



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:36 am BST

PDB ID : 5TTH  
Title : Heterodimeric SpyCatcher/SpyTag-fused zebrafish TRAP1 in ATP/ADP-hybrid state  
Authors : Elnatan, D.; Betegon, M.; Liu, Y.; Agard, D.A.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2016-11-03  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

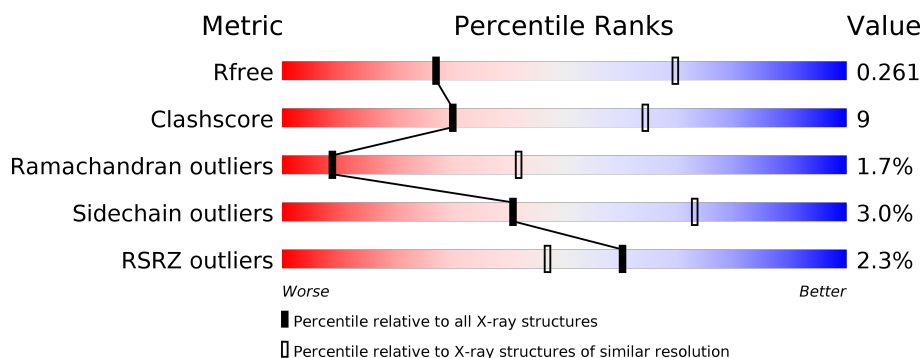
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	738	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>• 9%</div> </div> </div>
2	B	672	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•• 8%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10447 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 C-terminal SpyCatcher fusion of wildtype zebrafish TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	2	0
			5371	3399	923	1026	23			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	GLY	-	expression tag	UNP A8WFFV1
A	68	ILE	-	expression tag	UNP A8WFFV1
A	69	ASP	-	expression tag	UNP A8WFFV1
A	70	PRO	-	expression tag	UNP A8WFFV1
A	71	PHE	-	expression tag	UNP A8WFFV1
A	72	THR	-	expression tag	UNP A8WFFV1
A	720	GLY	-	linker	UNP A8WFFV1
A	721	SER	-	linker	UNP A8WFFV1
A	734	GLU	ILE	engineered mutation	UNP Q8G9G1
A	769	TYR	MET	engineered mutation	UNP Q8G9G1

- Molecule 2 is a protein called C-terminal Spytag fusion of R417A zebrafish TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	621	Total	C	N	O	S	0	4	0
			5012	3182	862	945	23			

There are 13 discrepancies between the modelled and reference sequences:

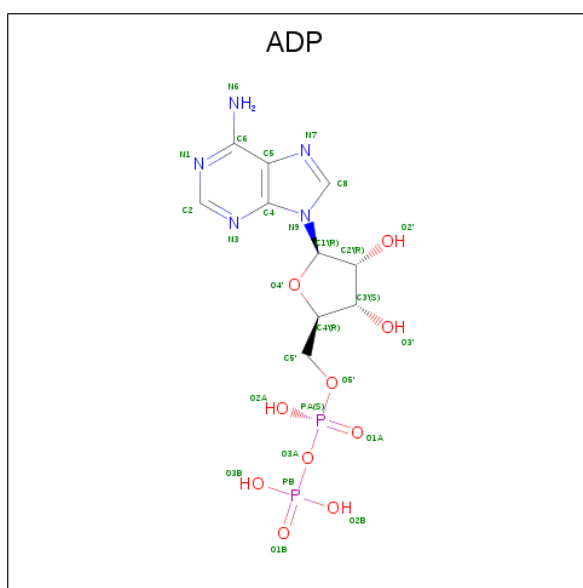
Chain	Residue	Modelled	Actual	Comment	Reference
B	67	GLY	-	expression tag	UNP A8WFFV1
B	68	ILE	-	expression tag	UNP A8WFFV1
B	69	ASP	-	expression tag	UNP A8WFFV1
B	70	PRO	-	expression tag	UNP A8WFFV1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	71	PHE	-	expression tag	UNP A8WV1
B	72	THR	-	expression tag	UNP A8WV1
B	417	ALA	ARG	engineered mutation	UNP A8WV1
B	720	GLY	-	linker	UNP A8WV1
B	721	GLY	-	linker	UNP A8WV1
B	722	SER	-	linker	UNP A8WV1
B	723	GLY	-	linker	UNP A8WV1
B	724	SER	-	linker	UNP A8WV1
B	725	SER	-	linker	UNP A8WV1

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $BeF_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		
4	B	1	Total	Be	F	0	0
			4	1	3		

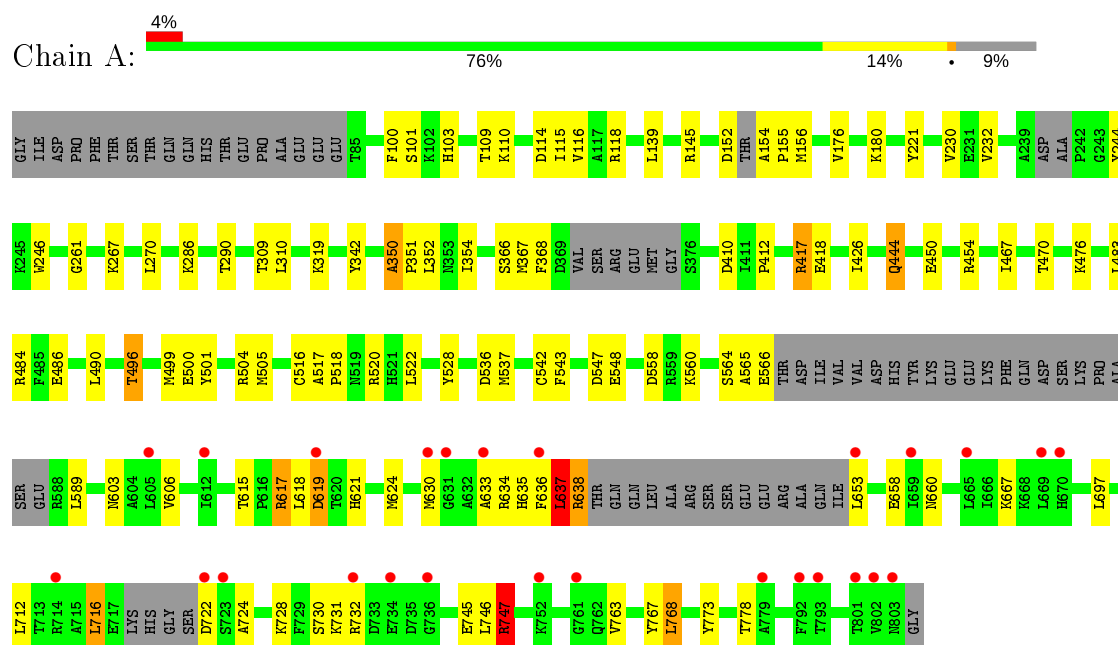
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

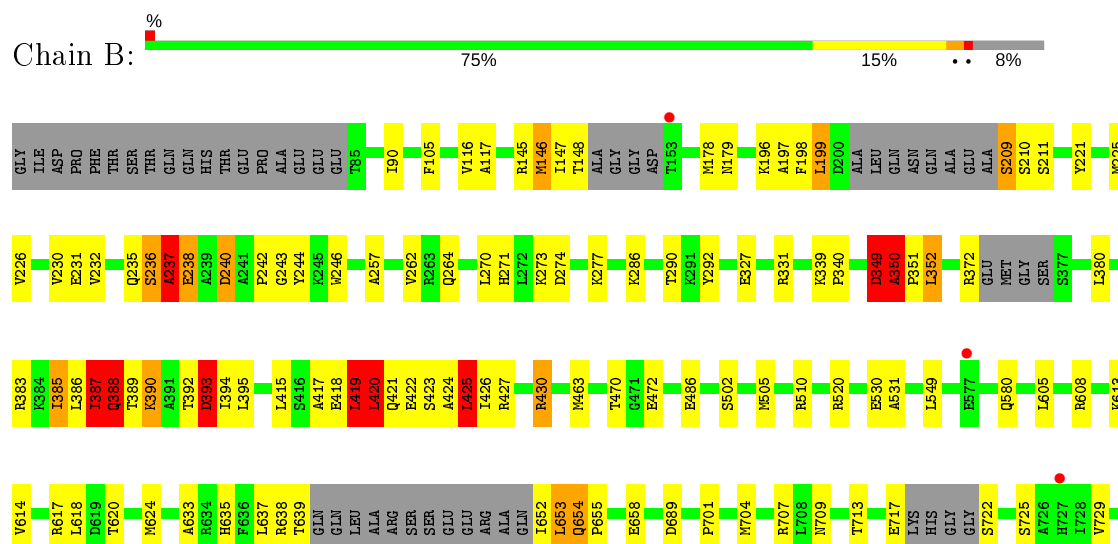
### 3 Residue-property plots

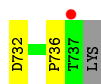
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: C-terminal SpyCatcher fusion of wildtype zebrafish TNF receptor-associated protein 1



- Molecule 2: C-terminal Spytag fusion of R417A zebrafish TNF receptor-associated protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.09 Å   95.71 Å   126.56 Å 90.00°   134.59°   90.00°	Depositor
Resolution (Å)	49.00 – 3.20 49.09 – 3.20	Depositor EDS
% Data completeness (in resolution range)	83.0 (49.00-3.20) 83.0 (49.09-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.228 , 0.261 0.227 , 0.261	Depositor DCC
$R_{free}$ test set	1014 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.015 for h+2*l,k,-h-l 0.028 for h,-k,-h-l 0.039 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.61	1/5473 (0.0%)	0.79	6/7377 (0.1%)
2	B	0.63	1/5116 (0.0%)	0.80	14/6895 (0.2%)
All	All	0.62	2/10589 (0.0%)	0.79	20/14272 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	393	ASP	CB-CG	-5.77	1.39	1.51
1	A	261	GLY	N-CA	-5.40	1.38	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	ARG	NE-CZ-NH2	15.85	128.22	120.30
1	A	417	ARG	NE-CZ-NH1	-10.06	115.27	120.30
2	B	349	ASP	CB-CG-OD1	-8.49	110.66	118.30
2	B	393	ASP	CB-CG-OD2	-7.42	111.62	118.30
2	B	352	LEU	CB-CG-CD1	-7.05	99.01	111.00
2	B	425	LEU	CB-CG-CD1	-6.64	99.72	111.00
2	B	237	ALA	CB-CA-C	-6.61	100.18	110.10
1	A	747	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	B	420	LEU	CB-CG-CD2	6.36	121.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	349	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	637	LEU	CB-CG-CD1	-5.92	100.93	111.00
2	B	430	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	747	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	B	510	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	427	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	350	ALA	C-N-CD	5.11	139.13	128.40
2	B	388	GLN	N-CA-C	5.09	124.74	111.00
2	B	387	ILE	CB-CG1-CD1	5.08	128.13	113.90
2	B	372	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	716	LEU	CB-CG-CD1	-5.01	102.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	393	ASP	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	5371	0	5343	90	2
2	B	5012	0	5028	111	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	10447	0	10395	193	2

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 9.

All (193) 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:745:GLU:OE1	1:A:747:ARG:NH2	1.61	1.31
2:B:419:LEU:HD21	2:B:422:GLU:OE1	1.29	1.29
2:B:419:LEU:CD2	2:B:420:LEU:HD22	1.64	1.27
1:A:712:LEU:O	1:A:716:LEU:HD12	1.28	1.27
2:B:385:ILE:O	2:B:387:ILE:CD1	1.83	1.25
2:B:393:ASP:OD2	2:B:430:ARG:CZ	1.88	1.22
2:B:419:LEU:O	2:B:421:GLN:HG2	1.32	1.21
2:B:393:ASP:CG	2:B:430:ARG:HH21	1.41	1.20
2:B:393:ASP:OD2	2:B:430:ARG:NH2	1.76	1.19
2:B:393:ASP:CG	2:B:430:ARG:NH2	1.98	1.17
1:A:712:LEU:O	1:A:716:LEU:CD1	1.93	1.14
2:B:178:MET:C	2:B:236:SER:OG	1.86	1.12
2:B:419:LEU:HD23	2:B:420:LEU:HD22	1.32	1.09
1:A:634:ARG:O	1:A:638:ARG:HB2	1.56	1.03
2:B:385:ILE:O	2:B:387:ILE:HD13	1.57	1.03
2:B:653:LEU:O	2:B:655:PRO:N	1.91	1.03
2:B:419:LEU:CD2	2:B:422:GLU:OE1	2.08	1.00
2:B:393:ASP:OD1	2:B:430:ARG:NH2	1.94	0.99
2:B:419:LEU:HD22	2:B:420:LEU:HD22	1.44	0.99
2:B:178:MET:C	2:B:236:SER:HG	1.61	0.99
2:B:179:ASN:N	2:B:236:SER:OG	1.95	0.98
1:A:768:LEU:HD23	1:A:773:TYR:CE2	2.00	0.97
2:B:386:LEU:C	2:B:387:ILE:HD12	1.86	0.96
1:A:768:LEU:HD23	1:A:773:TYR:CZ	2.01	0.95
2:B:209:SER:O	2:B:211:SER:N	1.99	0.94
1:A:635:HIS:HA	1:A:638:ARG:HB3	1.52	0.91
1:A:768:LEU:CD2	1:A:773:TYR:CE2	2.60	0.85
2:B:393:ASP:CG	2:B:430:ARG:HD3	1.98	0.84
2:B:385:ILE:O	2:B:387:ILE:HD12	1.79	0.82
2:B:393:ASP:OD2	2:B:430:ARG:NE	2.12	0.80
2:B:419:LEU:HD23	2:B:420:LEU:N	1.97	0.79
1:A:350:ALA:CB	1:A:351:PRO:HD3	2.13	0.78
2:B:237:ALA:HB2	2:B:264:GLN:HE22	1.49	0.78
2:B:146:MET:HA	2:B:146:MET:CE	2.14	0.77
2:B:237:ALA:HB2	2:B:264:GLN:NE2	2.00	0.77
2:B:419:LEU:O	2:B:421:GLN:CG	2.25	0.76
1:A:768:LEU:CD2	1:A:773:TYR:CZ	2.69	0.75
1:A:617:ARG:O	1:A:619:ASP:N	2.20	0.74
2:B:393:ASP:OD2	2:B:430:ARG:HD3	1.87	0.73
2:B:418:GLU:O	2:B:420:LEU:N	2.21	0.73
1:A:589:LEU:HD13	1:A:667:LYS:HG2	1.71	0.72
1:A:152:ASP:O	1:A:154:ALA:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ASP:OD2	2:B:430:ARG:CD	2.38	0.72
2:B:653:LEU:O	2:B:655:PRO:CD	2.39	0.71
1:A:505:MET:SD	1:A:560:LYS:NZ	2.56	0.71
2:B:196:LYS:O	2:B:199:LEU:HD13	1.91	0.71
2:B:209:SER:C	2:B:211:SER:H	1.95	0.70
1:A:350:ALA:CB	1:A:351:PRO:CD	2.69	0.70
1:A:635:HIS:HA	1:A:638:ARG:CB	2.21	0.69
2:B:385:ILE:HG22	2:B:387:ILE:HD11	1.74	0.69
2:B:349:ASP:N	2:B:349:ASP:OD1	2.23	0.68
1:A:350:ALA:HB3	1:A:351:PRO:CD	2.24	0.68
2:B:419:LEU:CG	2:B:422:GLU:OE1	2.43	0.67
2:B:116:VAL:HG11	2:B:221:TYR:HB2	1.76	0.67
2:B:419:LEU:HD23	2:B:420:LEU:CD2	2.19	0.66
1:A:100:PHE:HB3	2:B:257:ALA:HB2	1.77	0.66
1:A:712:LEU:O	1:A:716:LEU:HD11	1.92	0.65
2:B:240:ASP:N	2:B:240:ASP:OD1	2.28	0.65
2:B:701:PRO:O	2:B:704:MET:HG2	1.97	0.65
1:A:618:LEU:HB3	1:A:621:HIS:O	1.97	0.65
1:A:548:GLU:OE1	1:A:634:ARG:NH1	2.30	0.64
1:A:350:ALA:HB1	1:A:351:PRO:HD3	1.79	0.64
1:A:350:ALA:HB3	1:A:351:PRO:HD3	1.79	0.63
2:B:232:VAL:HB	2:B:246:TRP:HB3	1.81	0.61
2:B:385:ILE:O	2:B:387:ILE:HD11	1.93	0.60
1:A:633:ALA:O	1:A:637:LEU:CD1	2.49	0.60
1:A:101:SER:OG	1:A:103:HIS:NE2	2.23	0.59
2:B:243:GLY:O	2:B:244:TYR:CG	2.55	0.59
1:A:486:GLU:OE1	1:A:520:ARG:NH1	2.35	0.59
2:B:327:GLU:OE1	2:B:331:ARG:NH2	2.34	0.59
1:A:730:SER:HB2	2:B:729[A]:VAL:HG22	1.85	0.59
2:B:147:ILE:HD13	2:B:147:ILE:N	2.17	0.58
2:B:419:LEU:HD11	2:B:422:GLU:OE1	2.03	0.58
1:A:115:ILE:CG2	2:B:415:LEU:HD22	2.33	0.58
2:B:117:ALA:O	2:B:225:MET:HG2	2.04	0.57
2:B:231:GLU:OE2	2:B:271:HIS:NE2	2.32	0.57
1:A:116:VAL:HG11	1:A:221:TYR:HB2	1.87	0.56
1:A:636:PHE:CD2	1:A:653:LEU:HD22	2.40	0.56
2:B:419:LEU:HD23	2:B:420:LEU:CA	2.34	0.56
2:B:386:LEU:O	2:B:387:ILE:HD12	2.04	0.56
2:B:380:LEU:HD23	2:B:387:ILE:HB	1.87	0.56
2:B:386:LEU:C	2:B:387:ILE:CD1	2.70	0.55
2:B:653:LEU:O	2:B:654:GLN:C	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:O	1:A:352:LEU:HG	2.08	0.54
2:B:709:ASN:O	2:B:713:THR:HG23	2.08	0.54
2:B:388:GLN:O	2:B:420:LEU:HB2	2.07	0.54
2:B:531:ALA:O	2:B:617:ARG:NH2	2.40	0.54
2:B:419:LEU:CD2	2:B:420:LEU:CD2	2.60	0.53
1:A:768:LEU:CD2	1:A:773:TYR:CD2	2.92	0.53
1:A:558:ASP:O	1:A:560:LYS:HG3	2.09	0.52
1:A:634:ARG:O	1:A:638:ARG:CB	2.44	0.52
1:A:730:SER:HB2	2:B:729[B]:VAL:HB	1.91	0.52
1:A:522:LEU:HD11	1:A:697:LEU:HD13	1.92	0.52
1:A:232:VAL:HB	1:A:246:TRP:HB3	1.91	0.52
2:B:350:ALA:HB3	2:B:351:PRO:CD	2.40	0.52
2:B:393:ASP:CG	2:B:430:ARG:CD	2.75	0.52
1:A:638:ARG:NE	1:A:638:ARG:HA	2.24	0.52
1:A:417:ARG:HG3	1:A:417:ARG:HH11	1.75	0.51
1:A:109:THR:HG21	2:B:105:PHE:HB2	1.93	0.51
2:B:633:ALA:HB1	2:B:653:LEU:HD13	1.93	0.51
2:B:652:ILE:O	2:B:654:GLN:N	2.43	0.51
2:B:502:SER:HA	2:B:505:MET:CE	2.41	0.51
2:B:274:ASP:HA	2:B:277:LYS:HE3	1.93	0.50
2:B:196:LYS:O	2:B:197:ALA:C	2.48	0.50
1:A:366:SER:OG	1:A:367:MET:N	2.44	0.50
1:A:638:ARG:HE	1:A:638:ARG:HA	1.77	0.50
1:A:115:ILE:HG21	2:B:415:LEU:HD22	1.94	0.49
1:A:518:PRO:HD2	1:A:630:MET:HE2	1.94	0.49
2:B:389:THR:HG22	2:B:420:LEU:HG	1.95	0.49
1:A:114:ASP:OD2	1:A:118:ARG:NH2	2.44	0.49
2:B:425:LEU:HD23	2:B:426:ILE:HD12	1.94	0.49
2:B:502:SER:HA	2:B:505:MET:HE3	1.95	0.48
2:B:605:LEU:HD23	2:B:608:ARG:HH21	1.77	0.48
1:A:230:VAL:HG22	1:A:270:LEU:HD22	1.94	0.48
2:B:653:LEU:C	2:B:655:PRO:HD3	2.32	0.48
1:A:309:THR:HG22	1:A:309:THR:O	2.13	0.48
1:A:618:LEU:HD23	1:A:618:LEU:N	2.28	0.48
1:A:635:HIS:CA	1:A:638:ARG:HB3	2.33	0.48
2:B:385:ILE:C	2:B:387:ILE:HD12	2.32	0.48
2:B:419:LEU:CD1	2:B:422:GLU:OE1	2.61	0.48
1:A:603:ASN:O	1:A:606:VAL:HG23	2.14	0.48
1:A:528:TYR:CD1	1:A:566:GLU:HA	2.49	0.47
2:B:197:ALA:O	2:B:199:LEU:N	2.47	0.47
2:B:470:THR:HG22	2:B:472:GLU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:HE3	2:B:90:ILE:HG23	1.97	0.47
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.75	0.47
1:A:724:ALA:HB1	1:A:767:TYR:HB3	1.97	0.47
2:B:419:LEU:HD23	2:B:420:LEU:HA	1.96	0.47
1:A:450:GLU:HG3	1:A:454:ARG:HH21	1.79	0.46
1:A:139:LEU:HD22	1:A:156:MET:HB3	1.97	0.46
1:A:634:ARG:HA	1:A:637:LEU:CD1	2.46	0.46
2:B:243:GLY:O	2:B:244:TYR:CD2	2.68	0.46
1:A:470:THR:O	1:A:476:LYS:HE3	2.14	0.46
1:A:542[B]:CYS:HB2	1:A:547:ASP:HB3	1.96	0.46
1:A:768:LEU:HD22	1:A:773:TYR:CE1	2.51	0.46
1:A:501:TYR:O	1:A:505:MET:HG3	2.16	0.46
2:B:339:LYS:HB2	2:B:340:PRO:HD2	1.98	0.46
1:A:319:LYS:H	1:A:319:LYS:HE2	1.82	0.45
2:B:230:VAL:HG22	2:B:270:LEU:HD22	1.98	0.45
2:B:235:GLN:HB2	2:B:262:VAL:HG12	1.98	0.45
2:B:350:ALA:HB3	2:B:351:PRO:HD3	1.97	0.45
1:A:536:ASP:O	1:A:537:MET:SD	2.75	0.45
1:A:517:ALA:O	1:A:543:PHE:HA	2.17	0.45
1:A:145:ARG:HE	1:A:176:VAL:HG21	1.82	0.45
2:B:653:LEU:C	2:B:655:PRO:N	2.67	0.45
2:B:419:LEU:HD22	2:B:420:LEU:CD2	2.30	0.44
1:A:286:LYS:O	1:A:290:THR:HG23	2.17	0.44
1:A:490:LEU:HD11	1:A:496:THR:HG21	1.98	0.44
2:B:393:ASP:O	2:B:395:LEU:N	2.50	0.44
2:B:387:ILE:CD1	2:B:387:ILE:N	2.81	0.44
2:B:618:LEU:HD11	2:B:624:MET:SD	2.58	0.44
2:B:689:ASP:OD2	2:B:707:ARG:NH2	2.46	0.44
2:B:145:ARG:O	2:B:148:THR:OG1	2.31	0.44
2:B:179:ASN:CA	2:B:236:SER:OG	2.65	0.43
2:B:385:ILE:C	2:B:387:ILE:CD1	2.76	0.43
1:A:412:PRO:HD2	1:A:426:ILE:HD11	2.01	0.43
2:B:387:ILE:HD12	2:B:387:ILE:N	2.33	0.43
1:A:564:SER:O	1:A:566:GLU:N	2.51	0.43
2:B:637:LEU:O	2:B:639:THR:N	2.51	0.43
2:B:286:LYS:O	2:B:290:THR:HG23	2.19	0.43
1:A:746:LEU:HD21	1:A:768:LEU:HD11	2.01	0.43
1:A:518:PRO:HD2	1:A:630:MET:CE	2.49	0.42
2:B:236:SER:O	2:B:237:ALA:C	2.58	0.42
1:A:728:LYS:HE2	1:A:763:VAL:HG11	2.00	0.42
1:A:768:LEU:HD22	1:A:773:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LEU:HA	2:B:420:LEU:HD13	1.80	0.42
1:A:483:LEU:O	1:A:484:ARG:HD3	2.20	0.42
1:A:633:ALA:O	1:A:637:LEU:HD12	2.19	0.42
1:A:615:THR:HG21	1:A:658:GLU:OE1	2.20	0.42
1:A:697:LEU:HD12	1:A:697:LEU:HA	1.85	0.42
2:B:292:TYR:O	2:B:385:ILE:HD12	2.19	0.42
2:B:549:LEU:HD13	2:B:635:HIS:CE1	2.55	0.42
2:B:209:SER:C	2:B:211:SER:N	2.60	0.42
1:A:712:LEU:C	1:A:716:LEU:CD1	2.79	0.42
1:A:618:LEU:HD12	1:A:660:ASN:HB2	2.01	0.41
1:A:731:LYS:NZ	2:B:732:ASP:CG	2.73	0.41
2:B:425:LEU:HD23	2:B:425:LEU:C	2.40	0.41
2:B:530:GLU:OE2	2:B:620:THR:HB	2.20	0.41
1:A:516:CYS:SG	1:A:542[A]:CYS:HB2	2.60	0.41
2:B:350:ALA:CB	2:B:351:PRO:CD	2.98	0.41
2:B:486:GLU:OE1	2:B:520:ARG:HD3	2.21	0.41
1:A:500:GLU:O	1:A:504:ARG:HG3	2.20	0.41
1:A:180:LYS:HB2	1:A:244:TYR:CZ	2.55	0.41
1:A:467:ILE:O	1:A:476:LYS:HE2	2.21	0.41
2:B:388:GLN:HG2	2:B:390:LYS:HE2	2.03	0.41
1:A:633:ALA:O	1:A:637:LEU:HD11	2.21	0.41
1:A:352:LEU:O	1:A:354:ILE:HG13	2.21	0.40
1:A:618:LEU:HD21	1:A:624:MET:HG2	2.03	0.40
1:A:712:LEU:C	1:A:716:LEU:HD12	2.24	0.40
2:B:226:VAL:O	2:B:273:LYS:HG2	2.20	0.40
2:B:613:LYS:O	2:B:658:GLU:HA	2.21	0.40
1:A:342:TYR:CE1	1:A:444:GLN:HG2	2.56	0.40
1:A:410:ASP:OD1	1:A:410:ASP:N	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:CD	1:A:778:THR:O[1_454]	1.76	0.44
1:A:155:PRO:CG	1:A:778:THR:O[1_454]	1.83	0.37

## 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	659/738 (89%)	631 (96%)	24 (4%)	4 (1%)	25	64
2	B	613/672 (91%)	568 (93%)	27 (4%)	18 (3%)	4	28
All	All	1272/1410 (90%)	1199 (94%)	51 (4%)	22 (2%)	9	42

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ALA
2	B	198	PHE
2	B	210	SER
2	B	350	ALA
2	B	394	ILE
2	B	419	LEU
2	B	420	LEU
2	B	654	GLN
2	B	417	ALA
2	B	424	ALA
2	B	638	ARG
2	B	236	SER
2	B	237	ALA
2	B	725	SER
2	B	736	PRO
1	A	368	PHE
1	A	619	ASP
2	B	393	ASP
2	B	653	LEU
1	A	565	ALA
2	B	238	GLU
2	B	242	PRO



### 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	586/643 (91%)	574 (98%)	12 (2%)	55	80
2	B	553/587 (94%)	531 (96%)	22 (4%)	31	66
All	All	1139/1230 (93%)	1105 (97%)	34 (3%)	41	73

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LYS
1	A	418	GLU
1	A	444	GLN
1	A	496	THR
1	A	499	MET
1	A	617	ARG
1	A	637	LEU
1	A	638	ARG
1	A	722	ASP
1	A	732	ARG
1	A	747	ARG
1	A	768	LEU
2	B	146	MET
2	B	199	LEU
2	B	209	SER
2	B	238	GLU
2	B	240	ASP
2	B	349	ASP
2	B	352	LEU
2	B	383	ARG
2	B	385	ILE
2	B	387	ILE
2	B	388	GLN
2	B	390	LYS
2	B	392	THR
2	B	393	ASP
2	B	419	LEU

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Mol	Chain	Res	Type
2	B	423	SER
2	B	425	LEU
2	B	463	MET
2	B	580	GLN
2	B	614	VAL
2	B	717	GLU
2	B	722	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	97	GLN
2	B	235	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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
4	BEF	A	902	3	0,3,3	0.00	-	-		
3	ADP	B	801	5,4	24,29,29	1.02	2 (8%)	29,45,45	1.42	6 (20%)
3	ADP	A	901	5,4	24,29,29	1.01	2 (8%)	29,45,45	1.38	4 (13%)
4	BEF	B	802	3	0,3,3	0.00	-	-		

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	ADP	B	801	5,4	-	3/12/32/32	0/3/3/3
3	ADP	A	901	5,4	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	ADP	C2-N3	2.43	1.36	1.32
3	B	801	ADP	C5-C4	2.18	1.46	1.40
3	A	901	ADP	C2-N3	2.07	1.35	1.32
3	A	901	ADP	O4'-C4'	-2.00	1.40	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ADP	N3-C2-N1	-3.67	122.94	128.68
3	B	801	ADP	N3-C2-N1	-3.28	123.55	128.68
3	B	801	ADP	C4-C5-N7	-2.73	106.55	109.40
3	A	901	ADP	C4-C5-N7	-2.51	106.78	109.40
3	A	901	ADP	PA-O3A-PB	-2.29	124.96	132.83
3	B	801	ADP	C3'-C2'-C1'	2.21	104.31	100.98
3	A	901	ADP	O2A-PA-O1A	2.12	122.73	112.24
3	B	801	ADP	O3B-PB-O2B	2.09	115.61	107.64
3	B	801	ADP	O2B-PB-O3A	2.06	111.55	104.64
3	B	801	ADP	O3A-PB-O1B	-2.04	99.90	111.19

There are no chirality outliers.

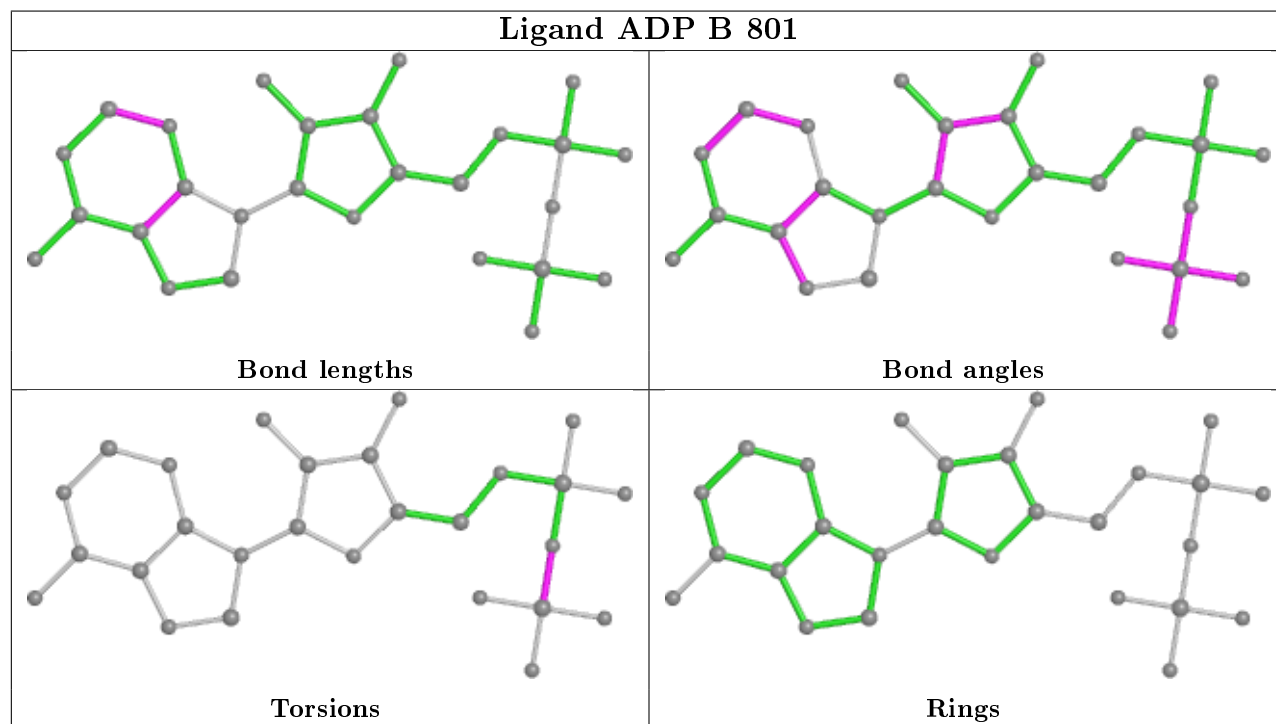
All (5) torsion outliers are listed below:

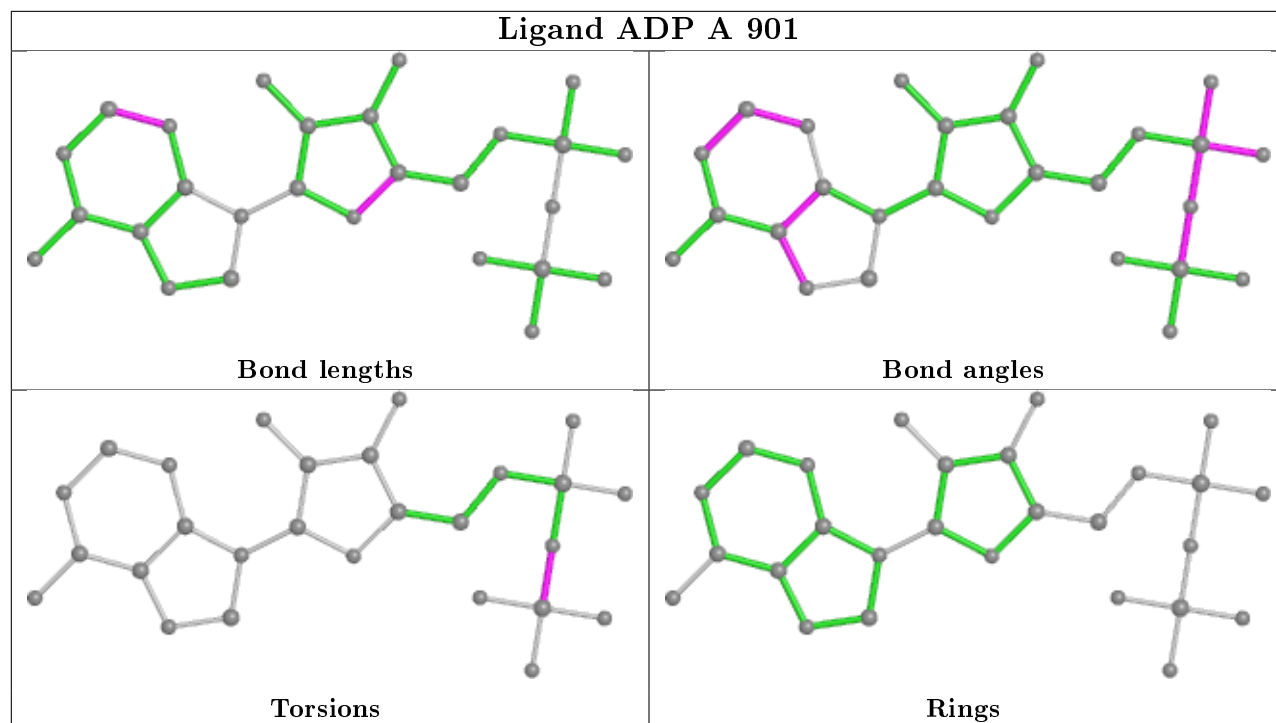
Mol	Chain	Res	Type	Atoms
3	B	801	ADP	PA-O3A-PB-O2B
3	A	901	ADP	PA-O3A-PB-O2B
3	B	801	ADP	PA-O3A-PB-O1B
3	B	801	ADP	PA-O3A-PB-O3B
3	A	901	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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.





## 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	671/738 (90%)	0.20	26 (3%) 39 25	63, 134, 204, 250	0
2	B	621/672 (92%)	-0.13	4 (0%) 89 83	57, 114, 176, 281	0
All	All	1292/1410 (91%)	0.04	30 (2%) 60 47	57, 124, 196, 281	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	803	ASN	5.1
2	B	737	THR	5.0
1	A	723	SER	4.5
1	A	633	ALA	4.3
1	A	779	ALA	3.7
1	A	802	VAL	3.6
1	A	665	LEU	3.4
1	A	752	LYS	3.3
1	A	630	MET	3.1
1	A	722	ASP	3.0
1	A	732	ARG	2.9
1	A	793	THR	2.9
1	A	670	HIS	2.9
1	A	659	ILE	2.8
1	A	801	THR	2.7
2	B	153	THR	2.7
1	A	792	PHE	2.6
1	A	714	ARG	2.6
1	A	636	PHE	2.5
1	A	612	ILE	2.4
1	A	653	LEU	2.4
1	A	631	GLY	2.3
1	A	736	GLY	2.3
2	B	577	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	761	GLY	2.3
1	A	669	LEU	2.2
1	A	619	ASP	2.2
1	A	734	GLU	2.1
2	B	727	HIS	2.1
1	A	605	LEU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

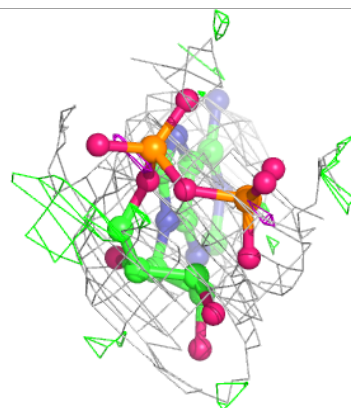
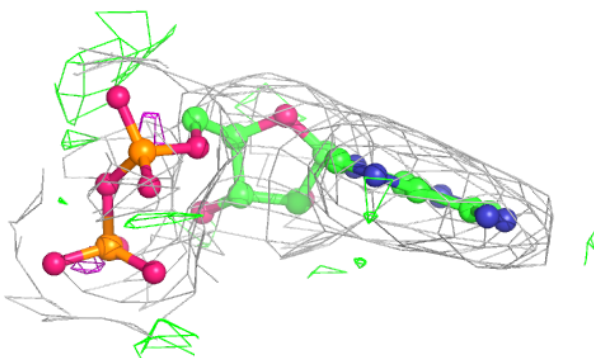
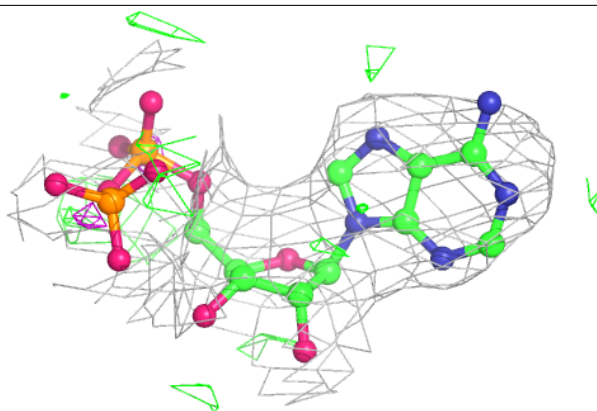
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BEF	A	902	4/4	0.95	0.15	57,64,66,72	0
4	BEF	B	802	4/4	0.95	0.14	55,55,55,58	0
3	ADP	B	801	27/27	0.96	0.14	47,54,74,79	0
5	MG	B	803	1/1	0.96	0.12	38,38,38,38	0
3	ADP	A	901	27/27	0.96	0.15	50,57,66,70	0
5	MG	A	903	1/1	0.97	0.20	48,48,48,48	0

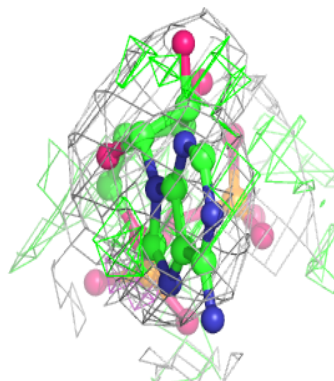
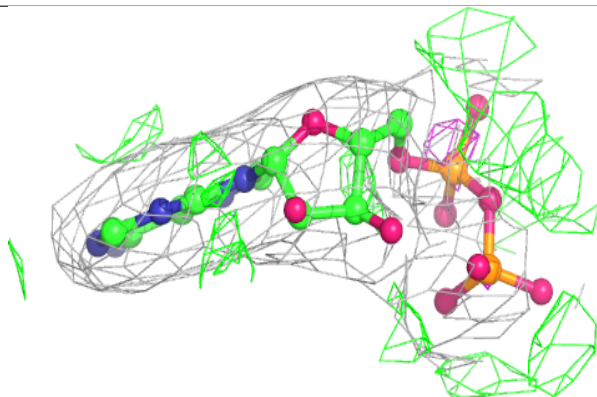
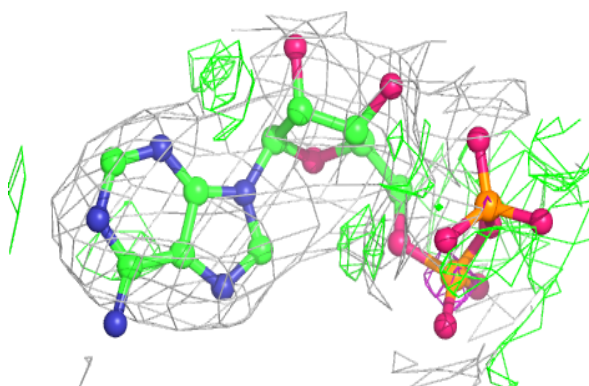
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP B 801:**

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

**Electron density around ADP A 901:**

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





## 6.5 Other polymers

There are no such residues in this entry.