Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:28 PM UTC

PDB ID	:	2OIB / pdb_00002oib
Title	:	Crystal structure of IRAK4 kinase domain apo form
Authors	:	Kuglstatter, A.; Villasenor, A.G.; Browner, M.F.
Deposited on	:	2007-01-10
Resolution	:	2.00 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 ⓘ 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:

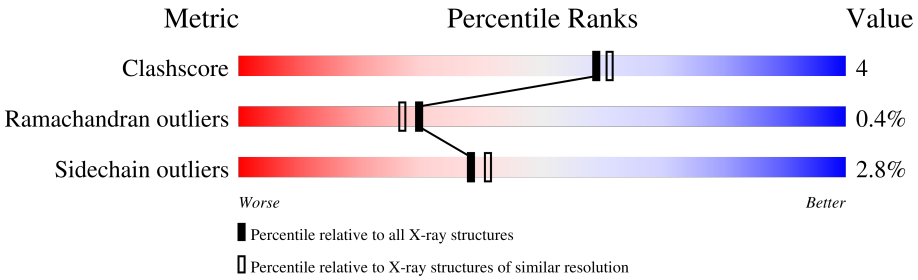
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	301	82% 10% • 6%
1	B	301	80% 12% • 7%
1	C	301	82% 11% • 7%
1	D	301	87% 9% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9747 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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	P	S	0	0	0
			2246	1402	377	450	3	14			
1	B	280	Total	C	N	O	P	S	0	1	0
			2228	1395	375	442	2	14			
1	C	281	Total	C	N	O	P	S	0	1	0
			2241	1403	376	445	3	14			
1	D	291	Total	C	N	O	P	S	0	1	0
			2316	1449	388	462	3	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	TPO	THR	modified residue	UNP Q9NWZ3
A	345	TPO	THR	modified residue	UNP Q9NWZ3
A	346	SEP	SER	modified residue	UNP Q9NWZ3
B	342	TPO	THR	modified residue	UNP Q9NWZ3
B	345	TPO	THR	modified residue	UNP Q9NWZ3
B	346	SEP	SER	modified residue	UNP Q9NWZ3
C	342	TPO	THR	modified residue	UNP Q9NWZ3
C	345	TPO	THR	modified residue	UNP Q9NWZ3
C	346	SEP	SER	modified residue	UNP Q9NWZ3
D	342	TPO	THR	modified residue	UNP Q9NWZ3
D	345	TPO	THR	modified residue	UNP Q9NWZ3
D	346	SEP	SER	modified residue	UNP Q9NWZ3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	209	Total	O	0	0
			209	209		
2	B	185	Total	O	0	0
			185	185		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	147	Total O 147 147	0	0
2	D	175	Total O 175 175	0	0

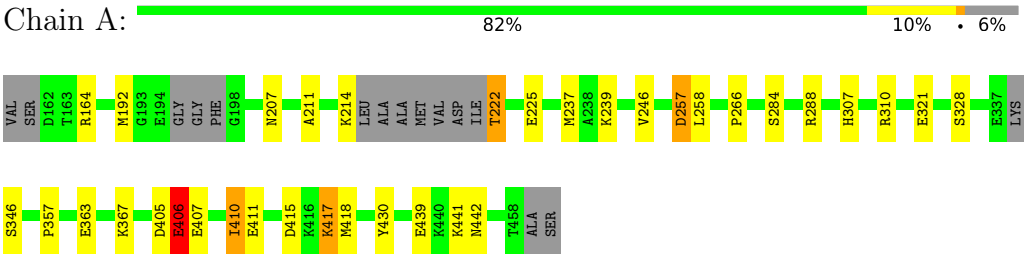
3 Residue-property plots (i)

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.

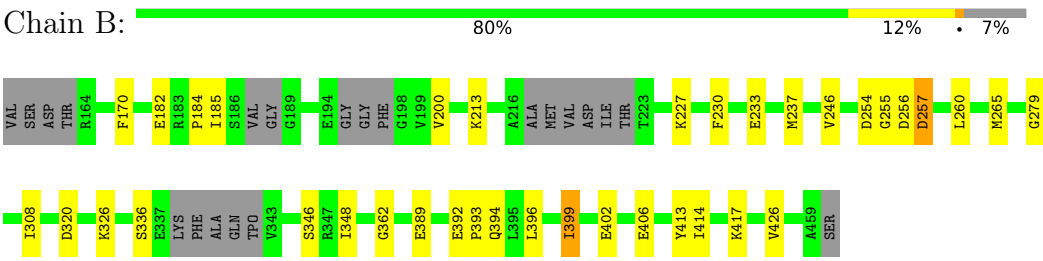
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



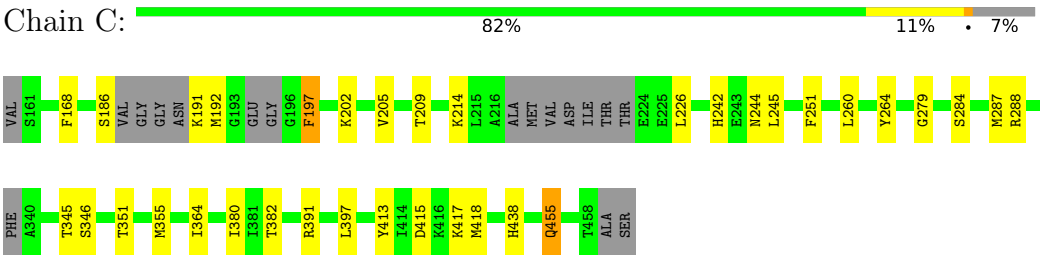
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:



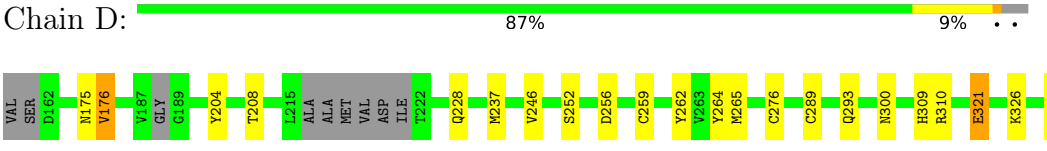
• Molecule 1: Interleukin-1 receptor-associated kinase 4

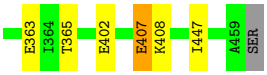
Chain C:



• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D:




E363
I364
T365
E402
E407
K408
I447
A459
SER

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.07Å 138.75Å 87.94Å 90.00° 123.95° 90.00°	Depositor
Resolution (Å)	48.56 – 2.00	Depositor
% Data completeness (in resolution range)	92.5 (48.56-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	9.30	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9747	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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, 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	0.51	0/2248	0.80	1/3027 (0.0%)
1	B	0.49	0/2240	0.80	0/3014
1	C	0.48	0/2242	0.80	0/3015
1	D	0.48	0/2320	0.76	0/3123
All	All	0.49	0/9050	0.79	1/12179 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	406	GLU	N-CA-C	5.08	121.61	110.80

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	2246	0	2201	20	0
1	B	2228	0	2185	21	0
1	C	2241	0	2194	23	0
1	D	2316	0	2265	17	0
2	A	209	0	0	2	0
2	B	185	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	147	0	0	4	0
2	D	175	0	0	1	0
All	All	9747	0	8845	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 4.

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:D:237:MET:HE1	1:D:246:VAL:HG23	1.46	0.96
1:D:176:VAL:HG13	1:D:204:TYR:H	1.46	0.78
1:B:246:VAL:HG23	2:B:1261:HOH:O	1.86	0.74
1:A:405:ASP:O	1:A:407:GLU:HG3	1.90	0.72
1:C:242:HIS:CD2	1:C:244:ASN:H	2.09	0.70
1:A:405:ASP:O	1:A:407:GLU:N	2.28	0.66
1:B:256:ASP:O	1:B:257:ASP:HB2	1.95	0.66
1:B:237:MET:HA	1:B:237:MET:HE2	1.80	0.64
1:C:345:TPO:HB	1:C:364:ILE:HD11	1.80	0.63
1:C:242:HIS:HD2	1:C:244:ASN:H	1.47	0.62
1:C:192:MET:HE1	1:C:264:TYR:HE2	1.66	0.61
1:B:237:MET:SD	2:B:1261:HOH:O	2.56	0.60
1:D:237:MET:HE3	1:D:262:TYR:HE1	1.67	0.59
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.84	0.58
1:B:417:LYS:O	1:C:279:GLY:HA2	2.05	0.56
1:C:168:PHE:HE2	1:C:205:VAL:HG11	1.69	0.56
1:D:264:TYR:O	1:D:265:MET:HE2	2.06	0.56
1:C:455:GLN:NE2	2:C:1077:HOH:O	2.28	0.55
1:C:168:PHE:CE2	1:C:205:VAL:HG11	2.41	0.55
1:A:357:PRO:HG2	1:A:439:GLU:HG3	1.88	0.54
1:B:265:MET:HE1	1:B:320:ASP:HB3	1.89	0.54
1:A:222:THR:HB	1:A:225:GLU:HB2	1.90	0.53
1:D:237:MET:HE1	1:D:246:VAL:CG2	2.30	0.53
1:C:197:PHE:H	1:C:197:PHE:HD2	1.57	0.53
1:B:200:VAL:HG22	1:B:213:LYS:HG3	1.89	0.53
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.91	0.53
1:A:266:PRO:HG2	1:A:321:GLU:HG3	1.92	0.52
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.90	0.52
1:D:176:VAL:CG1	1:D:204:TYR:H	2.20	0.52
1:C:192:MET:HE1	1:C:264:TYR:CE2	2.44	0.52
1:D:321:GLU:HG2	2:D:1116:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LYS:HD3	1:D:276:CYS:HB2	1.93	0.51
1:A:214:LYS:HE3	1:A:257:ASP:OD2	2.11	0.50
1:B:265:MET:CE	1:B:320:ASP:HB3	2.42	0.49
1:A:321:GLU:H	1:A:321:GLU:CD	2.19	0.49
1:B:308:ILE:HD11	1:B:336:SER:HB3	1.92	0.49
1:C:251:PHE:HB3	1:C:260:LEU:HD23	1.95	0.49
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.94	0.48
1:C:186:SER:HB2	2:C:2043:HOH:O	2.14	0.48
1:A:239:LYS:HD3	1:A:307:HIS:HE1	1.78	0.47
1:A:439:GLU:HB2	2:A:1299:HOH:O	2.15	0.47
1:B:396:LEU:HD12	1:B:399:ILE:HD13	1.97	0.46
1:B:402:GLU:OE2	1:B:413:TYR:OH	2.29	0.46
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.97	0.46
1:C:284:SER:OG	1:C:287:MET:HG3	2.16	0.45
1:A:363:GLU:OE2	1:A:441:LYS:HE2	2.16	0.45
1:B:265:MET:HE2	1:B:326:LYS:HB2	1.98	0.45
1:C:191:LYS:N	2:C:1347:HOH:O	2.50	0.44
1:A:246:VAL:HG21	1:A:328:SER:HB3	2.00	0.44
1:D:402:GLU:HB3	1:D:408:LYS:HE3	1.99	0.44
1:C:202:LYS:HE3	1:C:209:THR:HG21	2.00	0.43
1:D:309:HIS:O	1:D:310:ARG:HB2	2.19	0.43
1:B:287:MET:HE3	1:B:290:LYS:HB2	2.01	0.43
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.01	0.43
1:A:310:ARG:HD2	2:A:3011:HOH:O	2.19	0.43
1:B:414:ILE:HG12	1:B:426:VAL:HG11	2.01	0.43
1:D:344:MET:SD	1:D:363:GLU:HG2	2.59	0.43
1:A:367:LYS:HE2	1:A:442:ASN:ND2	2.34	0.42
1:A:192:MET:HE1	1:A:211:ALA:CB	2.50	0.42
1:A:284:SER:O	1:A:288:ARG:HG3	2.20	0.42
1:B:389:GLU:HA	1:B:394:GLN:CD	2.45	0.42
1:A:164:ARG:HA	1:A:164:ARG:NH1	2.35	0.42
1:B:348:ILE:HG12	1:B:362:GLY:HA2	2.01	0.42
1:D:402:GLU:O	1:D:407:GLU:HG3	2.20	0.42
1:A:192:MET:HE1	1:A:211:ALA:HA	2.00	0.41
1:B:170:PHE:CB	1:B:255:GLY:HA3	2.50	0.41
1:B:392:GLU:HA	1:B:393:PRO:HA	1.85	0.41
1:D:289:CYS:O	1:D:293:GLN:HG3	2.19	0.41
1:C:391:ARG:HD3	2:C:1281:HOH:O	2.19	0.41
1:D:237:MET:HE3	1:D:262:TYR:CE1	2.53	0.41
1:A:410:ILE:HG12	1:A:430:TYR:CD1	2.56	0.41
1:B:279:GLY:HA2	1:C:417:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:VAL:HG22	1:D:344:MET:H	1.86	0.41
1:C:382:THR:HG22	1:C:413:TYR:HB3	2.03	0.41
1:C:242:HIS:HB3	1:C:245:LEU:HG	2.03	0.40
1:C:284:SER:O	1:C:288:ARG:HG3	2.21	0.40
1:C:351:THR:O	1:C:355:MET:HG3	2.21	0.40
1:B:227:LYS:O	1:B:230:PHE:HB3	2.21	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	273/301 (91%)	263 (96%)	9 (3%)	1 (0%)	30 27
1	B	269/301 (89%)	257 (96%)	9 (3%)	3 (1%)	11 7
1	C	269/301 (89%)	261 (97%)	8 (3%)	0	100 100
1	D	283/301 (94%)	264 (93%)	19 (7%)	0	100 100
All	All	1094/1204 (91%)	1045 (96%)	45 (4%)	4 (0%)	30 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	B	184	PRO
1	B	257	ASP

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	247/259 (95%)	238 (96%)	9 (4%)	31	31
1	B	245/259 (95%)	241 (98%)	4 (2%)	55	62
1	C	245/259 (95%)	239 (98%)	6 (2%)	43	47
1	D	253/259 (98%)	244 (96%)	9 (4%)	31	31
All	All	990/1036 (96%)	962 (97%)	28 (3%)	38	41

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	222	THR
1	A	237	MET
1	A	257	ASP
1	A	258	LEU
1	A	406	GLU
1	A	410	ILE
1	A	411	GLU
1	A	417	LYS
1	B	182	GLU
1	B	185	ILE
1	B	254	ASP
1	B	399	ILE
1	C	197	PHE
1	C	214	LYS
1	C	226	LEU
1	C	397	LEU
1	C	438	HIS
1	C	455	GLN
1	D	175	ASN
1	D	176	VAL
1	D	208	THR
1	D	228	GLN
1	D	256	ASP
1	D	321	GLU
1	D	326	LYS
1	D	365	THR
1	D	407	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	207	ASN
1	A	228	GLN
1	A	229	GLN
1	A	293	GLN
1	A	307	HIS
1	A	442	ASN
1	B	179	ASN
1	B	207	ASN
1	B	293	GLN
1	B	394	GLN
1	B	451	GLN
1	B	455	GLN
1	C	166	HIS
1	C	242	HIS
1	C	244	ASN
1	C	390	HIS
1	C	394	GLN
1	D	206	ASN
1	D	229	GLN
1	D	293	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 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	C	346	1	8,9,10	1.63	1 (12%)	7,12,14	1.66	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SEP	A	346	1	8,9,10	1.65	1 (12%)	7,12,14	1.49	1 (14%)
1	TPO	A	342	1	8,10,11	0.70	0	10,14,16	1.02	0
1	TPO	D	342	1	8,10,11	0.77	0	10,14,16	0.98	0
1	TPO	D	345	1	8,10,11	0.97	0	10,14,16	1.01	0
1	SEP	D	346	1	8,9,10	1.66	1 (12%)	7,12,14	1.97	1 (14%)
1	SEP	B	346	1	8,9,10	1.65	1 (12%)	7,12,14	1.38	1 (14%)
1	TPO	C	342	1	8,10,11	0.74	0	10,14,16	1.03	0
1	TPO	B	345	1	8,10,11	0.90	0	10,14,16	1.01	0
1	TPO	C	345	1	8,10,11	0.86	0	10,14,16	0.90	0
1	TPO	A	345	1	8,10,11	0.87	0	10,14,16	0.94	0

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	C	346	1	-	0/6/8/10	-
1	SEP	A	346	1	-	2/6/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	D	342	1	-	0/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	2/6/8/10	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	C	345	1	-	4/9/11/13	-
1	TPO	A	345	1	-	2/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	346	SEP	P-O1P	3.59	1.61	1.50
1	A	346	SEP	P-O1P	3.59	1.61	1.50
1	C	346	SEP	P-O1P	3.53	1.61	1.50
1	D	346	SEP	P-O1P	3.52	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	346	SEP	OG-CB-CA	4.88	112.90	108.14
1	C	346	SEP	OG-CB-CA	3.90	111.94	108.14
1	A	346	SEP	OG-CB-CA	3.26	111.31	108.14
1	B	346	SEP	OG-CB-CA	3.05	111.11	108.14

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	346	SEP	N-CA-CB-OG
1	A	346	SEP	C-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	CA-CB-OG1-P
1	D	346	SEP	C-CA-CB-OG
1	B	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	CB-OG1-P-O1P
1	D	346	SEP	N-CA-CB-OG
1	C	345	TPO	CA-CB-OG1-P
1	C	345	TPO	CB-OG1-P-O2P
1	A	342	TPO	C-CA-CB-CG2
1	C	342	TPO	C-CA-CB-CG2
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	B	345	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	345	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.