Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 02:11 PM EDT

PDB ID	:	2I0E
Title	:	Structure of catalytic domain of human protein kinase C beta II complexed with a bisindolylmaleimide inhibitor
Authors	:	Grodsky, N.B.; Love, R.L.
Deposited on	:	2006-08-10
Resolution	:	2.60 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 (1)) were used in the production of this report:

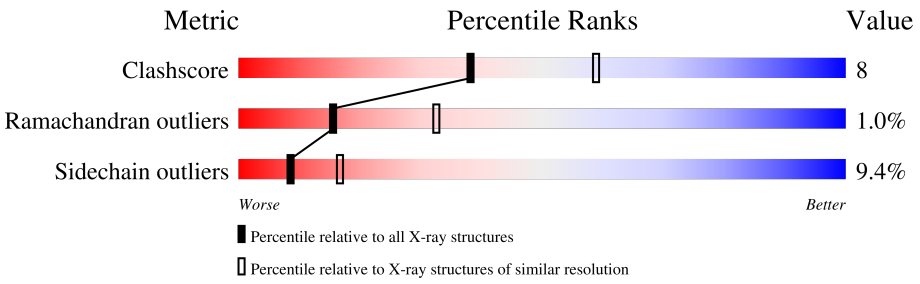
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	353	72% 18% • 7%
1	B	353	69% 14% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5293 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 Protein Kinase C-beta II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	329	2672	1721	434	495	3	19	0	0	0
1	B	302	2440	1578	390	452	2	18	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	TPO	THR	modified residue	UNP P05771
A	?	-	ARG	SEE REMARK 999	UNP P05771
A	622	CYS	ASP	SEE REMARK 999	UNP P05771
A	623	GLY	LYS	SEE REMARK 999	UNP P05771
A	625	ASN	ASP	SEE REMARK 999	UNP P05771
A	626	ALA	THR	SEE REMARK 999	UNP P05771
A	627	GLU	SER	SEE REMARK 999	UNP P05771
A	631	ARG	LYS	SEE REMARK 999	UNP P05771
A	632	PHE	GLU	SEE REMARK 999	UNP P05771
A	636	HIS	GLN	SEE REMARK 999	UNP P05771
A	638	PRO	VAL	SEE REMARK 999	UNP P05771
A	639	VAL	GLU	SEE REMARK 999	UNP P05771
A	641	TPO	THR	modified residue	UNP P05771
A	643	PRO	THR	SEE REMARK 999	UNP P05771
A	645	GLN	LYS	SEE REMARK 999	UNP P05771
A	646	GLU	LEU	SEE REMARK 999	UNP P05771
A	647	VAL	PHE	SEE REMARK 999	UNP P05771
A	649	ARG	MET	SEE REMARK 999	UNP P05771
A	651	ILE	LEU	SEE REMARK 999	UNP P05771
A	654	SER	ASN	SEE REMARK 999	UNP P05771
A	657	GLU	ALA	SEE REMARK 999	UNP P05771
A	660	SEP	SER	modified residue	UNP P05771
A	661	PHE	TYR	SEE REMARK 999	UNP P05771
A	662	VAL	THR	SEE REMARK 999	UNP P05771
A	664	SER	PRO	SEE REMARK 999	UNP P05771

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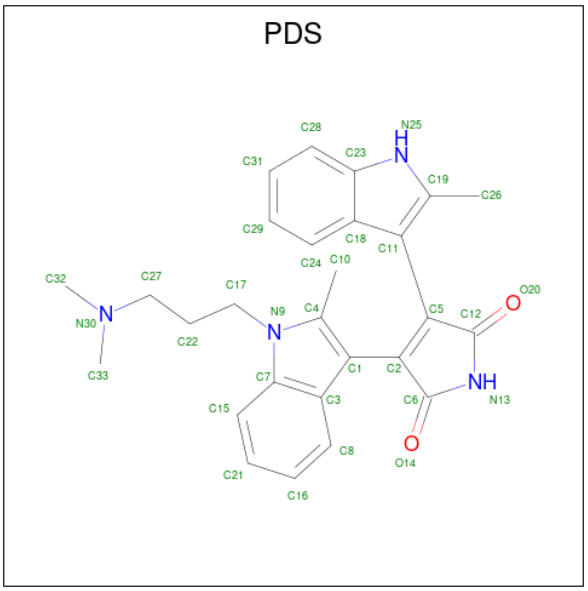
Chain	Residue	Modelled	Actual	Comment	Reference
A	667	LEU	VAL	SEE REMARK 999	UNP P05771
A	668	LYS	ILE	SEE REMARK 999	UNP P05771
A	669	PRO	ASN	SEE REMARK 999	UNP P05771
A	670	GLU	VAL	SEE REMARK 999	UNP P05771
A	671	VAL	-	SEE REMARK 999	UNP P05771
A	672	LYS	-	SEE REMARK 999	UNP P05771
A	673	SER	-	SEE REMARK 999	UNP P05771
B	500	TPO	THR	modified residue	UNP P05771
B	?	-	ARG	SEE REMARK 999	UNP P05771
B	622	CYS	ASP	SEE REMARK 999	UNP P05771
B	623	GLY	LYS	SEE REMARK 999	UNP P05771
B	625	ASN	ASP	SEE REMARK 999	UNP P05771
B	626	ALA	THR	SEE REMARK 999	UNP P05771
B	627	GLU	SER	SEE REMARK 999	UNP P05771
B	631	ARG	LYS	SEE REMARK 999	UNP P05771
B	632	PHE	GLU	SEE REMARK 999	UNP P05771
B	636	HIS	GLN	SEE REMARK 999	UNP P05771
B	638	PRO	VAL	SEE REMARK 999	UNP P05771
B	639	VAL	GLU	SEE REMARK 999	UNP P05771
B	641	TPO	THR	modified residue	UNP P05771
B	643	PRO	THR	SEE REMARK 999	UNP P05771
B	645	GLN	LYS	SEE REMARK 999	UNP P05771
B	646	GLU	LEU	SEE REMARK 999	UNP P05771
B	647	VAL	PHE	SEE REMARK 999	UNP P05771
B	649	ARG	MET	SEE REMARK 999	UNP P05771
B	651	ILE	LEU	SEE REMARK 999	UNP P05771
B	654	SER	ASN	SEE REMARK 999	UNP P05771
B	657	GLU	ALA	SEE REMARK 999	UNP P05771
B	660	SEP	SER	modified residue	UNP P05771
B	661	PHE	TYR	SEE REMARK 999	UNP P05771
B	662	VAL	THR	SEE REMARK 999	UNP P05771
B	664	SER	PRO	SEE REMARK 999	UNP P05771
B	667	LEU	VAL	SEE REMARK 999	UNP P05771
B	668	LYS	ILE	SEE REMARK 999	UNP P05771
B	669	PRO	ASN	SEE REMARK 999	UNP P05771
B	670	GLU	VAL	SEE REMARK 999	UNP P05771
B	671	VAL	-	SEE REMARK 999	UNP P05771
B	672	LYS	-	SEE REMARK 999	UNP P05771
B	673	SER	-	SEE REMARK 999	UNP P05771

- Molecule 2 is 3-{1-[3-(DIMETHYLAMINO)PROPYL]-2-METHYL-1H-INDOL-3-YL}-4-(2-METHYL-1H-INDOL-3-YL)-1H-PYRROLE-2,5-DIONE (three-letter code: PDS) (formula: $C_{27}H_{28}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	27	4	2	0	0
			Total	C	N	O		
2	B	1	33	27	4	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	63	63	63	0	0
			Total	O		
3	B	52	52	52	0	0

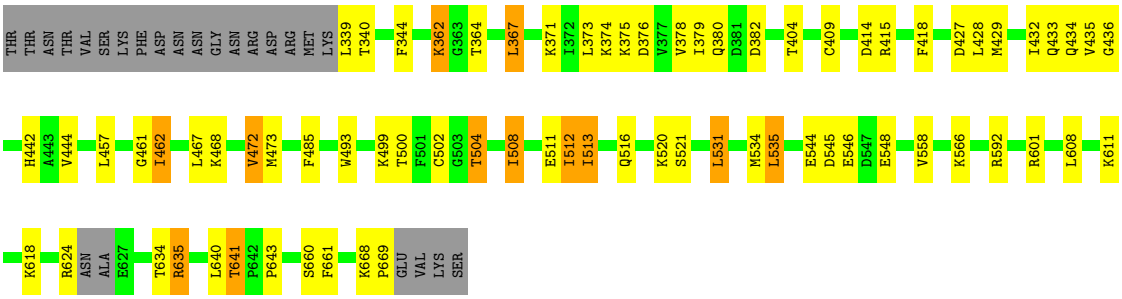
3 Residue-property plots (i)

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. 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.

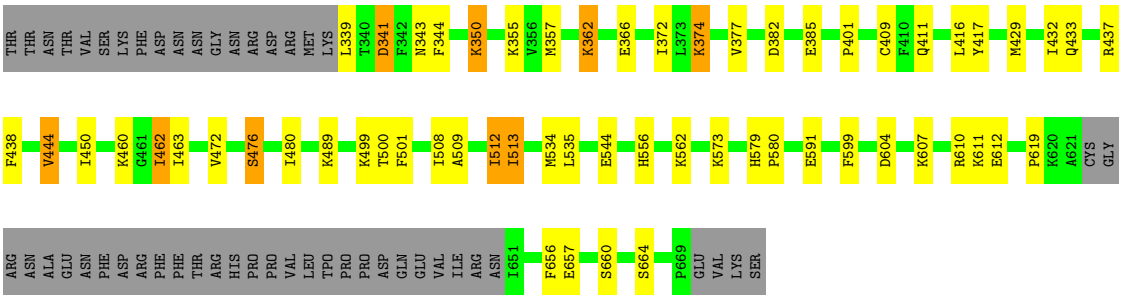
• Molecule 1: Protein Kinase C-beta II

Chain A: 72% 18% • 7%



• Molecule 1: Protein Kinase C-beta II

Chain B: 69% 14% • 14%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	93.10Å 131.42Å 83.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.9 (30.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.235 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5293	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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: PDS, SEP, TPO

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	0.49	0/2707	0.62	0/3644
1	B	0.49	0/2479	0.63	0/3336
All	All	0.49	0/5186	0.63	0/6980

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	GLY	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	2672	0	2606	44	0
1	B	2440	0	2391	33	0
2	A	33	0	28	2	0
2	B	33	0	28	0	0
3	A	63	0	0	2	0
3	B	52	0	0	0	0
All	All	5293	0	5053	78	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 8.

All (78) 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:635:ARG:HG3	1:A:635:ARG:HH21	1.02	1.13
1:A:635:ARG:HG3	1:A:635:ARG:NH2	1.83	0.85
1:A:635:ARG:HH21	1:A:635:ARG:CG	1.91	0.81
1:A:428:LEU:HD21	1:A:534:MET:CE	2.16	0.74
1:B:350:LYS:HB2	1:B:355:LYS:HG3	1.72	0.71
1:A:511:GLU:OE2	1:A:521:SER:HB3	1.98	0.63
1:A:428:LEU:HD21	1:A:534:MET:HE1	1.83	0.61
1:A:508:ILE:CD1	1:A:512:ILE:HG12	2.31	0.61
1:A:367:LEU:HD21	1:A:624:ARG:HD3	1.84	0.59
1:A:428:LEU:HD21	1:A:534:MET:HE3	1.84	0.58
1:B:544:GLU:CD	1:B:544:GLU:H	2.07	0.57
1:A:545:ASP:HB3	1:A:548:GLU:H	1.68	0.57
1:A:339:LEU:HD11	1:A:344:PHE:CZ	2.40	0.56
1:A:434:GLN:HG3	1:A:435:VAL:HG13	1.88	0.56
1:A:457:LEU:HD22	1:A:462:ILE:HD12	1.87	0.56
1:B:509:ALA:O	1:B:513:ILE:HG23	2.06	0.56
1:B:450:ILE:HG13	1:B:480:ILE:HD13	1.87	0.55
1:B:460:LYS:HB2	1:B:462:ILE:HG23	1.89	0.54
1:A:641:TPO:H	1:A:641:TPO:P	2.30	0.54
1:B:508:ILE:CD1	1:B:513:ILE:HG22	2.39	0.53
1:A:340:THR:HG22	1:A:362:LYS:NZ	2.24	0.52
1:A:502:CYS:H	1:A:512:ILE:HD11	1.73	0.52
1:A:468:LYS:NZ	1:A:504:THR:HG21	2.24	0.52
1:A:415:ARG:NH1	1:A:640:LEU:HD22	2.25	0.52
1:A:531:LEU:HD22	1:A:535:LEU:HD22	1.92	0.52
1:A:428:LEU:HD22	1:A:472:VAL:CG2	2.41	0.51
1:B:401:PRO:CB	1:B:611:LYS:HE2	2.40	0.51
1:B:508:ILE:HD12	1:B:513:ILE:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:GLN:OE1	1:B:656:PHE:HB2	2.11	0.50
1:A:404:THR:HG22	1:A:485:PHE:HE2	1.77	0.49
1:B:501:PHE:HA	1:B:512:ILE:HD12	1.94	0.49
1:B:432:ILE:HD11	1:B:437:ARG:HA	1.95	0.49
1:A:508:ILE:HD11	1:A:512:ILE:HG12	1.94	0.49
1:B:476:SER:O	1:B:619:PRO:HD2	2.13	0.48
1:B:372:ILE:HG12	1:B:417:TYR:CD2	2.49	0.48
1:B:604:ASP:HB3	1:B:607:LYS:HG2	1.96	0.48
1:A:457:LEU:HB3	1:A:462:ILE:HD13	1.95	0.48
1:B:610:ARG:HD2	1:B:612:GLU:OE2	2.15	0.47
1:B:344:PHE:HB3	1:B:357:MET:CE	2.45	0.46
1:A:404:THR:HG21	3:A:58:HOH:O	2.15	0.46
1:A:427:ASP:HA	1:A:473:MET:HA	1.98	0.46
1:B:374:LYS:HD2	1:B:377:VAL:HG21	1.98	0.46
1:A:544:GLU:N	1:A:548:GLU:OE1	2.46	0.45
1:A:376:ASP:O	1:A:380:GLN:HB2	2.17	0.45
1:A:635:ARG:NH2	1:A:635:ARG:CG	2.61	0.45
1:A:508:ILE:HG13	1:A:512:ILE:HG23	1.99	0.45
1:A:624:ARG:HA	1:A:624:ARG:HD2	1.78	0.44
1:A:375:LYS:O	1:A:379:ILE:HG13	2.17	0.44
1:A:428:LEU:CD2	1:A:534:MET:HE3	2.47	0.44
1:A:508:ILE:HD11	1:A:513:ILE:HG23	1.99	0.44
2:A:901:PDS:H24	2:A:901:PDS:C1	2.48	0.44
1:A:414:ASP:OD1	1:A:414:ASP:N	2.48	0.43
1:B:411:GLN:HG3	1:B:416:LEU:HD23	2.00	0.43
1:B:438:PHE:CD2	1:B:534:MET:HB2	2.53	0.43
1:A:493:TRP:CH2	1:B:460:LYS:HB3	2.54	0.43
1:B:344:PHE:HB3	1:B:357:MET:HE2	2.01	0.43
1:B:462:ILE:O	1:B:462:ILE:HG13	2.16	0.43
1:B:401:PRO:HB2	1:B:611:LYS:HE2	2.00	0.43
1:A:339:LEU:CD1	1:A:344:PHE:CZ	3.02	0.43
1:A:468:LYS:HZ2	1:A:504:THR:HG21	1.83	0.43
1:B:444:VAL:HG12	1:B:599:PHE:CZ	2.54	0.42
1:A:508:ILE:HD12	1:A:512:ILE:HG12	2.00	0.42
1:A:668:LYS:HA	1:A:669:PRO:HD3	1.87	0.42
1:B:432:ILE:HD13	1:B:534:MET:HA	2.02	0.42
1:B:438:PHE:HD2	1:B:534:MET:HB2	1.84	0.42
2:A:901:PDS:C11	2:A:901:PDS:H103	2.50	0.42
1:A:371:LYS:HB3	1:A:418:PHE:HB2	2.02	0.41
1:B:374:LYS:HD2	1:B:377:VAL:CG2	2.50	0.41
1:B:438:PHE:CD2	1:B:534:MET:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:PHE:CE2	1:B:534:MET:HE2	2.56	0.41
1:B:463:ILE:CG1	1:B:489:LYS:HB3	2.51	0.41
1:A:511:GLU:O	1:A:516:GLN:HB2	2.21	0.41
1:A:432:ILE:O	1:A:436:GLY:N	2.54	0.41
1:A:611:LYS:HA	3:A:22:HOH:O	2.21	0.41
1:B:339:LEU:C	1:B:341:ASP:H	2.24	0.41
1:B:579:HIS:HA	1:B:580:PRO:HD2	1.92	0.40
1:A:409:CYS:HB2	1:A:661:PHE:HB3	2.02	0.40
1:B:562:LYS:HA	1:B:562:LYS:HD3	1.82	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	322/353 (91%)	307 (95%)	12 (4%)	3 (1%)	17 35
1	B	296/353 (84%)	283 (96%)	10 (3%)	3 (1%)	15 32
All	All	618/706 (88%)	590 (96%)	22 (4%)	6 (1%)	15 32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	LYS
1	A	362	LYS
1	B	382	ASP
1	B	573	LYS
1	A	643	PRO
1	A	520	LYS

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	284/306 (93%)	255 (90%)	29 (10%)	7 14
1	B	259/306 (85%)	237 (92%)	22 (8%)	10 21
All	All	543/612 (89%)	492 (91%)	51 (9%)	8 17

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	THR
1	A	367	LEU
1	A	373	LEU
1	A	374	LYS
1	A	378	VAL
1	A	382	ASP
1	A	429	MET
1	A	433	GLN
1	A	442	HIS
1	A	444	VAL
1	A	462	ILE
1	A	467	LEU
1	A	472	VAL
1	A	499	LYS
1	A	504	THR
1	A	508	ILE
1	A	512	ILE
1	A	513	ILE
1	A	531	LEU
1	A	535	LEU
1	A	546	GLU
1	A	558	VAL
1	A	566	LYS
1	A	592	ARG
1	A	601	ARG
1	A	608	LEU
1	A	618	LYS

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Mol	Chain	Res	Type
1	A	634	THR
1	A	635	ARG
1	B	341	ASP
1	B	343	ASN
1	B	350	LYS
1	B	362	LYS
1	B	366	GLU
1	B	374	LYS
1	B	385	GLU
1	B	409	CYS
1	B	429	MET
1	B	433	GLN
1	B	444	VAL
1	B	462	ILE
1	B	472	VAL
1	B	476	SER
1	B	499	LYS
1	B	512	ILE
1	B	513	ILE
1	B	535	LEU
1	B	556	HIS
1	B	591	GLU
1	B	657	GLU
1	B	664	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	614	GLN
1	B	343	ASN
1	B	433	GLN
1	B	434	GLN
1	B	557	ASN
1	B	579	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)

5 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	TPO	B	500	1	8,10,11	0.67	0	10,14,16	1.21	1 (10%)
1	SEP	A	660	1	8,9,10	1.69	3 (37%)	8,12,14	1.28	1 (12%)
1	TPO	A	641	1	8,10,11	1.05	1 (12%)	10,14,16	1.19	0
1	SEP	B	660	1	8,9,10	1.72	1 (12%)	8,12,14	1.53	2 (25%)
1	TPO	A	500	1	8,10,11	0.66	0	10,14,16	1.05	1 (10%)

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	TPO	B	500	1	-	1/9/11/13	-
1	SEP	A	660	1	-	2/5/8/10	-
1	TPO	A	641	1	-	5/9/11/13	-
1	SEP	B	660	1	-	4/5/8/10	-
1	TPO	A	500	1	-	1/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	660	SEP	P-O1P	3.75	1.62	1.50
1	A	660	SEP	P-O1P	3.50	1.61	1.50
1	A	641	TPO	P-OG1	2.17	1.63	1.59
1	A	660	SEP	P-O2P	2.04	1.62	1.54
1	A	660	SEP	P-O3P	2.00	1.62	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	660	SEP	P-OG-CB	-2.81	110.56	118.30
1	B	660	SEP	OG-CB-CA	2.56	110.64	108.14
1	B	500	TPO	O3P-P-O2P	2.56	117.43	107.64
1	A	660	SEP	P-OG-CB	-2.37	111.77	118.30
1	A	500	TPO	O3P-P-O2P	2.12	115.72	107.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	500	TPO	O-C-CA-CB
1	A	641	TPO	N-CA-CB-CG2
1	A	641	TPO	N-CA-CB-OG1
1	A	641	TPO	C-CA-CB-CG2
1	A	641	TPO	O-C-CA-CB
1	A	660	SEP	N-CA-CB-OG
1	B	500	TPO	CB-OG1-P-O2P
1	B	660	SEP	CB-OG-P-O3P
1	B	660	SEP	CB-OG-P-O1P
1	B	660	SEP	CB-OG-P-O2P
1	B	660	SEP	CA-CB-OG-P
1	A	641	TPO	CG2-CB-OG1-P
1	A	660	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	641	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	PDS	B	902	-	30,37,37	2.03	10 (33%)	36,55,55	1.97	6 (16%)
2	PDS	A	901	-	30,37,37	2.03	10 (33%)	36,55,55	2.32	7 (19%)

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	PDS	B	902	-	-	3/6/30/30	0/5/5/5
2	PDS	A	901	-	-	2/6/30/30	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	PDS	C5-C12	-3.91	1.41	1.50
2	B	902	PDS	C5-C12	-3.76	1.42	1.50
2	A	901	PDS	C16-C8	3.65	1.45	1.36
2	B	902	PDS	C16-C8	3.54	1.44	1.36
2	B	902	PDS	C12-N13	3.35	1.45	1.38
2	B	902	PDS	C29-C24	3.34	1.44	1.36
2	A	901	PDS	C12-N13	3.29	1.44	1.38
2	B	902	PDS	C6-N13	3.27	1.44	1.38
2	A	901	PDS	C6-N13	3.16	1.44	1.38
2	A	901	PDS	C29-C24	3.12	1.43	1.36
2	B	902	PDS	C21-C15	3.12	1.43	1.36
2	A	901	PDS	C21-C15	3.01	1.43	1.36
2	B	902	PDS	C2-C6	-2.69	1.44	1.50
2	A	901	PDS	C31-C28	2.62	1.42	1.36
2	B	902	PDS	C21-C16	2.56	1.44	1.38
2	B	902	PDS	C31-C28	2.54	1.42	1.36
2	A	901	PDS	C21-C16	2.53	1.44	1.38
2	A	901	PDS	C2-C6	-2.48	1.44	1.50
2	A	901	PDS	C1-C4	2.10	1.44	1.40
2	B	902	PDS	C1-C4	2.03	1.44	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	PDS	C2-C6-N13	-9.08	101.12	106.62
2	A	901	PDS	C5-C12-N13	-7.54	102.06	106.62
2	B	902	PDS	C2-C6-N13	-7.16	102.28	106.62
2	B	902	PDS	C5-C12-N13	-6.68	102.58	106.62
2	A	901	PDS	C12-N13-C6	3.29	114.77	111.29
2	B	902	PDS	C1-C4-N9	2.97	110.62	107.06
2	A	901	PDS	C1-C4-N9	2.94	110.59	107.06
2	B	902	PDS	C17-N9-C4	2.90	129.59	124.72
2	A	901	PDS	C17-N9-C4	2.75	129.34	124.72
2	A	901	PDS	C10-C4-N9	-2.14	120.00	122.69
2	A	901	PDS	O14-C6-N13	2.12	130.01	125.08
2	B	902	PDS	O14-C6-N13	2.09	129.95	125.08
2	B	902	PDS	C12-N13-C6	2.04	113.44	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	902	PDS	N9-C17-C22-C27
2	B	902	PDS	C17-C22-C27-N30
2	A	901	PDS	C17-C22-C27-N30
2	A	901	PDS	C22-C27-N30-C33
2	B	902	PDS	C22-C27-N30-C33

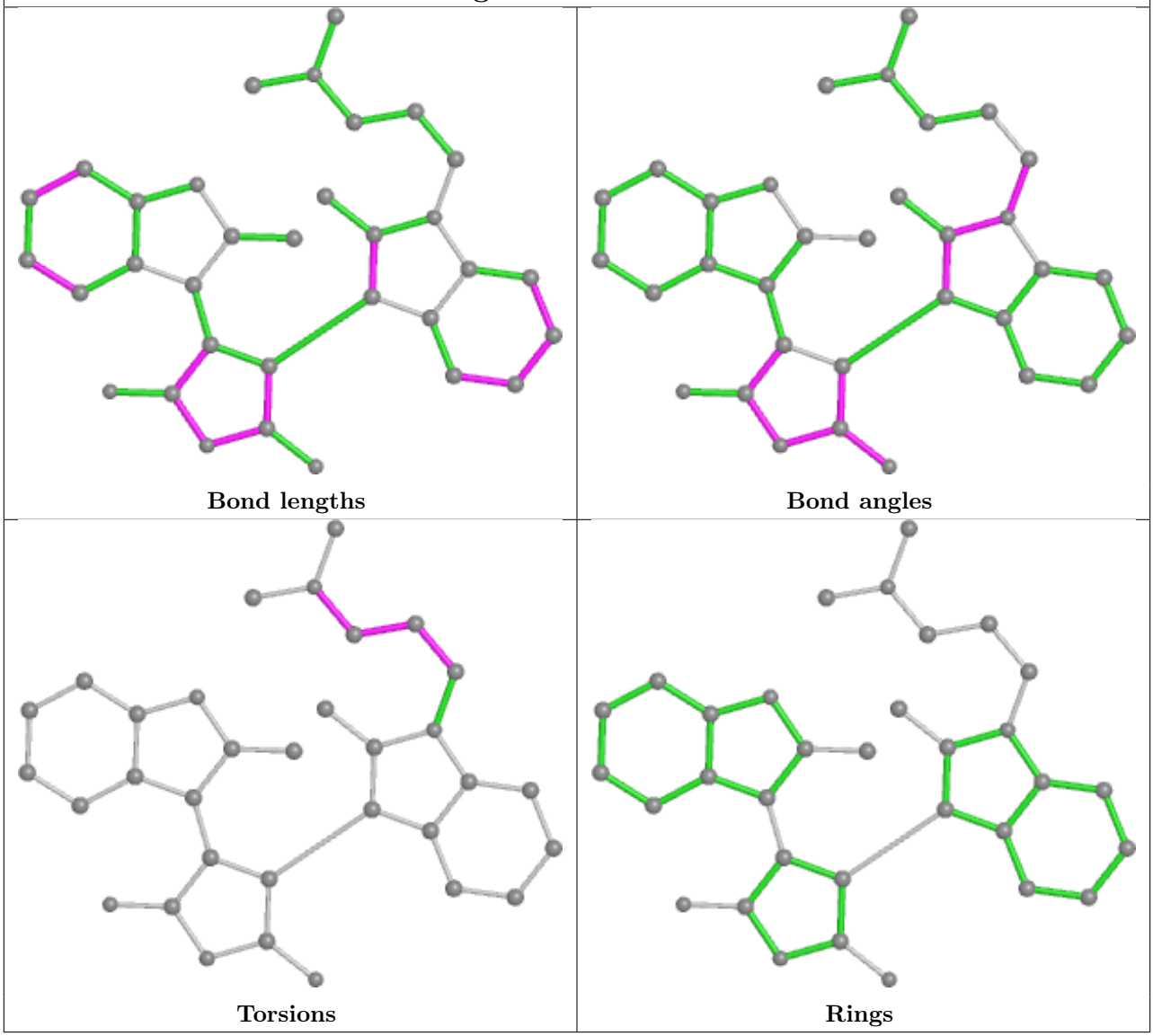
There are no ring outliers.

1 monomer is involved in 2 short contacts:

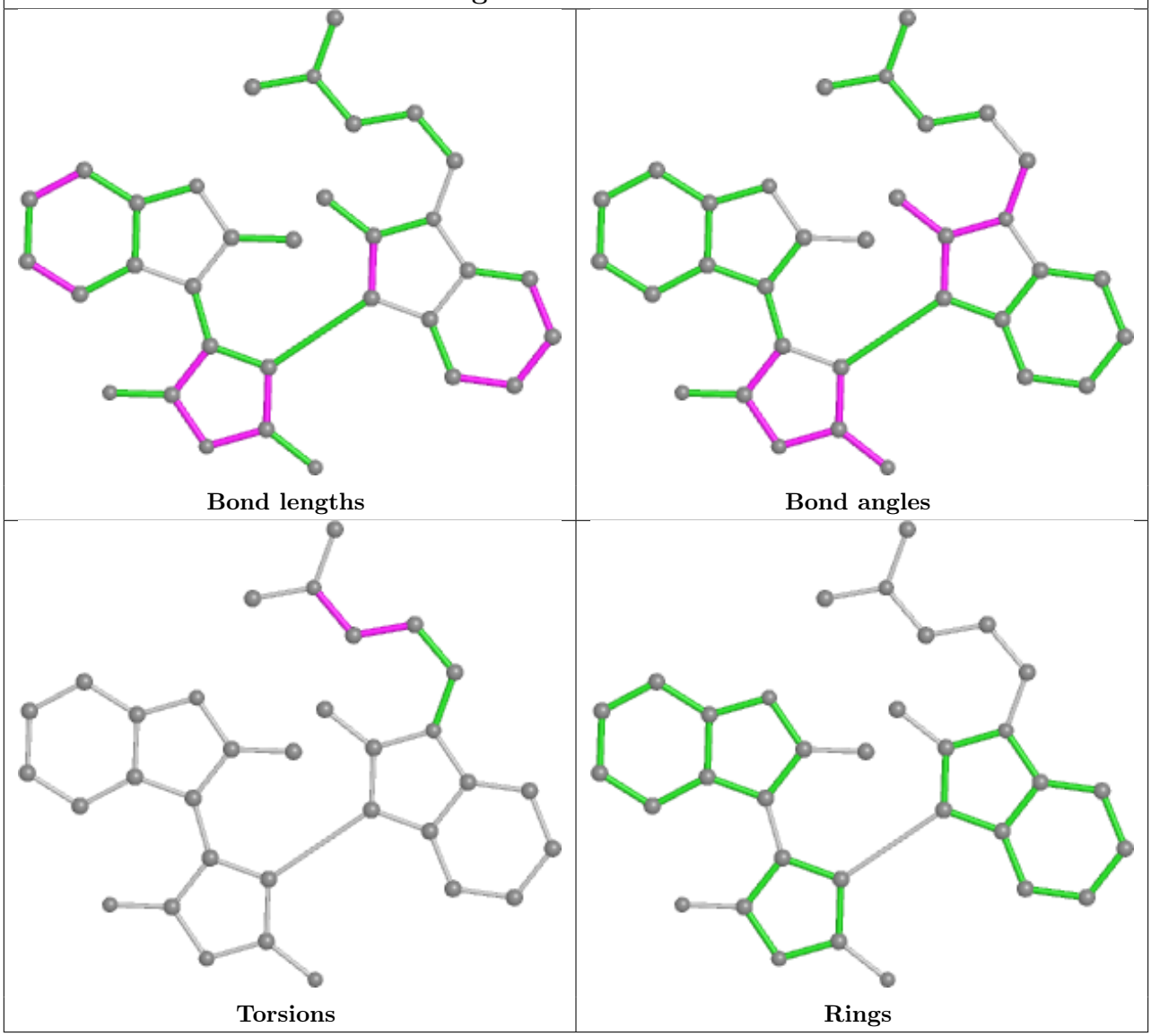
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	PDS	2	0

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 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 PDS B 902



Ligand PDS A 901



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.