



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:51 AM UTC

PDB ID : 9PSS / pdb_00009pss
Title : IRAK4 in Complex with Compound 3
Authors : Ferrao, R.
Deposited on : 2025-07-26
Resolution : 1.93 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

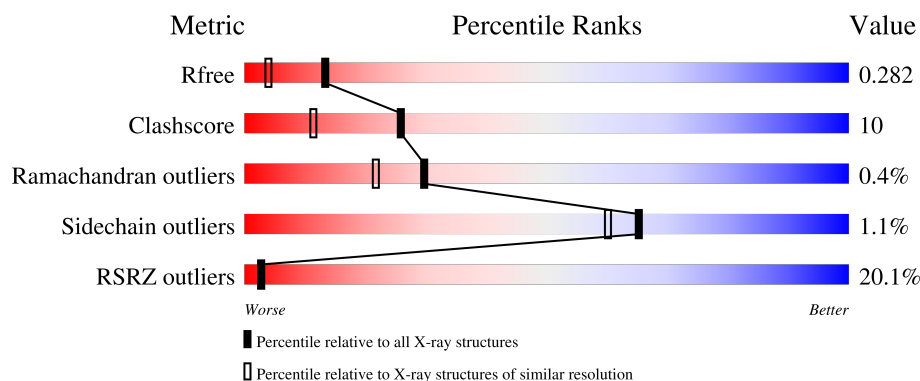
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	304	22% 73% 20% 7%
1	B	304	15% 72% 20% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4705 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.

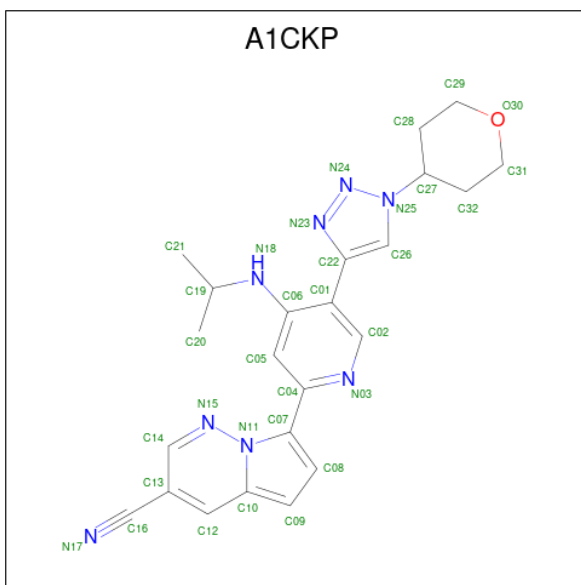
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	P	S	0	0	0
			2205	1380	372	436	3	14			
1	B	284	Total	C	N	O	P	S	0	0	0
			2217	1389	372	439	3	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	expression tag	UNP Q9NWZ3
A	158	ALA	-	expression tag	UNP Q9NWZ3
A	159	MET	-	expression tag	UNP Q9NWZ3
B	157	GLY	-	expression tag	UNP Q9NWZ3
B	158	ALA	-	expression tag	UNP Q9NWZ3
B	159	MET	-	expression tag	UNP Q9NWZ3

- Molecule 2 is (7P,8S)-7-{(5M)-5-[1-(oxan-4-yl)-1H-1,2,3-triazol-4-yl]-4-[(propan-2-yl)amino]pyridin-2-yl}pyrrolo[1,2-b]pyridazine-3-carbonitrile (CCD ID: A1CKP) (formula: C₂₃H₂₄N₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	23	8	1		
2	B	1	Total	C	N	O	0	0
			32	23	8	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

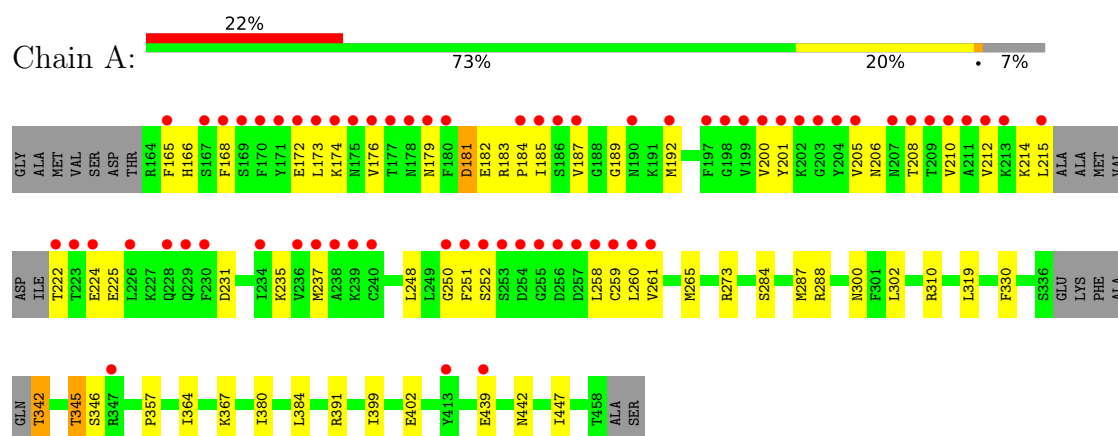
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	110	Total	O	0	0
			110	110		

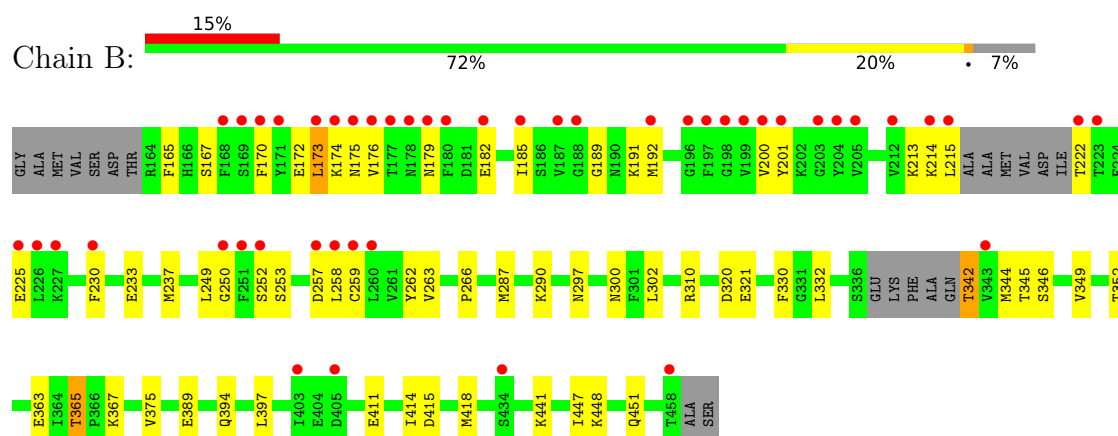
3 Residue-property plots

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 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.

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.63Å 109.42Å 141.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 1.93 48.93 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.93-1.93) 91.3 (48.93-1.93)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.247 , 0.283 0.247 , 0.282	Depositor DCC
R_{free} test set	1997 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4705	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9705e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO, SO4, A1CKP

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	0/2206	0.63	0/2973
1	B	0.59	0/2221	0.71	0/2996
All	All	0.55	0/4427	0.68	0/5969

There are no bond length outliers.

There are no bond angle outliers.

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	2205	0	2159	43	0
1	B	2217	0	2152	41	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	94	0	0	3	0
4	B	110	0	0	4	0
All	All	4705	0	4311	84	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 10.

All (84) 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:284:SER:H	1:A:287:MET:HE3	1.13	1.13
1:B:174:LYS:HG2	1:B:179:ASN:HA	1.59	0.83
1:A:357:PRO:HG3	1:A:439:GLU:HG3	1.61	0.80
1:B:266:PRO:HG2	1:B:321:GLU:HG2	1.65	0.76
1:A:284:SER:N	1:A:287:MET:HE3	1.98	0.71
1:A:172:GLU:HG2	1:A:173:LEU:HD12	1.76	0.67
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.78	0.65
1:A:165:PHE:HB3	1:A:250:GLY:HA2	1.78	0.65
1:A:222:THR:HG22	1:A:224:GLU:H	1.62	0.64
1:B:253:SER:HA	1:B:258:LEU:HD22	1.81	0.63
1:B:174:LYS:HD2	1:B:179:ASN:OD1	2.00	0.61
1:A:342:TPO:O2P	1:A:367:LYS:NZ	2.35	0.60
1:A:205:VAL:O	1:A:208:THR:N	2.29	0.59
1:A:185:ILE:HD11	1:A:192:MET:HG2	1.83	0.59
1:B:165:PHE:HB3	1:B:250:GLY:HA2	1.85	0.59
1:B:411:GLU:O	1:B:414:ILE:HG22	2.04	0.58
1:B:192:MET:HE2	1:B:201:TYR:C	2.29	0.58
1:B:287:MET:HE1	1:B:290:LYS:NZ	2.20	0.57
1:A:174:LYS:HG2	1:A:179:ASN:HA	1.86	0.56
1:A:215:LEU:HD12	1:A:258:LEU:HB2	1.86	0.56
1:B:344:MET:SD	1:B:363:GLU:HG2	2.47	0.55
1:A:251:PHE:HB3	1:A:260:LEU:HD23	1.87	0.55
1:A:384:LEU:HB3	1:A:391:ARG:NH1	2.21	0.55
1:A:237:MET:HE3	1:A:330:PHE:CE2	2.42	0.55
1:B:185:ILE:HG13	1:B:192:MET:HG2	1.87	0.55
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.89	0.53
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.90	0.53
1:B:182:GLU:HA	1:B:191:LYS:HB2	1.90	0.53
1:B:237:MET:HA	1:B:237:MET:HE2	1.90	0.53
1:B:389:GLU:HA	1:B:394:GLN:OE1	2.09	0.53
1:B:222:THR:N	1:B:225:GLU:OE2	2.42	0.53
1:A:168:PHE:HB3	1:A:173:LEU:HD11	1.90	0.52
1:A:182:GLU:HG3	1:A:201:TYR:HE2	1.74	0.52
1:A:248:LEU:HD11	1:A:260:LEU:HD22	1.91	0.52
1:B:365:THR:OG1	1:B:367:LYS:HD2	2.10	0.51
1:B:213:LYS:HE3	1:B:215:LEU:HD21	1.91	0.51
1:A:184:PRO:O	1:A:187:VAL:HG22	2.10	0.51
1:A:231:ASP:HB3	1:A:235:LYS:NZ	2.25	0.51
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.92	0.50
1:B:332:LEU:HD13	1:B:349:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HB	1:A:225:GLU:HG2	1.94	0.49
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.78	0.49
1:A:367:LYS:HE2	1:A:442:ASN:OD1	2.13	0.48
1:A:399:ILE:HA	1:A:402:GLU:HG3	1.96	0.48
1:A:310:ARG:HD3	1:A:364:ILE:HG23	1.96	0.48
1:B:170:PHE:N	4:B:610:HOH:O	2.44	0.47
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.95	0.47
1:B:389:GLU:HA	1:B:394:GLN:CD	2.40	0.47
1:A:345:TPO:CG2	1:A:364:ILE:HD11	2.44	0.47
1:B:297:ASN:OD1	1:B:451:GLN:NE2	2.38	0.46
1:B:192:MET:HE3	1:B:200:VAL:HG12	1.98	0.46
1:B:310:ARG:HD2	4:B:701:HOH:O	2.16	0.46
1:B:320:ASP:HB2	4:B:648:HOH:O	2.16	0.45
1:A:182:GLU:HG3	1:A:201:TYR:CE2	2.51	0.45
1:A:273:ARG:HG3	1:A:319:LEU:HD12	1.99	0.45
1:B:448:LYS:HD3	1:B:448:LYS:HA	1.74	0.45
1:B:172:GLU:O	1:B:176:VAL:HG22	2.17	0.44
1:A:250:GLY:C	1:A:261:VAL:HG12	2.43	0.44
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.44
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.83	0.43
1:B:249:LEU:HD11	1:B:263:VAL:HG22	2.00	0.43
1:B:185:ILE:HD13	1:B:189:GLY:O	2.18	0.43
1:A:166:HIS:HD2	4:A:688:HOH:O	2.01	0.43
1:B:173:LEU:HA	1:B:176:VAL:HG22	2.00	0.43
1:A:345:TPO:HG21	1:A:364:ILE:HD11	2.01	0.42
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.61	0.42
1:B:266:PRO:HD2	1:B:320:ASP:HA	2.01	0.42
1:A:166:HIS:O	1:A:250:GLY:HA3	2.20	0.42
1:B:342:TPO:O2P	1:B:441:LYS:NZ	2.37	0.42
1:A:174:LYS:CG	1:A:179:ASN:HA	2.50	0.41
1:A:201:TYR:CE1	1:A:214:LYS:HE3	2.55	0.41
1:A:287:MET:HG2	4:A:690:HOH:O	2.20	0.41
1:B:252:SER:OG	1:B:259:CYS:HB2	2.19	0.41
1:B:375:VAL:HG22	1:B:397:LEU:HD21	2.02	0.41
1:B:230:PHE:CZ	1:B:253:SER:HB3	2.56	0.41
1:B:230:PHE:CD2	1:B:258:LEU:HB3	2.55	0.41
1:A:181:ASP:OD2	1:A:189:GLY:HA2	2.20	0.41
1:B:233:GLU:OE2	1:B:262:TYR:OH	2.38	0.41
1:A:183:ARG:HB2	1:A:189:GLY:HA3	2.03	0.41
1:A:273:ARG:HA	1:A:273:ARG:NE	2.37	0.40
1:A:265:MET:HE3	4:A:608:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LYS:HG3	1:B:257:ASP:HB3	2.03	0.40
1:A:200:VAL:HA	1:A:212:VAL:O	2.22	0.40
1:B:175:ASN:ND2	4:B:618:HOH:O	2.53	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	276/304 (91%)	264 (96%)	10 (4%)	2 (1%)	18	9
1	B	276/304 (91%)	265 (96%)	11 (4%)	0	100	100
All	All	552/608 (91%)	529 (96%)	21 (4%)	2 (0%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	ASP
1	A	206	ASN

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	236/260 (91%)	235 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	238/260 (92%)	234 (98%)	4 (2%)	53 44
All	All	474/520 (91%)	469 (99%)	5 (1%)	65 60

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	VAL
1	B	167	SER
1	B	173	LEU
1	B	352	THR
1	B	365	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	232	GLN
1	A	293	GLN
1	A	306	HIS
1	A	455	GLN
1	B	166	HIS
1	B	293	GLN
1	B	305	ASN
1	B	452	GLN

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	TPO	A	342	1	8,10,11	2.62	1 (12%)	10,14,16	1.15	1 (10%)
1	SEP	B	346	1	8,9,10	1.79	2 (25%)	7,12,14	1.91	1 (14%)
1	TPO	B	345	1	8,10,11	2.77	1 (12%)	10,14,16	1.20	1 (10%)
1	SEP	A	346	1	8,9,10	1.92	3 (37%)	7,12,14	0.89	1 (14%)
1	TPO	A	345	1	8,10,11	3.02	2 (25%)	10,14,16	1.04	1 (10%)
1	TPO	B	342	1	8,10,11	3.03	2 (25%)	10,14,16	1.19	2 (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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	342	1	-	4/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	B	342	1	-	7/9/11/13	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	TPO	P-OG1	8.11	1.73	1.59
1	A	345	TPO	P-OG1	8.10	1.73	1.59
1	B	345	TPO	P-OG1	7.41	1.72	1.59
1	A	342	TPO	P-OG1	7.18	1.72	1.59
1	A	346	SEP	P-O1P	4.15	1.63	1.50
1	B	346	SEP	P-O1P	3.97	1.62	1.50
1	A	346	SEP	P-O3P	2.17	1.62	1.54
1	A	345	TPO	CB-CA	2.17	1.58	1.53
1	A	346	SEP	P-O2P	2.13	1.62	1.54
1	B	346	SEP	P-O2P	2.06	1.62	1.54
1	B	342	TPO	CB-CA	2.00	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-CB-CA	4.52	112.54	108.14
1	A	342	TPO	OG1-P-O1P	-2.40	100.77	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	TPO	OG1-P-O1P	-2.29	101.17	109.33
1	B	342	TPO	OG1-P-O1P	-2.29	101.17	109.33
1	A	346	SEP	O3P-P-OG	2.15	112.27	106.67
1	B	342	TPO	O3P-P-O2P	2.05	115.49	107.80
1	A	345	TPO	OG1-P-O1P	-2.01	102.18	109.33

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	342	TPO	1	0
1	A	345	TPO	2	0
1	B	342	TPO	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 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	$\# Z > 2$
3	SO4	B	502	-	4,4,4	1.03	0	6,6,6	0.48	0
3	SO4	A	503	-	4,4,4	1.04	0	6,6,6	0.65	0
3	SO4	A	502	-	4,4,4	0.75	0	6,6,6	0.34	0
2	A1CKP	B	501	-	35,36,36	1.04	1 (2%)	44,51,51	1.52	12 (27%)
2	A1CKP	A	501	-	35,36,36	1.17	3 (8%)	44,51,51	1.44	5 (11%)

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	A1CKP	B	501	-	-	2/16/26/26	0/5/5/5
2	A1CKP	A	501	-	-	3/16/26/26	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1CKP	C14-C13	4.34	1.48	1.42
2	B	501	A1CKP	C14-C13	3.69	1.47	1.42
2	A	501	A1CKP	C12-C13	-2.50	1.33	1.38
2	A	501	A1CKP	N25-N24	-2.38	1.32	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1CKP	C06-N18-C19	-5.15	117.33	124.66
2	A	501	A1CKP	O30-C31-C32	-3.87	105.06	111.74
2	B	501	A1CKP	C09-C08-C07	3.85	111.44	107.48
2	B	501	A1CKP	C27-N25-N24	-2.70	117.28	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	A1CKP	C06-N18-C19	-2.60	120.96	124.66
2	B	501	A1CKP	C13-C16-N17	-2.46	174.91	178.10
2	B	501	A1CKP	C22-C26-N25	-2.38	103.04	105.31
2	B	501	A1CKP	C32-C27-C28	-2.29	106.00	111.17
2	B	501	A1CKP	C08-C09-C10	-2.23	104.33	106.81
2	B	501	A1CKP	C28-C27-N25	2.23	114.00	110.95
2	B	501	A1CKP	C21-C19-N18	-2.18	105.67	109.95
2	B	501	A1CKP	C05-C06-N18	-2.18	118.48	121.90
2	B	501	A1CKP	C26-N25-N24	2.15	112.65	110.63
2	B	501	A1CKP	C31-O30-C29	2.11	116.70	109.88
2	A	501	A1CKP	C27-N25-N24	-2.11	118.08	120.94
2	A	501	A1CKP	C05-C06-N18	-2.08	118.63	121.90
2	A	501	A1CKP	C20-C19-N18	-2.01	106.00	109.95

There are no chirality outliers.

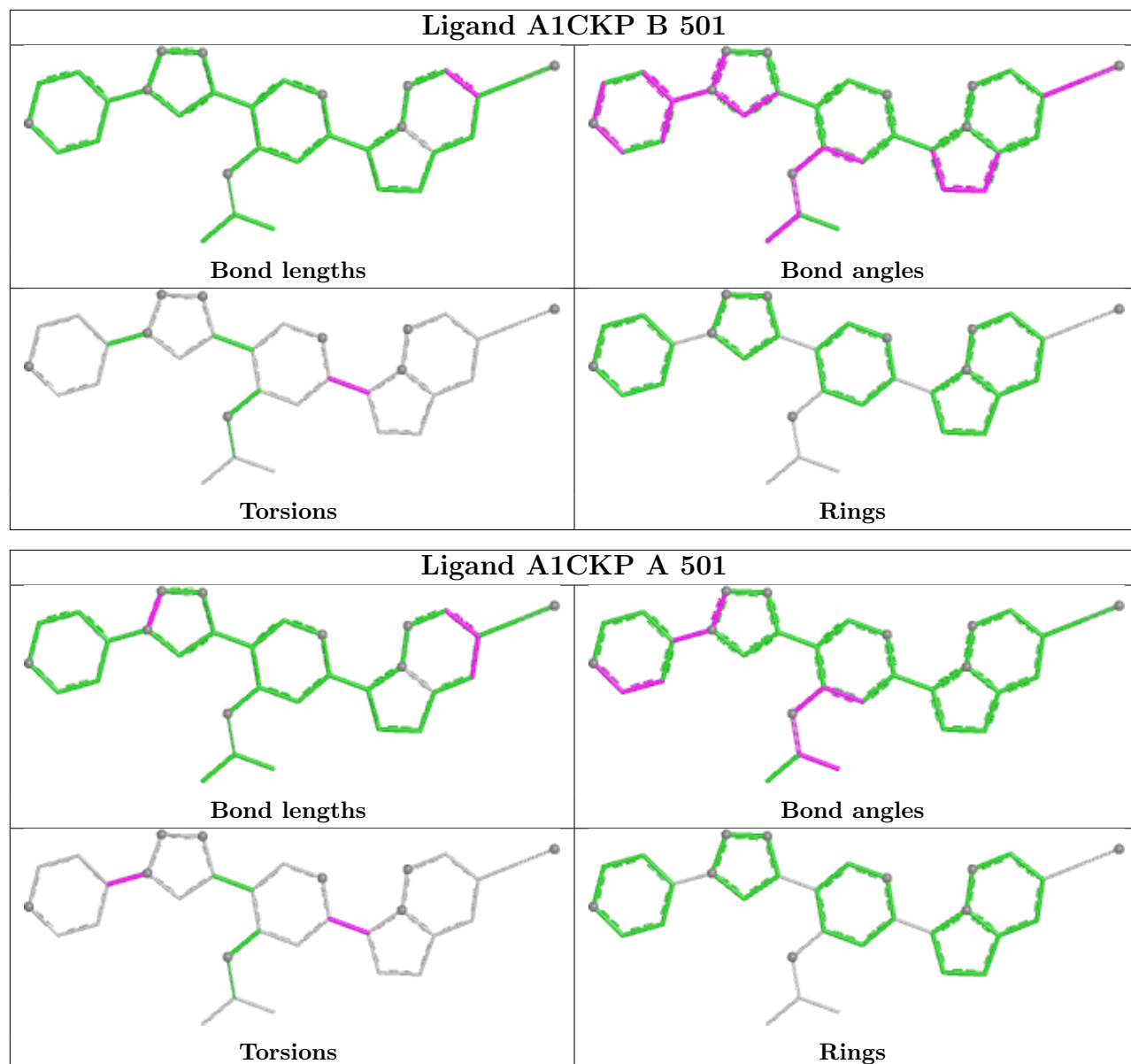
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1CKP	C05-C04-C07-N11
2	A	501	A1CKP	N03-C04-C07-N11
2	B	501	A1CKP	C05-C04-C07-N11
2	B	501	A1CKP	N03-C04-C07-N11
2	A	501	A1CKP	C28-C27-N25-C26

There are no ring outliers.

No monomer is involved in short contacts.

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.



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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/304 (92%)	1.36	66 (23%) 2 1	25, 45, 98, 134	0
1	B	281/304 (92%)	1.25	47 (16%) 4 4	26, 45, 70, 100	0
All	All	562/608 (92%)	1.31	113 (20%) 3 3	25, 45, 91, 134	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PHE	8.7
1	A	170	PHE	7.5
1	A	258	LEU	6.8
1	B	222	THR	6.6
1	A	205	VAL	6.4
1	B	187	VAL	6.3
1	B	170	PHE	6.1
1	B	258	LEU	5.7
1	A	173	LEU	5.6
1	B	201	TYR	5.3
1	A	251	PHE	5.3
1	A	180	PHE	5.1
1	A	257	ASP	5.1
1	B	250	GLY	5.1
1	A	176	VAL	5.1
1	A	201	TYR	5.0
1	B	176	VAL	4.9
1	A	260	LEU	4.9
1	B	230	PHE	4.8
1	A	226	LEU	4.8
1	B	251	PHE	4.8
1	A	208	THR	4.6
1	B	226	LEU	4.5
1	B	168	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	212	VAL	4.5
1	A	215	LEU	4.4
1	B	173	LEU	4.4
1	B	205	VAL	4.4
1	A	171	TYR	4.3
1	A	207	ASN	4.3
1	A	204	TYR	4.2
1	A	172	GLU	4.1
1	A	254	ASP	4.1
1	B	223	THR	4.0
1	B	171	TYR	3.9
1	A	177	THR	3.8
1	A	199	VAL	3.8
1	B	200	VAL	3.7
1	A	223	THR	3.7
1	A	234	ILE	3.7
1	B	180	PHE	3.7
1	A	222	THR	3.7
1	A	203	GLY	3.6
1	B	199	VAL	3.6
1	B	185	ILE	3.6
1	A	168	PHE	3.5
1	A	187	VAL	3.5
1	B	188	GLY	3.5
1	A	256	ASP	3.4
1	B	179	ASN	3.4
1	B	259	CYS	3.4
1	A	178	ASN	3.4
1	B	257	ASP	3.3
1	B	215	LEU	3.3
1	A	209	THR	3.2
1	A	184	PRO	3.2
1	A	179	ASN	3.2
1	A	210	VAL	3.2
1	B	198	GLY	3.2
1	B	203	GLY	3.1
1	A	228	GLN	3.1
1	A	229	GLN	3.0
1	A	192	MET	3.0
1	A	165	PHE	3.0
1	A	169	SER	3.0
1	A	211	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	212	VAL	3.0
1	A	174	LYS	3.0
1	B	177	THR	3.0
1	B	403	ILE	2.9
1	A	250	GLY	2.9
1	A	240	CYS	2.9
1	B	204	TYR	2.8
1	A	197	PHE	2.8
1	A	259	CYS	2.8
1	B	458	THR	2.7
1	A	237	MET	2.7
1	A	261	VAL	2.7
1	A	238	ALA	2.6
1	B	227	LYS	2.6
1	B	169	SER	2.6
1	A	200	VAL	2.6
1	A	252	SER	2.6
1	B	260	LEU	2.6
1	B	182	GLU	2.6
1	A	255	GLY	2.6
1	B	174	LYS	2.6
1	A	236	VAL	2.6
1	A	185	ILE	2.5
1	A	413	TYR	2.4
1	B	175	ASN	2.4
1	A	198	GLY	2.4
1	B	197	PHE	2.4
1	A	253	SER	2.4
1	A	213	LYS	2.3
1	B	343	VAL	2.3
1	B	178	ASN	2.3
1	B	196	GLY	2.3
1	B	192	MET	2.3
1	B	405	ASP	2.2
1	A	202	LYS	2.2
1	A	186	SER	2.2
1	B	434	SER	2.1
1	A	239	LYS	2.1
1	A	439	GLU	2.1
1	A	175	ASN	2.1
1	B	252	SER	2.1
1	B	225	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	347	ARG	2.1
1	A	224	GLU	2.0
1	A	167	SER	2.0
1	B	214	LYS	2.0
1	A	190	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	B	346	10/11	0.66	0.14	54,65,80,84	0
1	SEP	A	346	10/11	0.69	0.14	55,72,88,91	0
1	TPO	B	342	11/12	0.73	0.17	64,68,86,87	0
1	TPO	A	342	11/12	0.86	0.12	57,62,69,76	0
1	TPO	B	345	11/12	0.90	0.10	46,51,59,59	0
1	TPO	A	345	11/12	0.92	0.09	48,52,58,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

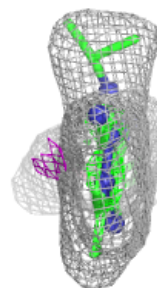
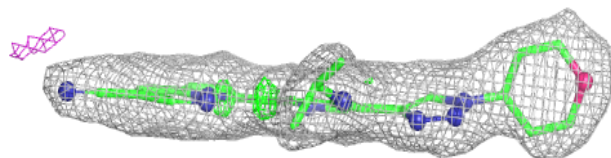
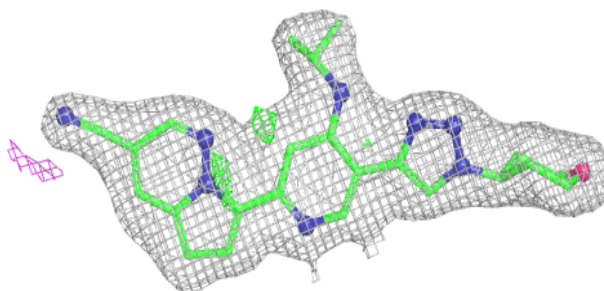
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	502	5/5	0.69	0.12	55,58,68,78	0
3	SO4	A	503	5/5	0.81	0.11	51,58,67,70	0
3	SO4	A	502	5/5	0.88	0.11	44,52,60,64	0
2	A1CKP	B	501	32/32	0.93	0.09	31,37,45,47	0
2	A1CKP	A	501	32/32	0.93	0.10	33,38,45,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

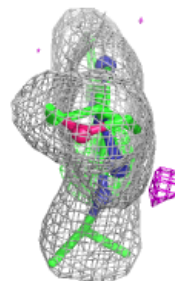
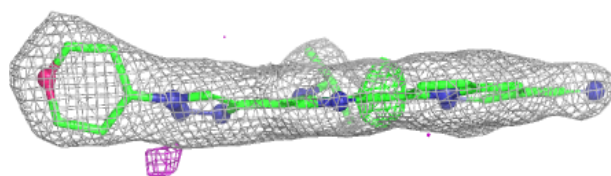
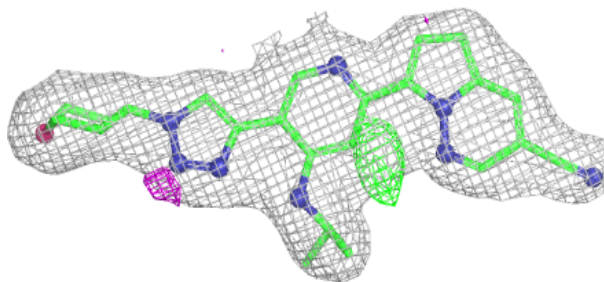
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1CKP B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around A1CKP A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.