



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:59 PM UTC

PDB ID : 4BE7 / pdb_00004be7
Title : MUTANT (K220R) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP
Authors : Csefalvay, E.; Lapkouski, M.; Guzanova, A.; Csefalvay, L.; Baikova, T.; Shevelev, I.; Janscak, P.; Smatanova, I.K.; Panjikar, S.; Carey, J.; Weiserova, M.; Ettrich, R.
Deposited on : 2013-03-06
Resolution : 2.74 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](#) ①) were used in the production of this report:

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

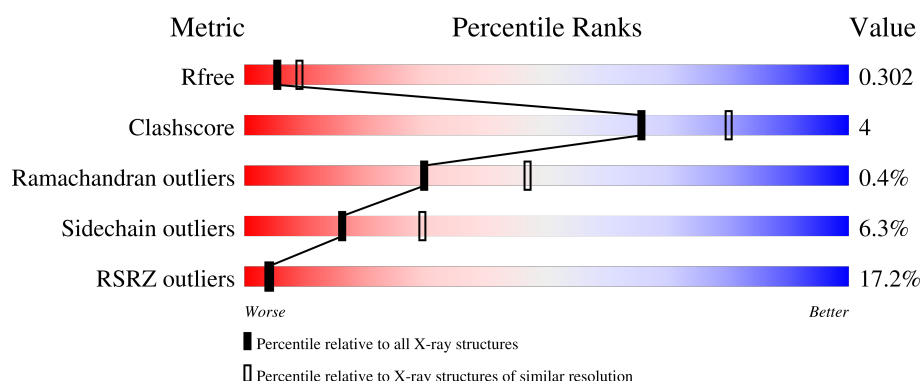
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	B	1038	11% 70% 9% 19%
1	D	1038	17% 69% 10% 20%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13387 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.

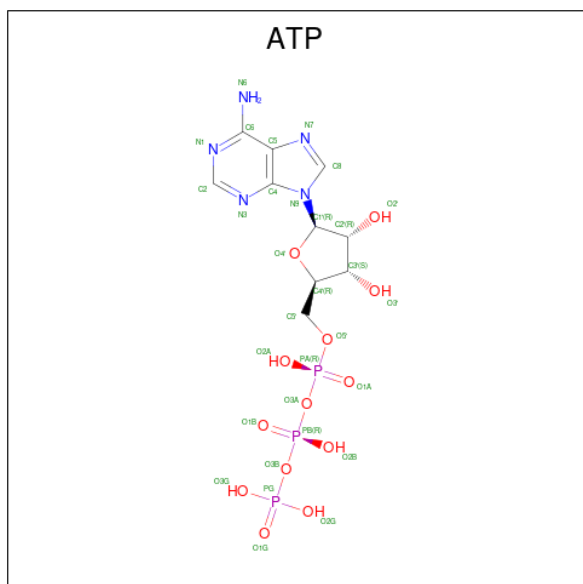
- Molecule 1 is a protein called TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	837	Total	C	N	O	S	0	0	0
			6631	4226	1112	1277	16			
1	D	835	Total	C	N	O	S	0	0	0
			6594	4204	1106	1268	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	220	ARG	LYS	engineered mutation	UNP Q304R3
D	220	ARG	LYS	engineered mutation	UNP Q304R3

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	45	Total 45	O 45	0	0
5	D	33	Total 33	O 33	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.05Å 124.35Å 128.01Å 90.00° 108.86° 90.00°	Depositor
Resolution (Å)	32.36 – 2.74 32.36 – 2.74	Depositor EDS
% Data completeness (in resolution range)	93.2 (32.36-2.74) 93.4 (32.36-2.74)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.249 , 0.292 0.263 , 0.302	Depositor DCC
R_{free} test set	3200 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13387	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% 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: PO4, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.34	0/6760	0.81	7/9146 (0.1%)
1	D	0.34	0/6721	0.85	15/9097 (0.2%)
All	All	0.34	0/13481	0.83	22/18243 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	441	PRO	CA-C-N	8.54	137.08	121.70
1	D	441	PRO	C-N-CA	8.54	137.08	121.70
1	D	826	ASP	CA-C-N	6.99	134.27	121.70
1	D	826	ASP	C-N-CA	6.99	134.27	121.70
1	D	581	SER	N-CA-C	6.94	119.68	107.61
1	D	509	HIS	CA-C-N	6.65	126.90	119.32
1	D	509	HIS	C-N-CA	6.65	126.90	119.32
1	D	441	PRO	N-CA-C	6.55	124.39	113.78
1	B	509	HIS	CA-C-N	6.44	126.66	119.32
1	B	509	HIS	C-N-CA	6.44	126.66	119.32
1	B	769	ILE	N-CA-C	-6.03	96.79	109.34
1	D	626	ASN	N-CA-C	5.96	120.56	112.88
1	D	441	PRO	CA-C-O	-5.95	110.65	120.05
1	B	626	ASN	N-CA-C	5.94	120.54	112.88
1	D	531	THR	N-CA-C	5.74	118.64	111.24
1	B	769	ILE	CA-C-N	5.71	131.97	121.70
1	B	769	ILE	C-N-CA	5.71	131.97	121.70
1	D	396	LEU	CA-C-N	5.53	125.62	119.32
1	D	396	LEU	C-N-CA	5.53	125.62	119.32
1	B	769	ILE	CB-CA-C	5.50	120.30	111.29
1	D	828	LYS	N-CA-C	-5.31	104.47	111.96
1	D	533	PRO	N-CA-C	5.09	119.09	111.14

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	B	6631	0	6305	48	0
1	D	6594	0	6268	50	0
2	B	31	0	12	1	0
2	D	31	0	12	1	0
3	B	10	0	0	0	0
3	D	10	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	45	0	0	1	0
5	D	33	0	0	1	0
All	All	13387	0	12597	98	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 4.

All (98) 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:D:824:VAL:HG13	1:D:828:LYS:HB3	1.54	0.90
1:D:27:GLY:HA2	1:D:28:ASP:HB2	1.59	0.85
1:D:169:ARG:HH11	1:D:169:ARG:HG3	1.52	0.73
1:D:465:ASP:OD1	1:D:468:ARG:NH2	2.22	0.71
1:D:322:ARG:NH2	5:D:2021:HOH:O	2.25	0.69
1:B:770:GLU:N	1:B:770:GLU:OE1	2.25	0.68
1:D:440:PHE:O	1:D:443:ASN:ND2	2.28	0.66
1:D:801:LEU:HG	1:D:837:LEU:HD11	1.78	0.65
1:B:322:ARG:NH2	5:B:2025:HOH:O	2.29	0.65
1:B:769:ILE:HG22	1:B:770:GLU:HA	1.79	0.65
1:B:213:ALA:HB2	1:B:271:VAL:HG23	1.81	0.63
1:D:54:VAL:HG11	1:D:60:MET:HG3	1.82	0.62
1:D:440:PHE:N	1:D:443:ASN:OD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:O	1:B:471:LYS:NZ	2.30	0.62
1:D:684:GLN:O	1:D:688:ARG:NH1	2.32	0.62
1:D:213:ALA:HB2	1:D:271:VAL:HG23	1.82	0.62
1:D:688:ARG:NH2	2:D:1887:ATP:O1G	2.30	0.61
1:B:154:ILE:HB	1:B:162:VAL:HB	1.81	0.60
1:D:154:ILE:HB	1:D:162:VAL:HB	1.83	0.60
1:D:678:ARG:NH1	1:D:711:SER:OG	2.34	0.60
1:B:298:LYS:O	1:B:301:SER:OG	2.21	0.58
1:B:65:ARG:HG3	1:B:81:TRP:CD2	2.39	0.58
1:B:110:ASP:HB2	1:B:118:LEU:HD21	1.86	0.57
1:B:313:LYS:NZ	1:B:409:GLU:OE1	2.32	0.57
1:B:443:ASN:HB3	1:B:718:LEU:HD11	1.86	0.57
1:D:309:THR:HA	1:D:313:LYS:HE2	1.86	0.56
1:B:13:ASN:HD22	1:B:13:ASN:N	2.04	0.56
1:B:89:LEU:O	1:B:99:LYS:NZ	2.38	0.55
1:D:313:LYS:NZ	1:D:409:GLU:OE1	2.37	0.55
1:D:54:VAL:HG11	1:D:60:MET:CG	2.37	0.55
1:B:44:LEU:HD13	1:B:136:ILE:HG21	1.89	0.54
1:B:54:VAL:HG11	1:B:60:MET:HG3	1.90	0.53
1:B:688:ARG:NH2	2:B:1887:ATP:O1G	2.34	0.53
1:B:824:VAL:HG13	1:B:828:LYS:HB3	1.89	0.53
1:B:838:PRO:HG2	1:B:843:ILE:HD11	1.92	0.52
1:D:189:ASN:HA	1:D:192:ASN:OD1	2.10	0.51
1:B:801:LEU:HG	1:B:837:LEU:HD11	1.91	0.51
1:B:54:VAL:HG11	1:B:60:MET:CG	2.41	0.51
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.38	0.51
1:B:204:SER:HB2	1:B:209:THR:HG23	1.94	0.50
1:D:325:THR:HG21	1:D:378:ILE:HB	1.94	0.50
1:D:88:TYR:CE1	1:D:109:CYS:HB2	2.47	0.49
1:D:125:ASP:OD2	1:D:131:ARG:NH1	2.45	0.49
1:B:541:MET:HE2	1:B:653:LEU:HD23	1.94	0.48
1:B:686:PHE:CZ	1:B:702:ILE:HG21	2.49	0.48
1:D:110:ASP:HB2	1:D:118:LEU:HD21	1.95	0.48
1:B:26:THR:OG1	1:B:27:GLY:HA2	2.13	0.48
1:D:679:TYR:CD1	1:D:718:LEU:HD12	2.49	0.48
1:B:256:VAL:HA	1:B:260:TYR:HB2	1.94	0.47
1:D:581:SER:O	1:D:597:GLU:HB3	2.15	0.47
1:D:211:TYR:CE2	1:D:227:MET:HE2	2.48	0.47
1:D:581:SER:OG	1:D:598:THR:O	2.23	0.47
1:D:528:THR:OG1	1:D:530:ARG:HD2	2.14	0.46
1:B:125:ASP:OD2	1:B:131:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:VAL:HA	1:D:260:TYR:HB2	1.96	0.46
1:B:112:ILE:HD13	1:B:118:LEU:HD23	1.98	0.46
1:D:531:THR:HG23	1:D:532:PHE:H	1.80	0.46
1:D:227:MET:HE3	1:D:273:ARG:HG3	1.98	0.46
1:D:441:PRO:HB2	1:D:442:GLU:HB2	1.98	0.46
1:D:825:ASP:O	1:D:828:LYS:HB2	2.15	0.46
1:D:224:ASP:OD1	1:D:224:ASP:N	2.48	0.46
1:D:838:PRO:HG2	1:D:843:ILE:HD11	1.98	0.46
1:D:686:PHE:CZ	1:D:702:ILE:HG21	2.52	0.45
1:D:328:ASP:OD1	1:D:329:PHE:N	2.49	0.45
1:B:684:GLN:O	1:B:688:ARG:NH1	2.47	0.45
1:D:89:LEU:HD21	1:D:159:LEU:HD21	1.98	0.44
1:D:354:SER:HB3	1:D:357:SER:OG	2.17	0.44
1:D:637:TYR:O	1:D:641:LEU:HB2	2.18	0.44
1:B:342:LEU:O	1:B:638:TYR:OH	2.32	0.44
1:B:57:GLN:OE1	1:B:192:ASN:HB3	2.17	0.44
1:B:99:LYS:HD2	1:B:197:TYR:CZ	2.52	0.44
1:B:637:TYR:O	1:B:641:LEU:HB2	2.18	0.44
1:B:60:MET:HE2	1:B:194:LEU:HD13	2.00	0.43
1:B:440:PHE:N	1:B:443:ASN:OD1	2.50	0.43
1:D:176:ALA:HB1	1:D:203:ILE:HD11	1.99	0.43
1:B:99:LYS:HD2	1:B:197:TYR:CE2	2.52	0.43
1:B:704:THR:HG21	1:B:708:LEU:HD12	2.01	0.43
1:B:769:ILE:CG2	1:B:770:GLU:HA	2.46	0.43
1:D:57:GLN:HB2	1:D:191:GLU:O	2.19	0.43
1:D:204:SER:HB2	1:D:209:THR:HG23	1.99	0.43
1:D:394:SER:HA	1:D:425:LYS:NZ	2.33	0.43
1:D:839:ALA:O	1:D:843:ILE:HG12	2.19	0.43
1:B:763:PHE:HA	1:B:768:SER:CB	2.49	0.43
1:B:544:VAL:HA	1:B:674:ASP:O	2.19	0.42
1:D:490:GLU:HG2	1:D:512:ARG:HH21	1.83	0.42
1:D:90:ASP:O	1:D:91:ASN:C	2.63	0.42
1:B:60:MET:HE2	1:B:60:MET:HB3	1.93	0.42
1:B:763:PHE:HA	1:B:768:SER:HB3	2.01	0.42
1:D:44:LEU:HD13	1:D:136:ILE:HG21	2.02	0.42
1:B:640:ASP:OD2	1:B:644:ARG:NE	2.50	0.41
1:D:40:LEU:HD11	1:D:164:ILE:HG21	2.01	0.41
1:B:847:ARG:NH2	1:B:886:GLN:OE1	2.40	0.41
1:B:386:LEU:HG	1:B:390:MET:HE2	2.01	0.41
1:D:65:ARG:HG3	1:D:81:TRP:CD2	2.54	0.41
1:D:476:LYS:NZ	1:D:478:ASP:OD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLN:C	1:B:91:ASN:HD21	2.28	0.41
1:B:90:ASP:O	1:B:91:ASN:C	2.64	0.40
1:B:679:TYR:CD1	1:B:718:LEU:HD12	2.56	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	B	827/1038 (80%)	798 (96%)	26 (3%)	3 (0%)	30	47
1	D	825/1038 (80%)	785 (95%)	37 (4%)	3 (0%)	30	47
All	All	1652/2076 (80%)	1583 (96%)	63 (4%)	6 (0%)	30	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	810	SER
1	B	807	ILE
1	B	810	SER
1	D	807	ILE
1	B	769	ILE
1	D	769	ILE

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	B	690/927 (74%)	649 (94%)	41 (6%)	18	32
1	D	684/927 (74%)	638 (93%)	46 (7%)	15	27
All	All	1374/1854 (74%)	1287 (94%)	87 (6%)	16	29

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	21	ILE
1	B	40	LEU
1	B	65	ARG
1	B	71	LEU
1	B	89	LEU
1	B	118	LEU
1	B	163	GLN
1	B	165	GLU
1	B	221	ASN
1	B	240	LEU
1	B	253	LEU
1	B	282	ARG
1	B	298	LYS
1	B	301	SER
1	B	307	HIS
1	B	332	LYS
1	B	336	VAL
1	B	346	THR
1	B	356	ASP
1	B	379	ILE
1	B	393	GLU
1	B	402	GLN
1	B	422	LEU
1	B	464	THR
1	B	472	VAL
1	B	482	VAL
1	B	641	LEU
1	B	652	LEU
1	B	655	VAL
1	B	688	ARG
1	B	718	LEU
1	B	722	LYS
1	B	731	LYS
1	B	753	MET

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Mol	Chain	Res	Type
1	B	765	ASP
1	B	769	ILE
1	B	781	LEU
1	B	804	LEU
1	B	824	VAL
1	B	840	ASP
1	D	21	ILE
1	D	26	THR
1	D	40	LEU
1	D	65	ARG
1	D	71	LEU
1	D	89	LEU
1	D	118	LEU
1	D	134	VAL
1	D	163	GLN
1	D	169	ARG
1	D	192	ASN
1	D	217	LYS
1	D	224	ASP
1	D	227	MET
1	D	240	LEU
1	D	253	LEU
1	D	307	HIS
1	D	309	THR
1	D	336	VAL
1	D	346	THR
1	D	356	ASP
1	D	393	GLU
1	D	402	GLN
1	D	422	LEU
1	D	442	GLU
1	D	443	ASN
1	D	464	THR
1	D	472	VAL
1	D	482	VAL
1	D	532	PHE
1	D	581	SER
1	D	626	ASN
1	D	641	LEU
1	D	647	ASN
1	D	652	LEU
1	D	655	VAL

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Mol	Chain	Res	Type
1	D	688	ARG
1	D	710	ARG
1	D	718	LEU
1	D	731	LYS
1	D	753	MET
1	D	765	ASP
1	D	781	LEU
1	D	804	LEU
1	D	805	GLN
1	D	824	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	GLN
1	B	228	ASN
1	B	249	GLN
1	B	307	HIS
1	B	363	ASN
1	B	387	ASN
1	B	402	GLN
1	B	414	GLN
1	B	419	GLN
1	B	431	GLN
1	B	648	GLN
1	D	57	GLN
1	D	91	ASN
1	D	234	ASN
1	D	249	GLN
1	D	259	ASN
1	D	267	GLN
1	D	307	HIS
1	D	387	ASN
1	D	414	GLN
1	D	421	ASN
1	D	514	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PO4	D	1890	-	4,4,4	0.99	0	6,6,6	0.47	0
2	ATP	D	1887	4	32,33,33	1.41	5 (15%)	48,52,52	1.77	8 (16%)
2	ATP	B	1887	4	32,33,33	1.40	5 (15%)	48,52,52	1.77	8 (16%)
3	PO4	B	1889	-	4,4,4	0.97	0	6,6,6	0.39	0
3	PO4	D	1889	-	4,4,4	0.93	0	6,6,6	0.40	0
3	PO4	B	1888	-	4,4,4	0.93	0	6,6,6	0.45	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
2	ATP	D	1887	4	-	1/22/38/38	0/3/3/3
2	ATP	B	1887	4	-	0/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1887	ATP	C5-C4	4.57	1.47	1.39
2	D	1887	ATP	C5-C4	4.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1887	ATP	C5-C6	2.71	1.48	1.41
2	D	1887	ATP	C5-C6	2.64	1.48	1.41
2	D	1887	ATP	PB-O3B	2.59	1.62	1.59
2	D	1887	ATP	C5-N7	-2.36	1.34	1.39
2	B	1887	ATP	C5-N7	-2.30	1.34	1.39
2	B	1887	ATP	PB-O3B	2.30	1.62	1.59
2	D	1887	ATP	C8-N7	2.24	1.36	1.31
2	B	1887	ATP	C8-N7	2.16	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1887	ATP	C5-C4-N3	-5.75	118.80	126.72
2	D	1887	ATP	C5-C4-N3	-5.73	118.83	126.72
2	B	1887	ATP	N3-C4-N9	4.73	135.22	127.17
2	D	1887	ATP	N3-C4-N9	4.68	135.12	127.17
2	D	1887	ATP	C2-N3-C4	3.65	120.75	111.83
2	B	1887	ATP	C2-N3-C4	3.63	120.70	111.83
2	B	1887	ATP	C4-C5-N7	-3.37	106.73	110.58
2	D	1887	ATP	C4-C5-N7	-3.33	106.78	110.58
2	D	1887	ATP	N3-C2-N1	-3.25	123.66	128.58
2	B	1887	ATP	N3-C2-N1	-3.13	123.84	128.58
2	B	1887	ATP	C4-N9-C8	2.98	108.86	105.74
2	D	1887	ATP	C4-N9-C8	2.89	108.78	105.74
2	B	1887	ATP	C5-N7-C8	2.58	107.51	103.45
2	D	1887	ATP	C5-N7-C8	2.53	107.43	103.45
2	B	1887	ATP	N9-C8-N7	-2.13	110.92	113.94
2	D	1887	ATP	N9-C8-N7	-2.09	110.97	113.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

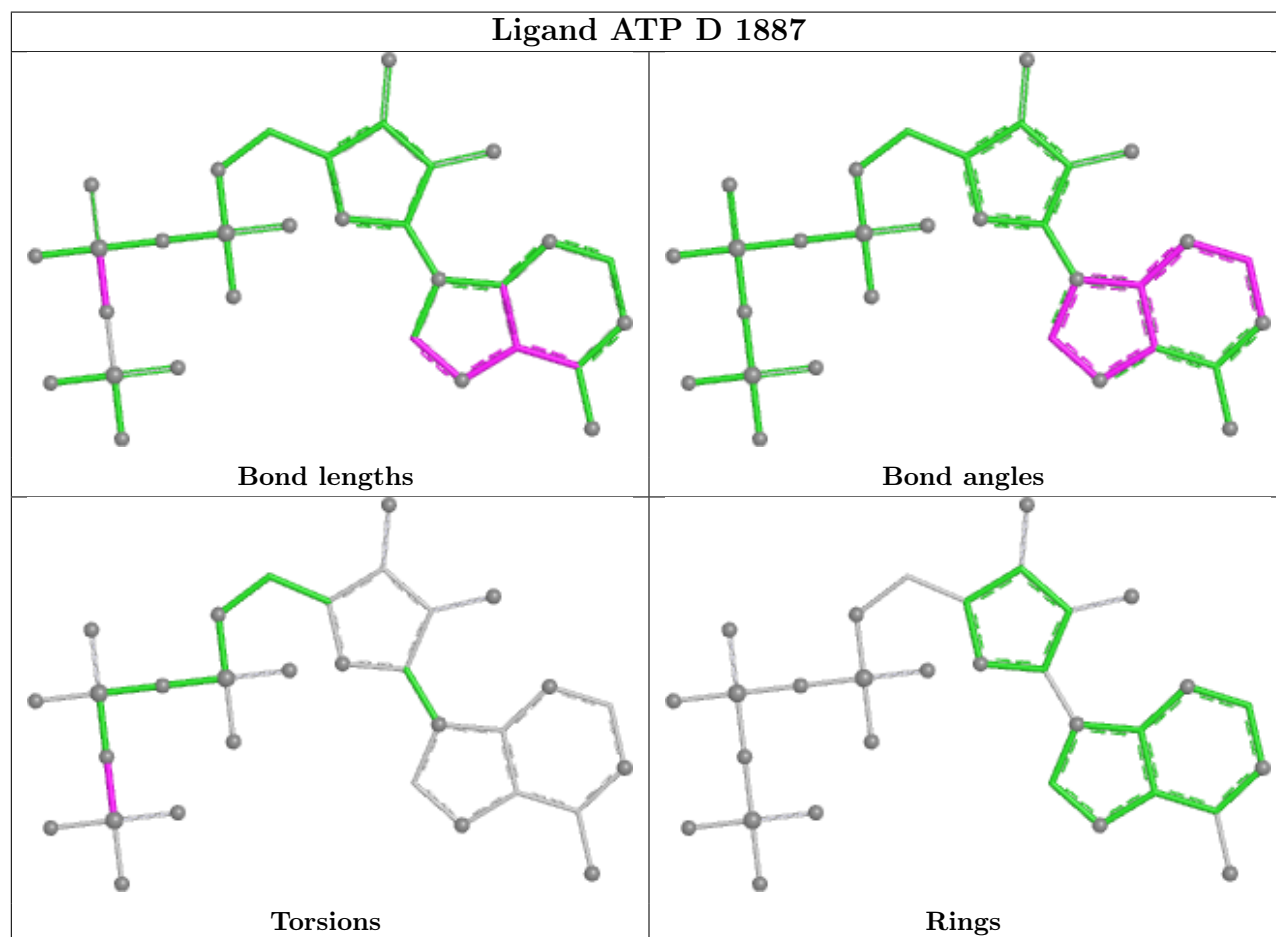
Mol	Chain	Res	Type	Atoms
2	D	1887	ATP	PB-O3B-PG-O1G

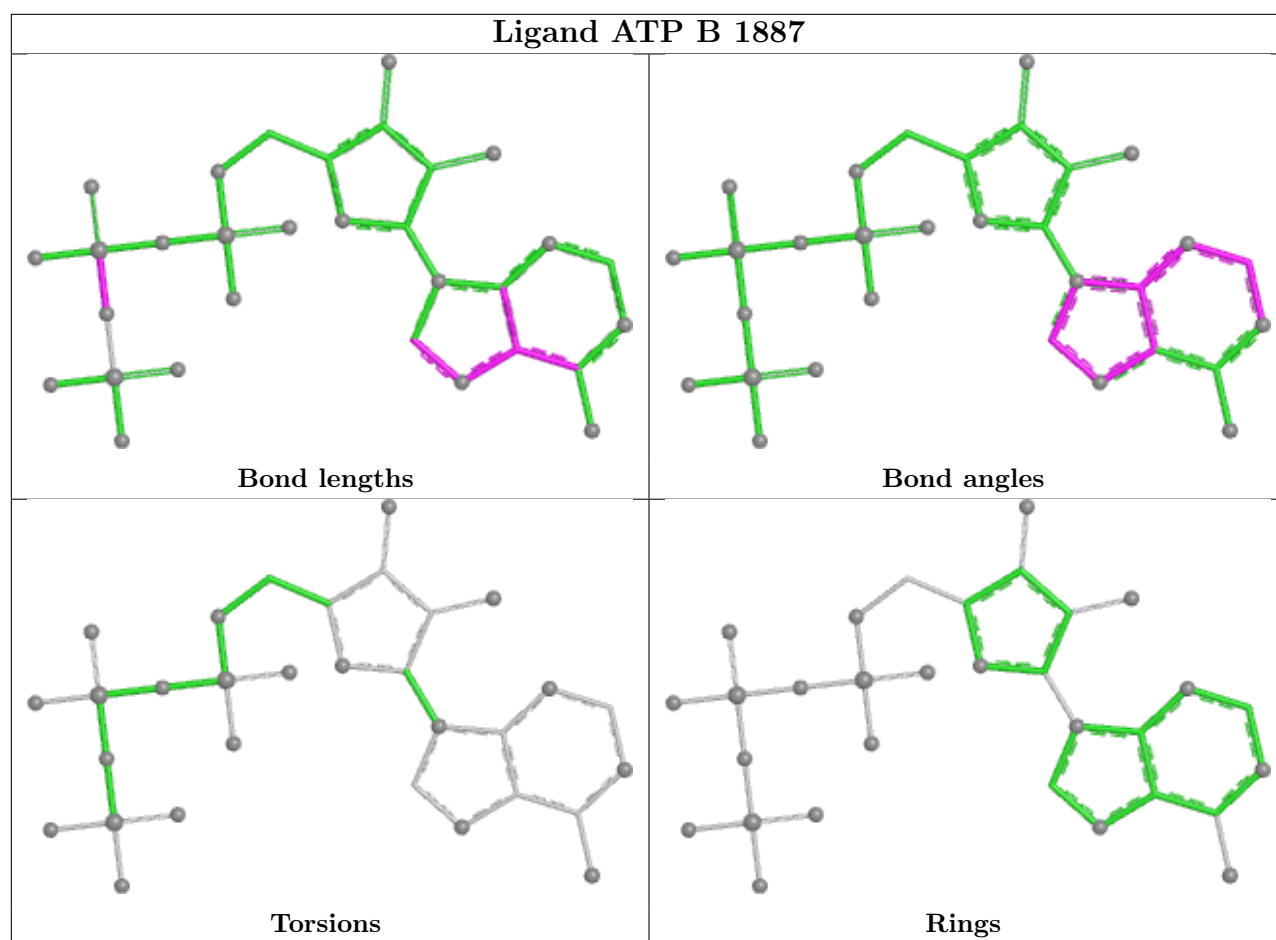
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1887	ATP	1	0
2	B	1887	ATP	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	B	837/1038 (80%)	0.88	110 (13%) 7 7	13, 33, 71, 121	0
1	D	835/1038 (80%)	1.18	178 (21%) 2 2	17, 40, 84, 114	0
All	All	1672/2076 (80%)	1.03	288 (17%) 4 4	13, 36, 78, 121	0

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	809	LEU	9.5
1	B	566	ASN	9.3
1	B	814	ALA	8.2
1	D	534	GLY	7.3
1	D	815	VAL	7.1
1	B	808	ASP	6.9
1	D	810	SER	6.8
1	B	813	VAL	6.7
1	D	811	ASP	6.6
1	D	768	SER	6.4
1	D	533	PRO	6.4
1	B	567	LYS	6.3
1	D	819	LYS	6.2
1	D	809	LEU	6.1
1	D	814	ALA	6.0
1	B	810	SER	5.8
1	D	565	ALA	5.6
1	B	811	ASP	5.5
1	D	769	ILE	5.4
1	D	566	ASN	5.3
1	D	874	ASP	5.1
1	D	818	PHE	5.1
1	D	603	ALA	5.0
1	D	807	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	769	ILE	4.6
1	B	806	GLN	4.6
1	D	506	ALA	4.5
1	D	562	GLU	4.5
1	B	807	ILE	4.5
1	D	570	THR	4.5
1	B	498	LEU	4.4
1	B	568	SER	4.4
1	D	808	ASP	4.4
1	D	766	PRO	4.4
1	D	813	VAL	4.4
1	B	767	THR	4.3
1	D	558	LYS	4.3
1	B	570	THR	4.3
1	B	565	ALA	4.3
1	B	745	THR	4.2
1	D	563	GLU	4.2
1	B	28	ASP	4.1
1	B	821	GLU	4.1
1	D	532	PHE	4.1
1	B	502	GLU	4.1
1	B	744	ALA	4.0
1	D	650	ILE	4.0
1	D	568	SER	4.0
1	B	563	GLU	4.0
1	D	767	THR	4.0
1	D	635	GLN	4.0
1	D	479	TYR	4.0
1	D	508	LEU	4.0
1	D	21	ILE	4.0
1	D	511	MET	4.0
1	B	812	PRO	3.9
1	B	818	PHE	3.9
1	B	564	ALA	3.9
1	B	21	ILE	3.9
1	B	508	LEU	3.9
1	D	502	GLU	3.8
1	D	446	GLY	3.8
1	D	505	GLN	3.8
1	D	806	GLN	3.8
1	D	569	ALA	3.8
1	D	604	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	880	VAL	3.8
1	D	812	PRO	3.8
1	D	772	GLU	3.8
1	D	824	VAL	3.8
1	D	482	VAL	3.7
1	B	189	ASN	3.7
1	B	815	VAL	3.7
1	B	522	ASN	3.6
1	D	344	TYR	3.6
1	B	190	SER	3.6
1	B	535	SER	3.6
1	B	506	ALA	3.6
1	D	191	GLU	3.6
1	D	774	GLU	3.6
1	D	623	PHE	3.5
1	D	178	ASN	3.5
1	D	447	SER	3.5
1	D	816	GLU	3.5
1	D	805	GLN	3.5
1	D	822	HIS	3.5
1	B	170	GLY	3.4
1	D	714	ASP	3.4
1	D	765	ASP	3.4
1	D	560	LEU	3.4
1	D	817	LYS	3.4
1	D	803	ALA	3.4
1	D	831	GLU	3.4
1	D	28	ASP	3.4
1	B	770	GLU	3.3
1	D	804	LEU	3.3
1	D	615	ALA	3.3
1	D	559	ARG	3.2
1	D	838	PRO	3.2
1	B	828	LYS	3.2
1	B	832	LEU	3.2
1	D	445	LEU	3.2
1	B	500	ALA	3.2
1	D	444	ALA	3.2
1	B	827	GLU	3.2
1	D	851	ASN	3.2
1	D	531	THR	3.1
1	D	535	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	27	GLY	3.1
1	D	180	ILE	3.1
1	D	853	ILE	3.1
1	B	823	TYR	3.1
1	B	511	MET	3.0
1	D	500	ALA	3.0
1	B	880	VAL	3.0
1	D	859	ARG	3.0
1	D	190	SER	3.0
1	D	496	LYS	3.0
1	D	567	LYS	3.0
1	D	494	ASP	3.0
1	D	617	ARG	3.0
1	D	614	ALA	3.0
1	D	744	ALA	2.9
1	B	533	PRO	2.9
1	D	679	TYR	2.9
1	B	824	VAL	2.9
1	D	510	PRO	2.9
1	D	606	SER	2.9
1	D	607	SER	2.9
1	B	790	ASN	2.9
1	B	826	ASP	2.9
1	D	605	ASP	2.9
1	D	850	TYR	2.9
1	B	765	ASP	2.9
1	D	825	ASP	2.9
1	D	855	ASP	2.9
1	B	569	ALA	2.9
1	D	829	PHE	2.9
1	B	618	GLU	2.8
1	D	827	GLU	2.8
1	B	179	GLN	2.8
1	D	481	ASP	2.8
1	B	611	PHE	2.8
1	B	829	PHE	2.8
1	B	817	LYS	2.8
1	D	629	THR	2.8
1	D	823	TYR	2.8
1	D	572	LYS	2.8
1	B	572	LYS	2.8
1	D	842	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	501	ALA	2.8
1	B	571	TYR	2.8
1	D	780	LYS	2.7
1	B	221	ASN	2.7
1	D	374	ASP	2.7
1	D	492	GLU	2.7
1	D	564	ALA	2.7
1	D	218	ARG	2.7
1	D	836	ARG	2.7
1	D	857	GLN	2.7
1	D	770	GLU	2.7
1	D	826	ASP	2.7
1	B	746	GLY	2.7
1	B	374	ASP	2.7
1	B	627	PHE	2.7
1	B	825	ASP	2.7
1	D	840	ASP	2.7
1	D	523	ASN	2.7
1	D	497	LYS	2.7
1	B	606	SER	2.6
1	B	820	ALA	2.6
1	B	59	ALA	2.6
1	B	134	VAL	2.6
1	D	875	ASP	2.6
1	D	27	GLY	2.6
1	D	416	GLY	2.6
1	B	357	SER	2.6
1	B	834	THR	2.6
1	D	748	ALA	2.6
1	B	757	SER	2.5
1	D	596	ASP	2.5
1	D	495	GLU	2.5
1	D	627	PHE	2.5
1	B	26	THR	2.5
1	D	771	SER	2.5
1	D	561	GLN	2.5
1	D	582	PHE	2.5
1	D	32	SER	2.5
1	B	375	ASP	2.5
1	B	612	LEU	2.5
1	B	29	SER	2.5
1	D	858	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	855	ASP	2.5
1	D	747	GLU	2.5
1	B	751	GLY	2.5
1	D	504	GLN	2.5
1	D	601	THR	2.4
1	B	595	SER	2.4
1	D	394	SER	2.4
1	D	544	VAL	2.4
1	B	505	GLN	2.4
1	B	560	LEU	2.4
1	B	460	SER	2.4
1	D	548	ASP	2.4
1	D	773	LYS	2.4
1	D	751	GLY	2.4
1	B	743	ALA	2.4
1	D	571	TYR	2.4
1	B	629	THR	2.4
1	D	631	SER	2.4
1	B	558	LYS	2.4
1	D	95	GLY	2.4
1	B	830	ALA	2.4
1	D	365	ALA	2.4
1	B	30	TYR	2.3
1	D	760	GLU	2.3
1	D	546	SER	2.3
1	B	634	PHE	2.3
1	B	883	LEU	2.3
1	D	820	ALA	2.3
1	B	493	THR	2.3
1	D	26	THR	2.3
1	B	610	GLU	2.3
1	B	290	SER	2.3
1	D	608	ALA	2.3
1	D	834	THR	2.3
1	B	218	ARG	2.3
1	B	804	LEU	2.3
1	D	781	LEU	2.3
1	D	517	THR	2.3
1	B	747	GLU	2.3
1	D	821	GLU	2.3
1	D	501	ALA	2.2
1	B	819	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	387	ASN	2.2
1	B	613	ASP	2.2
1	D	882	LEU	2.2
1	D	509	HIS	2.2
1	D	835	ILE	2.2
1	D	50	GLU	2.2
1	B	859	ARG	2.2
1	B	180	ILE	2.2
1	D	245	ALA	2.2
1	D	743	ALA	2.2
1	B	831	GLU	2.2
1	D	503	ASN	2.2
1	D	595	SER	2.2
1	D	641	LEU	2.2
1	D	507	PHE	2.2
1	D	555	ALA	2.2
1	B	510	PRO	2.2
1	D	355	PRO	2.2
1	D	573	PRO	2.2
1	B	494	ASP	2.2
1	B	796	ASP	2.2
1	D	881	ASP	2.2
1	B	835	ILE	2.2
1	D	856	TRP	2.1
1	D	764	PRO	2.1
1	D	529	HIS	2.1
1	D	611	PHE	2.1
1	B	593	GLU	2.1
1	D	618	GLU	2.1
1	D	793	GLN	2.1
1	B	718	LEU	2.1
1	B	509	HIS	2.1
1	D	439	ILE	2.1
1	D	779	VAL	2.1
1	B	140	PHE	2.1
1	D	551	LYS	2.1
1	B	805	GLN	2.1
1	D	443	ASN	2.1
1	D	796	ASP	2.1
1	D	848	SER	2.1
1	D	515	GLU	2.1
1	B	496	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	22	LYS	2.1
1	D	498	LEU	2.1
1	D	189	ASN	2.1
1	D	513	ILE	2.1
1	B	54	VAL	2.1
1	D	639	ARG	2.0
1	D	493	THR	2.0
1	D	46	ASN	2.0
1	D	23	ALA	2.0
1	D	204	SER	2.0
1	B	521	LEU	2.0
1	B	723	ASN	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.

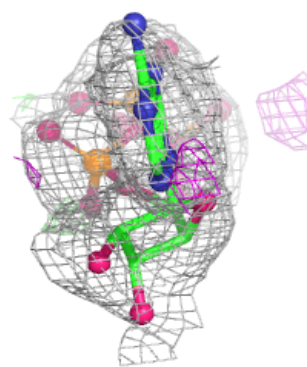
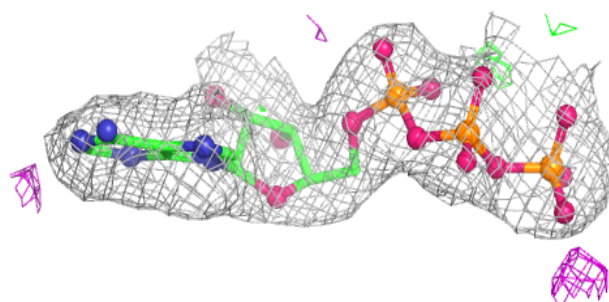
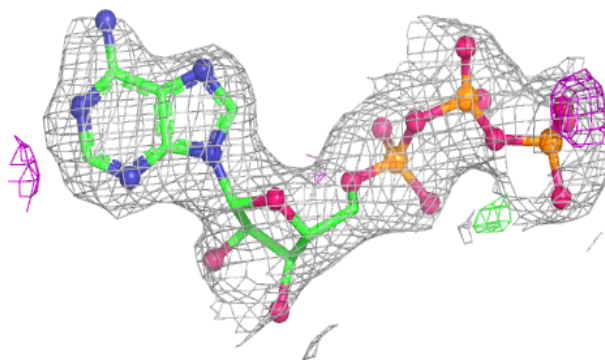
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	D	1889	5/5	0.81	0.11	36,53,55,82	0
3	PO4	B	1889	5/5	0.86	0.15	52,55,69,83	0
4	MG	B	1890	1/1	0.92	0.08	23,23,23,23	0
4	MG	D	1886	1/1	0.92	0.10	25,25,25,25	0
2	ATP	D	1887	31/31	0.96	0.09	13,21,27,33	0
2	ATP	B	1887	31/31	0.97	0.07	11,18,23,25	0
3	PO4	B	1888	5/5	0.97	0.08	24,24,27,32	0
3	PO4	D	1890	5/5	0.98	0.06	16,17,21,23	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.

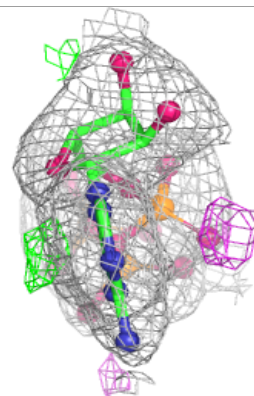
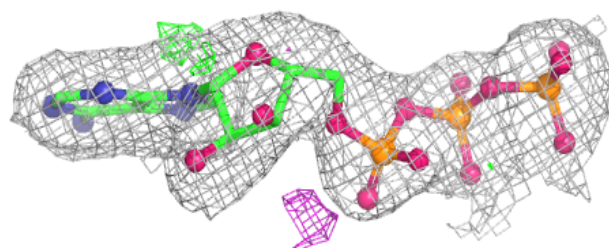
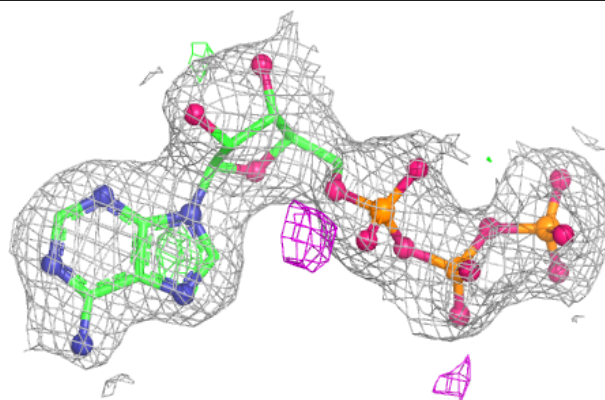
Electron density around ATP D 1887:

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



Electron density around ATP B 1887:

$2mF_o-DF_c$ (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.