



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 06:37 PM UTC

PDB ID : 2QKY / pdb_00002qky
Title : complex structure of dipeptidyl peptidase IV and a oxadiazolyl ketone
Authors : Kim, K.-H.; Hong, S.Y.; Koo, K.D.; Lee, C.-S.; Kim, G.T.; Han, H.O.
Deposited on : 2007-07-12
Resolution : 3.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

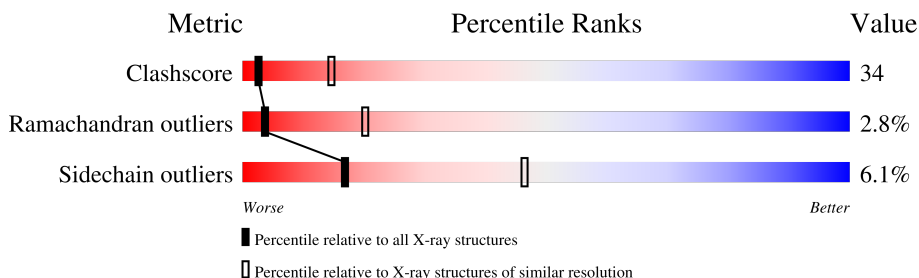
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	42% 49% 9%
1	B	728	42% 50% 7%
1	C	728	42% 50% 7%
1	D	728	43% 49% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24275 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.

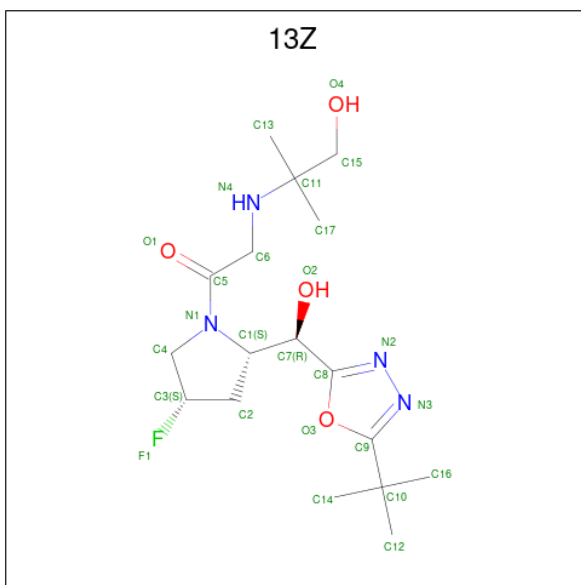
- Molecule 1 is a protein called Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	B	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	C	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	D	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	-	expression tag	UNP P27487
B	39	THR	-	expression tag	UNP P27487
C	39	THR	-	expression tag	UNP P27487
D	39	THR	-	expression tag	UNP P27487

- Molecule 2 is 2-[(2-{(2S,4S)-2-[(R)-(5-tert-butyl-1,3,4-oxadiazol-2-yl)(hydroxy)methyl]-4-fluoropyrrolidin-1-yl}-2-oxoethyl)amino]-2-methylpropan-1-ol (CCD ID: 13Z) (formula: C₁₇H₂₉FN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	B	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	C	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	D	1	Total 26	C 17	F 1	N 4	O 4	0	0

- Molecule 3 is water.

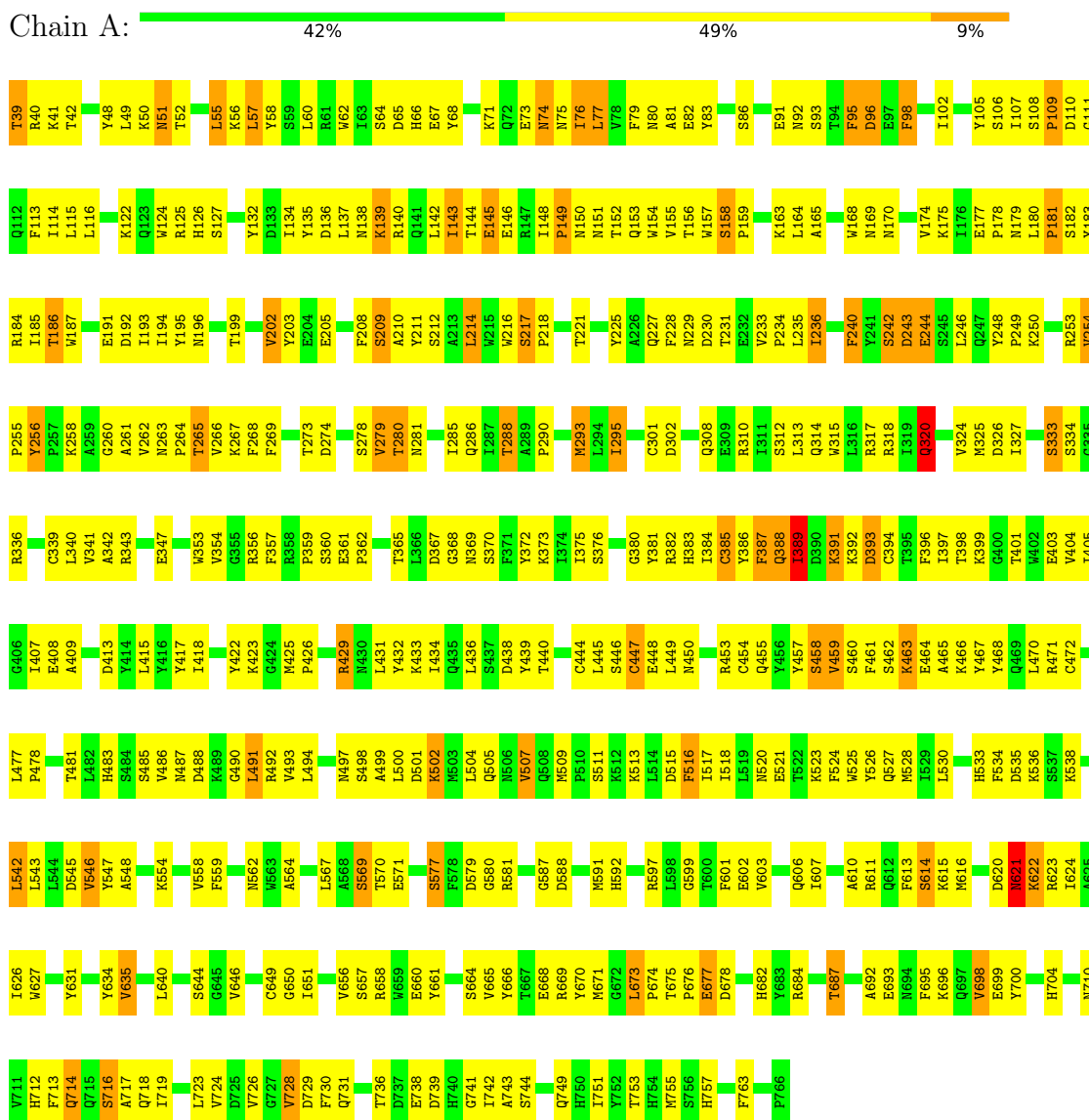
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	72	Total	O	0	0
			72	72		
3	C	66	Total	O	0	0
			66	66		
3	D	92	Total	O	0	0
			92	92		

3 Residue-property plots

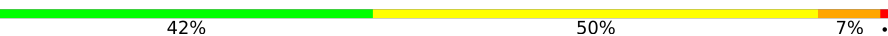
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

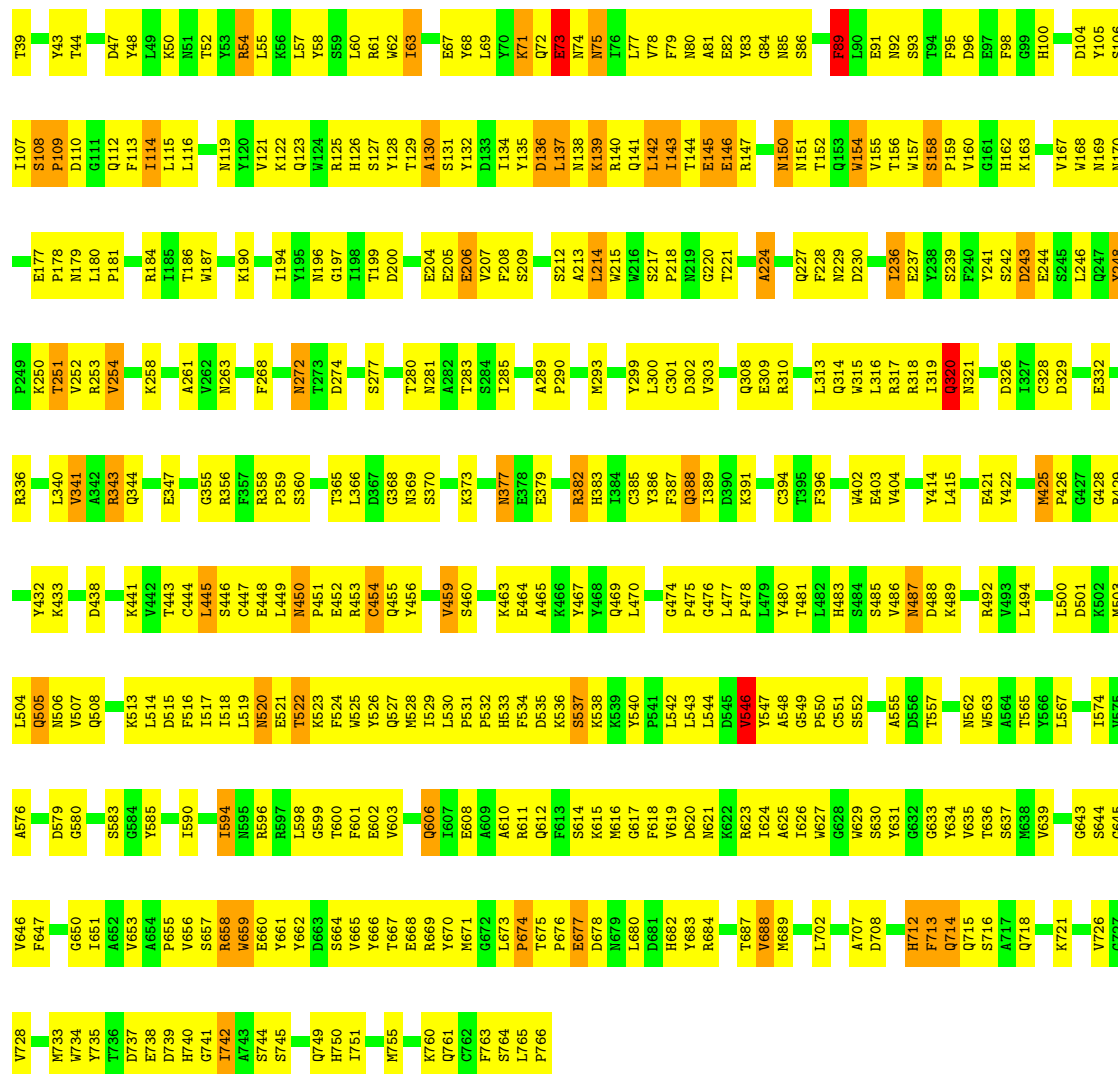
Note EDS was not executed.

- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

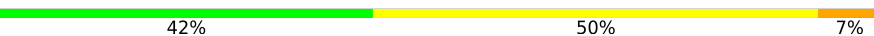


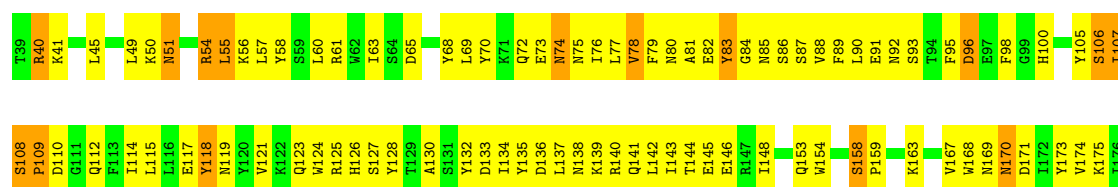
- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

Chain B: 



- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

Chain C: 





M733	M734	D737	E738	D739	H740	G741	I742	A743	S744	S745	Q749	H750	I751	Y752	M755	I759	K760	Q761	C762	F763	S764	L765	P766		
S642	G643	F647	K648	G649	G650	V653	A654	P655	V656	S657	R658	W659	E660	Y661	D663	S664	V665	Y666	T667	E668	R669	E677	D678	N679	
W663	L667	E571	N572	I573	S577	R581	Y585	Q586	K589	I590	M591	I594	N595	R596	R597	L598	F601	E602	D605	Q606	I607	R611	Q612	F613	
T481	L482	H483	S484	S485	W486	M487	L491	R492	V493	L494	D501	L504	Q505	N506	V507	Q508	M509	P510	S511	K512	K513	L514	D515	F516	I517
N520	E521	T522	K523	Y526	Q527	L530	P531	P532	H533	P541	L544	D545	V546	Y547	A548	G549	P550	C551	S552	T557	L561	N562			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.18Å 106.11Å 132.05Å 76.30° 78.62° 80.11°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	86.7 (20.00-3.10)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24275	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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:
13Z

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	0.67	0/6137	1.09	35/8346 (0.4%)
1	B	0.67	0/6137	1.11	47/8346 (0.6%)
1	C	0.66	2/6137 (0.0%)	1.06	29/8346 (0.3%)
1	D	0.69	0/6137	1.10	47/8346 (0.6%)
All	All	0.67	2/24548 (0.0%)	1.09	158/33384 (0.5%)

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	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	319	ILE	CA-CB	6.30	1.60	1.53
1	C	107	ILE	CA-CB	5.41	1.59	1.54

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	335	GLY	N-CA-C	-8.79	103.04	115.43
1	B	415	LEU	N-CA-C	-8.61	95.89	109.50
1	A	546	VAL	N-CA-C	8.57	120.83	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	454	CYS	N-CA-C	8.42	122.14	108.34
1	D	546	VAL	N-CA-C	8.36	119.73	108.27

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	TYR	Sidechain
1	A	700	TYR	Sidechain
1	B	128	TYR	Sidechain
1	C	83	TYR	Sidechain
1	D	752	TYR	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	5965	0	5686	410	0
1	B	5965	0	5686	411	0
1	C	5965	0	5686	390	0
1	D	5965	0	5686	408	0
2	A	26	0	28	2	0
2	B	26	0	28	2	0
2	C	26	0	28	1	0
2	D	26	0	28	3	0
3	A	81	0	0	2	0
3	B	72	0	0	5	0
3	C	66	0	0	2	0
3	D	92	0	0	9	0
All	All	24275	0	22856	1587	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 34.

The worst 5 of 1587 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:D:173:TYR:HE2	1:D:184:ARG:HG2	1.07	1.12
1:D:173:TYR:CE2	1:D:184:ARG:HG2	1.89	1.06
1:A:253:ARG:HH21	1:B:253:ARG:NH1	1.55	1.05
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.41	1.03
1:A:154:TRP:CZ3	1:A:214:LEU:HD21	1.95	1.02

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	726/728 (100%)	593 (82%)	112 (15%)	21 (3%)	3	19
1	B	726/728 (100%)	622 (86%)	84 (12%)	20 (3%)	4	20
1	C	726/728 (100%)	620 (85%)	86 (12%)	20 (3%)	4	20
1	D	726/728 (100%)	634 (87%)	73 (10%)	19 (3%)	4	21
All	All	2904/2912 (100%)	2469 (85%)	355 (12%)	80 (3%)	4	20

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	320	GLN
1	A	439	TYR
1	B	137	LEU
1	B	320	GLN

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	653/653 (100%)	611 (94%)	42 (6%)	16	44
1	B	653/653 (100%)	620 (95%)	33 (5%)	21	52
1	C	653/653 (100%)	611 (94%)	42 (6%)	16	44
1	D	653/653 (100%)	610 (93%)	43 (7%)	15	43
All	All	2612/2612 (100%)	2452 (94%)	160 (6%)	17	46

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	728	VAL
1	D	284	SER
1	D	57	LEU
1	D	156	THR
1	D	507	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	169	ASN
1	D	714	GLN
1	D	227	GLN
1	D	487	ASN
1	B	298	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	13Z	C	767	1	25,27,27	1.54	3 (12%)	31,41,41	1.18	2 (6%)
2	13Z	D	767	1	25,27,27	1.01	2 (8%)	31,41,41	1.11	2 (6%)
2	13Z	B	767	1	25,27,27	1.46	3 (12%)	31,41,41	1.08	3 (9%)
2	13Z	A	767	1	25,27,27	1.58	5 (20%)	31,41,41	1.15	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	13Z	C	767	1	-	6/26/39/39	0/2/2/2
2	13Z	D	767	1	-	9/26/39/39	0/2/2/2
2	13Z	B	767	1	-	7/26/39/39	0/2/2/2
2	13Z	A	767	1	-	9/26/39/39	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	767	13Z	C9-N3	5.26	1.33	1.28
2	C	767	13Z	C9-N3	5.14	1.33	1.28
2	A	767	13Z	C9-N3	4.35	1.32	1.28
2	A	767	13Z	C11-N4	3.94	1.53	1.49
2	C	767	13Z	C8-N2	2.96	1.31	1.28

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	767	13Z	C3-C4-N1	2.75	107.16	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	767	13Z	C3-C4-N1	2.56	106.88	103.13
2	D	767	13Z	C4-N1-C5	-2.54	124.37	129.13
2	C	767	13Z	C4-N1-C5	-2.52	124.42	129.13
2	D	767	13Z	C3-C4-N1	2.42	106.68	103.13

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	767	13Z	C5-C6-N4-C11
2	A	767	13Z	O2-C7-C8-O3
2	A	767	13Z	C13-C11-N4-C6
2	A	767	13Z	C15-C11-N4-C6
2	A	767	13Z	C17-C11-N4-C6

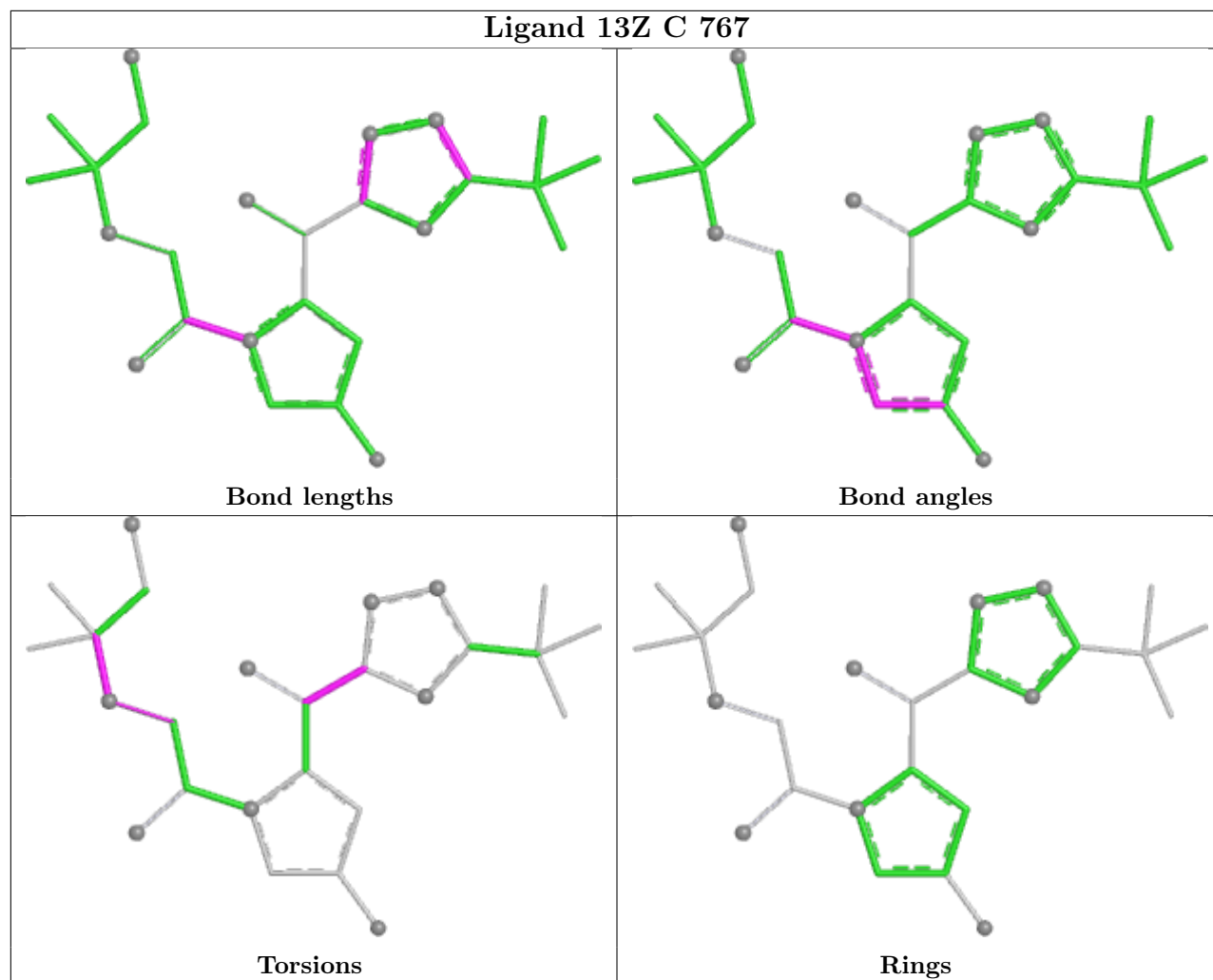
There are no ring outliers.

4 monomers are involved in 8 short contacts:

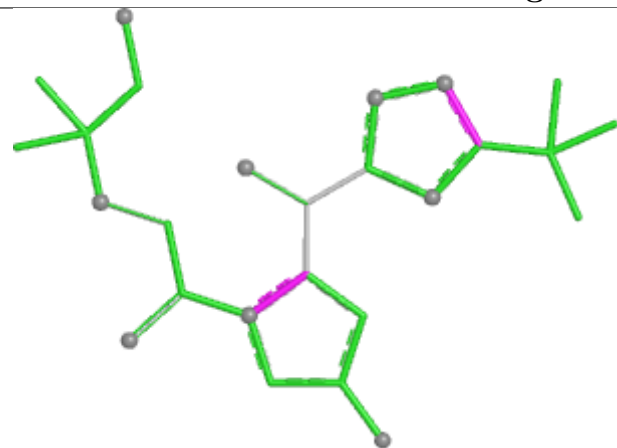
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	767	13Z	1	0
2	D	767	13Z	3	0
2	B	767	13Z	2	0
2	A	767	13Z	2	0

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.

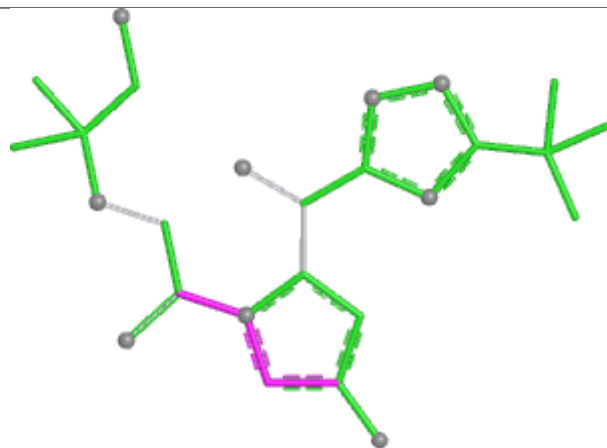
Ligand 13Z C 767



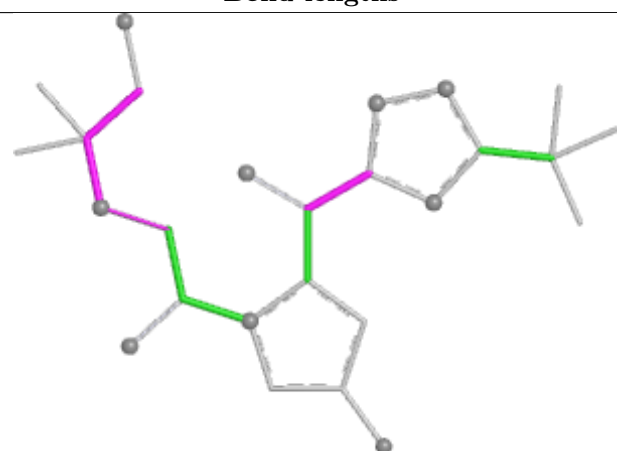
Ligand 13Z D 767



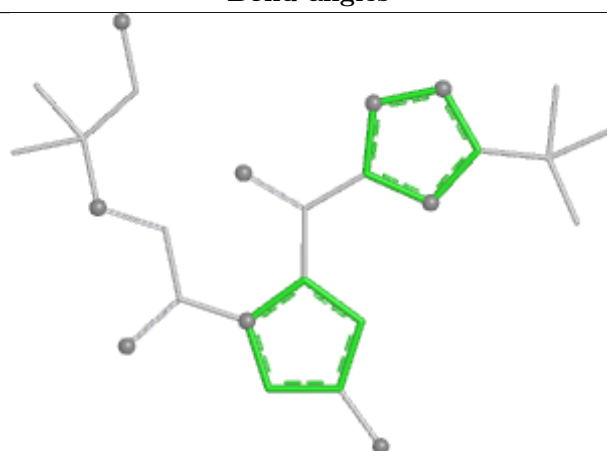
Bond lengths



Bond angles

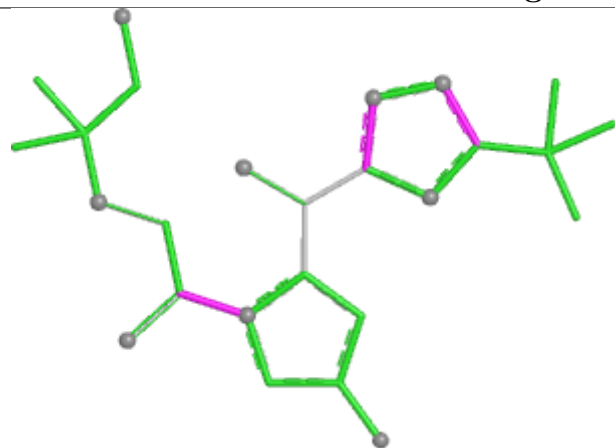


Torsions

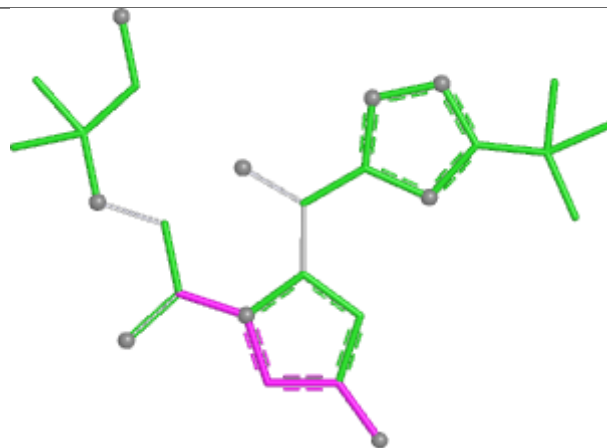


Rings

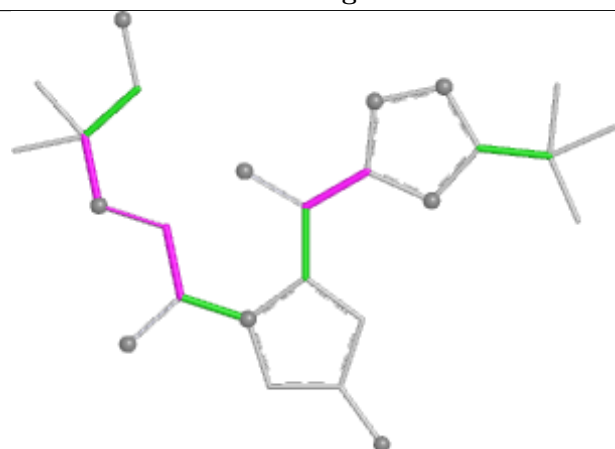
Ligand 13Z B 767



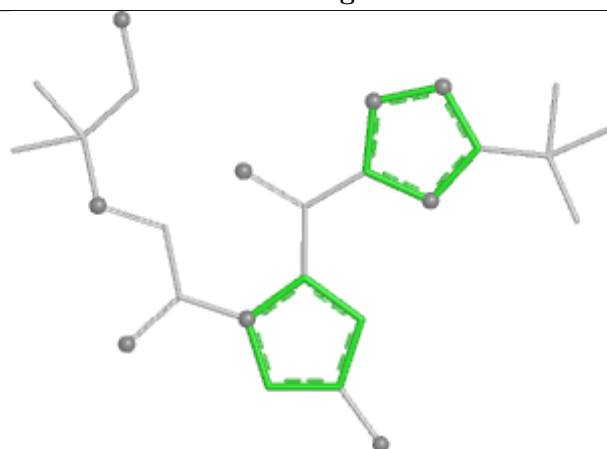
Bond lengths



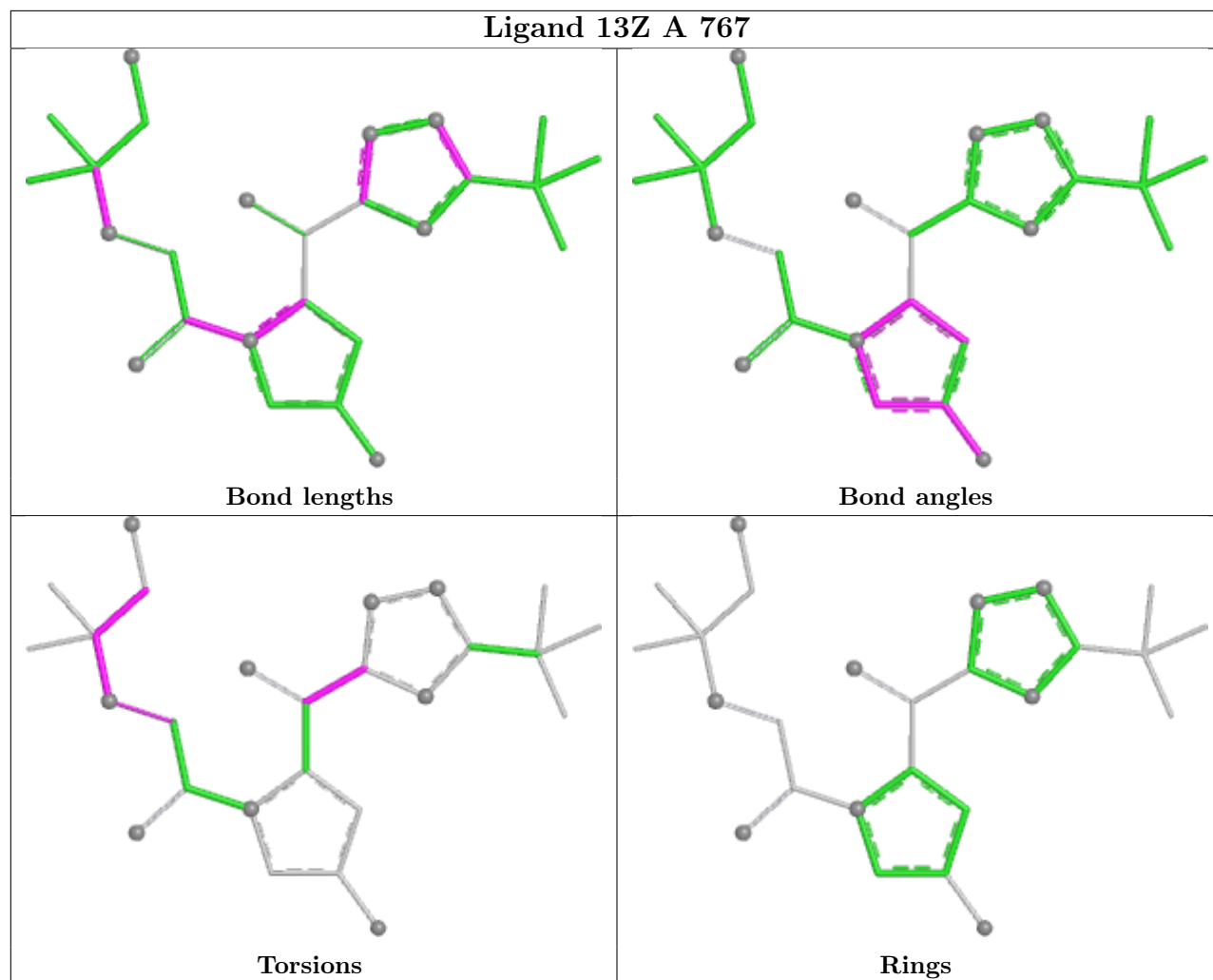
Bond angles



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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.