



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:59 AM UTC

PDB ID : 3O7L / pdb\_00003o7l  
Title : Crystal Structure of phospholamban (1-19):PKA C-subunit:AMP-PNP:Mg2  
+ complex  
Authors : Cheng, C.Y.; Taylor, S.S.  
Deposited on : 2010-07-30  
Resolution : 2.80 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

<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

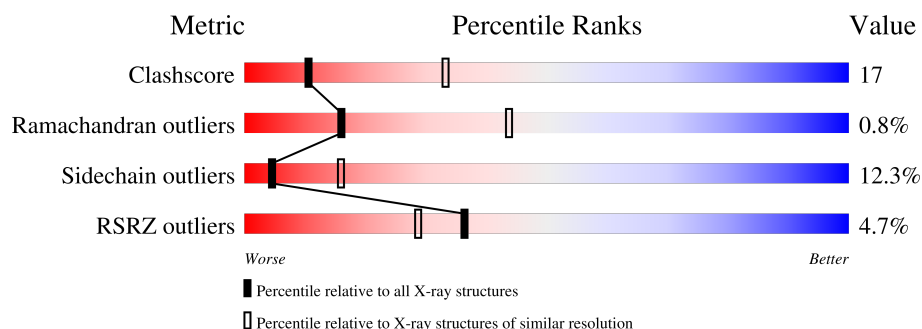
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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  $\geq 3$ , 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	B	350	<div> <div>5%</div> <div>58% 31% 7%</div> </div>
2	D	350	<div> <div>3%</div> <div>62% 27% 6%</div> </div>
3	I	15	<div> <div>13%</div> <div>80% 13% 7%</div> </div>

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
5	PEG	B	353	-	X	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5231 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	327	Total	C	N	O	P	S	20	0	0
			2470	1602	411	449	1	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	ILE	LEU	conflict	UNP P05132
B	211	ILE	LEU	conflict	UNP P05132

- Molecule 2 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	335	Total	C	N	O	P	S	27	0	0
			2594	1687	428	470	2	7			

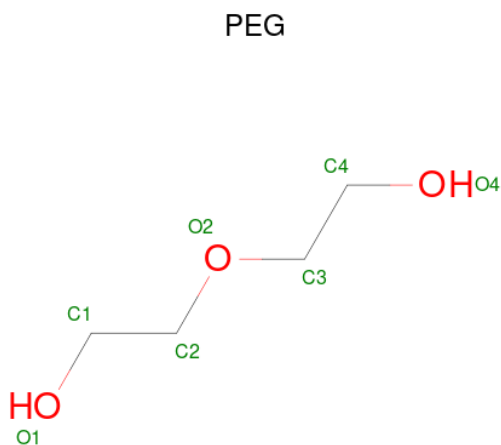
- Molecule 3 is a protein called Cardiac phospholamban.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	15	Total	C	N	O	0	0	0
			110	67	24	19			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

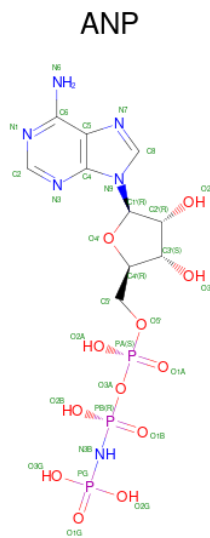
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	6	9	2		

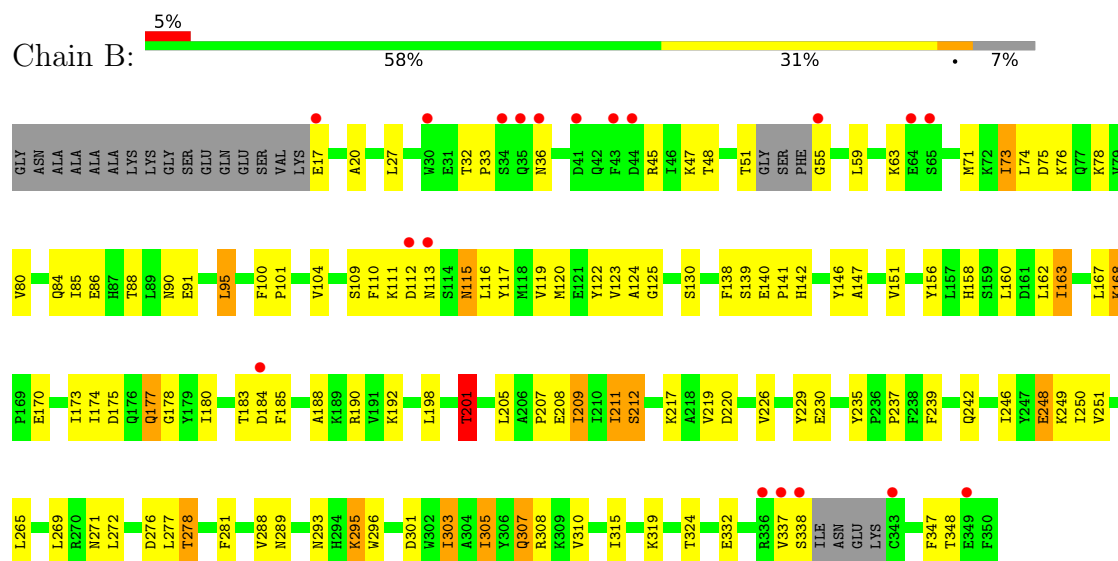
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	12	Total 12	O 12	0	0
7	D	9	Total 9	O 9	0	0

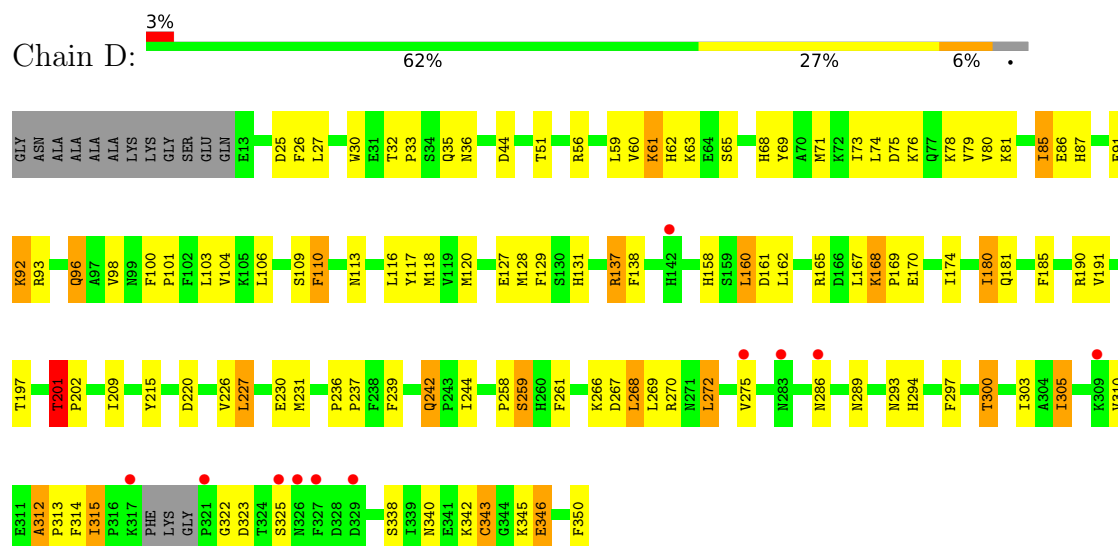
### 3 Residue-property plots

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.

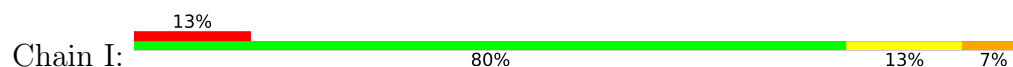
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

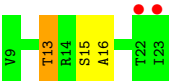


- Molecule 2: cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 3: Cardiac phospholamban







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.19Å 92.19Å 192.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.09 – 2.80 39.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.09-2.80) 94.5 (39.09-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.06 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.216 , 0.287 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SEP, TPO, MG, ANP

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	B	0.43	0/2519	0.81	6/3430 (0.2%)
2	D	0.39	0/2639	0.81	7/3581 (0.2%)
3	I	0.44	0/110	0.75	0/147
All	All	0.41	0/5268	0.80	13/7158 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	312	ALA	CA-C-N	5.96	125.84	119.28
2	D	312	ALA	C-N-CA	5.96	125.84	119.28
2	D	201	THR	CA-C-N	5.71	126.09	119.47
2	D	201	THR	C-N-CA	5.71	126.09	119.47
1	B	201	THR	CA-C-N	5.70	126.96	119.84
1	B	201	THR	C-N-CA	5.70	126.96	119.84
2	D	168	LYS	CA-C-N	5.41	126.60	119.84
2	D	168	LYS	C-N-CA	5.41	126.60	119.84
1	B	192	LYS	N-CA-C	-5.29	101.82	109.59
1	B	212	SER	N-CA-C	5.17	119.54	113.23
2	D	85	ILE	N-CA-C	5.05	115.48	110.23
1	B	168	LYS	CA-C-N	5.00	125.02	119.32
1	B	168	LYS	C-N-CA	5.00	125.02	119.32

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	B	2470	0	2255	95	0
2	D	2594	0	2413	73	0
3	I	110	0	104	4	0
4	B	2	0	0	0	0
5	B	7	0	10	6	0
6	B	27	0	12	1	0
7	B	12	0	0	1	0
7	D	9	0	0	0	0
All	All	5231	0	4794	166	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 17.

All (166) 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:B:75:ASP:N	5:B:353:PEG:O4	1.97	0.95
1:B:212:SER:HB3	2:D:81:LYS:NZ	1.87	0.88
2:D:33:PRO:HA	2:D:96:GLN:NE2	1.89	0.88
2:D:165:ARG:NH1	2:D:197:TPO:O2P	2.06	0.87
1:B:212:SER:HB3	2:D:81:LYS:HZ2	1.45	0.82
2:D:131:HIS:HD2	2:D:174:ILE:HD12	1.43	0.82
2:D:118:MET:HB3	2:D:120:MET:CE	2.11	0.81
2:D:80:VAL:HG22	2:D:85:ILE:HD11	1.63	0.81
2:D:71:MET:HE3	2:D:73:ILE:HD11	1.61	0.81
1:B:75:ASP:H	5:B:353:PEG:HO4	1.29	0.80
2:D:242:GLN:HE21	2:D:242:GLN:N	1.81	0.78
2:D:242:GLN:HE21	2:D:242:GLN:H	1.32	0.78
1:B:55:GLY:HA2	5:B:353:PEG:H42	1.66	0.77
1:B:177:GLN:HE21	1:B:177:GLN:N	1.81	0.77
1:B:147:ALA:O	1:B:151:VAL:HG23	1.85	0.77
2:D:131:HIS:CD2	2:D:174:ILE:HD12	2.23	0.73
1:B:80:VAL:HG22	1:B:85:ILE:HD11	1.75	0.68
1:B:168:LYS:HD3	1:B:201:THR:HG21	1.76	0.66
2:D:118:MET:HB3	2:D:120:MET:HE3	1.76	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LYS:HG3	1:B:115:ASN:HA	1.79	0.65
1:B:303:ILE:O	1:B:307:GLN:HG3	1.97	0.65
2:D:60:VAL:HG11	2:D:71:MET:HE2	1.78	0.64
2:D:128:MET:HE1	2:D:180:ILE:HD11	1.78	0.64
1:B:146:TYR:HB3	1:B:180:ILE:HD11	1.80	0.63
1:B:73:ILE:O	1:B:73:ILE:HG13	1.98	0.63
2:D:297:PHE:HD1	2:D:300:THR:HG21	1.62	0.63
1:B:104:VAL:HG21	1:B:183:THR:HG23	1.81	0.62
2:D:226:VAL:HG13	2:D:237:PRO:HD2	1.81	0.62
1:B:75:ASP:HA	1:B:115:ASN:HB3	1.83	0.61
1:B:198:LEU:HA	1:B:209:ILE:HD11	1.82	0.61
2:D:103:LEU:HD22	2:D:185:PHE:HZ	1.65	0.61
1:B:86:GLU:O	1:B:90:ASN:HB2	1.99	0.61
2:D:62:HIS:CD2	2:D:65:SER:H	2.19	0.60
1:B:276:ASP:OD2	1:B:278:THR:HG22	2.01	0.60
1:B:212:SER:HB3	2:D:81:LYS:HZ1	1.63	0.60
1:B:84:GLN:O	1:B:88:THR:HG23	2.02	0.60
1:B:55:GLY:N	5:B:353:PEG:HO1	1.98	0.60
1:B:75:ASP:N	5:B:353:PEG:HO4	1.91	0.59
2:D:137:ARG:C	2:D:138:PHE:HD1	2.09	0.59
1:B:55:GLY:HA2	5:B:353:PEG:C4	2.31	0.59
2:D:92:LYS:HG3	2:D:93:ARG:N	2.18	0.59
1:B:177:GLN:HE21	1:B:177:GLN:H	1.51	0.58
2:D:268:LEU:HD22	2:D:272:LEU:HD22	1.84	0.58
1:B:125:GLY:HA3	1:B:174:ILE:O	2.04	0.58
2:D:314:PHE:C	2:D:315:ILE:HG12	2.30	0.57
2:D:62:HIS:HD2	2:D:65:SER:H	1.53	0.57
2:D:35:GLN:HG2	2:D:350:PHE:O	2.05	0.57
1:B:32:THR:N	1:B:33:PRO:HD3	2.19	0.56
1:B:198:LEU:HA	1:B:209:ILE:CD1	2.35	0.56
2:D:73:ILE:HD12	2:D:117:TYR:CE1	2.40	0.56
1:B:74:LEU:O	1:B:115:ASN:HB2	2.06	0.56
1:B:239:PHE:O	1:B:249:LYS:HE3	2.07	0.55
2:D:30:TRP:CZ3	2:D:93:ARG:HG3	2.40	0.55
1:B:158:HIS:HE1	1:B:220:ASP:OD2	1.90	0.55
2:D:227:LEU:HD22	2:D:231:MET:HG3	1.88	0.54
2:D:297:PHE:O	2:D:300:THR:HG23	2.07	0.54
1:B:122:TYR:CE2	1:B:124:ALA:HB2	2.42	0.53
1:B:271:ASN:HB3	1:B:281:PHE:CD1	2.43	0.53
2:D:266:LYS:O	2:D:270:ARG:HG3	2.07	0.53
2:D:244:ILE:HD13	3:I:16:ALA:HB2	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ASP:CG	1:B:278:THR:HG22	2.33	0.53
1:B:162:LEU:HD23	1:B:190:ARG:HA	1.90	0.53
2:D:76:LYS:HG3	2:D:116:LEU:HG	1.91	0.53
1:B:36:ASN:HA	1:B:109:SER:O	2.10	0.52
2:D:74:LEU:HB2	2:D:116:LEU:HB2	1.93	0.51
2:D:75:ASP:O	2:D:79:VAL:HG23	2.10	0.51
2:D:230:GLU:OE2	2:D:236:PRO:HD3	2.10	0.51
1:B:207:PRO:O	1:B:211:ILE:HB	2.11	0.50
2:D:26:PHE:CD2	2:D:160:LEU:HG	2.46	0.50
1:B:230:GLU:HA	1:B:235:TYR:O	2.12	0.50
2:D:91:GLU:HG3	2:D:185:PHE:C	2.38	0.49
2:D:236:PRO:HG2	2:D:239:PHE:HB2	1.94	0.49
2:D:128:MET:CE	2:D:180:ILE:HD11	2.42	0.49
1:B:239:PHE:CZ	3:I:15:SER:HB3	2.47	0.49
1:B:91:GLU:HB3	1:B:185:PHE:O	2.12	0.49
1:B:177:GLN:H	1:B:177:GLN:NE2	2.10	0.49
2:D:35:GLN:HG2	2:D:350:PHE:C	2.36	0.49
1:B:239:PHE:CE1	3:I:15:SER:HB3	2.48	0.49
1:B:295:LYS:H	1:B:295:LYS:CE	2.25	0.49
2:D:158:HIS:HE1	2:D:220:ASP:OD2	1.95	0.49
1:B:175:ASP:OD1	1:B:175:ASP:C	2.54	0.48
1:B:158:HIS:CG	1:B:217:LYS:HD2	2.48	0.48
1:B:158:HIS:CE1	1:B:217:LYS:HB2	2.49	0.48
2:D:44:ASP:OD2	2:D:63:LYS:HE2	2.14	0.48
1:B:115:ASN:ND2	1:B:117:TYR:CZ	2.81	0.48
1:B:123:VAL:HB	1:B:173:ILE:HG21	1.96	0.48
1:B:90:ASN:ND2	1:B:188:ALA:O	2.47	0.48
2:D:100:PHE:HB3	2:D:103:LEU:HD12	1.96	0.48
1:B:104:VAL:HG21	1:B:183:THR:CG2	2.44	0.47
1:B:17:GLU:O	1:B:20:ALA:HB3	2.14	0.47
1:B:71:MET:HG3	1:B:119:VAL:HG22	1.95	0.47
2:D:305:ILE:HG13	2:D:310:VAL:HG21	1.96	0.47
1:B:156:TYR:O	1:B:160:LEU:HD22	2.13	0.47
2:D:27:LEU:HA	2:D:27:LEU:HD23	1.74	0.47
1:B:48:THR:HB	1:B:332:GLU:OE2	2.15	0.47
1:B:88:THR:C	1:B:90:ASN:N	2.72	0.47
1:B:100:PHE:CG	1:B:101:PRO:HD2	2.51	0.46
1:B:301:ASP:OD1	1:B:303:ILE:HG23	2.15	0.46
1:B:146:TYR:CB	1:B:180:ILE:HD11	2.44	0.46
1:B:115:ASN:ND2	1:B:117:TYR:OH	2.46	0.46
1:B:90:ASN:O	1:B:91:GLU:C	2.59	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLN:N	1:B:177:GLN:NE2	2.57	0.46
1:B:347:PHE:O	1:B:348:THR:C	2.59	0.46
2:D:342:LYS:O	2:D:343:CYS:C	2.59	0.46
1:B:289:ASN:O	1:B:293:ASN:HB2	2.15	0.46
1:B:36:ASN:HA	1:B:110:PHE:HB3	1.98	0.45
1:B:116:LEU:HD23	7:B:365:HOH:O	2.15	0.45
2:D:100:PHE:CG	2:D:101:PRO:HD2	2.52	0.45
2:D:312:ALA:HA	2:D:313:PRO:HD3	1.81	0.45
1:B:205:LEU:HD22	1:B:209:ILE:HG12	1.98	0.45
1:B:305:ILE:HG13	1:B:310:VAL:HG21	1.98	0.45
2:D:75:ASP:CG	2:D:78:LYS:HG3	2.41	0.45
2:D:286:ASN:O	2:D:289:ASN:HB2	2.17	0.45
2:D:96:GLN:CD	2:D:96:GLN:C	2.84	0.45
1:B:111:LYS:C	1:B:113:ASN:H	2.26	0.45
1:B:112:ASP:CB	1:B:117:TYR:CE1	3.00	0.44
2:D:103:LEU:HD22	2:D:185:PHE:CZ	2.49	0.44
1:B:167:LEU:O	1:B:168:LYS:HB3	2.17	0.44
2:D:209:ILE:HG12	2:D:215:TYR:CD1	2.53	0.43
1:B:138:PHE:HB3	1:B:142:HIS:HB3	2.00	0.43
2:D:109:SER:O	2:D:110:PHE:HB3	2.18	0.43
2:D:160:LEU:O	2:D:161:ASP:HB2	2.19	0.43
1:B:112:ASP:H	1:B:117:TYR:HE1	1.66	0.43
1:B:175:ASP:OD2	1:B:308:ARG:NH2	2.52	0.43
2:D:162:LEU:HD23	2:D:190:ARG:HA	2.01	0.43
1:B:74:LEU:HB2	1:B:116:LEU:HB2	2.01	0.42
1:B:229:TYR:C	1:B:229:TYR:CD1	2.97	0.42
1:B:265:LEU:HD13	1:B:296:TRP:CE2	2.54	0.42
1:B:198:LEU:HD12	1:B:209:ILE:HD11	2.01	0.42
1:B:246:ILE:O	1:B:250:ILE:HG13	2.19	0.42
2:D:322:GLY:HA3	2:D:323:ASP:HA	1.87	0.42
2:D:323:ASP:C	2:D:325:SER:H	2.26	0.42
2:D:60:VAL:HG22	2:D:69:TYR:O	2.20	0.42
2:D:138:PHE:HB2	2:D:231:MET:O	2.20	0.42
1:B:140:GLU:N	1:B:141:PRO:CD	2.82	0.42
1:B:303:ILE:O	1:B:307:GLN:CG	2.67	0.42
1:B:163:ILE:HG23	1:B:217:LYS:HA	2.02	0.42
2:D:258:PRO:O	2:D:259:SER:C	2.61	0.42
2:D:113:ASN:HB3	2:D:340:ASN:O	2.20	0.42
2:D:201:THR:HA	2:D:202:PRO:HD3	1.87	0.42
1:B:74:LEU:O	1:B:115:ASN:CB	2.67	0.41
1:B:139:SER:OG	1:B:141:PRO:HD2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:HA	1:B:251:VAL:HG22	2.02	0.41
2:D:258:PRO:HD2	2:D:261:PHE:CE2	2.55	0.41
1:B:226:VAL:HG13	1:B:237:PRO:HD2	2.01	0.41
1:B:74:LEU:O	1:B:116:LEU:N	2.53	0.41
2:D:61:LYS:HG3	2:D:68:HIS:CE1	2.55	0.41
2:D:167:LEU:HD12	2:D:168:LYS:H	1.86	0.41
3:I:13:THR:C	3:I:15:SER:H	2.29	0.41
1:B:174:ILE:CG2	1:B:178:GLY:HA2	2.51	0.41
2:D:104:VAL:HA	2:D:181:GLN:OE1	2.20	0.41
2:D:129:PHE:HB2	2:D:169:PRO:HB2	2.03	0.41
2:D:346:GLU:CD	2:D:346:GLU:H	2.29	0.41
1:B:100:PHE:CD2	1:B:101:PRO:HD2	2.55	0.41
1:B:208:GLU:HG2	1:B:277:LEU:HD11	2.03	0.41
1:B:337:VAL:HG12	1:B:338:SER:N	2.36	0.41
2:D:293:ASN:O	2:D:294:HIS:C	2.63	0.41
1:B:88:THR:C	1:B:90:ASN:H	2.29	0.40
1:B:112:ASP:CB	1:B:117:TYR:HE1	2.34	0.40
2:D:138:PHE:N	2:D:138:PHE:CD1	2.89	0.40
1:B:184:ASP:CG	6:B:354:ANP:O1B	2.64	0.40
1:B:242:GLN:HE21	1:B:242:GLN:HB3	1.69	0.40
2:D:267:ASP:HB3	2:D:294:HIS:HE2	1.87	0.40
1:B:47:LYS:HE3	1:B:324:THR:OG1	2.21	0.40
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.81	0.40
2:D:35:GLN:HG2	2:D:350:PHE:OXT	2.22	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	B	320/350 (91%)	292 (91%)	26 (8%)	2 (1%)	21 51

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	329/350 (94%)	299 (91%)	27 (8%)	3 (1%)	14	41
3	I	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	662/715 (93%)	602 (91%)	55 (8%)	5 (1%)	16	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ARG
1	B	63	LYS
2	D	36	ASN
2	D	110	PHE
2	D	343	CYS

### 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	B	230/304 (76%)	203 (88%)	27 (12%)	5	18
2	D	248/303 (82%)	216 (87%)	32 (13%)	4	14
3	I	9/13 (69%)	8 (89%)	1 (11%)	6	20
All	All	487/620 (78%)	427 (88%)	60 (12%)	4	16

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	LEU
1	B	51	THR
1	B	59	LEU
1	B	73	ILE
1	B	78	LYS
1	B	95	LEU
1	B	115	ASN
1	B	120	MET
1	B	130	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	163	ILE
1	B	170	GLU
1	B	177	GLN
1	B	201	THR
1	B	209	ILE
1	B	211	ILE
1	B	219	VAL
1	B	248	GLU
1	B	269	LEU
1	B	272	LEU
1	B	278	THR
1	B	288	VAL
1	B	295	LYS
1	B	303	ILE
1	B	305	ILE
1	B	307	GLN
1	B	315	ILE
1	B	319	LYS
2	D	25	ASP
2	D	32	THR
2	D	51	THR
2	D	56	ARG
2	D	59	LEU
2	D	61	LYS
2	D	86	GLU
2	D	87	HIS
2	D	92	LYS
2	D	96	GLN
2	D	98	VAL
2	D	106	LEU
2	D	127	GLU
2	D	137	ARG
2	D	160	LEU
2	D	170	GLU
2	D	180	ILE
2	D	191	VAL
2	D	201	THR
2	D	227	LEU
2	D	242	GLN
2	D	259	SER
2	D	268	LEU
2	D	269	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	272	LEU
2	D	275	VAL
2	D	300	THR
2	D	303	ILE
2	D	305	ILE
2	D	315	ILE
2	D	345	LYS
2	D	346	GLU
3	I	13	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	B	115	ASN
1	B	158	HIS
1	B	171	ASN
1	B	176	GLN
1	B	177	GLN
1	B	242	GLN
1	B	274	GLN
1	B	307	GLN
2	D	36	ASN
2	D	62	HIS
2	D	87	HIS
2	D	96	GLN
2	D	158	HIS
2	D	242	GLN
2	D	271	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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
2	TPO	D	197	2	8,10,11	0.96	0	10,14,16	1.05	0
2	SEP	D	338	2	8,9,10	1.60	1 (12%)	7,12,14	1.60	1 (14%)
1	TPO	B	197	1	8,10,11	1.03	0	10,14,16	1.16	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
2	TPO	D	197	2	-	1/9/11/13	-
2	SEP	D	338	2	-	5/6/8/10	-
1	TPO	B	197	1	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	338	SEP	P-O1P	3.45	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	338	SEP	OG-CB-CA	3.29	111.35	108.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	197	TPO	O-C-CA-CB
2	D	338	SEP	CB-OG-P-O1P
2	D	338	SEP	CB-OG-P-O2P
2	D	338	SEP	CB-OG-P-O3P
2	D	338	SEP	CA-CB-OG-P
2	D	338	SEP	N-CA-CB-OG
1	B	197	TPO	CB-OG1-P-O3P
2	D	197	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	197	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
6	ANP	B	354	4	28,29,33	4.61	14 (50%)	40,45,52	3.09	19 (47%)
5	PEG	B	353	-	6,6,6	1.89	2 (33%)	5,5,5	2.80	2 (40%)

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
6	ANP	B	354	4	-	7/13/32/38	0/3/3/3
5	PEG	B	353	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	354	ANP	PB-O1B	13.33	1.66	1.46
6	B	354	ANP	PB-O3A	10.38	1.72	1.59
6	B	354	ANP	PA-O3A	8.70	1.68	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	354	ANP	PA-O2A	7.85	1.91	1.55
6	B	354	ANP	PB-O2B	5.89	1.72	1.56
6	B	354	ANP	C5-C4	5.68	1.49	1.39
6	B	354	ANP	C5-C6	4.34	1.53	1.41
6	B	354	ANP	C4-N3	4.17	1.42	1.34
6	B	354	ANP	C8-N7	3.55	1.38	1.31
6	B	354	ANP	C6-N6	3.35	1.42	1.34
6	B	354	ANP	C2-N1	2.84	1.39	1.33
6	B	354	ANP	C2'-C1'	-2.64	1.45	1.53
6	B	354	ANP	O3'-C3'	2.46	1.49	1.43
5	B	353	PEG	O4-C4	2.39	1.54	1.42
6	B	354	ANP	C3'-C4'	2.08	1.58	1.53
5	B	353	PEG	C3-C4	2.08	1.60	1.49

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	354	ANP	O4'-C1'-N9	7.41	122.31	108.09
6	B	354	ANP	O5'-C5'-C4'	-5.94	88.78	108.99
6	B	354	ANP	O2B-PB-O3A	-5.80	85.29	104.64
5	B	353	PEG	O2-C2-C1	-5.62	85.35	110.11
6	B	354	ANP	O2'-C2'-C1'	-5.34	91.71	110.10
6	B	354	ANP	C2'-C1'-N9	-5.11	100.60	113.30
6	B	354	ANP	C5-C4-N3	-5.07	119.74	126.72
6	B	354	ANP	O5'-PA-O1A	4.73	127.67	108.94
6	B	354	ANP	O3A-PA-O1A	-4.44	97.36	110.70
6	B	354	ANP	N3-C4-N9	3.91	133.82	127.17
6	B	354	ANP	O3'-C3'-C4'	-3.91	99.84	111.08
6	B	354	ANP	PB-O3A-PA	-3.85	119.80	132.10
6	B	354	ANP	O2A-PA-O5'	-3.34	92.41	107.57
6	B	354	ANP	C4-C5-N7	-2.88	107.29	110.58
6	B	354	ANP	O4'-C4'-C5'	2.66	117.87	109.33
6	B	354	ANP	O2A-PA-O1A	2.63	124.67	112.44
6	B	354	ANP	O2B-PB-O1B	-2.60	103.52	110.26
6	B	354	ANP	C4-N9-C1'	-2.55	120.67	126.63
6	B	354	ANP	C2'-C3'-C4'	2.54	107.52	102.61
5	B	353	PEG	O1-C1-C2	-2.37	97.90	111.82
6	B	354	ANP	C1'-N9-C8	2.20	131.97	127.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

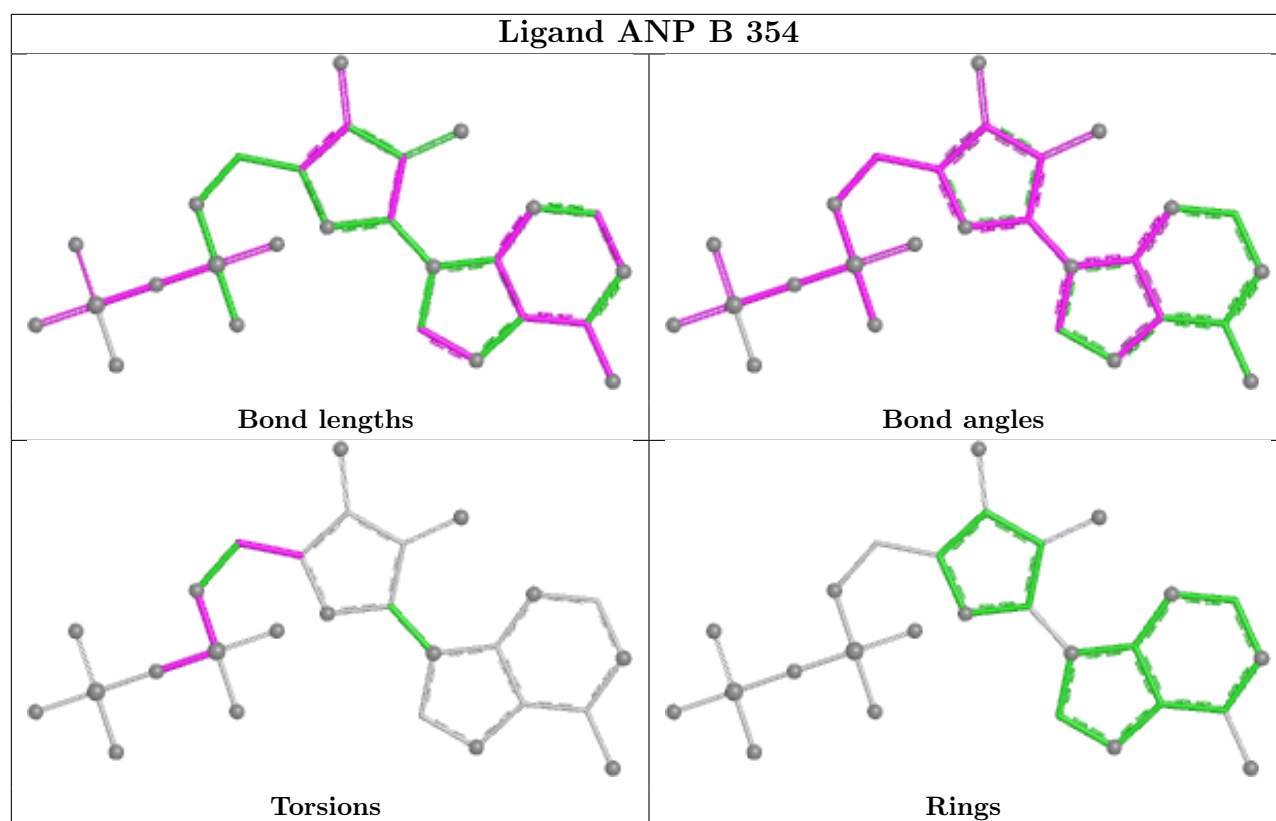
Mol	Chain	Res	Type	Atoms
6	B	354	ANP	C5'-O5'-PA-O1A
6	B	354	ANP	O4'-C4'-C5'-O5'
6	B	354	ANP	C3'-C4'-C5'-O5'
5	B	353	PEG	O1-C1-C2-O2
6	B	354	ANP	PB-O3A-PA-O1A
6	B	354	ANP	C5'-O5'-PA-O2A
6	B	354	ANP	C5'-O5'-PA-O3A
6	B	354	ANP	PB-O3A-PA-O2A
5	B	353	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	354	ANP	1	0
5	B	353	PEG	6	0

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, 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	B	326/350 (93%)	0.42	19 (5%) 29 22	30, 52, 96, 117	7 (2%)
2	D	333/350 (95%)	0.26	11 (3%) 49 39	33, 54, 76, 94	11 (3%)
3	I	15/15 (100%)	0.76	2 (13%) 7 5	43, 51, 68, 77	0
All	All	674/715 (94%)	0.35	32 (4%) 36 29	30, 53, 88, 117	18 (2%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	GLY	5.6
1	B	338	SER	4.8
1	B	113	ASN	3.9
1	B	43	PHE	3.3
1	B	337	VAL	3.0
1	B	349	GLU	2.9
1	B	41	ASP	2.8
2	D	325	SER	2.8
2	D	329	ASP	2.8
1	B	35	GLN	2.7
1	B	17	GLU	2.6
2	D	326	ASN	2.6
1	B	64	GLU	2.5
1	B	112	ASP	2.5
1	B	184	ASP	2.4
1	B	44	ASP	2.4
2	D	317	LYS	2.3
1	B	343	CYS	2.3
2	D	327	PHE	2.3
3	I	23	ILE	2.3
1	B	34	SER	2.3
3	I	22	THR	2.2
1	B	36	ASN	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	65	SER	2.2
1	B	336	ARG	2.1
2	D	283	ASN	2.1
1	B	30	TRP	2.1
2	D	286	ASN	2.1
2	D	275	VAL	2.0
2	D	309	LYS	2.0
2	D	142	HIS	2.0
2	D	321	PRO	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	B	197	11/12	0.81	0.16	29,41,49,61	0
2	TPO	D	197	11/12	0.88	0.14	33,33,47,52	0
2	SEP	D	338	10/11	0.89	0.09	41,61,71,91	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

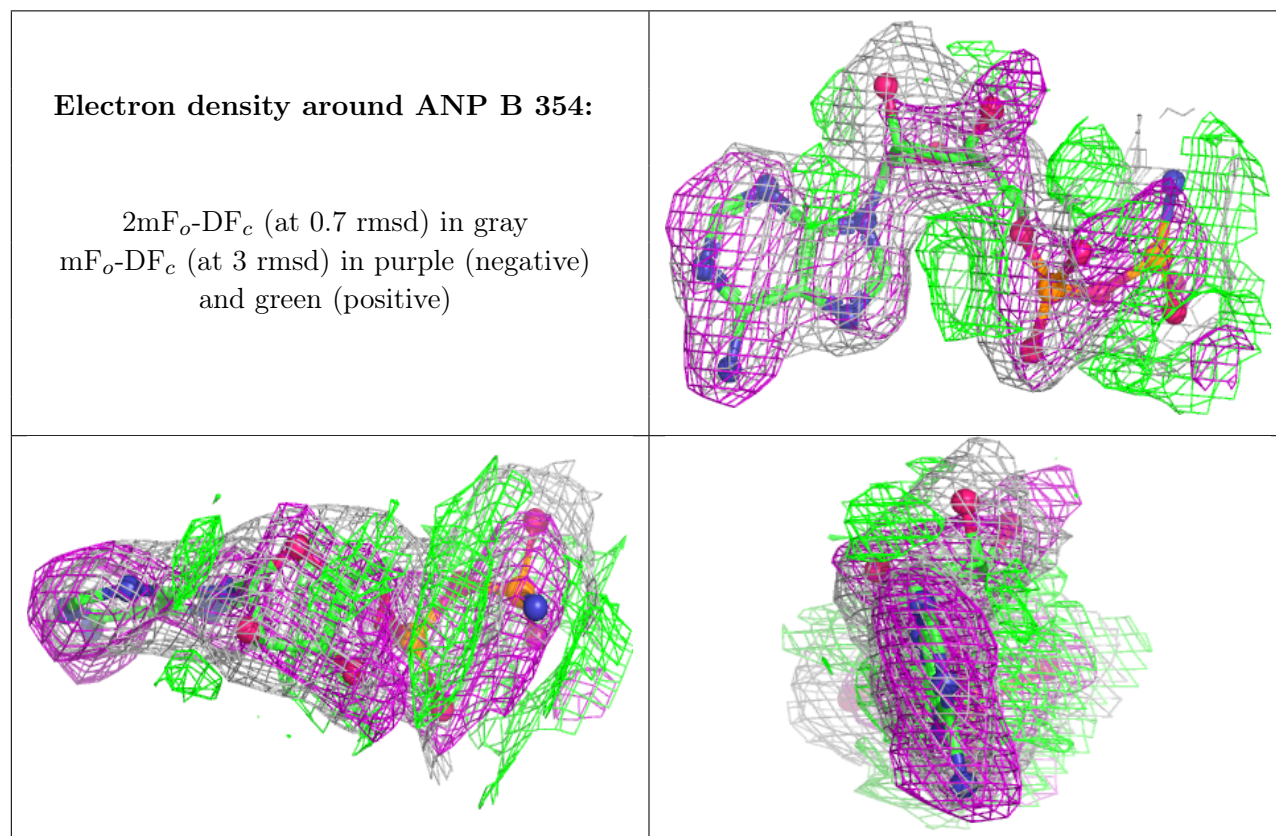
## 6.4 Ligands [i](#)

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	PEG	B	353	7/7	0.83	0.23	2,2,2,2	0
6	ANP	B	354	27/31	0.88	0.13	2,2,2,2	0
4	MG	B	352	1/1	0.94	0.12	2,2,2,2	0
4	MG	B	351	1/1	0.97	0.15	2,2,2,2	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.