Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 02:13 PM EDT

PDB ID	:	4RIX
Title	:	Crystal structure of an EGFR/HER3 kinase domain heterodimer containing the cancer-associated HER3-Q790R mutation
Authors	:	Littlefield, P.; Liu, L.; Jura, N.
Deposited on	:	2014-10-07
Resolution	:	3.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

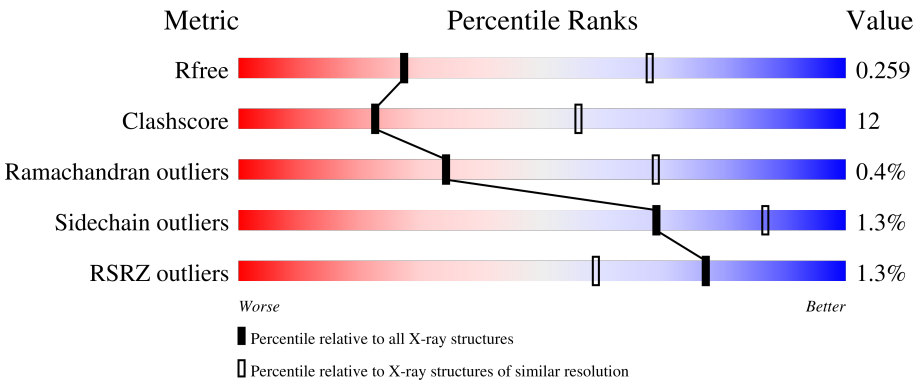
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	326	% 60% 21% • 17%
1	C	326	% 63% 21% • 16%
2	B	345	2% 62% 22% • 15%
2	D	345	64% 21% • 14%

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
4	MG	B	1002	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9147 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	2132	1378	371	370	13	0	0	0
1	C	275	2183	1413	375	382	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	676	GLY	-	expression tag	UNP P21860
A	677	ALA	-	expression tag	UNP P21860
A	678	GLY	-	expression tag	UNP P21860
A	790	ARG	GLN	engineered mutation	UNP P21860
C	676	GLY	-	expression tag	UNP P21860
C	677	ALA	-	expression tag	UNP P21860
C	678	GLY	-	expression tag	UNP P21860
C	790	ARG	GLN	engineered mutation	UNP P21860

- Molecule 2 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	293	2343	1510	397	421	15	0	0	0
2	D	297	2369	1525	402	427	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	654	GLY	-	expression tag	UNP P00533
B	655	ALA	-	expression tag	UNP P00533
B	656	MET	-	expression tag	UNP P00533
B	657	GLY	-	expression tag	UNP P00533

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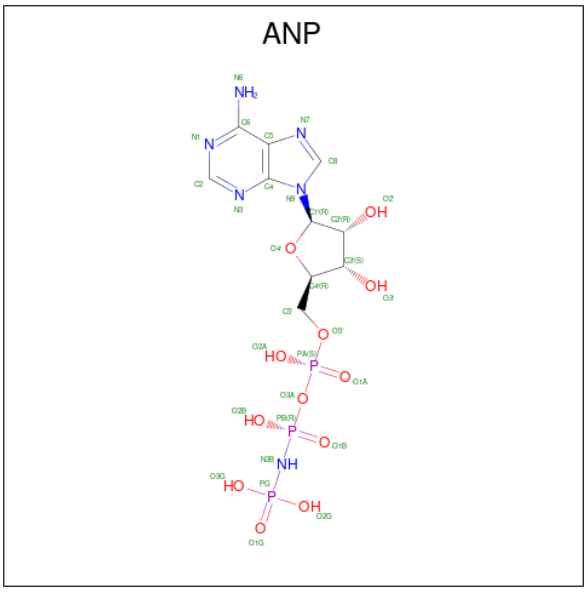
Chain	Residue	Modelled	Actual	Comment	Reference
B	924	ARG	VAL	engineered mutation	UNP P00533
B	973	ALA	PHE	engineered mutation	UNP P00533
B	977	ALA	LEU	engineered mutation	UNP P00533
D	654	GLY	-	expression tag	UNP P00533
D	655	ALA	-	expression tag	UNP P00533
D	656	MET	-	expression tag	UNP P00533
D	657	GLY	-	expression tag	UNP P00533
D	924	ARG	VAL	engineered mutation	UNP P00533
D	973	ALA	PHE	engineered mutation	UNP P00533
D	977	ALA	LEU	engineered mutation	UNP P00533

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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

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

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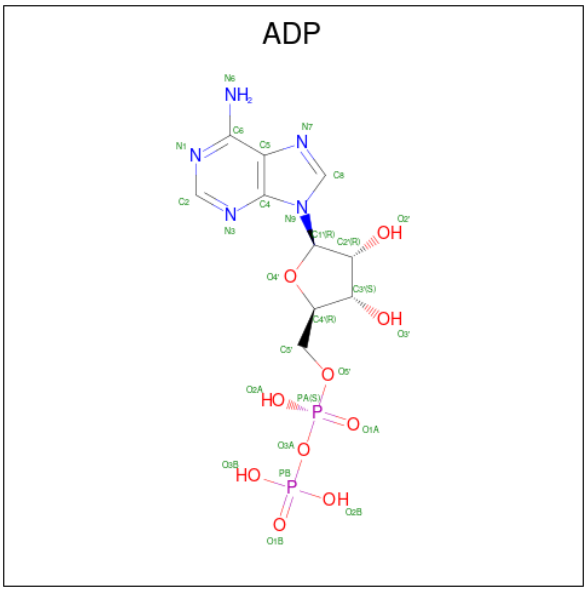
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	1	1	0	0
			Total	Mg		
4	C	1	1	1	0	0
			Total	Mg		
4	D	1	1	1	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

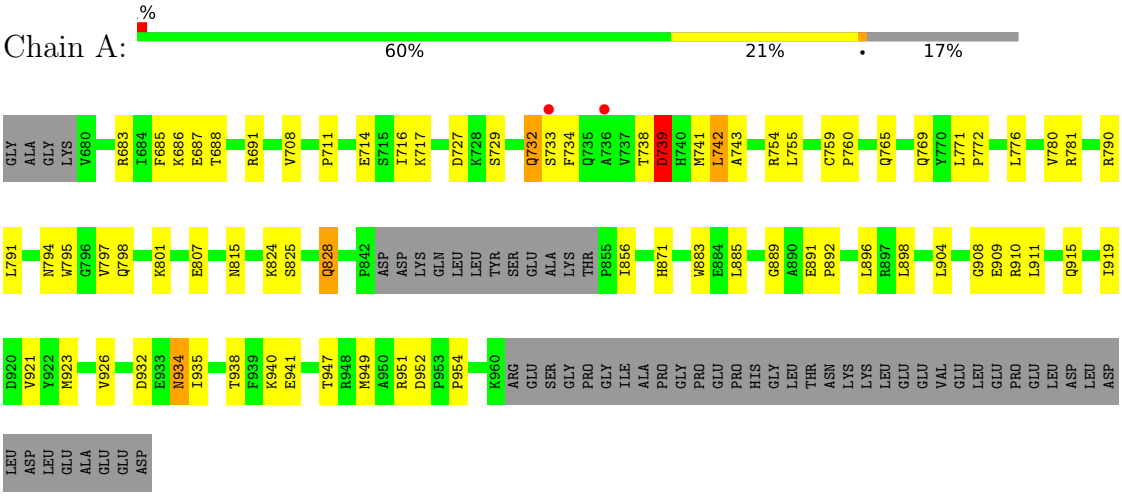


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
5	D	1	27	10	5	10	2	0	0

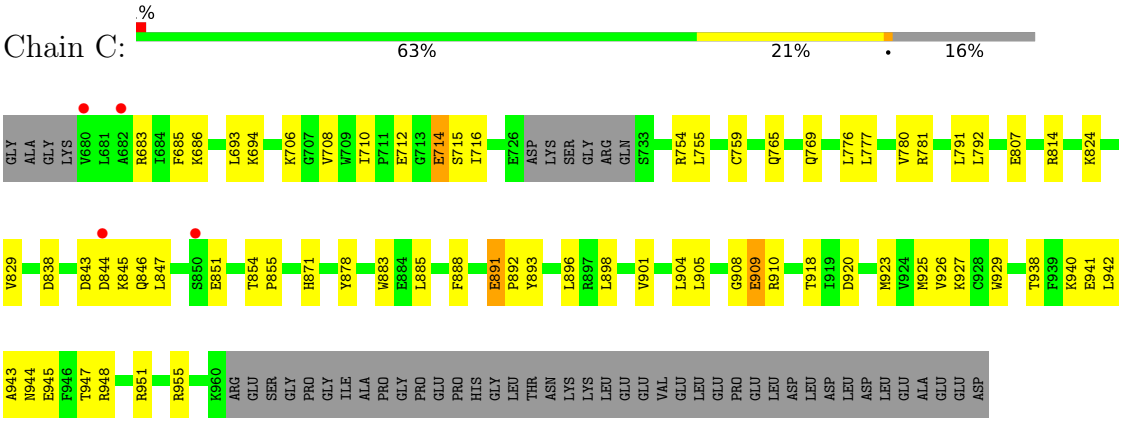
3 Residue-property plots (i)

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.

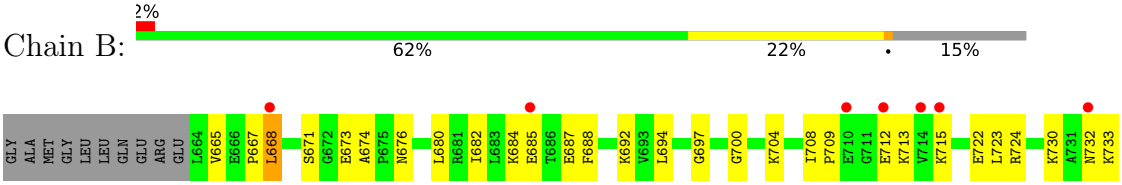
• Molecule 1: Receptor tyrosine-protein kinase erbB-3

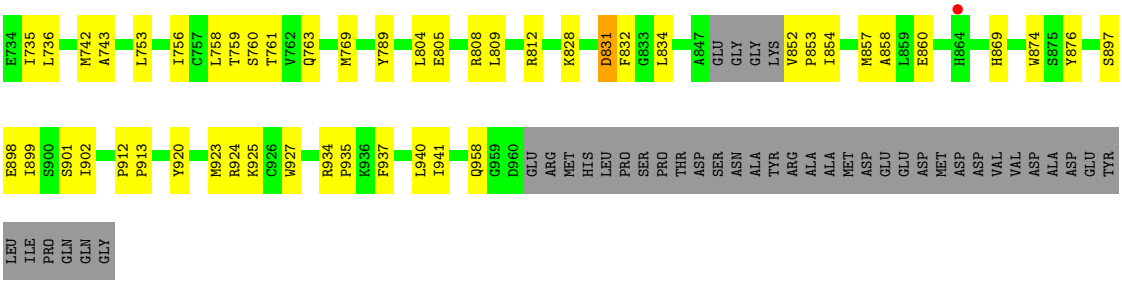


• Molecule 1: Receptor tyrosine-protein kinase erbB-3



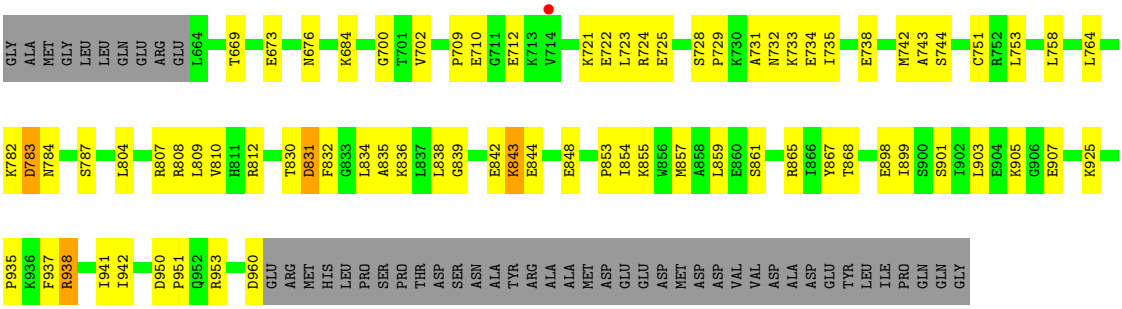
• Molecule 2: Epidermal growth factor receptor





- Molecule 2: Epidermal growth factor receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.65Å 155.05Å 86.86Å 90.00° 111.09° 90.00°	Depositor
Resolution (Å)	59.77 – 3.10 59.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (59.77-3.10) 88.4 (59.77-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.207 , 0.258 0.211 , 0.259	Depositor DCC
R_{free} test set	1390 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9147	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	0/2183	0.62	4/2958 (0.1%)
1	C	0.26	0/2235	0.53	1/3031 (0.0%)
2	B	0.30	0/2395	0.59	1/3243 (0.0%)
2	D	0.31	0/2422	0.59	1/3279 (0.0%)
All	All	0.30	0/9235	0.58	7/12511 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	739	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	A	742	LEU	CB-CG-CD2	6.90	122.72	111.00
1	A	739	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	934	ASN	N-CA-CB	-5.24	101.17	110.60
1	C	714	GLU	N-CA-C	5.23	125.13	111.00
2	D	733	LYS	CA-CB-CG	5.12	124.67	113.40
2	B	668	LEU	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	739	ASP	Peptide
1	A	934	ASN	Sidechain
2	B	667	PRO	Peptide

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	2132	0	2185	61	0
1	C	2183	0	2234	51	0
2	B	2343	0	2402	57	0
2	D	2369	0	2428	62	0
3	A	31	0	13	1	0
3	C	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	27	0	12	0	0
5	D	27	0	12	1	0
All	All	9147	0	9299	214	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 12.

All (214) 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)
2:D:684:LYS:NZ	2:D:710:GLU:OE2	1.61	1.33
1:A:732:GLN:HA	1:A:732:GLN:HE21	1.20	1.00
1:A:739:ASP:OD1	1:A:743:ALA:N	2.03	0.92
1:C:686:LYS:NZ	1:C:712:GLU:OE2	2.06	0.88
1:C:754:ARG:NH1	1:C:755:LEU:O	2.05	0.87
1:A:739:ASP:CG	1:A:742:LEU:HB2	1.97	0.85
1:A:708:VAL:HG21	1:A:717:LYS:HB3	1.59	0.83
1:C:769:GLN:OE1	1:C:824:LYS:NZ	2.12	0.83
1:C:945:GLU:HG3	1:C:948:ARG:NH1	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:721:LYS:NZ	2:D:738:GLU:OE2	2.13	0.81
2:B:713:LYS:NZ	2:B:715:LYS:HE3	1.96	0.80
1:A:754:ARG:NH1	1:A:755:LEU:O	2.15	0.80
1:C:814:ARG:NH1	1:C:838:ASP:OD1	2.16	0.79
1:A:769:GLN:OE1	1:A:824:LYS:NZ	2.15	0.79
2:D:723:LEU:HD11	2:D:731:ALA:HB1	1.65	0.78
2:D:728:SER:O	2:D:732:ASN:ND2	2.17	0.78
2:B:730:LYS:HA	2:B:733:LYS:HB3	1.66	0.78
1:C:940:LYS:O	1:C:944:ASN:ND2	2.15	0.78
2:D:722:GLU:HG2	2:D:724:ARG:HH22	1.49	0.77
2:B:854:ILE:HG22	2:B:899:ILE:HD11	1.67	0.76
1:A:739:ASP:OD1	1:A:742:LEU:HB2	1.84	0.76
2:B:713:LYS:HZ1	2:B:715:LYS:HE3	1.47	0.76
2:D:787:SER:HB2	2:D:951:PRO:HB2	1.66	0.76
2:B:692:LYS:HE3	2:B:704:LYS:HD3	1.69	0.75
2:D:925:LYS:HG2	2:D:935:PRO:HD3	1.69	0.75
2:B:697:GLY:O	2:B:724:ARG:NH1	2.19	0.75
2:B:759:THR:HG22	2:B:760:SER:H	1.50	0.74
2:B:925:LYS:HG2	2:B:935:PRO:HD3	1.71	0.73
1:A:732:GLN:HE21	1:A:732:GLN:CA	1.98	0.72
2:B:709:PRO:HB2	2:B:712:GLU:HB2	1.71	0.71
2:D:722:GLU:OE1	2:D:724:ARG:NH1	2.23	0.70
1:A:686:LYS:HD2	1:A:687:GLU:H	1.56	0.70
1:A:732:GLN:HA	1:A:732:GLN:NE2	2.02	0.69
1:C:714:GLU:O	1:C:716:ILE:N	2.25	0.69
2:D:804:LEU:HD22	2:D:809:LEU:HD23	1.73	0.69
1:A:754:ARG:HH11	1:A:754:ARG:HG3	1.58	0.68
2:B:700:GLY:HA2	2:B:724:ARG:HB2	1.77	0.67
2:B:722:GLU:HG3	2:B:761:THR:HG21	1.77	0.66
2:B:854:ILE:HA	2:B:857:MET:HE2	1.76	0.66
1:C:776:LEU:HD21	1:C:885:LEU:HD13	1.78	0.65
2:B:708:ILE:HG22	2:B:715:LYS:HG2	1.79	0.65
2:B:732:ASN:HA	2:B:735:ILE:HG12	1.78	0.65
2:B:808:ARG:HH12	2:D:942:ILE:HD13	1.61	0.65
2:D:700:GLY:HA2	2:D:724:ARG:CG	2.27	0.65
2:D:744:SER:HB3	2:D:807:ARG:HH22	1.62	0.64
2:B:723:LEU:HD13	2:B:735:ILE:HD11	1.81	0.63
1:A:908:GLY:HA2	2:B:758:LEU:O	1.98	0.63
1:C:951:ARG:HB3	2:D:669:THR:HG22	1.80	0.63
1:A:711:PRO:HG2	1:A:714:GLU:HB2	1.80	0.63
1:C:893:TYR:HB3	1:C:896:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:898:GLU:O	2:D:901:SER:OG	2.18	0.61
1:C:943:ALA:O	1:C:947:THR:HG23	2.00	0.61
1:A:926:VAL:HG13	2:B:758:LEU:HD11	1.83	0.61
2:D:843:LYS:HB2	2:D:844:GLU:OE1	2.00	0.60
2:B:804:LEU:HD22	2:B:809:LEU:HD11	1.82	0.60
2:D:700:GLY:HA2	2:D:724:ARG:HG2	1.83	0.60
1:A:733:SER:OG	1:A:734:PHE:N	2.35	0.59
2:B:812:ARG:NH1	2:B:834:LEU:HB3	2.16	0.59
1:C:926:VAL:HG13	2:D:758:LEU:HD11	1.84	0.59
1:A:688:THR:O	1:A:691:ARG:NH1	2.36	0.59
1:A:932:ASP:HB3	1:A:935:ILE:HD12	1.85	0.59
1:C:777:LEU:HD11	1:C:781:ARG:HH21	1.67	0.59
1:C:951:ARG:HG2	1:C:951:ARG:HH11	1.67	0.59
1:A:923:MET:HE1	2:B:736:LEU:HB3	1.85	0.59
2:D:830:THR:OG1	2:D:831:ASP:N	2.33	0.58
2:D:808:ARG:NE	2:D:838:LEU:O	2.35	0.58
1:C:851:GLU:HG2	1:C:898:LEU:HD13	1.86	0.57
2:D:812:ARG:NH1	2:D:834:LEU:O	2.35	0.57
1:C:923:MET:O	1:C:927:LYS:HG3	2.05	0.57
2:D:844:GLU:HG3	2:D:868:THR:HG22	1.86	0.57
1:A:738:THR:O	1:A:741:MET:HB2	2.04	0.57
2:B:898:GLU:O	2:B:901:SER:OG	2.19	0.57
1:A:807:GLU:OE2	1:A:871:HIS:HB3	2.04	0.57
1:A:729:SER:HB3	1:A:733:SER:HB3	1.86	0.56
2:B:899:ILE:O	2:B:902:ILE:HG12	2.06	0.56
1:C:694:LYS:HE2	1:C:706:LYS:HD3	1.87	0.56
1:A:780:VAL:HG11	1:A:885:LEU:HD12	1.87	0.56
2:D:855:LYS:HG2	2:D:899:ILE:HD12	1.87	0.56
2:D:810:VAL:HG12	2:D:812:ARG:HG3	1.86	0.55
1:A:915:GLN:CD	1:A:915:GLN:H	2.09	0.55
1:C:843:ASP:OD2	1:C:846:GLN:NE2	2.39	0.55
1:A:951:ARG:HH11	1:A:951:ARG:HG2	1.72	0.55
2:B:769:MET:HE3	2:B:828:LYS:HD2	1.88	0.55
2:B:722:GLU:HB2	2:B:763:GLN:HG2	1.88	0.55
2:D:724:ARG:HD3	2:D:725:GLU:HG3	1.90	0.54
1:A:825:SER:HB3	1:A:828:GLN:HB2	1.90	0.54
2:D:731:ALA:O	2:D:735:ILE:HG12	2.08	0.54
1:A:904:LEU:HD11	1:A:909:GLU:HB3	1.91	0.53
1:C:909:GLU:CG	2:D:684:LYS:HG2	2.38	0.53
2:D:844:GLU:HG3	2:D:868:THR:CG2	2.38	0.53
1:A:807:GLU:HG3	1:A:871:HIS:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:807:GLU:HA	1:C:871:HIS:CE1	2.44	0.52
1:C:918:THR:HG23	1:C:920:ASP:H	1.75	0.52
1:A:921:VAL:HG22	1:A:949:MET:SD	2.50	0.52
2:B:694:LEU:HD11	2:B:704:LYS:HB2	1.91	0.52
1:C:955:ARG:NH1	2:D:673:GLU:HG2	2.25	0.52
2:D:812:ARG:NH1	2:D:834:LEU:HB3	2.26	0.51
1:A:947:THR:O	1:A:951:ARG:HG3	2.11	0.50
2:D:724:ARG:HA	2:D:725:GLU:HG3	1.92	0.50
2:B:673:GLU:OE2	2:B:674:ALA:N	2.43	0.50
2:B:920:TYR:HA	2:B:923:MET:HG2	1.93	0.50
1:A:776:LEU:HD11	1:A:795:TRP:CE3	2.46	0.50
1:A:919:ILE:HG22	2:B:676:ASN:HB3	1.94	0.50
2:D:950:ASP:OD2	2:D:953:ARG:NE	2.43	0.49
1:C:776:LEU:HD12	1:C:829:VAL:HG11	1.94	0.49
1:C:909:GLU:HG3	2:D:684:LYS:HG2	1.94	0.49
2:D:702:VAL:HG11	5:D:1001:ADP:C8	2.47	0.49
1:A:754:ARG:NH1	1:A:754:ARG:HG3	2.27	0.49
2:D:723:LEU:O	2:D:725:GLU:HA	2.12	0.49
1:C:847:LEU:HD22	1:C:855:PRO:HG2	1.95	0.49
1:A:798:GLN:HA	1:A:801:LYS:HE2	1.95	0.49
2:B:673:GLU:CD	2:B:674:ALA:H	2.16	0.48
2:B:730:LYS:CA	2:B:733:LYS:HB3	2.40	0.48
2:D:743:ALA:HB2	2:D:753:LEU:HD23	1.95	0.48
2:D:808:ARG:HH11	2:D:839:GLY:HA2	1.77	0.48
1:A:938:THR:OG1	1:A:940:LYS:HG3	2.14	0.48
2:B:897:SER:HB2	2:B:898:GLU:OE2	2.14	0.48
1:A:797:VAL:O	1:A:801:LYS:HG2	2.14	0.48
1:C:759:CYS:HB3	1:C:765:GLN:HB2	1.96	0.48
2:B:958:GLN:OE1	2:B:958:GLN:HA	2.14	0.47
1:C:710:ILE:HG23	1:C:716:ILE:O	2.14	0.47
1:A:896:LEU:HD21	1:A:904:LEU:HD22	1.97	0.47
1:C:854:THR:HG21	1:C:898:LEU:HD11	1.96	0.47
1:A:938:THR:OG1	1:A:941:GLU:HG3	2.15	0.47
2:B:713:LYS:HZ1	2:B:715:LYS:CE	2.22	0.47
2:D:722:GLU:CG	2:D:724:ARG:HH22	2.23	0.47
2:D:721:LYS:HD3	2:D:764:LEU:HD12	1.97	0.47
2:D:839:GLY:N	2:D:842:GLU:OE1	2.32	0.47
2:B:805:GLU:HG3	2:B:869:HIS:CG	2.50	0.46
1:A:727:ASP:OD2	1:A:733:SER:OG	2.34	0.46
1:C:844:ASP:O	1:C:847:LEU:HB2	2.15	0.46
2:D:835:ALA:O	2:D:836:LYS:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:918:THR:HG23	1:C:920:ASP:N	2.30	0.46
1:A:739:ASP:OD1	1:A:739:ASP:O	2.34	0.46
1:C:908:GLY:HA2	2:D:758:LEU:O	2.15	0.46
2:D:855:LYS:HG2	2:D:899:ILE:CD1	2.45	0.46
1:A:683:ARG:HE	1:A:685:PHE:HE1	1.64	0.46
1:C:780:VAL:HG11	1:C:885:LEU:HD12	1.97	0.46
2:B:684:LYS:HG3	2:B:687:GLU:HG3	1.97	0.46
2:B:743:ALA:HB2	2:B:753:LEU:HD23	1.98	0.46
2:D:723:LEU:HD13	2:D:735:ILE:CG1	2.47	0.46
1:A:904:LEU:CD1	1:A:909:GLU:HB3	2.46	0.45
1:C:683:ARG:HE	1:C:685:PHE:HE1	1.63	0.45
2:D:854:ILE:HD12	2:D:854:ILE:H	1.81	0.45
1:C:878:TYR:CD2	1:C:942:LEU:HD13	2.51	0.45
1:C:918:THR:OG1	2:D:676:ASN:O	2.27	0.45
2:B:937:PHE:O	2:B:941:ILE:HG13	2.16	0.45
2:D:937:PHE:O	2:D:941:ILE:HG13	2.16	0.45
1:A:781:ARG:HG3	1:A:889:GLY:HA3	1.99	0.45
1:A:729:SER:CB	1:A:733:SER:HB3	2.46	0.45
1:A:815:ASN:ND2	3:A:1101:ANP:O3G	2.50	0.45
2:B:742:MET:HG2	2:B:832:PHE:CD2	2.52	0.45
1:A:791:LEU:HD23	1:A:791:LEU:HA	1.86	0.44
1:C:951:ARG:HG2	1:C:951:ARG:NH1	2.31	0.44
2:D:853:PRO:O	2:D:857:MET:HG3	2.16	0.44
1:C:938:THR:OG1	1:C:941:GLU:HG3	2.17	0.44
2:B:722:GLU:HG3	2:B:761:THR:CG2	2.44	0.44
2:B:831:ASP:HB3	2:B:832:PHE:H	1.55	0.44
1:A:952:ASP:OD1	1:A:954:PRO:HD2	2.18	0.44
2:D:859:LEU:HD13	2:D:903:LEU:HB2	2.00	0.44
2:B:668:LEU:HD23	2:D:953:ARG:NH2	2.34	0.43
1:C:791:LEU:HD23	1:C:791:LEU:HA	1.85	0.43
1:C:845:LYS:HD2	1:C:845:LYS:N	2.32	0.43
2:D:787:SER:CB	2:D:951:PRO:HB2	2.43	0.43
2:D:861:SER:O	2:D:865:ARG:HA	2.19	0.43
2:D:938:ARG:H	2:D:938:ARG:HG3	1.57	0.43
1:A:919:ILE:CD1	2:B:680:LEU:HB2	2.48	0.43
1:A:759:CYS:HB3	1:A:765:GLN:HB2	2.00	0.43
1:A:856:ILE:HG21	1:A:898:LEU:HG	2.00	0.43
2:B:753:LEU:HD21	2:B:756:ILE:HG23	2.00	0.43
1:A:790:ARG:O	1:A:794:ASN:ND2	2.22	0.43
2:B:685:GLU:HA	2:B:688:PHE:CE1	2.54	0.43
1:C:883:TRP:HD1	1:C:925:MET:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:920:TYR:HA	2:B:923:MET:CG	2.49	0.43
2:D:684:LYS:H	2:D:684:LYS:HG3	1.63	0.43
1:A:794:ASN:O	1:A:798:GLN:HG3	2.18	0.42
1:A:910:ARG:HB2	2:B:682:ILE:HD12	2.00	0.42
1:A:951:ARG:HG2	1:A:951:ARG:NH1	2.32	0.42
2:B:858:ALA:HA	2:B:874:TRP:CD2	2.54	0.42
1:C:901:VAL:O	1:C:905:LEU:HG	2.18	0.42
1:C:904:LEU:HD23	1:C:904:LEU:HA	1.84	0.42
1:C:910:ARG:NH2	1:C:929:TRP:O	2.52	0.42
2:D:905:LYS:NZ	2:D:907:GLU:OE1	2.45	0.42
1:A:727:ASP:OD1	1:A:727:ASP:C	2.57	0.42
1:A:807:GLU:OE2	1:A:871:HIS:CB	2.67	0.42
1:C:693:LEU:HD11	1:C:708:VAL:HG13	2.01	0.42
1:A:952:ASP:OD2	2:B:671:SER:N	2.45	0.42
2:D:709:PRO:HB2	2:D:712:GLU:HB2	2.01	0.41
1:C:955:ARG:HH12	2:D:673:GLU:HG2	1.85	0.41
2:B:860:GLU:CD	2:B:934:ARG:HH12	2.23	0.41
1:C:807:GLU:HG3	1:C:871:HIS:CG	2.55	0.41
2:D:728:SER:HA	2:D:729:PRO:HD3	1.92	0.41
2:D:812:ARG:HG2	2:D:867:TYR:CD1	2.54	0.41
1:A:754:ARG:NH1	1:A:755:LEU:C	2.74	0.41
2:D:742:MET:HG2	2:D:832:PHE:CD2	2.56	0.41
1:A:883:TRP:CD2	1:A:911:LEU:HD13	2.55	0.41
2:B:708:ILE:CG2	2:B:715:LYS:HG2	2.48	0.41
2:B:713:LYS:HZ3	2:B:715:LYS:HE3	1.81	0.41
2:B:852:VAL:HA	2:B:853:PRO:HD3	1.94	0.41
2:B:876:TYR:CE2	2:B:940:LEU:HD13	2.55	0.41
2:D:751:CYS:SG	2:D:830:THR:HB	2.60	0.41
1:C:792:LEU:HD11	1:C:888:PHE:HE1	1.85	0.41
1:A:771:LEU:HA	1:A:772:PRO:HD3	1.78	0.41
2:B:854:ILE:HD13	2:B:857:MET:HE1	2.03	0.41
1:C:923:MET:HG3	1:C:927:LYS:HE3	2.02	0.41
2:D:831:ASP:HB3	2:D:832:PHE:H	1.68	0.41
1:C:891:GLU:HA	1:C:892:PRO:HD3	1.78	0.41
2:D:848:GLU:O	2:D:865:ARG:NH1	2.54	0.41
1:A:891:GLU:HA	1:A:892:PRO:HD3	1.97	0.40
2:B:924:ARG:HA	2:B:927:TRP:CE3	2.57	0.40
1:C:754:ARG:HH11	1:C:754:ARG:HG2	1.86	0.40
1:A:759:CYS:HA	1:A:760:PRO:HD3	1.87	0.40
2:B:912:PRO:HA	2:B:913:PRO:HD3	1.89	0.40
1:C:947:THR:O	1:C:951:ARG:HG3	2.21	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	A	265/326 (81%)	259 (98%)	6 (2%)	0	100	100
1	C	271/326 (83%)	264 (97%)	6 (2%)	1 (0%)	34	69
2	B	289/345 (84%)	279 (96%)	9 (3%)	1 (0%)	41	73
2	D	295/345 (86%)	285 (97%)	7 (2%)	3 (1%)	15	49
All	All	1120/1342 (84%)	1087 (97%)	28 (2%)	5 (0%)	34	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	715	SER
2	D	783	ASP
2	D	784	ASN
2	B	831	ASP
2	D	831	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/278 (83%)	228 (99%)	3 (1%)	69	87
1	C	237/278 (85%)	235 (99%)	2 (1%)	81	92
2	B	258/300 (86%)	256 (99%)	2 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	260/300 (87%)	254 (98%)	6 (2%)	50 77
All	All	986/1156 (85%)	973 (99%)	13 (1%)	69 87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	716	ILE
1	A	732	GLN
1	A	828	GLN
2	B	665	VAL
2	B	789	TYR
1	C	891	GLU
1	C	909	GLU
2	D	734	GLU
2	D	782	LYS
2	D	783	ASP
2	D	843	LYS
2	D	938	ARG
2	D	960	ASP

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

Mol	Chain	Res	Type
1	A	732	GLN
1	A	735	GLN
2	D	763	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	ANP	A	1101	4	29,33,33	1.12	4 (13%)	31,52,52	1.08	3 (9%)
5	ADP	B	1001	4	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
5	ADP	D	1001	4	24,29,29	0.97	1 (4%)	29,45,45	1.50	4 (13%)
3	ANP	C	1101	4	29,33,33	1.09	4 (13%)	31,52,52	1.06	3 (9%)

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	ANP	A	1101	4	-	5/14/38/38	0/3/3/3
5	ADP	B	1001	4	-	3/12/32/32	0/3/3/3
5	ADP	D	1001	4	-	1/12/32/32	0/3/3/3
3	ANP	C	1101	4	-	7/14/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ANP	PG-N3B	2.72	1.70	1.63
3	C	1101	ANP	PG-N3B	2.64	1.70	1.63
5	D	1001	ADP	C5-C4	2.58	1.47	1.40
5	B	1001	ADP	C5-C4	2.58	1.47	1.40
3	A	1101	ANP	PG-O1G	2.51	1.50	1.46
3	C	1101	ANP	PG-O1G	2.38	1.49	1.46
3	A	1101	ANP	PB-O1B	2.37	1.49	1.46
3	C	1101	ANP	PB-O1B	2.32	1.49	1.46
3	C	1101	ANP	PB-N3B	2.16	1.69	1.63
3	A	1101	ANP	PB-N3B	2.13	1.68	1.63

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1001	ADP	PA-O3A-PB	-3.63	120.38	132.83
5	D	1001	ADP	C3'-C2'-C1'	3.62	106.44	100.98
5	B	1001	ADP	C3'-C2'-C1'	3.59	106.39	100.98
5	D	1001	ADP	PA-O3A-PB	-3.31	121.46	132.83
5	D	1001	ADP	N3-C2-N1	-3.05	123.92	128.68
5	B	1001	ADP	N3-C2-N1	-2.93	124.10	128.68
3	A	1101	ANP	PB-O3A-PA	-2.78	122.83	132.62
5	D	1001	ADP	C4-C5-N7	-2.71	106.57	109.40
3	C	1101	ANP	O1B-PB-N3B	-2.70	107.79	111.77
5	B	1001	ADP	C4-C5-N7	-2.68	106.61	109.40
3	A	1101	ANP	O1B-PB-N3B	-2.41	108.22	111.77
3	C	1101	ANP	C5-C6-N6	2.35	123.92	120.35
3	A	1101	ANP	C5-C6-N6	2.15	123.63	120.35
3	C	1101	ANP	O2B-PB-O3A	2.05	111.47	104.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	ANP	PA-O3A-PB-O1B
3	A	1101	ANP	PA-O3A-PB-O2B
3	A	1101	ANP	O4'-C4'-C5'-O5'
3	C	1101	ANP	PG-N3B-PB-O3A
3	C	1101	ANP	PA-O3A-PB-O1B
3	C	1101	ANP	O4'-C4'-C5'-O5'
5	B	1001	ADP	C5'-O5'-PA-O1A
5	B	1001	ADP	C5'-O5'-PA-O2A
5	D	1001	ADP	C5'-O5'-PA-O1A
3	A	1101	ANP	C3'-C4'-C5'-O5'
3	C	1101	ANP	C3'-C4'-C5'-O5'
3	A	1101	ANP	PB-O3A-PA-O1A
3	C	1101	ANP	PB-O3A-PA-O1A
3	C	1101	ANP	PA-O3A-PB-O2B
3	C	1101	ANP	PB-O3A-PA-O2A
5	B	1001	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	ANP	1	0

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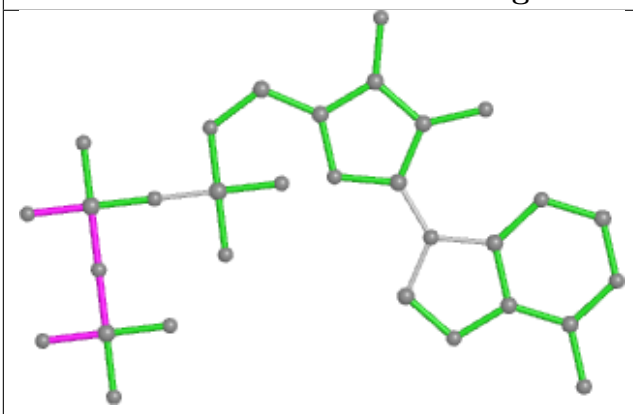
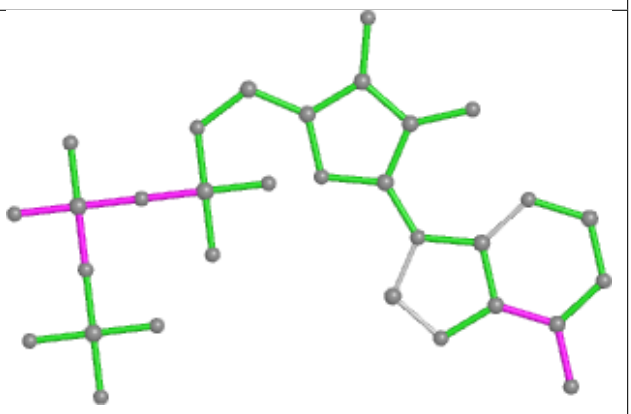
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1001	ADP	1	0

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 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.

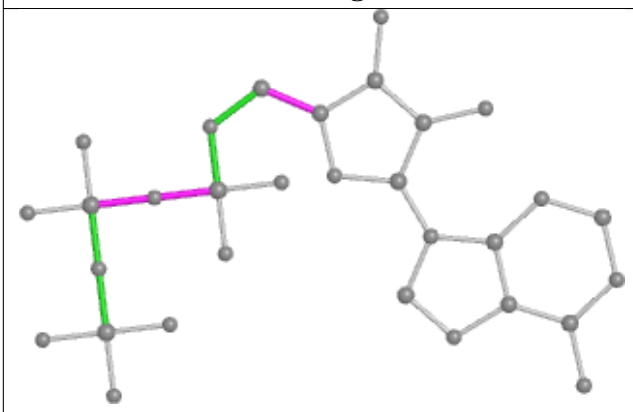
Ligand ANP A 1101



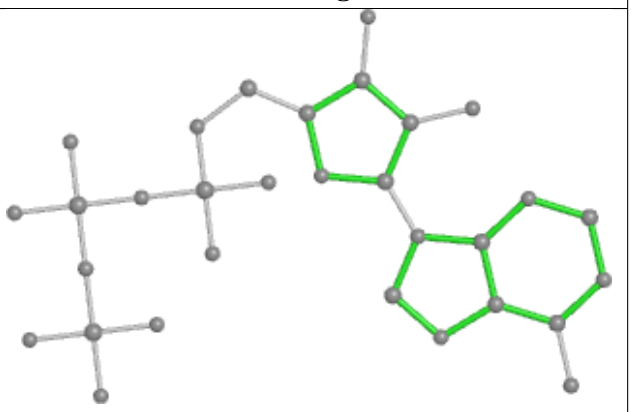
Bond lengths



Bond angles

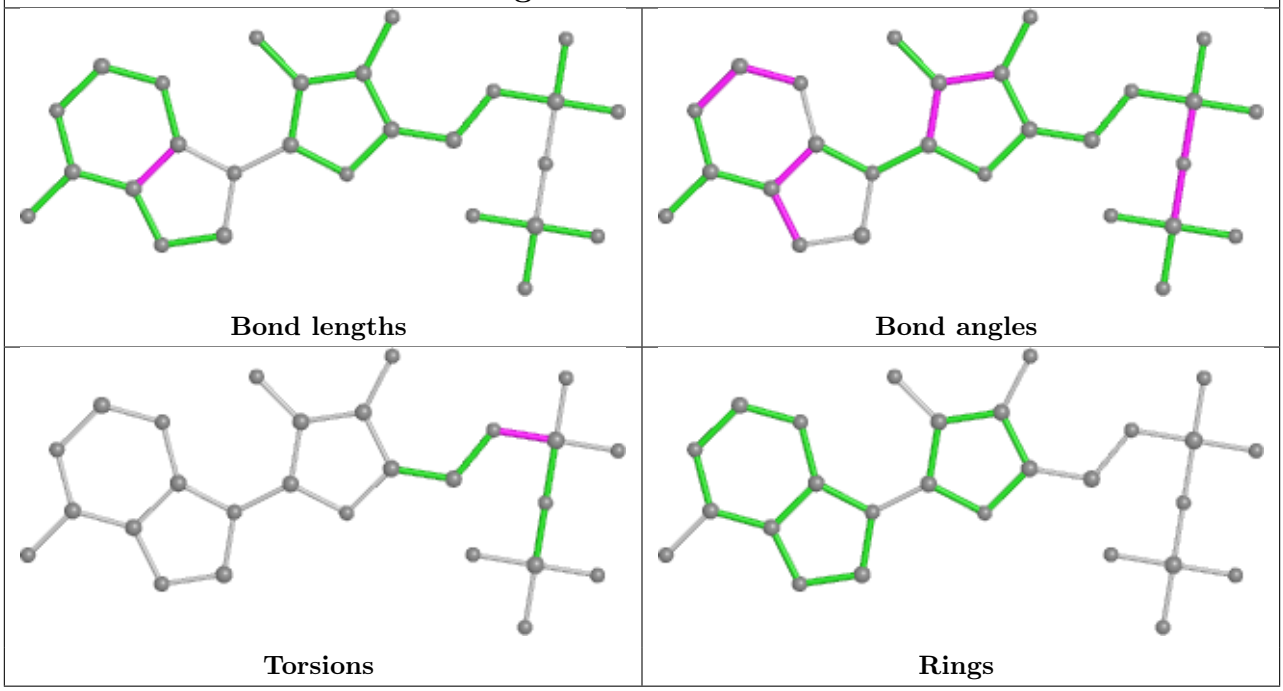


Torsions

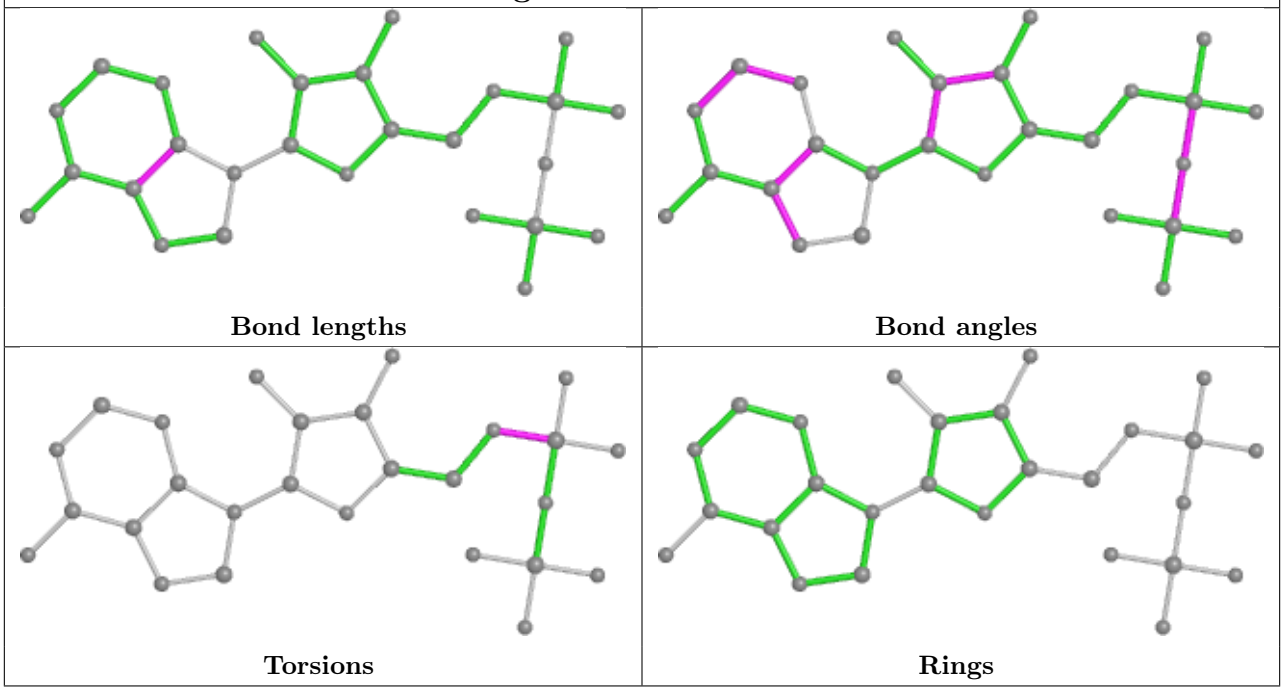


Rings

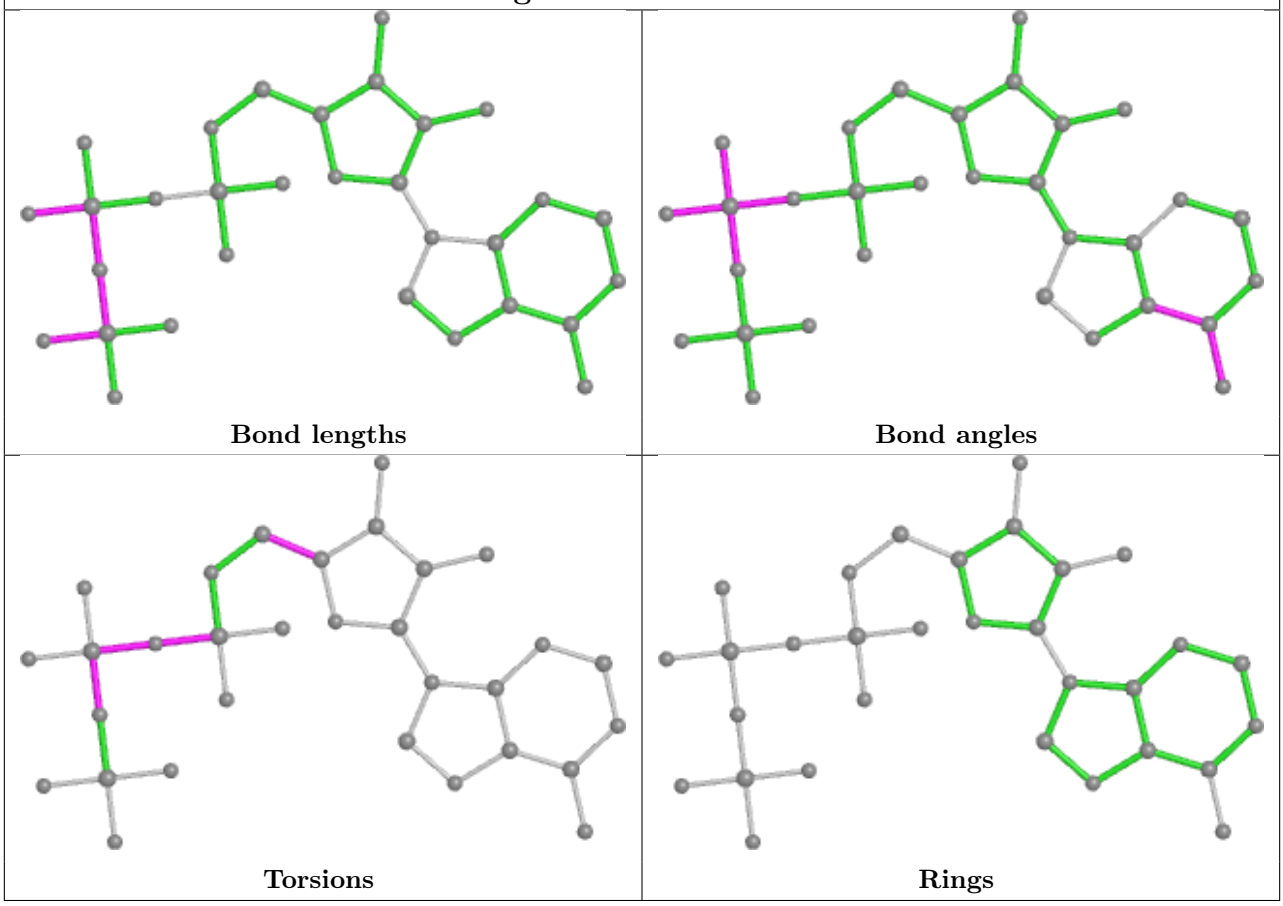
Ligand ADP B 1001



Ligand ADP D 1001



Ligand ANP C 1101



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	269/326 (82%)	0.12	2 (0%)	87	75	28, 56, 96, 149	0
1	C	275/326 (84%)	0.08	4 (1%)	73	54	24, 51, 88, 123	0
2	B	293/345 (84%)	0.29	8 (2%)	54	31	30, 56, 100, 141	0
2	D	297/345 (86%)	0.09	1 (0%)	94	88	31, 58, 104, 130	0
All	All	1134/1342 (84%)	0.15	15 (1%)	77	59	24, 56, 100, 149	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	714	VAL	4.4
2	B	732	ASN	3.6
2	B	710	GLU	3.3
2	D	714	VAL	3.3
1	C	680	VAL	3.1
1	A	733	SER	2.8
1	C	682	ALA	2.5
2	B	715	LYS	2.4
2	B	712	GLU	2.3
2	B	864	HIS	2.3
1	C	850	SER	2.1
2	B	668	LEU	2.1
1	A	736	ALA	2.1
1	C	844	ASP	2.1
2	B	685	GLU	2.1

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)

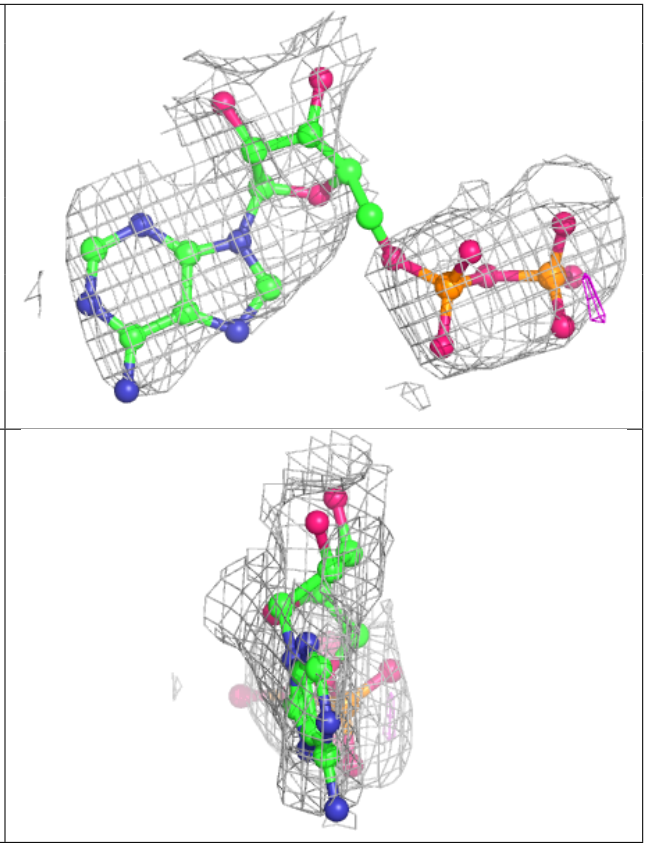
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	1002	1/1	0.56	0.40	72,72,72,72	0
4	MG	D	1002	1/1	0.76	0.23	67,67,67,67	0
5	ADP	B	1001	27/27	0.76	0.35	88,113,160,170	0
5	ADP	D	1001	27/27	0.83	0.28	79,105,167,167	0
4	MG	C	1102	1/1	0.89	0.10	20,20,20,20	0
4	MG	A	1102	1/1	0.92	0.08	34,34,34,34	0
3	ANP	A	1101	31/31	0.94	0.19	40,66,84,90	0
3	ANP	C	1101	31/31	0.96	0.17	35,45,53,67	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.

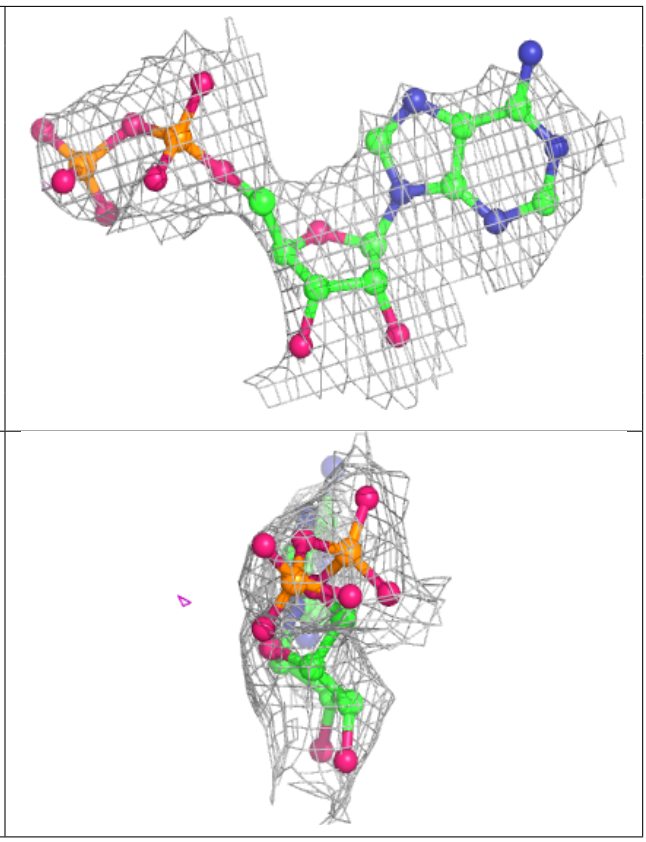
Electron density around ADP B 1001:

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



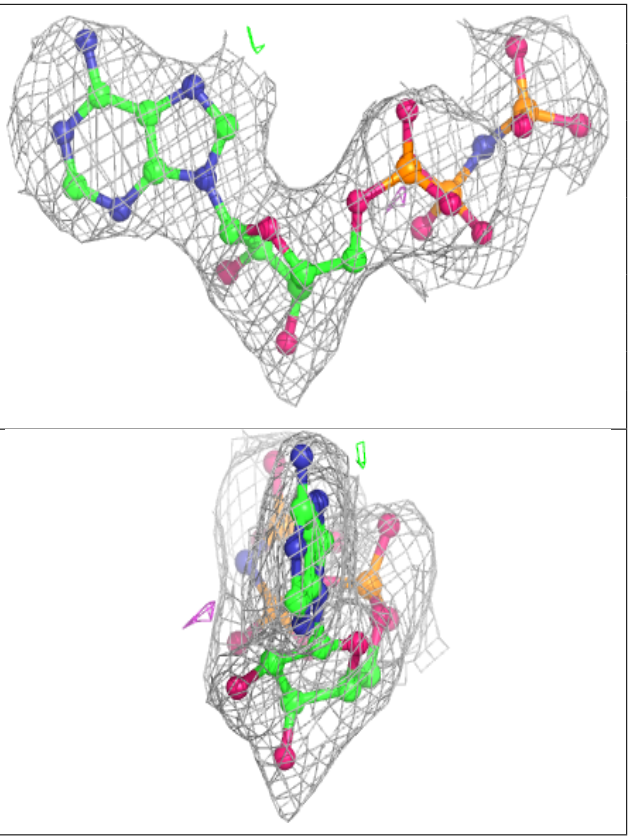
Electron density around ADP D 1001:

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



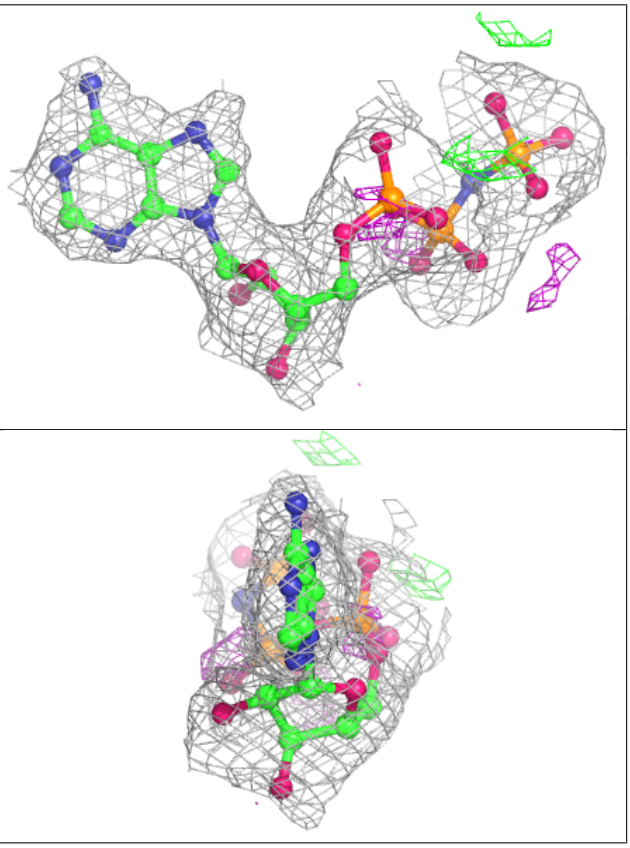
Electron density around ANP A 1101:

$2mF_o$-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 C 1101:

$2mF_o$-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.