



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 01:09 pm BST

PDB ID : 8ATN
Title : Discovery of IRAK4 Inhibitor 38
Authors : Schafer, M.; Bothe, U.; Schmidt, N.; Gunther, J.; Nubbemeyer, R.; Siebeneicher, H.; Ring, S.; Boemer, U.; Peters, M.; Denner, K.; Himmel, H.; Sutter, A.; Terebesi, I.; Lange, M.; Wenger, A.M.; Guimond, N.; Thaler, T.; Platzek, J.; Eberspaecher, U.; Steuber, H.; Steinmeyer, A.; Zollner, T.M.
Deposited on : 2022-08-23
Resolution : 2.17 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

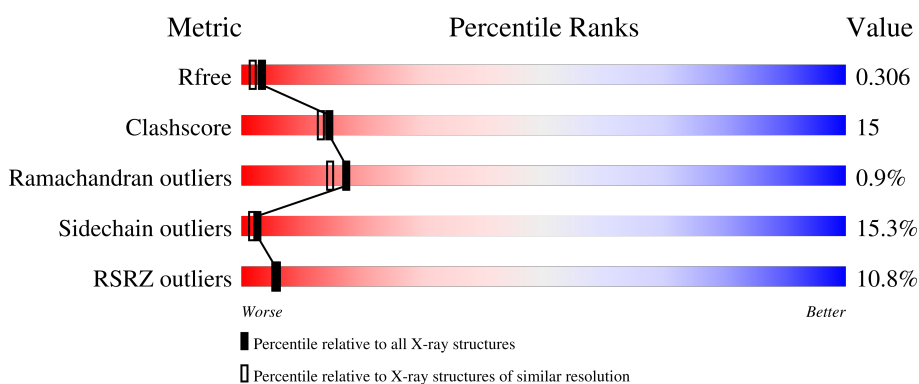
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


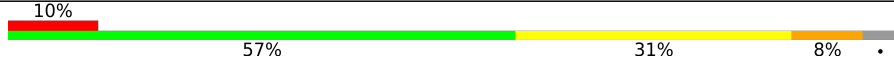
The reported resolution of this entry is 2.17 Å.

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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	AAA	298	
1	BBB	298	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4545 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.

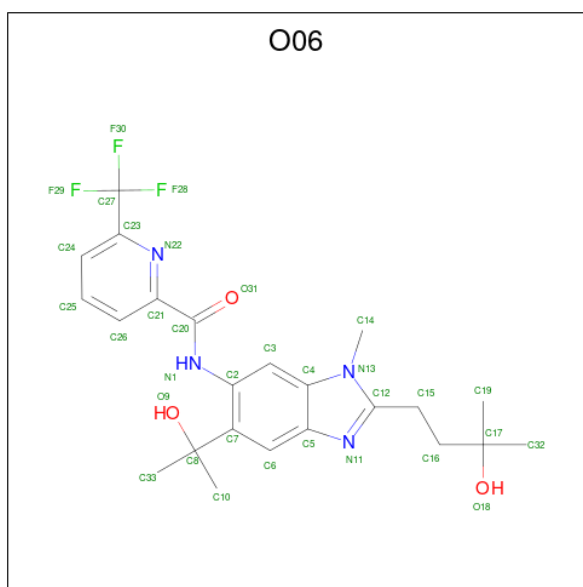
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	AAA	282	2215	1393	372	433	2	15	0	1	0
1	BBB	286	2241	1406	377	442	2	14	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	163	GLY	-	expression tag	UNP Q9NWZ3
AAA	164	SER	-	expression tag	UNP Q9NWZ3
AAA	400	ALA	LYS	engineered mutation	UNP Q9NWZ3
AAA	401	ALA	GLU	engineered mutation	UNP Q9NWZ3
AAA	402	ALA	GLU	engineered mutation	UNP Q9NWZ3
BBB	163	GLY	-	expression tag	UNP Q9NWZ3
BBB	164	SER	-	expression tag	UNP Q9NWZ3
BBB	400	ALA	LYS	engineered mutation	UNP Q9NWZ3
BBB	401	ALA	GLU	engineered mutation	UNP Q9NWZ3
BBB	402	ALA	GLU	engineered mutation	UNP Q9NWZ3

- Molecule 2 is {N}-[3-methyl-2-(3-methyl-3-oxidanyl-butyl)-6-(2-oxidanylpropan-2-yl)benzimidazol-5-yl]-6-(trifluoromethyl)pyridine-2-carboxamide (three-letter code: O06) (formula: C₂₃H₂₇F₃N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	AAA	1	33	23	3	4	3	0	0
2	BBB	1	33	23	3	4	3	0	0

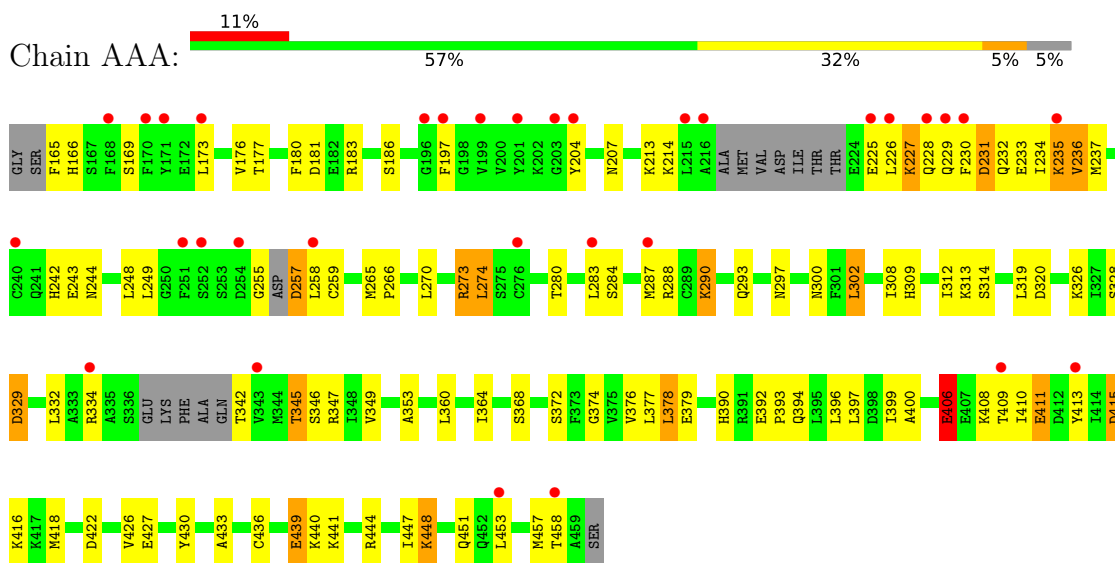
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	AAA	12	12	12	0	0
3	BBB	11	11	11	0	0

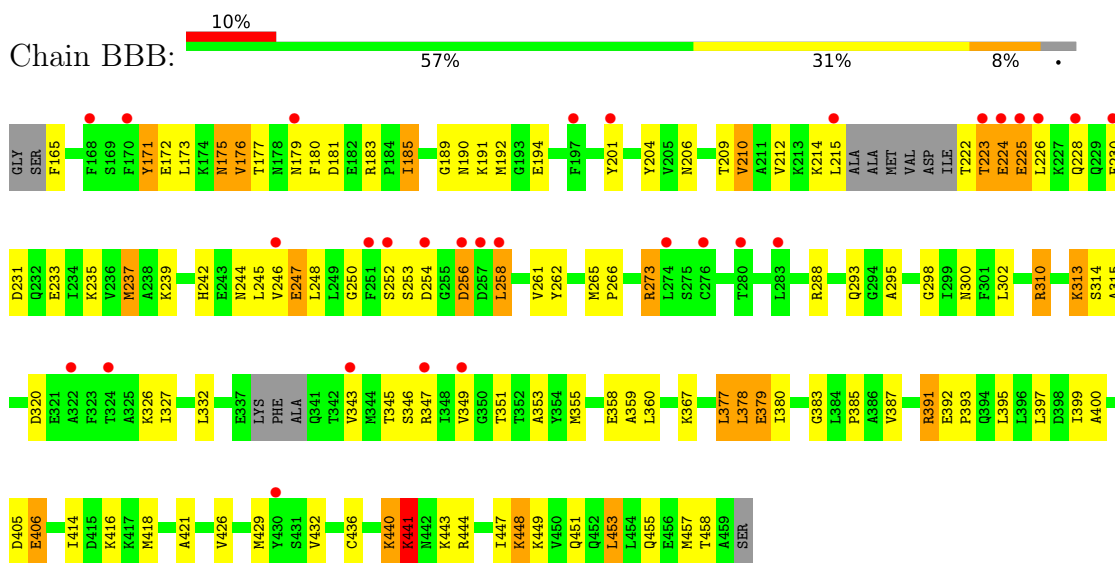
3 Residue-property plots [i](#)

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 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	88.19Å 118.90Å 140.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.17 49.88 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.88-2.17) 99.9 (49.88-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.306 0.244 , 0.306	Depositor DCC
R_{free} test set	1965 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	1.204	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.38 % 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 5.7723e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: O06, 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	AAA	1.01	9/2232 (0.4%)	0.97	2/3006 (0.1%)
1	BBB	0.94	3/2256 (0.1%)	0.96	2/3042 (0.1%)
All	All	0.98	12/4488 (0.3%)	0.97	4/6048 (0.1%)

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	AAA	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	374	GLY	C-O	10.30	1.40	1.23
1	BBB	379	GLU	CD-OE2	9.18	1.35	1.25
1	BBB	206	ASN	C-O	7.48	1.37	1.23
1	AAA	376	VAL	C-O	7.36	1.37	1.23
1	AAA	439	GLU	C-O	6.68	1.36	1.23
1	AAA	353	ALA	C-O	6.38	1.35	1.23
1	AAA	396	LEU	C-O	6.25	1.35	1.23
1	AAA	415	ASP	CG-OD1	6.00	1.39	1.25
1	AAA	374	GLY	C-N	5.81	1.47	1.34
1	AAA	406	GLU	C-O	5.78	1.34	1.23
1	AAA	399	ILE	C-O	5.76	1.34	1.23
1	BBB	247	GLU	C-O	5.03	1.32	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	415	ASP	CB-CG-OD2	-10.49	108.86	118.30
1	AAA	284	SER	O-C-N	6.31	132.80	122.70
1	BBB	310	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	BBB	391	ARG	NE-CZ-NH2	-5.33	117.63	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	406	GLU	Mainchain
1	AAA	439	GLU	Mainchain

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	AAA	2215	0	2187	73	2
1	BBB	2241	0	2202	64	2
2	AAA	33	0	0	0	0
2	BBB	33	0	0	0	0
3	AAA	12	0	0	1	0
3	BBB	11	0	0	0	0
All	All	4545	0	4389	137	2

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 15.

All (137) 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:BBB:177:THR:HG23	1:BBB:180:PHE:H	1.27	0.98
1:AAA:288:ARG:HD2	1:AAA:418:MET:HE1	1.58	0.85
1:AAA:293:GLN:HE22	1:AAA:458:THR:HG21	1.49	0.78
1:AAA:265:MET:HE3	1:AAA:319:LEU:C	2.12	0.70
1:AAA:410:ILE:HD11	1:AAA:427:GLU:OE1	1.91	0.70
1:AAA:288:ARG:CD	1:AAA:418:MET:HE1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:201:TYR:HB2	1:BBB:212:VAL:HG13	1.75	0.68
1:AAA:257:ASP:N	1:AAA:257:ASP:OD1	2.25	0.67
1:AAA:293:GLN:HE22	1:AAA:458:THR:CG2	2.08	0.66
1:AAA:378:LEU:HD21	1:AAA:400:ALA:HB2	1.76	0.65
1:AAA:231:ASP:HA	1:AAA:234:ILE:HD12	1.78	0.64
1:AAA:288:ARG:CZ	1:AAA:418:MET:HE3	2.28	0.64
1:AAA:176:VAL:HG21	1:AAA:204:TYR:O	1.98	0.63
1:BBB:172:GLU:O	1:BBB:176:VAL:HG23	1.98	0.63
1:BBB:173:LEU:O	1:BBB:177:THR:HG22	1.98	0.62
1:AAA:288:ARG:NE	1:AAA:418:MET:CE	2.63	0.62
1:AAA:410:ILE:HG21	1:AAA:430:TYR:CG	2.35	0.62
1:AAA:177:THR:HG23	1:AAA:180:PHE:H	1.66	0.61
1:BBB:298:GLY:HA3	1:BBB:327:ILE:HD12	1.82	0.60
1:BBB:177:THR:HG23	1:BBB:180:PHE:N	2.08	0.60
1:AAA:255:GLY:O	1:AAA:257:ASP:N	2.35	0.60
1:AAA:458:THR:O	1:AAA:458:THR:HG23	2.03	0.59
1:BBB:181:ASP:HB3	1:BBB:190:ASN:HD22	1.67	0.58
1:BBB:378:LEU:HD21	1:BBB:400:ALA:HB2	1.87	0.57
1:BBB:387:VAL:CG2	1:BBB:395:LEU:HD23	2.35	0.57
1:AAA:242:HIS:HE1	1:AAA:244:ASN:HD22	1.53	0.56
1:BBB:288:ARG:HB3	1:BBB:380:ILE:HG23	1.87	0.54
1:BBB:237:MET:HG2	1:BBB:248:LEU:CB	2.37	0.54
1:BBB:440:LYS:HB2	1:BBB:443:LYS:HG2	1.90	0.53
1:BBB:201:TYR:HB2	1:BBB:212:VAL:CG1	2.37	0.53
1:BBB:230:PHE:CD1	1:BBB:258:LEU:HB3	2.42	0.53
1:BBB:414:ILE:HG12	1:BBB:426:VAL:HG11	1.91	0.53
1:BBB:300:ASN:HA	1:BBB:447:ILE:HG21	1.91	0.52
1:BBB:351:THR:O	1:BBB:355:MET:HG3	2.09	0.52
1:BBB:266:PRO:HD2	1:BBB:320:ASP:HA	1.91	0.52
1:AAA:266:PRO:HD2	1:AAA:320:ASP:HA	1.93	0.51
1:AAA:181:ASP:OD1	1:AAA:183:ARG:HB2	2.10	0.51
1:AAA:237:MET:HG2	1:AAA:248:LEU:HB2	1.91	0.51
1:AAA:433:ALA:O	1:AAA:436:CYS:N	2.44	0.51
1:BBB:313:LYS:HG3	1:BBB:315:ALA:H	1.76	0.51
1:BBB:256:ASP:OD1	1:BBB:256:ASP:N	2.43	0.51
1:AAA:409:THR:HG22	1:AAA:411:GLU:HB3	1.91	0.51
1:AAA:334:ARG:NH1	1:AAA:345:TPO:O1P	2.44	0.50
1:AAA:422:ASP:O	1:AAA:426:VAL:HG23	2.11	0.50
1:BBB:436:CYS:O	1:BBB:444:ARG:HD3	2.10	0.50
1:AAA:232:GLN:O	1:AAA:236:VAL:HG12	2.11	0.50
1:BBB:295:ALA:O	1:BBB:327:ILE:HD11	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:410:ILE:O	1:AAA:413:TYR:N	2.41	0.50
1:AAA:173:LEU:O	1:AAA:177:THR:HG22	2.11	0.49
1:BBB:358:GLU:HG2	1:BBB:359:ALA:N	2.26	0.49
1:AAA:288:ARG:NE	1:AAA:418:MET:HE1	2.28	0.49
1:AAA:227:LYS:NZ	1:AAA:231:ASP:HB2	2.28	0.49
1:AAA:265:MET:CE	1:AAA:319:LEU:C	2.81	0.49
1:AAA:300:ASN:ND2	1:AAA:448:LYS:HD3	2.28	0.49
1:AAA:342:THR:HG22	1:AAA:441:LYS:NZ	2.28	0.48
1:BBB:177:THR:HG21	1:BBB:180:PHE:CD1	2.48	0.48
1:BBB:179:ASN:O	1:BBB:180:PHE:C	2.52	0.48
1:AAA:244:ASN:O	1:AAA:326:LYS:HA	2.13	0.48
1:AAA:308:ILE:HD13	1:AAA:364:ILE:HG22	1.94	0.48
1:AAA:312:ILE:O	1:AAA:372:SER:HB3	2.14	0.47
1:AAA:408:LYS:HD2	1:AAA:413:TYR:CE1	2.48	0.47
1:BBB:183:ARG:HB2	1:BBB:189:GLY:HA3	1.95	0.47
1:BBB:185:ILE:CD1	1:BBB:192:MET:HG2	2.44	0.47
1:BBB:406:GLU:HA	1:BBB:406:GLU:OE2	2.14	0.47
1:AAA:309:HIS:NE2	1:AAA:329:ASP:O	2.48	0.47
1:BBB:310:ARG:HD3	1:BBB:332:LEU:O	2.14	0.47
1:BBB:237:MET:HG2	1:BBB:248:LEU:HB2	1.97	0.47
1:BBB:273:ARG:HD3	1:BBB:273:ARG:HA	1.68	0.47
1:AAA:235:LYS:HE3	1:AAA:235:LYS:HB2	1.72	0.47
1:AAA:265:MET:HE3	1:AAA:320:ASP:N	2.30	0.47
1:BBB:242:HIS:HE1	1:BBB:244:ASN:OD1	1.98	0.47
1:AAA:273:ARG:HD3	1:AAA:273:ARG:HA	1.77	0.46
1:BBB:385:PRO:O	1:BBB:391:ARG:NH1	2.44	0.46
1:BBB:393:PRO:HG2	1:BBB:399:ILE:HG13	1.98	0.46
1:BBB:204:TYR:HE1	1:BBB:209:THR:HG1	1.64	0.46
1:AAA:288:ARG:NE	1:AAA:418:MET:HE3	2.31	0.46
1:AAA:297:ASN:ND2	1:AAA:451:GLN:HE21	2.14	0.46
1:BBB:223:THR:HG22	1:BBB:224:GLU:N	2.30	0.46
1:AAA:265:MET:CE	1:AAA:320:ASP:N	2.79	0.45
1:BBB:379:GLU:O	1:BBB:383:GLY:N	2.44	0.45
1:AAA:392:GLU:HA	1:AAA:393:PRO:HA	1.75	0.45
1:BBB:418:MET:HE3	1:BBB:421:ALA:HB2	1.98	0.45
1:BBB:448:LYS:HA	1:BBB:448:LYS:HD3	1.76	0.45
1:AAA:302:LEU:HD12	1:AAA:302:LEU:HA	1.87	0.45
1:BBB:448:LYS:O	1:BBB:451:GLN:HB2	2.17	0.45
1:BBB:185:ILE:HD13	1:BBB:192:MET:HG2	1.98	0.45
1:BBB:231:ASP:O	1:BBB:235:LYS:HG2	2.17	0.45
1:AAA:287[B]:MET:CE	1:AAA:290:LYS:HD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:171:TYR:CD1	1:BBB:172:GLU:N	2.85	0.45
1:BBB:293:GLN:HE22	1:BBB:458:THR:HG21	1.82	0.45
1:AAA:225:GLU:O	1:AAA:228:GLN:HB3	2.17	0.44
1:AAA:436:CYS:O	1:AAA:444:ARG:HD3	2.17	0.44
1:AAA:300:ASN:HD22	1:AAA:447:ILE:HG23	1.81	0.44
1:BBB:387:VAL:HG23	1:BBB:395:LEU:HD23	1.98	0.44
1:AAA:300:ASN:HA	1:AAA:447:ILE:HG21	2.00	0.44
1:AAA:409:THR:CG2	1:AAA:411:GLU:HB3	2.48	0.44
1:BBB:244:ASN:O	1:BBB:245:LEU:HD23	2.18	0.44
1:AAA:390:HIS:HB2	3:AAA:1108:HOH:O	2.17	0.44
1:BBB:367:LYS:HD2	1:BBB:441:LYS:HG2	2.00	0.44
1:BBB:353:ALA:HB2	1:BBB:387:VAL:HG23	1.99	0.44
1:BBB:222:THR:HB	1:BBB:225:GLU:HB2	1.99	0.43
1:BBB:165:PHE:HB3	1:BBB:250:GLY:HA2	1.99	0.43
1:BBB:455:GLN:O	1:BBB:458:THR:HG22	2.18	0.43
1:AAA:332:LEU:HD21	1:AAA:349:VAL:HG22	1.99	0.43
1:AAA:273:ARG:NH1	1:AAA:280:THR:HG21	2.34	0.43
1:BBB:210:VAL:HG22	1:BBB:262:TYR:O	2.19	0.43
1:BBB:441:LYS:HB3	1:BBB:441:LYS:HE2	1.60	0.43
1:BBB:237:MET:HG2	1:BBB:248:LEU:HB3	2.00	0.43
1:BBB:440:LYS:HB3	1:BBB:440:LYS:HE3	1.87	0.43
1:AAA:283:LEU:HD12	1:AAA:283:LEU:N	2.34	0.43
1:AAA:415:ASP:OD1	1:AAA:416:LYS:N	2.51	0.43
1:BBB:432:VAL:HG22	1:BBB:453:LEU:HB3	2.00	0.43
1:BBB:387:VAL:HG22	1:BBB:395:LEU:HD23	2.00	0.42
1:AAA:177:THR:HG21	1:AAA:180:PHE:CD1	2.53	0.42
1:BBB:288:ARG:HB3	1:BBB:380:ILE:CG2	2.49	0.42
1:BBB:175:ASN:O	1:BBB:177:THR:N	2.52	0.42
1:BBB:429:MET:HB2	1:BBB:457:MET:CE	2.49	0.42
1:AAA:230:PHE:CD2	1:AAA:258:LEU:HD22	2.55	0.42
1:AAA:270:LEU:O	1:AAA:274:LEU:HB2	2.20	0.42
1:AAA:345:TPO:HB	1:AAA:364:ILE:HD11	2.02	0.42
1:AAA:177:THR:HG21	1:AAA:180:PHE:CE1	2.55	0.42
1:AAA:274:LEU:HD12	1:AAA:274:LEU:HA	1.79	0.42
1:BBB:377:LEU:HD12	1:BBB:429:MET:HE3	2.02	0.42
1:AAA:265:MET:HE3	1:AAA:319:LEU:O	2.20	0.41
1:AAA:287[B]:MET:HE3	1:AAA:287[B]:MET:HA	2.01	0.41
1:AAA:345:TPO:O	1:AAA:345:TPO:HG22	2.20	0.41
1:AAA:213:LYS:O	1:AAA:259:CYS:HA	2.20	0.41
1:BBB:265:MET:SD	1:BBB:326:LYS:HG3	2.61	0.41
1:BBB:214:LYS:HE2	1:BBB:214:LYS:HB3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:233:GLU:O	1:AAA:237:MET:HB2	2.20	0.41
1:AAA:314:SER:HB2	1:AAA:379:GLU:OE1	2.21	0.41
1:BBB:353:ALA:CB	1:BBB:387:VAL:HG23	2.51	0.41
1:AAA:447:ILE:HD12	1:AAA:447:ILE:HA	1.91	0.40
1:AAA:227:LYS:HA	1:AAA:227:LYS:HD2	1.82	0.40
1:AAA:309:HIS:HE1	1:AAA:328:SER:O	2.04	0.40
1:AAA:270:LEU:HG	1:AAA:274:LEU:HD22	2.03	0.40
1:AAA:288:ARG:CZ	1:AAA:418:MET:CE	2.94	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:390:HIS:NE2	1:BBB:392:GLU:O[3_555]	1.33	0.87
1:AAA:390:HIS:CD2	1:BBB:392:GLU:O[3_555]	1.69	0.51

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	AAA	273/298 (92%)	253 (93%)	19 (7%)	1 (0%)	34	35
1	BBB	278/298 (93%)	254 (91%)	20 (7%)	4 (1%)	11	8
All	All	551/596 (92%)	507 (92%)	39 (7%)	5 (1%)	17	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	176	VAL
1	BBB	258	LEU
1	BBB	441	LYS
1	BBB	247	GLU

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Mol	Chain	Res	Type
1	AAA	329	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	AAA	241/253 (95%)	207 (86%)	34 (14%)	3 2
1	BBB	244/253 (96%)	204 (84%)	40 (16%)	2 1
All	All	485/506 (96%)	411 (85%)	74 (15%)	2 2

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	165	PHE
1	AAA	166	HIS
1	AAA	169	SER
1	AAA	186	SER
1	AAA	197	PHE
1	AAA	207	ASN
1	AAA	214	LYS
1	AAA	226	LEU
1	AAA	227	LYS
1	AAA	229	GLN
1	AAA	231	ASP
1	AAA	235	LYS
1	AAA	236	VAL
1	AAA	243	GLU
1	AAA	249	LEU
1	AAA	257	ASP
1	AAA	273	ARG
1	AAA	274	LEU
1	AAA	290	LYS
1	AAA	302	LEU
1	AAA	313	LYS
1	AAA	347	ARG

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Mol	Chain	Res	Type
1	AAA	360	LEU
1	AAA	368	SER
1	AAA	377	LEU
1	AAA	378	LEU
1	AAA	394	GLN
1	AAA	397	LEU
1	AAA	406	GLU
1	AAA	411	GLU
1	AAA	440	LYS
1	AAA	448	LYS
1	AAA	453	LEU
1	AAA	457	MET
1	BBB	171	TYR
1	BBB	175	ASN
1	BBB	185	ILE
1	BBB	191	LYS
1	BBB	194	GLU
1	BBB	210	VAL
1	BBB	215	LEU
1	BBB	223	THR
1	BBB	224	GLU
1	BBB	225	GLU
1	BBB	226	LEU
1	BBB	228	GLN
1	BBB	233	GLU
1	BBB	237	MET
1	BBB	239	LYS
1	BBB	246	VAL
1	BBB	252	SER
1	BBB	253	SER
1	BBB	254	ASP
1	BBB	256	ASP
1	BBB	261	VAL
1	BBB	273	ARG
1	BBB	302	LEU
1	BBB	313	LYS
1	BBB	314	SER
1	BBB	343	VAL
1	BBB	347	ARG
1	BBB	349	VAL
1	BBB	360	LEU
1	BBB	377	LEU

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Mol	Chain	Res	Type
1	BBB	378	LEU
1	BBB	397	LEU
1	BBB	405	ASP
1	BBB	406	GLU
1	BBB	416	LYS
1	BBB	440	LYS
1	BBB	441	LYS
1	BBB	448	LYS
1	BBB	449	LYS
1	BBB	453	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	BBB	345	1	8,10,11	0.94	1 (12%)	10,14,16	0.84	0
1	SEP	AAA	346	1	8,9,10	0.56	0	8,12,14	1.20	1 (12%)
1	TPO	AAA	345	1	8,10,11	0.95	1 (12%)	10,14,16	0.87	1 (10%)
1	SEP	BBB	346	1	8,9,10	0.70	0	8,12,14	1.13	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	BBB	345	1	-	3/9/11/13	-
1	SEP	AAA	346	1	-	1/5/8/10	-
1	TPO	AAA	345	1	-	2/9/11/13	-
1	SEP	BBB	346	1	-	2/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	345	TPO	P-OG1	2.35	1.63	1.59
1	AAA	345	TPO	P-OG1	2.18	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	346	SEP	OG-CB-CA	2.99	111.06	108.14
1	BBB	346	SEP	OG-CB-CA	2.84	110.91	108.14
1	AAA	345	TPO	O-C-CA	-2.05	119.42	124.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	345	TPO	N-CA-CB-OG1
1	AAA	345	TPO	CB-OG1-P-O1P
1	AAA	346	SEP	N-CA-CB-OG
1	BBB	345	TPO	N-CA-CB-OG1
1	BBB	345	TPO	O-C-CA-CB
1	BBB	345	TPO	CB-OG1-P-O1P
1	BBB	346	SEP	N-CA-CB-OG
1	BBB	346	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	345	TPO	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	O06	BBB	1001	-	33,35,35	1.80	9 (27%)	45,55,55	1.78	8 (17%)
2	O06	AAA	1001	-	33,35,35	1.45	3 (9%)	45,55,55	1.59	8 (17%)

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	O06	BBB	1001	-	-	2/26/26/26	0/3/3/3
2	O06	AAA	1001	-	-	5/26/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	1001	O06	C14-N13	5.27	1.58	1.47
2	BBB	1001	O06	C27-C23	4.80	1.58	1.50
2	BBB	1001	O06	C2-C7	3.32	1.44	1.40
2	BBB	1001	O06	C10-C8	3.28	1.56	1.52
2	BBB	1001	O06	C14-N13	2.99	1.53	1.47
2	AAA	1001	O06	C2-N1	-2.67	1.36	1.41
2	BBB	1001	O06	C8-C7	-2.65	1.52	1.54
2	BBB	1001	O06	C3-C2	2.42	1.42	1.37
2	BBB	1001	O06	C21-N22	-2.42	1.31	1.34
2	AAA	1001	O06	C33-C8	-2.27	1.50	1.52
2	BBB	1001	O06	C25-C24	2.11	1.43	1.38
2	BBB	1001	O06	C33-C8	-2.07	1.50	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	1001	O06	F29-C27-C23	-5.37	103.29	112.47
2	BBB	1001	O06	C16-C15-C12	-4.66	101.83	112.16
2	BBB	1001	O06	C27-C23-N22	4.56	119.73	114.56
2	BBB	1001	O06	C21-N22-C23	4.49	124.80	118.83
2	AAA	1001	O06	C27-C23-N22	3.83	118.91	114.56
2	BBB	1001	O06	F29-C27-C23	-3.53	106.44	112.47
2	BBB	1001	O06	C26-C21-N22	-3.35	118.99	122.92
2	AAA	1001	O06	C33-C8-C7	-3.21	106.44	111.55
2	AAA	1001	O06	C16-C15-C12	-3.02	105.46	112.16
2	BBB	1001	O06	C33-C8-C7	-2.43	107.68	111.55
2	BBB	1001	O06	C25-C24-C23	-2.42	115.62	118.81
2	AAA	1001	O06	C20-C21-N22	2.31	121.10	117.42
2	BBB	1001	O06	C3-C2-C7	-2.28	117.22	120.09
2	AAA	1001	O06	C26-C21-N22	-2.27	120.26	122.92
2	AAA	1001	O06	C3-C2-C7	-2.14	117.39	120.09
2	AAA	1001	O06	O31-C20-N1	2.06	128.41	123.71

There are no chirality outliers.

All (7) torsion outliers are listed below:

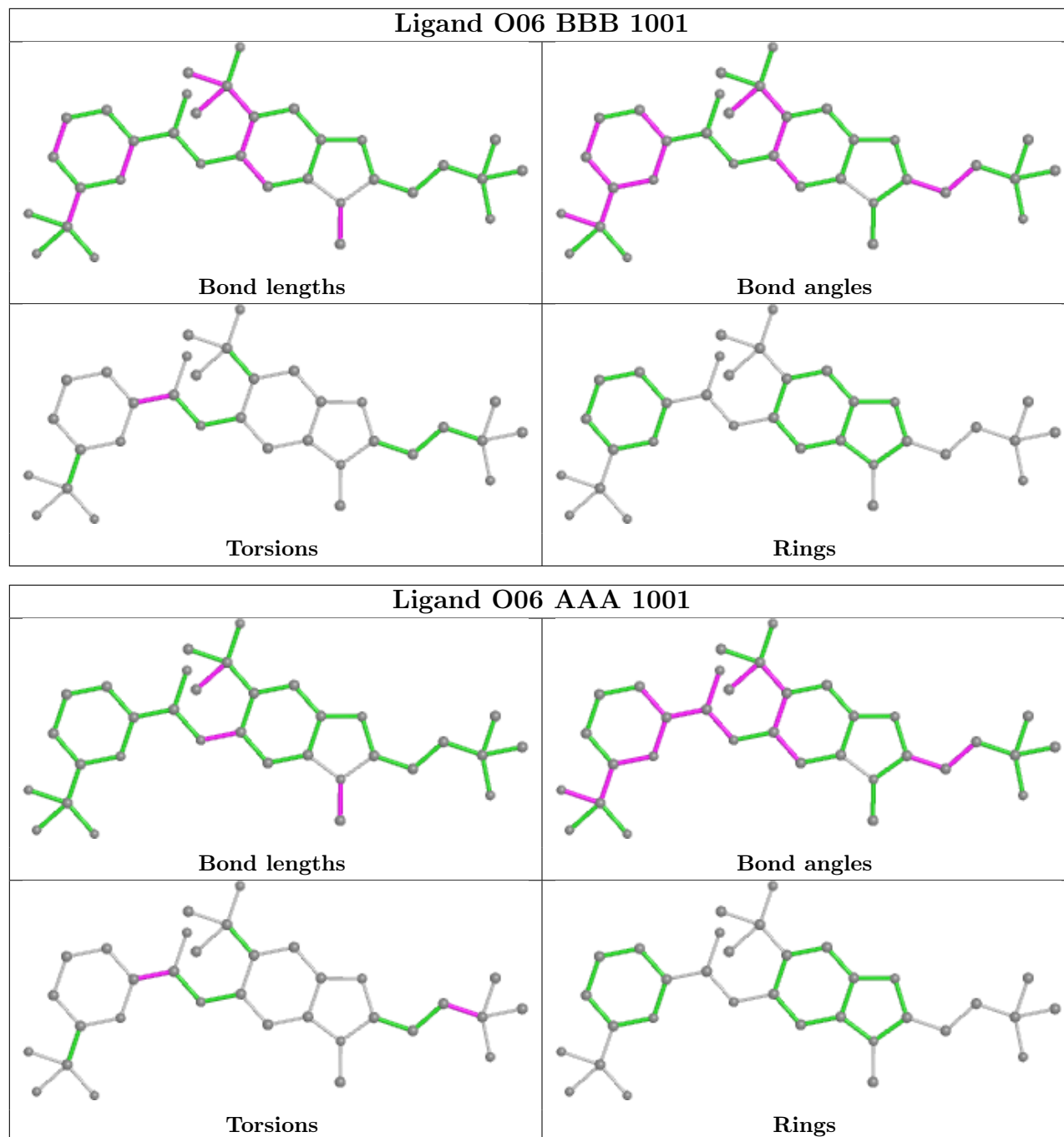
Mol	Chain	Res	Type	Atoms
2	AAA	1001	O06	C15-C16-C17-C19
2	BBB	1001	O06	N1-C20-C21-C26
2	AAA	1001	O06	C15-C16-C17-O18
2	AAA	1001	O06	O31-C20-C21-C26
2	AAA	1001	O06	O31-C20-C21-N22
2	BBB	1001	O06	N1-C20-C21-N22
2	AAA	1001	O06	C15-C16-C17-C32

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	AAA	280/298 (93%)	0.89	32 (11%) 5 5	56, 84, 126, 168	0
1	BBB	284/298 (95%)	0.75	29 (10%) 6 7	48, 72, 117, 144	0
All	All	564/596 (94%)	0.82	61 (10%) 5 6	48, 78, 124, 168	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	197	PHE	11.5
1	BBB	197	PHE	7.7
1	AAA	226	LEU	6.5
1	AAA	215	LEU	6.2
1	AAA	230	PHE	5.9
1	AAA	228	GLN	5.3
1	BBB	230	PHE	5.1
1	AAA	204	TYR	4.5
1	AAA	229	GLN	4.4
1	AAA	216	ALA	4.2
1	BBB	256	ASP	4.1
1	BBB	258	LEU	3.9
1	BBB	223	THR	3.9
1	BBB	343	VAL	3.9
1	AAA	409	THR	3.8
1	AAA	254	ASP	3.6
1	BBB	347	ARG	3.3
1	BBB	179	ASN	3.2
1	AAA	168	PHE	3.2
1	AAA	251	PHE	3.1
1	AAA	171	TYR	3.1
1	BBB	215	LEU	3.1
1	AAA	334	ARG	3.0
1	BBB	226	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	BBB	251	PHE	3.0
1	AAA	196	GLY	3.0
1	BBB	257	ASP	2.9
1	AAA	170	PHE	2.9
1	BBB	225	GLU	2.9
1	BBB	201	TYR	2.9
1	BBB	349	VAL	2.8
1	AAA	252	SER	2.8
1	BBB	170	PHE	2.8
1	AAA	240	CYS	2.8
1	AAA	343	VAL	2.7
1	AAA	173	LEU	2.7
1	AAA	453	LEU	2.7
1	AAA	276	CYS	2.7
1	BBB	252	SER	2.7
1	AAA	258	LEU	2.7
1	BBB	254	ASP	2.5
1	AAA	203	GLY	2.5
1	BBB	168	PHE	2.4
1	BBB	276	CYS	2.4
1	BBB	322	ALA	2.4
1	BBB	246	VAL	2.3
1	BBB	228	GLN	2.3
1	BBB	283	LEU	2.3
1	BBB	430	TYR	2.2
1	AAA	235	LYS	2.2
1	AAA	287[A]	MET	2.2
1	BBB	224	GLU	2.2
1	AAA	413	TYR	2.2
1	AAA	458	THR	2.2
1	AAA	283	LEU	2.2
1	BBB	324	THR	2.2
1	AAA	225	GLU	2.1
1	AAA	201	TYR	2.1
1	AAA	199	VAL	2.0
1	BBB	274	LEU	2.0
1	BBB	280	THR	2.0

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

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	AAA	346	10/11	0.85	0.11	109,131,162,164	0
1	SEP	BBB	346	10/11	0.85	0.17	93,117,153,158	0
1	TPO	AAA	345	11/12	0.88	0.15	107,120,152,157	0
1	TPO	BBB	345	11/12	0.94	0.12	82,95,101,104	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

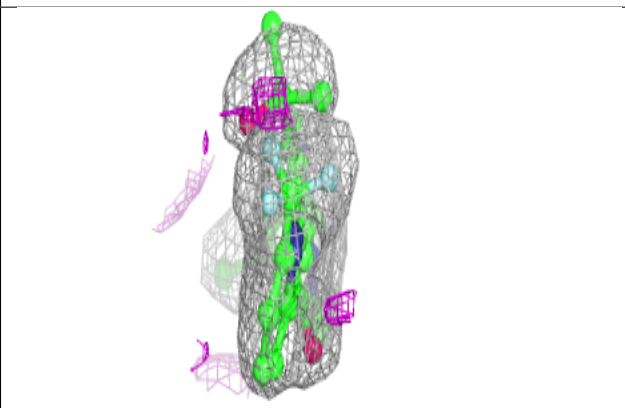
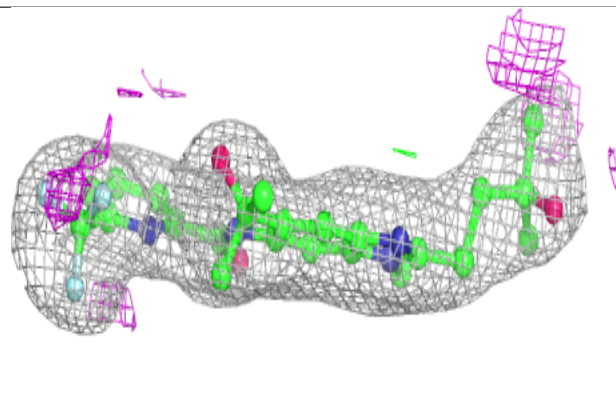
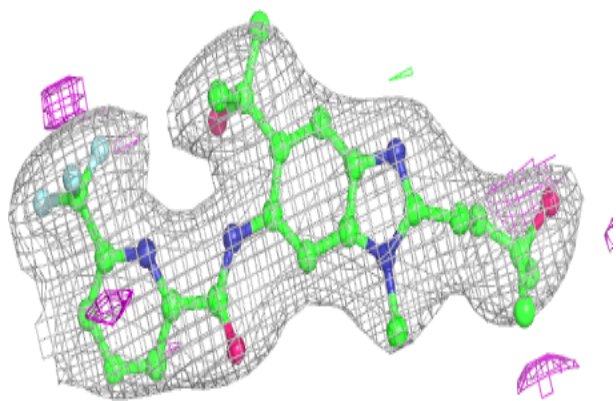
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	O06	AAA	1001	33/33	0.95	0.12	63,70,75,76	0
2	O06	BBB	1001	33/33	0.96	0.14	51,64,74,79	0

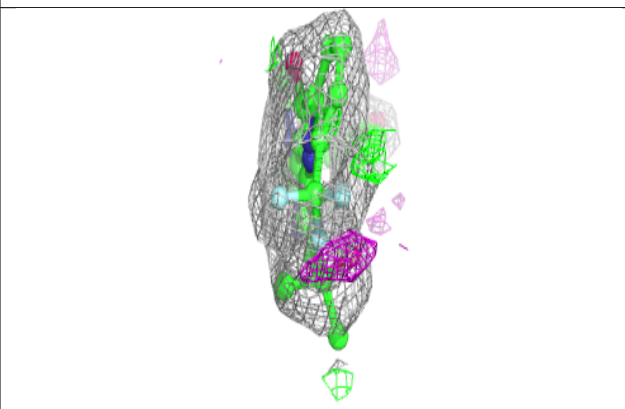
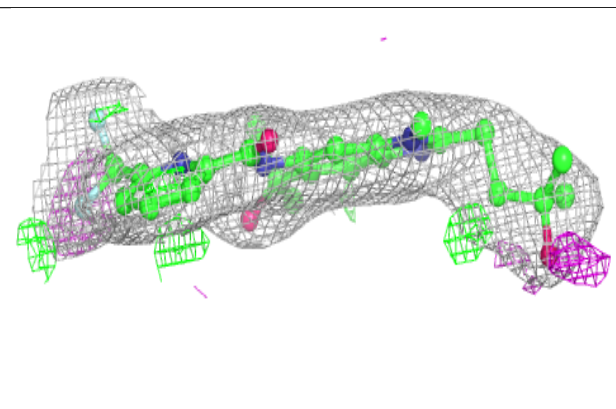
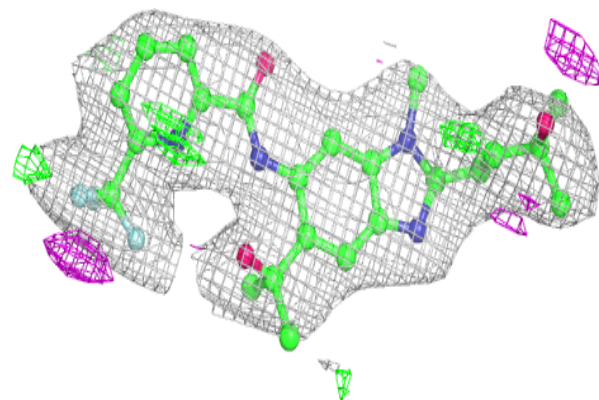
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around O06 AAA 1001:

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

**Electron density around O06 BBB 1001:**

$2mF_o-DF_c$ (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.