



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:14 am BST

PDB ID : 4RIW
Title : Crystal structure of an EGFR/HER3 kinase domain heterodimer
Authors : Littlefield, P.; 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 ⓘ symbol.

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

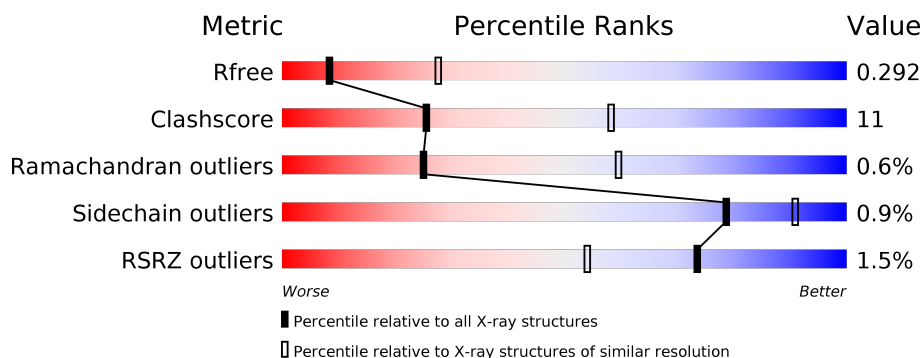
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	<div> <div></div> <div>63%19%17%</div> </div>
1	C	326	<div> <div>%</div> <div>64%20%16%</div> </div>
2	B	345	<div> <div>3%</div> <div>66%18%15%</div> </div>
2	D	345	<div> <div>%</div> <div>67%17%14%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9143 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
1	A	269	Total	C	N	O	S	0	0	0
			2130	1377	369	371	13			
1	C	275	Total	C	N	O	S	0	0	0
			2181	1412	373	383	13			

There are 6 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
C	676	GLY	-	EXPRESSION TAG	UNP P21860
C	677	ALA	-	EXPRESSION TAG	UNP P21860
C	678	GLY	-	EXPRESSION TAG	UNP P21860

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

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

There are 14 discrepancies between the modelled and reference sequences:

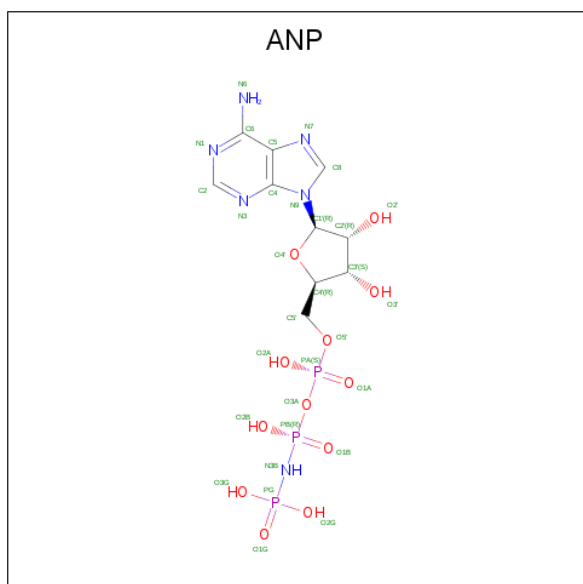
Chain	Residue	Modelled	Actual	Comment	Reference
B	654	GLY	-	EXPRESSION TAG	UNP P00533
B	655	ALA	-	EXPRESSION TAG	UNP P00533
B	656	MET	-	EXPRESSION TAG	UNP P00533
B	657	GLY	-	EXPRESSION TAG	UNP P00533
B	924	ARG	VAL	ENGINEERED MUTATION	UNP P00533
B	973	ALA	PHE	ENGINEERED MUTATION	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
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
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

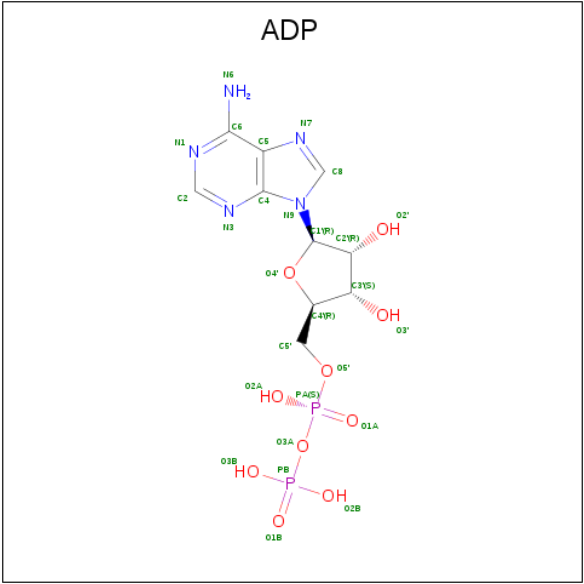
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

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

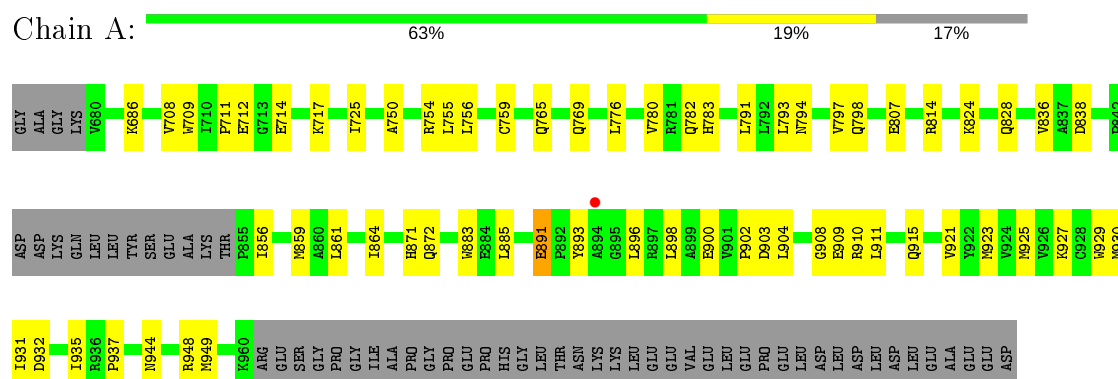
- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



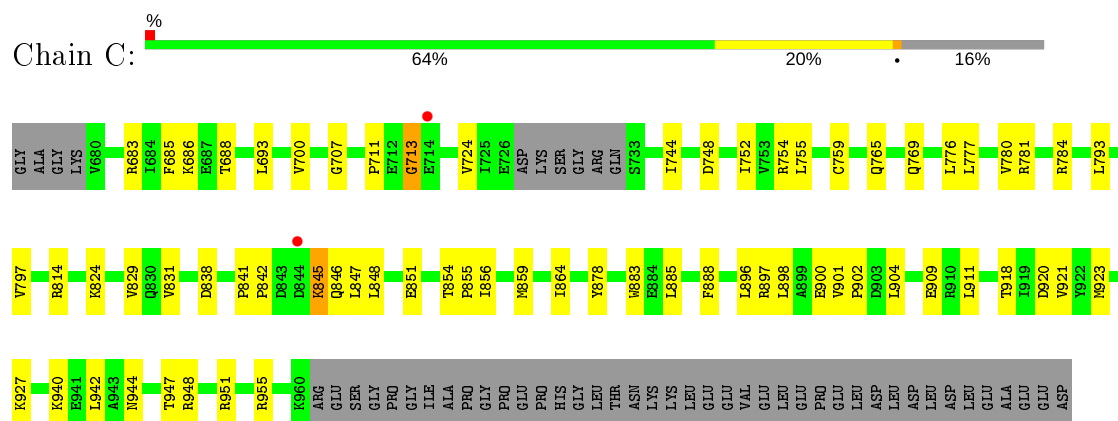
3 Residue-property plots

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.

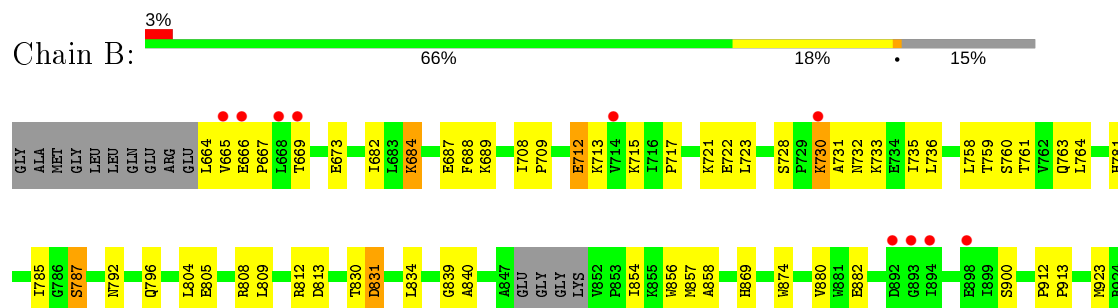
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

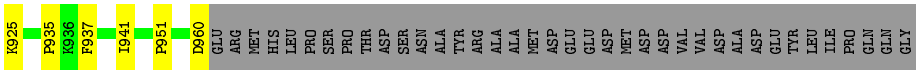


- Molecule 1: Receptor tyrosine-protein kinase erbB-3

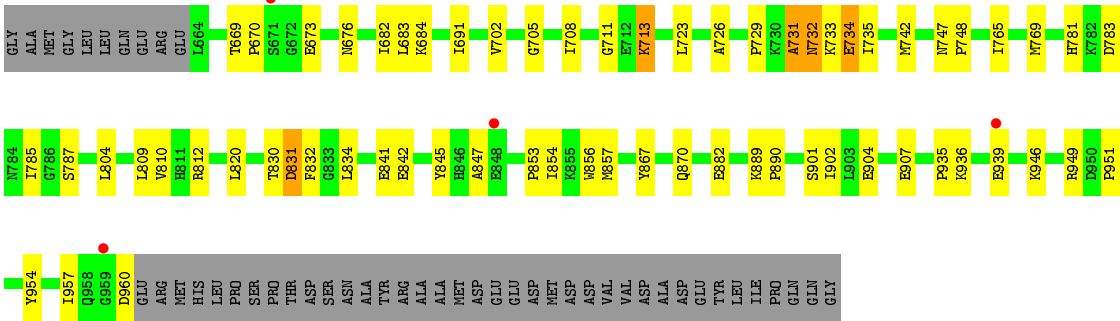


- Molecule 2: Epidermal growth factor receptor





● Molecule 2: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.78Å 154.64Å 86.97Å 90.00° 110.89° 90.00°	Depositor
Resolution (Å)	60.48 – 3.10 60.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (60.48-3.10) 91.0 (60.48-3.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.227 , 0.287 0.235 , 0.292	Depositor DCC
R_{free} test set	2865 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9143	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/2181	0.44	0/2956
1	C	0.26	0/2233	0.51	0/3029
2	B	0.28	0/2395	0.52	0/3243
2	D	0.33	1/2422 (0.0%)	0.52	2/3279 (0.1%)
All	All	0.28	1/9231 (0.0%)	0.50	2/12507 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	734	GLU	CB-CG	7.11	1.65	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	783	ASP	CB-CG-OD1	5.81	123.53	118.30
2	D	783	ASP	CB-CG-OD2	-5.41	113.43	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	713	GLY	Peptide

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	2130	0	2180	47	1
1	C	2181	0	2229	49	0
2	B	2343	0	2402	56	1
2	D	2369	0	2428	55	0
3	A	31	0	13	1	0
3	C	31	0	13	1	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	3	0
All	All	9143	0	9289	195	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 11.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:ARG:NH1	1:A:838:ASP:OD1	2.01	0.94
2:D:731:ALA:O	2:D:734:GLU:N	2.01	0.93
2:D:812:ARG:NH1	2:D:834:LEU:O	2.00	0.93
2:B:808:ARG:NH2	2:B:839:GLY:O	2.11	0.84
2:D:734:GLU:HG2	2:D:735:ILE:N	1.93	0.83
2:D:787:SER:HB2	2:D:951:PRO:HB2	1.61	0.81
1:A:754:ARG:HH11	1:A:754:ARG:HG3	1.46	0.79
2:D:734:GLU:HG2	2:D:735:ILE:H	1.47	0.79
1:C:814:ARG:NH1	1:C:838:ASP:OD1	2.16	0.79
1:C:940:LYS:O	1:C:944:ASN:ND2	2.13	0.78
2:B:812:ARG:NH1	2:B:834:LEU:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:709:PRO:HB2	2:B:712:GLU:HG3	1.67	0.75
1:C:845:LYS:HE3	1:C:848:LEU:HB2	1.68	0.74
1:C:909:GLU:HB2	2:D:684:LYS:HG2	1.70	0.74
2:B:722:GLU:HB2	2:B:763:GLN:HG2	1.71	0.73
2:D:936:LYS:N	2:D:939:GLU:OE1	2.21	0.71
1:C:904:LEU:HD22	2:D:684:LYS:HZ1	1.56	0.69
1:C:759:CYS:HB3	1:C:765:GLN:HB2	1.74	0.69
2:B:733:LYS:HG3	2:B:736:LEU:HD12	1.76	0.68
1:A:769:GLN:OE1	1:A:824:LYS:NZ	2.25	0.68
1:A:708:VAL:HG21	1:A:717:LYS:HB3	1.75	0.68
2:B:787:SER:HB2	2:B:951:PRO:HB2	1.75	0.68
1:A:750:ALA:O	1:A:828:GLN:NE2	2.27	0.67
1:C:904:LEU:HD22	2:D:684:LYS:NZ	2.09	0.67
2:D:830:THR:OG1	2:D:831:ASP:N	2.27	0.67
2:D:936:LYS:HB2	2:D:939:GLU:OE2	1.94	0.67
2:B:684:LYS:HG3	2:B:687:GLU:HG3	1.77	0.66
2:D:734:GLU:HG3	2:D:735:ILE:HD13	1.78	0.66
2:D:787:SER:CB	2:D:951:PRO:HB2	2.26	0.66
2:D:856:TRP:NE1	2:D:882:GLU:OE2	2.26	0.65
1:A:782:GLN:HG2	1:A:783:HIS:ND1	2.11	0.65
2:B:787:SER:CB	2:B:951:PRO:HB2	2.26	0.65
1:C:851:GLU:HG2	1:C:898:LEU:HD13	1.78	0.64
2:B:713:LYS:HG2	2:B:715:LYS:HZ2	1.63	0.63
1:A:891:GLU:OE1	1:A:891:GLU:N	2.25	0.63
2:B:854:ILE:HA	2:B:857:MET:HE2	1.80	0.63
2:B:804:LEU:HD22	2:B:809:LEU:HD11	1.80	0.62
2:D:734:GLU:CG	2:D:735:ILE:N	2.63	0.62
1:A:754:ARG:HH12	1:A:756:LEU:HA	1.64	0.62
1:A:927:LYS:HE2	1:A:937:PRO:HG3	1.80	0.62
1:C:776:LEU:HD12	1:C:829:VAL:HG11	1.81	0.61
2:B:730:LYS:HD3	2:B:733:LYS:HB3	1.81	0.61
2:B:856:TRP:NE1	2:B:882:GLU:OE2	2.29	0.60
5:D:1001:ADP:H5'2	5:D:1001:ADP:C8	2.37	0.60
2:B:713:LYS:HG2	2:B:715:LYS:NZ	2.16	0.60
1:A:915:GLN:CD	1:A:915:GLN:H	2.06	0.59
2:B:732:ASN:O	2:B:735:ILE:HB	2.03	0.59
1:A:754:ARG:NH1	1:A:754:ARG:HG3	2.17	0.59
1:A:759:CYS:HB3	1:A:765:GLN:HB2	1.84	0.59
2:B:728:SER:H	2:B:731:ALA:HB3	1.67	0.58
1:C:918:THR:OG1	2:D:676:ASN:O	2.15	0.58
1:C:777:LEU:HD11	1:C:781:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:927:LYS:HD3	2:D:733:LYS:NZ	2.19	0.57
1:A:904:LEU:HD11	2:B:684:LYS:HD2	1.87	0.57
1:C:955:ARG:NH1	2:D:673:GLU:OE1	2.37	0.56
2:D:731:ALA:O	2:D:732:ASN:C	2.43	0.56
2:B:759:THR:OG1	2:B:760:SER:N	2.38	0.56
5:D:1001:ADP:H5'2	5:D:1001:ADP:H8	1.70	0.56
1:A:932:ASP:HB3	1:A:935:ILE:HD12	1.86	0.55
1:A:754:ARG:NH1	1:A:755:LEU:O	2.40	0.55
2:D:711:GLY:H	2:D:713:LYS:HE2	1.71	0.55
1:A:927:LYS:HD2	2:B:733:LYS:HD2	1.88	0.55
2:D:810:VAL:HG12	2:D:812:ARG:HG3	1.89	0.55
2:B:713:LYS:HA	2:B:715:LYS:NZ	2.23	0.54
1:C:845:LYS:CE	1:C:848:LEU:HB2	2.35	0.54
1:C:700:VAL:O	1:C:846:GLN:NE2	2.42	0.54
2:D:769:MET:HG3	2:D:820:LEU:HB3	1.89	0.54
1:C:776:LEU:HD21	1:C:885:LEU:HD13	1.89	0.53
1:A:904:LEU:HG	1:A:909:GLU:HB3	1.90	0.53
2:D:708:ILE:HD11	2:D:713:LYS:HD3	1.90	0.53
1:C:923:MET:O	1:C:927:LYS:HG3	2.09	0.53
3:C:1101:ANP:O2B	3:C:1101:ANP:O1G	2.26	0.53
1:A:872:GLN:OE1	1:A:872:GLN:N	2.41	0.53
1:C:927:LYS:HB3	2:D:733:LYS:NZ	2.24	0.53
2:B:728:SER:HB2	2:B:731:ALA:HB2	1.90	0.52
1:A:864:ILE:HG21	1:A:902:PRO:HG3	1.90	0.52
1:C:927:LYS:HD3	2:D:733:LYS:HZ1	1.73	0.52
1:A:780:VAL:HG11	1:A:885:LEU:HD12	1.91	0.52
2:D:902:ILE:HG23	2:D:907:GLU:HB3	1.91	0.52
1:C:944:ASN:O	1:C:947:THR:HG22	2.10	0.52
1:A:944:ASN:O	1:A:948:ARG:HG3	2.11	0.51
1:C:854:THR:HG21	1:C:898:LEU:HD11	1.92	0.51
2:D:723:LEU:HD22	2:D:735:ILE:CD1	2.40	0.51
1:A:776:LEU:HD21	1:A:885:LEU:HD13	1.93	0.51
1:A:686:LYS:NZ	1:A:712:GLU:HG2	2.26	0.50
1:A:864:ILE:HD13	1:A:902:PRO:HG3	1.93	0.50
2:D:742:MET:HG2	2:D:832:PHE:HD2	1.76	0.50
3:A:1101:ANP:O2B	3:A:1101:ANP:O1A	2.30	0.50
2:B:733:LYS:HA	2:B:736:LEU:HB2	1.92	0.50
2:D:691:ILE:HG13	2:D:705:GLY:HA2	1.94	0.49
2:D:731:ALA:O	2:D:733:LYS:N	2.44	0.49
1:A:904:LEU:HD21	1:A:909:GLU:OE2	2.12	0.49
2:B:925:LYS:HG2	2:B:935:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:769:GLN:OE1	1:C:824:LYS:NZ	2.45	0.49
2:B:781:HIS:O	2:B:785:ILE:HG13	2.12	0.49
2:B:880:VAL:HG12	2:B:923:MET:HE2	1.94	0.49
2:B:666:GLU:OE1	2:B:666:GLU:N	2.45	0.49
2:B:937:PHE:O	2:B:941:ILE:HG13	2.12	0.49
1:C:897:ARG:O	1:C:901:VAL:HG23	2.12	0.49
2:B:722:GLU:OE2	2:B:761:THR:HG21	2.12	0.48
1:A:900:GLU:HB3	1:A:903:ASP:HB2	1.96	0.48
2:D:946:LYS:NZ	2:D:954:TYR:OH	2.40	0.48
1:A:883:TRP:HD1	1:A:925:MET:HE1	1.79	0.48
2:D:734:GLU:HG3	2:D:735:ILE:CD1	2.44	0.48
1:A:893:TYR:HB3	1:A:896:LEU:HD12	1.95	0.47
2:D:723:LEU:HD22	2:D:735:ILE:HD11	1.96	0.47
2:D:845:TYR:CE2	2:D:847:ALA:HB2	2.50	0.47
2:B:723:LEU:HD22	2:B:735:ILE:HD11	1.95	0.47
1:A:910:ARG:HB2	2:B:682:ILE:HD12	1.96	0.47
1:A:908:GLY:HA2	2:B:758:LEU:O	2.13	0.47
1:C:693:LEU:HG	1:C:707:GLY:HA2	1.95	0.47
1:C:784:ARG:HG2	1:C:888:PHE:HB3	1.97	0.47
1:C:896:LEU:HD23	1:C:904:LEU:HD12	1.97	0.47
1:C:864:ILE:HG21	1:C:902:PRO:HB3	1.97	0.47
2:D:901:SER:HA	2:D:904:GLU:OE2	2.15	0.47
1:A:709:TRP:CZ2	1:A:711:PRO:HB3	2.50	0.46
2:B:689:LYS:N	2:B:689:LYS:HD3	2.30	0.46
2:B:715:LYS:HA	2:B:715:LYS:HE3	1.96	0.46
1:A:807:GLU:OE2	1:A:871:HIS:HB3	2.14	0.46
1:C:944:ASN:O	1:C:948:ARG:HG3	2.15	0.46
2:B:673:GLU:HA	2:D:949:ARG:HH11	1.81	0.46
2:D:830:THR:HG1	2:D:831:ASP:H	1.58	0.46
2:B:808:ARG:NH2	2:B:840:ALA:HA	2.31	0.46
2:D:731:ALA:O	2:D:734:GLU:CB	2.64	0.46
1:A:911:LEU:HB2	1:A:929:TRP:CH2	2.50	0.46
2:B:688:PHE:C	2:B:689:LYS:HD3	2.36	0.45
1:A:927:LYS:HD2	2:B:733:LYS:CD	2.46	0.45
2:B:813:ASP:HB2	2:B:834:LEU:HD13	1.98	0.45
1:A:930:MET:HG3	1:A:935:ILE:HG22	1.98	0.45
2:D:702:VAL:HG11	5:D:1001:ADP:C8	2.51	0.45
2:D:804:LEU:HD22	2:D:809:LEU:HD23	1.98	0.45
1:C:683:ARG:HE	1:C:685:PHE:HE1	1.64	0.45
2:D:781:HIS:O	2:D:785:ILE:HG13	2.17	0.45
1:C:686:LYS:NZ	1:C:688:THR:OG1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:VAL:HG22	1:C:765:GLN:HG2	1.99	0.45
2:D:853:PRO:O	2:D:857:MET:HG3	2.17	0.45
2:B:713:LYS:HA	2:B:715:LYS:HZ2	1.80	0.45
1:A:923:MET:O	1:A:927:LYS:HG3	2.17	0.44
1:A:921:VAL:HG22	1:A:949:MET:SD	2.56	0.44
1:C:947:THR:O	1:C:951:ARG:HG2	2.17	0.44
1:A:864:ILE:HG21	1:A:902:PRO:CG	2.47	0.44
1:A:856:ILE:HD12	1:A:859:MET:HE3	2.00	0.44
2:B:830:THR:HB	2:B:831:ASP:H	1.42	0.44
2:D:889:LYS:HA	2:D:890:PRO:HD3	1.85	0.44
1:A:900:GLU:HA	1:A:902:PRO:HD2	2.00	0.44
2:D:726:ALA:HB1	2:D:731:ALA:HB3	1.99	0.44
1:C:845:LYS:HZ1	1:C:848:LEU:HD13	1.83	0.44
2:D:842:GLU:HG2	2:D:842:GLU:H	1.48	0.44
2:B:723:LEU:O	2:B:761:THR:OG1	2.29	0.43
1:A:754:ARG:NH1	1:A:756:LEU:HA	2.30	0.43
2:B:792:ASN:O	2:B:796:GLN:HG3	2.19	0.43
2:B:812:ARG:NH1	2:B:834:LEU:HB3	2.34	0.43
2:B:858:ALA:HA	2:B:874:TRP:CD2	2.54	0.43
2:D:683:LEU:HD12	2:D:765:ILE:HD12	2.00	0.43
2:B:664:LEU:HD23	2:B:665:VAL:HG22	2.00	0.43
1:A:794:ASN:O	1:A:798:GLN:HG3	2.19	0.43
1:C:744:ILE:HG22	1:C:755:LEU:HD22	2.00	0.42
1:C:855:PRO:O	1:C:859:MET:HG3	2.19	0.42
2:D:854:ILE:HD12	2:D:854:ILE:H	1.84	0.42
1:A:793:LEU:O	1:A:797:VAL:HG23	2.19	0.42
1:A:725:ILE:HD11	1:A:836:VAL:HG13	2.00	0.42
2:B:721:LYS:HD3	2:B:764:LEU:HD12	2.01	0.42
1:C:900:GLU:O	1:C:904:LEU:HG	2.19	0.42
2:D:747:ASN:OD1	2:D:748:PRO:HD2	2.19	0.42
2:D:957:ILE:HB	2:D:960:ASP:OD2	2.18	0.42
2:B:912:PRO:HA	2:B:913:PRO:HD3	1.87	0.42
1:C:883:TRP:CD2	1:C:911:LEU:HD13	2.55	0.42
1:C:918:THR:HG22	1:C:921:VAL:HG12	2.01	0.42
2:D:729:PRO:O	2:D:733:LYS:HG2	2.19	0.42
1:C:711:PRO:HG2	1:C:713:GLY:O	2.20	0.42
1:A:856:ILE:HG21	1:A:898:LEU:HG	2.01	0.42
2:B:733:LYS:CG	2:B:736:LEU:HB2	2.50	0.42
1:C:748:ASP:HB2	1:C:754:ARG:HD2	2.02	0.42
1:C:841:PRO:HA	1:C:842:PRO:HD3	1.94	0.42
2:B:708:ILE:HG23	2:B:715:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:780:VAL:HG11	1:C:885:LEU:HD12	2.01	0.41
2:B:708:ILE:HG23	2:B:715:LYS:HZ3	1.85	0.41
1:C:878:TYR:CD2	1:C:942:LEU:HD13	2.55	0.41
1:C:752:ILE:HA	1:C:831:VAL:H	1.86	0.41
2:B:715:LYS:O	2:B:717:PRO:HD3	2.20	0.41
1:A:861:LEU:HD12	1:A:931:ILE:HG12	2.01	0.41
1:A:927:LYS:HD2	2:B:733:LYS:CE	2.51	0.41
2:B:730:LYS:HZ3	2:B:733:LYS:HZ3	1.69	0.41
1:C:793:LEU:O	1:C:797:VAL:HG23	2.21	0.41
1:C:909:GLU:OE2	2:D:682:ILE:O	2.39	0.41
2:B:787:SER:OG	2:B:960:ASP:OD2	2.39	0.41
1:C:856:ILE:HG21	1:C:898:LEU:HG	2.03	0.41
2:B:805:GLU:HG3	2:B:869:HIS:CG	2.56	0.41
1:C:845:LYS:HA	1:C:847:LEU:HG	2.03	0.41
2:D:669:THR:N	2:D:670:PRO:HD3	2.35	0.41
2:D:812:ARG:NH1	2:D:834:LEU:HB3	2.36	0.40
2:B:787:SER:HB3	2:B:951:PRO:HB2	2.00	0.40
2:D:870:GLN:NE2	2:D:935:PRO:O	2.42	0.40
1:C:918:THR:HG23	1:C:920:ASP:N	2.37	0.40
2:D:812:ARG:HG2	2:D:867:TYR:CD1	2.56	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:714:GLU:OE1	2:B:925:LYS:NZ[2_545]	2.18	0.02

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%)	258 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	271/326 (83%)	267 (98%)	4 (2%)	0	100	100
2	B	289/345 (84%)	275 (95%)	11 (4%)	3 (1%)	15	49
2	D	295/345 (86%)	285 (97%)	6 (2%)	4 (1%)	11	40
All	All	1120/1342 (84%)	1085 (97%)	28 (2%)	7 (1%)	25	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	667	PRO
2	D	713	LYS
2	D	732	ASN
2	D	731	ALA
2	B	831	ASP
2	D	831	ASP
2	B	669	THR

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	231/278 (83%)	229 (99%)	2 (1%)	78	91
1	C	237/278 (85%)	236 (100%)	1 (0%)	91	96
2	B	258/300 (86%)	253 (98%)	5 (2%)	57	81
2	D	260/300 (87%)	259 (100%)	1 (0%)	91	96
All	All	986/1156 (85%)	977 (99%)	9 (1%)	78	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	791	LEU
1	A	891	GLU
2	B	684	LYS
2	B	712	GLU

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Mol	Chain	Res	Type
2	B	730	LYS
2	B	787	SER
2	B	900	SER
1	C	845	LYS
2	D	841	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	732	ASN

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 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	C	1101	4	29,33,33	1.08	4 (13%)	31,52,52	1.07	2 (6%)
5	ADP	B	1001	4	24,29,29	0.96	1 (4%)	29,45,45	1.39	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	D	1001	4	24,29,29	0.98	1 (4%)	29,45,45	1.53	5 (17%)
3	ANP	A	1101	4	29,33,33	1.08	4 (13%)	31,52,52	1.13	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
3	ANP	C	1101	4	-	7/14/38/38	0/3/3/3
5	ADP	B	1001	4	-	5/12/32/32	0/3/3/3
5	ADP	D	1001	4	-	2/12/32/32	0/3/3/3
3	ANP	A	1101	4	-	4/14/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1001	ADP	C5-C4	2.64	1.47	1.40
3	A	1101	ANP	PG-N3B	2.58	1.70	1.63
3	C	1101	ANP	PG-N3B	2.54	1.70	1.63
5	B	1001	ADP	C5-C4	2.50	1.47	1.40
3	A	1101	ANP	PG-O1G	2.43	1.50	1.46
3	C	1101	ANP	PG-O1G	2.40	1.50	1.46
3	A	1101	ANP	PB-O1B	2.31	1.49	1.46
3	C	1101	ANP	PB-O1B	2.28	1.49	1.46
3	A	1101	ANP	PB-O3A	-2.03	1.56	1.59
3	C	1101	ANP	PB-N3B	2.02	1.68	1.63

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	ADP	C3'-C2'-C1'	3.68	106.52	100.98
5	D	1001	ADP	PA-O3A-PB	-3.46	120.97	132.83
3	A	1101	ANP	PA-O3A-PB	-3.32	120.93	132.62
5	B	1001	ADP	N3-C2-N1	-3.23	123.64	128.68
5	D	1001	ADP	C3'-C2'-C1'	3.16	105.73	100.98
5	D	1001	ADP	N3-C2-N1	-2.98	124.03	128.68
3	C	1101	ANP	PA-O3A-PB	-2.78	122.82	132.62
5	B	1001	ADP	C4-C5-N7	-2.50	106.80	109.40
5	D	1001	ADP	C5'-C4'-C3'	-2.48	105.88	115.18
3	A	1101	ANP	C5-C6-N6	2.42	124.03	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1001	ADP	C4-C5-N7	-2.42	106.88	109.40
3	C	1101	ANP	C5-C6-N6	2.29	123.83	120.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1101	ANP	PG-N3B-PB-O1B
3	C	1101	ANP	PA-O3A-PB-O1B
3	C	1101	ANP	O4'-C4'-C5'-O5'
5	B	1001	ADP	PA-O3A-PB-O3B
5	B	1001	ADP	C5'-O5'-PA-O3A
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	C3'-C4'-C5'-O5'
5	D	1001	ADP	C3'-C4'-C5'-O5'
3	A	1101	ANP	C3'-C4'-C5'-O5'
5	D	1001	ADP	O4'-C4'-C5'-O5'
5	B	1001	ADP	PB-O3A-PA-O1A
5	B	1001	ADP	C5'-O5'-PA-O1A
5	B	1001	ADP	PB-O3A-PA-O2A
3	C	1101	ANP	PA-O3A-PB-O2B
3	C	1101	ANP	PB-O3A-PA-O2A
3	C	1101	ANP	C5'-O5'-PA-O1A

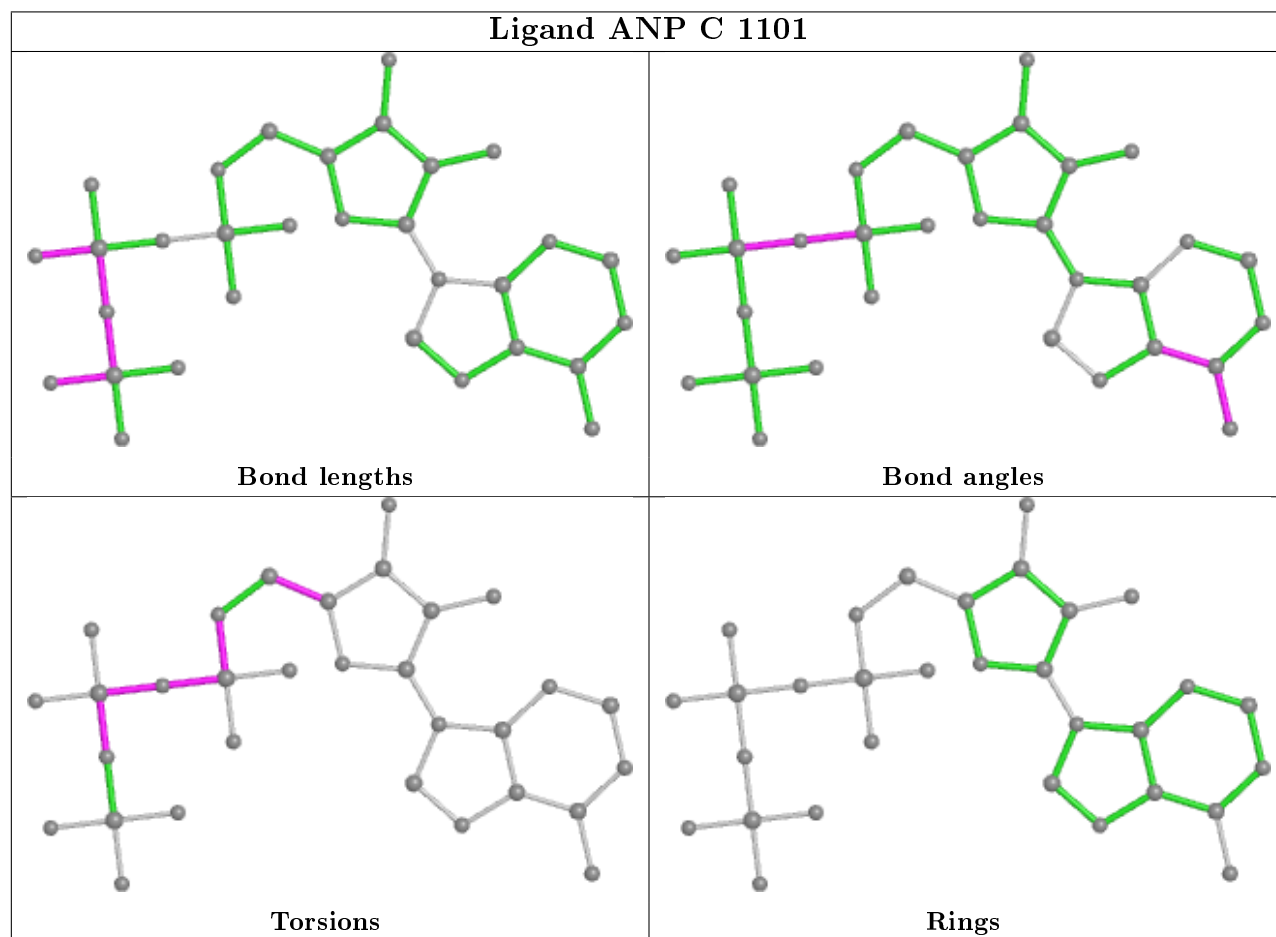
There are no ring outliers.

3 monomers are involved in 5 short contacts:

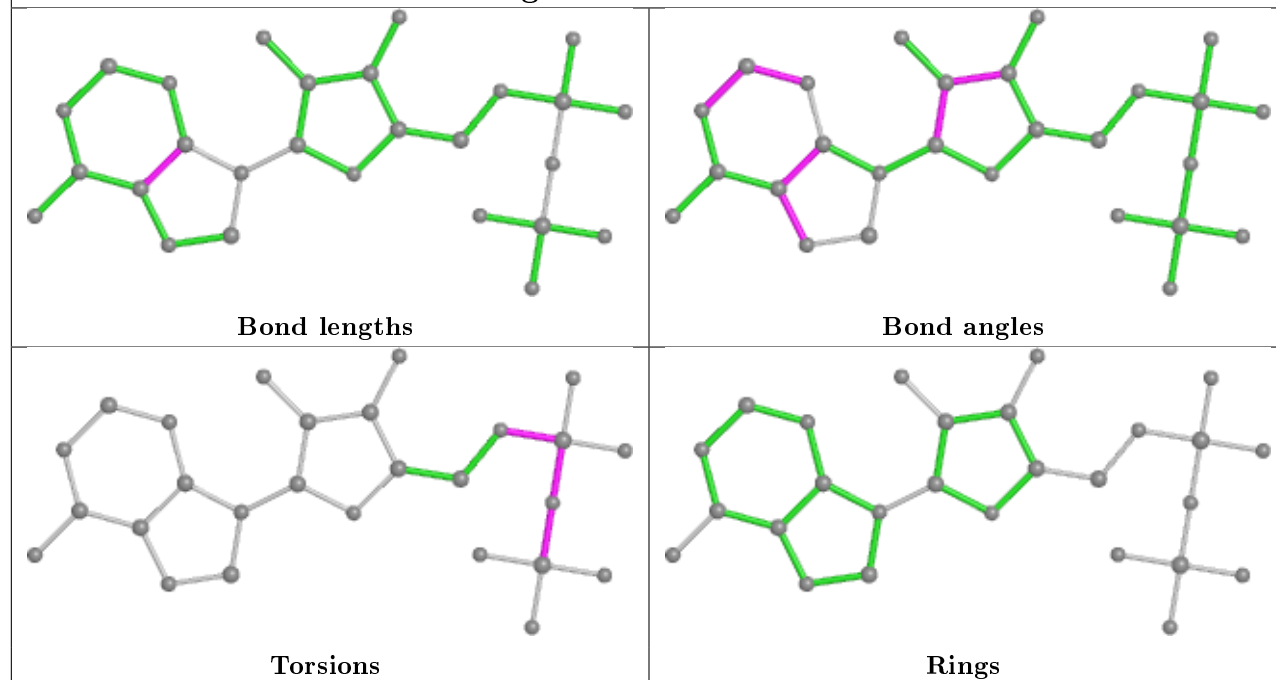
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	ANP	1	0
5	D	1001	ADP	3	0
3	A	1101	ANP	1	0

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

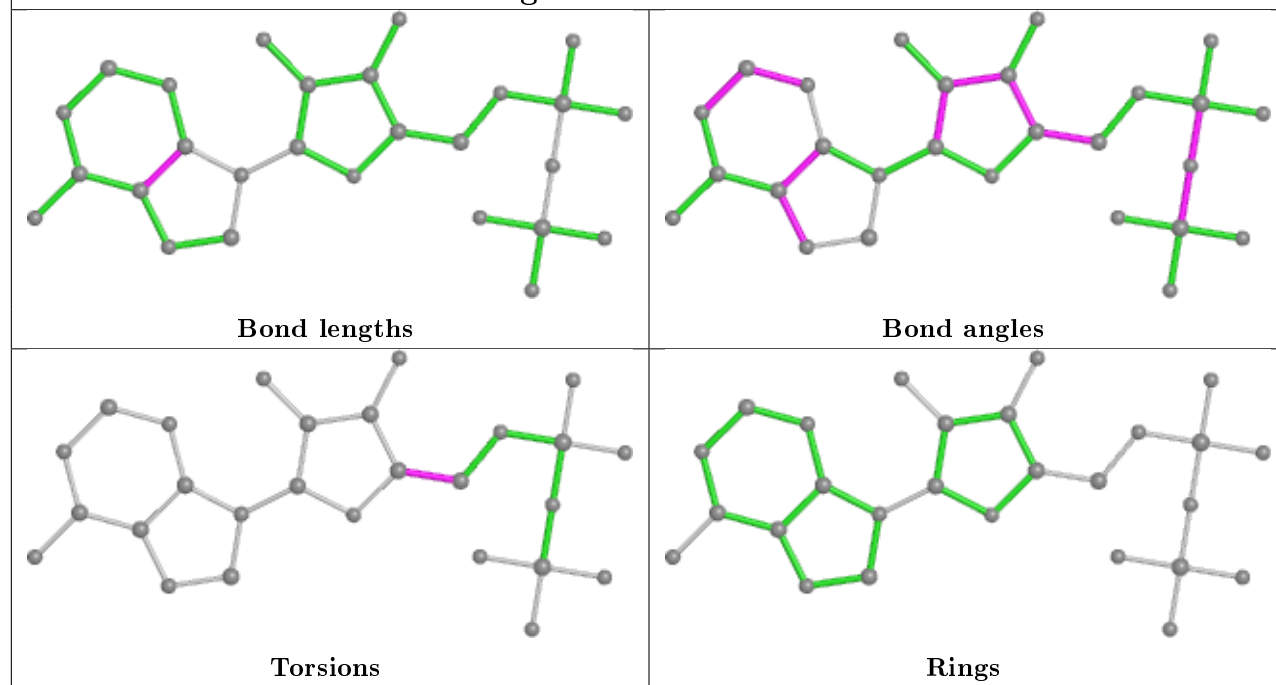
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

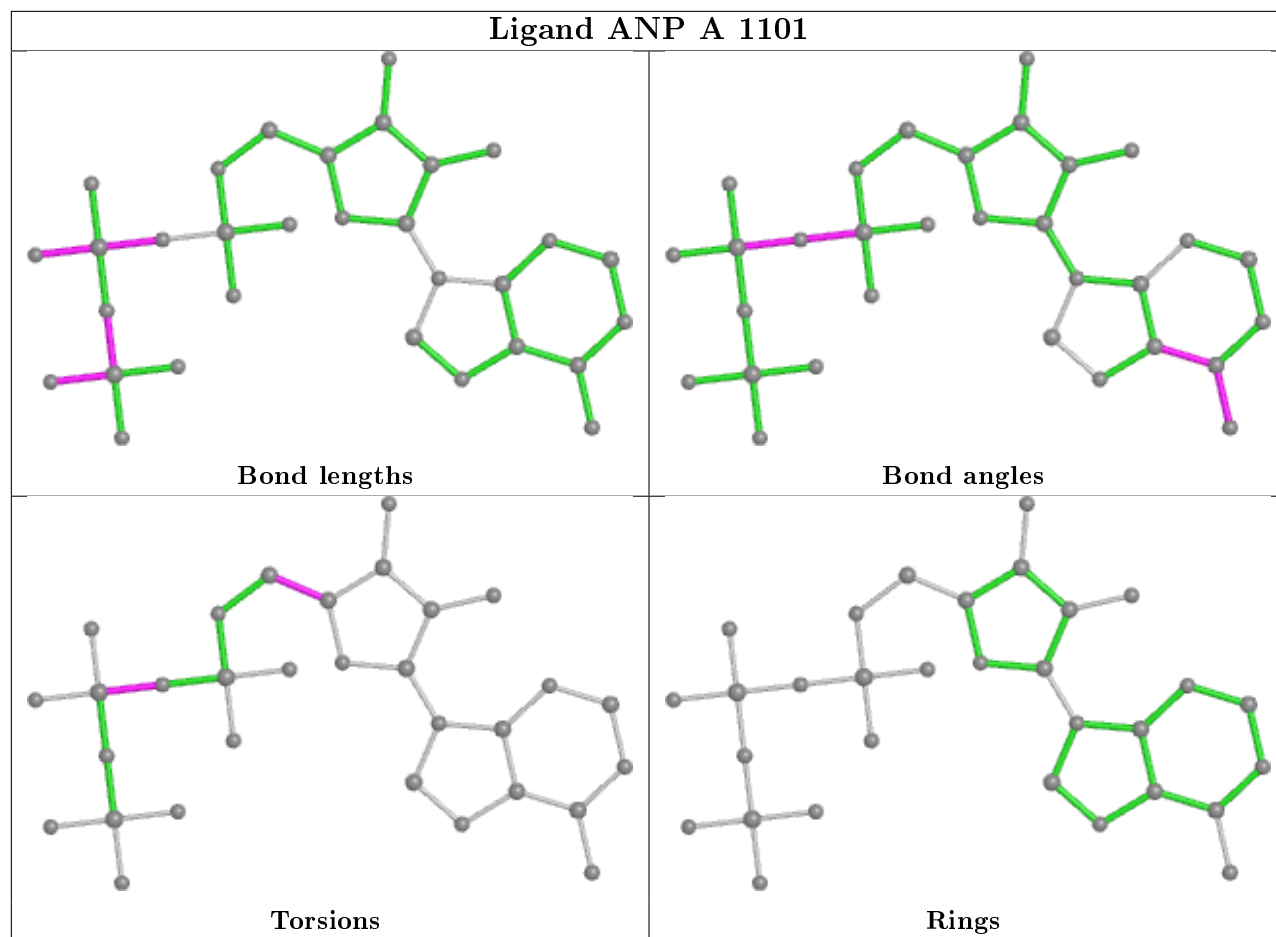


Ligand ADP B 1001



Ligand ADP D 1001





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, 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%)	-0.05	1 (0%) 92 84	11, 38, 63, 85	0
1	C	275/326 (84%)	-0.02	2 (0%) 87 75	17, 37, 69, 97	0
2	B	293/345 (84%)	0.15	10 (3%) 45 24	16, 39, 79, 100	0
2	D	297/345 (86%)	0.04	4 (1%) 77 59	16, 37, 78, 94	0
All	All	1134/1342 (84%)	0.04	17 (1%) 73 54	11, 38, 75, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	893	GLY	3.8
1	C	844	ASP	3.8
2	B	665	VAL	3.3
2	B	730	LYS	3.1
2	B	668	LEU	2.9
2	D	959	GLY	2.7
2	D	848	GLU	2.7
2	B	892	ASP	2.5
2	B	714	VAL	2.4
2	B	666	GLU	2.3
1	C	714	GLU	2.3
2	D	939	GLU	2.2
2	D	671	SER	2.1
2	B	898	GLU	2.0
1	A	894	ALA	2.0
2	B	894	ILE	2.0
2	B	669	THR	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

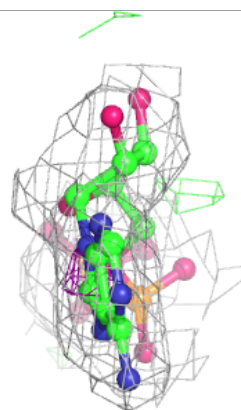
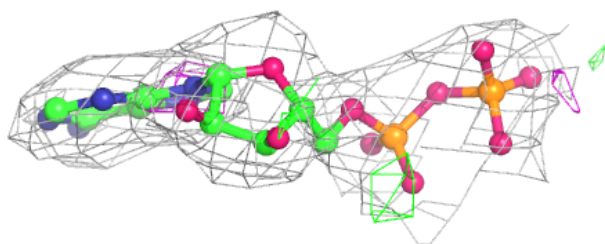
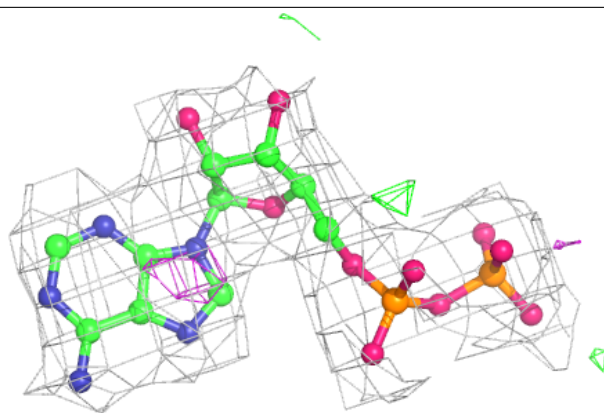
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	1102	1/1	0.89	0.12	42,42,42,42	0
4	MG	B	1002	1/1	0.91	0.17	37,37,37,37	0
4	MG	C	1102	1/1	0.92	0.13	10,10,10,10	0
4	MG	D	1002	1/1	0.92	0.21	38,38,38,38	0
5	ADP	B	1001	27/27	0.93	0.16	17,35,47,50	0
5	ADP	D	1001	27/27	0.93	0.17	4,23,42,44	0
3	ANP	A	1101	31/31	0.93	0.18	21,45,55,58	0
3	ANP	C	1101	31/31	0.96	0.18	8,27,38,75	0

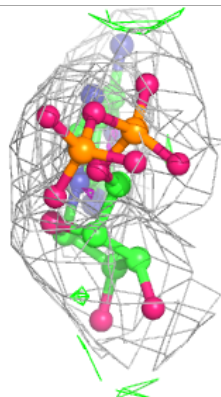
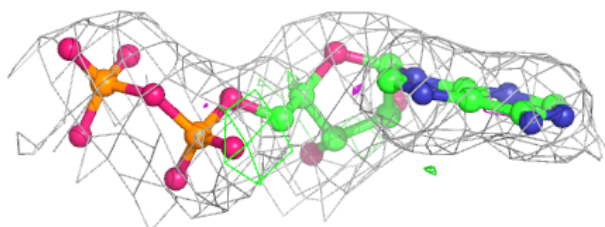
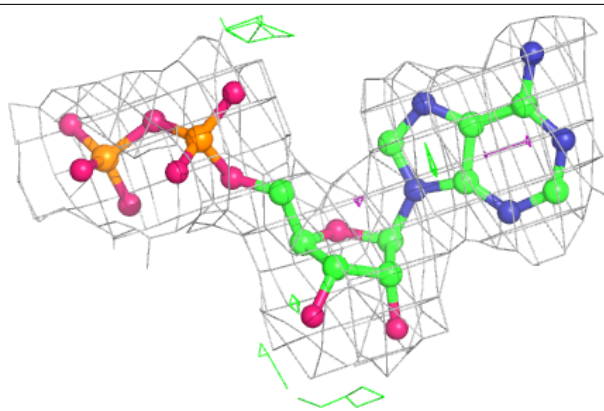
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

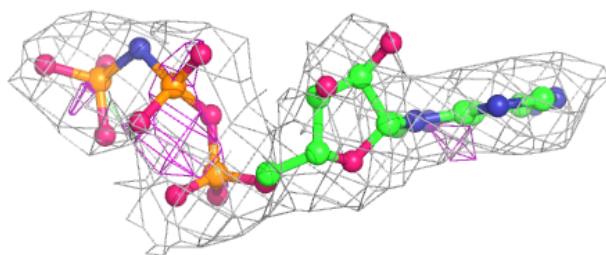
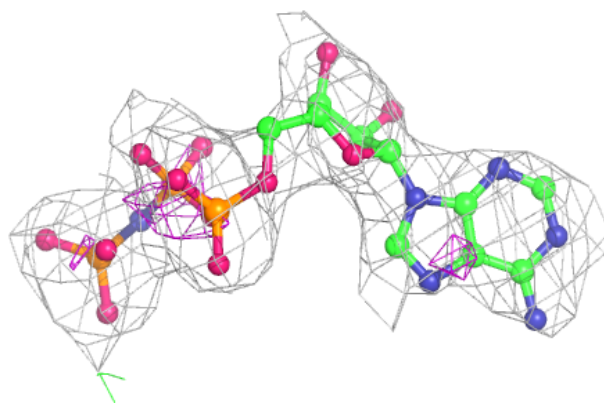
**Electron density around ADP D 1001:**

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

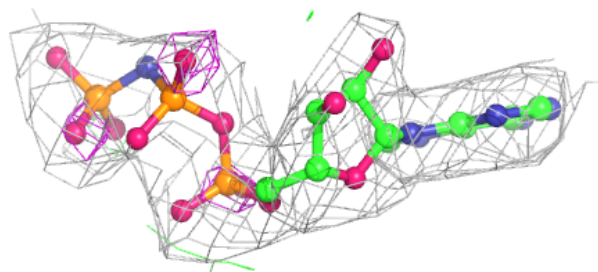
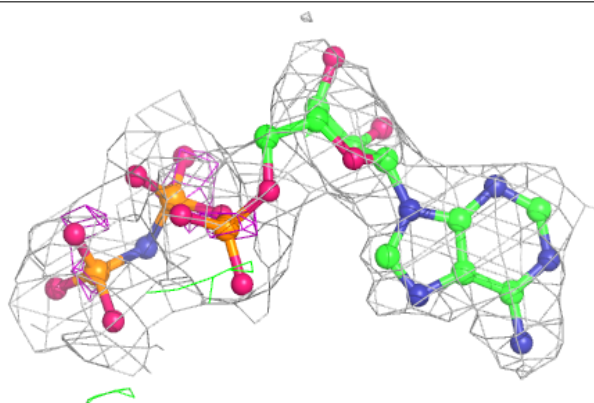


Electron density around ANP A 1101:

$2mF_o-DF_c$ (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.