



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 10:11 PM UTC

PDB ID : 6GEL / pdb_00006gel
Title : The structure of TWITCH-2B
Authors : Trigo Mourino, P.; Paulat, M.; Thestrup, T.; Griesbeck, O.; Griesinger, C.;
Becker, S.
Deposited on : 2018-04-26
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

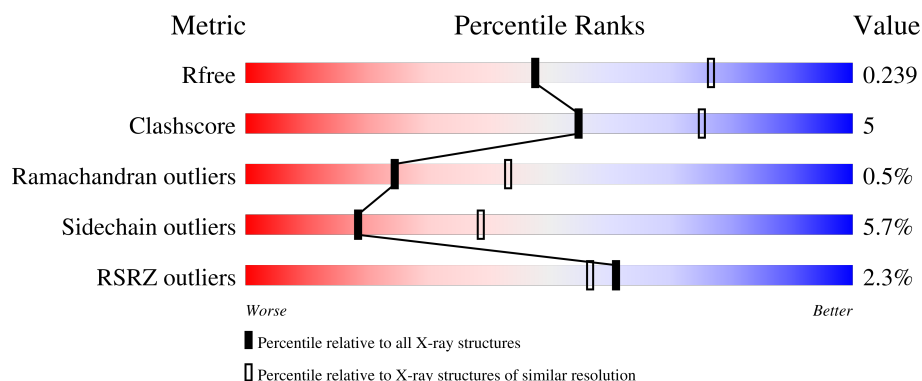
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

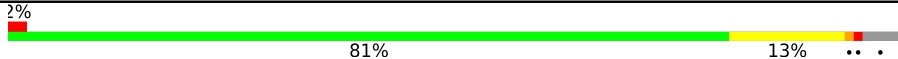
The reported resolution of this entry is 2.51 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of 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 $\leq 5\%$. 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	552	
1	B	552	

2 Entry composition

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	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	3	0
			4278	2710	720	832	16			
1	B	530	Total	C	N	O	S	0	1	0
			4249	2696	713	823	17			

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	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
B	2	VAL	-	insertion	UNP P42212
B	65	LEU	PHE	conflict	UNP P42212
B	66	CRF	SER	chromophore	UNP P42212
B	66	CRF	TYR	chromophore	UNP P42212
B	66	CRF	GLY	chromophore	UNP P42212
B	73	ALA	SER	conflict	UNP P42212
B	146	ALA	TYR	conflict	UNP P42212
B	147	ILE	ASN	conflict	UNP P42212
B	148	HIS	SER	conflict	UNP P42212
B	149	GLY	HIS	conflict	UNP P42212

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

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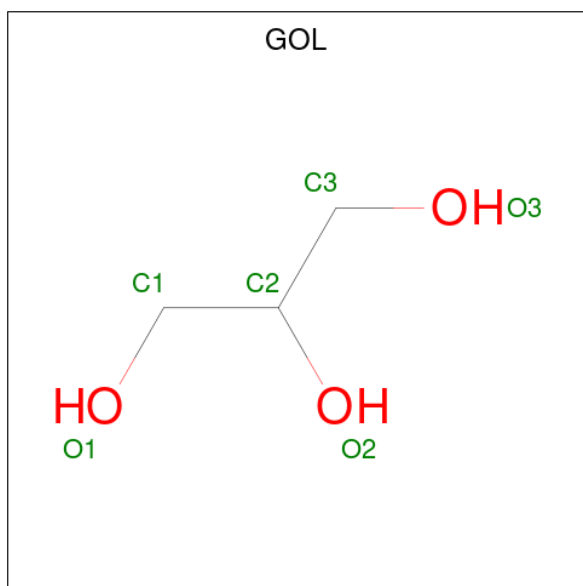
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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	MET	GLN	conflict	UNP P42212
B	455	ALA	SER	conflict	UNP P42212
B	536	THR	MET	conflict	UNP P42212
B	546	ALA	VAL	conflict	UNP P42212

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

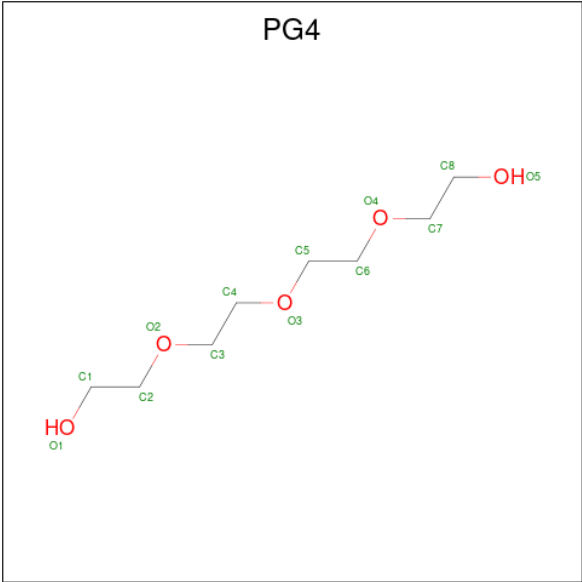
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



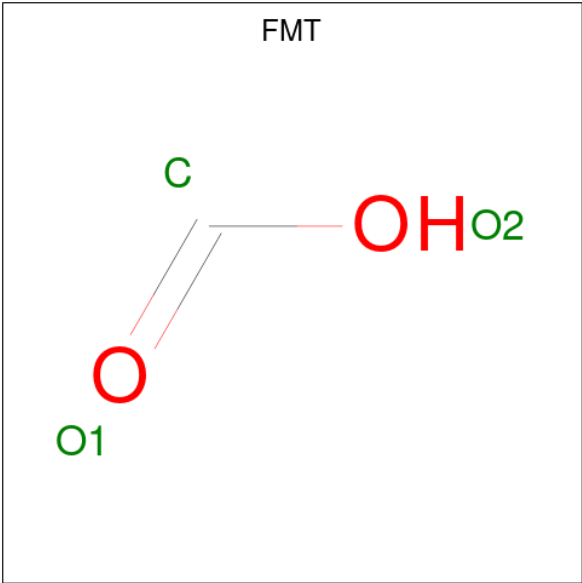
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

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

- Molecule 6 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.08Å 156.77Å 169.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.51 47.93 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.93-2.51) 98.7 (47.93-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.195 , 0.240 0.199 , 0.239	Depositor DCC
R_{free} test set	2656 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8685	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, PG4, CA, CRF, CR2, GOL

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	1.21	23/4323 (0.5%)	1.18	11/5837 (0.2%)
1	B	1.21	24/4293 (0.6%)	1.26	26/5795 (0.4%)
All	All	1.21	47/8616 (0.5%)	1.22	37/11632 (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	5
1	B	0	10
All	All	0	15

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	GLU	C-O	-8.40	1.13	1.24
1	B	253	GLY	N-CA	-8.32	1.33	1.45
1	A	531	HIS	CE1-NE2	7.43	1.40	1.32
1	A	532	ASN	N-CA	-7.29	1.37	1.46
1	A	331	VAL	C-O	-7.24	1.15	1.23

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	THR	CA-CB-OG1	-9.00	96.10	109.60
1	A	40	TYR	N-CA-C	-8.64	97.67	110.46
1	B	40	TYR	N-CA-C	7.44	121.20	112.72
1	B	361	PHE	CA-CB-CG	7.11	120.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	GLY	CA-C-N	7.08	134.44	121.70

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

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	33	0
1	B	4249	0	4098	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
4	A	8	0	10	1	0
5	A	6	0	2	0	0
5	B	9	0	3	0	0
6	A	66	0	0	1	0
6	B	47	0	0	5	0
All	All	8685	0	8254	80	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 80 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:B:260:PHE:CE1	1:B:299:MET:HE1	2.03	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:SER:O	1:B:245[A]:ARG:HG3	1.78	0.82
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

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	525/552 (95%)	508 (97%)	16 (3%)	1 (0%)	43	63
1	B	519/552 (94%)	499 (96%)	16 (3%)	4 (1%)	16	31
All	All	1044/1104 (95%)	1007 (96%)	32 (3%)	5 (0%)	24	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	41	GLY
1	B	146	ALA
1	B	172	ILE
1	B	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	Outliers	Percentiles	
1	A	462/476 (97%)	438 (95%)	24 (5%)	21	42
1	B	459/476 (96%)	430 (94%)	29 (6%)	16	34
All	All	921/952 (97%)	868 (94%)	53 (6%)	18	38

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	119	THR
1	B	264	ILE
1	B	491	THR
1	B	134	ASP
1	B	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	488	ASN
1	B	460	HIS
1	B	78	HIS
1	B	205	GLN
1	A	532	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CR2	A	448	1	20,20,21	3.38	8 (40%)	25,27,29	3.48	12 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRF	A	66	1	25,26,27	2.06	8 (32%)	34,37,39	3.98	17 (50%)
1	CRF	B	66	1	25,26,27	2.42	10 (40%)	34,37,39	3.38	16 (47%)
1	CR2	B	448	1	20,20,21	3.75	6 (30%)	25,27,29	3.32	12 (48%)

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	-	1/12/31/32	0/3/3/3
1	CRF	B	66	1	-	1/12/31/32	0/3/3/3
1	CR2	B	448	1	-	0/6/25/26	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	448	CR2	CB2-CA2	14.39	1.49	1.35
1	A	448	CR2	CB2-CA2	12.17	1.46	1.35
1	B	66	CRF	CD2-CE2	4.69	1.47	1.41
1	B	448	CR2	C1-N2	4.55	1.40	1.32
1	A	66	CRF	CD2-CE2	4.24	1.46	1.41

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRF	O2-C2-CA2	-12.68	122.92	131.02
1	B	448	CR2	O2-C2-CA2	-10.25	124.48	131.02
1	A	448	CR2	C2-N3-C1	-10.05	103.56	108.08
1	A	448	CR2	CA2-C2-N3	8.98	111.04	103.50
1	B	66	CRF	O2-C2-CA2	-8.88	125.36	131.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRF	N2-C1-CA1-CB1
1	B	66	CRF	N2-C1-CA1-CB1

There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FMT	A	606	-	2,2,2	0.88	0	1,1,1	0.68	0
4	PG4	A	605	-	3,3,12	0.76	0	2,2,11	0.23	0
5	FMT	B	605	-	2,2,2	1.23	0	1,1,1	0.18	0
3	GOL	A	603	-	5,5,5	0.72	0	5,5,5	0.76	0
5	FMT	A	607	-	2,2,2	1.11	0	1,1,1	0.41	0
5	FMT	B	606	-	2,2,2	0.79	0	1,1,1	0.80	0
5	FMT	B	607	-	2,2,2	1.08	0	1,1,1	0.54	0
3	GOL	B	603	-	5,5,5	0.47	0	5,5,5	0.89	0
3	GOL	B	604	-	5,5,5	0.42	0	5,5,5	0.85	0
4	PG4	A	604	-	3,3,12	0.63	0	2,2,11	0.88	0

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	A	603	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	B	604	-	-	2/4/4/4	-
4	PG4	A	604	-	-	1/1/1/10	-

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	A	603	GOL	C1-C2-C3-O3
3	B	603	GOL	C1-C2-C3-O3
3	B	604	GOL	O1-C1-C2-C3
3	B	604	GOL	O1-C1-C2-O2
3	A	603	GOL	O2-C2-C3-O3

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, 95th 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 ²)	Q<0.9
1	A	530/552 (96%)	-0.00	11 (2%) 63 59	19, 61, 95, 123	3 (0%)
1	B	528/552 (95%)	0.16	13 (2%) 58 54	25, 65, 100, 123	1 (0%)
All	All	1058/1104 (95%)	0.08	24 (2%) 61 57	19, 63, 97, 123	4 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	MET	6.0
1	B	5	GLY	4.6
1	A	386	LYS	3.8
1	A	224	PHE	3.7
1	B	386	LYS	3.6

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, 95th 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(Å ²)	Q<0.9
1	CRF	A	66	24/25	0.96	0.07	51,56,65,71	0
1	CR2	B	448	19/20	0.96	0.07	43,46,51,53	0
1	CRF	B	66	24/25	0.97	0.07	40,43,56,58	0
1	CR2	A	448	19/20	0.97	0.05	37,39,44,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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(Å ²)	Q<0.9
5	FMT	B	607	3/3	0.81	0.20	53,53,84,84	0
4	PG4	A	604	4/13	0.82	0.16	59,68,70,74	0
5	FMT	A	606	3/3	0.84	0.17	70,70,74,76	0
3	GOL	B	604	6/6	0.86	0.14	74,81,84,85	0
5	FMT	A	607	3/3	0.87	0.16	57,57,75,76	0
4	PG4	A	605	4/13	0.90	0.14	45,58,63,63	0
3	GOL	A	603	6/6	0.90	0.12	56,59,65,67	0
5	FMT	B	606	3/3	0.92	0.12	65,65,72,73	0
5	FMT	B	605	3/3	0.94	0.10	59,59,68,78	0
2	CA	A	602	1/1	0.95	0.07	64,64,64,64	0
3	GOL	B	603	6/6	0.95	0.10	51,60,67,68	0
2	CA	B	602	1/1	0.97	0.07	68,68,68,68	0
2	CA	B	601	1/1	0.98	0.06	52,52,52,52	0
2	CA	A	601	1/1	0.99	0.05	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.