



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:04 am GMT

PDB ID : 3UIM  
Title : Structural basis for the impact of phosphorylation on plant receptor-like kinase  
BAK1 activation  
Authors : Lou, Z.Y.; Yan, L.M.; Ma, Y.Y.  
Deposited on : 2011-11-05  
Resolution : 2.20 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

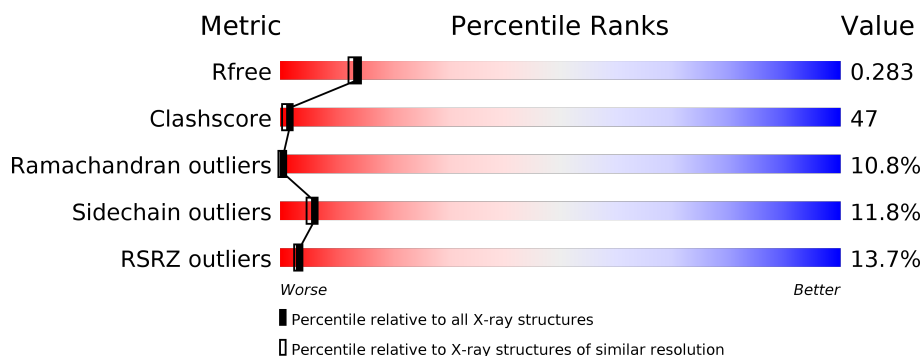
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	290	-	-	X	-
1	TPO	A	446	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2508 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 BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	297	2366	1477	413	456	6	14	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0

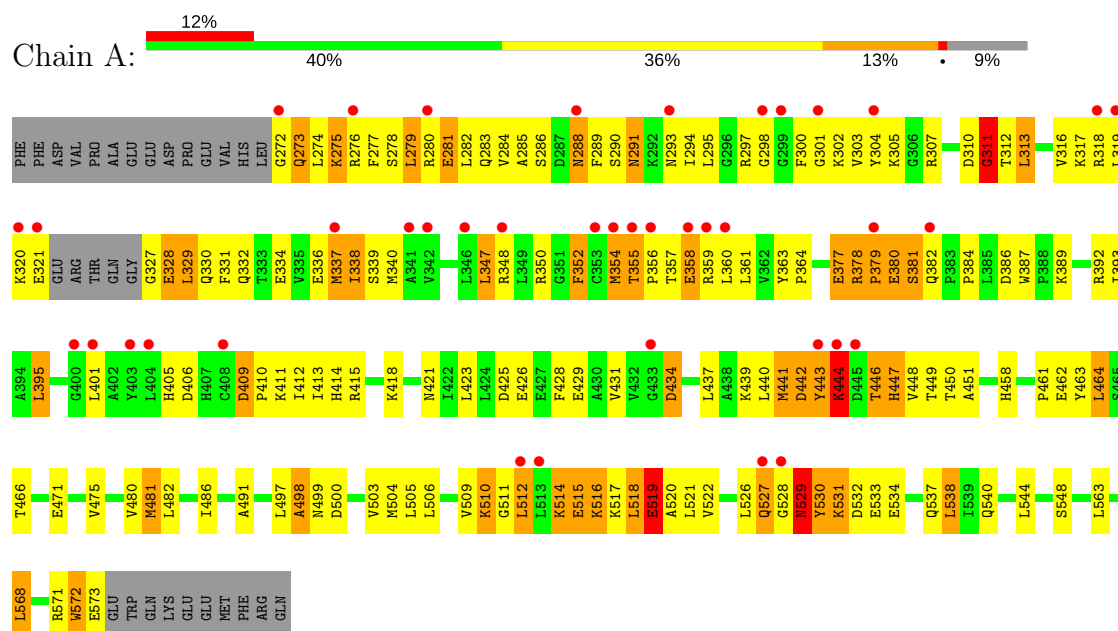
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.11Å 74.70Å 71.92Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	37.35 – 2.20 37.35 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.35-2.20) 89.0 (37.35-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.17 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.234 , 0.277 0.239 , 0.283	Depositor DCC
$R_{free}$ test set	957 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 68.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TPO, ANP, 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	0.45	1/2333 (0.0%)	0.67	1/3130 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	LEU	C-N	-6.67	1.18	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	ASP	CB-CG-OD2	5.21	122.98	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	GLY	Mainchain
1	A	446	TPO	Mainchain

## 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	2366	0	2362	225	1
2	A	31	0	12	3	0
3	A	111	0	0	5	1
All	All	2508	0	2374	226	1

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 47.

All (226) 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:377:GLU:CB	1:A:378:ARG:HA	1.77	1.12
1:A:378:ARG:HB3	1:A:379:PRO:HD2	1.35	1.09
1:A:377:GLU:HB3	1:A:378:ARG:HA	1.37	1.03
1:A:273:GLN:OE1	1:A:275:LYS:NZ	1.99	0.96
1:A:354:MET:HG2	1:A:355:THR:H	1.28	0.96
1:A:446:TPO:P	1:A:447:HIS:HB2	2.05	0.95
1:A:447:HIS:NE2	1:A:449:TPO:OG1	2.02	0.92
1:A:405:HIS:O	1:A:411:LYS:HG2	1.73	0.88
1:A:280:ARG:HA	1:A:283:GLN:HG3	1.55	0.87
1:A:377:GLU:HB2	1:A:378:ARG:HA	1.60	0.84
1:A:518:LEU:O	1:A:520:ALA:N	2.16	0.79
1:A:377:GLU:HB3	1:A:378:ARG:CA	2.11	0.79
1:A:310:ASP:OD1	1:A:312:TPO:O1P	2.00	0.79
1:A:497:LEU:O	1:A:499:ASN:N	2.18	0.77
1:A:518:LEU:HB3	1:A:522:VAL:HG23	1.65	0.77
1:A:347:LEU:HD22	1:A:363:TYR:HD1	1.50	0.77
1:A:441:MET:HG2	1:A:448:VAL:CG2	2.16	0.75
1:A:446:TPO:O	1:A:447:HIS:HB3	1.84	0.75
1:A:295:LEU:HB2	1:A:303:VAL:HG23	1.68	0.75
1:A:279:LEU:HG	1:A:283:GLN:HE21	1.52	0.74
1:A:290:SEP:HA	1:A:304:TYR:HE2	1.52	0.74
1:A:450:TPO:O3P	1:A:451:ALA:N	2.21	0.74
1:A:387:TRP:H	1:A:529:ASN:HD22	1.37	0.72
1:A:300:PHE:O	1:A:319:LEU:HA	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLY:O	1:A:273:GLN:HB2	1.89	0.71
1:A:285:ALA:HB1	1:A:307:ARG:O	1.92	0.70
1:A:275:LYS:HD2	1:A:275:LYS:N	2.08	0.68
1:A:347:LEU:HD22	1:A:363:TYR:CD1	2.28	0.68
1:A:378:ARG:CB	1:A:379:PRO:HD2	2.19	0.68
1:A:283:GLN:HG2	1:A:289:PHE:CE2	2.29	0.67
1:A:378:ARG:HB3	1:A:379:PRO:CD	2.20	0.67
2:A:1000:ANP:O1A	3:A:171:HOH:O	2.12	0.67
1:A:347:LEU:HD21	1:A:364:PRO:HD2	1.75	0.67
1:A:446:TPO:O1P	1:A:447:HIS:HB2	1.94	0.67
1:A:283:GLN:O	1:A:288:ASN:N	2.28	0.67
1:A:273:GLN:HA	1:A:275:LYS:HZ1	1.60	0.67
1:A:497:LEU:O	1:A:499:ASN:O	2.12	0.67
1:A:290:SEP:HA	1:A:304:TYR:CE2	2.29	0.66
1:A:425:ASP:OD1	1:A:429:GLU:HB2	1.94	0.66
1:A:516:LYS:O	1:A:517:LYS:HB2	1.97	0.65
1:A:446:TPO:P	1:A:447:HIS:CB	2.85	0.64
1:A:380:GLU:CD	1:A:381:SER:H	2.01	0.64
1:A:572:TRP:N	1:A:572:TRP:CD1	2.64	0.64
1:A:354:MET:CG	1:A:355:THR:H	2.07	0.64
1:A:298:GLY:HA2	2:A:1000:ANP:O2A	1.97	0.64
1:A:512:LEU:HG	1:A:521:LEU:HD21	1.79	0.64
1:A:506:LEU:O	1:A:510:LYS:HG3	1.98	0.64
1:A:386:ASP:HB2	1:A:529:ASN:ND2	2.13	0.63
1:A:409:ASP:HB3	1:A:410:PRO:CD	2.28	0.63
1:A:276:ARG:NH2	3:A:60:HOH:O	2.31	0.63
1:A:540:GLN:OE1	1:A:568:LEU:HD11	1.98	0.63
1:A:282:LEU:HD11	1:A:360:LEU:HD13	1.80	0.63
1:A:328:GLU:HG3	1:A:329:LEU:H	1.63	0.63
1:A:275:LYS:HB3	1:A:277:PHE:CE1	2.34	0.63
1:A:415:ARG:NH1	1:A:439:LYS:HG2	2.14	0.62
1:A:486:ILE:HD11	1:A:538:LEU:HB3	1.80	0.62
1:A:504:MET:HA	1:A:504:MET:HE3	1.82	0.62
1:A:533:GLU:O	1:A:537:GLN:HG3	2.00	0.62
1:A:318:ARG:HA	1:A:360:LEU:HD23	1.82	0.61
1:A:529:ASN:O	1:A:530:TYR:O	2.18	0.61
1:A:441:MET:HE2	1:A:448:VAL:HG23	1.83	0.61
1:A:447:HIS:HE2	1:A:449:TPO:CB	2.12	0.61
1:A:301:GLY:HA3	1:A:318:ARG:O	2.00	0.61
1:A:280:ARG:C	1:A:282:LEU:H	2.05	0.60
1:A:302:LYS:HB2	1:A:304:TYR:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD23	1:A:320:LYS:N	2.16	0.60
1:A:274:LEU:H	1:A:275:LYS:NZ	2.00	0.60
1:A:497:LEU:C	1:A:499:ASN:N	2.55	0.60
1:A:310:ASP:OD1	1:A:312:TPO:P	2.59	0.60
1:A:512:LEU:HG	1:A:521:LEU:CD2	2.32	0.59
1:A:337:MET:O	1:A:339:SER:N	2.36	0.59
1:A:354:MET:HG2	1:A:355:THR:N	2.10	0.59
1:A:279:LEU:O	1:A:282:LEU:HG	2.02	0.59
1:A:509:VAL:C	1:A:511:GLY:N	2.56	0.59
1:A:278:SER:OG	1:A:281:GLU:OE2	2.20	0.58
1:A:442:ASP:O	1:A:443:TYR:C	2.40	0.58
1:A:337:MET:O	1:A:340:MET:N	2.28	0.58
1:A:310:ASP:OD1	1:A:312:TPO:O3P	2.22	0.58
1:A:272:GLY:O	1:A:273:GLN:CB	2.51	0.58
1:A:409:ASP:HB3	1:A:410:PRO:HD3	1.84	0.58
1:A:446:TPO:O1P	1:A:447:HIS:CB	2.51	0.58
1:A:347:LEU:HD21	1:A:363:TYR:HB3	1.85	0.58
1:A:446:TPO:O2P	1:A:447:HIS:HB2	2.04	0.57
1:A:379:PRO:O	1:A:381:SER:N	2.36	0.56
1:A:350:ARG:HD2	1:A:364:PRO:HG3	1.86	0.56
1:A:442:ASP:O	1:A:444:LYS:N	2.38	0.56
1:A:509:VAL:C	1:A:511:GLY:H	2.09	0.56
1:A:534:GLU:O	1:A:537:GLN:HB2	2.05	0.56
1:A:471:GLU:O	1:A:475:VAL:HG23	2.05	0.56
1:A:319:LEU:HD22	1:A:358:GLU:HG3	1.87	0.55
1:A:283:GLN:HG2	1:A:289:PHE:HE2	1.71	0.55
1:A:355:THR:C	1:A:357:THR:H	2.11	0.55
1:A:380:GLU:CG	1:A:381:SER:N	2.69	0.55
1:A:354:MET:N	1:A:354:MET:SD	2.74	0.55
1:A:531:LYS:HB3	1:A:534:GLU:HG2	1.89	0.55
1:A:280:ARG:HG2	1:A:283:GLN:NE2	2.21	0.54
1:A:434:ASP:HB2	3:A:171:HOH:O	2.06	0.54
1:A:293:ASN:ND2	1:A:305:LYS:O	2.39	0.54
1:A:286:SER:HB2	1:A:289:PHE:HA	1.90	0.54
1:A:386:ASP:HB2	1:A:529:ASN:HD21	1.71	0.54
1:A:412:ILE:HG12	1:A:440:LEU:CD2	2.37	0.54
1:A:531:LYS:HD3	1:A:533:GLU:H	1.72	0.54
1:A:312:TPO:P	1:A:312:TPO:H	2.31	0.54
1:A:540:GLN:O	1:A:544:LEU:HG	2.08	0.53
1:A:387:TRP:HE1	1:A:534:GLU:HB3	1.73	0.53
1:A:310:ASP:OD1	1:A:311:GLY:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:N	1:A:431:VAL:HG13	2.23	0.53
1:A:409:ASP:CB	1:A:410:PRO:CD	2.87	0.53
1:A:415:ARG:HG3	1:A:415:ARG:HH11	1.74	0.53
1:A:568:LEU:O	1:A:568:LEU:HD22	2.09	0.53
1:A:280:ARG:HA	1:A:283:GLN:CG	2.33	0.52
1:A:295:LEU:HB2	1:A:303:VAL:CG2	2.39	0.52
1:A:518:LEU:HA	1:A:521:LEU:HG	1.91	0.52
1:A:423:LEU:HD12	1:A:423:LEU:N	2.25	0.52
1:A:510:LYS:C	1:A:512:LEU:H	2.13	0.52
1:A:497:LEU:C	1:A:499:ASN:H	2.13	0.52
1:A:290:SEP:CA	1:A:304:TYR:HE2	2.21	0.52
1:A:337:MET:O	1:A:338:ILE:C	2.48	0.52
1:A:336:GLU:O	1:A:339:SER:OG	2.22	0.52
1:A:415:ARG:HH11	1:A:439:LYS:HG2	1.75	0.52
1:A:415:ARG:NH1	1:A:437:LEU:O	2.43	0.51
1:A:447:HIS:HD2	1:A:448:VAL:N	2.08	0.51
1:A:409:ASP:CB	1:A:410:PRO:HD3	2.40	0.51
1:A:572:TRP:N	1:A:572:TRP:HD1	2.07	0.51
1:A:514:LYS:O	1:A:515:GLU:C	2.49	0.51
1:A:280:ARG:O	1:A:282:LEU:N	2.44	0.51
1:A:297:ARG:O	3:A:174:HOH:O	2.18	0.51
1:A:347:LEU:CD2	1:A:364:PRO:HD2	2.40	0.51
1:A:481:MET:C	1:A:481:MET:CE	2.79	0.51
1:A:447:HIS:CE1	1:A:449:TPO:P	3.04	0.51
1:A:293:ASN:OD1	1:A:305:LYS:N	2.44	0.50
1:A:303:VAL:HG21	2:A:1000:ANP:O4'	2.11	0.50
1:A:328:GLU:CG	1:A:329:LEU:H	2.23	0.50
1:A:526:LEU:O	1:A:527:GLN:C	2.49	0.50
1:A:278:SER:O	1:A:280:ARG:N	2.44	0.50
1:A:274:LEU:H	1:A:275:LYS:HZ1	1.58	0.50
1:A:518:LEU:HB3	1:A:522:VAL:CG2	2.40	0.50
1:A:509:VAL:O	1:A:511:GLY:N	2.44	0.50
1:A:276:ARG:O	1:A:276:ARG:HG3	2.11	0.49
1:A:540:GLN:NE2	1:A:572:TRP:CZ2	2.80	0.49
1:A:274:LEU:N	1:A:275:LYS:HZ1	2.10	0.49
1:A:298:GLY:H	1:A:302:LYS:HA	1.76	0.49
1:A:380:GLU:HG2	1:A:381:SER:N	2.27	0.49
1:A:481:MET:HE1	1:A:482:LEU:HD23	1.94	0.49
1:A:425:ASP:OD2	1:A:428:PHE:N	2.46	0.48
1:A:318:ARG:CZ	1:A:320:LYS:HE3	2.43	0.48
1:A:409:ASP:OD2	1:A:409:ASP:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MET:CE	1:A:448:VAL:HG23	2.44	0.48
1:A:280:ARG:CA	1:A:283:GLN:HG3	2.35	0.48
1:A:355:THR:C	1:A:357:THR:N	2.67	0.47
1:A:278:SER:O	1:A:279:LEU:C	2.52	0.47
1:A:405:HIS:O	1:A:411:LYS:CG	2.54	0.47
1:A:491:ALA:HA	1:A:505:LEU:HB2	1.97	0.47
1:A:414:HIS:O	1:A:415:ARG:HB2	2.15	0.47
1:A:466:THR:HG22	1:A:466:THR:O	2.14	0.47
1:A:441:MET:HG2	1:A:448:VAL:HG23	1.97	0.47
1:A:307:ARG:HG2	1:A:313:LEU:HD23	1.96	0.47
1:A:338:ILE:HG23	1:A:339:SER:N	2.30	0.47
1:A:317:LYS:O	1:A:360:LEU:HD23	2.14	0.46
1:A:540:GLN:CD	1:A:572:TRP:CZ2	2.88	0.46
1:A:280:ARG:C	1:A:282:LEU:N	2.69	0.46
1:A:379:PRO:O	1:A:380:GLU:C	2.54	0.46
1:A:458:HIS:CD2	1:A:480:VAL:HB	2.49	0.46
1:A:462:GLU:HG2	1:A:463:TYR:N	2.31	0.46
1:A:319:LEU:HD23	1:A:319:LEU:C	2.36	0.46
1:A:355:THR:O	1:A:357:THR:N	2.48	0.46
1:A:290:SEP:O	1:A:291:ASN:HB2	2.15	0.46
1:A:337:MET:O	1:A:340:MET:HG2	2.16	0.46
1:A:378:ARG:HD2	1:A:382:GLN:O	2.16	0.45
1:A:447:HIS:CD2	1:A:448:VAL:N	2.84	0.45
1:A:481:MET:HE3	1:A:481:MET:C	2.37	0.45
1:A:328:GLU:C	1:A:330:GLN:H	2.18	0.45
1:A:531:LYS:HD3	1:A:531:LYS:C	2.37	0.45
1:A:413:ILE:HG22	1:A:415:ARG:HG2	1.98	0.45
1:A:328:GLU:C	1:A:330:GLN:N	2.69	0.45
1:A:294:ILE:HD11	1:A:304:TYR:CZ	2.52	0.45
1:A:329:LEU:HB2	1:A:332:GLN:NE2	2.32	0.45
1:A:350:ARG:NH2	3:A:160:HOH:O	2.51	0.44
1:A:418:LYS:HE2	1:A:421:ASN:ND2	2.32	0.44
1:A:509:VAL:O	1:A:512:LEU:HB2	2.17	0.44
1:A:481:MET:HE2	1:A:482:LEU:N	2.32	0.44
1:A:441:MET:HE1	1:A:447:HIS:C	2.37	0.44
1:A:481:MET:HE3	1:A:481:MET:O	2.16	0.44
1:A:334:GLU:CD	1:A:361:LEU:HD13	2.38	0.44
1:A:538:LEU:HA	1:A:538:LEU:HD23	1.79	0.44
1:A:441:MET:O	1:A:442:ASP:CB	2.66	0.43
1:A:531:LYS:HD3	1:A:532:ASP:N	2.34	0.43
1:A:572:TRP:HD1	1:A:572:TRP:H	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:CD	1:A:321:GLU:H	2.21	0.43
1:A:531:LYS:H	1:A:534:GLU:HG3	1.83	0.43
1:A:389:LYS:O	1:A:393:ILE:HG13	2.18	0.43
1:A:509:VAL:CG1	1:A:512:LEU:HD12	2.48	0.43
1:A:302:LYS:HB2	1:A:304:TYR:CE1	2.51	0.43
1:A:331:PHE:CZ	1:A:359:ARG:HB3	2.54	0.43
1:A:352:PHE:HD2	1:A:352:PHE:H	1.67	0.43
1:A:516:LYS:O	1:A:517:LYS:CB	2.63	0.43
1:A:531:LYS:O	1:A:532:ASP:C	2.57	0.43
1:A:347:LEU:HD13	1:A:363:TYR:CD1	2.54	0.43
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.76	0.42
1:A:348:ARG:HH22	1:A:350:ARG:CZ	2.32	0.42
1:A:447:HIS:CE1	1:A:449:TPO:O1P	2.72	0.42
1:A:517:LYS:HD2	1:A:519:GLU:OE1	2.20	0.42
1:A:497:LEU:O	1:A:498:ALA:C	2.59	0.41
1:A:395:LEU:HA	1:A:563:LEU:HD12	2.02	0.41
1:A:293:ASN:OD1	1:A:305:LYS:O	2.37	0.41
1:A:329:LEU:C	1:A:331:PHE:N	2.73	0.41
1:A:329:LEU:C	1:A:331:PHE:H	2.24	0.41
1:A:378:ARG:CB	1:A:379:PRO:CD	2.89	0.41
1:A:380:GLU:O	1:A:381:SER:HB2	2.21	0.41
1:A:461:PRO:O	1:A:464:LEU:HD12	2.21	0.41
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.68	0.41
1:A:387:TRP:HE1	1:A:534:GLU:CB	2.34	0.41
1:A:481:MET:HE2	1:A:481:MET:HB3	1.87	0.41
1:A:540:GLN:NE2	1:A:572:TRP:HZ2	2.19	0.41
1:A:378:ARG:HH12	1:A:384:PRO:HG3	1.86	0.41
1:A:409:ASP:CG	1:A:410:PRO:HD3	2.41	0.41
1:A:279:LEU:HG	1:A:283:GLN:NE2	2.30	0.40
1:A:307:ARG:HG2	1:A:313:LEU:CD2	2.51	0.40
1:A:352:PHE:N	1:A:352:PHE:CD2	2.88	0.40
1:A:450:TPO:O3P	1:A:450:TPO:HG22	2.21	0.40
1:A:482:LEU:HD13	1:A:538:LEU:HD22	2.03	0.40
1:A:352:PHE:N	1:A:352:PHE:HD2	2.20	0.40
1:A:380:GLU:CD	1:A:381:SER:N	2.72	0.40
1:A:447:HIS:NE2	1:A:449:TPO:P	2.94	0.40
1:A:284:VAL:HG13	1:A:285:ALA:N	2.36	0.40
1:A:481:MET:HE2	1:A:481:MET:C	2.42	0.40

All (1) 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:A:327:GLY:N	3:A:92:HOH:O[3_445]	1.98	0.22

## 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	287/326 (88%)	227 (79%)	29 (10%)	31 (11%)	<b>0</b> <b>0</b>

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	279	LEU
1	A	291	ASN
1	A	338	ILE
1	A	380	GLU
1	A	381	SER
1	A	443	TYR
1	A	498	ALA
1	A	514	LYS
1	A	518	LEU
1	A	519	GLU
1	A	527	GLN
1	A	530	TYR
1	A	281	GLU
1	A	434	ASP
1	A	442	ASP
1	A	447	HIS
1	A	516	LYS
1	A	311	GLY
1	A	329	LEU
1	A	377	GLU
1	A	409	ASP
1	A	444	LYS

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Mol	Chain	Res	Type
1	A	328	GLU
1	A	355	THR
1	A	356	PRO
1	A	510	LYS
1	A	515	GLU
1	A	529	ASN
1	A	379	PRO
1	A	528	GLY

### 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	246/273 (90%)	217 (88%)	29 (12%)	<b>6</b> <b>5</b>

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	LYS
1	A	288	ASN
1	A	316	VAL
1	A	337	MET
1	A	347	LEU
1	A	352	PHE
1	A	354	MET
1	A	358	GLU
1	A	378	ARG
1	A	392	ARG
1	A	395	LEU
1	A	401	LEU
1	A	426	GLU
1	A	441	MET
1	A	444	LYS
1	A	464	LEU
1	A	481	MET
1	A	500	ASP

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Mol	Chain	Res	Type
1	A	503	VAL
1	A	512	LEU
1	A	519	GLU
1	A	529	ASN
1	A	531	LYS
1	A	538	LEU
1	A	548	SER
1	A	568	LEU
1	A	571	ARG
1	A	572	TRP
1	A	573	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	332	GLN
1	A	529	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	290	1	9,9,10	0.96	0	9,12,14	3.08	1 (11%)
1	TPO	A	312	1	9,10,11	1.35	2 (22%)	10,14,16	1.02	1 (10%)
1	TPO	A	446	1	9,10,11	1.08	1 (11%)	10,14,16	1.16	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	A	449	1	9,10,11	1.10	1 (11%)	10,14,16	1.15	1 (10%)
1	TPO	A	450	1	9,10,11	1.22	1 (11%)	10,14,16	1.06	1 (10%)
1	TPO	A	455	1	9,10,11	1.05	1 (11%)	10,14,16	0.74	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	A	290	1	-	0/5/8/10	0/0/0/0
1	TPO	A	312	1	-	0/8/11/13	0/0/0/0
1	TPO	A	446	1	-	0/8/11/13	0/0/0/0
1	TPO	A	449	1	-	0/8/11/13	0/0/0/0
1	TPO	A	450	1	-	0/8/11/13	0/0/0/0
1	TPO	A	455	1	-	0/8/11/13	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	TPO	CB-CA	-2.58	1.49	1.53
1	A	450	TPO	CB-CA	-2.55	1.49	1.53
1	A	449	TPO	CB-CA	-2.22	1.50	1.53
1	A	446	TPO	CB-CA	-2.19	1.50	1.53
1	A	455	TPO	CB-CA	-2.06	1.50	1.53
1	A	312	TPO	CA-N	-2.04	1.40	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	TPO	CG2-CB-CA	-2.69	108.22	113.22
1	A	449	TPO	CG2-CB-CA	-2.67	108.26	113.22
1	A	312	TPO	O-C-CA	-2.49	119.34	125.15
1	A	450	TPO	O-C-CA	-2.49	119.35	125.15
1	A	290	SEP	OG-CB-CA	9.04	117.08	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	290	SEP	4	0
1	A	312	TPO	4	0
1	A	446	TPO	6	0
1	A	449	TPO	5	0
1	A	450	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	ANP	A	1000	-	29,33,33	3.07	10 (34%)	28,52,52	2.11	5 (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	ANP	A	1000	-	-	0/13/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	ANP	O2'-C2'	-3.01	1.36	1.43
2	A	1000	ANP	C5'-C4'	-2.84	1.42	1.51
2	A	1000	ANP	C2'-C1'	-2.35	1.49	1.53
2	A	1000	ANP	PG-O3G	-2.26	1.50	1.56
2	A	1000	ANP	C3'-C4'	-2.23	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	ANP	C2'-C3'	-2.23	1.47	1.53
2	A	1000	ANP	O3'-C3'	-2.17	1.38	1.43
2	A	1000	ANP	C6-N6	2.20	1.43	1.34
2	A	1000	ANP	PG-O1G	10.23	1.57	1.46
2	A	1000	ANP	PB-O1B	10.31	1.57	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ANP	N3-C2-N1	-8.52	121.44	128.86
2	A	1000	ANP	PA-O3A-PB	-2.86	122.28	132.38
2	A	1000	ANP	C4'-O4'-C1'	-2.82	106.77	109.77
2	A	1000	ANP	C5'-C4'-C3'	-2.61	105.35	115.29
2	A	1000	ANP	C4-C5-N7	-2.42	107.07	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	ANP	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	291/326 (89%)	0.87	40 (13%) 3 3	33, 74, 136, 154	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	LEU	6.7
1	A	445	ASP	6.5
1	A	298	GLY	4.8
1	A	443	TYR	4.8
1	A	319	LEU	4.4
1	A	318	ARG	4.3
1	A	528	GLY	4.1
1	A	299	GLY	4.1
1	A	304	TYR	3.8
1	A	360	LEU	3.7
1	A	276	ARG	3.6
1	A	354	MET	3.3
1	A	444	LYS	3.2
1	A	346	LEU	3.2
1	A	301	GLY	3.0
1	A	512	LEU	2.9
1	A	280	ARG	2.8
1	A	356	PRO	2.8
1	A	382	GLN	2.7
1	A	293	ASN	2.7
1	A	403	TYR	2.7
1	A	341	ALA	2.6
1	A	359	ARG	2.6
1	A	355	THR	2.5
1	A	320	LYS	2.5
1	A	358	GLU	2.4
1	A	353	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	337	MET	2.3
1	A	401	LEU	2.3
1	A	527	GLN	2.2
1	A	272	GLY	2.2
1	A	408	CYS	2.2
1	A	433	GLY	2.2
1	A	321	GLU	2.2
1	A	288	ASN	2.2
1	A	342	VAL	2.1
1	A	379	PRO	2.1
1	A	400	GLY	2.1
1	A	348	ARG	2.0
1	A	404	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	A	446	11/12	0.56	0.29	-	73,84,112,116	0
1	TPO	A	455	11/12	0.91	0.12	-	79,95,114,124	0
1	TPO	A	449	11/12	0.87	0.17	-	73,84,112,116	0
1	TPO	A	312	11/12	0.80	0.23	-	70,88,110,111	0
1	SEP	A	290	10/11	0.67	0.24	-	112,143,180,186	0
1	TPO	A	450	11/12	0.91	0.13	-	70,88,110,111	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	A	1000	31/31	0.86	0.15	-0.67	57,114,167,198	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.