Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 07:04 PM EDT

PDB ID	:	4Q5J
Title	:	Crystal structure of SeMet derivative BRI1 in complex with BKI1
Authors	:	Wang, J.; Wang, J.; Chen, L.; Wu, J.W.; Wang, Z.X.
Deposited on	:	2014-04-17
Resolution	:	2.77 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:

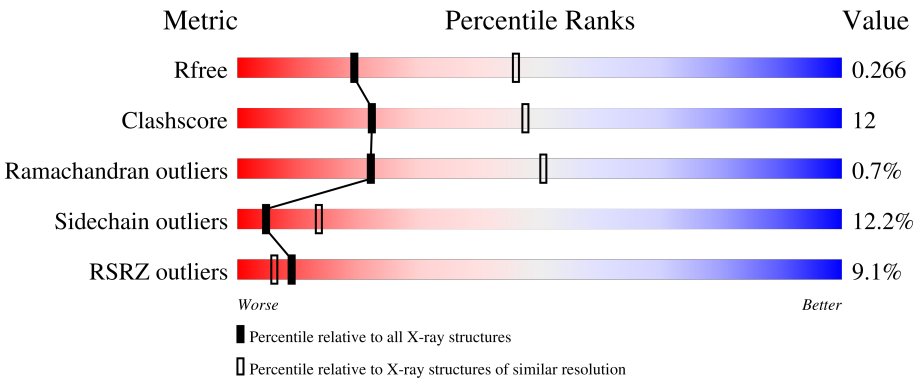
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	341	7%, 61%, 25%, •, 13%
1	B	341	6%, 58%, 24%, •, 14%
2	E	21	24%, 38%, 29%, 5%, 29%
2	F	21	19%, 38%, 33%, 5%, 24%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4912 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 Protein BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S	Se			
1	A	298	2319	1468	397	434	4	4	12	0	0	0
1	B	294	2304	1463	398	423	4	4	12	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	840	MSE	-	expression tag	UNP O22476
A	841	GLY	-	expression tag	UNP O22476
A	842	SER	-	expression tag	UNP O22476
A	843	SER	-	expression tag	UNP O22476
A	844	HIS	-	expression tag	UNP O22476
A	845	HIS	-	expression tag	UNP O22476
A	846	HIS	-	expression tag	UNP O22476
A	847	HIS	-	expression tag	UNP O22476
A	848	HIS	-	expression tag	UNP O22476
A	849	HIS	-	expression tag	UNP O22476
A	850	SER	-	expression tag	UNP O22476
A	851	GLN	-	expression tag	UNP O22476
A	852	ASP	-	expression tag	UNP O22476
A	853	LEU	-	expression tag	UNP O22476
A	854	GLU	-	expression tag	UNP O22476
A	855	VAL	-	expression tag	UNP O22476
A	856	LEU	-	expression tag	UNP O22476
A	857	PHE	-	expression tag	UNP O22476
A	858	GLN	-	expression tag	UNP O22476
A	859	GLY	-	expression tag	UNP O22476
A	860	PRO	-	expression tag	UNP O22476
A	861	HIS	-	expression tag	UNP O22476
A	862	MSE	-	expression tag	UNP O22476
B	840	MSE	-	expression tag	UNP O22476
B	841	GLY	-	expression tag	UNP O22476

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	842	SER	-	expression tag	UNP O22476
B	843	SER	-	expression tag	UNP O22476
B	844	HIS	-	expression tag	UNP O22476
B	845	HIS	-	expression tag	UNP O22476
B	846	HIS	-	expression tag	UNP O22476
B	847	HIS	-	expression tag	UNP O22476
B	848	HIS	-	expression tag	UNP O22476
B	849	HIS	-	expression tag	UNP O22476
B	850	SER	-	expression tag	UNP O22476
B	851	GLN	-	expression tag	UNP O22476
B	852	ASP	-	expression tag	UNP O22476
B	853	LEU	-	expression tag	UNP O22476
B	854	GLU	-	expression tag	UNP O22476
B	855	VAL	-	expression tag	UNP O22476
B	856	LEU	-	expression tag	UNP O22476
B	857	PHE	-	expression tag	UNP O22476
B	858	GLN	-	expression tag	UNP O22476
B	859	GLY	-	expression tag	UNP O22476
B	860	PRO	-	expression tag	UNP O22476
B	861	HIS	-	expression tag	UNP O22476
B	862	MSE	-	expression tag	UNP O22476

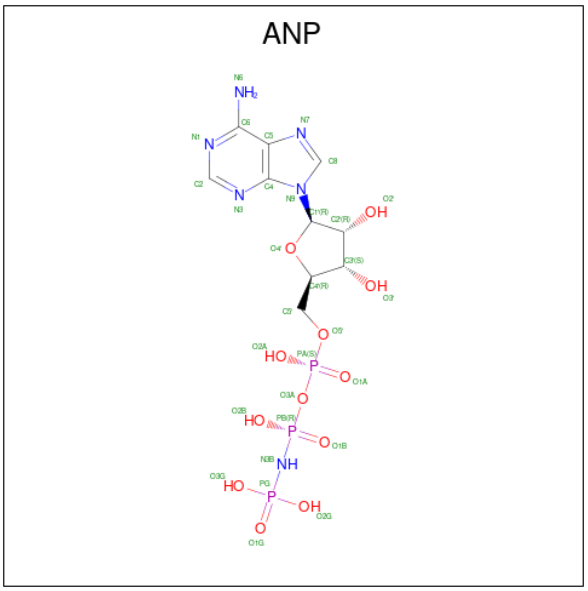
- Molecule 2 is a protein called BRI1 kinase inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	16	116	71	20	23	2	0	0	0
			Total	C	N	O	S			
2	E	15	109	67	19	21	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	326	TYR	-	expression tag	UNP Q9FMZ0
E	326	TYR	-	expression tag	UNP Q9FMZ0

- 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	B	1	31	10	6	12	3	0	0

- Molecule 4 is water.

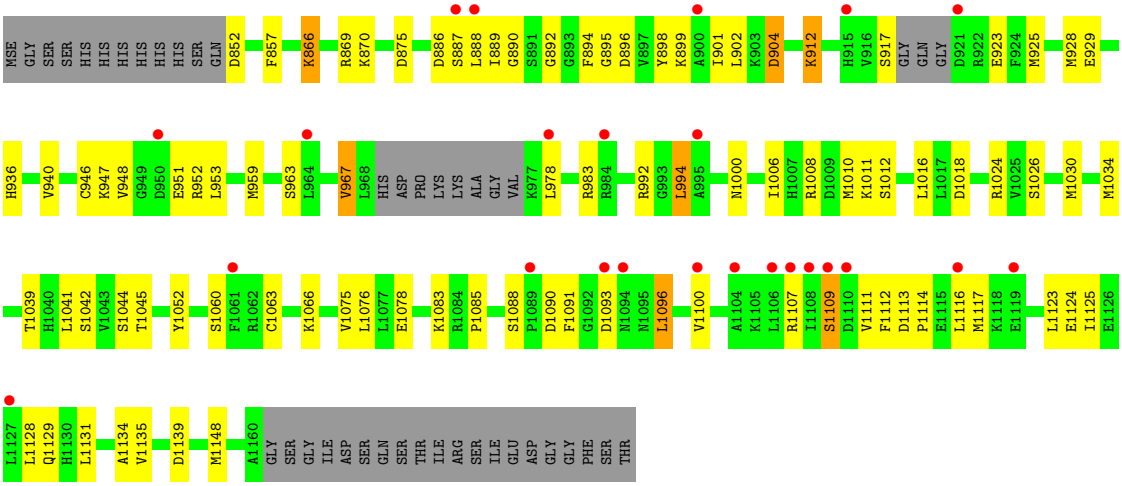
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	2	2	2	0	0

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.

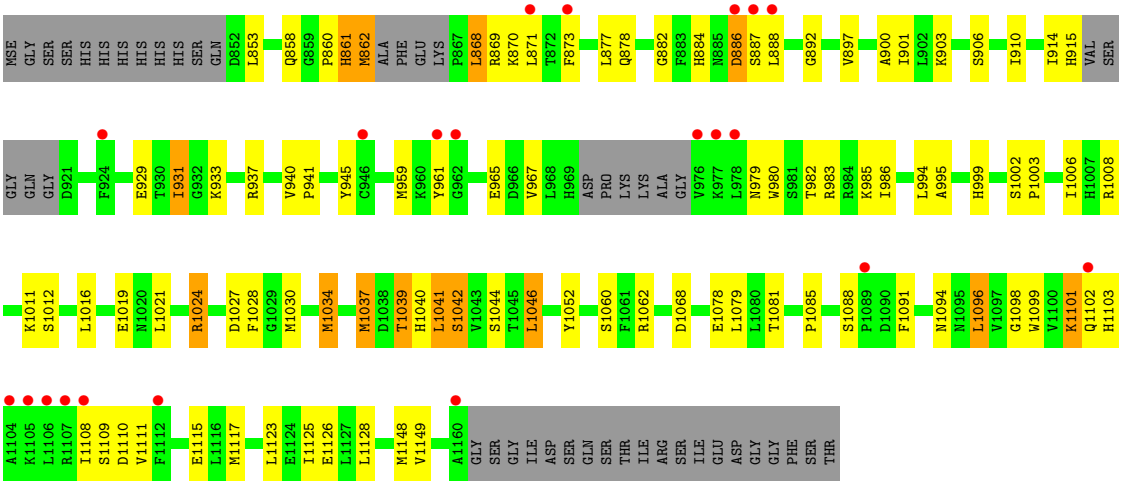
• Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1

Chain A: 7% 61% 25% • 13%



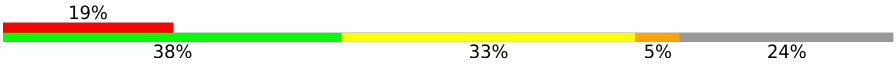
• Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1

Chain B: 6% 58% 24% • 14%



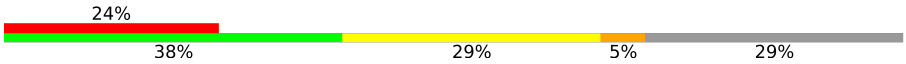
• Molecule 2: BRI1 kinase inhibitor 1

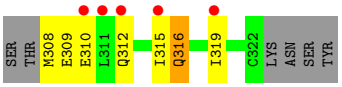
Chain F:



- Molecule 2: BRI1 kinase inhibitor 1

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.72Å 80.29Å 80.56Å 90.00° 109.55° 90.00°	Depositor
Resolution (Å)	38.41 – 2.77 38.41 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.41-2.77) 98.8 (38.41-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.66 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.201 , 0.259 0.207 , 0.266	Depositor DCC
R_{free} test set	990 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4912	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: ANP, SEP, TPO

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	0.62	0/2309	0.77	0/3096
1	B	0.61	0/2294	0.76	4/3070 (0.1%)
2	E	0.32	0/109	0.50	0/146
2	F	0.31	0/116	0.55	0/156
All	All	0.60	0/4828	0.76	4/6468 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1041	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	B	1008	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	1068	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	1037	MSE	CG-SE-CE	-5.28	87.29	98.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2319	0	2250	49	0
1	B	2304	0	2275	55	0
2	E	109	0	106	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	116	0	113	5	0
3	A	31	0	13	2	0
3	B	31	0	13	2	0
4	A	2	0	0	0	0
All	All	4912	0	4770	113	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 (113) 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:B:1091:PHE:HB3	1:B:1094:ASN:O	1.80	0.81
1:B:940:VAL:HG11	1:B:1016:LEU:HD12	1.60	0.81
1:A:1125:ILE:HA	1:A:1128:LEU:HD12	1.66	0.77
1:B:1098:GLY:HA2	1:B:1101:LYS:HD2	1.65	0.77
3:A:1201:ANP:O2B	3:A:1201:ANP:H5'1	1.88	0.73
1:A:1076:LEU:HD23	1:A:1134:ALA:HB2	1.71	0.73
1:A:888:LEU:HD11	1:A:896:ASP:HB3	1.71	0.72
1:B:995:ALA:O	1:B:999:HIS:HB2	1.89	0.71
1:A:940:VAL:HG11	1:A:1016:LEU:HD12	1.72	0.71
1:B:1039:TPO:O2P	1:B:1040:HIS:ND1	2.18	0.71
1:A:994:LEU:HD11	1:A:1010:MSE:HG3	1.74	0.70
1:B:1101:LYS:HE3	2:F:308:MET:HE2	1.80	0.64
1:A:1088:SER:HB2	1:A:1091:PHE:CZ	2.33	0.63
1:A:994:LEU:HB3	1:A:1148:MSE:HG3	1.81	0.62
1:B:1103:HIS:CE1	1:B:1110:ASP:HB3	2.34	0.61
1:A:852:ASP:N	1:A:852:ASP:OD1	2.33	0.60
1:A:959:MSE:CE	1:A:1024:ARG:HG3	2.32	0.59
1:A:1006:ILE:HD11	1:A:1034:MSE:HE2	1.83	0.59
1:B:873:PHE:HE1	1:B:877:LEU:HG	1.67	0.59
1:B:982:THR:O	1:B:986:ILE:HG13	2.03	0.59
1:A:1131:LEU:O	1:A:1135:VAL:HG23	2.03	0.59
1:B:1128:LEU:HD22	2:F:315:ILE:HG23	1.84	0.59
1:B:914:ILE:O	1:B:915:HIS:HB2	2.03	0.59
1:B:1108:ILE:O	1:B:1111:VAL:HG12	2.03	0.57
1:A:1112:PHE:HE1	1:A:1131:LEU:HD22	1.68	0.57
1:A:925:MSE:O	1:A:929:GLU:HG2	2.04	0.57
1:B:861:HIS:CD2	1:B:862:MSE:H	2.23	0.56
2:F:312:GLN:HG2	2:F:313:ALA:N	2.21	0.56
1:A:857:PHE:CD2	1:A:1000:ASN:HB2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:ILE:HD11	1:A:899:LYS:HB2	1.88	0.56
1:B:873:PHE:CE1	1:B:877:LEU:HG	2.41	0.56
1:B:892:GLY:HA2	3:B:1201:ANP:HNB1	1.71	0.55
1:B:1099:TRP:CZ3	1:B:1111:VAL:HG23	2.41	0.55
1:B:1088:SER:HB3	1:B:1091:PHE:CE2	2.41	0.55
1:A:936:HIS:HE1	1:A:992:ARG:HG2	1.72	0.54
1:A:959:MSE:HE1	1:A:1018:ASP:HB3	1.88	0.54
1:B:1103:HIS:HE1	1:B:1110:ASP:HB3	1.73	0.54
1:A:1008:ARG:HD3	1:A:1063:CYS:SG	2.47	0.54
1:A:1011:LYS:HB2	1:A:1052:TYR:CZ	2.42	0.54
1:A:1078:GLU:HG3	1:A:1083:LYS:O	2.08	0.54
1:B:1011:LYS:NZ	3:B:1201:ANP:O1G	2.42	0.53
2:E:315:ILE:O	2:E:319:ILE:HG13	2.09	0.53
1:B:931:ILE:HD13	1:B:1028:PHE:CE1	2.44	0.52
1:B:1052:TYR:CE2	1:B:1085:PRO:HG3	2.44	0.52
1:B:994:LEU:HB3	1:B:1148:MSE:HG3	1.92	0.52
1:A:963:SER:O	1:A:967:VAL:HG23	2.10	0.51
1:A:1010:MSE:HE3	1:A:1075:VAL:HG21	1.92	0.51
1:B:870:LYS:HD3	1:B:945:TYR:CZ	2.45	0.51
1:A:959:MSE:HE2	1:A:1024:ARG:HG3	1.93	0.51
2:E:316:GLN:HA	2:E:319:ILE:HD12	1.92	0.51
1:A:1085:PRO:HA	1:A:1096:LEU:HD22	1.91	0.51
1:A:1034:MSE:HG3	1:A:1041:LEU:HB2	1.93	0.51
1:B:861:HIS:CG	1:B:862:MSE:H	2.29	0.51
1:B:1034:MSE:HG3	1:B:1041:LEU:HB2	1.93	0.50
1:A:1139:ASP:HA	2:E:308:MET:HE1	1.94	0.49
1:B:980:TRP:HE1	1:B:1126:GLU:CD	2.16	0.49
1:B:1034:MSE:CG	1:B:1041:LEU:HB2	2.43	0.48
1:B:1042:SEP:O1P	1:B:1062:ARG:NH2	2.46	0.48
1:B:877:LEU:HD23	1:B:882:GLY:HA2	1.95	0.48
1:B:982:THR:HG21	1:B:1021:LEU:HD13	1.96	0.48
1:A:959:MSE:HE1	1:A:1024:ARG:HG3	1.95	0.47
1:B:1002:SER:HA	1:B:1003:PRO:C	2.34	0.47
1:A:912:LYS:HE3	1:A:951:GLU:OE1	2.15	0.47
1:A:904:ASP:N	1:A:904:ASP:OD1	2.46	0.47
1:B:961:TYR:HB3	1:B:967:VAL:HG21	1.96	0.47
1:A:1006:ILE:CD1	1:A:1034:MSE:HE2	2.44	0.47
1:A:940:VAL:CG1	1:A:1016:LEU:HD12	2.42	0.46
1:A:983:ARG:HD2	1:A:1116:LEU:HD21	1.96	0.46
1:B:937:ARG:O	1:B:1024:ARG:HD3	2.16	0.46
1:B:861:HIS:CG	1:B:862:MSE:N	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:TYR:HE2	1:A:912:LYS:HB2	1.81	0.46
1:A:1113:ASP:HA	1:A:1114:PRO:HD2	1.82	0.45
1:B:1098:GLY:O	1:B:1102:GLN:HG2	2.16	0.45
1:B:884:HIS:ND1	1:B:886:ASP:HB2	2.32	0.44
2:E:308:MET:HB3	2:E:309:GLU:OE1	2.16	0.44
1:B:929:GLU:OE1	1:B:933:LYS:HE3	2.17	0.44
1:B:983:ARG:NH1	1:B:1079:LEU:O	2.50	0.44
1:B:1081:THR:HG22	1:B:1111:VAL:HG22	1.99	0.44
3:A:1201:ANP:H5'1	3:A:1201:ANP:PB	2.57	0.44
1:B:1016:LEU:O	1:B:1024:ARG:N	2.45	0.44
1:B:1099:TRP:O	1:B:1103:HIS:HB2	2.18	0.44
1:A:959:MSE:CE	1:A:1018:ASP:HB3	2.48	0.44
1:A:1066:LYS:HD3	1:A:1066:LYS:HA	1.80	0.44
1:B:1012:SER:OG	1:B:1078:GLU:OE2	2.21	0.44
1:A:866:LYS:HE2	1:A:866:LYS:HB2	1.70	0.43
1:A:946:CYS:HB3	1:A:953:LEU:HB2	1.99	0.43
1:B:1006:ILE:HD11	1:B:1034:MSE:HG3	2.00	0.43
1:A:936:HIS:CE1	1:A:992:ARG:HG2	2.51	0.43
1:A:948:VAL:HG23	1:A:951:GLU:HB2	2.01	0.43
1:B:999:HIS:ND1	1:B:1149:VAL:HG23	2.33	0.43
1:A:1011:LYS:HB2	1:A:1052:TYR:CE2	2.53	0.43
1:B:940:VAL:HG12	1:B:959:MSE:HE3	2.00	0.43
1:B:900:ALA:CB	1:B:910:ILE:HD11	2.49	0.42
1:B:940:VAL:HA	1:B:941:PRO:HD3	1.84	0.42
1:B:1085:PRO:HA	1:B:1096:LEU:HB2	2.00	0.42
1:A:890:GLY:O	1:A:896:ASP:HA	2.20	0.42
1:A:928:MSE:HE3	1:A:928:MSE:HB3	1.98	0.42
1:B:994:LEU:HA	1:B:994:LEU:HD23	1.63	0.42
1:A:894:PHE:CD2	1:A:923:GLU:HG2	2.55	0.42
1:B:868:LEU:HA	1:B:868:LEU:HD22	1.83	0.42
1:A:857:PHE:CE2	1:A:1000:ASN:HB2	2.55	0.41
1:A:1128:LEU:HB3	2:E:319:ILE:HG12	2.03	0.41
1:B:869:ARG:O	1:B:871:LEU:HD12	2.20	0.41
1:B:931:ILE:O	1:B:931:ILE:HG13	2.20	0.41
2:F:309:GLU:HA	2:F:312:GLN:CD	2.41	0.41
2:E:309:GLU:OE1	2:E:309:GLU:N	2.46	0.41
1:A:892:GLY:HA3	1:A:895:GLY:O	2.21	0.41
1:B:1046:LEU:HD12	1:B:1046:LEU:HA	1.85	0.40
2:F:309:GLU:HA	2:F:312:GLN:OE1	2.21	0.40
1:A:1109:SER:O	1:A:1117:MSE:HE2	2.21	0.40
1:B:900:ALA:HB3	1:B:910:ILE:HD11	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1109:SER:HB3	1:B:1117:MSE:CE	2.52	0.40
1:A:947:LYS:HE3	1:A:952:ARG:NH2	2.36	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	288/341 (84%)	270 (94%)	17 (6%)	1 (0%)	41	70
1	B	282/341 (83%)	268 (95%)	11 (4%)	3 (1%)	14	38
2	E	13/21 (62%)	13 (100%)	0	0	100	100
2	F	14/21 (67%)	14 (100%)	0	0	100	100
All	All	597/724 (82%)	565 (95%)	28 (5%)	4 (1%)	22	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	860	PRO
1	B	1027	ASP
1	B	861	HIS
1	A	967	VAL

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	239/273 (88%)	212 (89%)	27 (11%)	6 16
1	B	240/273 (88%)	213 (89%)	27 (11%)	6 16
2	E	10/16 (62%)	7 (70%)	3 (30%)	0 0
2	F	11/16 (69%)	7 (64%)	4 (36%)	0 0
All	All	500/578 (86%)	439 (88%)	61 (12%)	5 13

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	866	LYS
1	A	869	ARG
1	A	870	LYS
1	A	875	ASP
1	A	886	ASP
1	A	887	SER
1	A	901	ILE
1	A	902	LEU
1	A	904	ASP
1	A	912	LYS
1	A	917	SER
1	A	978	LEU
1	A	994	LEU
1	A	1012	SER
1	A	1026	SER
1	A	1030	MSE
1	A	1045	THR
1	A	1090	ASP
1	A	1093	ASP
1	A	1096	LEU
1	A	1100	VAL
1	A	1107	ARG
1	A	1109	SER
1	A	1111	VAL
1	A	1123	LEU
1	A	1124	GLU
1	A	1129	GLN
1	B	853	LEU
1	B	858	GLN
1	B	862	MSE
1	B	868	LEU
1	B	878	GLN
1	B	886	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	887	SER
1	B	888	LEU
1	B	897	VAL
1	B	901	ILE
1	B	903	LYS
1	B	906	SER
1	B	931	ILE
1	B	965	GLU
1	B	979	ASN
1	B	985	LYS
1	B	1019	GLU
1	B	1024	ARG
1	B	1030	MSE
1	B	1034	MSE
1	B	1037	MSE
1	B	1046	LEU
1	B	1096	LEU
1	B	1101	LYS
1	B	1115	GLU
1	B	1123	LEU
1	B	1125	ILE
2	F	307	THR
2	F	312	GLN
2	F	316	GLN
2	F	322	CYS
2	E	310	GLU
2	E	312	GLN
2	E	316	GLN

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	936	HIS
1	A	1103	HIS
1	B	861	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	SEP	B	1042	1	8,9,10	1.62	2 (25%)	8,12,14	1.53	1 (12%)
1	SEP	A	1044	1	8,9,10	1.52	1 (12%)	8,12,14	1.61	1 (12%)
1	SEP	A	1060	1	8,9,10	1.64	1 (12%)	8,12,14	1.31	0
1	SEP	A	1042	1	8,9,10	1.61	1 (12%)	8,12,14	0.87	1 (12%)
1	SEP	B	1060	1	8,9,10	1.72	1 (12%)	8,12,14	3.25	5 (62%)
1	TPO	A	1039	1	8,10,11	1.12	0	10,14,16	2.23	2 (20%)
1	TPO	B	1039	1	8,10,11	1.01	0	10,14,16	2.19	2 (20%)
1	SEP	B	1044	1	8,9,10	1.66	1 (12%)	8,12,14	1.04	0

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
1	SEP	B	1042	1	-	1/5/8/10	-
1	SEP	A	1044	1	-	4/5/8/10	-
1	SEP	A	1060	1	-	2/5/8/10	-
1	SEP	A	1042	1	-	1/5/8/10	-
1	SEP	B	1060	1	-	4/5/8/10	-
1	TPO	A	1039	1	-	2/9/11/13	-
1	TPO	B	1039	1	-	1/9/11/13	-
1	SEP	B	1044	1	-	3/5/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1060	SEP	P-O1P	3.56	1.62	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1042	SEP	P-O1P	3.53	1.61	1.50
1	A	1060	SEP	P-O1P	3.49	1.61	1.50
1	B	1044	SEP	P-O1P	3.46	1.61	1.50
1	B	1042	SEP	P-O1P	3.28	1.61	1.50
1	A	1044	SEP	P-O1P	3.20	1.60	1.50
1	B	1042	SEP	P-O2P	2.11	1.63	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1060	SEP	OG-CB-CA	7.06	115.02	108.14
1	B	1039	TPO	P-OG1-CB	-5.83	105.61	123.21
1	A	1039	TPO	P-OG1-CB	-5.58	106.34	123.21
1	A	1039	TPO	CG2-CB-CA	-3.59	106.07	113.16
1	A	1044	SEP	OG-CB-CA	3.51	111.56	108.14
1	B	1060	SEP	O2P-P-OG	3.25	115.38	106.73
1	B	1042	SEP	P-OG-CB	-3.01	110.00	118.30
1	B	1039	TPO	CG2-CB-CA	-2.78	107.68	113.16
1	B	1060	SEP	OG-P-O1P	2.60	113.75	106.47
1	B	1060	SEP	O3P-P-OG	2.43	113.21	106.73
1	B	1060	SEP	P-OG-CB	-2.41	111.66	118.30
1	A	1042	SEP	P-OG-CB	-2.08	112.57	118.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1039	TPO	O-C-CA-CB
1	A	1039	TPO	CB-OG1-P-O1P
1	A	1044	SEP	CB-OG-P-O1P
1	A	1044	SEP	CB-OG-P-O2P
1	A	1044	SEP	CB-OG-P-O3P
1	B	1060	SEP	CA-CB-OG-P
1	B	1060	SEP	CB-OG-P-O2P
1	B	1060	SEP	CB-OG-P-O3P
1	B	1060	SEP	CB-OG-P-O1P
1	A	1044	SEP	CA-CB-OG-P
1	A	1060	SEP	CA-CB-OG-P
1	B	1044	SEP	CA-CB-OG-P
1	A	1060	SEP	N-CA-CB-OG
1	B	1044	SEP	N-CA-CB-OG
1	B	1039	TPO	N-CA-CB-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	1042	SEP	CB-OG-P-O3P
1	B	1042	SEP	CB-OG-P-O2P
1	B	1044	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1042	SEP	1	0
1	B	1039	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	1201	-	29,33,33	1.78	3 (10%)	31,52,52	1.39	5 (16%)
3	ANP	B	1201	-	29,33,33	1.88	5 (17%)	31,52,52	1.04	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	1201	-	-	8/14/38/38	0/3/3/3
3	ANP	B	1201	-	-	7/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	ANP	PG-O1G	8.13	1.59	1.46
3	A	1201	ANP	PG-O1G	7.84	1.58	1.46
3	A	1201	ANP	PG-N3B	2.67	1.70	1.63
3	B	1201	ANP	PG-N3B	2.65	1.70	1.63
3	B	1201	ANP	PG-O3G	-2.53	1.49	1.56
3	A	1201	ANP	PG-O3G	-2.41	1.50	1.56
3	B	1201	ANP	PB-N3B	2.30	1.69	1.63
3	B	1201	ANP	PB-O1B	2.26	1.49	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1201	ANP	C3'-C2'-C1'	2.76	105.13	100.98
3	A	1201	ANP	O1B-PB-N3B	-2.66	107.85	111.77
3	B	1201	ANP	C5-C6-N6	2.29	123.83	120.35
3	A	1201	ANP	O2G-PG-O1G	-2.27	107.74	113.45
3	B	1201	ANP	O2B-PB-O3A	2.23	112.09	104.64
3	A	1201	ANP	O2B-PB-O3A	2.15	111.83	104.64
3	B	1201	ANP	O1B-PB-N3B	-2.08	108.71	111.77
3	A	1201	ANP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	ANP	PB-N3B-PG-O1G
3	A	1201	ANP	PG-N3B-PB-O1B
3	A	1201	ANP	PG-N3B-PB-O3A
3	A	1201	ANP	C5'-O5'-PA-O3A
3	B	1201	ANP	PB-N3B-PG-O1G
3	B	1201	ANP	PG-N3B-PB-O1B
3	B	1201	ANP	PG-N3B-PB-O3A
3	B	1201	ANP	C5'-O5'-PA-O1A
3	B	1201	ANP	O4'-C4'-C5'-O5'
3	B	1201	ANP	C3'-C4'-C5'-O5'
3	B	1201	ANP	C5'-O5'-PA-O3A
3	A	1201	ANP	C5'-O5'-PA-O1A
3	A	1201	ANP	C5'-O5'-PA-O2A
3	A	1201	ANP	O4'-C4'-C5'-O5'
3	A	1201	ANP	C3'-C4'-C5'-O5'

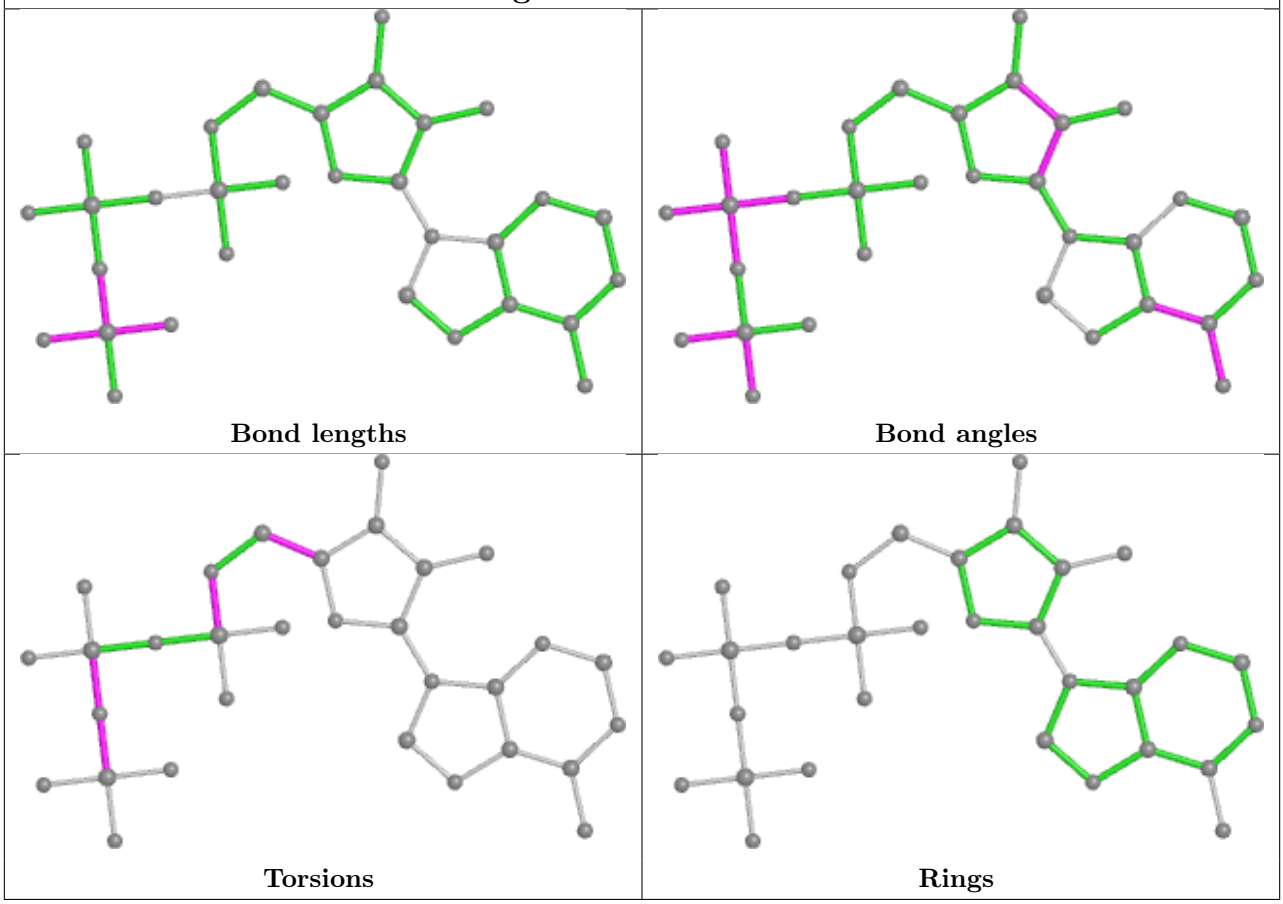
There are no ring outliers.

2 monomers are involved in 4 short contacts:

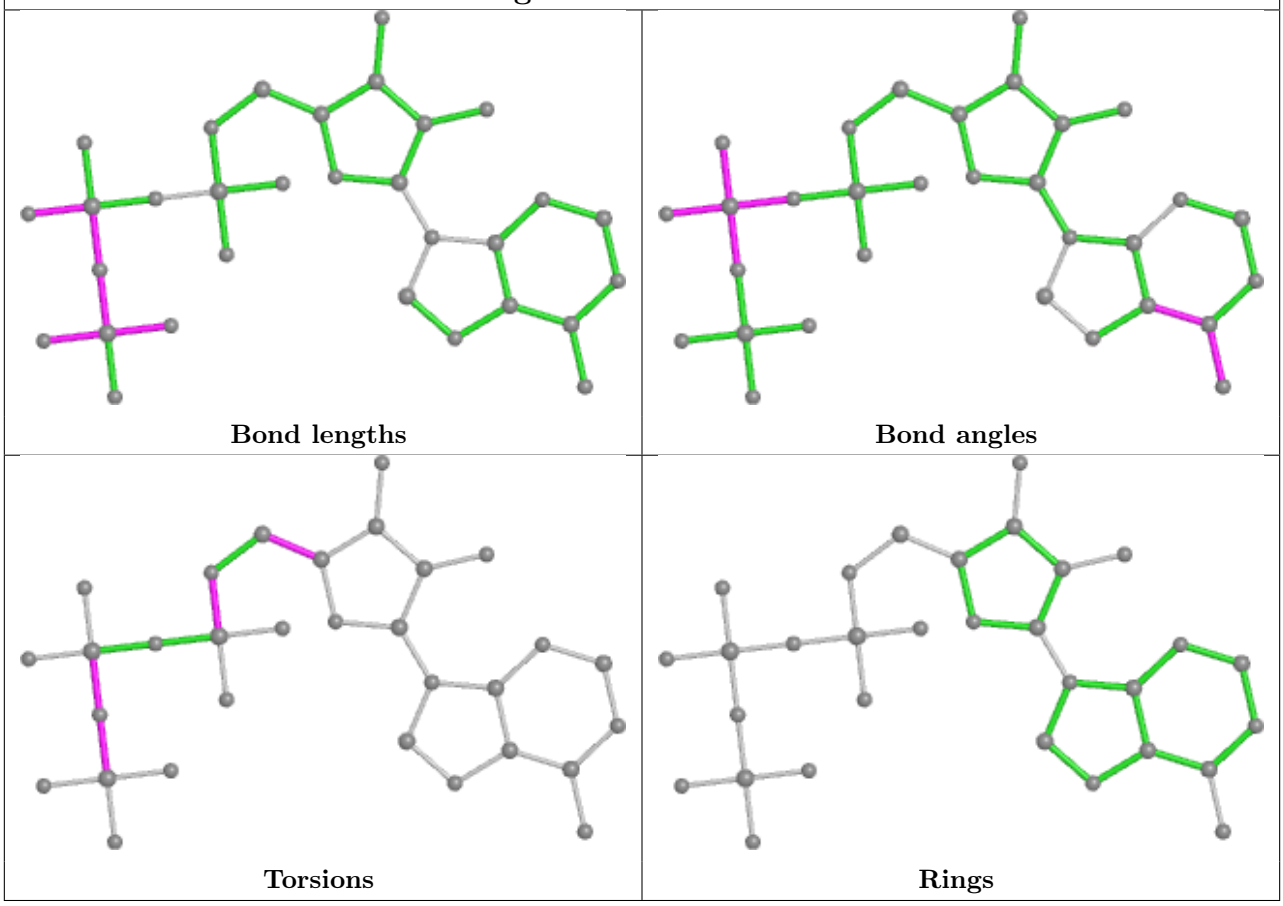
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	ANP	2	0
3	B	1201	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ANP A 1201



Ligand ANP B 1201



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	282/341 (82%)	0.50	24 (8%)	10	7	21, 71, 128, 155	0
1	B	278/341 (81%)	0.49	21 (7%)	13	9	26, 73, 127, 143	0
2	E	15/21 (71%)	2.12	5 (33%)	0	0	108, 118, 128, 134	0
2	F	16/21 (76%)	1.72	4 (25%)	0	0	109, 118, 126, 136	0
All	All	591/724 (81%)	0.57	54 (9%)	9	6	21, 76, 128, 155	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1102	GLN	8.1
1	A	1094	ASN	5.8
1	A	1100	VAL	5.7
1	B	1160	ALA	5.3
2	E	315	ILE	5.0
1	B	1108	ILE	4.9
1	A	1108	ILE	4.9
1	A	1106	LEU	4.8
2	E	319	ILE	4.6
2	E	312	GLN	4.5
1	A	1089	PRO	4.4
1	B	978	LEU	4.3
2	F	311	LEU	4.2
2	E	310	GLU	4.0
1	B	1105	LYS	3.7
1	A	978	LEU	3.6
1	B	961	TYR	3.6
2	F	307	THR	3.5
2	F	310	GLU	3.5
1	A	887	SER	3.5
1	A	1119	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1106	LEU	3.3
2	F	320	ALA	3.3
1	B	871	LEU	3.2
1	B	1112	PHE	3.2
1	B	962	GLY	3.1
1	A	900	ALA	3.0
1	A	888	LEU	2.9
1	A	1110	ASP	2.9
1	B	924	PHE	2.9
1	A	1127	LEU	2.9
1	B	1104	ALA	2.9
2	E	311	LEU	2.9
1	B	887	SER	2.7
1	A	915	HIS	2.7
1	B	873	PHE	2.6
1	A	1061	PHE	2.6
1	A	1093	ASP	2.5
1	A	984	ARG	2.4
1	B	976	VAL	2.4
1	B	1107	ARG	2.4
1	A	1107	ARG	2.3
1	B	977	LYS	2.3
1	B	886	ASP	2.3
1	B	946	CYS	2.3
1	A	1104	ALA	2.2
1	B	1089	PRO	2.2
1	A	1109	SER	2.1
1	B	888	LEU	2.1
1	A	921	ASP	2.1
1	A	950	ASP	2.1
1	A	995	ALA	2.1
1	A	964	LEU	2.1
1	A	1116	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	A	1060	10/11	0.90	0.15	62,71,143,195	0
1	SEP	B	1060	10/11	0.91	0.12	45,53,85,131	0
1	SEP	A	1044	10/11	0.92	0.19	61,74,112,136	0
1	SEP	B	1044	10/11	0.93	0.15	57,62,110,120	0
1	TPO	A	1039	11/12	0.96	0.12	38,46,70,86	0
1	SEP	B	1042	10/11	0.96	0.14	39,48,62,68	0
1	TPO	B	1039	11/12	0.97	0.12	32,42,56,100	0
1	SEP	A	1042	10/11	0.97	0.09	46,62,79,98	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

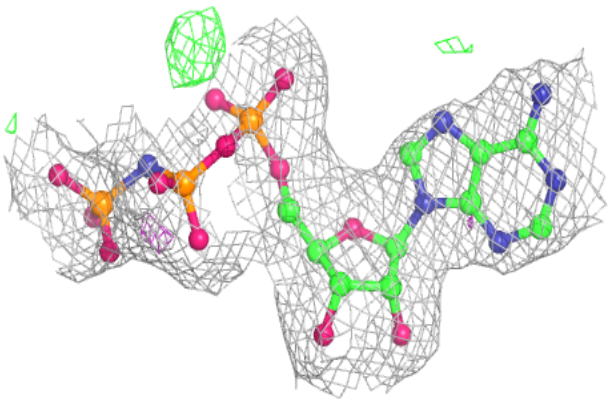
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

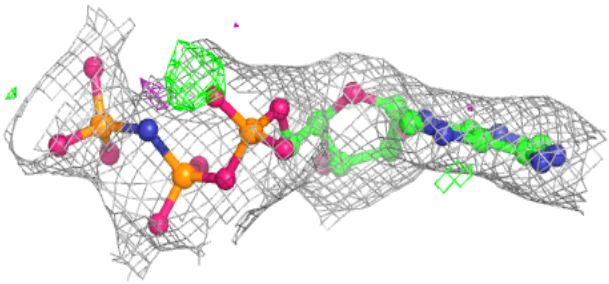
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ANP	A	1201	31/31	0.85	0.17	44,52,187,195	0
3	ANP	B	1201	31/31	0.89	0.18	47,62,171,182	0

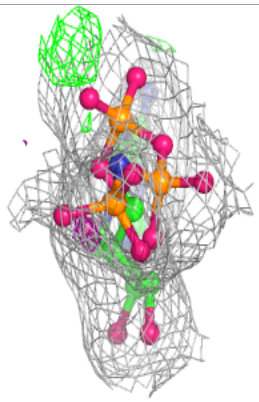
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 1201:

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

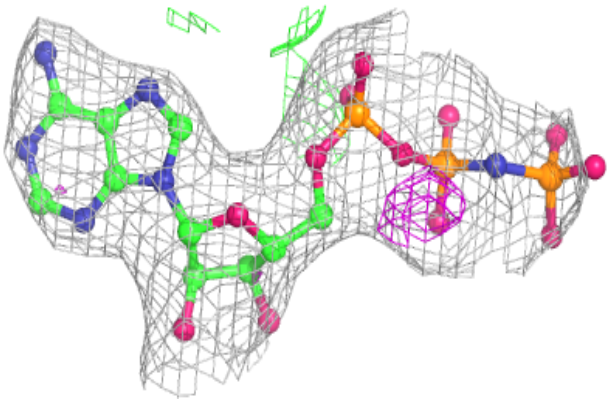


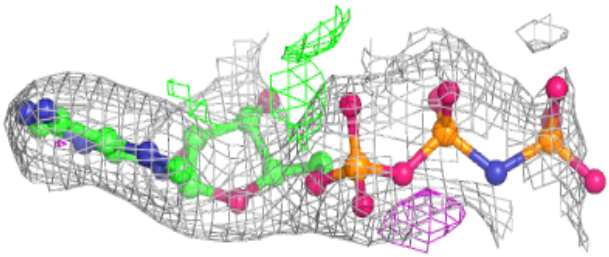


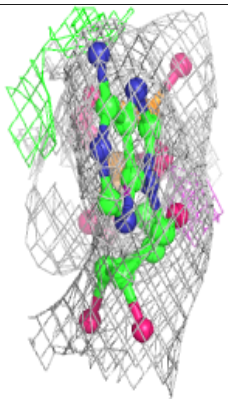


Electron density around ANP B 1201:

$2mF_o$-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.