Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 09:44 am BST

PDB ID	:	7NN0
Title	:	Crystal structure of the SARS-CoV-2 helicase in complex with AMP-PNP
Authors	:	Newman, J.A.; Yosaatmadja, Y.; Douangamath, A.; Bountra, C.; Gileadi, O.
Deposited on	:	2021-02-23
Resolution	:	3.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

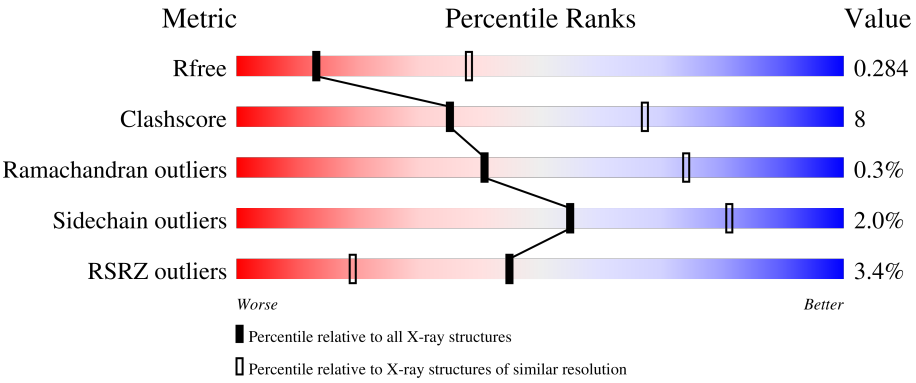
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	603	3% 72% 24%
1	B	603	% 83% 15%
1	C	603	6% 73% 23%
1	D	603	2% 82% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18199 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.

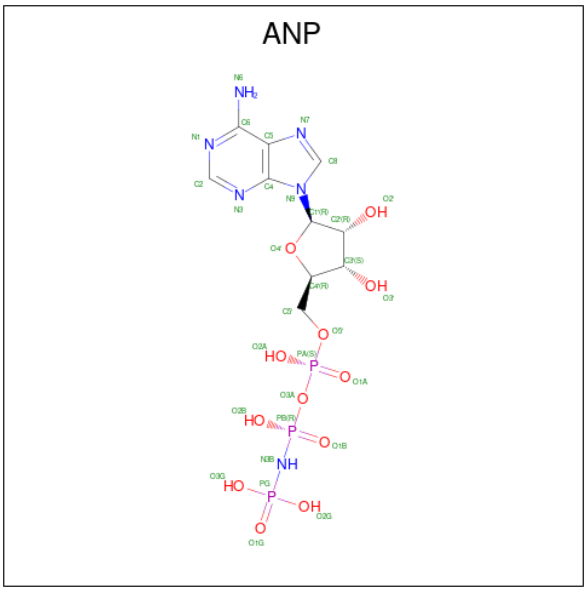
- Molecule 1 is a protein called SARS-CoV-2 helicase NSP13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4523	2882	757	850	34			
1	B	590	Total	C	N	O	S	0	0	0
			4550	2899	764	852	35			
1	C	585	Total	C	N	O	S	0	0	0
			4486	2861	744	847	34			
1	D	585	Total	C	N	O	S	0	0	0
			4500	2870	749	847	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P0DTD1
A	0	MET	-	expression tag	UNP P0DTD1
B	-1	SER	-	expression tag	UNP P0DTD1
B	0	MET	-	expression tag	UNP P0DTD1
C	-1	SER	-	expression tag	UNP P0DTD1
C	0	MET	-	expression tag	UNP P0DTD1
D	-1	SER	-	expression tag	UNP P0DTD1
D	0	MET	-	expression tag	UNP P0DTD1

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		
3	B	3	Total	Zn	0	0
			3	3		
3	C	3	Total	Zn	0	0
			3	3		
3	D	3	Total	Zn	0	0
			3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

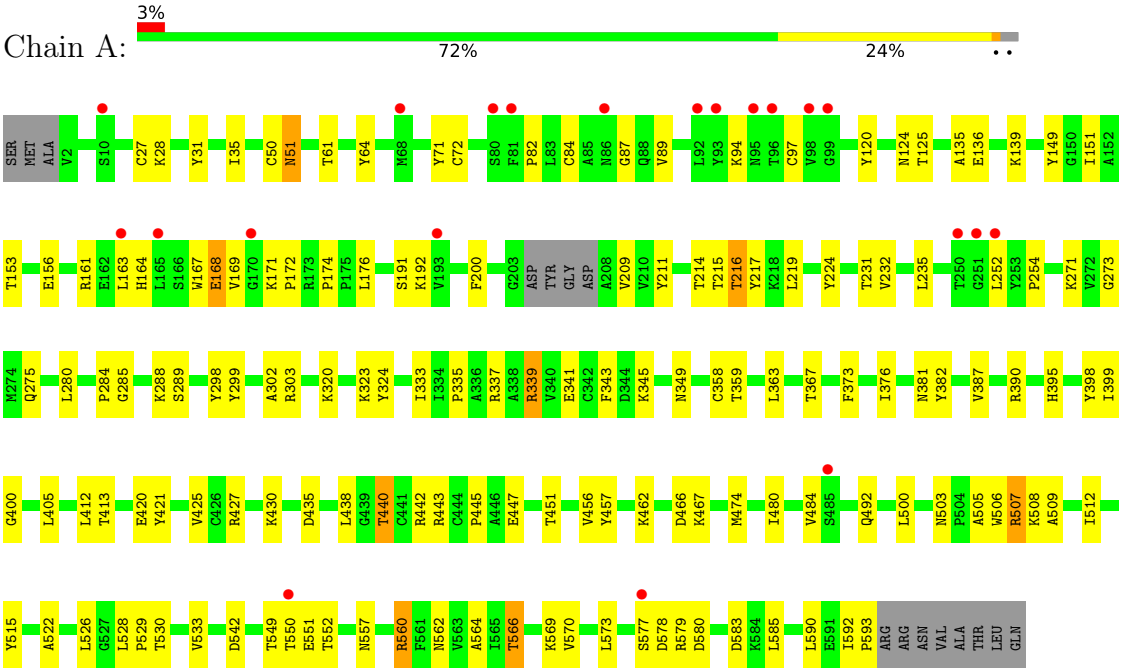
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

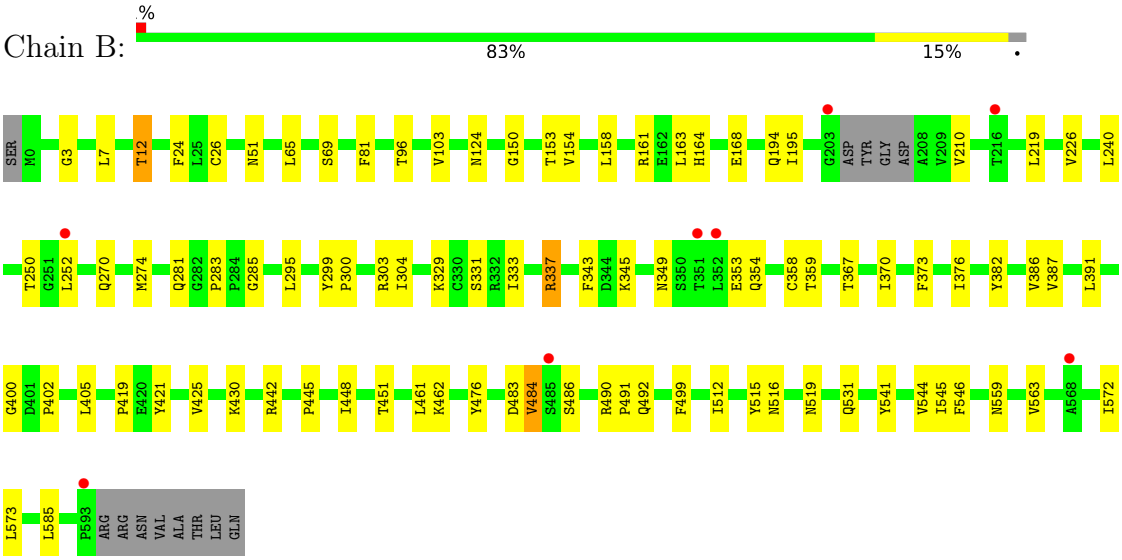
• Molecule 1: SARS-CoV-2 helicase NSP13

Chain A:



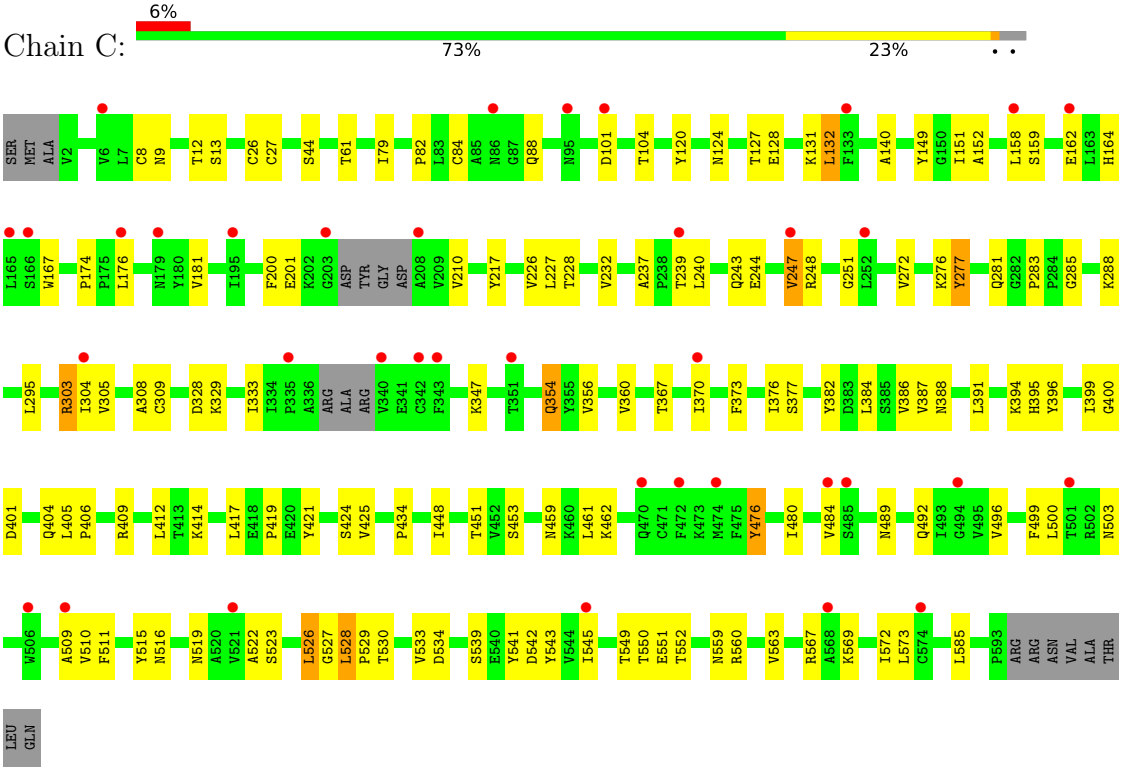
• Molecule 1: SARS-CoV-2 helicase NSP13

Chain B:



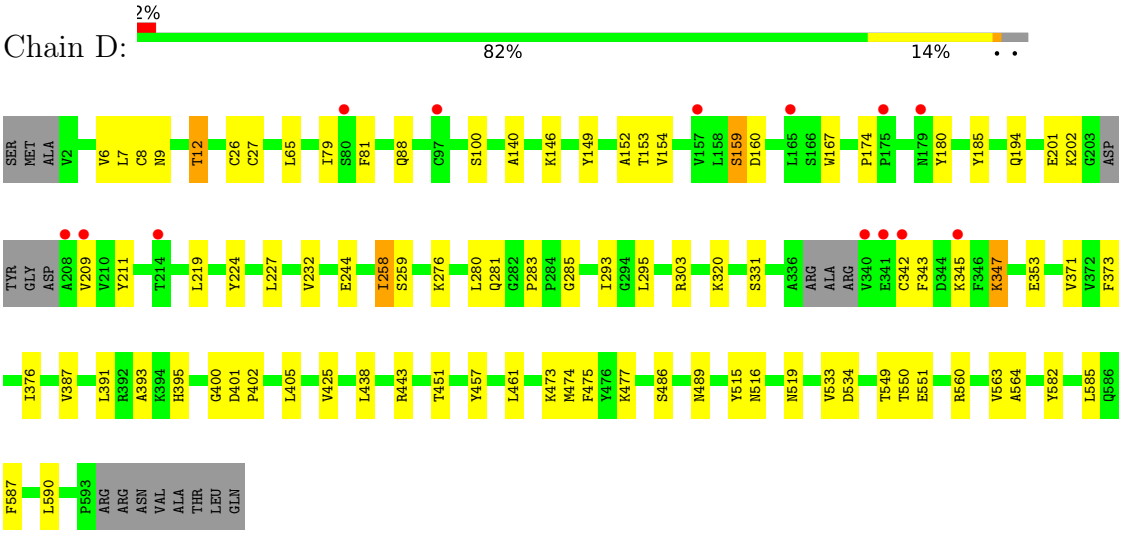
• Molecule 1: SARS-CoV-2 helicase NSP13

Chain C:



• Molecule 1: SARS-CoV-2 helicase NSP13

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	324.89Å 59.50Å 132.38Å 90.00° 93.89° 90.00°	Depositor
Resolution (Å)	81.03 – 3.04 81.03 – 3.04	Depositor EDS
% Data completeness (in resolution range)	97.3 (81.03-3.04) 97.3 (81.03-3.04)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.244 , 0.284 0.244 , 0.284	Depositor DCC
R_{free} test set	2347 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	60.2	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	18199	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9697e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ANP, ZN, MG

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	0.33	0/4626	0.52	0/6307
1	B	0.29	0/4653	0.49	0/6339
1	C	0.28	0/4588	0.51	0/6258
1	D	0.28	0/4602	0.48	0/6273
All	All	0.30	0/18469	0.50	0/25177

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4523	0	4435	95	1
1	B	4550	0	4486	57	0
1	C	4486	0	4382	96	0
1	D	4500	0	4415	56	0
2	A	31	0	13	4	0
2	B	31	0	13	2	0
2	C	31	0	13	2	0
2	D	31	0	13	4	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
All	All	18199	0	17770	295	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 8.

All (295) 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:C:528:LEU:HB2	1:C:529:PRO:HD2	1.45	0.99
1:C:528:LEU:HB2	1:C:529:PRO:CD	1.94	0.98
1:A:285:GLY:H	2:A:701:ANP:HNB1	1.13	0.96
1:C:522:ALA:O	1:C:526:LEU:HB2	1.78	0.84
1:A:284:PRO:HB2	1:A:566:THR:HG21	1.65	0.79
1:C:451:THR:HG21	1:C:585:LEU:HD23	1.65	0.78
1:C:528:LEU:HD23	1:C:528:LEU:N	1.99	0.77
1:C:528:LEU:CB	1:C:529:PRO:CD	2.63	0.77
1:C:523:SER:HB2	1:C:530:THR:HG21	1.68	0.75
1:C:243:GLN:HB2	1:C:277:TYR:HE1	1.53	0.73
1:A:509:ALA:O	1:A:529:PRO:HD2	1.89	0.72
1:C:124:ASN:O	1:C:131:LYS:NZ	2.22	0.72
1:C:303:ARG:NH2	1:C:367:THR:O	2.19	0.71
1:C:528:LEU:HD23	1:C:528:LEU:H	1.54	0.70
1:B:419:PRO:HG3	1:B:559:ASN:HD21	1.56	0.69
1:C:489:ASN:HB2	1:C:549:THR:HG23	1.74	0.69
1:C:149:TYR:HB3	1:C:174:PRO:HD3	1.74	0.69
1:C:405:LEU:HG	1:C:563:VAL:HG21	1.74	0.68
1:C:448:ILE:HD11	1:C:572:ILE:HG21	1.73	0.68
1:C:476:TYR:O	1:C:492:GLN:NE2	2.25	0.68
1:B:331:SER:HB2	1:B:353:GLU:HG3	1.74	0.68
1:B:531:GLN:OE1	1:B:541:TYR:OH	2.13	0.67
1:A:480:ILE:HB	1:C:480:ILE:HB	1.77	0.67
1:A:579:ARG:NH1	1:A:583:ASP:OD2	2.27	0.67
1:C:545:ILE:HG23	1:C:573:LEU:HD23	1.77	0.66
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.77	0.66
1:A:500:LEU:HB3	1:A:507:ARG:HD2	1.77	0.65
1:B:163:LEU:HD21	1:B:219:LEU:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ASN:HD22	1:C:421:TYR:HA	1.61	0.64
1:C:247:VAL:HG13	1:C:248:ARG:HH21	1.63	0.64
1:D:387:VAL:HG13	1:D:391:LEU:HD12	1.79	0.64
1:A:124:ASN:ND2	1:A:421:TYR:O	2.31	0.63
1:C:251:GLY:HA3	1:C:394:LYS:HE2	1.79	0.63
1:A:214:THR:HA	1:A:339:ARG:HB3	1.80	0.63
1:D:477:LYS:NZ	1:D:551:GLU:OE2	2.23	0.63
1:D:533:VAL:HG11	1:D:560:ARG:HG3	1.81	0.63
1:C:533:VAL:HG11	1:C:560:ARG:HG3	1.82	0.62
1:A:451:THR:HG21	1:A:585:LEU:HD23	1.81	0.62
2:D:704:ANP:O1A	2:D:704:ANP:N3B	2.31	0.62
1:D:342:CYS:SG	1:D:343:PHE:N	2.71	0.62
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.82	0.62
1:A:153:THR:HG22	1:A:224:TYR:HB3	1.82	0.62
1:A:303:ARG:NH2	1:A:367:THR:O	2.33	0.61
1:A:343:PHE:CZ	1:A:345:LYS:HB2	2.35	0.61
1:B:303:ARG:NH2	1:B:367:THR:O	2.33	0.61
1:D:320:LYS:NZ	2:D:704:ANP:O2'	2.25	0.60
1:A:515:TYR:HH	1:A:552:THR:HG1	1.48	0.60
1:B:387:VAL:HG13	1:B:391:LEU:HD12	1.84	0.60
1:C:499:PHE:CD2	1:C:573:LEU:HD22	2.38	0.59
1:B:3:GLY:HA3	1:B:24:PHE:CE1	2.37	0.59
1:D:475:PHE:HB2	1:D:582:TYR:CE2	2.37	0.59
1:A:474:MET:HE3	1:A:573:LEU:HD11	1.85	0.59
1:A:163:LEU:HD11	1:A:219:LEU:HD11	1.83	0.58
1:D:516:ASN:HA	1:D:519:ASN:HB2	1.85	0.58
1:B:333:ILE:HB	1:B:358:CYS:HB2	1.86	0.58
1:A:341:GLU:N	1:A:341:GLU:OE1	2.37	0.58
1:A:376:ILE:HG22	1:A:400:GLY:HA3	1.86	0.57
1:D:27:CYS:HB3	1:D:88:GLN:HB3	1.86	0.57
1:D:373:PHE:HE1	1:D:387:VAL:HG21	1.69	0.57
1:B:329:LYS:HG3	1:B:354:GLN:HB3	1.86	0.57
1:C:27:CYS:HB3	1:C:88:GLN:HB3	1.86	0.57
1:C:328:ASP:HA	1:C:347:LYS:NZ	2.20	0.57
1:A:288:LYS:N	2:A:701:ANP:O1B	2.32	0.57
1:D:281:GLN:HG3	1:D:402:PRO:HD2	1.87	0.57
1:B:154:VAL:HG21	1:B:219:LEU:HD13	1.86	0.57
1:A:530:THR:HG23	1:A:530:THR:O	2.04	0.56
1:C:61:THR:HA	1:C:84:CYS:SG	2.45	0.56
1:C:329:LYS:HB3	1:C:354:GLN:HB3	1.88	0.56
1:D:473:LYS:NZ	1:D:585:LEU:O	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.40	0.56
1:C:128:GLU:OE2	1:C:239:THR:N	2.28	0.56
1:D:12:THR:OG1	1:D:26:CYS:HA	2.06	0.56
1:A:285:GLY:N	2:A:701:ANP:HNB1	1.95	0.56
1:B:51:ASN:OD1	1:B:69:SER:OG	2.24	0.56
1:D:376:ILE:HG22	1:D:400:GLY:HA3	1.88	0.56
1:B:499:PHE:CD2	1:B:573:LEU:HD22	2.41	0.56
1:A:51:ASN:O	1:A:51:ASN:ND2	2.33	0.55
1:B:405:LEU:HG	1:B:563:VAL:HG21	1.89	0.55
1:C:406:PRO:HB2	1:C:409:ARG:HH12	1.72	0.55
1:C:419:PRO:HG3	1:C:559:ASN:HD21	1.71	0.55
1:D:443:ARG:NH2	2:D:704:ANP:O2B	2.40	0.55
1:A:167:TRP:CZ3	1:A:174:PRO:HD2	2.41	0.55
1:B:158:LEU:HD11	1:B:164:HIS:ND1	2.21	0.55
1:A:569:LYS:HG3	1:A:570:VAL:HG23	1.89	0.55
1:C:509:ALA:HA	1:C:543:TYR:HB2	1.87	0.55
1:C:542:ASP:HA	1:C:569:LYS:HB2	1.89	0.55
1:D:486:SER:OG	1:D:515:TYR:HB3	2.07	0.55
1:C:239:THR:O	1:C:388:ASN:ND2	2.40	0.54
1:A:443:ARG:HB2	2:A:701:ANP:H4'	1.88	0.54
1:A:440:THR:HG23	1:A:462:LYS:HB2	1.90	0.54
1:B:451:THR:HG21	1:B:585:LEU:HD23	1.90	0.54
1:B:285:GLY:HA2	2:B:701:ANP:H5'1	1.89	0.54
1:C:405:LEU:HD13	1:C:534:ASP:HA	1.89	0.54
1:C:376:ILE:HG22	1:C:400:GLY:HA3	1.89	0.54
1:A:27:CYS:SG	1:A:94:LYS:HA	2.48	0.53
1:C:510:VAL:HG11	1:C:541:TYR:CD2	2.43	0.53
1:A:216:THR:HG22	1:B:195:ILE:HA	1.91	0.53
1:B:445:PRO:HD2	1:B:448:ILE:HD12	1.91	0.53
1:B:476:TYR:O	1:B:492:GLN:NE2	2.41	0.53
1:C:239:THR:HG21	1:C:424:SER:HB2	1.91	0.53
1:C:244:GLU:HG2	1:C:276:LYS:HB2	1.90	0.53
1:B:12:THR:OG1	1:B:26:CYS:HA	2.09	0.53
1:D:185:TYR:CE2	1:D:194:GLN:HG2	2.44	0.53
1:A:252:LEU:HD22	1:A:302:ALA:HB2	1.90	0.53
1:C:328:ASP:HA	1:C:347:LYS:HZ2	1.75	0.52
1:D:373:PHE:CE1	1:D:387:VAL:HG21	2.44	0.52
1:A:156:GLU:HB3	1:A:164:HIS:HB2	1.91	0.52
1:A:474:MET:HG2	1:A:590:LEU:HB2	1.91	0.52
1:D:201:GLU:OE1	1:D:516:ASN:ND2	2.43	0.52
1:C:82:PRO:HG3	1:D:345:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:PRO:HD3	1:A:457:TYR:CZ	2.45	0.51
1:C:391:LEU:O	1:C:396:TYR:OH	2.19	0.51
1:C:151:ILE:HG12	1:C:226:VAL:HG22	1.93	0.51
1:C:285:GLY:H	2:C:704:ANP:HNB1	1.59	0.51
1:D:258:ILE:HG23	1:D:259:SER:H	1.75	0.51
1:D:283:PRO:HG2	1:D:461:LEU:HD13	1.93	0.51
1:A:552:THR:HG22	1:C:551:GLU:HG3	1.92	0.51
1:A:562:ASN:O	1:A:566:THR:OG1	2.25	0.51
1:D:154:VAL:HG21	1:D:219:LEU:HD13	1.92	0.51
1:C:132:LEU:HD11	1:C:237:ALA:O	2.10	0.51
1:C:240:LEU:HD21	1:C:425:VAL:HG22	1.93	0.51
1:A:512:ILE:HG21	1:A:564:ALA:HB1	1.93	0.50
1:C:283:PRO:HG2	1:C:461:LEU:HD13	1.92	0.50
1:D:343:PHE:CZ	1:D:345:LYS:HB2	2.46	0.50
1:A:163:LEU:HG	1:A:211:TYR:CD2	2.47	0.50
1:A:50:CYS:SG	1:A:72:CYS:N	2.81	0.50
1:B:486:SER:OG	1:B:515:TYR:HB3	2.12	0.50
1:A:176:LEU:HD22	1:A:200:PHE:HB2	1.93	0.49
1:A:335:PRO:HB2	1:B:337:ARG:NH1	2.27	0.49
1:A:522:ALA:O	1:A:526:LEU:HB2	2.12	0.49
1:A:580:ASP:HA	1:C:414:LYS:HG2	1.94	0.49
1:A:456:VAL:HG13	1:A:457:TYR:CD2	2.48	0.49
1:D:159:SER:OG	1:D:160:ASP:N	2.45	0.49
1:B:283:PRO:HG2	1:B:461:LEU:HD13	1.94	0.49
1:C:373:PHE:CE1	1:C:387:VAL:HG21	2.47	0.49
1:A:124:ASN:OD1	1:A:381:ASN:ND2	2.46	0.49
1:A:405:LEU:HD22	1:A:560:ARG:HH21	1.77	0.49
1:C:120:TYR:CE1	1:C:412:LEU:HD12	2.47	0.49
1:D:401:ASP:OD2	1:D:457:TYR:OH	2.25	0.49
1:D:280:LEU:HD11	1:D:438:LEU:HG	1.95	0.48
1:A:191:SER:OG	1:A:192:LYS:N	2.45	0.48
1:A:503:ASN:HB3	1:A:506:TRP:CD1	2.48	0.48
1:B:373:PHE:CE1	1:B:387:VAL:HG21	2.48	0.48
1:B:343:PHE:CZ	1:B:345:LYS:HB2	2.49	0.48
1:D:473:LYS:HD3	1:D:587:PHE:HB2	1.94	0.48
1:A:551:GLU:HB2	1:C:552:THR:HG22	1.96	0.48
1:B:419:PRO:HG3	1:B:559:ASN:ND2	2.27	0.48
1:B:483:ASP:OD1	1:B:484:VAL:N	2.39	0.48
1:C:272:VAL:HG11	1:C:295:LEU:HD11	1.96	0.48
1:D:7:LEU:HB3	1:D:100:SER:CB	2.44	0.48
1:D:65:LEU:HD23	1:D:81:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PRO:HB3	1:A:298:TYR:CZ	2.48	0.47
1:C:499:PHE:CE2	1:C:573:LEU:HD22	2.49	0.47
1:A:288:LYS:HB3	1:A:399:ILE:CG2	2.43	0.47
1:B:373:PHE:HE1	1:B:387:VAL:HG21	1.79	0.47
1:C:162:GLU:HG2	1:C:210:VAL:HG22	1.96	0.47
1:C:523:SER:HB2	1:C:530:THR:CG2	2.39	0.47
1:C:201:GLU:O	1:C:210:VAL:N	2.34	0.47
1:B:3:GLY:HA3	1:B:24:PHE:CD1	2.50	0.47
1:A:333:ILE:HB	1:A:358:CYS:HB2	1.96	0.47
1:A:31:TYR:CE2	1:A:35:ILE:HD13	2.50	0.47
1:A:84:CYS:HB3	1:A:89:VAL:HG22	1.95	0.47
1:A:289:SER:HB2	1:A:320:LYS:HE3	1.96	0.47
1:D:285:GLY:HA2	2:D:704:ANP:H5'1	1.97	0.47
1:B:295:LEU:HD21	1:B:370:ILE:HG21	1.97	0.47
1:B:376:ILE:HG12	1:B:425:VAL:HG11	1.97	0.47
1:A:275:GLN:NE2	1:A:435:ASP:OD2	2.47	0.47
1:C:496:VAL:CG1	1:C:526:LEU:HD11	2.45	0.47
1:D:451:THR:HG21	1:D:585:LEU:HD23	1.97	0.47
1:C:541:TYR:O	1:C:569:LYS:N	2.43	0.46
1:C:304:ILE:HD12	1:C:370:ILE:HB	1.97	0.46
1:C:376:ILE:HD11	1:C:384:LEU:HD21	1.98	0.46
1:A:139:LYS:HG2	1:A:232:VAL:HG22	1.98	0.46
1:A:363:LEU:O	1:A:390:ARG:NE	2.46	0.46
1:B:7:LEU:HD13	1:B:103:VAL:HG22	1.96	0.46
1:D:473:LYS:HG3	1:D:582:TYR:HE1	1.81	0.46
1:C:453:SER:OG	1:C:459:ASN:HA	2.16	0.46
1:D:474:MET:HG2	1:D:590:LEU:HB2	1.97	0.46
1:A:31:TYR:CE2	1:A:87:GLY:HA2	2.51	0.45
1:B:516:ASN:HA	1:B:519:ASN:HB2	1.99	0.45
1:C:305:VAL:HA	1:C:356:VAL:HB	1.98	0.45
1:A:557:ASN:HB3	1:A:560:ARG:HB3	1.98	0.45
1:C:404:GLN:NE2	2:C:704:ANP:O3G	2.49	0.45
1:D:276:LYS:O	1:D:395:HIS:HA	2.16	0.45
1:A:136:GLU:OE2	1:A:235:LEU:N	2.30	0.45
1:A:578:ASP:OD2	1:A:580:ASP:HB3	2.16	0.45
1:B:150:GLY:HA3	1:B:168:GLU:HB3	1.99	0.45
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.51	0.45
1:B:240:LEU:HD21	1:B:425:VAL:HG22	1.98	0.45
1:C:563:VAL:O	1:C:567:ARG:HG2	2.16	0.45
1:D:180:TYR:HB3	1:D:227:LEU:HD21	1.97	0.45
1:A:542:ASP:HA	1:A:569:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:GLN:O	1:B:274:MET:HG3	2.17	0.45
1:C:12:THR:HG21	1:C:26:CYS:HA	1.98	0.44
1:C:295:LEU:HD21	1:C:370:ILE:HD12	1.98	0.44
1:B:462:LYS:HA	1:B:462:LYS:HD3	1.85	0.44
1:A:323:LYS:HD3	1:A:324:TYR:CZ	2.53	0.44
1:D:149:TYR:HB3	1:D:174:PRO:HD3	1.99	0.44
1:D:152:ALA:HB2	1:D:167:TRP:CZ3	2.53	0.44
1:A:398:TYR:HB3	1:A:425:VAL:HG11	2.00	0.44
1:A:61:THR:HA	1:A:84:CYS:SG	2.57	0.44
1:A:492:GLN:NE2	1:A:577:SER:OG	2.49	0.44
1:A:420:GLU:HB2	1:A:430:LYS:HG3	1.98	0.44
1:D:489:ASN:HB2	1:D:549:THR:HG23	2.00	0.44
1:C:528:LEU:N	1:C:528:LEU:CD2	2.73	0.44
1:D:202:LYS:HA	1:D:209:VAL:HG23	2.00	0.44
1:C:528:LEU:CB	1:C:529:PRO:HD3	2.44	0.44
1:A:125:THR:HG22	1:A:427:ARG:NH1	2.33	0.44
1:A:273:GLY:HA2	1:A:395:HIS:CE1	2.53	0.44
1:A:271:LYS:HE3	1:A:435:ASP:HB3	2.00	0.43
1:A:474:MET:CG	1:A:590:LEU:HB2	2.48	0.43
1:B:382:TYR:O	1:B:386:VAL:HG23	2.18	0.43
1:C:152:ALA:HB2	1:C:167:TRP:CZ3	2.53	0.43
1:A:333:ILE:HD13	1:A:349:ASN:HA	1.99	0.43
1:C:462:LYS:HD3	1:C:462:LYS:HA	1.82	0.43
1:D:405:LEU:HG	1:D:563:VAL:HG21	1.99	0.43
1:D:533:VAL:HG22	1:D:564:ALA:HB2	1.99	0.43
1:C:176:LEU:HD23	1:C:200:PHE:HB2	2.01	0.43
1:A:505:ALA:O	1:A:508:LYS:NZ	2.46	0.43
1:D:293:ILE:HG13	1:D:320:LYS:HG3	2.01	0.43
1:C:281:GLN:HA	1:C:400:GLY:O	2.19	0.43
1:A:216:THR:HG21	1:B:195:ILE:HG12	2.01	0.43
1:A:217:TYR:HE1	1:A:219:LEU:HA	1.83	0.43
1:A:373:PHE:CE1	1:A:387:VAL:HG21	2.54	0.43
1:C:523:SER:O	1:C:527:GLY:HA2	2.19	0.43
1:C:281:GLN:OE1	1:C:434:PRO:HG3	2.19	0.43
1:A:549:THR:HG22	1:A:550:THR:HG23	2.01	0.42
1:D:8:CYS:O	1:D:9:ASN:HB2	2.19	0.42
1:C:251:GLY:HA3	1:C:394:LYS:CE	2.47	0.42
1:C:549:THR:HG22	1:C:550:THR:HG23	2.01	0.42
1:A:337:ARG:HG2	1:B:194:GLN:OE1	2.20	0.42
1:C:382:TYR:O	1:C:386:VAL:HG23	2.18	0.42
1:D:153:THR:HA	1:D:224:TYR:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HB2	1:A:447:GLU:OE1	2.19	0.42
1:B:442:ARG:HD3	2:B:701:ANP:N7	2.34	0.42
1:A:405:LEU:HD21	1:A:533:VAL:HG12	2.02	0.42
1:B:544:VAL:O	1:B:572:ILE:HA	2.19	0.42
1:C:384:LEU:HD13	1:C:425:VAL:HG23	2.00	0.42
1:D:244:GLU:O	1:D:276:LYS:N	2.45	0.42
1:D:258:ILE:HG23	1:D:259:SER:N	2.34	0.42
1:A:135:ALA:HB1	1:A:382:TYR:HB2	2.01	0.42
1:A:528:LEU:HB3	1:A:529:PRO:CD	2.50	0.42
1:B:154:VAL:HG13	1:B:163:LEU:HD22	2.00	0.42
1:C:333:ILE:HD13	1:C:356:VAL:HG13	2.00	0.42
1:C:516:ASN:HA	1:C:519:ASN:HB2	2.01	0.42
1:A:219:LEU:HD23	1:A:219:LEU:H	1.85	0.42
1:B:512:ILE:O	1:B:546:PHE:HA	2.20	0.42
1:A:231:THR:OG1	1:B:349:ASN:HB3	2.20	0.42
1:C:127:THR:O	1:C:131:LYS:HG3	2.20	0.42
1:C:515:TYR:OH	1:C:552:THR:OG1	2.36	0.42
1:D:140:ALA:HA	1:D:232:VAL:HG21	2.01	0.42
1:B:281:GLN:HG3	1:B:402:PRO:HD2	2.01	0.42
1:C:8:CYS:O	1:C:9:ASN:HB2	2.20	0.42
1:D:376:ILE:HG12	1:D:425:VAL:HG11	2.02	0.42
1:A:28:LYS:N	1:A:97:CYS:SG	2.82	0.41
1:C:158:LEU:HD21	1:C:164:HIS:ND1	2.35	0.41
1:C:276:LYS:O	1:C:395:HIS:HA	2.19	0.41
1:D:347:LYS:HE2	1:D:347:LYS:HB2	1.73	0.41
1:B:329:LYS:HA	1:B:329:LYS:HD3	1.86	0.41
1:D:303:ARG:NH1	1:D:353:GLU:O	2.53	0.41
1:D:405:LEU:HD13	1:D:534:ASP:HA	2.02	0.41
1:A:217:TYR:CE1	1:A:219:LEU:HA	2.55	0.41
1:C:140:ALA:HA	1:C:232:VAL:HG21	2.02	0.41
1:A:500:LEU:HD11	1:A:528:LEU:HD11	2.02	0.41
1:A:592:ILE:HA	1:A:593:PRO:HD3	1.92	0.41
1:C:377:SER:OG	1:C:401:ASP:O	2.29	0.41
1:D:146:LYS:HA	1:D:149:TYR:CD2	2.56	0.41
1:C:308:ALA:O	1:C:360:VAL:HG23	2.21	0.41
1:D:549:THR:HG22	1:D:550:THR:HG23	2.03	0.41
1:A:215:THR:HG23	1:A:217:TYR:H	1.86	0.41
1:C:328:ASP:O	1:C:329:LYS:HE2	2.20	0.41
1:C:500:LEU:HD23	1:C:500:LEU:HA	1.86	0.41
1:B:304:ILE:HG12	1:B:370:ILE:HB	2.03	0.41
1:A:64:TYR:CE2	1:A:82:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:O	1:A:168:GLU:HB3	2.21	0.41
1:B:124:ASN:HD22	1:B:421:TYR:HA	1.86	0.41
1:B:300:PRO:O	1:B:354:GLN:NE2	2.54	0.41
1:C:511:PHE:O	1:C:530:THR:HA	2.20	0.41
1:D:6:VAL:HG23	1:D:7:LEU:CD2	2.51	0.41
1:A:149:TYR:CD1	1:A:172:PRO:HG2	2.56	0.41
1:A:466:ASP:OD1	1:A:467:LYS:N	2.53	0.41
1:B:402:PRO:HB2	1:B:430:LYS:HD3	2.03	0.41
1:D:331:SER:HB2	1:D:353:GLU:HG3	2.02	0.41
1:B:161:ARG:O	1:B:210:VAL:HA	2.21	0.40
1:C:288:LYS:HD2	1:C:399:ILE:HG22	2.02	0.40
1:A:31:TYR:CD2	1:A:87:GLY:HA2	2.56	0.40
1:A:120:TYR:CD1	1:A:412:LEU:HD12	2.56	0.40
1:B:545:ILE:HG23	1:B:573:LEU:HD23	2.04	0.40
1:C:13:SER:O	1:C:44:SER:HA	2.21	0.40
1:C:174:PRO:HB3	1:C:227:LEU:HD11	2.02	0.40
1:C:499:PHE:HE1	1:C:503:ASN:ND2	2.19	0.40
1:C:539:SER:O	1:C:567:ARG:HD3	2.21	0.40
1:A:252:LEU:HB3	1:A:299:TYR:CD1	2.57	0.40
1:B:490:ARG:HB2	1:B:491:PRO:HD3	2.03	0.40
1:D:371:VAL:HG23	1:D:393:ALA:HB2	2.04	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:71:TYR:OH	1:A:171:LYS:NZ[4_445]	1.83	0.37

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	584/603 (97%)	555 (95%)	27 (5%)	2 (0%)	41 74
1	B	586/603 (97%)	551 (94%)	35 (6%)	0	100 100
1	C	579/603 (96%)	545 (94%)	30 (5%)	4 (1%)	22 57
1	D	579/603 (96%)	547 (94%)	30 (5%)	2 (0%)	41 74
All	All	2328/2412 (96%)	2198 (94%)	122 (5%)	8 (0%)	41 74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	ARG
1	C	217	TYR
1	C	101	ASP
1	A	484	VAL
1	C	159	SER
1	C	484	VAL
1	D	159	SER
1	D	258	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	498/525 (95%)	485 (97%)	13 (3%)	46 76
1	B	502/525 (96%)	494 (98%)	8 (2%)	62 85
1	C	494/525 (94%)	480 (97%)	14 (3%)	43 75
1	D	497/525 (95%)	492 (99%)	5 (1%)	76 91
All	All	1991/2100 (95%)	1951 (98%)	40 (2%)	55 81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	168	GLU
1	A	169	VAL

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Mol	Chain	Res	Type
1	A	209	VAL
1	A	216	THR
1	A	339	ARG
1	A	359	THR
1	A	413	THR
1	A	440	THR
1	A	442	ARG
1	A	507	ARG
1	A	560	ARG
1	A	566	THR
1	B	12	THR
1	B	96	THR
1	B	153	THR
1	B	226	VAL
1	B	250	THR
1	B	337	ARG
1	B	359	THR
1	B	484	VAL
1	C	79	ILE
1	C	104	THR
1	C	132	LEU
1	C	181	VAL
1	C	228	THR
1	C	247	VAL
1	C	277	TYR
1	C	303	ARG
1	C	309	CYS
1	C	354	GLN
1	C	417	LEU
1	C	476	TYR
1	C	526	LEU
1	C	528	LEU
1	D	12	THR
1	D	79	ILE
1	D	211	TYR
1	D	295	LEU
1	D	347	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	HIS

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Mol	Chain	Res	Type
1	B	559	ASN
1	C	124	ASN
1	C	459	ASN
1	C	531	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 13 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	$\#\|Z\| > 2$
2	ANP	C	704	-	29,33,33	1.07	3 (10%)	31,52,52	1.03	2 (6%)
2	ANP	A	701	4	29,33,33	0.90	1 (3%)	31,52,52	1.26	5 (16%)
2	ANP	D	704	-	29,33,33	1.10	4 (13%)	31,52,52	1.14	2 (6%)
2	ANP	B	701	-	29,33,33	1.07	4 (13%)	31,52,52	1.02	2 (6%)

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	C	704	-	-	9/14/38/38	0/3/3/3
2	ANP	A	701	4	-	1/14/38/38	0/3/3/3
2	ANP	D	704	-	-	6/14/38/38	0/3/3/3
2	ANP	B	701	-	-	9/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ANP	PB-O3A	-2.80	1.55	1.59
2	C	704	ANP	PG-O1G	2.56	1.50	1.46
2	C	704	ANP	PG-N3B	2.56	1.70	1.63
2	D	704	ANP	PB-O1B	2.50	1.50	1.46
2	D	704	ANP	PG-O1G	2.49	1.50	1.46
2	B	701	ANP	PG-O1G	2.45	1.50	1.46
2	D	704	ANP	PG-N3B	2.45	1.69	1.63
2	B	701	ANP	PB-O1B	2.44	1.50	1.46
2	B	701	ANP	PG-N3B	2.38	1.69	1.63
2	C	704	ANP	PB-O1B	2.37	1.49	1.46
2	D	704	ANP	PB-O3A	-2.27	1.56	1.59
2	B	701	ANP	PB-O3A	-2.05	1.56	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	704	ANP	PA-O3A-PB	-3.89	118.90	132.62
2	B	701	ANP	PA-O3A-PB	-3.29	121.03	132.62
2	A	701	ANP	O1G-PG-N3B	-3.25	106.98	111.77
2	C	704	ANP	PA-O3A-PB	-3.18	121.41	132.62
2	A	701	ANP	PA-O3A-PB	-2.74	122.97	132.62
2	A	701	ANP	O2B-PB-O1B	-2.61	104.44	109.92
2	A	701	ANP	O3G-PG-O2G	2.39	114.01	107.64
2	B	701	ANP	C5-C6-N6	2.32	123.88	120.35
2	C	704	ANP	C5-C6-N6	2.28	123.82	120.35
2	D	704	ANP	C5-C6-N6	2.27	123.80	120.35
2	A	701	ANP	C5-C6-N6	2.23	123.74	120.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	B	701	ANP	PB-N3B-PG-O1G
2	B	701	ANP	PG-N3B-PB-O1B
2	B	701	ANP	PG-N3B-PB-O3A
2	B	701	ANP	C5'-O5'-PA-O1A
2	B	701	ANP	C5'-O5'-PA-O2A
2	B	701	ANP	C5'-O5'-PA-O3A
2	C	704	ANP	PB-N3B-PG-O1G
2	C	704	ANP	PG-N3B-PB-O1B
2	C	704	ANP	PG-N3B-PB-O3A
2	C	704	ANP	PA-O3A-PB-O1B
2	C	704	ANP	PA-O3A-PB-O2B
2	C	704	ANP	C5'-O5'-PA-O1A
2	C	704	ANP	C5'-O5'-PA-O2A
2	C	704	ANP	C5'-O5'-PA-O3A
2	D	704	ANP	PG-N3B-PB-O1B
2	D	704	ANP	C5'-O5'-PA-O3A
2	B	701	ANP	O4'-C4'-C5'-O5'
2	D	704	ANP	C5'-O5'-PA-O1A
2	D	704	ANP	C5'-O5'-PA-O2A
2	B	701	ANP	C3'-C4'-C5'-O5'
2	B	701	ANP	C4'-C5'-O5'-PA
2	C	704	ANP	O4'-C4'-C5'-O5'
2	D	704	ANP	C4'-C5'-O5'-PA
2	D	704	ANP	PB-N3B-PG-O1G

There are no ring outliers.

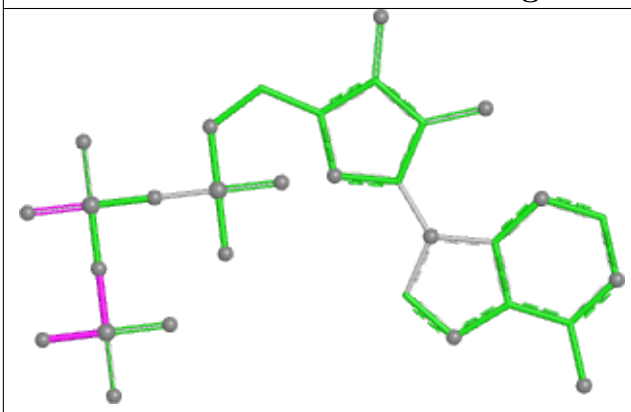
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	704	ANP	2	0
2	A	701	ANP	4	0
2	D	704	ANP	4	0
2	B	701	ANP	2	0

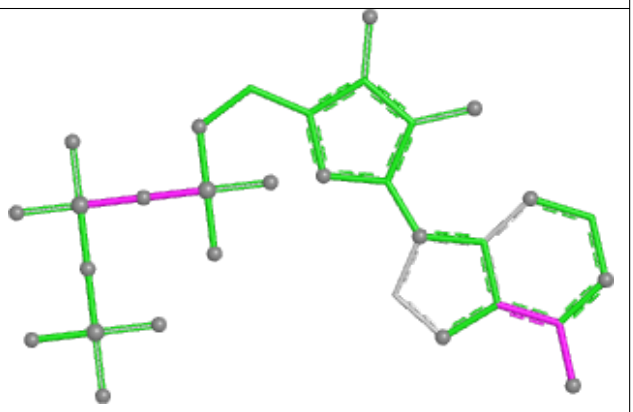
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

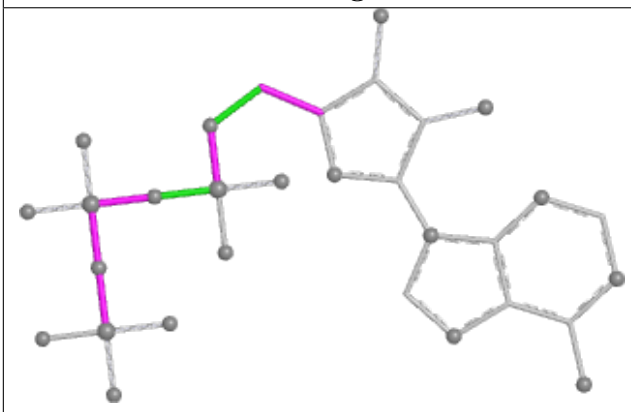
Ligand ANP C 704



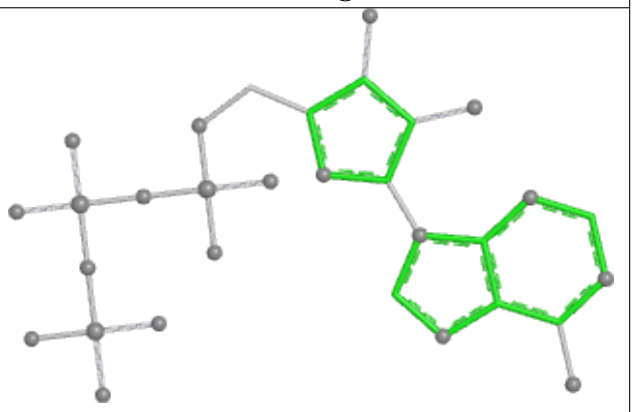
Bond lengths



Bond angles

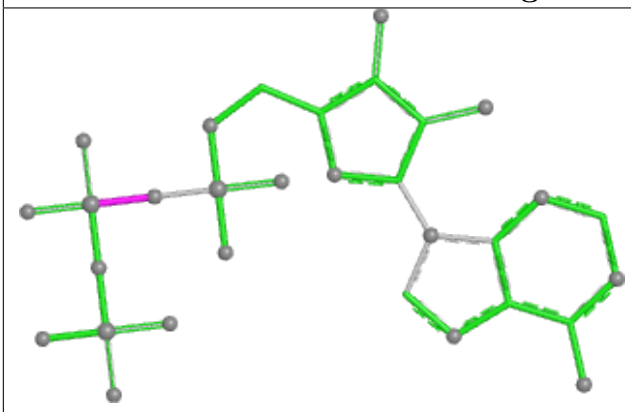


Torsions

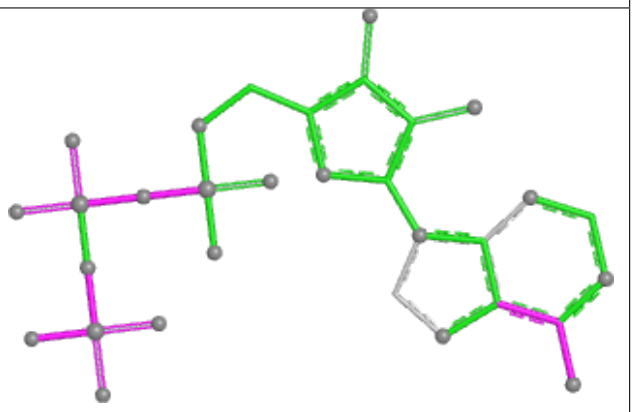


Rings

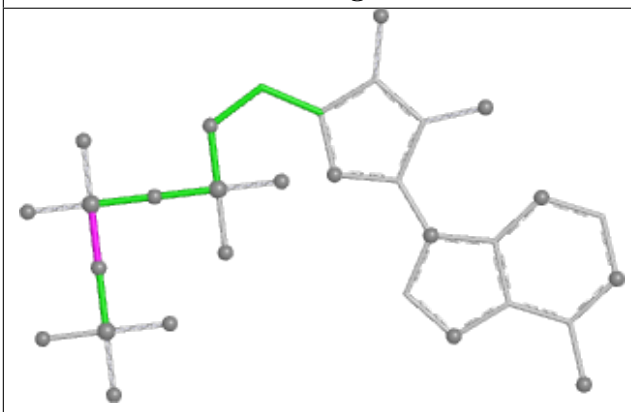
Ligand ANP A 701



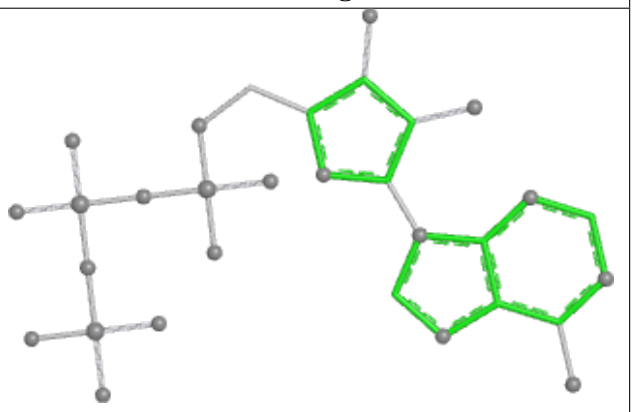
Bond lengths



Bond angles

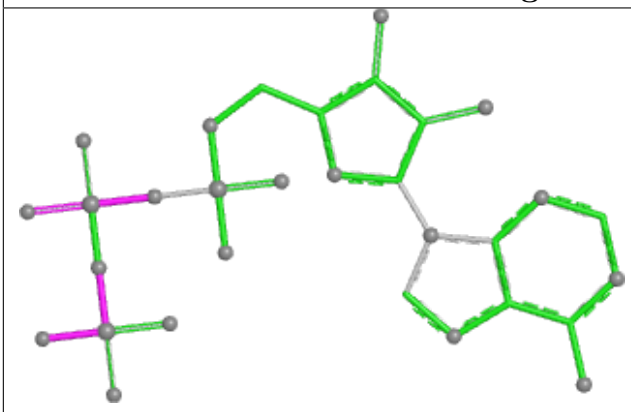


Torsions

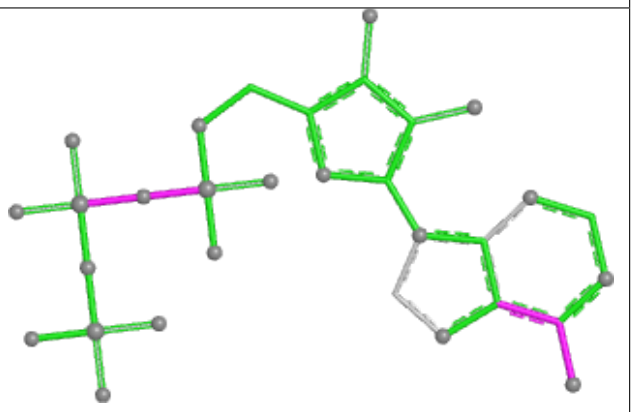


Rings

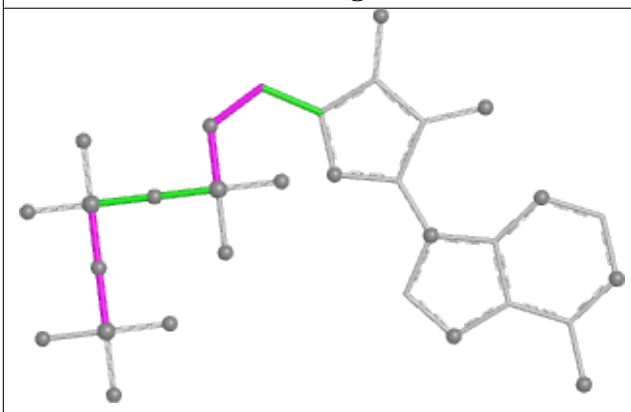
Ligand ANP D 704



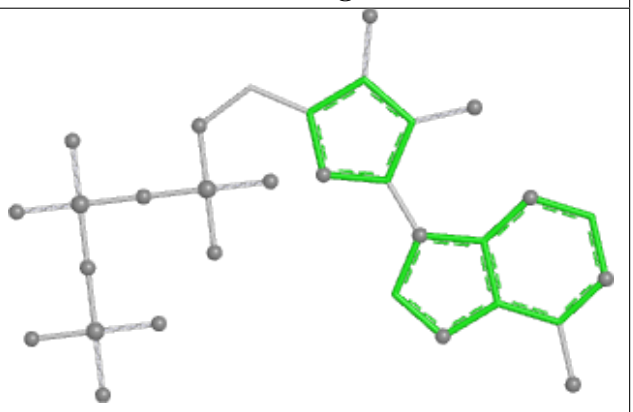
Bond lengths



Bond angles

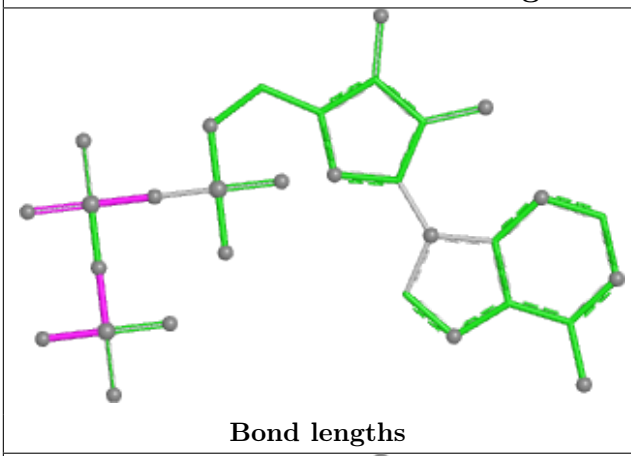


Torsions

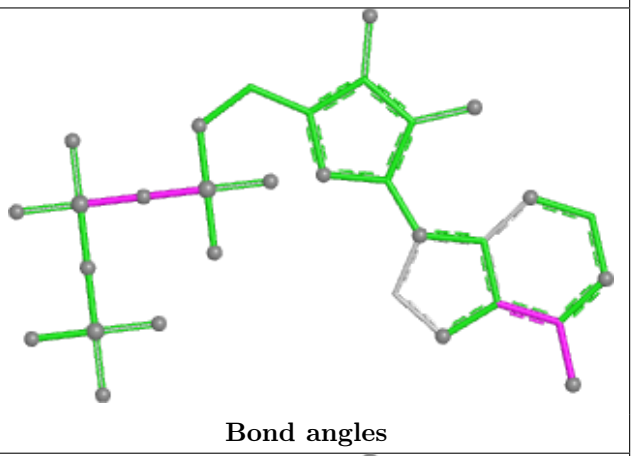


Rings

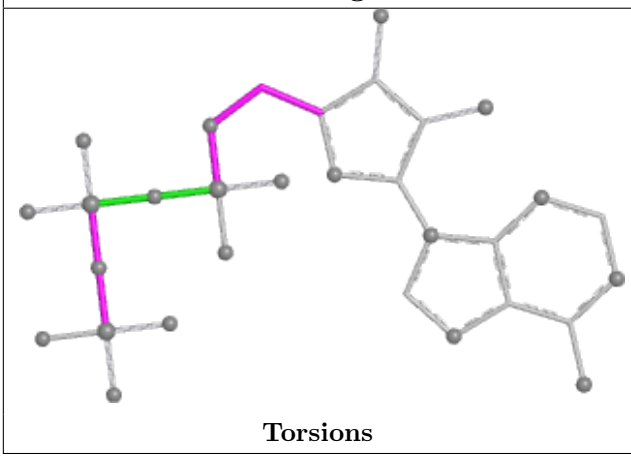
Ligand ANP B 701



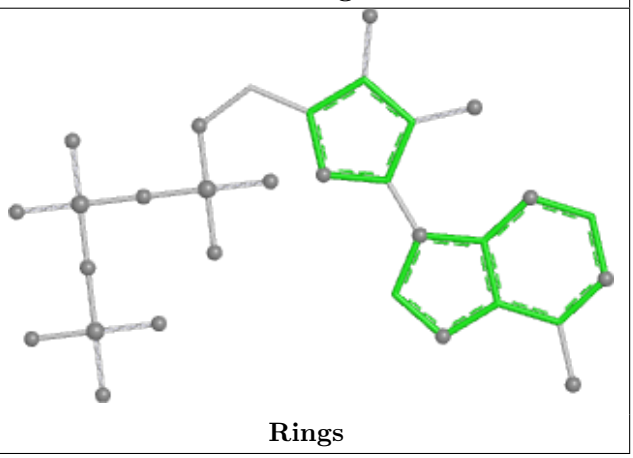
Bond lengths



Bond angles



Torsions



Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	588/603 (97%)	0.23	21 (3%) 42 18	25, 53, 87, 118	0
1	B	590/603 (97%)	0.14	8 (1%) 75 49	24, 51, 77, 116	0
1	C	585/603 (97%)	0.55	37 (6%) 20 6	46, 78, 101, 114	0
1	D	585/603 (97%)	0.24	13 (2%) 62 33	32, 59, 96, 115	0
All	All	2348/2412 (97%)	0.29	79 (3%) 45 19	24, 61, 95, 118	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	ALA	6.5
1	A	250	THR	5.9
1	C	203	GLY	5.5
1	A	251	GLY	4.7
1	A	95	ASN	4.7
1	A	96	THR	4.2
1	D	340	VAL	4.0
1	A	92	LEU	3.9
1	C	335	PRO	3.9
1	A	93	TYR	3.7
1	C	247	VAL	3.7
1	C	484	VAL	3.6
1	A	252	LEU	3.5
1	C	506	TRP	3.5
1	C	166	SER	3.4
1	D	341	GLU	3.3
1	C	472	PHE	3.3
1	C	574	CYS	3.2
1	C	158	LEU	3.2
1	C	485	SER	3.2
1	A	193	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	485	SER	3.1
1	B	352	LEU	3.1
1	C	252	LEU	3.1
1	C	521	VAL	3.0
1	A	10	SER	3.0
1	C	501	THR	3.0
1	C	162	GLU	3.0
1	C	509	ALA	2.9
1	C	545	ILE	2.9
1	D	175	PRO	2.9
1	D	214	THR	2.8
1	A	68	MET	2.8
1	B	252	LEU	2.8
1	C	568	ALA	2.8
1	C	340	VAL	2.8
1	B	216	THR	2.8
1	C	86	ASN	2.8
1	D	209	VAL	2.7
1	A	98	VAL	2.7
1	B	351	THR	2.7
1	A	81	PHE	2.6
1	C	474	MET	2.6
1	C	370	ILE	2.6
1	C	176	LEU	2.6
1	C	101	ASP	2.5
1	D	179	ASN	2.5
1	C	95	ASN	2.5
1	A	577	SER	2.5
1	C	470	GLN	2.4
1	B	203	GLY	2.4
1	C	304	ILE	2.4
1	D	80	SER	2.3
1	D	97	CYS	2.3
1	B	568	ALA	2.3
1	C	165	LEU	2.3
1	B	593	PRO	2.3
1	A	80	SER	2.3
1	A	163	LEU	2.3
1	D	157	VAL	2.3
1	A	485	SER	2.2
1	C	494	GLY	2.2
1	C	6	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	342	CYS	2.2
1	D	165	LEU	2.2
1	C	239	THR	2.2
1	C	351	THR	2.2
1	C	133	PHE	2.2
1	A	99	GLY	2.2
1	C	195	ILE	2.1
1	A	550	THR	2.1
1	A	86	ASN	2.1
1	C	343	PHE	2.1
1	C	208	ALA	2.0
1	D	345	LYS	2.0
1	C	179	ASN	2.0
1	C	342	CYS	2.0
1	A	170	GLY	2.0
1	A	165	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	702	1/1	0.76	0.11	77,77,77,77	0
2	ANP	C	704	31/31	0.77	0.33	83,101,112,125	0
3	ZN	A	704	1/1	0.80	0.14	74,74,74,74	0
2	ANP	B	701	31/31	0.84	0.24	70,84,94,101	0
2	ANP	D	704	31/31	0.85	0.25	54,84,99,102	0
3	ZN	C	703	1/1	0.87	0.09	73,73,73,73	0
4	MG	A	705	1/1	0.87	0.14	39,39,39,39	0

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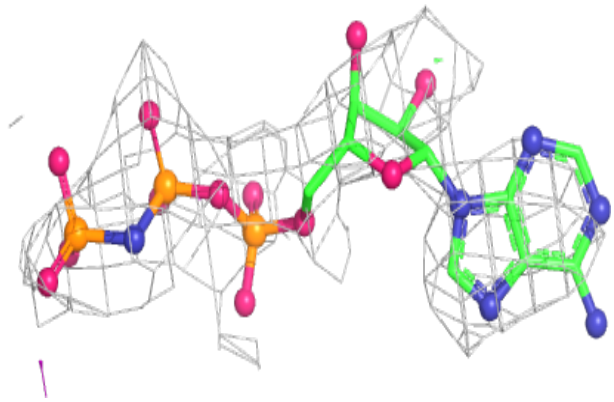
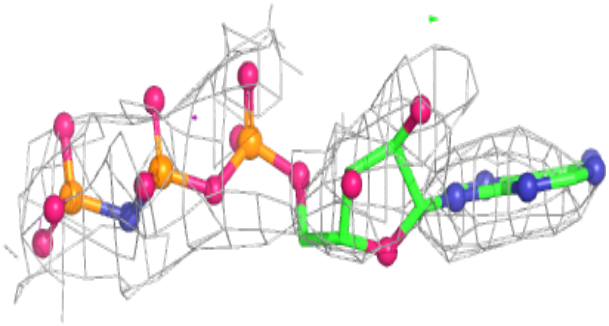
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	703	1/1	0.90	0.10	66,66,66,66	0
3	ZN	B	703	1/1	0.92	0.12	39,39,39,39	0
3	ZN	B	704	1/1	0.92	0.15	37,37,37,37	0
2	ANP	A	701	31/31	0.93	0.18	34,44,56,61	0
3	ZN	C	702	1/1	0.93	0.09	95,95,95,95	0
3	ZN	D	701	1/1	0.94	0.12	60,60,60,60	0
3	ZN	A	703	1/1	0.95	0.08	61,61,61,61	0
3	ZN	A	702	1/1	0.96	0.07	58,58,58,58	0
3	ZN	C	701	1/1	0.96	0.08	76,76,76,76	0
3	ZN	B	702	1/1	0.97	0.14	39,39,39,39	0

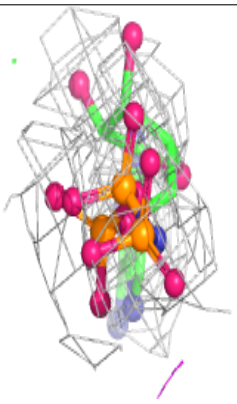
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP C 704:

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

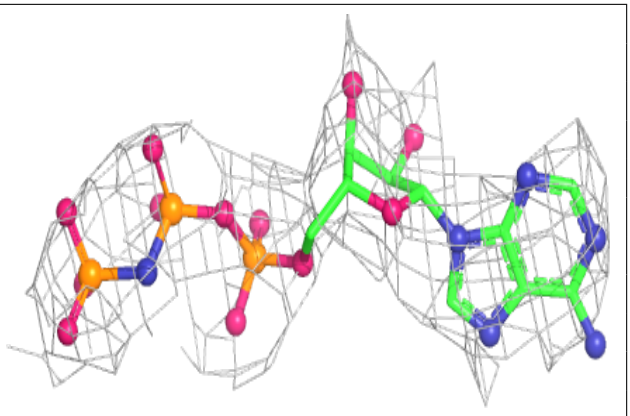


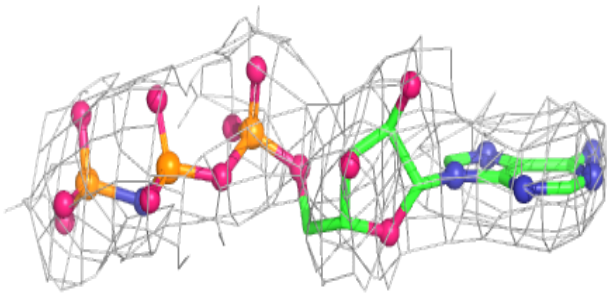


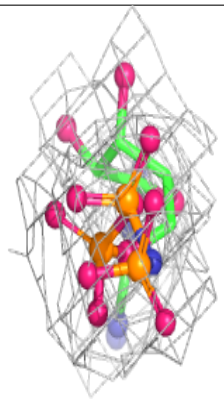


Electron density around ANP B 701:

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

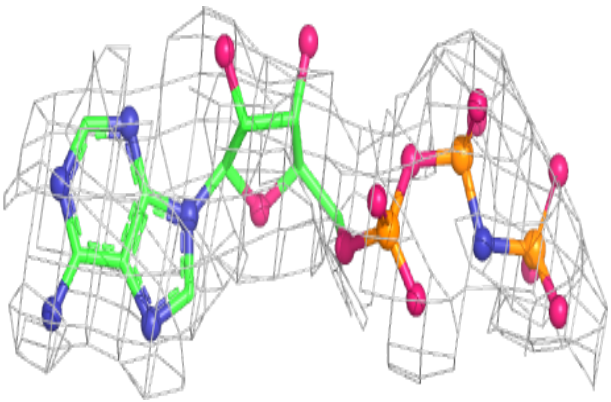


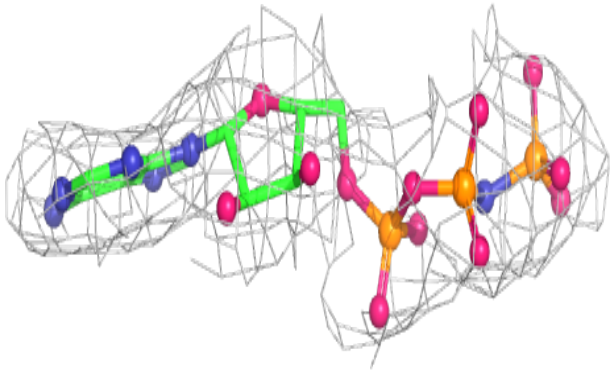


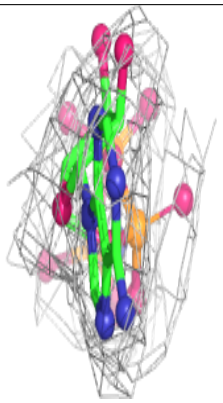


Electron density around ANP D 704:

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

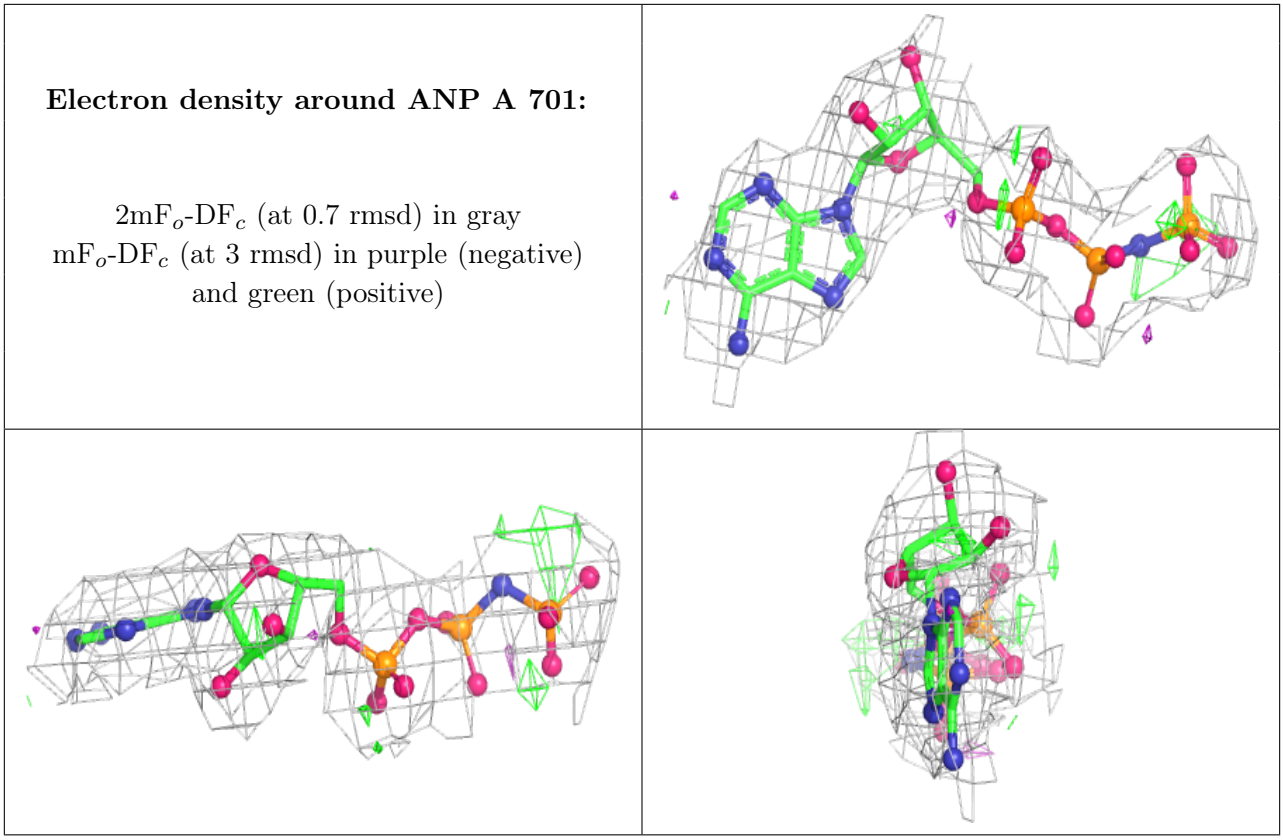






Electron density around ANP A 701:

$2mF_o$-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.