GOL	C1-C2-C3-O3
3	В	604	GOL	O1-C1-C2-O2
4	A	605	PG4	O4-C7-C8-O5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	PG4	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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	530/552~(96%)	-0.19	4 (0%) 86 87	36, 61, 95, 123	0
1	В	528/552~(95%)	-0.10	6 (1%) 80 82	38, 65, 100, 123	0
All	All	1058/1104 (95%)	-0.15	10 (0%) 84 86	36, 63, 97, 123	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	8	LEU	2.7
1	В	13	VAL	2.7
1	A	16	LEU	2.4
1	В	398	LEU	2.3
1	A	118	ASP	2.3

## 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	$\operatorname{B-factors}({\rm \AA}^2)$	Q < 0.9
1	CRF	A	66	24/25	0.97	0.14	51,56,65,71	0
1	CRF	В	66	24/25	0.98	0.15	40,43,56,58	0
1	CR2	В	448	19/20	0.98	0.13	43,46,51,53	0
1	CR2	A	448	19/20	0.99	0.13	37,39,44,45	0

## 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	PG4	A	604	4/13	0.84	0.18	59,68,70,74	0
3	GOL	В	604	6/6	0.85	0.17	74,81,84,85	0
5	FMT	A	606	3/3	0.86	0.13	70,70,74,76	0
5	FMT	A	607	3/3	0.87	0.14	57,57,75,76	0
3	GOL	A	603	6/6	0.89	0.22	56,59,65,67	0
5	FMT	В	606	3/3	0.89	0.14	65,65,72,73	0
2	CA	В	602	1/1	0.90	0.07	68,68,68,68	0
5	FMT	В	607	3/3	0.91	0.35	53,53,84,84	0
5	FMT	В	605	3/3	0.91	0.24	59,59,68,78	0
2	CA	A	602	1/1	0.91	0.07	64,64,64,64	0
2	CA	В	601	1/1	0.93	0.09	52,52,52,52	0
4	PG4	A	605	4/13	0.93	0.16	45,58,63,63	0
3	GOL	В	603	6/6	0.95	0.18	51,60,67,68	0
2	CA	A	601	1/1	0.97	0.08	50,50,50,50	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

