



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:18 AM EDT

PDB ID : 4J0B / pdb_00004j0b
Title : Structure of mitochondrial Hsp90 (TRAP1) with ADP-BeF3
Authors : Partridge, J.R.; Lavery, L.A.; Agard, D.A.
Deposited on : 2013-01-30
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

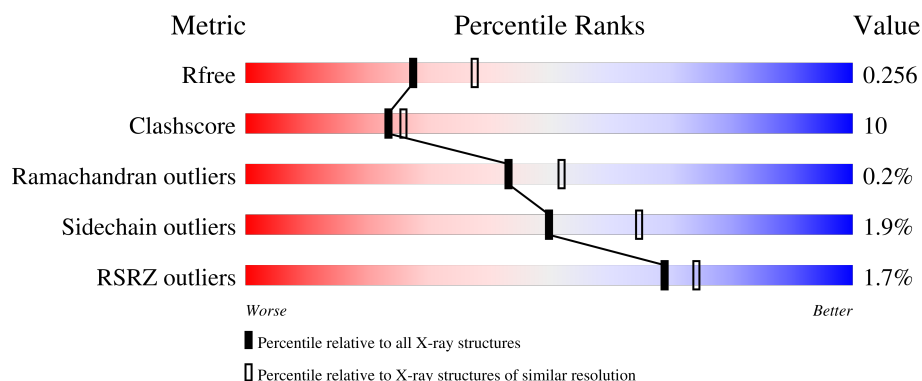
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	647	
1	B	647	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9953 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.

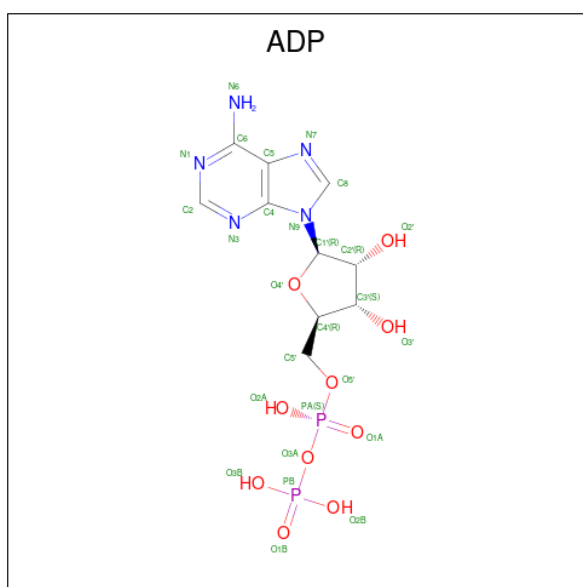
- Molecule 1 is a protein called TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4764	3017	826	900	21			
1	B	609	Total	C	N	O	S	0	4	0
			4934	3130	853	927	24			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

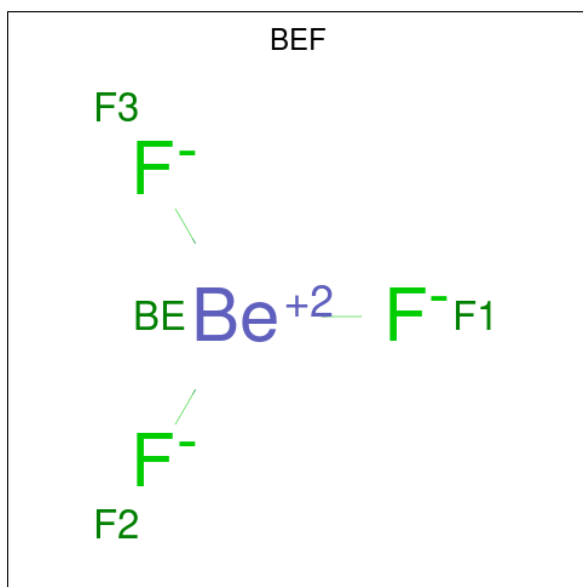
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	B	2	Total	Co	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 (CCD ID: BEF) (formula: BeF₃).



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

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

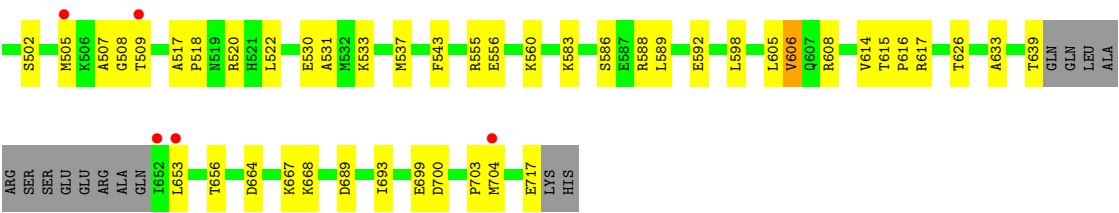
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	97	Total	O	0	0
			97	97		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.78Å 96.57Å 124.98Å 90.00° 134.29° 90.00°	Depositor
Resolution (Å)	29.82 – 2.35 29.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.82-2.35) 90.9 (29.82-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1278)	Depositor
R, R_{free}	0.205 , 0.248 0.219 , 0.256	Depositor DCC
R_{free} test set	2030 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.011 for h,-k,-h-l 0.015 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9953	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.52	0/4849	0.92	14/6536 (0.2%)
1	B	0.52	1/5035 (0.0%)	0.87	14/6780 (0.2%)
All	All	0.52	1/9884 (0.0%)	0.90	28/13316 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	491	PRO	N-CD	5.17	1.54	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	HIS	N-CA-C	-12.72	98.27	114.04
1	A	608	ARG	N-CA-C	9.28	124.56	112.12
1	B	215	GLN	N-CA-CB	-8.03	100.31	111.00
1	A	260	SER	N-CA-C	-7.45	97.86	108.96
1	B	606	VAL	N-CA-C	7.26	117.78	110.23
1	A	214	GLY	N-CA-C	7.07	125.09	111.31
1	B	423	SER	N-CA-C	6.58	120.17	111.75
1	B	214	GLY	N-CA-C	6.29	128.08	113.18
1	B	147	ILE	CB-CA-C	-6.17	104.83	110.63
1	B	249	ASP	N-CA-C	5.98	118.70	111.40
1	B	639	THR	N-CA-CB	5.95	121.61	111.50
1	A	405	VAL	N-CA-C	5.66	115.82	108.35
1	A	118	ARG	N-CA-CB	-5.58	101.05	110.49
1	A	519	ASN	N-CA-C	5.57	115.60	108.24
1	A	608	ARG	CB-CA-C	-5.57	102.01	111.26
1	B	147	ILE	N-CA-C	-5.49	108.49	113.71
1	B	490	LEU	CA-C-N	-5.47	113.00	119.84
1	B	490	LEU	C-N-CA	-5.47	113.00	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	SER	CB-CA-C	-5.38	110.36	116.54
1	B	699	GLU	N-CA-C	5.36	119.75	111.56
1	B	411	ILE	CA-C-N	-5.30	115.11	120.31
1	B	411	ILE	C-N-CA	-5.30	115.11	120.31
1	A	654	GLN	CA-C-N	-5.21	115.36	120.52
1	A	654	GLN	C-N-CA	-5.21	115.36	120.52
1	A	122	SER	N-CA-C	-5.20	106.78	113.23
1	A	590	SER	N-CA-C	5.17	116.17	108.31
1	A	426	ILE	CB-CA-C	-5.17	105.16	112.14
1	B	384	LYS	N-CA-CB	-5.02	102.70	110.98

There are no chirality outliers.

There are no planarity outliers.

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	4764	0	4770	108	0
1	B	4934	0	4950	102	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	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
6	A	90	0	0	1	0
6	B	97	0	0	0	0
All	All	9953	0	9744	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (198) 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:414:ASN:ND2	1:B:419:LEU:HB2	1.43	1.30
1:A:490:LEU:CD1	1:A:496:THR:CG2	2.31	1.09
1:A:490:LEU:CD1	1:A:496:THR:HG21	1.84	1.06
1:B:509:THR:HG21	1:B:537:MET:SD	1.96	1.06
1:B:664:ASP:O	1:B:668:LYS:HG2	1.58	1.03
1:A:490:LEU:HD11	1:A:496:THR:HG21	1.40	1.00
1:B:352:LEU:HD11	1:B:425:LEU:CD1	2.01	0.91
1:A:608:ARG:O	1:A:652:ILE:HD11	1.71	0.89
1:B:352:LEU:CD1	1:B:425:LEU:HD11	2.04	0.88
1:A:490:LEU:CD1	1:A:496:THR:HG23	2.06	0.86
1:B:313:LEU:HA	1:B:316:MET:HE2	1.58	0.85
1:B:414:ASN:ND2	1:B:419:LEU:CB	2.36	0.82
1:B:507:ALA:HB3	1:B:508:GLY:HA2	1.62	0.81
1:A:423:SER:HB3	1:A:426:ILE:HG12	1.61	0.81
1:B:493:GLY:HA2	1:B:494:GLN:O	1.82	0.80
1:B:352:LEU:HD13	1:B:425:LEU:HD11	1.62	0.80
1:B:414:ASN:HD21	1:B:419:LEU:HB2	1.46	0.78
1:B:352:LEU:CD1	1:B:425:LEU:CD1	2.62	0.77
1:B:352:LEU:HD11	1:B:425:LEU:HD12	1.67	0.76
1:B:393:ASP:O	1:B:430:ARG:HD2	1.87	0.75
1:B:509:THR:CG2	1:B:537:MET:SD	2.75	0.75
1:A:490:LEU:HD12	1:A:496:THR:CG2	2.18	0.74
1:A:545:GLN:HG2	1:A:546:PHE:CD2	2.24	0.73
1:B:394:ILE:O	1:B:430:ARG:HG2	1.89	0.73
1:B:493:GLY:HA2	1:B:494:GLN:C	2.15	0.72
1:B:693:ILE:HD11	1:B:704:MET:HE1	1.71	0.72
1:B:116:VAL:HG11	1:B:221:TYR:HB2	1.73	0.70
1:A:601:MET:HE1	1:A:659:ILE:HG13	1.74	0.70
1:B:232:VAL:HB	1:B:246:TRP:HB3	1.73	0.70
1:B:126:VAL:HG13	1:B:129:ARG:CZ	2.21	0.70
1:A:119:SER:O	1:B:415:LEU:N	2.24	0.70
1:A:490:LEU:HD11	1:A:496:THR:CG2	2.07	0.69
1:B:507:ALA:N	1:B:508:GLY:HA3	2.07	0.68
1:B:505:MET:SD	1:B:560:LYS:HD3	2.35	0.67
1:A:114:ASP:O	1:A:118:ARG:HB2	1.95	0.67
1:A:118:ARG:O	1:B:421:GLN:NE2	2.22	0.66
1:A:680:ALA:O	1:A:683:LEU:N	2.27	0.66
1:A:445:SER:OG	1:A:484:ARG:NH2	2.29	0.66
1:A:589:LEU:HD13	1:A:667:LYS:HG2	1.78	0.65
1:A:490:LEU:HD13	1:A:496:THR:HG23	1.79	0.65
1:A:376:SER:O	1:A:403:ARG:CZ	2.45	0.65
1:B:507:ALA:HB3	1:B:508:GLY:CA	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:HD12	1:A:496:THR:HG21	1.75	0.63
1:B:664:ASP:O	1:B:668:LYS:CG	2.43	0.62
1:B:126:VAL:CG1	1:B:129:ARG:NH2	2.62	0.62
1:A:634:ARG:HG2	1:A:634:ARG:O	1.99	0.61
1:B:388:GLN:O	1:B:389:THR:OG1	2.14	0.61
1:B:139:LEU:HD22	1:B:156:MET:HB3	1.81	0.61
1:B:364:LYS:NZ	1:B:458:ASP:OD1	2.33	0.61
1:B:493:GLY:HA2	1:B:494:GLN:HB3	1.82	0.61
1:A:111:LYS:HE2	1:B:196:LYS:HD2	1.82	0.61
1:A:545:GLN:HG2	1:A:546:PHE:CE2	2.36	0.61
1:A:294:ASN:ND2	1:A:332:TYR:OH	2.34	0.61
1:B:238:GLU:OE1	1:B:240:ASP:N	2.32	0.60
1:B:117:ALA:O	1:B:225:MET:HG2	2.01	0.60
1:A:104:GLU:O	1:A:106:GLN:NE2	2.33	0.60
1:A:196:LYS:HD3	1:A:215:GLN:HB3	1.84	0.60
1:B:693:ILE:CD1	1:B:704:MET:HE1	2.32	0.59
1:B:583:LYS:O	1:B:588:ARG:NH1	2.35	0.59
1:A:464:ARG:NH2	1:A:547:ASP:OD1	2.36	0.58
1:B:616:PRO:HD2	1:B:617:ARG:HG3	1.86	0.58
1:A:329:PHE:CZ	1:A:333:VAL:HG21	2.38	0.58
1:A:637:LEU:HB3	1:A:638:ARG:HA	1.86	0.58
1:A:689:ASP:OD2	1:A:707:ARG:NH2	2.26	0.58
1:A:96:VAL:HG21	1:A:100:PHE:CE1	2.39	0.58
1:A:400:ARG:O	1:A:403:ARG:NH2	2.38	0.57
1:A:504:ARG:NH2	1:A:538:GLU:OE2	2.37	0.57
1:B:689:ASP:HB3	1:B:704:MET:SD	2.44	0.57
1:A:228:ASP:OD1	1:A:273:LYS:HG2	2.04	0.57
1:A:440:PHE:O	1:A:444:GLN:HG2	2.05	0.57
1:A:542:CYS:HB2	1:A:547:ASP:HB3	1.86	0.56
1:B:126:VAL:CG1	1:B:129:ARG:CZ	2.83	0.56
1:B:555[B]:ARG:NH2	1:B:556:GLU:OE2	2.39	0.56
1:A:512:ILE:HD11	1:A:562:LEU:HG	1.89	0.55
1:B:230:VAL:HG22	1:B:270:LEU:HD22	1.89	0.55
1:A:215:GLN:O	1:B:111:LYS:NZ	2.30	0.54
1:A:377:SER:OG	1:A:390:LYS:HG2	2.07	0.54
1:A:442:LEU:HD23	1:A:482:LEU:HD23	1.89	0.54
1:A:490:LEU:HD13	1:A:496:THR:CG2	2.30	0.54
1:B:414:ASN:CG	1:B:419:LEU:HB2	2.26	0.54
1:A:158:ILE:HB	1:A:300:ILE:HD13	1.89	0.54
1:A:139:LEU:HD22	1:A:156:MET:HB3	1.88	0.54
1:B:530:GLU:HA	1:B:533:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:SER:OG	1:A:538:GLU:OE1	2.23	0.54
1:A:512:ILE:N	1:A:561:LYS:O	2.36	0.54
1:B:470:THR:HG21	1:B:475:VAL:HB	1.90	0.54
1:A:232:VAL:HB	1:A:246:TRP:HB3	1.90	0.54
1:A:257:ALA:HB2	1:B:100:PHE:HB3	1.88	0.54
1:A:412:PRO:HD2	1:A:426:ILE:HD11	1.90	0.54
1:A:115:ILE:HG21	1:B:415:LEU:HD22	1.89	0.53
1:A:700:ASP:OD1	1:A:702:ARG:HD3	2.08	0.53
1:A:703:PRO:HA	1:B:522:LEU:HD21	1.91	0.53
1:A:545:GLN:NE2	1:A:546:PHE:CZ	2.76	0.53
1:A:554:LEU:HD23	1:A:562:LEU:HD21	1.90	0.53
1:A:546:PHE:O	1:A:550:THR:HG23	2.08	0.53
1:B:414:ASN:HD22	1:B:419:LEU:HB2	1.61	0.53
1:A:522:LEU:HB3	1:A:630:MET:HE2	1.90	0.53
1:B:337:TYR:CZ	1:B:363:MET:HE1	2.44	0.53
1:B:249:ASP:N	1:B:250:GLY:HA2	2.23	0.53
1:A:191:ALA:O	1:B:111:LYS:HD3	2.09	0.53
1:B:426:ILE:O	1:B:430:ARG:HG3	2.09	0.52
1:A:330:TYR:OH	1:A:361:PRO:HB3	2.09	0.52
1:A:434:GLN:NE2	1:A:475:VAL:HG21	2.24	0.52
1:A:590:SER:OG	1:A:591:SER:N	2.40	0.52
1:A:608:ARG:O	1:A:652:ILE:CD1	2.53	0.52
1:B:190:ILE:HD13	1:B:221:TYR:CZ	2.44	0.52
1:B:518:PRO:HG2	1:B:522:LEU:HD12	1.92	0.52
1:A:673:LYS:NZ	1:A:674:ASP:OD2	2.43	0.51
1:A:483:LEU:O	1:A:484:ARG:HD3	2.11	0.51
1:A:597:LEU:HD11	1:A:669:LEU:HD23	1.92	0.51
1:A:699:GLU:OE1	1:A:699:GLU:N	2.32	0.51
1:A:316:MET:HB2	1:A:321:ILE:HD11	1.91	0.51
1:B:180:LYS:HB2	1:B:244:TYR:CZ	2.46	0.51
1:A:140:GLU:OE1	1:A:143:ARG:NH1	2.44	0.51
1:A:242:PRO:HG2	1:A:244:TYR:CZ	2.46	0.51
1:A:376:SER:O	1:A:403:ARG:NH2	2.44	0.51
1:B:299:PRO:HB3	1:B:306:ARG:CZ	2.41	0.51
1:A:511:ASN:OD1	1:A:513:TYR:CZ	2.64	0.50
1:B:352:LEU:HD22	1:B:410:ASP:OD2	2.11	0.50
1:B:232:VAL:HG22	1:B:268:ILE:HG12	1.92	0.50
1:A:230:VAL:HG22	1:A:270:LEU:HD22	1.93	0.50
1:B:486:GLU:CD	1:B:493:GLY:H	2.20	0.49
1:B:486:GLU:CD	1:B:493:GLY:HA3	2.36	0.49
1:A:490:LEU:HD12	1:A:496:THR:HG23	1.87	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LEU:HD23	1:B:608:ARG:HH21	1.78	0.49
1:A:680:ALA:O	1:A:681:GLN:C	2.56	0.48
1:B:394:ILE:C	1:B:430:ARG:HG2	2.37	0.48
1:A:546:PHE:CE1	1:B:368:PHE:HB2	2.49	0.48
1:A:701:PRO:HG2	1:B:693:ILE:HD13	1.95	0.48
1:B:633:ALA:HB1	1:B:653:LEU:HD13	1.95	0.48
1:B:493:GLY:CA	1:B:494:GLN:C	2.86	0.48
1:A:180:LYS:HB2	1:A:244:TYR:CZ	2.48	0.48
1:A:528:TYR:CD1	1:A:566:GLU:HA	2.49	0.48
1:A:291:LYS:O	6:A:942:HOH:O	2.20	0.47
1:B:183:LEU:O	1:B:187:LEU:HB2	2.15	0.47
1:A:232:VAL:HG22	1:A:268:ILE:HG12	1.97	0.47
1:B:598:LEU:HD11	1:B:614:VAL:HG23	1.95	0.47
1:A:635:HIS:O	1:A:639:THR:HG23	2.14	0.47
1:B:483:LEU:O	1:B:484:ARG:NH1	2.46	0.47
1:B:700:ASP:O	1:B:703:PRO:HD2	2.15	0.47
1:A:196:LYS:HD3	1:A:215:GLN:CB	2.44	0.46
1:A:361:PRO:HG2	1:A:459:TYR:OH	2.16	0.46
1:B:231:GLU:OE2	1:B:271:HIS:NE2	2.49	0.46
1:A:702:ARG:NH2	1:B:518:PRO:HD3	2.30	0.46
1:B:509:THR:HG21	1:B:537:MET:CE	2.46	0.46
1:A:618:LEU:HB2	1:A:660:ASN:HB2	1.98	0.45
1:A:609:VAL:HG12	1:A:655:PRO:HG2	1.98	0.45
1:A:294:ASN:ND2	1:A:332:TYR:CZ	2.84	0.45
1:A:213:ILE:HD13	1:A:385:ILE:HD11	1.98	0.45
1:B:100:PHE:HE2	1:B:102:LYS:HE3	1.81	0.45
1:B:505:MET:SD	1:B:560:LYS:CE	3.04	0.45
1:B:589:LEU:HG	1:B:667:LYS:HG2	1.99	0.45
1:B:422:GLU:O	1:B:425:LEU:HB3	2.16	0.45
1:B:493:GLY:CA	1:B:494:GLN:HB3	2.47	0.44
1:B:592:GLU:OE1	1:B:592:GLU:N	2.44	0.44
1:B:277:LYS:HD3	1:B:277:LYS:HA	1.82	0.44
1:A:478:ASP:HA	1:A:481:LYS:HE3	1.99	0.44
1:A:114:ASP:OD2	1:A:118:ARG:NH1	2.51	0.44
1:A:598:LEU:O	1:A:602:ARG:HG3	2.18	0.44
1:A:550:THR:O	1:A:554:LEU:N	2.50	0.44
1:B:242:PRO:HG2	1:B:244:TYR:CZ	2.52	0.44
1:B:626:THR:OG1	1:B:656:THR:HB	2.18	0.44
1:B:505:MET:SD	1:B:560:LYS:CD	3.05	0.43
1:B:517:ALA:O	1:B:543:PHE:HA	2.18	0.43
1:B:486:GLU:OE1	1:B:520:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:OD1	1:A:118:ARG:HD3	2.18	0.43
1:A:545:GLN:NE2	1:A:546:PHE:CE2	2.86	0.43
1:A:637:LEU:CB	1:A:638:ARG:HA	2.46	0.43
1:A:464:ARG:HG2	1:A:550:THR:HG21	2.01	0.43
1:A:668:LYS:HD3	1:A:668:LYS:HA	1.76	0.43
1:A:396:PRO:HD2	1:A:399:LEU:HD12	2.00	0.43
1:A:199:LEU:CD2	1:A:209:SER:HA	2.50	0.42
1:A:601:MET:HE3	1:A:612:ILE:HG21	2.01	0.42
1:A:198:PHE:CE2	1:A:202:LEU:HD11	2.55	0.42
1:A:330:TYR:CD2	1:A:340:PRO:HD3	2.54	0.42
1:B:502:SER:O	1:B:505:MET:HB2	2.19	0.42
1:A:551:LEU:HB3	1:A:562:LEU:HD23	2.02	0.42
1:A:363:MET:HE3	1:A:363:MET:HB3	1.82	0.41
1:A:679:LEU:C	1:A:679:LEU:HD23	2.45	0.41
1:B:186:ASN:HB3	3:B:803:ADP:H4'	2.01	0.41
1:B:531:ALA:O	1:B:617:ARG:NH2	2.49	0.41
1:B:489:ALA:O	1:B:490:LEU:HD23	2.21	0.41
1:B:172:GLN:HA	1:B:266:THR:O	2.20	0.41
1:A:289:VAL:HG11	1:A:307:LEU:HD12	2.02	0.41
1:B:178:MET:N	1:B:234:SER:OG	2.53	0.41
1:B:290:THR:O	1:B:294:ASN:HB2	2.21	0.41
1:A:525:HIS:CD2	1:A:624:MET:HE1	2.55	0.41
1:A:467:ILE:HD12	1:A:483:LEU:HD11	2.01	0.41
1:B:227:ALA:HB2	1:B:270:LEU:HB3	2.03	0.41
1:A:252:GLY:O	1:B:104:GLU:HG3	2.20	0.41
1:A:274:ASP:OD1	1:A:277:LYS:NZ	2.51	0.41
1:B:411:ILE:CG2	1:B:420:LEU:HB2	2.51	0.41
1:B:509:THR:CG2	1:B:537:MET:HE1	2.51	0.41
1:B:615:THR:HA	1:B:616:PRO:HD3	1.93	0.40
1:B:366:SER:HB3	1:B:369:ASP:HB2	2.02	0.40
1:B:693:ILE:HD11	1:B:704:MET:CE	2.48	0.40
1:B:492:ALA:O	1:B:494:GLN:HB2	2.21	0.40
1:A:420:LEU:HD13	1:A:426:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/647 (90%)	551 (94%)	32 (6%)	1 (0%)	43	52
1	B	601/647 (93%)	572 (95%)	28 (5%)	1 (0%)	43	52
All	All	1185/1294 (92%)	1123 (95%)	60 (5%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	491	PRO
1	A	150	GLY

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	520/569 (91%)	510 (98%)	10 (2%)	50	65
1	B	543/569 (95%)	533 (98%)	10 (2%)	51	66
All	All	1063/1138 (93%)	1043 (98%)	20 (2%)	50	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	119	SER
1	A	126	VAL
1	A	212	ILE

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Mol	Chain	Res	Type
1	A	215	GLN
1	A	313	LEU
1	A	355	ARG
1	A	363	MET
1	A	639	THR
1	A	702	ARG
1	B	131	LEU
1	B	148	THR
1	B	231	GLU
1	B	378	VAL
1	B	394	ILE
1	B	435	GLN
1	B	490	LEU
1	B	586	SER
1	B	606	VAL
1	B	717	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	294	ASN
1	A	553	HIS
1	B	161	GLN
1	B	235	GLN
1	B	686	GLN
1	B	690	ASN
1	B	710	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	803	4,5	28,29,29	1.53	6 (21%)	43,45,45	1.81	9 (20%)
4	BEF	B	804	3	0,3,3	-	-	-		
4	BEF	A	804	3	0,3,3	-	-	-		
3	ADP	B	803	4,5	28,29,29	1.44	4 (14%)	43,45,45	1.85	10 (23%)

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	A	803	4,5	-	3/16/32/32	0/3/3/3
3	ADP	B	803	4,5	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	ADP	C5-C4	4.92	1.47	1.39
3	A	803	ADP	C5-C4	4.88	1.47	1.39
3	A	803	ADP	PA-O3A	3.29	1.63	1.59
3	B	803	ADP	C5-C6	2.79	1.48	1.41
3	A	803	ADP	C5-C6	2.38	1.47	1.41
3	A	803	ADP	C5-N7	-2.28	1.34	1.39
3	B	803	ADP	C5-N7	-2.25	1.35	1.39
3	B	803	ADP	C8-N7	2.18	1.35	1.31
3	A	803	ADP	C4-N9	-2.03	1.33	1.37
3	A	803	ADP	C8-N7	2.02	1.35	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	ADP	C5-C4-N3	-5.86	118.65	126.72
3	A	803	ADP	C5-C4-N3	-5.17	119.60	126.72
3	A	803	ADP	N3-C4-N9	4.82	135.36	127.17
3	B	803	ADP	N3-C4-N9	4.56	134.92	127.17
3	B	803	ADP	C2-N3-C4	3.72	120.93	111.83
3	A	803	ADP	C4-N9-C8	3.56	109.48	105.74
3	B	803	ADP	N3-C2-N1	-3.51	123.27	128.58
3	A	803	ADP	N3-C2-N1	-3.48	123.32	128.58
3	B	803	ADP	C4-C5-N7	-3.40	106.70	110.58
3	A	803	ADP	C2-N3-C4	3.31	119.93	111.83
3	A	803	ADP	C4-C5-N7	-2.70	107.49	110.58
3	A	803	ADP	C2-N1-C6	2.70	123.17	118.73
3	B	803	ADP	C2-N1-C6	2.46	122.77	118.73
3	B	803	ADP	C5-N7-C8	2.35	107.14	103.45
3	B	803	ADP	O3B-PB-O2B	2.34	116.56	107.80
3	B	803	ADP	C4-N9-C8	2.25	108.10	105.74
3	A	803	ADP	C5-N7-C8	2.24	106.97	103.45
3	A	803	ADP	N9-C8-N7	-2.06	111.01	113.94
3	B	803	ADP	C6-C5-N7	2.02	135.99	132.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	ADP	PA-O3A-PB-O2B
3	B	803	ADP	PA-O3A-PB-O2B
3	A	803	ADP	PA-O3A-PB-O1B
3	A	803	ADP	PA-O3A-PB-O3B
3	B	803	ADP	PA-O3A-PB-O3B

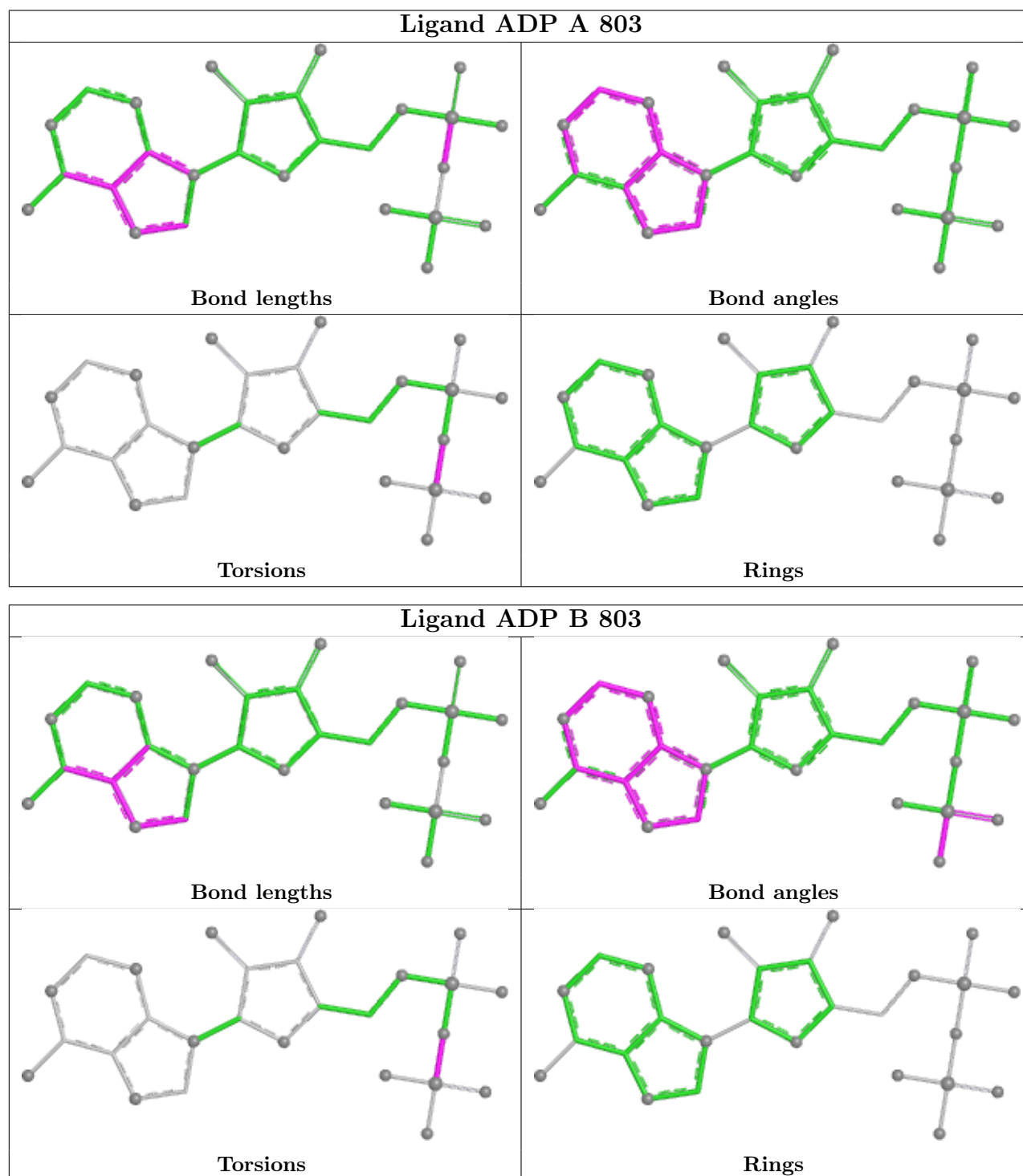
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/647 (91%)	0.10	13 (2%) 62 67	26, 79, 140, 185	0
1	B	609/647 (94%)	-0.02	8 (1%) 75 79	36, 74, 124, 154	4 (0%)
All	All	1203/1294 (92%)	0.04	21 (1%) 69 74	26, 76, 136, 185	4 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	PRO	7.7
1	A	679	LEU	4.0
1	A	680	ALA	3.9
1	A	374	MET	3.7
1	B	505	MET	3.4
1	B	149	ALA	3.0
1	B	653	LEU	2.9
1	A	324	TRP	2.8
1	B	352	LEU	2.6
1	A	100	PHE	2.6
1	B	704	MET	2.6
1	B	652	ILE	2.6
1	A	652	ILE	2.4
1	A	214	GLY	2.3
1	A	633	ALA	2.2
1	B	384	LYS	2.2
1	A	507	ALA	2.2
1	A	676	ASN	2.1
1	A	588	ARG	2.0
1	B	509	THR	2.0
1	A	154	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

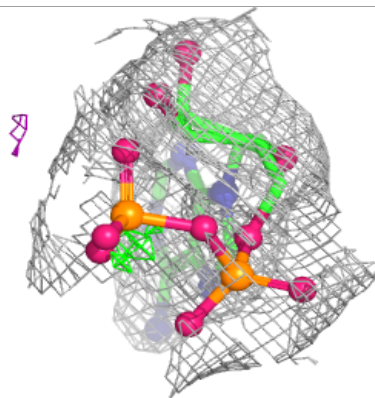
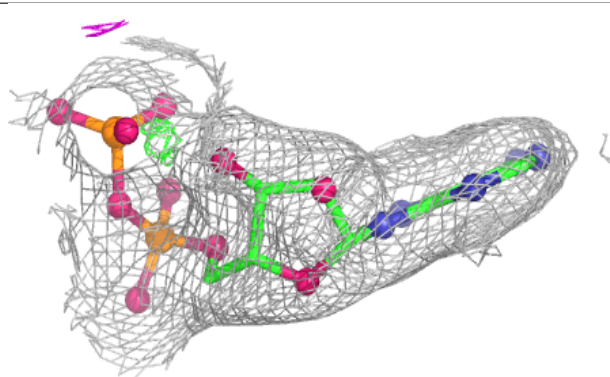
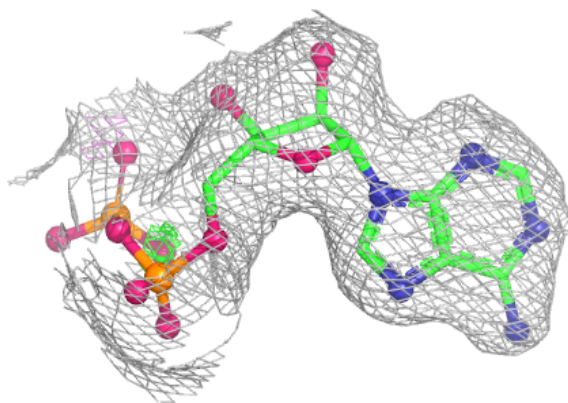
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO	A	802	1/1	0.85	0.08	113,113,113,113	1
2	CO	A	801	1/1	0.88	0.09	109,109,109,109	1
2	CO	B	801	1/1	0.92	0.08	94,94,94,94	0
2	CO	B	802	1/1	0.97	0.10	109,109,109,109	1
4	BEF	A	804	4/4	0.97	0.04	34,41,41,44	0
4	BEF	B	804	4/4	0.97	0.04	52,57,58,77	0
3	ADP	A	803	27/27	0.98	0.05	39,48,55,57	0
3	ADP	B	803	27/27	0.98	0.04	51,60,68,75	0
5	MG	A	805	1/1	0.99	0.05	51,51,51,51	0
5	MG	B	805	1/1	1.00	0.01	49,49,49,49	0

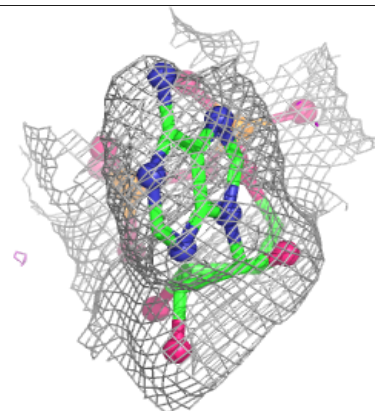
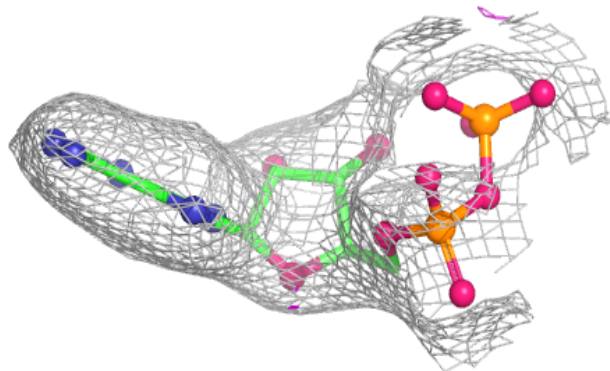
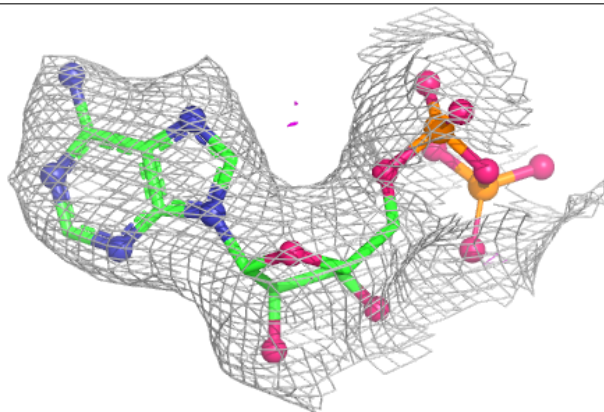
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 803:

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

**Electron density around ADP B 803:**

$2mF_o-DF_c$ (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.