Full wwPDB X-ray Structure Validation Report (i)

Jun 3, 2025 – 02:42 PM EDT

PDB ID	:	9BYS / pdb_00009bys
Title	:	Structure of human MAIT BV28 TCR in complex with human MR1-5-OP-RU
Authors	:	Awad, W.; Rossjohn, J.
Deposited on	:	2024-05-24
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

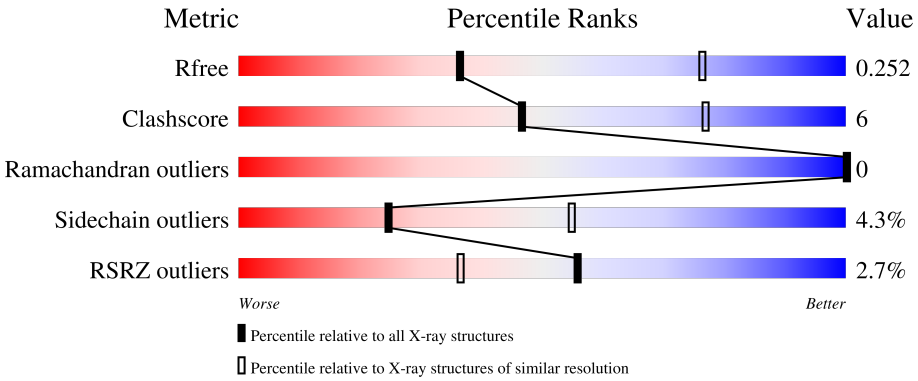
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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 <=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	271	83% 14%
2	AAAB	244	6% 77% 20%
3	AAAC	204	% 82% 15%
4	AAAD	100	2% 97%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5889 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	267	Total	C	N	O	S	0	2	0
			2177	1391	378	397	11			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AAAB	196	Total	C	N	O	S	0	0	0
			1453	921	239	284	9			

- Molecule 3 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AAAC	173	Total	C	N	O	S	0	0	0
			1318	829	212	268	9			

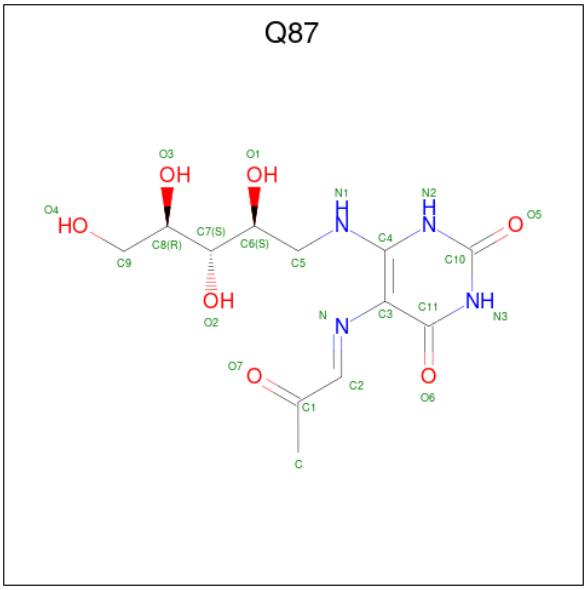
- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AAAD	99	Total	C	N	O	S	0	0	0
			797	509	136	149	3			

There is a discrepancy between the modelled and reference sequences:

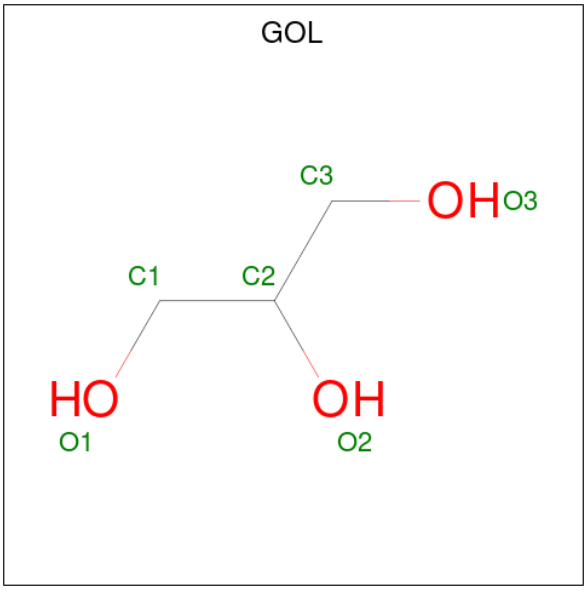
Chain	Residue	Modelled	Actual	Comment	Reference
AAAD	0	MET	-	initiating methionine	UNP P61769

- Molecule 5 is 1-deoxy-1-({2,6-dioxo-5-[(E)-(2-oxopropylidene)amino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-ribitol (CCD ID: Q87) (formula: $C_{12}H_{18}N_4O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	22	12	4	6	0	0

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



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

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

- Molecule 7 is water.

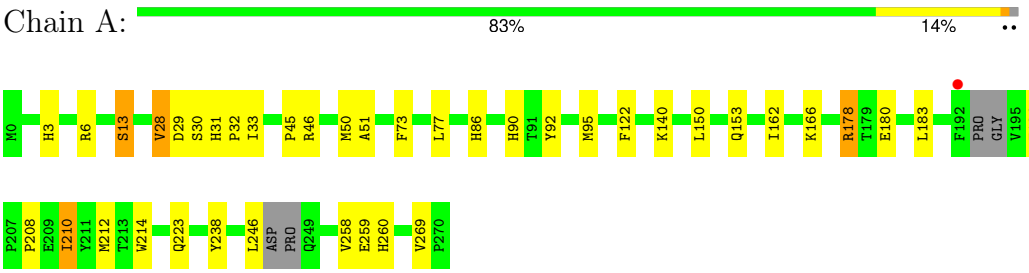
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	68	Total O 68 68	0	0
7	AAAB	7	Total O 7 7	0	0
7	AAAC	21	Total O 21 21	0	0
7	AAAD	8	Total O 8 8	0	0

3 Residue-property plots (i)

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.

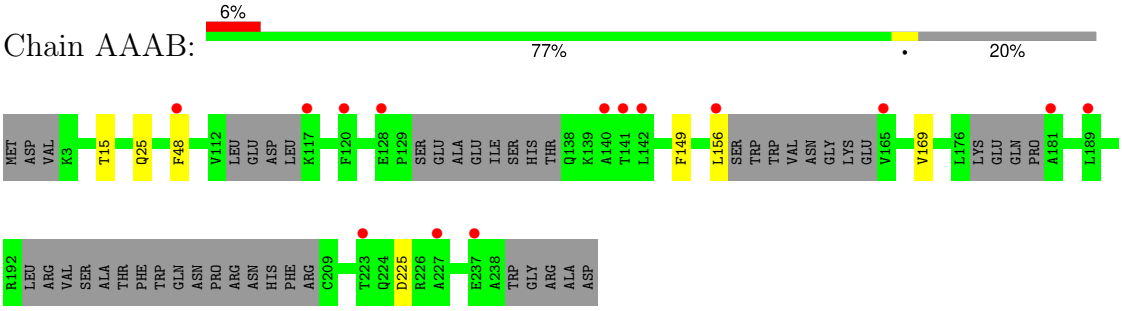
• Molecule 1: Major histocompatibility complex class I-related gene protein

Chain A:



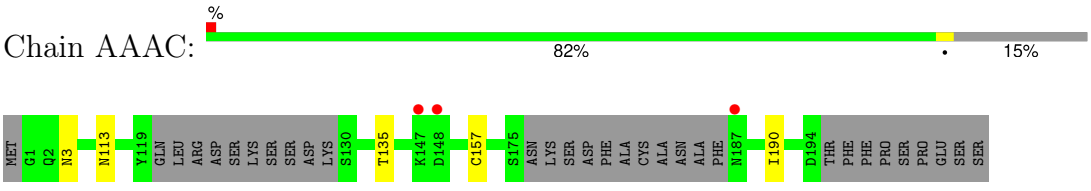
• Molecule 2: TCR beta chain

Chain AAAB:



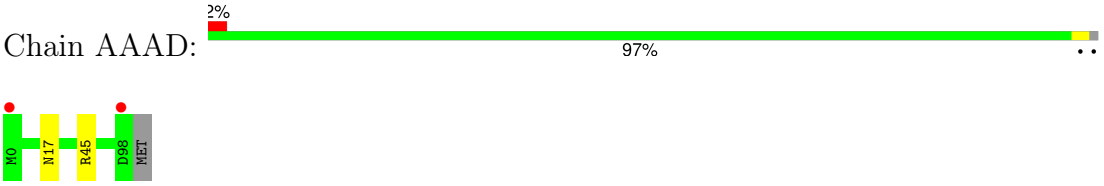
• Molecule 3: TCR alpha chain

Chain AAAC:



• Molecule 4: Beta-2-microglobulin

Chain AAAD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.35Å 111.35Å 206.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 3.10 46.83 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.83-3.10) 99.9 (46.83-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.252 0.222 , 0.252	Depositor DCC
R_{free} test set	1219 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 72.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5889	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, Q87

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	0.11	0/2246	0.34	2/3054 (0.1%)
2	AAAB	0.09	0/1486	0.27	0/2025
3	AAAC	0.07	0/1343	0.23	0/1821
4	AAAD	0.07	0/820	0.25	0/1117
All	All	0.09	0/5895	0.29	2/8017 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	SER	CA-C-N	5.25	128.91	121.61
1	A	30	SER	C-N-CA	5.25	128.91	121.61

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	VAL	Peptide

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	2177	0	2050	21	0
2	AAAB	1453	0	0	0	0
3	AAAC	1318	0	0	0	0
4	AAAD	797	0	0	0	0
5	A	22	0	0	0	0
6	A	18	0	24	0	0
7	A	68	0	0	2	0
7	AAAB	7	0	0	0	0
7	AAAC	21	0	0	0	0
7	AAAD	8	0	0	0	0
All	All	5889	0	2074	21	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 6.

All (21) 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:77:LEU:HD13	1:A:92:TYR:HB2	1.75	0.67
1:A:212:MET:HG2	1:A:258:VAL:HG22	1.78	0.65
1:A:28:VAL:HG23	1:A:33:ILE:HD13	1.79	0.63
1:A:153:GLN:NE2	7:A:401:HOH:O	2.36	0.58
1:A:3:HIS:HA	1:A:29:ASP:OD1	2.05	0.56
1:A:208:PRO:HG3	1:A:238:TYR:CE1	2.40	0.56
1:A:45:PRO:HG3	1:A:51:ALA:HB2	1.88	0.55
1:A:28:VAL:HG12	1:A:29:ASP:H	1.72	0.55
1:A:13:SER:HG	1:A:90:HIS:H	1.56	0.50
1:A:210:ILE:HG13	1:A:260:HIS:HB2	1.94	0.49
1:A:122:PHE:HE1	1:A:150:LEU:HD22	1.80	0.47
1:A:212:MET:HE3	1:A:212:MET:HB2	1.79	0.46
1:A:13:SER:OG	1:A:90:HIS:N	2.38	0.45
1:A:178:ARG:NH2	1:A:180:GLU:OE2	2.50	0.44
1:A:31:HIS:NE2	1:A:206:TYR:OH	2.36	0.44
1:A:86:HIS:HB3	1:A:90:HIS:NE2	2.33	0.43
1:A:200:CYS:HB2	1:A:214:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HB2	1:A:46:ARG:HD3	2.02	0.42
1:A:6[B]:ARG:NH2	7:A:403:HOH:O	2.48	0.41
1:A:162:ILE:HG22	1:A:166:LYS:HE3	2.03	0.41
1:A:33:ILE:HB	1:A:50:MET:HG3	2.04	0.40

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	263/271 (97%)	260 (99%)	3 (1%)	0	100	100
2	AAAB	184/244 (75%)	176 (96%)	8 (4%)	0	100	100
3	AAAC	167/204 (82%)	165 (99%)	2 (1%)	0	100	100
4	AAAD	97/100 (97%)	97 (100%)	0	0	100	100
All	All	711/819 (87%)	698 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	229/241 (95%)	217 (95%)	12 (5%)	19	48
2	AAAB	146/218 (67%)	139 (95%)	7 (5%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AAAC	142/181 (78%)	137 (96%)	5 (4%)	31 61
4	AAAD	86/95 (90%)	84 (98%)	2 (2%)	45 70
All	All	603/735 (82%)	577 (96%)	26 (4%)	25 55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	73	PHE
1	A	95	MET
1	A	140	LYS
1	A	178	ARG
1	A	183	LEU
1	A	196	THR
1	A	210	ILE
1	A	223	GLN
1	A	246	LEU
1	A	259	GLU
1	A	269	VAL
2	AAAB	15	THR
2	AAAB	25	GLN
2	AAAB	48	PHE
2	AAAB	149	PHE
2	AAAB	156	LEU
2	AAAB	169	VAL
2	AAAB	225	ASP
3	AAAC	3	ASN
3	AAAC	113	ASN
3	AAAC	135	THR
3	AAAC	157	CYS
3	AAAC	190	ILE
4	AAAD	17	ASN
4	AAAD	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	A	260	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
6	GOL	A	302	-	5,5,5	0.95	0	5,5,5	1.08	0
6	GOL	A	304	-	5,5,5	0.95	0	5,5,5	1.07	0
6	GOL	A	303	-	5,5,5	0.94	0	5,5,5	1.07	0
5	Q87	A	301	1	22,22,23	1.05	2 (9%)	24,29,31	0.72	1 (4%)

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
6	GOL	A	302	-	-	2/4/4/4	-
6	GOL	A	304	-	-	0/4/4/4	-
6	GOL	A	303	-	-	0/4/4/4	-
5	Q87	A	301	1	-	2/18/19/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	Q87	C4-N1	3.45	1.38	1.32
5	A	301	Q87	C1-C2	-3.06	1.46	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	301	Q87	C5-N1-C4	-2.34	121.74	126.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

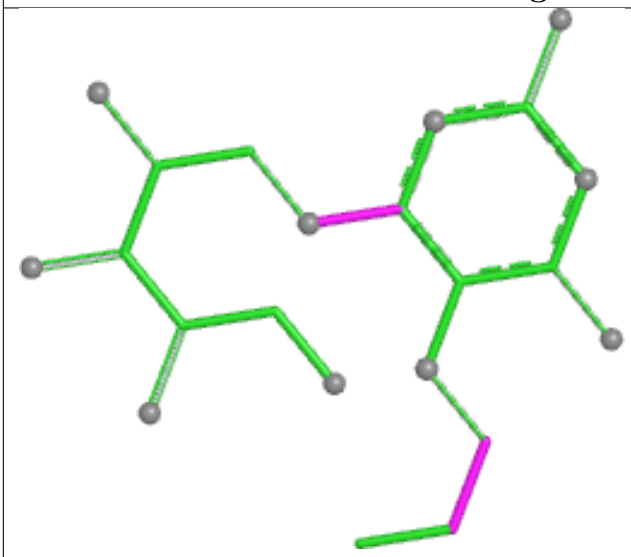
Mol	Chain	Res	Type	Atoms
6	A	302	GOL	O1-C1-C2-C3
6	A	302	GOL	O1-C1-C2-O2
5	A	301	Q87	N1-C5-C6-C7
5	A	301	Q87	C5-C6-C7-O2

There are no ring outliers.

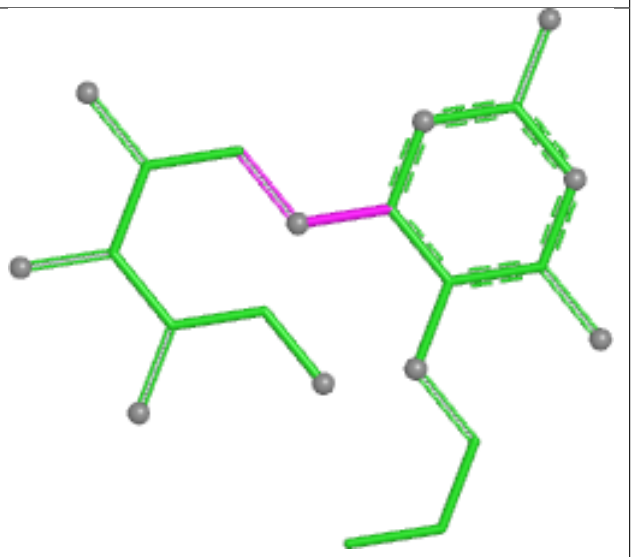
No monomer is involved in short contacts.

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 then 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.

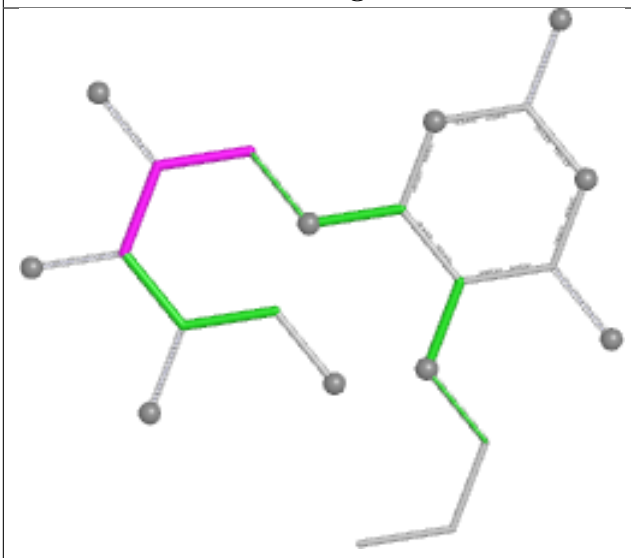
Ligand Q87 A 301



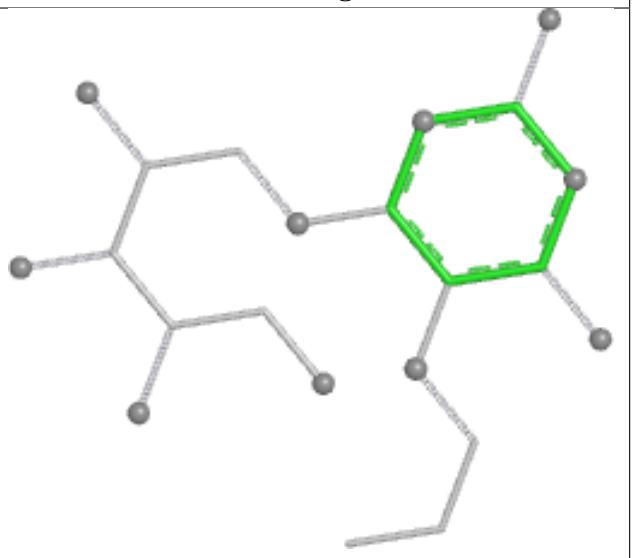
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	267/271 (98%)	-0.31	1 (0%)	89	77	25, 57, 102, 139	3 (1%)
2	AAAB	196/244 (80%)	0.50	14 (7%)	23	14	46, 107, 149, 216	2 (1%)
3	AAAC	173/204 (84%)	-0.01	3 (1%)	69	50	38, 67, 145, 175	0
4	AAAD	99/100 (99%)	-0.07	2 (2%)	64	45	43, 74, 106, 124	1 (1%)
All	All	735/819 (89%)	0.01	20 (2%)	56	36	25, 71, 133, 216	6 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AAAB	181	ALA	4.5
3	AAAC	148	ASP	4.2
1	A	192	PHE	3.8
2	AAAB	140	ALA	3.6
3	AAAC	187	ASN	3.2
3	AAAC	147	LYS	3.2
2	AAAB	165	VAL	3.0
4	AAAD	0	MET	2.9
2	AAAB	117	LYS	2.9
2	AAAB	48	PHE	2.6
2	AAAB	156	LEU	2.6
2	AAAB	223	THR	2.5
4	AAAD	98	ASP	2.5
2	AAAB	142	LEU	2.5
2	AAAB	237	GLU	2.5
2	AAAB	141	THR	2.3
2	AAAB	189	LEU	2.2
2	AAAB	227	ALA	2.1
2	AAAB	120	PHE	2.1
2	AAAB	128	GLU	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

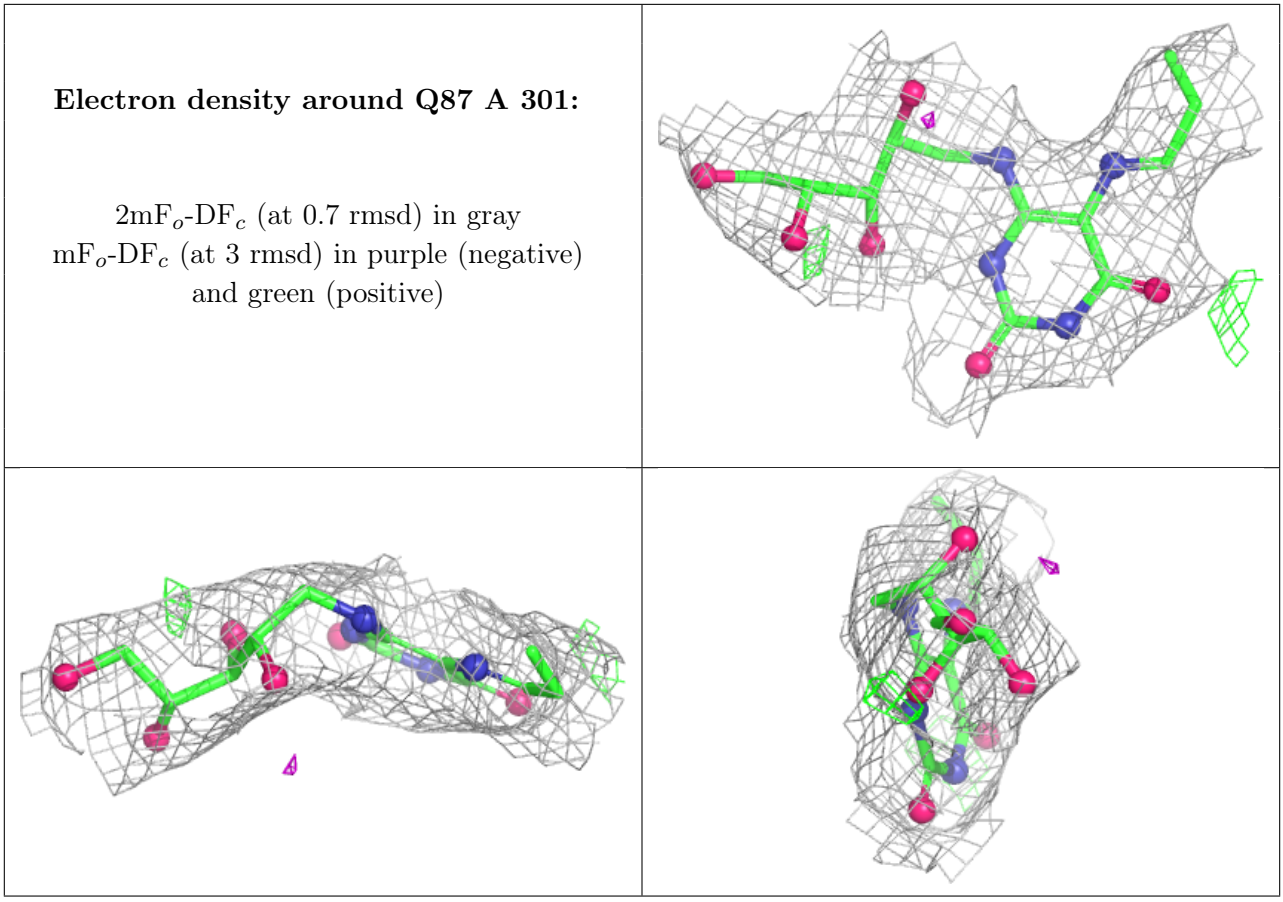
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	302	6/6	0.81	0.14	78,82,85,87	0
6	GOL	A	304	6/6	0.83	0.19	80,80,80,80	0
6	GOL	A	303	6/6	0.87	0.13	70,72,78,78	0
5	Q87	A	301	22/23	0.96	0.08	37,43,47,51	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 Q87 A 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

There are no such residues in this entry.