



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:24 AM GMT

PDB ID : 2QKY
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

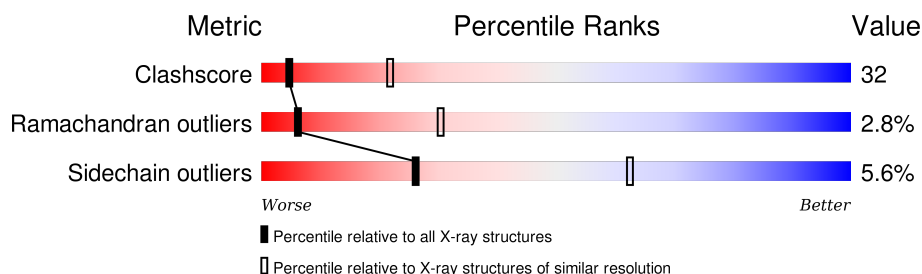
1 Overall quality at a glance

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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>44%</div> <div>51%</div> <div>5%</div> </div>
1	B	728	<div> <div>46%</div> <div>49%</div> <div>.</div> </div>
1	C	728	<div> <div>46%</div> <div>49%</div> <div>5%</div> </div>
1	D	728	<div> <div>47%</div> <div>48%</div> <div>5%</div> </div>

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.

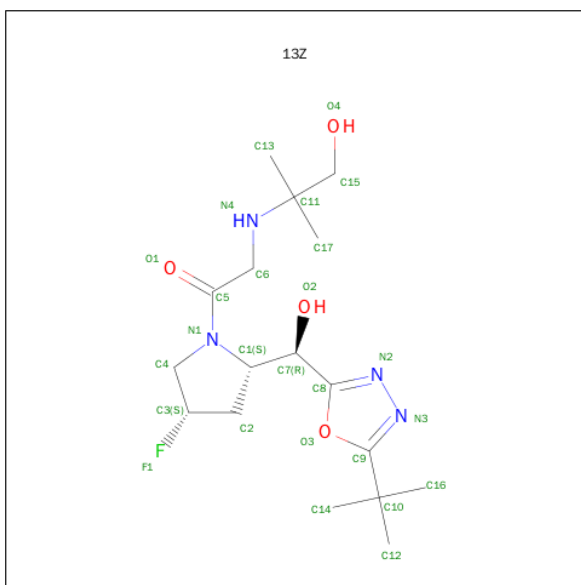
- Molecule 1 is a protein called Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form).

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-METHYLPAN-1-OL (three-letter code: 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.

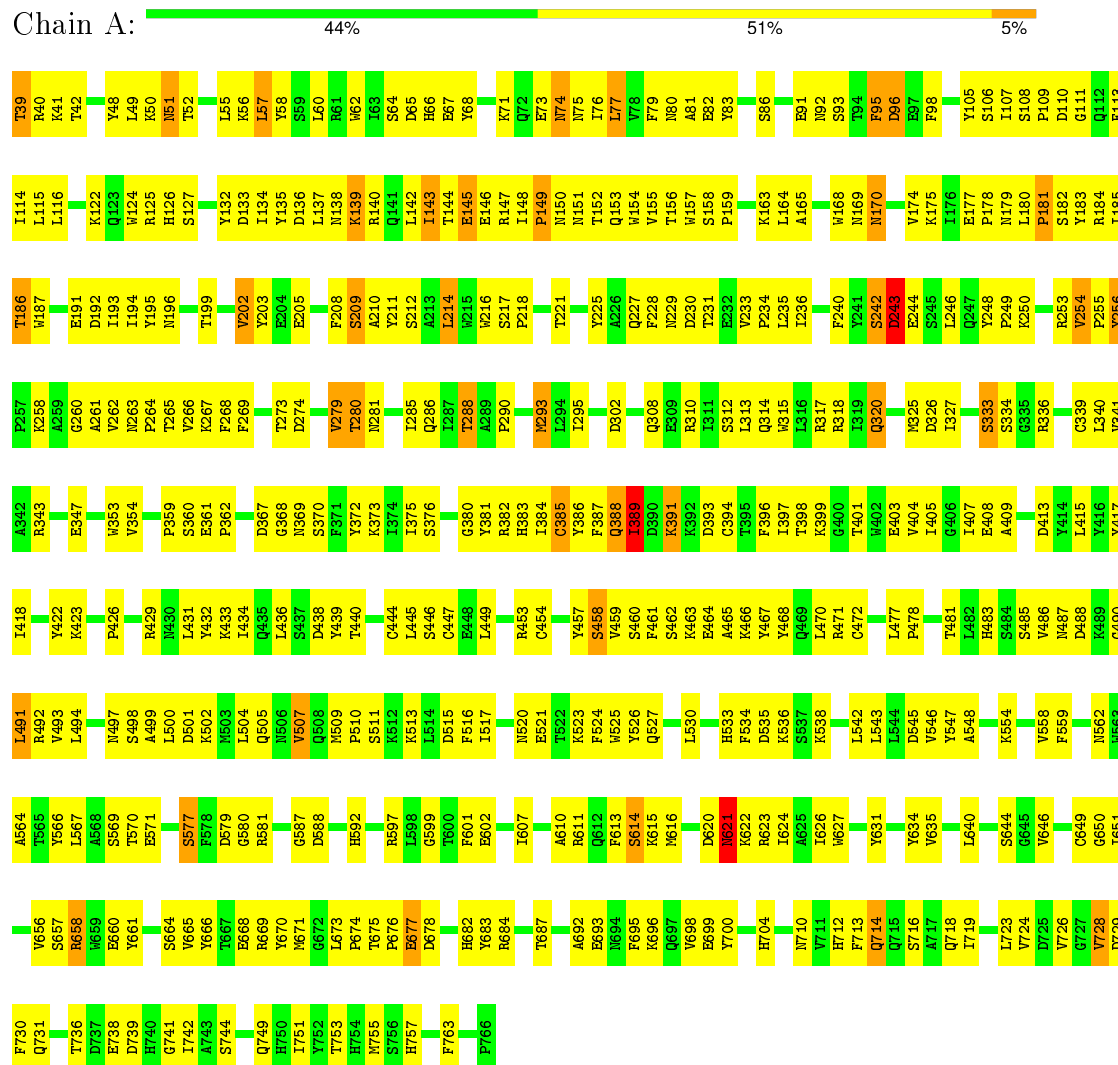
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	72	Total	O	0	0
			72	72		
3	C	66	Total	O	0	0
			66	66		
3	D	92	Total	O	0	0
			92	92		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

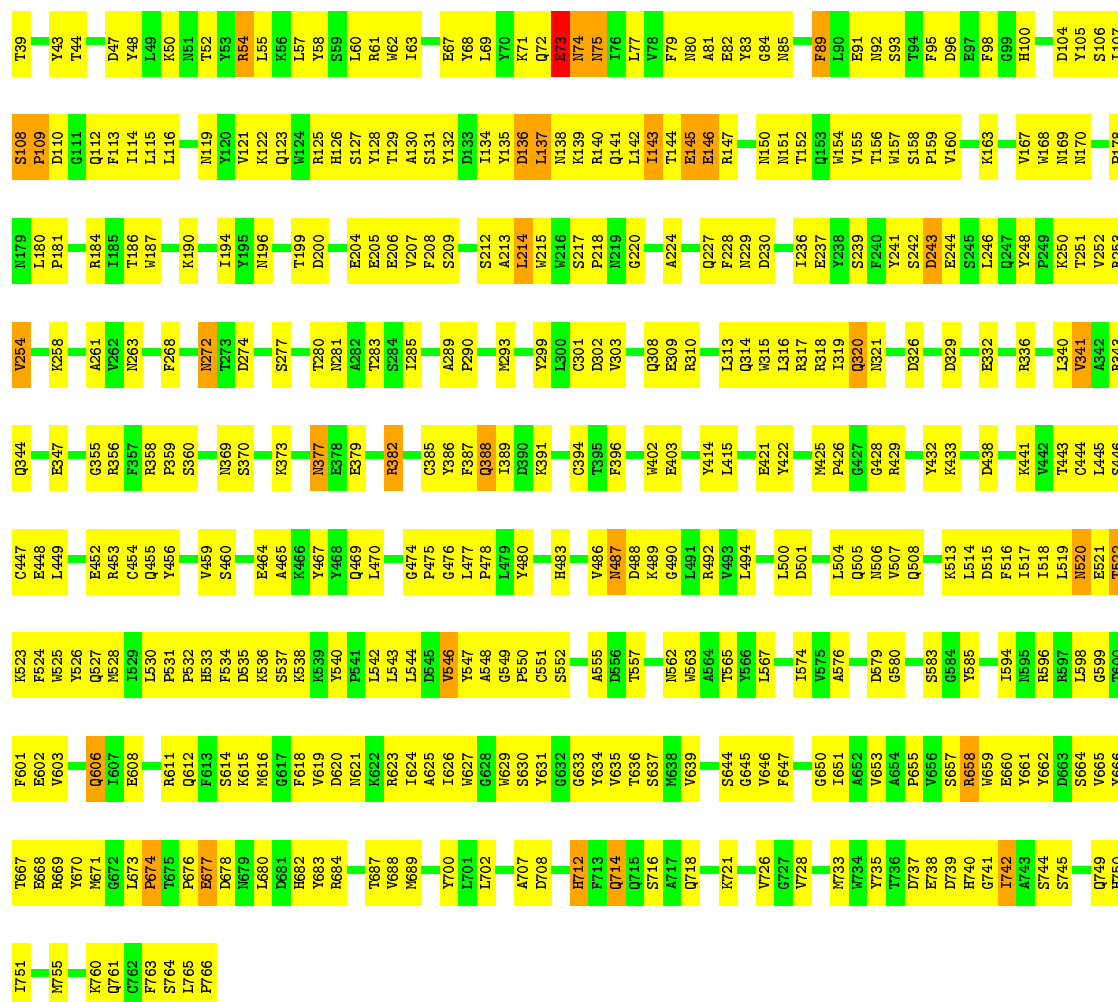
Note EDS was not executed.

- 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)



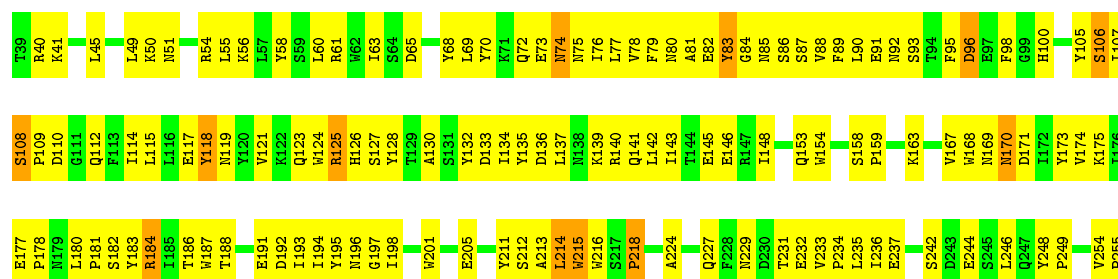
- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

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: 



P766	D678 M679 L680 D681 H682 Y683 R684 M685 M689 V688 E699 I703 H704 D708 W709 M710 V711 H712 F713 Q714 Q715 I719 S720 K721 V724 A732 M733 W734 D737 E738 D739 H740 G741 I742 A743 S744 S745 Q749 H750 Y752 M755 I759 K760 Q761 C762 F763 S764 I765
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.18 Å 106.11 Å 132.05 Å 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

5.1 Standard geometry

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	0.56	0/6137	0.76	0/8346
1	B	0.56	0/6137	0.75	2/8346 (0.0%)
1	C	0.56	0/6137	0.73	2/8346 (0.0%)
1	D	0.56	0/6137	0.75	0/8346
All	All	0.56	0/24548	0.75	4/33384 (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	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	415	LEU	N-CA-C	-5.60	95.89	111.00
1	C	388	GLN	N-CA-C	-5.33	96.60	111.00
1	B	388	GLN	N-CA-C	-5.11	97.20	111.00

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	385	0
1	B	5965	0	5686	389	0
1	C	5965	0	5686	364	0
1	D	5965	0	5686	383	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	1490	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 32.

The worst 5 of 1490 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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	6	29
1	B	726/728 (100%)	622 (86%)	84 (12%)	20 (3%)	6	30
1	C	726/728 (100%)	620 (85%)	86 (12%)	20 (3%)	6	30
1	D	726/728 (100%)	634 (87%)	73 (10%)	19 (3%)	7	32
All	All	2904/2912 (100%)	2469 (85%)	355 (12%)	80 (3%)	6	30

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 ⓘ

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%)	610 (93%)	43 (7%)	21	56
1	B	653/653 (100%)	624 (96%)	29 (4%)	35	71
1	C	653/653 (100%)	616 (94%)	37 (6%)	25	62
1	D	653/653 (100%)	616 (94%)	37 (6%)	25	62
All	All	2612/2612 (100%)	2466 (94%)	146 (6%)	26	62

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	546	VAL
1	C	215	TRP
1	D	351	THR
1	B	606	GLN
1	C	118	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	712	HIS
1	C	126	HIS
1	D	595	ASN
1	B	731	GLN
1	C	75	ASN

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 carbohydrates 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	A	767	1	22,27,27	1.68	6 (27%)	24,41,41	2.36	4 (16%)
2	13Z	B	767	1	22,27,27	1.48	4 (18%)	24,41,41	2.24	4 (16%)
2	13Z	C	767	1	22,27,27	1.73	3 (13%)	24,41,41	1.96	2 (8%)
2	13Z	D	767	1	22,27,27	1.44	5 (22%)	24,41,41	2.23	3 (12%)

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	A	767	1	-	0/20/39/39	0/1/2/2
2	13Z	B	767	1	-	0/20/39/39	0/1/2/2
2	13Z	C	767	1	-	0/20/39/39	0/1/2/2
2	13Z	D	767	1	-	0/20/39/39	0/1/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	767	13Z	F1-C3	-2.99	1.33	1.41
2	D	767	13Z	C8-N2	-2.94	1.30	1.33
2	A	767	13Z	F1-C3	-2.83	1.34	1.41
2	D	767	13Z	F1-C3	-2.78	1.34	1.41
2	B	767	13Z	F1-C3	-2.69	1.34	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	767	13Z	O2-C7-C8	-2.33	104.54	109.78
2	D	767	13Z	O2-C7-C8	-2.07	105.13	109.78
2	A	767	13Z	C2-C1-N1	2.02	104.77	101.68
2	B	767	13Z	C6-N4-C11	2.45	122.69	117.68
2	A	767	13Z	C6-N4-C11	2.46	122.72	117.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.