



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:17 PM GMT

PDB ID : 1SZM
Title : DUAL BINDING MODE OF BISINDOLYLMALEIMIDE 2 TO PROTEIN KINASE A (PKA)
Authors : Gassel, M.; Breitenlechner, C.B.; Koenig, N.; Huber, R.; Engh, R.A.; Bossemeyer, D.
Deposited on : 2004-04-06
Resolution : 2.50 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
<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

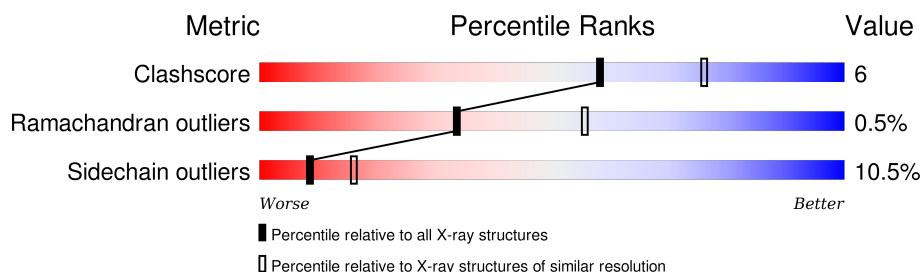
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	350	 71% 18% • 9%
1	B	350	 73% 17% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5326 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.

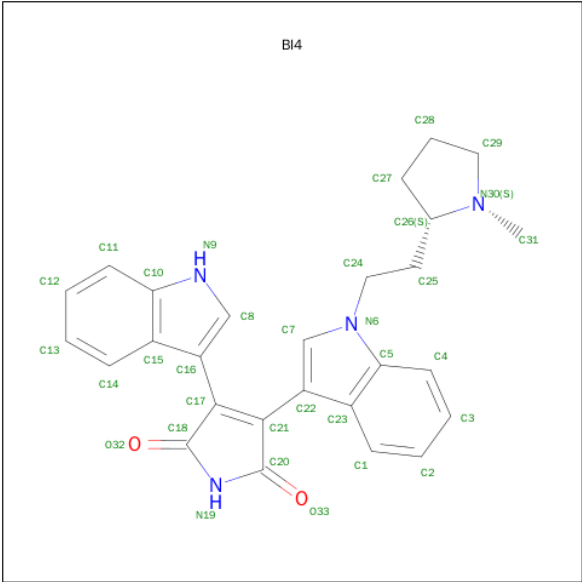
- Molecule 1 is a protein called cAMP-dependent protein kinase, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	P	S	0	0	0
			2565	1660	427	465	3	10			
1	B	323	Total	C	N	O	P	S	0	0	0
			2616	1697	432	474	3	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ALA	VAL	ENGINEERED	UNP P00517
A	139	SEP	SER	MODIFIED RESIDUE	UNP P00517
A	173	MET	LEU	ENGINEERED	UNP P00517
A	181	LYS	GLN	ENGINEERED	UNP P00517
A	197	TPO	THR	MODIFIED RESIDUE	UNP P00517
A	338	SEP	SER	MODIFIED RESIDUE	UNP P00517
B	123	ALA	VAL	ENGINEERED	UNP P00517
B	139	SEP	SER	MODIFIED RESIDUE	UNP P00517
B	173	MET	LEU	ENGINEERED	UNP P00517
B	181	LYS	GLN	ENGINEERED	UNP P00517
B	197	TPO	THR	MODIFIED RESIDUE	UNP P00517
B	338	SEP	SER	MODIFIED RESIDUE	UNP P00517

- Molecule 2 is 3-(1H-INDOL-3-YL)-4-{1-[2-(1-METHYLPYRROLIDIN-2-YL)ETHYL]-1H-INDOL-3-YL}-1H-PYRROLE-2,5-DIONE (three-letter code: BI4) (formula: C₂₇H₂₆N₄O₂).



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

- Molecule 3 is water.

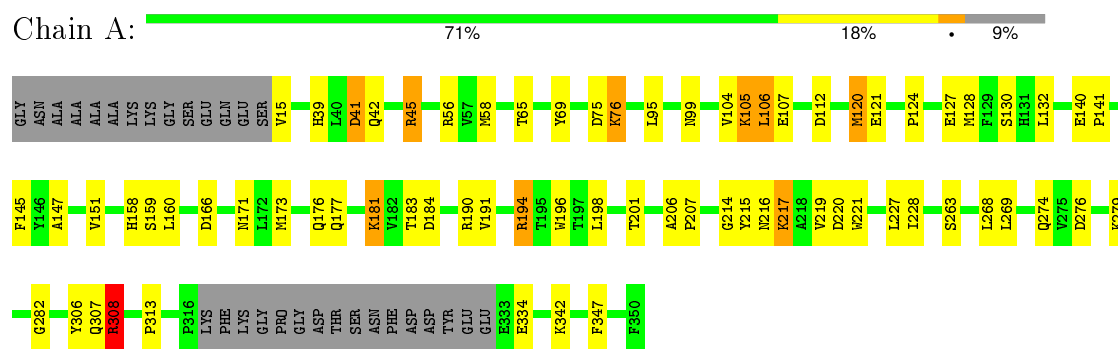
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	45	Total	O	0	0
			45	45		

3 Residue-property plots

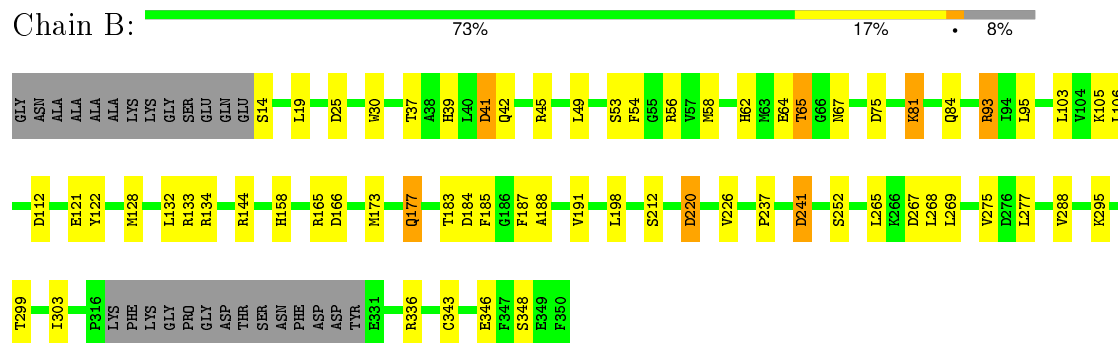
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: cAMP-dependent protein kinase, alpha-catalytic subunit



- Molecule 1: cAMP-dependent protein kinase, alpha-catalytic subunit



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.06 Å 89.00 Å 116.39 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.8 (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.231 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5326	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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: TPO, BI4, SEP

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	0/2599	0.86	7/3510 (0.2%)
1	B	0.74	0/2648	0.88	12/3573 (0.3%)
All	All	0.71	0/5247	0.87	19/7083 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ASP	CB-CG-OD2	8.01	125.51	118.30
1	A	75	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	112	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	166	ASP	CB-CG-OD2	6.73	124.36	118.30
1	B	25	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	173	MET	CG-SD-CE	-6.21	90.27	100.20
1	B	112	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	75	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	220	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	267	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	241	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	93	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	166	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	144	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	276	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	220	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	308	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	41	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	41	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2565	0	2446	34	0
1	B	2616	0	2533	27	0
2	A	33	0	26	2	0
2	B	33	0	26	3	0
3	A	34	0	0	0	0
3	B	45	0	0	1	0
All	All	5326	0	5031	61	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 (61) 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:173:MET:CE	2:A:351:BI4:H7	2.07	0.85
1:B:133:ARG:O	1:B:134:ARG:N	2.11	0.84
1:A:173:MET:HE2	2:A:351:BI4:H7	1.65	0.77
1:B:39:HIS:HD2	1:B:41:ASP:OD1	1.77	0.66
1:B:103:LEU:HD22	1:B:185:PHE:HZ	1.65	0.61
1:A:39:HIS:HD2	1:A:41:ASP:H	1.50	0.59
1:A:171:ASN:O	1:A:183:THR:HG22	2.03	0.59
1:B:62:HIS:HD2	1:B:64:GLU:H	1.48	0.59
1:A:147:ALA:O	1:A:151:VAL:HG23	2.04	0.58
1:A:221:TRP:CD1	1:A:282:GLY:HA3	2.38	0.58
1:B:39:HIS:H	1:B:42:GLN:HE21	1.52	0.58
1:B:105:LYS:HA	3:B:380:HOH:O	2.04	0.57
1:A:95:LEU:HD21	1:A:120:MET:HE2	1.87	0.57
1:B:30:TRP:CZ3	1:B:93:ARG:HG2	2.42	0.55
1:B:177:GLN:HG3	1:B:177:GLN:O	2.06	0.54
1:A:95:LEU:HD21	1:A:120:MET:CE	2.38	0.54
1:B:65:THR:CG2	1:B:67:ASN:H	2.21	0.53
1:B:158:HIS:HE1	1:B:220:ASP:OD2	1.92	0.52
1:A:128:MET:HE1	1:A:227:LEU:HD11	1.93	0.50
1:B:103:LEU:HD22	1:B:185:PHE:CZ	2.46	0.50
1:A:158:HIS:O	1:A:217:LYS:NZ	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:THR:HG22	1:B:67:ASN:H	1.76	0.50
1:A:45:ARG:HG3	1:A:58:MET:HE3	1.94	0.49
1:B:39:HIS:CD2	1:B:41:ASP:OD1	2.62	0.49
1:B:49:LEU:HD22	2:B:351:BI4:C2	2.42	0.48
1:A:104:VAL:HG22	1:A:181:LYS:HZ3	1.79	0.48
1:A:104:VAL:HG13	1:A:121:GLU:HB2	1.96	0.47
1:A:76:LYS:HG2	1:A:347:PHE:CD2	2.49	0.47
1:A:39:HIS:O	1:A:42:GLN:HG2	2.14	0.47
1:B:226:VAL:HG13	1:B:237:PRO:HD2	1.97	0.46
1:A:121:GLU:CD	1:A:181:LYS:NZ	2.69	0.46
1:A:95:LEU:HG	1:A:106:LEU:HB2	1.98	0.46
1:B:265:LEU:HD11	1:B:269:LEU:HD11	1.98	0.46
1:A:194:ARG:HB3	1:A:194:ARG:HH11	1.80	0.45
1:B:49:LEU:HD13	2:B:351:BI4:C1	2.47	0.45
1:B:54:PHE:HZ	1:B:84:GLN:HG3	1.82	0.45
1:A:196:TRP:CD1	1:A:214:GLY:HA2	2.52	0.45
1:A:105:LYS:HB2	1:A:121:GLU:HG3	1.98	0.45
1:A:45:ARG:HG3	1:A:58:MET:CE	2.47	0.45
1:B:62:HIS:HB3	1:B:65:THR:HG22	1.99	0.45
1:A:206:ALA:HB1	1:A:207:PRO:HD2	1.99	0.44
1:A:124:PRO:HG2	1:A:176:GLN:HE21	1.83	0.44
1:A:140:GLU:N	1:A:141:PRO:CD	2.81	0.44
1:B:58:MET:HB2	1:B:58:MET:HE3	1.89	0.43
1:A:145:PHE:CD2	1:A:313:PRO:HD3	2.53	0.43
1:A:228:ILE:CG2	1:A:269:LEU:HD21	2.49	0.43
1:A:128:MET:CE	1:A:227:LEU:HD11	2.48	0.42
1:B:187:PHE:O	1:B:188:ALA:C	2.56	0.42
1:A:274:GLN:HG2	1:A:279:LYS:O	2.20	0.42
1:B:133:ARG:CB	1:B:134:ARG:N	2.83	0.42
1:A:307:GLN:O	1:A:308:ARG:HB2	2.20	0.42
1:B:343:CYS:HB3	1:B:346:GLU:HG2	2.02	0.41
1:A:121:GLU:CD	1:A:181:LYS:HZ1	2.23	0.41
1:B:81:LYS:HE3	1:B:81:LYS:HB3	1.88	0.41
1:B:122:TYR:HE1	2:B:351:BI4:H2	1.84	0.41
1:A:194:ARG:CB	1:A:194:ARG:HH11	2.34	0.41
1:A:306:TYR:CD1	1:A:306:TYR:C	2.93	0.41
1:A:69:TYR:CE1	1:A:107:GLU:HG3	2.56	0.41
1:B:303:ILE:HD12	1:B:303:ILE:H	1.86	0.41
1:B:133:ARG:CA	1:B:134:ARG:N	2.84	0.40
1:A:215:TYR:CD2	1:A:219:VAL:HG11	2.56	0.40

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	313/350 (89%)	289 (92%)	22 (7%)	2 (1%)	30	50
1	B	314/350 (90%)	297 (95%)	16 (5%)	1 (0%)	46	68
All	All	627/700 (90%)	586 (94%)	38 (6%)	3 (0%)	34	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	LYS
1	B	165	ARG
1	A	184	ASP

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	256/301 (85%)	229 (90%)	27 (10%)	8	16
1	B	266/301 (88%)	238 (90%)	28 (10%)	8	16
All	All	522/602 (87%)	467 (90%)	55 (10%)	8	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	45	ARG
1	A	56	ARG

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Mol	Chain	Res	Type
1	A	65	THR
1	A	76	LYS
1	A	99	ASN
1	A	105	LYS
1	A	106	LEU
1	A	120	MET
1	A	127	GLU
1	A	130	SER
1	A	132	LEU
1	A	159	SER
1	A	160	LEU
1	A	177	GLN
1	A	181	LYS
1	A	190	ARG
1	A	191	VAL
1	A	194	ARG
1	A	198	LEU
1	A	201	THR
1	A	216	ASN
1	A	263	SER
1	A	268	LEU
1	A	308	ARG
1	A	334	GLU
1	A	342	LYS
1	B	14	SER
1	B	19	LEU
1	B	37	THR
1	B	45	ARG
1	B	53	SER
1	B	56	ARG
1	B	65	THR
1	B	81	LYS
1	B	95	LEU
1	B	106	LEU
1	B	121	GLU
1	B	128	MET
1	B	132	LEU
1	B	177	GLN
1	B	183	THR
1	B	191	VAL
1	B	198	LEU
1	B	212	SER

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Mol	Chain	Res	Type
1	B	241	ASP
1	B	252	SER
1	B	268	LEU
1	B	275	VAL
1	B	277	LEU
1	B	288	VAL
1	B	295	LYS
1	B	299	THR
1	B	336	ARG
1	B	348	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	42	GLN
1	A	158	HIS
1	A	176	GLN
1	A	216	ASN
1	B	39	HIS
1	B	42	GLN
1	B	62	HIS
1	B	67	ASN
1	B	68	HIS
1	B	158	HIS
1	B	245	GLN
1	B	283	ASN
1	B	293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 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	SEP	A	139	1	8,9,10	1.57	2 (25%)	8,12,14	2.20	2 (25%)
1	TPO	A	197	1	8,10,11	1.02	1 (12%)	7,14,16	1.12	1 (14%)
1	SEP	A	338	1	8,9,10	1.34	1 (12%)	8,12,14	2.14	2 (25%)
1	SEP	B	139	1	8,9,10	1.69	3 (37%)	8,12,14	1.76	2 (25%)
1	TPO	B	197	1	8,10,11	1.15	1 (12%)	7,14,16	0.98	0
1	SEP	B	338	1	8,9,10	1.40	2 (25%)	8,12,14	2.60	2 (25%)

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	SEP	A	139	1	-	0/6/8/10	0/0/0/0
1	TPO	A	197	1	-	0/8/11/13	0/0/0/0
1	SEP	A	338	1	-	0/6/8/10	0/0/0/0
1	SEP	B	139	1	-	0/6/8/10	0/0/0/0
1	TPO	B	197	1	-	0/8/11/13	0/0/0/0
1	SEP	B	338	1	-	0/6/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	SEP	P-O3P	2.00	1.61	1.54
1	B	338	SEP	P-O3P	2.08	1.62	1.54
1	B	139	SEP	P-O3P	2.15	1.62	1.54
1	B	197	TPO	P-O1P	2.16	1.58	1.51
1	B	139	SEP	P-O2P	2.19	1.62	1.54
1	A	197	TPO	P-O1P	2.24	1.58	1.51
1	B	338	SEP	P-O1P	2.25	1.58	1.51
1	A	338	SEP	P-O1P	2.76	1.60	1.51
1	A	139	SEP	P-O1P	3.12	1.61	1.51
1	B	139	SEP	P-O1P	3.20	1.61	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SEP	O-C-CA	-2.21	119.74	125.49
1	B	139	SEP	O-C-CA	-2.06	120.13	125.49
1	A	197	TPO	O-C-CA	-2.01	120.12	125.44
1	A	338	SEP	O2P-P-OG	2.96	115.10	106.56
1	B	139	SEP	OG-CB-CA	3.13	110.94	108.27
1	A	338	SEP	OG-CB-CA	4.42	112.05	108.27
1	B	338	SEP	OG-P-O1P	4.47	118.52	107.14
1	B	338	SEP	OG-CB-CA	5.08	112.61	108.27
1	A	139	SEP	OG-CB-CA	5.48	112.95	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	BI4	A	351	-	35,38,38	1.58	6 (17%)	40,56,56	1.87	5 (12%)
2	BI4	B	351	-	35,38,38	1.74	8 (22%)	40,56,56	1.65	8 (20%)

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	BI4	A	351	-	-	0/5/39/39	0/6/6/6
2	BI4	B	351	-	-	0/5/39/39	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	351	BI4	C18-N19	2.05	1.42	1.37
2	B	351	BI4	C31-N30	2.11	1.50	1.46
2	B	351	BI4	C26-N30	2.13	1.50	1.48
2	A	351	BI4	C22-C23	2.22	1.44	1.42
2	A	351	BI4	C20-N19	2.31	1.43	1.37
2	A	351	BI4	C5-N6	2.43	1.42	1.39
2	B	351	BI4	C8-N9	2.44	1.41	1.36
2	B	351	BI4	C12-C13	2.47	1.44	1.38
2	A	351	BI4	C18-N19	2.48	1.43	1.37
2	A	351	BI4	C8-N9	2.91	1.42	1.36
2	B	351	BI4	C7-N6	2.98	1.42	1.38
2	B	351	BI4	C22-C23	3.56	1.45	1.42
2	A	351	BI4	C16-C15	4.92	1.46	1.42
2	B	351	BI4	C16-C15	5.26	1.46	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	351	BI4	C20-N19-C18	-6.45	104.84	111.29
2	B	351	BI4	C20-N19-C18	-3.72	107.57	111.29
2	A	351	BI4	C25-C24-N6	-2.82	105.63	112.01
2	B	351	BI4	C25-C24-N6	-2.19	107.06	112.01
2	B	351	BI4	O32-C18-N19	-2.11	119.53	125.14
2	A	351	BI4	C16-C17-C21	2.11	131.31	128.37
2	B	351	BI4	C22-C21-C17	2.13	131.35	128.37
2	B	351	BI4	C24-N6-C7	2.53	128.82	124.31
2	B	351	BI4	C4-C5-C23	2.93	124.96	120.93
2	B	351	BI4	O32-C18-C17	3.34	132.98	128.07
2	A	351	BI4	C21-C20-N19	4.24	109.45	106.76
2	B	351	BI4	C21-C20-N19	4.37	109.53	106.76
2	A	351	BI4	C17-C18-N19	6.13	110.65	106.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	351	BI4	2	0
2	B	351	BI4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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