



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:04 pm BST

PDB ID : 4CZY  
Title : Complex of Neurospora crassa PAN2 (WD40-CS1) with PAN3 (pseudokinase and C-term)  
Authors : Jonas, S.; Izaurralde, E.; Weichenrieder, O.  
Deposited on : 2014-04-22  
Resolution : 3.40 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

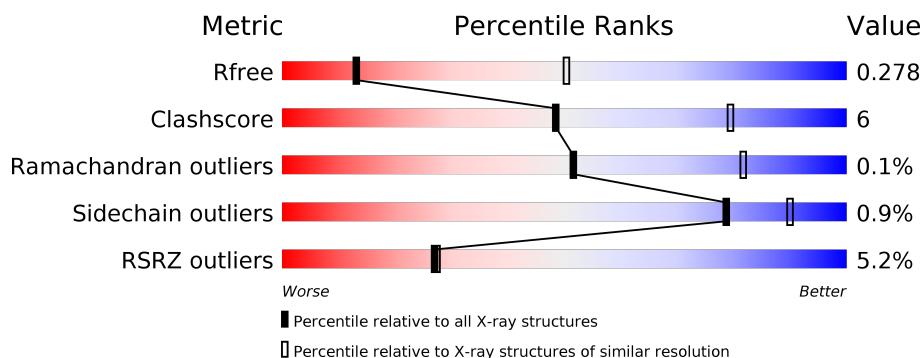
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	354	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	C	354	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>9%</div> </div> </div>
2	B	429	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> </div>
2	D	429	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11650 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 PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2516	1600	441	460	15			
1	C	323	Total	C	N	O	S	0	0	0
			2529	1609	444	461	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP P0C581
A	-1	HIS	-	expression tag	UNP P0C581
A	0	MET	-	expression tag	UNP P0C581
C	-2	PRO	-	expression tag	UNP P0C581
C	-1	HIS	-	expression tag	UNP P0C581
C	0	MET	-	expression tag	UNP P0C581

- Molecule 2 is a protein called PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3262	2073	580	598	11			
2	D	403	Total	C	N	O	S	0	0	0
			3255	2072	577	595	11			

There are 12 discrepancies between the modelled and reference sequences:

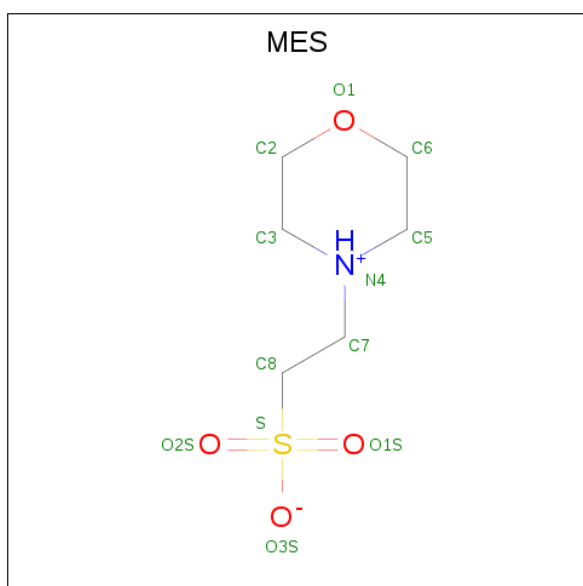
Chain	Residue	Modelled	Actual	Comment	Reference
B	228	GLY	-	expression tag	UNP Q7SDP4
B	229	PRO	-	expression tag	UNP Q7SDP4
B	230	HIS	-	expression tag	UNP Q7SDP4
B	231	MET	-	expression tag	UNP Q7SDP4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	232	LEU	-	expression tag	UNP Q7SDP4
B	233	GLU	-	expression tag	UNP Q7SDP4
D	228	GLY	-	expression tag	UNP Q7SDP4
D	229	PRO	-	expression tag	UNP Q7SDP4
D	230	HIS	-	expression tag	UNP Q7SDP4
D	231	MET	-	expression tag	UNP Q7SDP4
D	232	LEU	-	expression tag	UNP Q7SDP4
D	233	GLU	-	expression tag	UNP Q7SDP4

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	D	1	Total 31	C 10	N 6	O 12	P 3	0	0

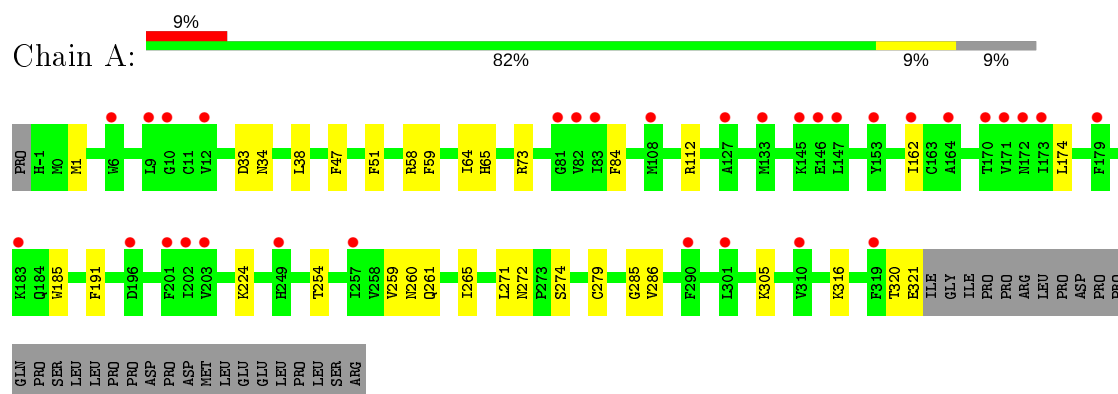
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

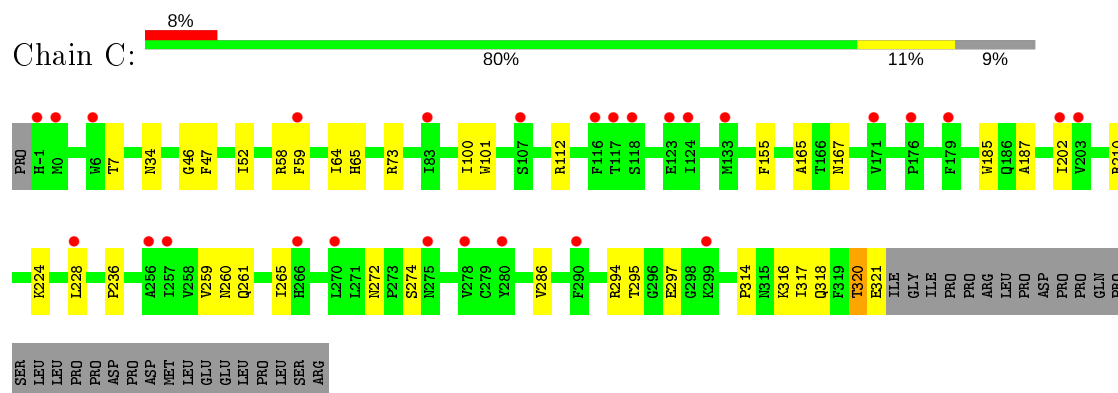
### 3 Residue-property plots

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.

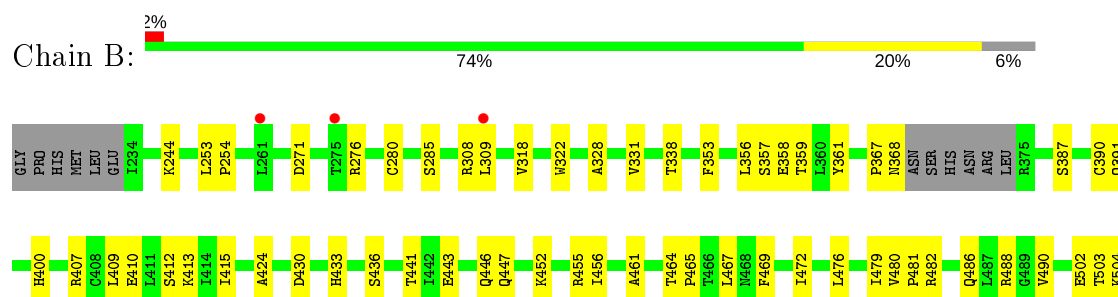
#### • Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN2

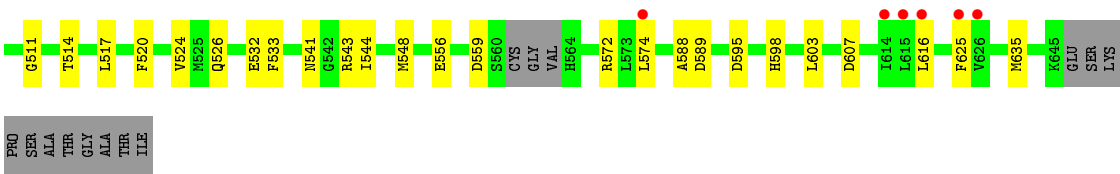


#### • Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN2

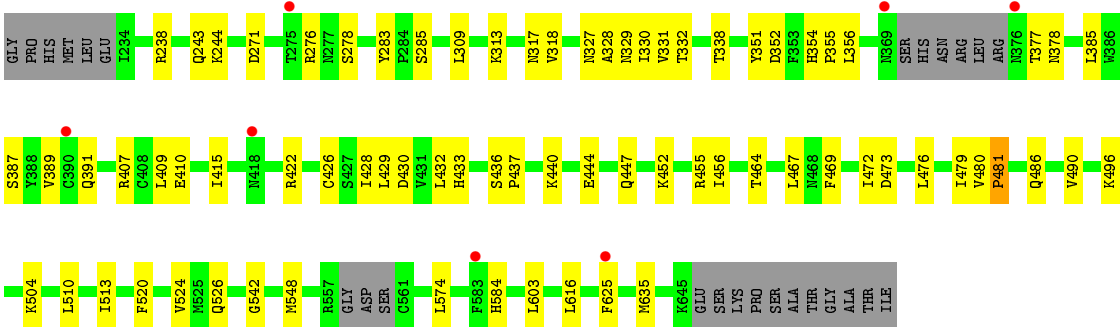
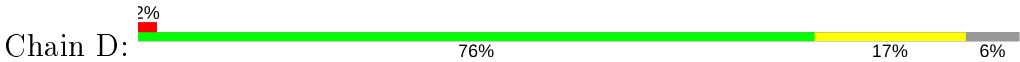


#### • Molecule 2: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3





● Molecule 2: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.27Å 139.98Å 157.44Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	48.74 – 3.40 48.74 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.74-3.40) 99.0 (48.74-3.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE 1.8.4_1496)	Depositor
R, $R_{free}$	0.221 , 0.263 0.239 , 0.278	Depositor DCC
$R_{free}$ test set	1677 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	106.6	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 77.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: MG, ANP, MES

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	0.24	0/2582	0.50	0/3512
1	C	0.25	0/2596	0.51	0/3530
2	B	0.26	0/3332	0.48	0/4512
2	D	0.26	0/3325	0.48	0/4504
All	All	0.25	0/11835	0.49	0/16058

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	A	2516	0	2461	16	0
1	C	2529	0	2479	23	0
2	B	3262	0	3233	58	0
2	D	3255	0	3226	48	0
3	A	12	0	12	1	0
3	C	12	0	12	1	0
4	B	31	0	13	7	0
4	D	31	0	13	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
All	All	11650	0	11449	139	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 6.

All (139) 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)
4:B:1650:ANP:H5'2	4:B:1650:ANP:H8	1.51	0.90
2:B:359:THR:HG23	4:B:1650:ANP:H3'	1.56	0.87
4:B:1650:ANP:C8	4:B:1650:ANP:H5'2	2.08	0.83
2:B:559:ASP:H	2:B:572:ARG:HH12	1.27	0.81
2:B:532:GLU:OE1	2:D:238:ARG:NH2	2.18	0.76
2:B:357:SER:O	4:B:1650:ANP:O2'	2.05	0.75
4:B:1650:ANP:C5'	4:B:1650:ANP:H8	2.23	0.68
2:D:377:THR:HG22	2:D:378:ASN:H	1.58	0.68
2:D:469:PHE:HA	2:D:472:ILE:HG23	1.78	0.65
2:B:556:GLU:HB2	2:D:584:HIS:NE2	2.13	0.63
2:B:574:LEU:HB3	2:B:635:MET:HE1	1.81	0.63
2:B:544:ILE:HD12	2:B:603:LEU:HB3	1.80	0.62
1:C:259:VAL:HG22	1:C:265:ILE:HG12	1.84	0.60
1:A:185:TRP:CZ2	1:A:224:LYS:HB3	2.37	0.59
2:D:473:ASP:OD1	2:D:496:LYS:NZ	2.32	0.59
2:B:461:ALA:O	2:B:482:ARG:NH2	2.29	0.57
2:B:452:LYS:O	2:B:456:ILE:HG13	2.06	0.56
2:B:328:ALA:HB2	2:D:526:GLN:HG3	1.88	0.55
2:B:253:LEU:HD12	2:B:254:PRO:HD2	1.87	0.55
2:B:447:GLN:HE22	2:B:504:LYS:H	1.56	0.54
2:B:556:GLU:HB2	2:D:584:HIS:CE1	2.43	0.54
2:B:520:PHE:O	2:B:524:VAL:HG23	2.07	0.54
2:D:574:LEU:HB3	2:D:635:MET:HE1	1.89	0.53
2:B:308:ARG:HD2	2:B:308:ARG:O	2.08	0.53
1:C:202:ILE:HG13	1:C:228:LEU:HG	1.90	0.53
2:D:616:LEU:HB2	2:D:625:PHE:HB2	1.90	0.53
2:B:400:HIS:CD2	2:B:446:GLN:HG2	2.44	0.52
2:B:616:LEU:HB2	2:B:625:PHE:HB2	1.90	0.52
1:A:1:MET:HG3	1:A:279:CYS:HB3	1.91	0.52
2:B:353:PHE:CD1	4:B:1650:ANP:H2	2.44	0.52
2:D:276:ARG:NH1	2:D:285:SER:O	2.42	0.52
2:B:548:MET:HB3	2:D:548:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:SER:O	2:D:391:GLN:HG3	2.11	0.51
2:D:407:ARG:NH1	2:D:430:ASP:OD2	2.43	0.51
2:B:543:ARG:CZ	2:D:243:GLN:HE22	2.25	0.50
1:C:297:GLU:HB3	1:C:317:ILE:HB	1.93	0.50
1:A:162:ILE:HB	1:A:174:LEU:HB2	1.92	0.49
2:B:441:THR:HG22	2:B:443:GLU:H	1.77	0.49
2:D:447:GLN:HE22	2:D:504:LYS:H	1.59	0.49
1:C:7:THR:HG21	1:C:314:PRO:HG3	1.94	0.49
2:D:351:TYR:OH	2:D:426:CYS:O	2.26	0.49
2:B:464:THR:OG1	2:B:464:THR:O	2.23	0.49
2:B:541:ASN:HD22	2:D:542:GLY:HA2	1.77	0.49
2:B:415:ILE:HG12	2:B:424:ALA:HB2	1.94	0.48
2:B:480:VAL:HG12	2:B:481:PRO:HD3	1.96	0.48
2:B:479:ILE:HD11	2:B:488:ARG:HG3	1.95	0.48
1:C:73:ARG:HD2	1:C:112:ARG:HA	1.95	0.48
2:D:313:LYS:O	2:D:317:ASN:HB2	2.14	0.48
1:C:46:GLY:O	1:C:64:ILE:HG13	2.14	0.48
2:D:377:THR:O	2:D:378:ASN:HB2	2.14	0.48
2:D:329:ASN:HA	2:D:422:ARG:HG2	1.95	0.48
1:C:187:ALA:O	1:C:224:LYS:HG3	2.13	0.48
1:C:34:ASN:HB3	1:C:294:ARG:CZ	2.43	0.48
1:A:73:ARG:HD2	1:A:112:ARG:HA	1.96	0.48
1:A:261:GLN:HB3	1:A:286:VAL:HG13	1.96	0.47
1:C:185:TRP:CZ2	1:C:224:LYS:HB3	2.49	0.47
1:A:58:ARG:HG2	1:A:59:PHE:N	2.30	0.47
2:B:433:HIS:HA	2:B:436:SER:HB2	1.97	0.47
2:D:510:LEU:HD23	2:D:513:ILE:HD11	1.96	0.47
2:D:520:PHE:O	2:D:524:VAL:HG23	2.15	0.47
1:C:167:ASN:HB2	1:C:210:ARG:NH2	2.30	0.47
1:A:320:THR:HG22	1:A:321:GLU:H	1.80	0.46
2:B:387:SER:O	2:B:391:GLN:HG3	2.15	0.46
1:C:228:LEU:HD23	1:C:228:LEU:HA	1.79	0.46
1:C:261:GLN:HB3	1:C:286:VAL:HG13	1.97	0.46
2:D:436:SER:OG	2:D:437:PRO:HD2	2.15	0.46
2:D:486:GLN:O	2:D:490:VAL:HG23	2.15	0.46
2:B:447:GLN:OE1	2:B:504:LYS:HB2	2.16	0.46
2:B:407:ARG:NH1	2:B:430:ASP:OD2	2.49	0.46
2:B:390:CYS:SG	2:B:517:LEU:HD23	2.56	0.46
1:C:272:ASN:ND2	1:C:274:SER:OG	2.49	0.46
1:C:34:ASN:O	1:C:320:THR:HG21	2.16	0.46
2:B:309:LEU:HB2	2:B:338:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:HH12	3:C:1330:MES:H82	1.81	0.45
2:D:318:VAL:HG11	2:D:430:ASP:HB2	1.98	0.45
2:D:548:MET:SD	2:D:603:LEU:HD11	2.56	0.45
2:B:588:ALA:O	2:B:589:ASP:HB2	2.16	0.45
2:D:433:HIS:HA	2:D:436:SER:HB2	1.98	0.45
1:A:272:ASN:ND2	1:A:274:SER:OG	2.48	0.45
1:A:259:VAL:HG22	1:A:265:ILE:HG12	1.99	0.45
2:B:276:ARG:HD3	2:B:285:SER:O	2.17	0.45
2:D:476:LEU:O	2:D:479:ILE:HG12	2.17	0.45
1:C:7:THR:CG2	1:C:314:PRO:HG3	2.47	0.45
2:B:318:VAL:HG12	2:B:322:TRP:HD1	1.82	0.45
2:D:409:LEU:O	2:D:456:ILE:HD11	2.16	0.45
1:A:34:ASN:O	1:A:320:THR:HG21	2.17	0.44
1:A:51:PHE:CD2	1:A:58:ARG:HA	2.52	0.44
1:A:285:GLY:HA3	1:A:305:LYS:HG2	1.99	0.44
2:D:309:LEU:HD22	2:D:338:THR:HG21	2.00	0.44
1:A:33:ASP:HB2	1:A:38:LEU:HB2	1.98	0.44
2:D:385:LEU:O	2:D:389:VAL:HG23	2.18	0.44
2:D:407:ARG:HD3	2:D:429:LEU:HB2	1.99	0.44
2:B:556:GLU:HB2	2:D:584:HIS:HE2	1.83	0.44
2:D:327:ASN:HB3	2:D:330:ILE:HB	2.00	0.43
1:C:320:THR:HG22	1:C:321:GLU:H	1.81	0.43
1:C:58:ARG:HG2	1:C:59:PHE:N	2.32	0.43
2:D:464:THR:OG1	2:D:464:THR:O	2.23	0.43
2:B:476:LEU:O	2:B:479:ILE:HG12	2.18	0.43
2:B:467:LEU:HD12	2:B:467:LEU:HA	1.81	0.43
2:D:410:GLU:OE2	2:D:455:ARG:NH1	2.52	0.43
2:B:280:CYS:SG	2:B:410:GLU:HG3	2.59	0.43
2:B:469:PHE:HA	2:B:472:ILE:HG23	2.01	0.43
2:B:412:SER:O	2:B:413:LYS:NZ	2.52	0.43
2:B:464:THR:HA	2:B:465:PRO:HD2	1.77	0.43
2:B:410:GLU:CD	2:B:455:ARG:HH22	2.22	0.43
2:B:502:GLU:O	2:B:503:THR:OG1	2.28	0.43
2:B:361:TYR:CE2	2:B:465:PRO:HB2	2.54	0.42
2:B:511:GLY:O	2:B:514:THR:HG23	2.20	0.42
1:C:155:PHE:HB2	1:C:165:ALA:HB3	2.01	0.42
2:D:278:SER:OG	2:D:283:TYR:O	2.26	0.42
2:D:331:VAL:HG21	2:D:415:ILE:HD11	2.00	0.42
2:B:309:LEU:HD12	2:B:309:LEU:HA	1.83	0.42
2:D:452:LYS:O	2:D:456:ILE:HG13	2.20	0.42
2:B:526:GLN:HG3	2:D:328:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:THR:HB	2:D:352:ASP:OD2	2.20	0.42
2:D:480:VAL:HG12	2:D:481:PRO:HD3	2.02	0.42
2:B:244:LYS:HB2	2:B:356:LEU:HD11	2.02	0.41
1:C:295:THR:OG1	1:C:318:GLN:O	2.29	0.41
2:D:244:LYS:HB2	2:D:356:LEU:HD11	2.02	0.41
2:D:428:ILE:O	2:D:432:LEU:HG	2.20	0.41
2:B:543:ARG:NH2	2:B:607:ASP:OD1	2.53	0.41
1:A:254:THR:HG21	1:A:271:LEU:HD11	2.01	0.41
2:B:409:LEU:O	2:B:456:ILE:HD11	2.21	0.41
2:B:407:ARG:HD2	2:B:430:ASP:CG	2.40	0.41
1:C:100:ILE:HG22	1:C:101:TRP:CD1	2.55	0.41
1:A:64:ILE:HG21	1:A:84:PHE:CG	2.56	0.41
2:B:595:ASP:HB3	2:B:598:HIS:HB3	2.03	0.41
2:B:358:GLU:HA	4:B:1650:ANP:O2'	2.21	0.40
2:B:356:LEU:HD23	2:B:356:LEU:HA	1.88	0.40
2:D:447:GLN:OE1	2:D:504:LYS:HB2	2.22	0.40
1:C:224:LYS:HD3	1:C:236:PRO:HB3	2.03	0.40
1:C:52:ILE:HG13	1:C:59:PHE:HB2	2.02	0.40
2:D:464:THR:OG1	2:D:467:LEU:HD13	2.21	0.40
2:B:331:VAL:HG21	2:B:415:ILE:HD11	2.03	0.40
2:B:367:PRO:O	2:B:368:ASN:HB2	2.21	0.40
2:D:440:LYS:HB3	2:D:444:GLU:OE2	2.21	0.40
1:A:191:PHE:CG	3:A:1330:MES:H32	2.56	0.40
2:B:486:GLN:O	2:B:490:VAL:HG23	2.22	0.40
2:D:354:HIS:HA	2:D:355:PRO:HD2	1.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	321/354 (91%)	311 (97%)	9 (3%)	1 (0%)	41 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	321/354 (91%)	310 (97%)	10 (3%)	1 (0%)	41	72
2	B	397/429 (92%)	381 (96%)	16 (4%)	0	100	100
2	D	397/429 (92%)	378 (95%)	19 (5%)	0	100	100
All	All	1436/1566 (92%)	1380 (96%)	54 (4%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	LYS
1	C	316	LYS

### 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	273/308 (89%)	270 (99%)	3 (1%)	73	86
1	C	275/308 (89%)	271 (98%)	4 (2%)	65	82
2	B	355/380 (93%)	353 (99%)	2 (1%)	86	94
2	D	353/380 (93%)	351 (99%)	2 (1%)	86	94
All	All	1256/1376 (91%)	1245 (99%)	11 (1%)	78	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	PHE
1	A	65	HIS
1	A	260	ASN
2	B	271	ASP
2	B	533	PHE
1	C	47	PHE
1	C	65	HIS
1	C	260	ASN
1	C	320	THR

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Mol	Chain	Res	Type
2	D	271	ASP
2	D	481	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
2	B	354	HIS
2	B	363	HIS
2	B	433	HIS
2	B	470	ASN
2	B	541	ASN
1	C	23	HIS
1	C	264	GLN
2	D	243	GLN
2	D	298	HIS
2	D	354	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
3	MES	A	1330	-	12,12,12	2.31	1 (8%)	14,16,16	1.86	4 (28%)
4	ANP	B	1650	5	29,33,33	1.72	8 (27%)	31,52,52	1.86	8 (25%)
4	ANP	D	1650	5	29,33,33	1.87	5 (17%)	31,52,52	1.88	8 (25%)
3	MES	C	1330	-	12,12,12	2.30	1 (8%)	14,16,16	1.79	2 (14%)

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
3	MES	A	1330	-	-	5/6/14/14	0/1/1/1
4	ANP	B	1650	5	-	3/14/38/38	0/3/3/3
4	ANP	D	1650	5	-	6/14/38/38	0/3/3/3
3	MES	C	1330	-	-	3/6/14/14	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1330	MES	C8-S	-7.76	1.66	1.77
3	C	1330	MES	C8-S	-7.73	1.66	1.77
4	D	1650	ANP	PG-N3B	4.62	1.75	1.63
4	D	1650	ANP	PB-N3B	4.62	1.75	1.63
4	B	1650	ANP	PB-N3B	4.20	1.74	1.63
4	B	1650	ANP	PG-N3B	4.13	1.74	1.63
4	D	1650	ANP	PB-O1B	3.35	1.51	1.46
4	D	1650	ANP	PG-O1G	3.32	1.51	1.46
4	B	1650	ANP	PG-O1G	3.01	1.50	1.46
4	B	1650	ANP	PB-O1B	2.99	1.50	1.46
4	D	1650	ANP	C5-C4	2.50	1.47	1.40
4	B	1650	ANP	PG-O2G	-2.22	1.50	1.56
4	B	1650	ANP	C5-C4	2.18	1.46	1.40
4	B	1650	ANP	PG-O3G	-2.17	1.50	1.56
4	B	1650	ANP	PB-O2B	-2.10	1.51	1.56

All (22) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1650	ANP	O1G-PG-N3B	-4.82	104.68	111.77
3	C	1330	MES	C5-N4-C3	4.79	119.62	108.83
3	A	1330	MES	C5-N4-C3	4.76	119.55	108.83
4	B	1650	ANP	PA-O3A-PB	-4.37	117.22	132.62
4	B	1650	ANP	O2B-PB-O1B	4.32	118.97	109.92
4	B	1650	ANP	O1G-PG-N3B	-4.19	105.61	111.77
4	D	1650	ANP	O2B-PB-O1B	4.07	118.46	109.92
4	D	1650	ANP	C3'-C2'-C1'	3.53	106.30	100.98
4	D	1650	ANP	PA-O3A-PB	-3.44	120.51	132.62
4	B	1650	ANP	N3-C2-N1	-3.19	123.70	128.68
4	D	1650	ANP	N3-C2-N1	-3.14	123.78	128.68
4	B	1650	ANP	C3'-C2'-C1'	2.84	105.25	100.98
4	D	1650	ANP	C4-C5-N7	-2.69	106.59	109.40
4	B	1650	ANP	C4-C5-N7	-2.61	106.68	109.40
4	B	1650	ANP	O3G-PG-O2G	2.60	114.57	107.64
3	A	1330	MES	O2S-S-C8	2.56	109.99	106.92
4	B	1650	ANP	O1B-PB-N3B	-2.54	108.03	111.77
4	D	1650	ANP	O1B-PB-N3B	-2.52	108.06	111.77
4	D	1650	ANP	O3G-PG-O2G	2.32	113.82	107.64
3	C	1330	MES	O2S-S-C8	2.24	109.61	106.92
3	A	1330	MES	O3S-S-C8	2.13	109.21	105.77
3	A	1330	MES	C6-C5-N4	-2.10	106.92	110.10

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1330	MES	N4-C7-C8-S
3	A	1330	MES	C7-C8-S-O2S
4	D	1650	ANP	PB-N3B-PG-O1G
4	D	1650	ANP	PG-N3B-PB-O1B
4	D	1650	ANP	PA-O3A-PB-O1B
4	D	1650	ANP	C5'-O5'-PA-O1A
4	D	1650	ANP	C5'-O5'-PA-O3A
4	B	1650	ANP	PG-N3B-PB-O1B
4	B	1650	ANP	C3'-C4'-C5'-O5'
3	C	1330	MES	N4-C7-C8-S
4	B	1650	ANP	O4'-C4'-C5'-O5'
3	A	1330	MES	C8-C7-N4-C3
3	C	1330	MES	C8-C7-N4-C3
3	A	1330	MES	C7-C8-S-O3S
3	A	1330	MES	C7-C8-S-O1S
3	C	1330	MES	C7-C8-S-O2S

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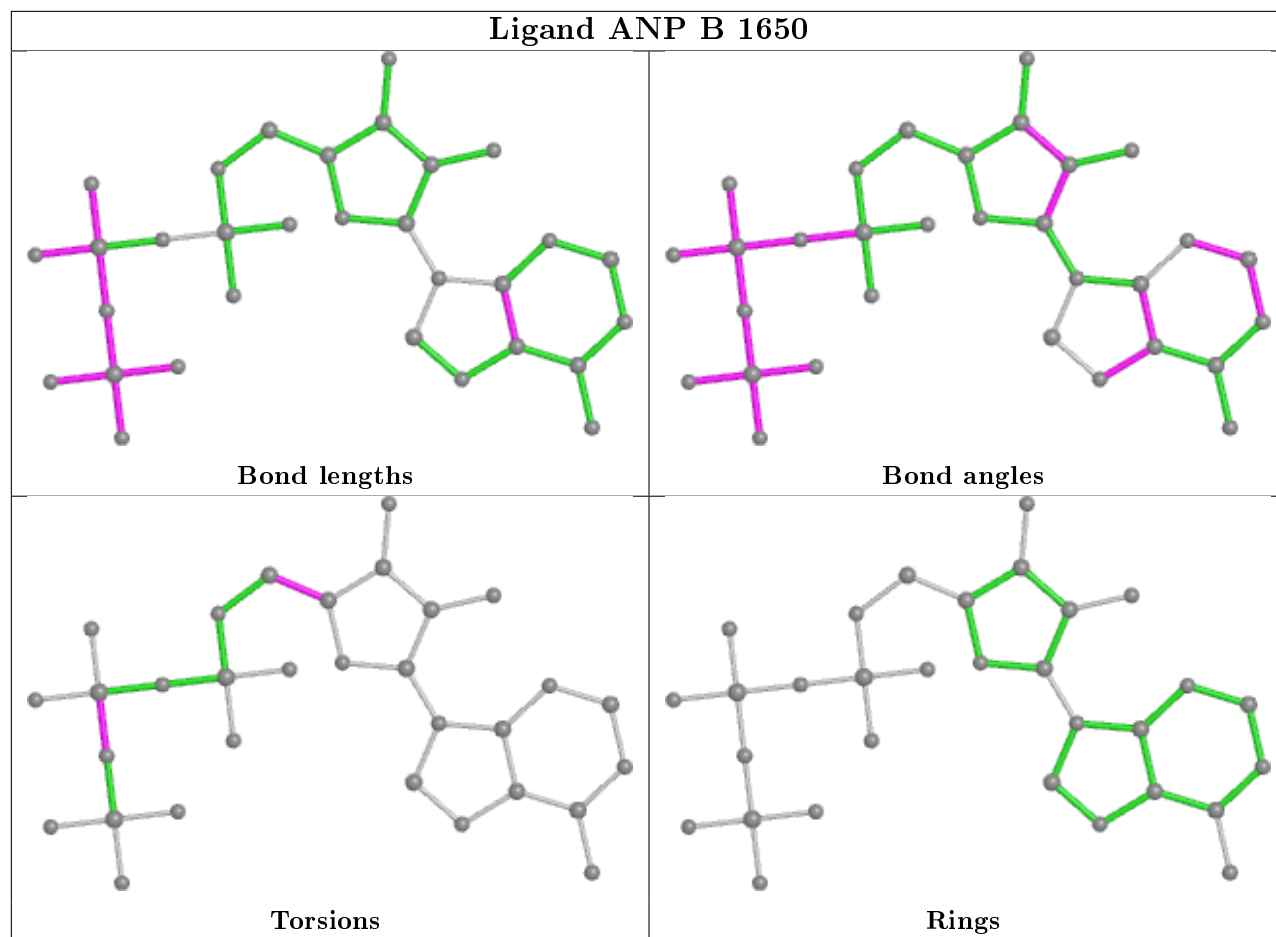
Mol	Chain	Res	Type	Atoms
4	D	1650	ANP	C4'-C5'-O5'-PA

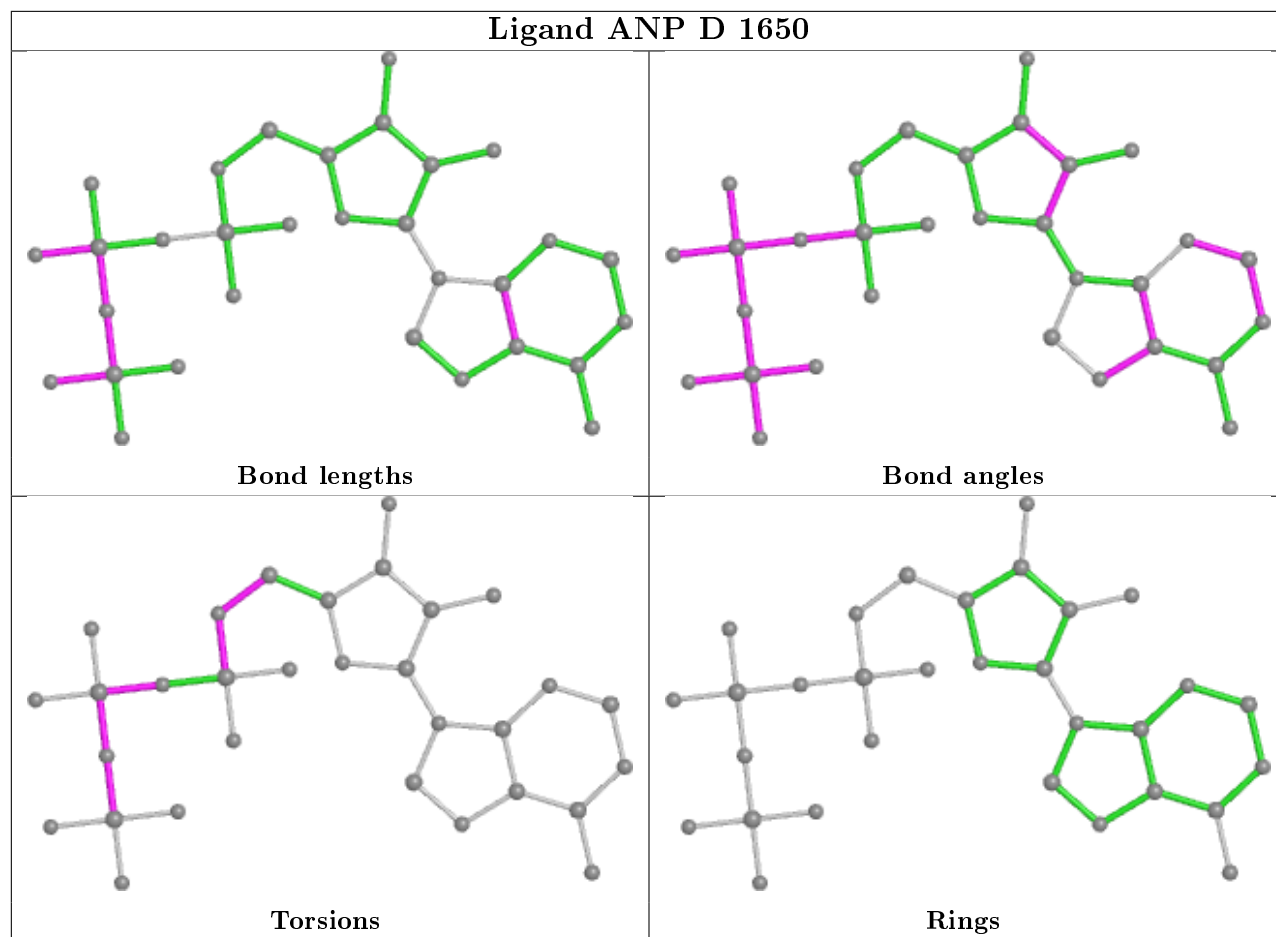
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1330	MES	1	0
4	B	1650	ANP	7	0
3	C	1330	MES	1	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	A	323/354 (91%)	0.52	32 (9%) 7 8	135, 163, 180, 197	0
1	C	323/354 (91%)	0.44	27 (8%) 11 13	131, 156, 182, 203	0
2	B	403/429 (93%)	0.32	9 (2%) 62 60	91, 122, 167, 191	0
2	D	403/429 (93%)	0.29	7 (1%) 70 68	91, 121, 167, 199	0
All	All	1452/1566 (92%)	0.38	75 (5%) 27 27	91, 147, 177, 203	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	ILE	5.1
1	A	202	ILE	4.3
1	C	299	LYS	4.3
1	A	172	ASN	4.0
2	B	616	LEU	4.0
1	A	183	LYS	3.9
1	C	280	TYR	3.9
1	A	201	PHE	3.8
1	A	9	LEU	3.8
1	A	145	LYS	3.8
2	D	275	THR	3.7
1	C	203	VAL	3.6
1	C	256	ALA	3.6
1	C	270	LEU	3.5
1	C	257	ILE	3.5
1	C	202	ILE	3.4
1	C	266	HIS	3.2
1	A	127	ALA	3.1
1	C	117	THR	3.1
1	C	6	TRP	3.0
2	B	626	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	133	MET	2.9
1	A	171	VAL	2.9
1	A	310	VAL	2.9
2	B	625	PHE	2.8
1	A	81	GLY	2.7
2	B	614	ILE	2.7
1	C	176	PRO	2.7
1	A	257	ILE	2.7
2	B	275	THR	2.6
2	D	418	ASN	2.6
1	A	82	VAL	2.6
1	C	123	GLU	2.6
1	C	133	MET	2.6
1	C	83	ILE	2.6
1	A	12	VAL	2.6
2	B	615	LEU	2.5
1	C	179	PHE	2.5
2	B	261	LEU	2.5
2	B	309	LEU	2.4
1	A	196	ASP	2.4
2	D	583	PHE	2.4
1	A	153	TYR	2.3
1	C	118	SER	2.3
1	A	170	THR	2.3
1	C	0	MET	2.3
2	B	574	LEU	2.3
1	C	290	PHE	2.3
2	D	625	PHE	2.3
1	C	275	ASN	2.3
1	C	228	LEU	2.2
1	C	-1	HIS	2.2
1	A	162	ILE	2.2
2	D	390	CYS	2.2
1	A	6	TRP	2.2
1	A	203	VAL	2.2
1	A	83	ILE	2.2
1	C	278	VAL	2.2
1	A	146	GLU	2.2
1	C	171	VAL	2.2
1	A	147	LEU	2.2
1	C	59	PHE	2.2
2	D	376	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	116	PHE	2.1
2	D	369	ASN	2.1
1	A	301	LEU	2.1
1	A	290	PHE	2.1
1	A	319	PHE	2.1
1	A	179	PHE	2.0
1	A	108	MET	2.0
1	A	164	ALA	2.0
1	A	10	GLY	2.0
1	A	249	HIS	2.0
1	C	107	SER	2.0
1	C	124	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

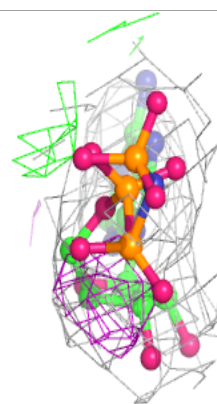
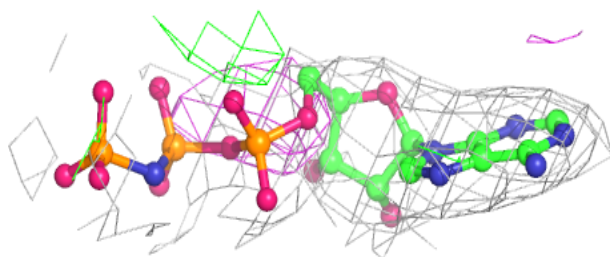
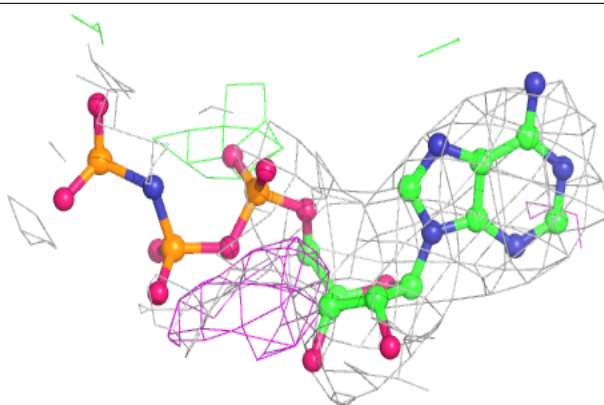
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	MES	C	1330	12/12	0.83	0.37	130,152,164,168	0
3	MES	A	1330	12/12	0.88	0.31	129,146,176,177	0
4	ANP	D	1650	31/31	0.90	0.25	90,111,136,153	0
4	ANP	B	1650	31/31	0.92	0.25	90,111,143,159	0
5	MG	B	1651	1/1	0.98	0.25	106,106,106,106	0
5	MG	D	1651	1/1	0.98	0.30	111,111,111,111	0

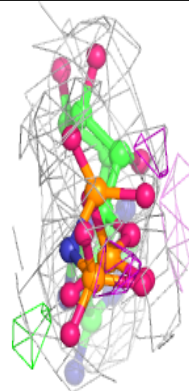
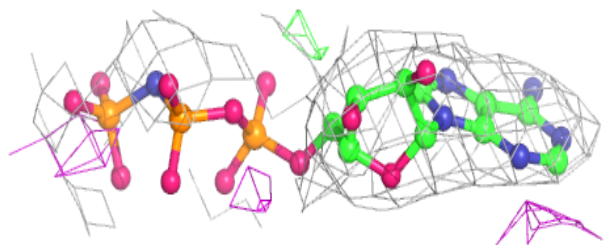
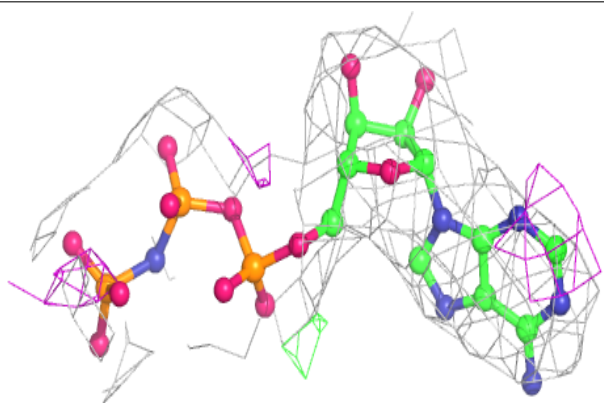
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ANP D 1650:**

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

**Electron density around ANP B 1650:**

$2mF_o-DF_c$  (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.