



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:16 AM UTC

PDB ID : 4RIY / pdb_00004riy
Title : Crystal structure of an EGFR/HER3 kinase domain heterodimer containing the cancer-associated HER3-E909G mutation
Authors : Littlefield, P.; Liu, L.; Jura, N.
Deposited on : 2014-10-07
Resolution : 2.98 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

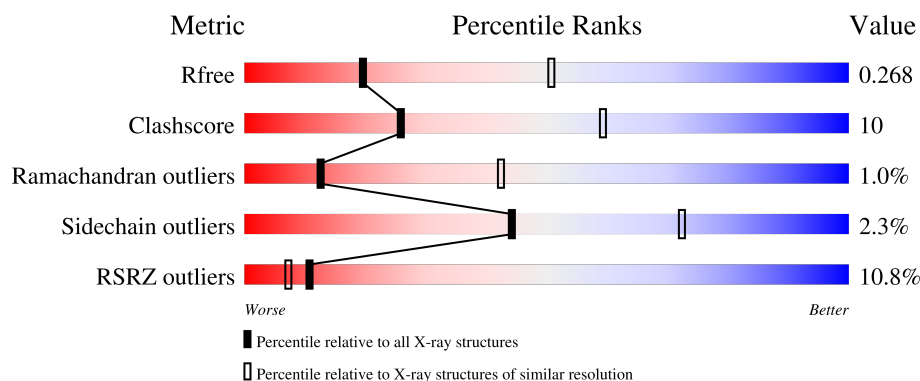
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 $\leq 5\%$. 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	4% 71% 11% • 17%
1	C	326	6% 71% 12% • 16%
2	B	345	13% 66% 16% •• 15%
2	D	345	13% 63% 18% 5% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9122 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
			2118	1371	369	365	13			
1	C	275	Total	C	N	O	S	0	0	0
			2172	1407	373	379	13			

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	909	GLY	GLU	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	909	GLY	GLU	engineered mutation	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:

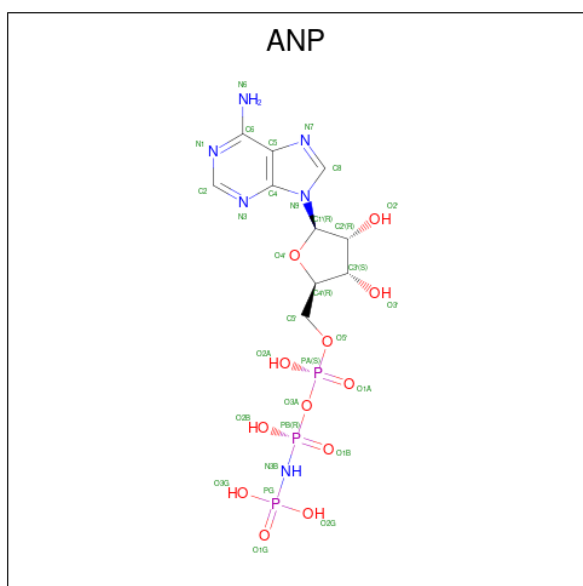
Chain	Residue	Modelled	Actual	Comment	Reference
B	654	GLY	-	expression tag	UNP P00533
B	655	ALA	-	expression tag	UNP P00533
B	656	MET	-	expression tag	UNP P00533
B	657	GLY	-	expression tag	UNP P00533

Continued on next page...

Continued from previous page...

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

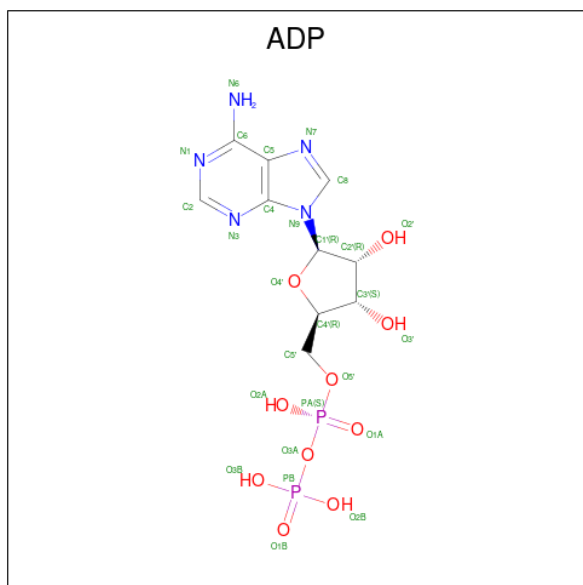
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

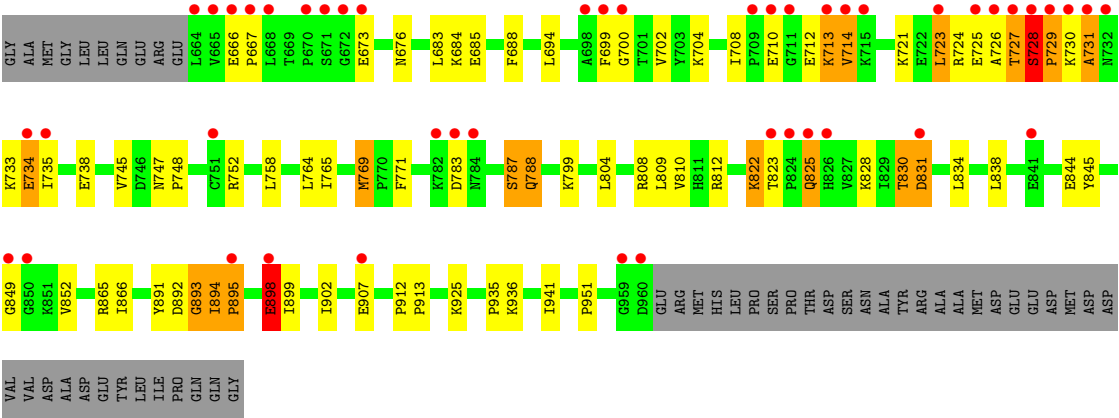
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

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





● 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	65.33Å 155.14Å 87.30Å 90.00° 110.93° 90.00°	Depositor
Resolution (Å)	56.20 – 2.98 56.20 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.6 (56.20-2.98) 93.2 (56.20-2.98)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.216 , 0.267 0.220 , 0.268	Depositor DCC
R_{free} test set	3254 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.52% 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: ANP, ADP, 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	0.34	0/2169	0.80	3/2940 (0.1%)
1	C	0.32	0/2224	0.82	5/3017 (0.2%)
2	B	0.41	0/2395	0.91	7/3243 (0.2%)
2	D	0.48	0/2422	1.00	17/3279 (0.5%)
All	All	0.39	0/9210	0.89	32/12479 (0.3%)

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
2	B	0	1
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	822	LYS	N-CA-C	-7.83	102.69	111.07
2	D	726	ALA	N-CA-C	-7.76	101.31	111.71
2	D	723	LEU	CB-CG-CD2	-7.42	88.44	110.70
2	D	734	GLU	CB-CG-CD	7.32	125.04	112.60
2	D	729	PRO	CA-C-N	7.24	130.57	120.29
2	D	729	PRO	C-N-CA	7.24	130.57	120.29
2	D	898	GLU	N-CA-C	7.13	123.06	111.37
2	B	714	VAL	N-CA-C	6.71	118.81	109.55
1	C	710	ILE	CA-C-N	6.70	127.09	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	710	ILE	C-N-CA	6.70	127.09	119.92
2	D	894	ILE	CA-C-N	6.44	127.89	119.84
2	D	894	ILE	C-N-CA	6.44	127.89	119.84
1	A	734	PHE	N-CA-C	-6.20	104.88	112.88
1	C	847	LEU	N-CA-C	-6.13	103.90	111.75
2	B	723	LEU	N-CA-C	6.04	119.55	109.95
2	B	769	MET	CA-C-N	6.01	126.18	119.32
2	B	769	MET	C-N-CA	6.01	126.18	119.32
2	D	714	VAL	N-CA-C	-5.89	103.63	110.05
2	D	731	ALA	N-CA-C	-5.85	104.82	111.14
2	B	958	GLN	N-CA-C	5.81	120.09	112.89
1	A	872	GLN	CA-CB-CG	-5.44	103.22	114.10
1	A	953	PRO	N-CA-C	5.40	117.29	110.70
2	D	830	THR	N-CA-C	5.38	115.14	108.19
2	B	726	ALA	N-CA-C	5.31	117.93	110.23
2	D	727	THR	N-CA-C	-5.29	102.65	110.48
2	D	899	ILE	N-CA-C	5.28	116.64	110.62
2	D	893	GLY	N-CA-C	-5.27	108.44	115.40
2	D	769	MET	CA-C-N	5.27	125.32	119.32
2	D	769	MET	C-N-CA	5.27	125.32	119.32
2	B	898	GLU	N-CA-C	5.22	121.91	110.80
1	C	953	PRO	N-CA-C	5.17	117.00	110.70
1	C	784	ARG	CB-CA-C	-5.03	109.31	116.34

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	751	CYS	Peptide
1	C	846	GLN	Peptide
2	D	728	SER	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	2118	0	2171	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2172	0	2222	30	0
2	B	2343	0	2402	46	0
2	D	2369	0	2428	76	0
3	A	31	0	13	0	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	1	0
5	D	27	0	12	2	0
All	All	9122	0	9273	175	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 10.

All (175) 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:B:751:CYS:HB2	2:B:828:LYS:HD3	1.57	0.84
2:D:734:GLU:HG2	2:D:735:ILE:N	1.91	0.84
2:D:723:LEU:HD21	2:D:734:GLU:OE2	1.77	0.83
1:C:945:GLU:HG2	1:C:948:ARG:NH1	1.96	0.80
1:A:712:GLU:H	1:A:712:GLU:CD	1.90	0.80
2:B:751:CYS:SG	2:B:752:ARG:N	2.56	0.78
2:D:731:ALA:O	2:D:734:GLU:N	2.17	0.78
2:D:788:GLN:HG3	2:D:951:PRO:HG3	1.67	0.75
2:D:745:VAL:O	2:D:752:ARG:NH2	2.20	0.74
1:C:932:ASP:OD2	1:C:935:ILE:HD13	1.87	0.73
2:D:723:LEU:HD23	2:D:735:ILE:HD13	1.72	0.72
2:D:734:GLU:CG	2:D:735:ILE:N	2.56	0.68
1:C:893:TYR:HB3	1:C:896:LEU:HD12	1.76	0.68
2:B:728:SER:HB2	2:B:730:LYS:HG2	1.77	0.67
2:B:787:SER:HB2	2:B:951:PRO:HB2	1.78	0.66
2:D:713:LYS:HE3	2:D:713:LYS:HA	1.78	0.66
2:B:854:ILE:HA	2:B:857:MET:HE2	1.77	0.66
2:D:734:GLU:HG2	2:D:735:ILE:H	1.61	0.65
2:B:897:SER:O	2:B:898:GLU:HG2	1.96	0.65
2:D:728:SER:HB2	2:D:730:LYS:N	2.12	0.65
1:C:945:GLU:HG2	1:C:948:ARG:HH11	1.62	0.65
1:C:859:MET:HE3	1:C:864:ILE:HG12	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:944:ASN:O	1:C:947:THR:HG22	1.97	0.64
1:C:918:THR:OG1	2:D:676:ASN:O	2.15	0.64
2:D:787:SER:HB2	2:D:951:PRO:HB2	1.78	0.63
2:B:897:SER:O	2:B:899:ILE:N	2.28	0.62
2:D:891:TYR:O	2:D:894:ILE:HB	2.00	0.61
2:D:673:GLU:CD	2:D:808:ARG:HH22	2.09	0.61
2:D:830:THR:OG1	2:D:831:ASP:N	2.32	0.60
2:D:925:LYS:HG2	2:D:935:PRO:HD3	1.83	0.60
2:D:710:GLU:HA	2:D:713:LYS:HZ3	1.66	0.60
2:D:730:LYS:HA	2:D:733:LYS:HB2	1.82	0.60
2:B:897:SER:C	2:B:898:GLU:HG2	2.27	0.60
1:C:944:ASN:O	1:C:948:ARG:HG3	2.02	0.60
2:D:728:SER:CB	2:D:730:LYS:H	2.14	0.60
2:D:723:LEU:CD2	2:D:735:ILE:HD13	2.31	0.59
2:D:708:ILE:HG22	2:D:713:LYS:HE3	1.84	0.59
1:A:893:TYR:HB3	1:A:896:LEU:HD12	1.84	0.59
2:D:721:LYS:NZ	2:D:738:GLU:OE1	2.33	0.59
1:C:814:ARG:NH1	1:C:838:ASP:OD1	2.34	0.58
1:C:777:LEU:HD11	1:C:781:ARG:HH21	1.69	0.58
2:D:684:LYS:NZ	2:D:710:GLU:OE1	2.18	0.58
2:D:723:LEU:CD2	2:D:734:GLU:OE2	2.49	0.58
2:B:957:ILE:HD11	2:B:960:ASP:CG	2.29	0.58
2:D:804:LEU:HD22	2:D:809:LEU:HD11	1.86	0.57
2:D:702:VAL:HG11	5:D:1001:ADP:C8	2.38	0.57
2:B:925:LYS:HG2	2:B:935:PRO:HD3	1.86	0.57
1:A:856:ILE:HA	1:A:859:MET:HE2	1.87	0.56
1:A:797:VAL:HG12	1:A:801:LYS:HE3	1.86	0.56
1:A:927:LYS:HG2	1:A:937:PRO:HD3	1.88	0.56
1:C:856:ILE:HA	1:C:859:MET:HE2	1.88	0.56
2:D:710:GLU:HA	2:D:713:LYS:NZ	2.20	0.56
1:A:945:GLU:OE2	1:A:948:ARG:NH1	2.40	0.55
2:D:812:ARG:NH1	2:D:834:LEU:O	2.37	0.55
1:A:945:GLU:OE1	1:A:948:ARG:NH1	2.40	0.55
3:C:1101:ANP:O1G	3:C:1101:ANP:O2B	2.24	0.55
2:B:727:THR:HB	2:B:731:ALA:HB2	1.88	0.55
2:B:751:CYS:HB2	2:B:828:LYS:CD	2.34	0.55
2:B:727:THR:H	2:B:731:ALA:HB3	1.71	0.55
2:D:731:ALA:O	2:D:734:GLU:HG2	2.06	0.55
2:D:699:PHE:O	2:D:723:LEU:HB2	2.07	0.54
2:D:844:GLU:HB2	2:D:866:ILE:HG23	1.89	0.54
1:C:904:LEU:HD12	2:D:684:LYS:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:880:VAL:HG12	2:B:923:MET:HE2	1.90	0.53
1:C:748:ASP:HB2	1:C:754:ARG:HH11	1.74	0.53
5:D:1001:ADP:C8	5:D:1001:ADP:H5'2	2.44	0.53
2:B:681:ARG:HG3	2:B:682:ILE:N	2.23	0.52
2:D:728:SER:CB	2:D:731:ALA:H	2.23	0.52
2:D:728:SER:HB3	2:D:730:LYS:H	1.73	0.52
1:A:927:LYS:HZ2	1:A:937:PRO:HG3	1.75	0.52
2:B:728:SER:HB3	2:B:730:LYS:NZ	2.25	0.52
2:D:721:LYS:HD3	2:D:764:LEU:HD12	1.90	0.51
1:C:739:ASP:OD1	1:C:739:ASP:N	2.43	0.51
1:C:940:LYS:O	1:C:944:ASN:ND2	2.42	0.51
2:D:728:SER:CB	2:D:730:LYS:N	2.74	0.51
2:B:671:SER:O	2:B:673:GLU:N	2.41	0.51
2:D:902:ILE:HG23	2:D:907:GLU:HG2	1.94	0.50
2:D:895:PRO:C	2:D:898:GLU:OE2	2.54	0.50
1:A:689:GLU:HG2	1:A:712:GLU:OE2	2.11	0.50
1:A:945:GLU:OE2	1:A:948:ARG:CZ	2.59	0.50
2:D:731:ALA:HB1	2:D:734:GLU:OE1	2.12	0.50
2:D:849:GLY:HA2	2:D:865:ARG:HD2	1.93	0.50
2:B:804:LEU:HD22	2:B:809:LEU:HD11	1.94	0.50
2:D:892:ASP:OD1	2:D:893:GLY:N	2.44	0.50
2:D:731:ALA:O	2:D:734:GLU:CG	2.61	0.49
2:B:895:PRO:N	2:B:898:GLU:OE2	2.45	0.49
1:A:780:VAL:HG11	1:A:885:LEU:HD12	1.95	0.49
1:A:872:GLN:H	1:A:872:GLN:HG2	1.23	0.49
1:C:930:MET:HE2	1:C:935:ILE:HG21	1.95	0.49
1:A:945:GLU:CD	1:A:948:ARG:NH1	2.71	0.48
2:D:727:THR:HG22	2:D:728:SER:OG	2.13	0.48
1:A:926:VAL:HG13	2:B:758:LEU:HD11	1.95	0.48
1:C:870:THR:HG22	1:C:871:HIS:H	1.79	0.48
2:D:936:LYS:N	2:D:936:LYS:HD2	2.29	0.48
2:D:724:ARG:HG3	2:D:725:GLU:OE2	2.14	0.47
1:A:712:GLU:OE2	1:A:712:GLU:N	2.44	0.47
2:B:727:THR:H	2:B:731:ALA:CB	2.27	0.47
2:B:957:ILE:HD11	2:B:960:ASP:OD2	2.15	0.47
2:D:723:LEU:CD1	2:D:734:GLU:OE2	2.62	0.47
1:A:908:GLY:HA2	2:B:758:LEU:O	2.14	0.47
2:B:683:LEU:HD12	2:B:765:ILE:HD12	1.98	0.46
2:B:805:GLU:HG3	2:B:869:HIS:ND1	2.30	0.46
2:B:918:ASP:O	2:B:921:MET:HB3	2.15	0.46
1:C:845:LYS:HZ2	1:C:846:GLN:HG3	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:666:GLU:CD	2:D:667:PRO:HD2	2.40	0.46
2:D:895:PRO:N	2:D:898:GLU:OE2	2.48	0.46
2:B:831:ASP:OD1	5:B:1001:ADP:O1B	2.34	0.46
1:C:846:GLN:C	1:C:848:LEU:N	2.72	0.46
2:B:730:LYS:N	2:B:730:LYS:HD3	2.31	0.46
2:D:823:THR:HG1	2:D:825:GLN:CD	2.23	0.46
2:D:723:LEU:HD11	2:D:734:GLU:OE2	2.16	0.45
2:B:728:SER:HB3	2:B:730:LYS:HZ2	1.82	0.45
2:D:728:SER:HB2	2:D:730:LYS:H	1.76	0.45
2:D:728:SER:HB2	2:D:731:ALA:H	1.82	0.45
1:C:855:PRO:O	1:C:859:MET:HG3	2.16	0.45
2:B:726:ALA:HB2	2:B:732:ASN:ND2	2.32	0.45
2:D:683:LEU:HD12	2:D:765:ILE:HD12	1.99	0.45
1:C:748:ASP:HB2	1:C:754:ARG:NH1	2.31	0.45
2:D:712:GLU:O	2:D:714:VAL:N	2.50	0.45
2:D:799:LYS:HA	2:D:941:ILE:HD11	1.98	0.45
2:D:823:THR:OG1	2:D:825:GLN:OE1	2.33	0.45
2:B:805:GLU:HG3	2:B:869:HIS:CG	2.52	0.44
2:B:852:VAL:HA	2:B:853:PRO:HD3	1.87	0.44
2:B:857:MET:HE3	2:B:862:ILE:HG12	1.98	0.44
1:C:693:LEU:HD11	1:C:708:VAL:HG13	1.98	0.44
2:D:895:PRO:O	2:D:898:GLU:OE2	2.35	0.44
1:A:923:MET:HE1	2:B:736:LEU:HB3	1.99	0.44
1:C:926:VAL:HG13	2:D:758:LEU:HD11	1.99	0.44
1:A:769:GLN:OE1	1:A:824:LYS:NZ	2.51	0.44
1:A:932:ASP:HB3	1:A:935:ILE:HD12	1.98	0.44
1:C:792:LEU:HD22	1:C:885:LEU:HG	1.99	0.44
2:B:742:MET:HG2	2:B:832:PHE:CD2	2.53	0.43
2:B:896:ALA:C	2:B:897:SER:O	2.61	0.43
2:B:912:PRO:HA	2:B:913:PRO:HD3	1.88	0.43
1:C:694:LYS:HD3	1:C:694:LYS:HA	1.65	0.43
2:D:694:LEU:HD11	2:D:704:LYS:HB2	2.00	0.43
2:B:787:SER:CB	2:B:951:PRO:HB2	2.48	0.43
2:B:894:ILE:HG22	2:B:898:GLU:OE2	2.19	0.43
2:D:728:SER:HB3	2:D:730:LYS:HB2	2.00	0.43
2:B:889:LYS:HA	2:B:890:PRO:HD3	1.87	0.43
2:D:685:GLU:HA	2:D:688:PHE:CE1	2.54	0.43
2:B:723:LEU:HD21	2:B:732:ASN:OD1	2.18	0.43
1:A:739:ASP:OD1	1:A:739:ASP:N	2.36	0.43
1:C:807:GLU:HG3	1:C:871:HIS:CG	2.54	0.43
1:C:896:LEU:HD11	1:C:904:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:894:ILE:HA	2:D:895:PRO:HD2	1.82	0.43
1:A:689:GLU:OE2	1:A:712:GLU:OE2	2.36	0.42
2:D:769:MET:HB3	2:D:822:LYS:HA	2.01	0.42
2:B:723:LEU:HD22	2:B:735:ILE:HG21	2.00	0.42
2:D:700:GLY:HA3	2:D:723:LEU:HA	2.01	0.42
1:A:745:GLY:HA2	1:A:755:LEU:HD23	2.01	0.42
2:D:771:PHE:CD1	2:D:823:THR:HA	2.54	0.42
1:A:793:LEU:O	1:A:797:VAL:HG23	2.19	0.42
1:C:710:ILE:HA	1:C:711:PRO:HD2	1.76	0.42
2:D:748:PRO:O	2:D:828:LYS:HE3	2.20	0.42
2:D:912:PRO:HA	2:D:913:PRO:HD3	1.85	0.42
2:B:782:LYS:HE2	2:B:782:LYS:HB2	1.88	0.42
2:D:747:ASN:OD1	2:D:748:PRO:HD2	2.19	0.42
1:A:741:MET:HE2	1:A:764:LEU:HD22	2.03	0.41
2:B:728:SER:CB	2:B:730:LYS:HZ2	2.34	0.41
2:D:838:LEU:HD21	2:D:845:TYR:HB2	2.02	0.41
1:A:901:VAL:HB	1:A:902:PRO:HD3	2.02	0.41
1:C:927:LYS:HZ3	2:D:733:LYS:HE3	1.85	0.41
2:D:810:VAL:HG12	2:D:812:ARG:HG3	2.03	0.41
2:D:787:SER:CB	2:D:951:PRO:HB2	2.49	0.41
1:A:896:LEU:HB3	1:A:900:GLU:HG3	2.03	0.41
1:A:759:CYS:HB3	1:A:765:GLN:HB2	2.03	0.41
2:B:781:HIS:O	2:B:785:ILE:HG13	2.21	0.41
2:B:919:VAL:HG12	2:B:923:MET:HE3	2.02	0.41
1:C:918:THR:HG23	1:C:921:VAL:H	1.85	0.41
2:D:825:GLN:H	2:D:825:GLN:HG3	1.71	0.40
2:D:892:ASP:C	2:D:894:ILE:H	2.26	0.40
2:D:898:GLU:H	2:D:898:GLU:HG3	1.29	0.40
2:D:902:ILE:CG2	2:D:907:GLU:HG2	2.52	0.40
1:A:791:LEU:HD23	1:A:791:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/326 (81%)	259 (98%)	5 (2%)	1 (0%)	30	62
1	C	271/326 (83%)	265 (98%)	6 (2%)	0	100	100
2	B	289/345 (84%)	271 (94%)	13 (4%)	5 (2%)	7	30
2	D	295/345 (86%)	276 (94%)	14 (5%)	5 (2%)	7	30
All	All	1120/1342 (84%)	1071 (96%)	38 (3%)	11 (1%)	12	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	747	LEU
2	B	897	SER
2	B	898	GLU
2	D	713	LYS
2	B	672	GLY
2	B	831	ASP
2	D	728	SER
2	D	831	ASP
2	D	895	PRO
2	D	729	PRO
2	B	728	SER

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	228/277 (82%)	223 (98%)	5 (2%)	45	73
1	C	235/277 (85%)	232 (99%)	3 (1%)	61	81
2	B	258/300 (86%)	250 (97%)	8 (3%)	35	66
2	D	260/300 (87%)	253 (97%)	7 (3%)	39	70
All	All	981/1154 (85%)	958 (98%)	23 (2%)	44	72

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	708	VAL
1	A	712	GLU
1	A	716	ILE
1	A	739	ASP
1	A	945	GLU
2	B	665	VAL
2	B	684	LYS
2	B	696	SER
2	B	723	LEU
2	B	733	LYS
2	B	787	SER
2	B	852	VAL
2	B	956	VAL
1	C	694	LYS
1	C	945	GLU
1	C	960	LYS
2	D	728	SER
2	D	783	ASP
2	D	787	SER
2	D	788	GLN
2	D	825	GLN
2	D	852	VAL
2	D	898	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	820	ASN
1	A	944	ASN
2	B	763	GLN
2	B	846	HIS
2	D	677	GLN
2	D	802	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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
5	ADP	D	1001	4	28,29,29	1.42	4 (14%)	43,45,45	1.82	7 (16%)
5	ADP	B	1001	4	28,29,29	1.42	4 (14%)	43,45,45	1.86	9 (20%)
3	ANP	C	1101	4	33,33,33	0.99	4 (12%)	45,52,52	0.79	0
3	ANP	A	1101	4	33,33,33	0.96	4 (12%)	45,52,52	0.79	2 (4%)

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
5	ADP	D	1001	4	-	1/16/32/32	0/3/3/3
5	ADP	B	1001	4	-	6/16/32/32	0/3/3/3
3	ANP	C	1101	4	-	4/18/38/38	0/3/3/3
3	ANP	A	1101	4	-	7/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1001	ADP	C5-C4	4.93	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	ADP	C5-C4	4.75	1.47	1.39
5	B	1001	ADP	C5-C6	2.75	1.48	1.41
3	C	1101	ANP	PG-N3B	2.69	1.70	1.63
5	D	1001	ADP	C5-C6	2.65	1.48	1.41
3	A	1101	ANP	PG-N3B	2.60	1.70	1.63
3	C	1101	ANP	PG-O1G	2.57	1.50	1.46
3	A	1101	ANP	PG-O1G	2.50	1.50	1.46
3	C	1101	ANP	PB-O1B	2.48	1.49	1.46
3	A	1101	ANP	PB-O1B	2.45	1.49	1.46
5	D	1001	ADP	C5-N7	-2.36	1.34	1.39
5	B	1001	ADP	C8-N7	2.36	1.36	1.31
5	B	1001	ADP	C5-N7	-2.24	1.35	1.39
5	D	1001	ADP	C8-N7	2.19	1.35	1.31
3	C	1101	ANP	PB-N3B	2.13	1.68	1.63
3	A	1101	ANP	PB-N3B	2.13	1.68	1.63

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1001	ADP	C5-C4-N3	-5.98	118.48	126.72
5	B	1001	ADP	C5-C4-N3	-5.84	118.68	126.72
5	D	1001	ADP	N3-C4-N9	4.71	135.18	127.17
5	B	1001	ADP	N3-C4-N9	4.69	135.15	127.17
5	B	1001	ADP	C2-N3-C4	3.72	120.91	111.83
5	D	1001	ADP	C2-N3-C4	3.65	120.74	111.83
5	B	1001	ADP	C4-C5-N7	-3.33	106.78	110.58
5	B	1001	ADP	N3-C2-N1	-3.29	123.60	128.58
5	D	1001	ADP	N3-C2-N1	-3.13	123.84	128.58
5	D	1001	ADP	C4-C5-N7	-3.10	107.03	110.58
5	B	1001	ADP	C4-N9-C8	2.63	108.50	105.74
5	B	1001	ADP	C3'-C2'-C1'	2.63	106.43	101.46
5	D	1001	ADP	C5'-C4'-C3'	-2.46	106.34	115.21
5	B	1001	ADP	C5-N7-C8	2.45	107.30	103.45
3	A	1101	ANP	O1B-PB-N3B	-2.16	108.58	111.77
5	D	1001	ADP	C5-N7-C8	2.08	106.72	103.45
3	A	1101	ANP	O2B-PB-O3A	2.03	111.42	104.64
5	B	1001	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

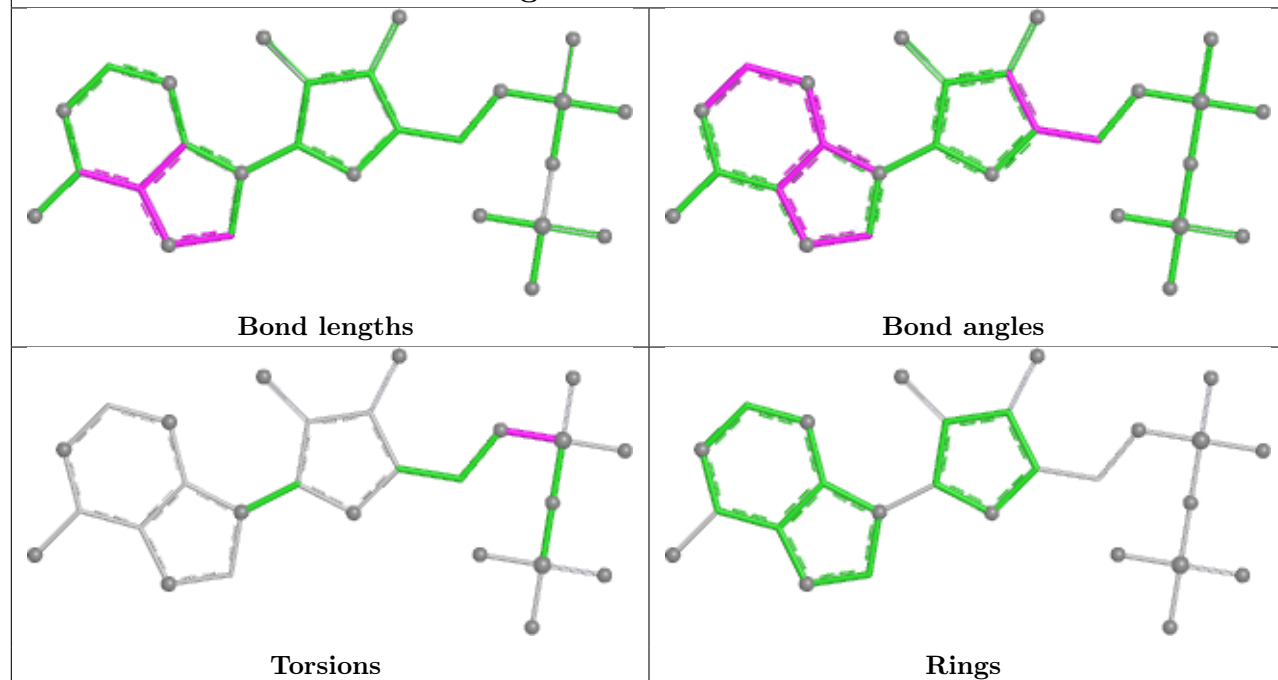
There are no ring outliers.

3 monomers are involved in 4 short contacts:

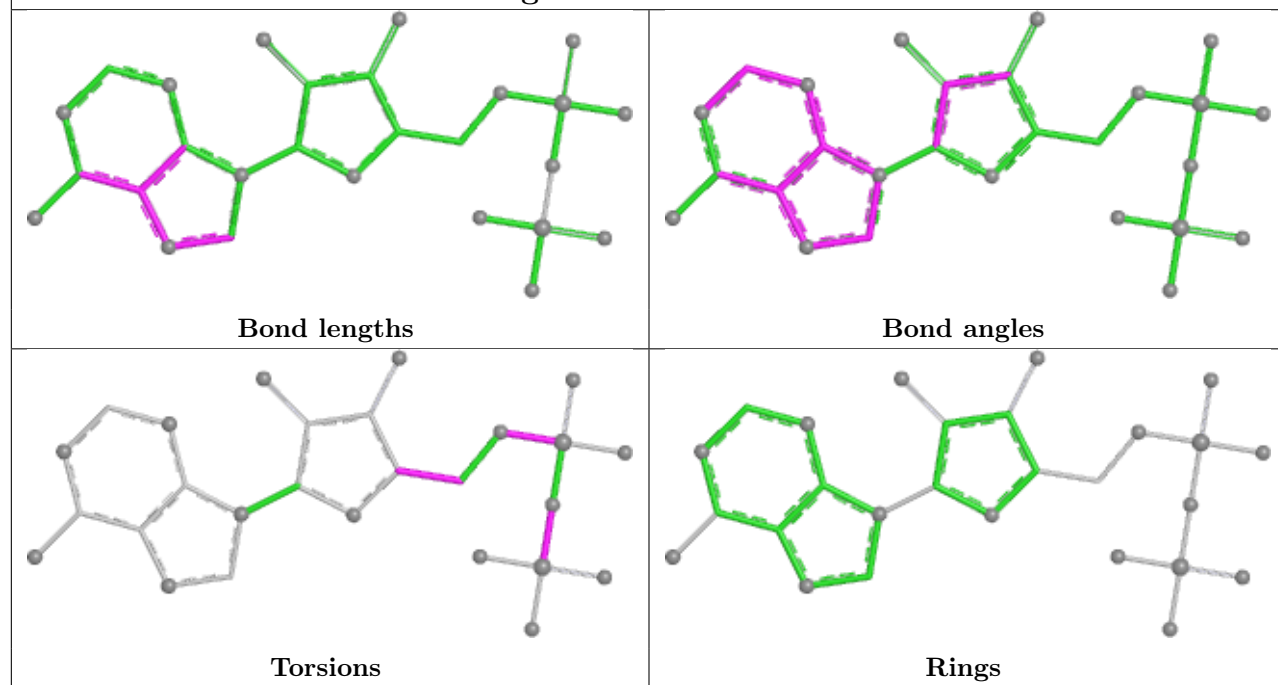
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1001	ADP	2	0
5	B	1001	ADP	1	0
3	C	1101	ANP	1	0

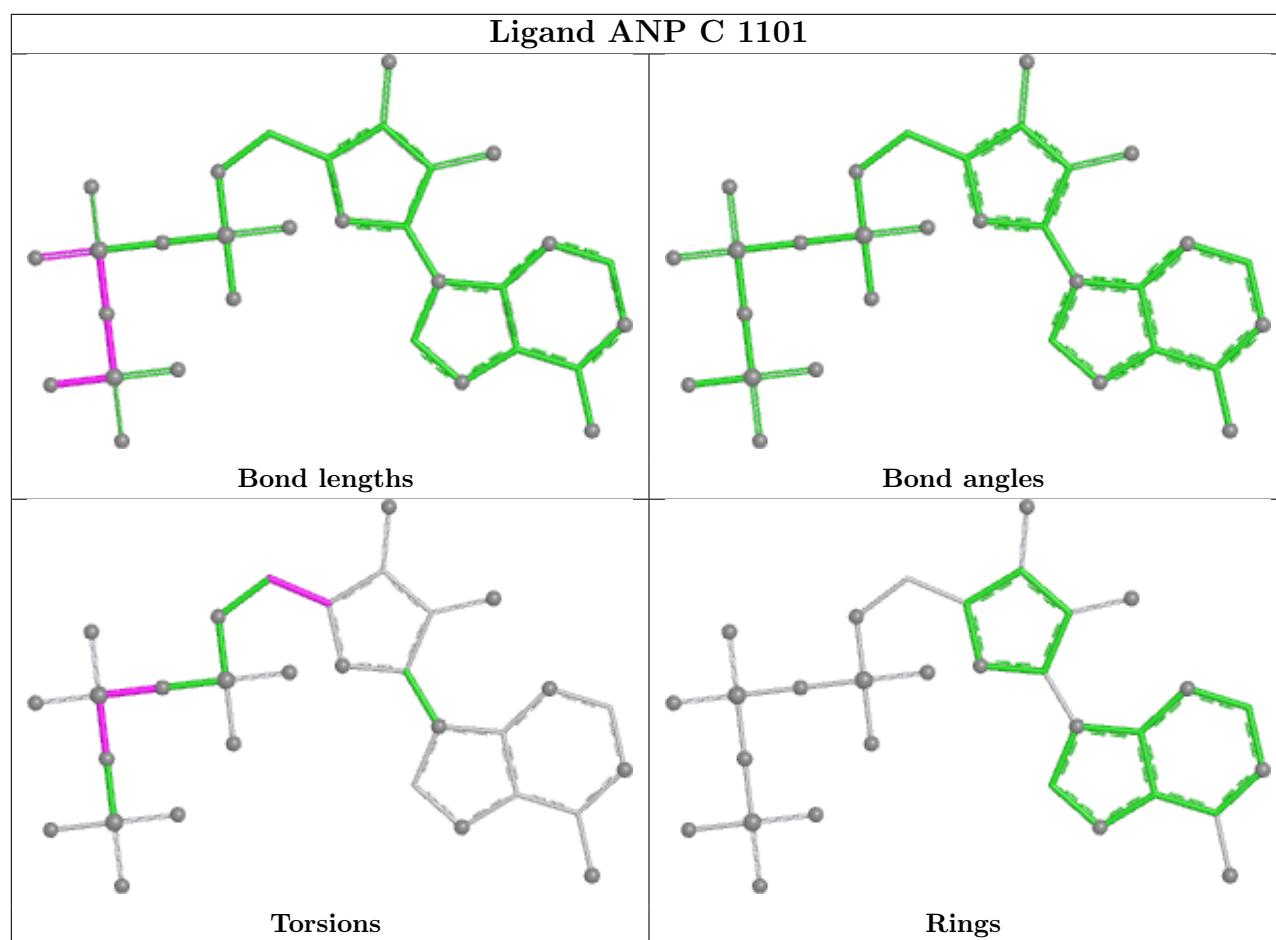
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

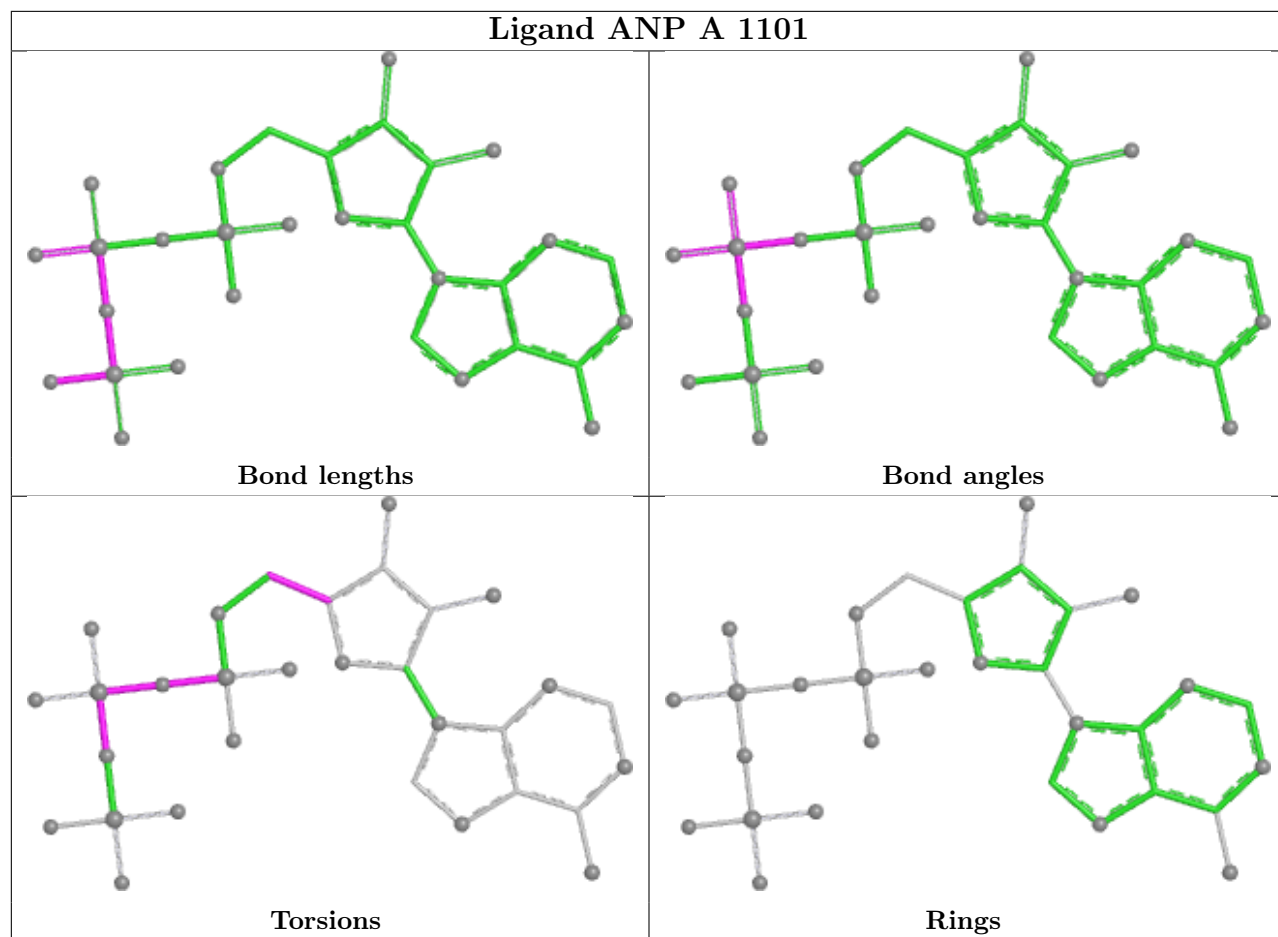
Ligand ADP D 1001



Ligand ADP B 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%)	0.48	12 (4%) 38 23	18, 38, 67, 110	0
1	C	275/326 (84%)	0.45	21 (7%) 20 12	17, 37, 72, 107	0
2	B	293/345 (84%)	0.91	44 (15%) 5 4	20, 42, 98, 123	0
2	D	297/345 (86%)	0.93	46 (15%) 5 3	20, 44, 93, 128	0
All	All	1134/1342 (84%)	0.70	123 (10%) 11 7	17, 41, 88, 128	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	729	PRO	6.7
2	B	730	LYS	6.4
2	B	729	PRO	5.9
2	B	664	LEU	5.6
2	B	751	CYS	5.3
1	A	680	VAL	4.9
2	B	732	ASN	4.8
2	B	668	LEU	4.8
2	B	731	ALA	4.7
2	D	710	GLU	4.6
2	D	727	THR	4.5
2	D	730	LYS	4.4
2	D	668	LEU	4.3
2	D	825	GLN	4.2
2	D	959	GLY	4.1
2	B	728	SER	4.1
1	C	680	VAL	4.0
2	D	666	GLU	3.9
2	B	714	VAL	3.8
2	D	711	GLY	3.8
2	D	849	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	696	SER	3.7
2	B	895	PRO	3.7
2	B	725	GLU	3.6
2	D	783	ASP	3.6
2	B	724	ARG	3.4
2	B	723	LEU	3.4
2	D	698	ALA	3.4
2	D	732	ASN	3.4
1	C	847	LEU	3.3
2	B	726	ALA	3.3
2	D	831	ASP	3.3
2	D	664	LEU	3.3
1	C	945	GLU	3.2
1	C	844	ASP	3.2
2	D	726	ALA	3.1
2	D	784	ASN	3.1
2	B	727	THR	3.1
2	B	958	GLN	3.1
1	A	960	LYS	3.1
2	B	825	GLN	3.0
2	D	671	SER	3.0
2	B	713	LYS	3.0
2	D	734	GLU	3.0
1	C	726	GLU	3.0
2	B	665	VAL	3.0
2	B	666	GLU	2.9
1	A	682	ALA	2.9
1	A	712	GLU	2.9
2	B	960	ASP	2.9
2	D	665	VAL	2.9
2	D	728	SER	2.9
2	D	823	THR	2.8
2	D	713	LYS	2.8
2	D	672	GLY	2.8
2	D	841	GLU	2.8
1	C	742	LEU	2.8
2	D	895	PRO	2.8
2	B	715	LYS	2.7
2	D	960	ASP	2.7
1	C	788	GLY	2.7
2	D	898	GLU	2.7
2	D	731	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	784	ASN	2.7
2	B	896	ALA	2.7
2	B	700	GLY	2.7
1	C	846	GLN	2.7
2	B	852	VAL	2.7
2	D	714	VAL	2.6
2	D	725	GLU	2.6
2	B	847	ALA	2.6
2	B	671	SER	2.6
1	A	945	GLU	2.6
2	D	699	PHE	2.6
2	B	699	PHE	2.5
2	B	667	PRO	2.5
1	A	746	SER	2.5
2	B	898	GLU	2.5
2	B	752	ARG	2.5
2	B	952	GLN	2.5
2	D	700	GLY	2.4
1	C	762	SER	2.4
1	C	852	ALA	2.4
2	B	831	ASP	2.4
2	D	667	PRO	2.4
2	B	907	GLU	2.4
2	D	723	LEU	2.4
2	D	735	ILE	2.4
1	C	808	GLU	2.4
2	D	709	PRO	2.3
2	B	806	ASP	2.3
1	C	682	ALA	2.3
1	A	681	LEU	2.3
1	A	742	LEU	2.2
1	C	733	SER	2.2
2	B	811	HIS	2.2
1	C	842	PRO	2.2
1	C	933	GLU	2.2
2	D	673	GLU	2.2
2	D	850	GLY	2.2
1	C	694	LYS	2.2
2	D	824	PRO	2.2
1	A	733	SER	2.2
1	C	960	LYS	2.1
1	C	681	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	837	LEU	2.1
1	C	712	GLU	2.1
2	B	897	SER	2.1
2	B	905	LYS	2.1
1	C	897	ARG	2.1
1	A	736	ALA	2.1
2	D	715	LYS	2.1
2	D	826	HIS	2.1
2	B	672	GLY	2.1
1	A	897	ARG	2.1
2	B	735	ILE	2.1
2	B	843	LYS	2.0
2	D	782	LYS	2.0
1	A	842	PRO	2.0
2	D	670	PRO	2.0
2	D	751	CYS	2.0
1	C	843	ASP	2.0
2	D	907	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
5	ADP	B	1001	27/27	0.77	0.19	62,74,145,146	0
5	ADP	D	1001	27/27	0.77	0.17	50,62,144,145	0
4	MG	B	1002	1/1	0.84	0.10	60,60,60,60	0
4	MG	D	1002	1/1	0.92	0.07	59,59,59,59	0
3	ANP	A	1101	31/31	0.94	0.10	25,42,62,89	0

Continued on next page...

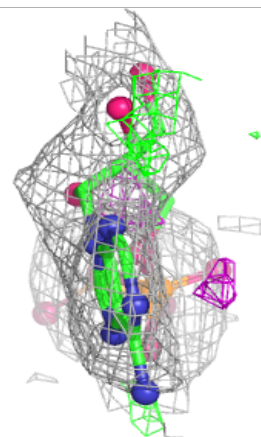
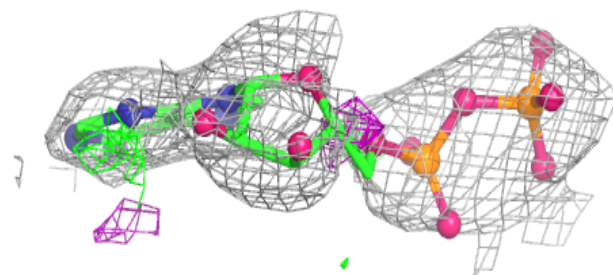
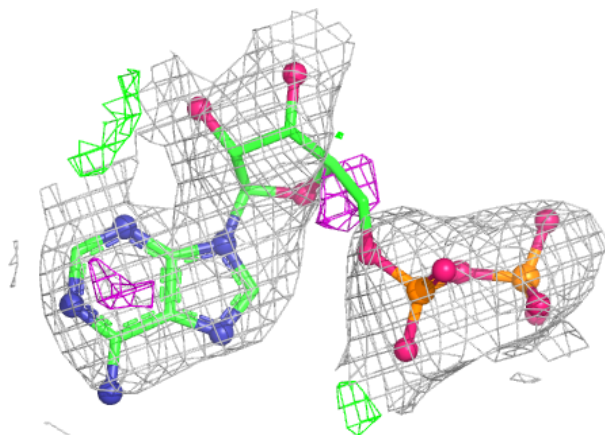
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	1102	1/1	0.96	0.09	23,23,23,23	0
3	ANP	C	1101	31/31	0.96	0.08	17,31,47,79	0
4	MG	C	1102	1/1	0.96	0.14	17,17,17,17	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.

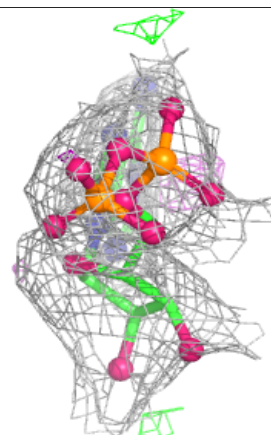
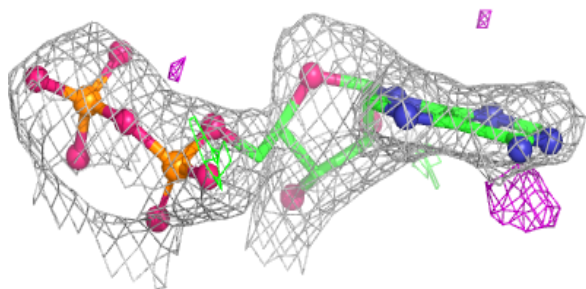
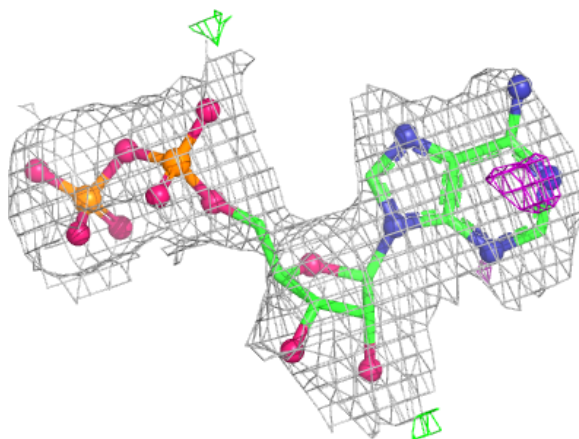
Electron density around ADP B 1001:

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

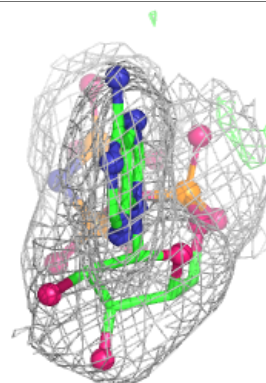
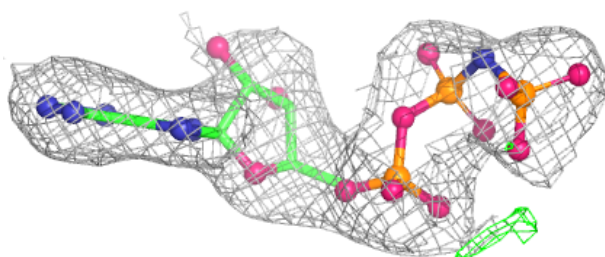
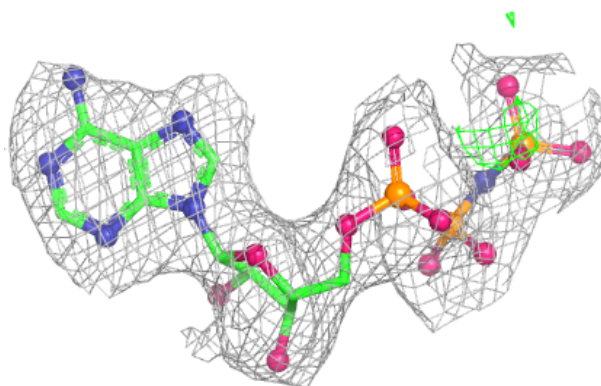


Electron density around ADP D 1001:

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

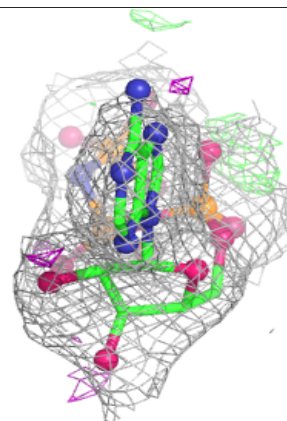
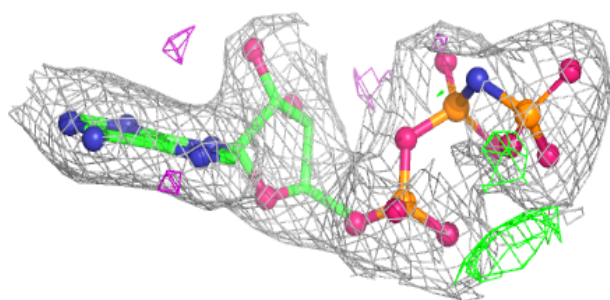
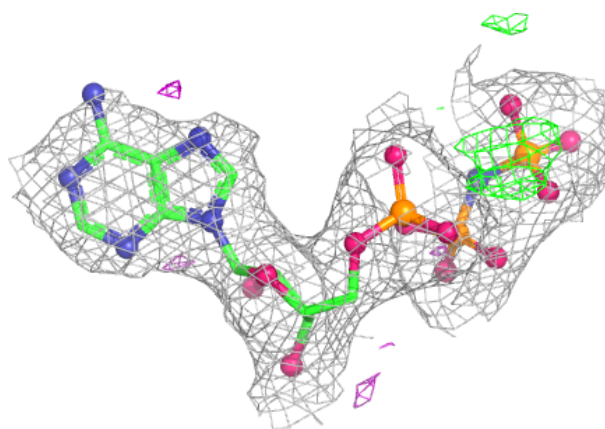
**Electron density around ANP A 1101:**

$2mF_o - DF_c$ (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.