



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2026 – 02:16 PM JST

PDB ID : 26SJ / pdb_000026sj
Title : Crystal structure of MAIT A-F7 TCR-MR1-xanthine
Authors : Awad, W.; Rossjohn, J.
Deposited on : 2026-05-13
Resolution : 2.60 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:

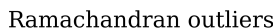
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

i

X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

Metric

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.

Mol

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Mol	Chain	Length	Quality of chain
4	E	246	 3% 76% 21% ..
4	H	246	 85% 14%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13396 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	4	0
			2174	1393	378	392	11			
1	C	266	Total	C	N	O	S	3	3	0
			2177	1400	374	392	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	engineered mutation	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	engineered mutation	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	1	0
			782	503	132	144	3			
2	F	100	Total	C	N	O	S	1	1	0
			813	519	137	153	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Human A-F7 TCR TRAV1-2_ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	191	Total	C	N	O	S	0	4	0
			1467	938	233	286	10			

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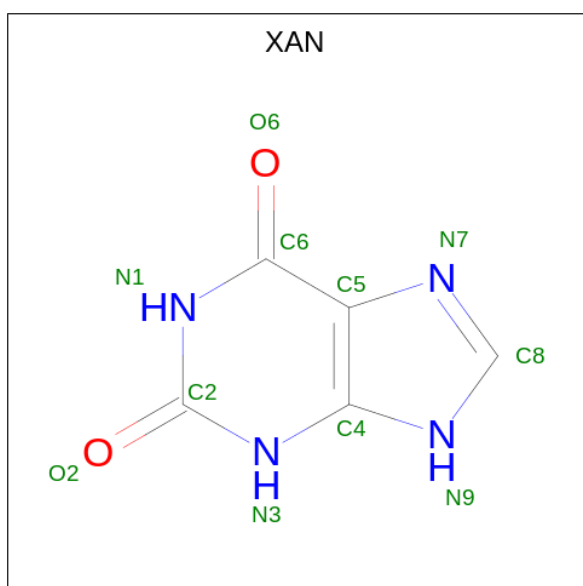
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	200	Total	C	N	O	S	1	12	0
			1616	1029	253	322	12			

- Molecule 4 is a protein called Human A-F7 TCR TRBV6-1_BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	240	Total	C	N	O	S	1	3	0
			1848	1168	316	355	9			
4	H	245	Total	C	N	O	S	1	13	0
			1971	1248	337	373	13			

- Molecule 5 is XANTHINE (CCD ID: XAN) (formula: $C_5H_4N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	5	4	2		
5	C	1	Total	C	N	O	0	0
			11	5	4	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total 1	Ca 1	0	0

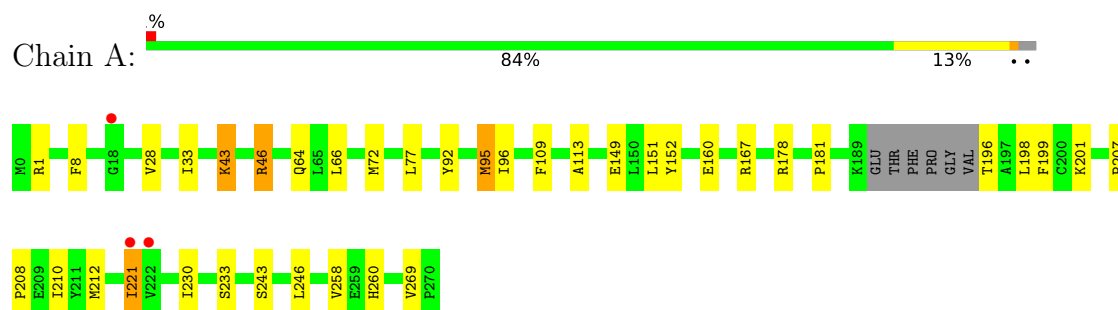
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	77	Total 77	O 77	0	0
9	B	23	Total 23	O 23	0	0
9	C	83	Total 83	O 83	0	0
9	D	40	Total 40	O 40	0	0
9	E	36	Total 36	O 36	0	0
9	F	37	Total 37	O 37	0	0
9	G	80	Total 80	O 80	0	0
9	H	99	Total 99	O 99	0	0

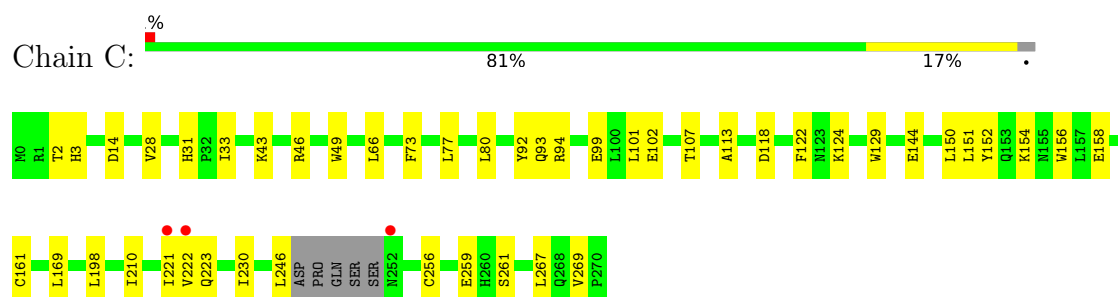
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

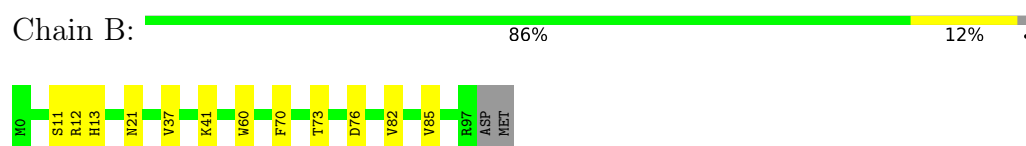
- Molecule 1: Major histocompatibility complex class I-related gene protein



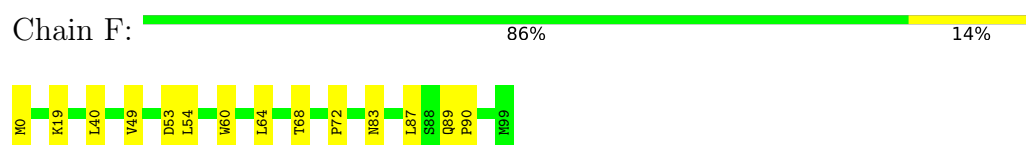
- Molecule 1: Major histocompatibility complex class I-related gene protein



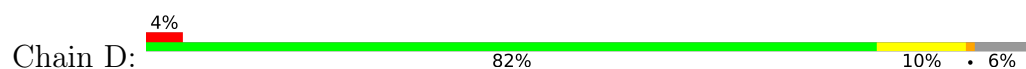
- Molecule 2: Beta-2-microglobulin

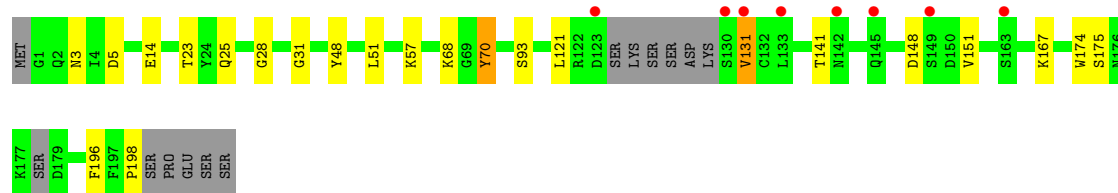


- Molecule 2: Beta-2-microglobulin



- Molecule 3: Human A-F7 TCR TRAV1-2_ALPHA





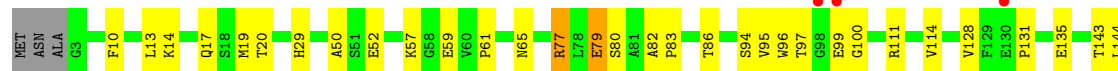
• Molecule 3: Human A-F7 TCR TRAV1-2_ALPHA

Chain G: 85% 12% ..



• Molecule 4: Human A-F7 TCR TRBV6-1_BETA

Chain E: 3% 76% 21% ..



• Molecule 4: Human A-F7 TCR TRBV6-1_BETA

Chain H: 85% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.64Å 70.17Å 143.71Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	46.38 – 2.60 46.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.38-2.60) 88.0 (46.38-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.61Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.177 , 0.222 0.177 , 0.222	Depositor DCC
R_{free} test set	1969 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13396	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, CA, XAN

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	0.39	0/2252	0.54	0/3063
1	C	0.40	0/2252	0.52	0/3064
2	B	0.33	0/808	0.49	0/1103
2	F	0.37	0/839	0.55	0/1141
3	D	0.34	0/1508	0.48	0/2049
3	G	0.39	0/1685	0.55	0/2285
4	E	0.34	0/1904	0.49	0/2600
4	H	0.42	0/2062	0.56	0/2804
All	All	0.38	0/13310	0.52	0/18109

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	2174	0	2055	30	1
1	C	2177	0	2065	34	0
2	B	782	0	721	8	0
2	F	813	0	756	7	0
3	D	1467	0	1356	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1616	0	1547	20	0
4	E	1848	0	1702	32	0
4	H	1971	0	1881	27	0
5	A	11	0	4	1	0
5	C	11	0	4	1	0
6	A	6	0	8	1	0
6	C	12	0	16	3	0
6	D	6	0	8	0	1
6	E	6	0	8	1	0
6	F	12	0	16	1	0
6	G	6	0	8	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	H	1	0	0	0	0
9	A	77	0	0	0	0
9	B	23	0	0	2	0
9	C	83	0	0	3	0
9	D	40	0	0	0	0
9	E	36	0	0	5	0
9	F	37	0	0	1	0
9	G	80	0	0	2	0
9	H	99	0	0	1	0
All	All	13396	0	12155	151	1

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 6.

The worst 5 of 151 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:C:46[A]:ARG:NH1	9:C:401:HOH:O	1.97	0.98
4:E:13:LEU:HB2	4:E:114:VAL:HG12	1.60	0.82
4:H:57:LYS:HD2	4:H:61:PRO:HG3	1.64	0.80
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.64	0.80
4:H:210:ARG:NH1	4:H:212:GLN:OE1	2.15	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:O	6:D:301:GOL:O1[2_554]	2.19	0.01

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	265/271 (98%)	259 (98%)	5 (2%)	1 (0%)	30	51
1	C	265/271 (98%)	258 (97%)	6 (2%)	1 (0%)	30	51
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	F	99/100 (99%)	99 (100%)	0	0	100	100
3	D	189/204 (93%)	187 (99%)	2 (1%)	0	100	100
3	G	210/204 (103%)	204 (97%)	6 (3%)	0	100	100
4	E	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
4	H	256/246 (104%)	253 (99%)	3 (1%)	0	100	100
All	All	1622/1642 (99%)	1592 (98%)	28 (2%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	VAL
1	A	221	ILE

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	228/241 (95%)	222 (97%)	6 (3%)	40	68
1	C	228/241 (95%)	223 (98%)	5 (2%)	45	72
2	B	83/95 (87%)	82 (99%)	1 (1%)	63	83
2	F	89/95 (94%)	86 (97%)	3 (3%)	32	60
3	D	154/181 (85%)	148 (96%)	6 (4%)	28	55
3	G	184/181 (102%)	177 (96%)	7 (4%)	29	56
4	E	193/212 (91%)	182 (94%)	11 (6%)	18	40
4	H	214/212 (101%)	208 (97%)	6 (3%)	38	66
All	All	1373/1458 (94%)	1328 (97%)	45 (3%)	35	61

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	225	THR
3	G	70[B]	TYR
2	F	0	MET
3	G	54	LEU
3	G	93[B]	SER

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

Mol	Chain	Res	Type
4	E	214	GLN
4	E	226	GLN
4	H	234	GLN
2	F	13	HIS
1	C	111	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 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	XAN	A	301	-	12,12,12	0.37	0	12,17,17	0.36	0
6	GOL	G	501	-	5,5,5	0.38	0	5,5,5	0.33	0
6	GOL	F	102	-	5,5,5	0.34	0	5,5,5	0.46	0
6	GOL	D	301	-	5,5,5	0.34	0	5,5,5	0.45	0
6	GOL	C	302	-	5,5,5	0.49	0	5,5,5	0.74	0
6	GOL	F	101	-	5,5,5	0.56	0	5,5,5	0.70	0
6	GOL	E	301	-	5,5,5	0.49	0	5,5,5	0.65	0
6	GOL	C	303	-	5,5,5	0.34	0	5,5,5	0.42	0
5	XAN	C	301	-	12,12,12	0.40	0	12,17,17	0.45	0
6	GOL	A	302	-	5,5,5	0.33	0	5,5,5	0.32	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
5	XAN	A	301	-	-	-	0/2/2/2
6	GOL	G	501	-	-	4/4/4/4	-
6	GOL	F	102	-	-	0/4/4/4	-
6	GOL	D	301	-	-	2/4/4/4	-
6	GOL	C	302	-	-	0/4/4/4	-
6	GOL	F	101	-	-	0/4/4/4	-
6	GOL	E	301	-	-	2/4/4/4	-
6	GOL	C	303	-	-	3/4/4/4	-
5	XAN	C	301	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	303	GOL	O1-C1-C2-C3
6	E	301	GOL	C1-C2-C3-O3
6	G	501	GOL	O1-C1-C2-C3
6	C	303	GOL	O1-C1-C2-O2
6	G	501	GOL	C1-C2-C3-O3

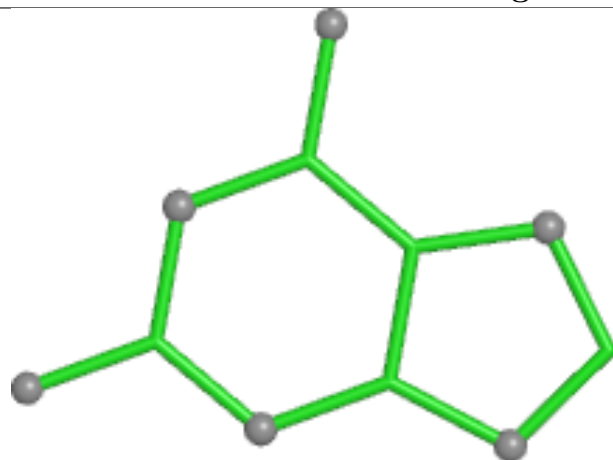
There are no ring outliers.

8 monomers are involved in 9 short contacts:

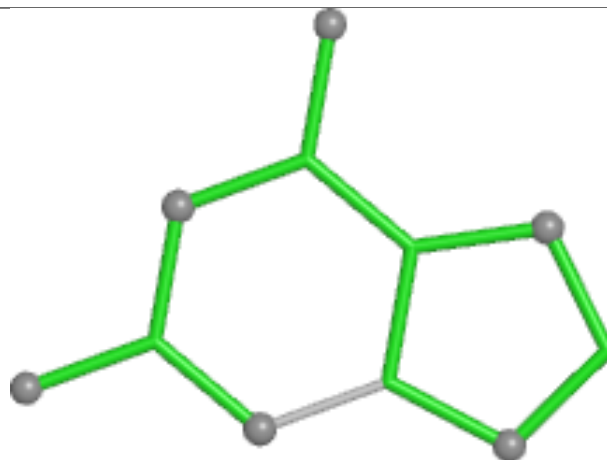
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	XAN	1	0
6	G	501	GOL	1	0
6	D	301	GOL	0	1
6	C	302	GOL	3	0
6	F	101	GOL	1	0
6	E	301	GOL	1	0
5	C	301	XAN	1	0
6	A	302	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

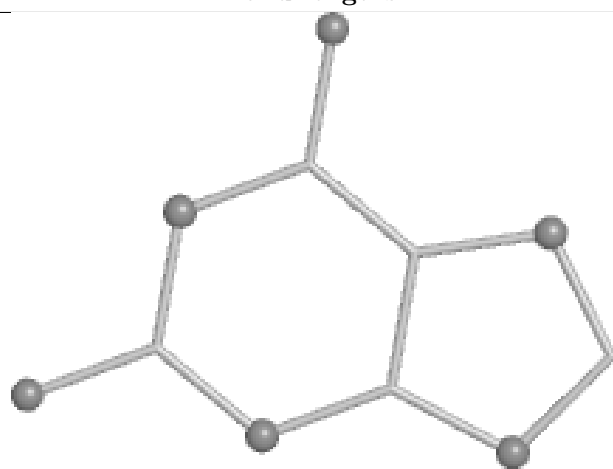
Ligand XAN A 301



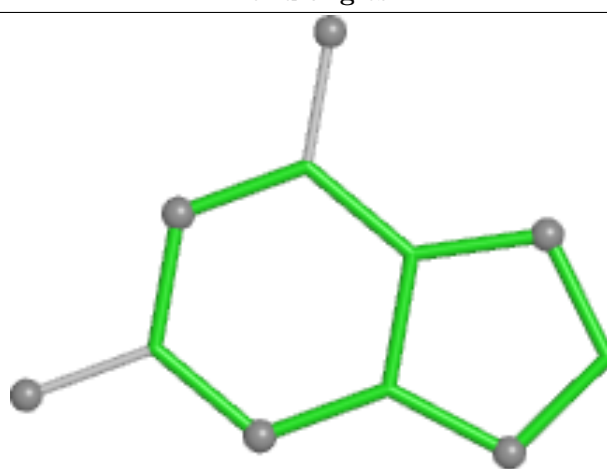
Bond lengths



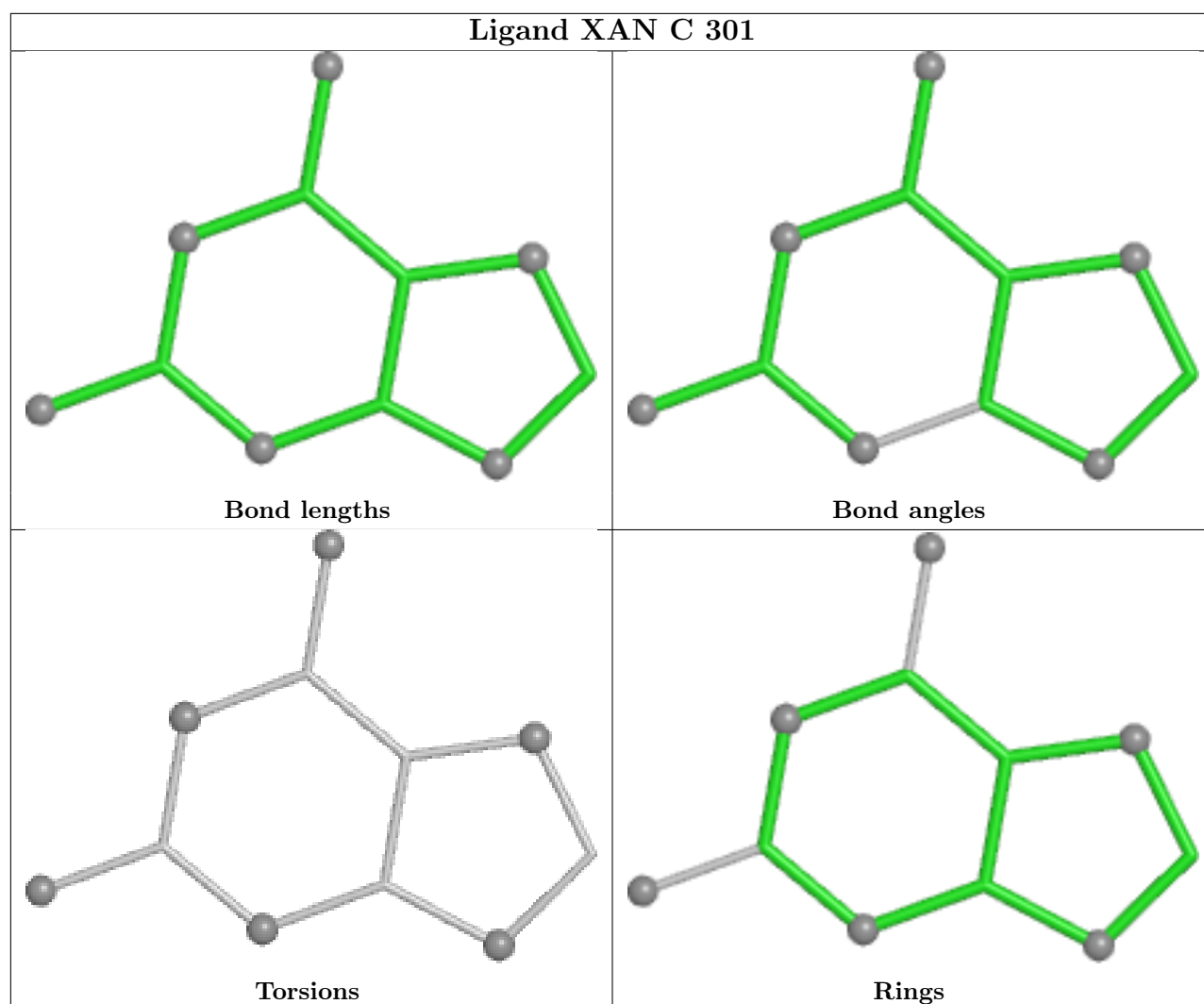
Bond angles



Torsions



Rings



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	265/271 (97%)	-0.23	3 (1%) 78 74	25, 48, 89, 117	6 (2%)
1	C	266/271 (98%)	-0.29	3 (1%) 78 74	29, 47, 75, 91	12 (4%)
2	B	98/100 (98%)	0.04	0 100 100	36, 65, 89, 96	2 (2%)
2	F	100/100 (100%)	-0.27	0 100 100	27, 53, 75, 95	3 (3%)
3	D	191/204 (93%)	0.25	8 (4%) 40 35	21, 60, 103, 125	7 (3%)
3	G	200/204 (98%)	-0.37	1 (0%) 87 85	26, 43, 71, 97	19 (9%)
4	E	240/246 (97%)	0.29	8 (3%) 49 43	26, 63, 100, 119	7 (2%)
4	H	245/246 (99%)	-0.36	1 (0%) 88 86	25, 43, 64, 96	19 (7%)
All	All	1605/1642 (97%)	-0.13	24 (1%) 72 68	21, 50, 89, 125	75 (4%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	149	SER	4.4
3	D	130	SER	3.4
4	E	99	GLU	3.2
1	C	222	VAL	3.1
3	D	123	ASP	2.9

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 oligosaccharides in this entry.

6.4 Ligands

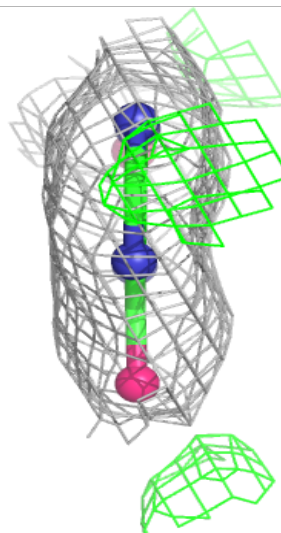
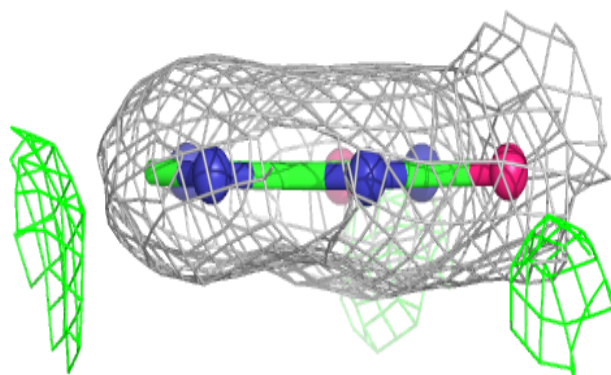
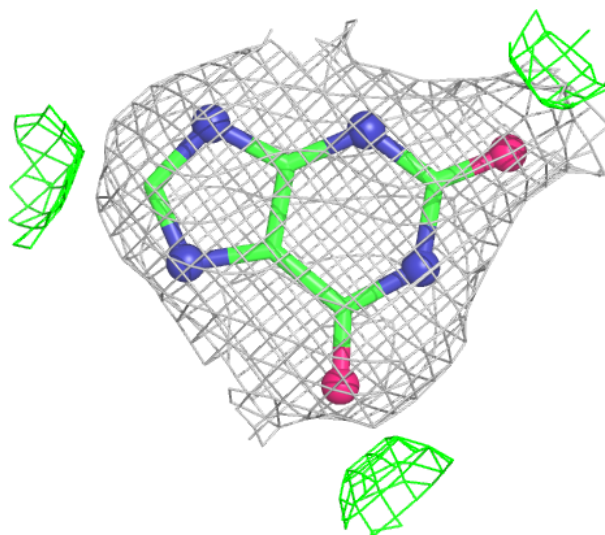
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

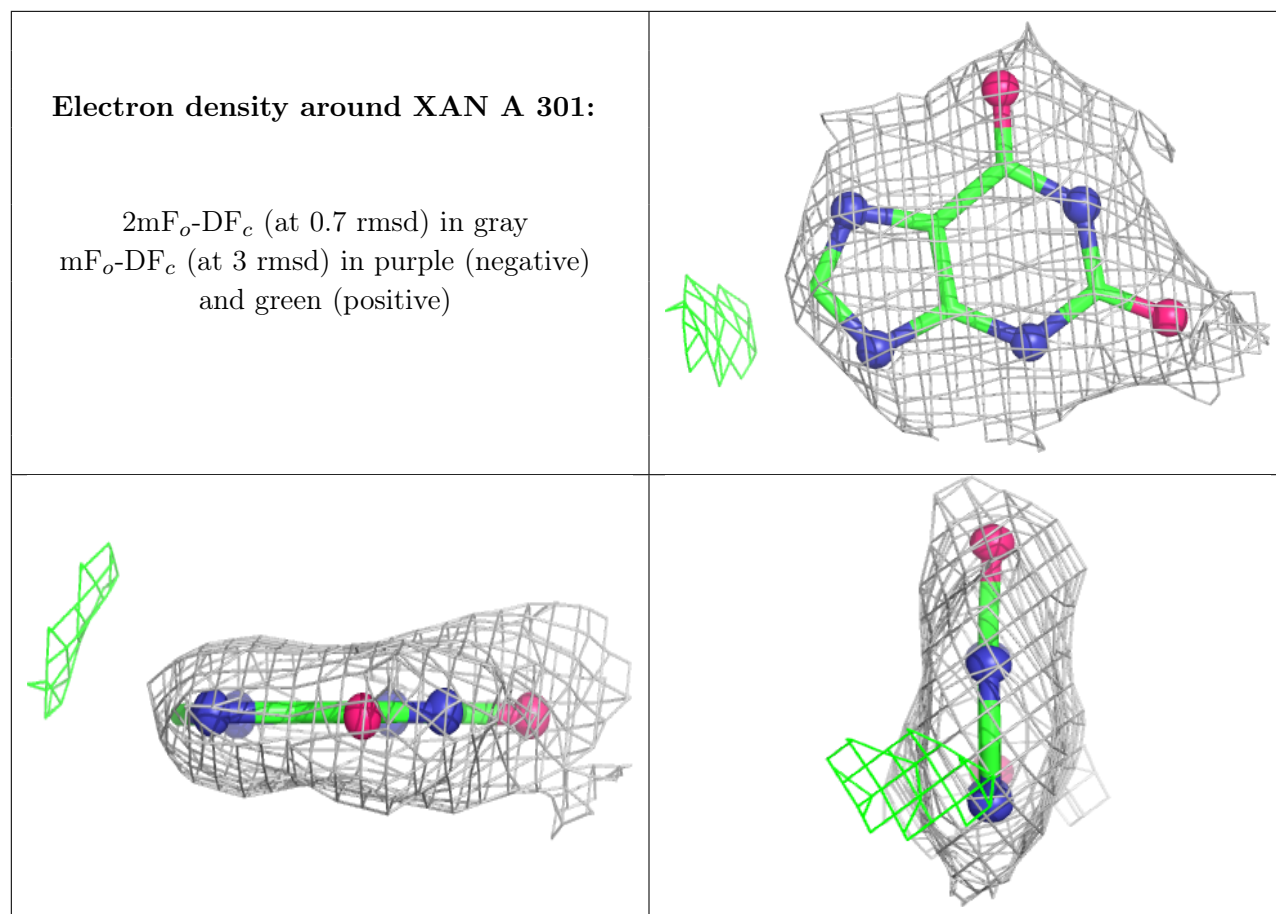
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	D	301	6/6	0.86	0.16	77,78,85,89	0
6	GOL	E	301	6/6	0.88	0.13	72,79,85,90	0
6	GOL	G	501	6/6	0.88	0.15	53,68,81,86	0
6	GOL	C	303	6/6	0.89	0.16	56,67,78,81	0
7	CL	C	304	1/1	0.89	0.13	69,69,69,69	0
6	GOL	C	302	6/6	0.90	0.16	53,61,72,74	6
5	XAN	C	301	11/11	0.91	0.10	46,52,61,61	11
6	GOL	A	302	6/6	0.93	0.16	45,56,67,67	6
6	GOL	F	102	6/6	0.93	0.11	42,51,55,63	0
7	CL	A	303	1/1	0.94	0.10	63,63,63,63	0
6	GOL	F	101	6/6	0.94	0.09	40,42,51,62	6
5	XAN	A	301	11/11	0.95	0.08	40,43,47,50	0
8	CA	H	301	1/1	0.96	0.07	83,83,83,83	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around XAN C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.