



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 PM GMT

PDB ID : 4OH4  
Title : Crystal structure of BRI1 in complex with BKI1  
Authors : Wang, J.; Wang, J.; Wu, J.W.; Wang, Z.X.  
Deposited on : 2014-01-17  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

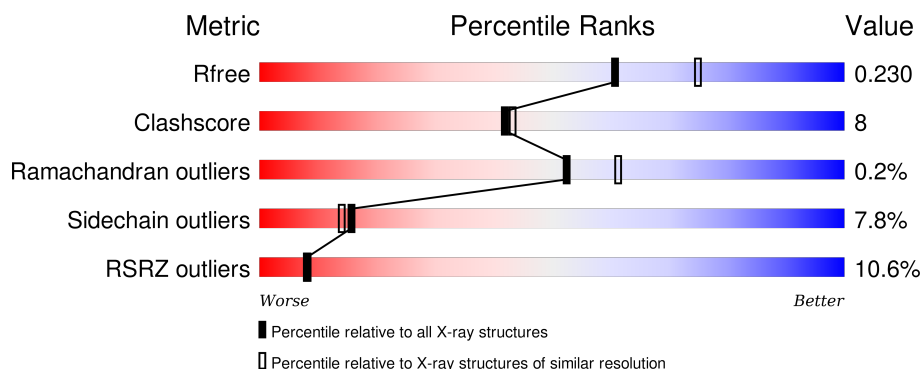
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	333	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	333	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>12%</div> </div> </div>
2	E	21	<div> <div>57%</div> <div> <div></div> <div>43%</div> <div>29%</div> <div>5%</div> <div>24%</div> </div> </div>
2	F	21	<div> <div>52%</div> <div> <div></div> <div>33%</div> <div>33%</div> <div>10%</div> <div>24%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5240 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
1	A	303	Total	C	N	O	P	S	0	0	0
			2404	1520	415	449	4	16			
1	B	293	Total	C	N	O	P	S	0	0	0
			2331	1476	403	433	4	15			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	840	MET	-	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	MET	-	EXPRESSION TAG	UNP O22476
B	840	MET	-	EXPRESSION TAG	UNP O22476
B	841	GLY	-	EXPRESSION TAG	UNP O22476

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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	MET	-	EXPRESSION TAG	UNP O22476

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	16	Total 116	C 71	N 20	O 23	S 2	0	0	0
2	E	16	Total 116	C 71	N 20	O 23	S 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<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

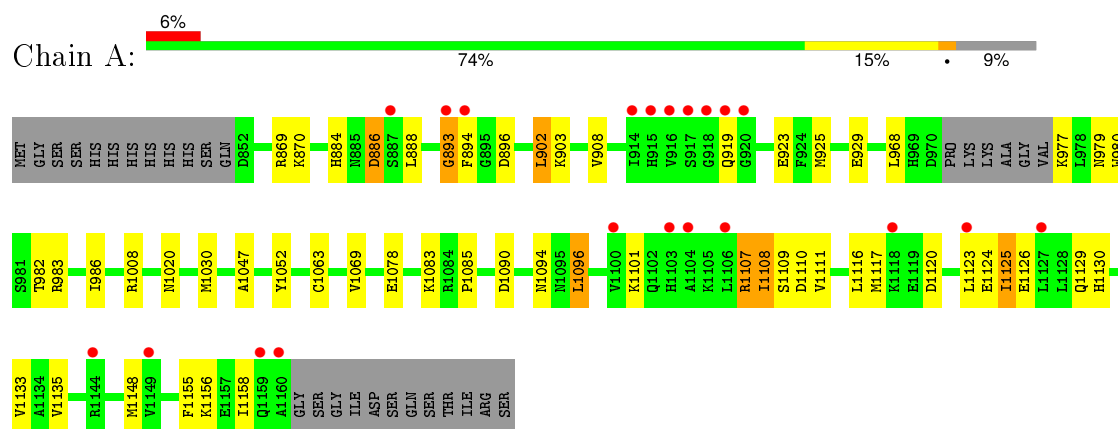
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	123	Total O 123 123	0	0
4	B	84	Total O 84 84	0	0
4	F	1	Total O 1 1	0	0
4	E	3	Total O 3 3	0	0

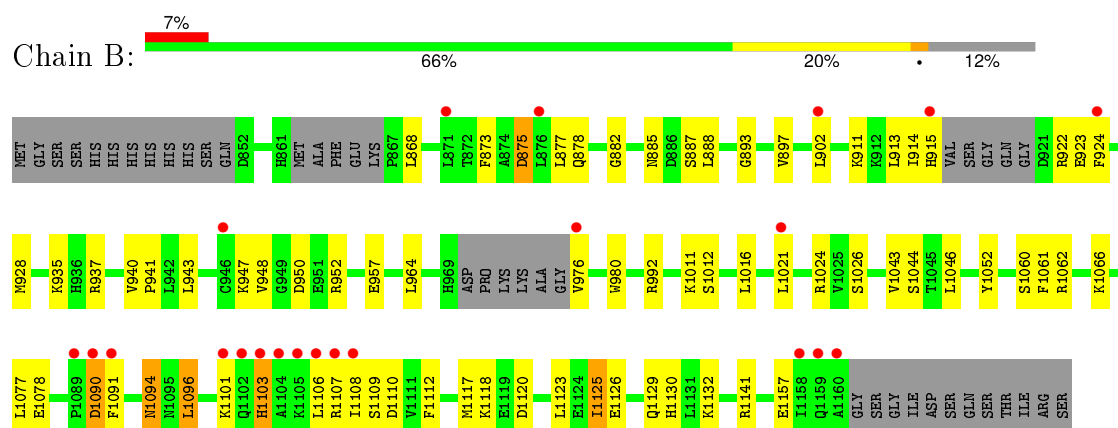
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

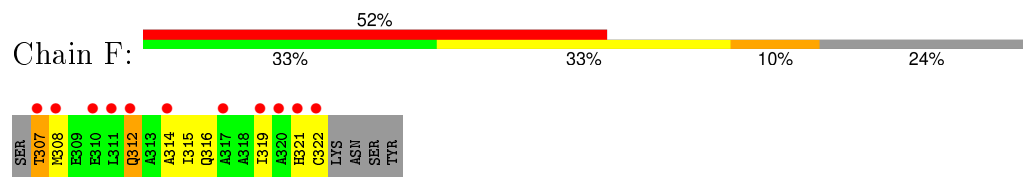
#### • Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1



#### • Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1

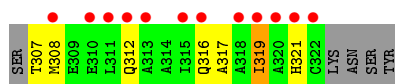


#### • Molecule 2: BRI1 kinase inhibitor 1



#### • Molecule 2: BRI1 kinase inhibitor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.91Å 80.14Å 79.62Å 90.00° 108.86° 90.00°	Depositor
Resolution (Å)	37.84 – 2.25 37.84 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.84-2.25) 97.9 (37.84-2.24)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.202 , 0.236 0.198 , 0.230	Depositor DCC
$R_{free}$ test set	1773 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 35187 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, ANP, SEP

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	0.45	0/2409	0.60	1/3242 (0.0%)
1	B	0.43	0/2333	0.58	0/3138
2	E	0.29	0/116	0.54	0/156
2	F	0.28	0/116	0.41	0/156
All	All	0.44	0/4974	0.59	1/6692 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	GLY	N-CA-C	5.54	126.95	113.10

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	2404	0	2385	33	0
1	B	2331	0	2320	45	0
2	E	116	0	113	5	0
2	F	116	0	113	5	0
3	A	31	0	12	0	0
3	B	31	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	123	0	0	1	0
4	B	84	0	0	1	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
All	All	5240	0	4956	84	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 8.

All (84) 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:893:GLY:O	1:A:894:PHE:CD1	2.23	0.91
1:B:940:VAL:HG11	1:B:1016:LEU:HD12	1.68	0.76
1:B:877:LEU:HD22	1:B:882:GLY:HA2	1.66	0.76
1:B:875:ASP:N	1:B:875:ASP:OD1	2.22	0.73
1:B:1011:LYS:NZ	3:B:1201:ANP:O3G	2.23	0.66
1:B:1091:PHE:O	1:B:1094:ASN:ND2	2.27	0.66
1:A:1108:ILE:H	1:A:1108:ILE:HD13	1.61	0.65
3:B:1201:ANP:O2A	3:B:1201:ANP:O1B	2.16	0.64
1:B:1101:LYS:HE2	2:F:308:MET:HG3	1.79	0.63
1:A:893:GLY:O	1:A:894:PHE:HD1	1.76	0.62
1:B:940:VAL:CG1	1:B:1016:LEU:HD12	2.30	0.61
1:B:1108:ILE:HD11	2:F:314:ALA:HB1	1.84	0.60
1:A:1085:PRO:HA	1:A:1096:LEU:HB2	1.84	0.58
1:A:983:ARG:HD2	1:A:1116:LEU:HD21	1.86	0.57
1:A:1117:MET:SD	1:A:1124:GLU:HG2	2.45	0.56
1:A:1083:LYS:NZ	1:A:1090:ASP:OD2	2.40	0.55
1:B:1077:LEU:HB3	1:B:1096:LEU:HD13	1.89	0.55
1:A:888:LEU:HD11	1:A:896:ASP:HB3	1.88	0.55
1:A:1030:MET:HG2	4:A:1408:HOH:O	2.07	0.53
1:A:902:LEU:HD22	1:A:908:VAL:HG11	1.91	0.52
1:B:1101:LYS:HB3	2:F:307:THR:HG22	1.90	0.52
1:B:1103:HIS:HE1	1:B:1110:ASP:CB	2.23	0.52
2:E:317:ALA:O	2:E:321:HIS:N	2.37	0.52
1:B:1107:ARG:NH2	1:B:1109:SER:HB2	2.24	0.52
1:B:893:GLY:H	3:B:1201:ANP:HNB1	1.58	0.52
1:B:914:ILE:HG22	1:B:915:HIS:H	1.76	0.51
1:B:992:ARG:HD3	4:B:1375:HOH:O	2.12	0.50
1:B:873:PHE:CE1	1:B:877:LEU:HG	2.46	0.50
1:B:1103:HIS:HE1	1:B:1110:ASP:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:THR:O	1:A:986:ILE:HG13	2.12	0.49
1:A:925:MET:O	1:A:929:GLU:HG2	2.12	0.49
1:B:943:LEU:HD21	1:B:957:GLU:HG3	1.95	0.48
1:B:1052:TYR:OH	1:B:1078:GLU:OE1	2.25	0.48
1:A:893:GLY:C	1:A:894:PHE:HD1	2.16	0.48
1:B:1094:ASN:N	1:B:1094:ASN:HD22	2.12	0.47
2:E:307:THR:OG1	2:E:308:MET:N	2.48	0.47
1:A:1069:VAL:HG22	1:A:1148:MET:SD	2.55	0.47
1:A:1108:ILE:HG12	1:A:1109:SER:N	2.29	0.47
1:A:893:GLY:C	1:A:894:PHE:CD1	2.88	0.47
1:B:1107:ARG:HH21	1:B:1109:SER:HB2	1.79	0.46
1:B:1090:ASP:OD1	1:B:1090:ASP:N	2.48	0.46
1:A:1030:MET:HE3	1:A:1047:ALA:HB1	1.97	0.46
1:B:980:TRP:HE1	1:B:1126:GLU:CD	2.19	0.46
1:A:979:ASN:H	1:A:979:ASN:ND2	2.13	0.46
1:A:1108:ILE:HG12	1:A:1109:SER:H	1.81	0.46
1:A:894:PHE:CD2	1:A:923:GLU:HG2	2.50	0.46
1:A:884:HIS:ND1	1:A:886:ASP:OD1	2.48	0.46
1:A:1125:ILE:O	1:A:1129:GLN:HG3	2.15	0.46
1:B:923:GLU:OE1	1:B:923:GLU:N	2.48	0.46
1:A:1052:TYR:OH	1:A:1078:GLU:OE2	2.32	0.45
1:A:1133:VAL:HG11	1:A:1155:PHE:CE1	2.52	0.45
2:F:315:ILE:O	2:F:319:ILE:HG13	2.16	0.45
1:A:1008:ARG:HD3	1:A:1063:CYS:SG	2.56	0.45
2:F:308:MET:O	2:F:312:GLN:HG2	2.17	0.45
1:B:940:VAL:HG21	1:B:1026:SER:OG	2.17	0.45
1:B:1120:ASP:HB3	1:B:1123:LEU:HG	1.98	0.45
1:B:1109:SER:HA	1:B:1112:PHE:CD2	2.51	0.45
1:A:968:LEU:HD21	1:A:1078:GLU:O	2.16	0.44
1:B:1125:ILE:O	1:B:1129:GLN:HG3	2.17	0.44
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.86	0.44
2:E:316:GLN:O	2:E:319:ILE:HG13	2.18	0.44
1:B:924:PHE:O	1:B:928:MET:HG2	2.19	0.43
1:B:980:TRP:HZ2	1:B:1130:HIS:CE1	2.36	0.43
1:A:888:LEU:CD1	1:A:896:ASP:HB3	2.48	0.43
1:B:1044:SEP:O1P	1:B:1044:SEP:N	2.45	0.43
1:A:980:TRP:HE1	1:A:1126:GLU:CD	2.22	0.42
2:E:308:MET:O	2:E:312:GLN:HG3	2.19	0.42
1:B:1060:SEP:O3P	1:B:1062:ARG:HD2	2.20	0.42
1:B:976:VAL:HG11	1:B:1021:LEU:HD21	2.01	0.42
1:A:1107:ARG:HG3	1:A:1110:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:937:ARG:O	1:B:1024:ARG:HD3	2.20	0.42
1:B:940:VAL:HA	1:B:941:PRO:HD3	1.95	0.41
1:B:1043:VAL:O	1:B:1061:PHE:HB3	2.20	0.41
1:B:964:LEU:HB3	1:B:1012:SER:O	2.20	0.41
1:B:868:LEU:HA	1:B:868:LEU:HD23	1.79	0.41
1:A:1130:HIS:CE1	1:A:1158:ILE:HG21	2.55	0.41
1:B:911:LYS:HE3	1:B:913:LEU:HD21	2.02	0.41
1:A:1135:VAL:HG13	2:E:308:MET:HE3	2.02	0.41
1:B:873:PHE:HB2	1:B:948:VAL:HG21	2.02	0.41
1:B:947:LYS:HG3	1:B:952:ARG:NH1	2.36	0.41
1:B:1107:ARG:O	1:B:1107:ARG:HG3	2.21	0.41
1:B:1066:LYS:HD2	1:B:1066:LYS:HA	1.60	0.41
1:A:1120:ASP:HB3	1:A:1123:LEU:HG	2.03	0.41
1:A:903:LYS:HG2	1:B:885:ASN:ND2	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	295/333 (89%)	282 (96%)	13 (4%)	0	100	100
1	B	281/333 (84%)	263 (94%)	17 (6%)	1 (0%)	39	43
2	E	14/21 (67%)	13 (93%)	1 (7%)	0	100	100
2	F	14/21 (67%)	14 (100%)	0	0	100	100
All	All	604/708 (85%)	572 (95%)	31 (5%)	1 (0%)	52	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1106	LEU

### 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	255/280 (91%)	240 (94%)	15 (6%)	24	24
1	B	248/280 (89%)	228 (92%)	20 (8%)	15	13
2	E	11/16 (69%)	10 (91%)	1 (9%)	12	9
2	F	11/16 (69%)	6 (54%)	5 (46%)	0	0
All	All	525/592 (89%)	484 (92%)	41 (8%)	16	14

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	869	ARG
1	A	870	LYS
1	A	886	ASP
1	A	902	LEU
1	A	919	GLN
1	A	977	LYS
1	A	1020	ASN
1	A	1094	ASN
1	A	1096	LEU
1	A	1101	LYS
1	A	1107	ARG
1	A	1108	ILE
1	A	1111	VAL
1	A	1125	ILE
1	A	1156	LYS
1	B	875	ASP
1	B	878	GLN
1	B	887	SER
1	B	888	LEU
1	B	897	VAL
1	B	902	LEU
1	B	922	ARG
1	B	935	LYS
1	B	950	ASP

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Mol	Chain	Res	Type
1	B	1046	LEU
1	B	1090	ASP
1	B	1094	ASN
1	B	1096	LEU
1	B	1103	HIS
1	B	1117	MET
1	B	1118	LYS
1	B	1125	ILE
1	B	1132	LYS
1	B	1141	ARG
1	B	1157	GLU
2	F	307	THR
2	F	312	GLN
2	F	316	GLN
2	F	321	HIS
2	F	322	CYS
2	E	319	ILE

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

Mol	Chain	Res	Type
1	A	919	GLN
1	A	979	ASN
1	B	1020	ASN
1	B	1094	ASN
1	B	1102	GLN
1	B	1103	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	TPO	A	1039	1	8,10,11	1.07	0	7,14,16	0.95	0
1	SEP	A	1042	1	8,9,10	1.53	1 (12%)	8,12,14	1.40	1 (12%)
1	SEP	A	1044	1	8,9,10	1.65	2 (25%)	8,12,14	1.60	2 (25%)
1	SEP	A	1060	1	8,9,10	1.35	1 (12%)	8,12,14	1.35	1 (12%)
1	TPO	B	1039	1	8,10,11	1.14	0	7,14,16	1.17	0
1	SEP	B	1042	1	8,9,10	1.50	1 (12%)	8,12,14	1.05	0
1	SEP	B	1044	1	8,9,10	1.63	2 (25%)	8,12,14	1.49	1 (12%)
1	SEP	B	1060	1	8,9,10	1.61	2 (25%)	8,12,14	1.88	1 (12%)

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	TPO	A	1039	1	-	0/8/11/13	0/0/0/0
1	SEP	A	1042	1	-	0/6/8/10	0/0/0/0
1	SEP	A	1044	1	-	0/6/8/10	0/0/0/0
1	SEP	A	1060	1	-	0/6/8/10	0/0/0/0
1	TPO	B	1039	1	-	0/8/11/13	0/0/0/0
1	SEP	B	1042	1	-	0/6/8/10	0/0/0/0
1	SEP	B	1044	1	-	0/6/8/10	0/0/0/0
1	SEP	B	1060	1	-	0/6/8/10	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1060	SEP	P-O3P	2.06	1.62	1.54
1	B	1044	SEP	P-O2P	2.07	1.62	1.54
1	A	1044	SEP	P-O2P	2.18	1.62	1.54
1	A	1060	SEP	P-O1P	2.90	1.60	1.51
1	B	1042	SEP	P-O1P	2.95	1.60	1.51
1	A	1042	SEP	P-O1P	3.10	1.61	1.51
1	B	1060	SEP	P-O1P	3.31	1.62	1.51
1	A	1044	SEP	P-O1P	3.41	1.62	1.51
1	B	1044	SEP	P-O1P	3.43	1.62	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1044	SEP	OG-P-O1P	2.02	112.28	107.14
1	A	1060	SEP	OG-CB-CA	2.75	110.62	108.27
1	A	1042	SEP	OG-CB-CA	2.82	110.68	108.27
1	A	1044	SEP	OG-CB-CA	2.96	110.80	108.27
1	B	1044	SEP	OG-CB-CA	3.18	110.99	108.27
1	B	1060	SEP	OG-CB-CA	4.36	111.99	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1044	SEP	1	0
1	B	1060	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	27,33,33	3.58	14 (51%)	30,52,52	3.29	11 (36%)
3	ANP	B	1201	-	27,33,33	3.29	12 (44%)	30,52,52	3.30	11 (36%)

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	-	-	0/12/38/38	0/3/3/3
3	ANP	B	1201	-	-	1/12/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	ANP	C5'-C4'	-2.88	1.42	1.51
3	A	1201	ANP	O3'-C3'	-2.83	1.36	1.43
3	B	1201	ANP	C5'-C4'	-2.81	1.42	1.51
3	B	1201	ANP	O3'-C3'	-2.45	1.37	1.43
3	B	1201	ANP	C2'-C3'	-2.43	1.46	1.53
3	B	1201	ANP	PG-O3G	-2.34	1.50	1.56
3	A	1201	ANP	O2'-C2'	-2.31	1.37	1.43
3	A	1201	ANP	C2'-C3'	-2.22	1.47	1.53
3	A	1201	ANP	PG-O3G	-2.17	1.50	1.56
3	B	1201	ANP	O2'-C2'	-2.15	1.37	1.43
3	A	1201	ANP	C3'-C4'	-2.04	1.47	1.53
3	B	1201	ANP	O4'-C4'	2.00	1.49	1.45
3	A	1201	ANP	O4'-C4'	2.10	1.49	1.45
3	A	1201	ANP	PG-N3B	2.28	1.69	1.63
3	B	1201	ANP	PB-O2B	3.47	1.66	1.56
3	B	1201	ANP	C6-N6	3.66	1.46	1.34
3	A	1201	ANP	PB-O2B	3.82	1.67	1.56
3	A	1201	ANP	C6-N6	4.10	1.47	1.34
3	B	1201	ANP	PB-N3B	5.09	1.76	1.63
3	A	1201	ANP	PB-N3B	5.34	1.77	1.63
3	B	1201	ANP	PB-O3A	6.29	1.66	1.59
3	B	1201	ANP	PG-O1G	7.37	1.54	1.46
3	A	1201	ANP	PG-O1G	7.43	1.54	1.46
3	A	1201	ANP	PB-O3A	8.39	1.69	1.59
3	B	1201	ANP	PB-O1B	9.92	1.57	1.46
3	A	1201	ANP	PB-O1B	10.47	1.58	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1201	ANP	N3-C2-N1	-9.70	121.47	128.89
3	B	1201	ANP	O2B-PB-O1B	-9.39	90.40	110.00
3	A	1201	ANP	N3-C2-N1	-8.83	122.14	128.89
3	A	1201	ANP	O2B-PB-O1B	-8.48	92.30	110.00
3	A	1201	ANP	O1B-PB-N3B	-8.18	99.35	111.90
3	B	1201	ANP	O1B-PB-N3B	-7.33	100.65	111.90
3	B	1201	ANP	PA-O3A-PB	-4.19	118.63	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1201	ANP	C4'-O4'-C1'	-3.29	106.10	109.72
3	A	1201	ANP	PA-O3A-PB	-3.24	121.79	132.67
3	B	1201	ANP	C4-C5-N7	-3.02	106.70	109.48
3	A	1201	ANP	C4-C5-N7	-2.99	106.73	109.48
3	B	1201	ANP	C1'-N9-C4	-2.17	123.67	126.94
3	A	1201	ANP	C1'-N9-C4	-2.11	123.75	126.94
3	A	1201	ANP	O2G-PG-O1G	-2.00	108.17	113.49
3	A	1201	ANP	O3A-PA-O5'	2.14	108.61	102.94
3	B	1201	ANP	O2A-PA-O3A	2.23	115.19	105.09
3	B	1201	ANP	O2B-PB-O3A	2.38	115.88	105.09
3	B	1201	ANP	O5'-C5'-C4'	2.42	118.03	109.12
3	A	1201	ANP	O5'-C5'-C4'	2.46	118.20	109.12
3	A	1201	ANP	O2B-PB-O3A	2.53	116.58	105.09
3	B	1201	ANP	O3A-PB-N3B	4.05	117.57	106.44
3	A	1201	ANP	O3A-PB-N3B	6.16	123.38	106.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1201	ANP	O1B-PB-N3B-PG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	299/333 (89%)	0.39	21 (7%) 19 21	10, 41, 106, 133	0
1	B	289/333 (86%)	0.44	22 (7%) 17 18	11, 47, 107, 145	0
2	E	16/21 (76%)	3.22	12 (75%) 0 0	91, 108, 134, 146	0
2	F	16/21 (76%)	2.68	11 (68%) 0 0	81, 91, 133, 138	0
All	All	620/708 (87%)	0.55	66 (10%) 8 8	10, 46, 115, 146	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	311	LEU	6.3
2	E	308	MET	6.3
2	F	321	HIS	6.1
1	B	1106	LEU	6.0
2	E	319	ILE	5.7
2	F	307	THR	4.9
1	A	1104	ALA	4.8
2	F	311	LEU	4.3
2	E	321	HIS	4.2
1	B	1102	GLN	4.0
1	B	1105	LYS	3.9
1	A	894	PHE	3.9
1	A	1160	ALA	3.9
1	A	917	SER	3.8
2	E	322	CYS	3.8
1	A	1106	LEU	3.6
2	E	312	GLN	3.5
1	A	919	GLN	3.5
1	B	876	LEU	3.5
2	E	315	ILE	3.4
2	E	320	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	893	GLY	3.2
1	B	1091	PHE	3.2
1	B	946	CYS	3.1
1	B	1104	ALA	3.1
1	A	918	GLY	3.1
1	A	920	GLY	3.1
1	B	1107	ARG	3.1
1	B	902	LEU	3.0
1	B	915	HIS	3.0
2	F	310	GLU	3.0
1	B	1101	LYS	3.0
1	A	1100	VAL	2.9
2	F	320	ALA	2.9
2	F	314	ALA	2.9
1	B	1108	ILE	2.8
1	A	915	HIS	2.7
2	E	316	GLN	2.7
1	A	1127	LEU	2.7
1	B	1159	GLN	2.7
1	B	1089	PRO	2.7
1	A	1123	LEU	2.6
1	A	916	VAL	2.5
1	B	1103	HIS	2.5
2	F	308	MET	2.4
2	F	312	GLN	2.4
2	F	317	ALA	2.4
2	E	313	ALA	2.4
2	F	322	CYS	2.4
1	A	914	ILE	2.4
1	A	1149	VAL	2.4
2	E	310	GLU	2.4
2	E	318	ALA	2.4
1	B	976	VAL	2.3
1	A	1159	GLN	2.2
2	F	319	ILE	2.2
1	B	871	LEU	2.2
1	A	887	SER	2.2
1	A	1118	LYS	2.2
1	A	1103	HIS	2.2
1	B	1021	LEU	2.1
1	B	1090	ASP	2.1
1	B	1160	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1158	ILE	2.0
1	B	924	PHE	2.0
1	A	1144	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	B	1042	10/11	0.97	0.07	-	37,42,51,54	0
1	SEP	A	1044	10/11	0.84	0.17	-	59,65,67,70	0
1	TPO	B	1039	11/12	0.97	0.12	-	32,38,43,47	0
1	SEP	B	1060	10/11	0.91	0.09	-	55,61,72,77	0
1	SEP	B	1044	10/11	0.86	0.18	-	90,97,100,103	0
1	TPO	A	1039	11/12	0.96	0.13	-	32,37,48,48	0
1	SEP	A	1060	10/11	0.66	0.21	-	61,67,79,82	0
1	SEP	A	1042	10/11	0.96	0.09	-	35,44,54,59	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ANP	B	1201	31/31	0.88	0.16	0.51	22,43,180,184	0
3	ANP	A	1201	31/31	0.92	0.12	-0.54	26,47,184,188	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.