



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:21 am BST

PDB ID : 4BEB  
Title : MUTANT (K220E) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP  
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Deposited on : 2013-03-07  
Resolution : 2.99 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

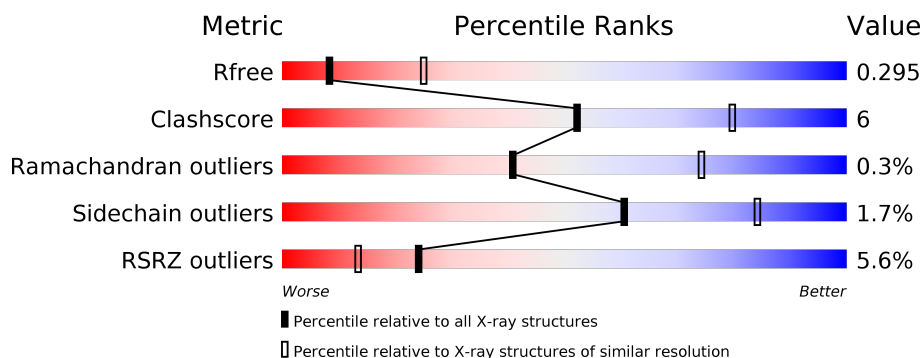
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	1038	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>12%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	1038	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	1038	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>10%</div> <div>•</div> <div>19%</div> </div> </div>
1	D	1038	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>12%</div> <div>•</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27369 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 HSDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6821	4340	1158	1307	16			
1	B	842	Total	C	N	O	S	0	0	0
			6846	4353	1158	1319	16			
1	C	838	Total	C	N	O	S	0	0	0
			6802	4326	1151	1309	16			
1	D	833	Total	C	N	O	S	0	0	0
			6772	4309	1146	1301	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLU	LYS	engineered mutation	UNP Q304R3
B	220	GLU	LYS	engineered mutation	UNP Q304R3
C	220	GLU	LYS	engineered mutation	UNP Q304R3
D	220	GLU	LYS	engineered mutation	UNP Q304R3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

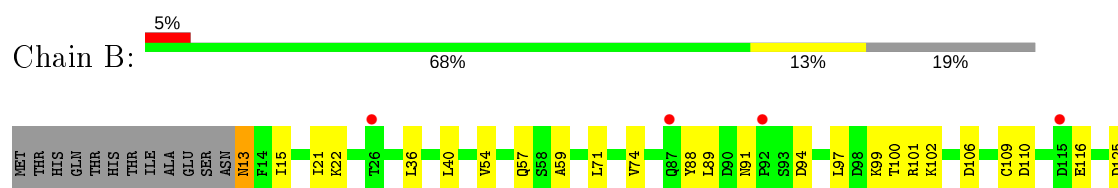
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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



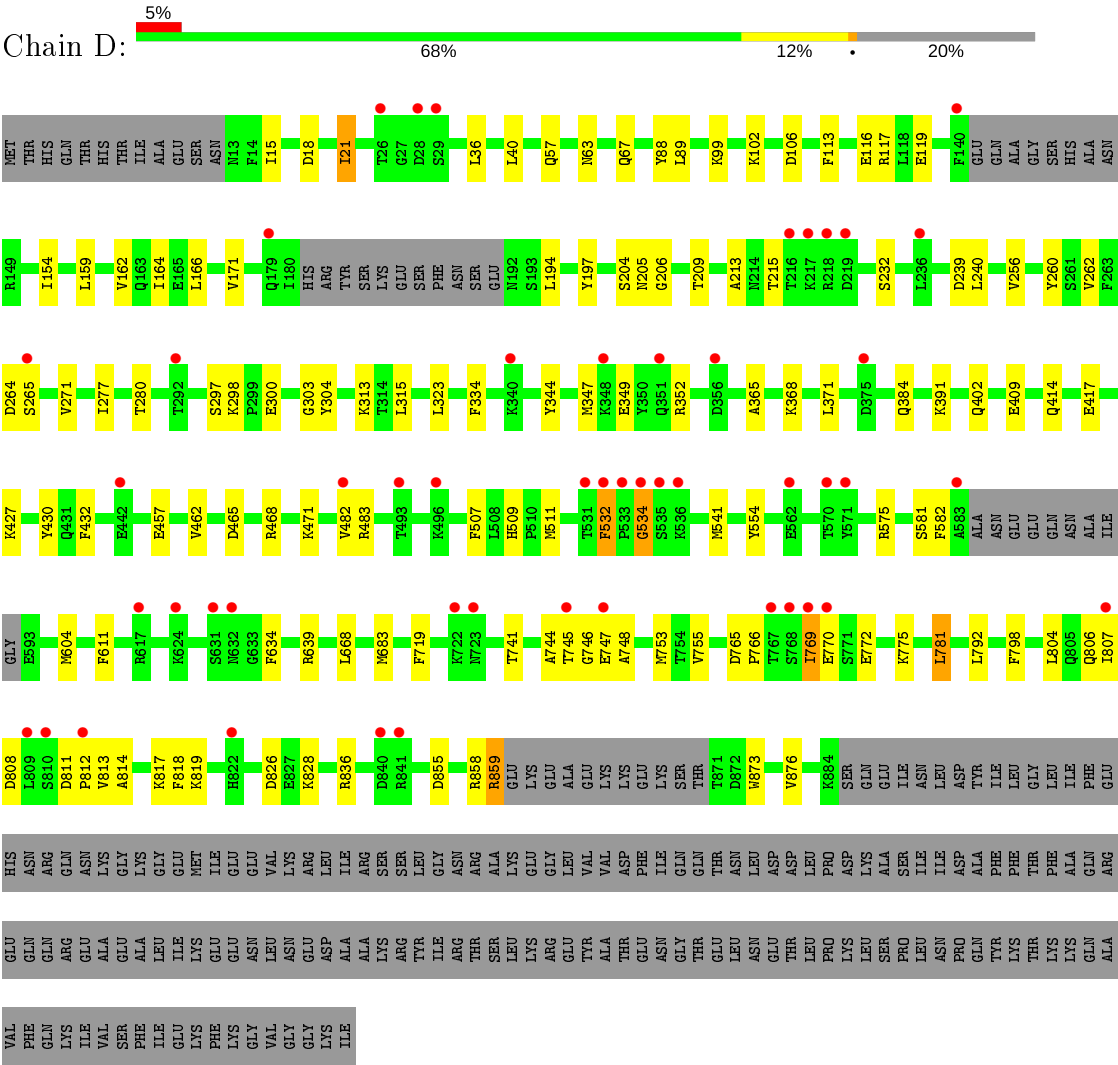
- Molecule 1: TYPE I RESTRICTION ENZYME HSDR





ASP	LEU	THR	LEU	PRO	GLN	ASP	LYS	LEU	ASP	SER	ALA	THR	ILE	ASP	GLU	ALA	PHE	PHE	LYS	THR	PHE	ALA	GLN	ARG	GLU	GLN	GLN	ARG	ILE	LYS	GLU	GLY	ASN	ALA	ALA	LYS	ARG	TYR	ILE	THR	ARG	THR	SER	LEU	LYS	ARG	GLU	TYR	ALA	THR	GLU	ASN	GLU
THR	LEU	PRO	LYS	LEU	SER	PRO	LEU	ASN	PRO	GLU	GLN	ALA	THR	LYS	THR	LYS	LYS	ALA	GLN	VAL	PHE	GLN	LYS	ILE	GLU	VAL	SER	PHE	ILE	GLU	LYS	PHE	GLY	VAL	GLY	GLY	LYS	ILE	LYS	THR	GLN	ARG	TYR	ILE	THR	GLU	GLY	ASN	GLU				

● Molecule 1: TYPE I RESTRICTION ENZYME HSDR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.11Å 123.11Å 160.11Å 90.00° 111.48° 90.00°	Depositor
Resolution (Å)	19.89 – 2.99 19.88 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.89-2.99) 98.4 (19.88-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.255 , 0.296 0.255 , 0.295	Depositor DCC
$R_{free}$ test set	970 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	1.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2132e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.27	0/6954	0.51	1/9383 (0.0%)
1	B	0.25	0/6979	0.50	1/9418 (0.0%)
1	C	0.27	0/6933	0.49	0/9355
1	D	0.25	0/6901	0.48	1/9309 (0.0%)
All	All	0.26	0/27767	0.50	3/37465 (0.0%)

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
1	A	0	4
1	B	0	4
1	C	0	2
1	D	0	3
All	All	0	13

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	813	VAL	N-CA-C	7.00	129.89	111.00
1	B	813	VAL	N-CA-C	6.66	128.98	111.00
1	D	534	GLY	N-CA-C	5.49	126.81	113.10

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ALA	Peptide
1	A	769	ILE	Peptide
1	A	806	GLN	Peptide
1	A	812	PRO	Peptide
1	B	144	GLY	Peptide
1	B	769	ILE	Peptide
1	B	806	GLN	Peptide
1	B	812	PRO	Peptide
1	C	769	ILE	Peptide
1	C	806	GLN	Peptide
1	D	769	ILE	Peptide
1	D	811	ASP	Peptide
1	D	812	PRO	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	6821	0	6660	83	0
1	B	6846	0	6672	78	0
1	C	6802	0	6636	67	0
1	D	6772	0	6607	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	0	0
All	All	27369	0	26623	297	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 6.

All (297) 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:147:ALA:HB1	1:A:148:ASN:HA	1.49	0.93
1:A:807:ILE:H	1:A:808:ASP:HB2	1.39	0.86
1:B:807:ILE:H	1:B:808:ASP:HB2	1.44	0.81
1:C:807:ILE:H	1:C:808:ASP:HB2	1.46	0.80
1:D:859:ARG:H	1:D:859:ARG:HH11	1.27	0.79
1:A:365:ALA:HB3	1:C:116:GLU:HB3	1.65	0.79
1:D:819:LYS:NZ	1:D:826:ASP:OD1	2.17	0.78
1:A:810:SER:HB3	1:A:812:PRO:HD3	1.67	0.76
1:B:810:SER:HB3	1:B:812:PRO:HD3	1.65	0.76
1:D:807:ILE:H	1:D:808:ASP:HB2	1.50	0.75
1:A:213:ALA:HB2	1:A:271:VAL:HG23	1.69	0.74
1:B:116:GLU:HB3	1:D:365:ALA:HB3	1.68	0.74
1:C:851:ASN:OD1	1:C:854:ARG:NH1	2.22	0.72
1:D:769:ILE:HG22	1:D:770:GLU:HA	1.70	0.72
1:A:807:ILE:N	1:A:808:ASP:HB2	2.05	0.71
1:C:810:SER:HB3	1:C:812:PRO:HD3	1.74	0.70
1:C:881:ASP:N	1:C:881:ASP:OD1	2.23	0.69
1:A:583:ALA:HB2	1:A:597:GLU:HG2	1.73	0.69
1:A:116:GLU:HB3	1:C:365:ALA:HB3	1.75	0.68
1:C:57:GLN:HE22	1:C:194:LEU:H	1.42	0.68
1:B:541:MET:HG3	1:B:668:LEU:HD11	1.76	0.67
1:B:807:ILE:N	1:B:808:ASP:HB2	2.09	0.67
1:A:94:ASP:OD2	1:A:102:LYS:NZ	2.27	0.66
1:B:125:ASP:OD2	1:B:131:ARG:NH1	2.27	0.66
1:D:154:ILE:HB	1:D:162:VAL:HB	1.75	0.66
1:A:811:ASP:H	1:A:814:ALA:HB3	1.60	0.66
1:B:855:ASP:OD1	1:B:858:ARG:NH1	2.28	0.66
1:D:57:GLN:HE22	1:D:194:LEU:H	1.44	0.66
1:B:97:LEU:HD21	1:B:267:GLN:HB3	1.78	0.66
1:C:632:ASN:O	1:C:636:ASN:ND2	2.28	0.66
1:C:812:PRO:HB3	1:C:815:VAL:HB	1.78	0.66
1:A:313:LYS:NZ	1:A:409:GLU:OE2	2.30	0.65
1:B:811:ASP:H	1:B:814:ALA:HB3	1.61	0.65
1:D:532:PHE:O	1:D:534:GLY:HA3	1.97	0.65
1:B:365:ALA:HB3	1:D:116:GLU:HB3	1.78	0.65
1:C:807:ILE:N	1:C:808:ASP:HB2	2.11	0.65
1:B:265:SER:HB3	1:B:352:ARG:HE	1.61	0.64
1:A:632:ASN:O	1:A:636:ASN:ND2	2.30	0.64
1:C:213:ALA:HB2	1:C:271:VAL:HG23	1.79	0.64
1:B:313:LYS:NZ	1:B:409:GLU:OE2	2.30	0.64
1:B:89:LEU:HD11	1:B:159:LEU:HD21	1.79	0.63
1:C:395:ASP:HB3	1:D:836:ARG:HE	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASP:OD2	1:C:131:ARG:NH1	2.32	0.62
1:A:110:ASP:OD1	1:A:120:ASN:ND2	2.33	0.62
1:A:154:ILE:HB	1:A:162:VAL:HB	1.82	0.62
1:C:313:LYS:NZ	1:C:409:GLU:OE2	2.26	0.62
1:C:87:GLN:O	1:C:91:ASN:ND2	2.32	0.62
1:B:819:LYS:NZ	1:B:826:ASP:OD1	2.23	0.61
1:D:807:ILE:N	1:D:808:ASP:HB2	2.14	0.61
1:D:40:LEU:HD12	1:D:240:LEU:HD21	1.82	0.61
1:C:613:ASP:OD1	1:C:629:THR:OG1	2.13	0.61
1:B:554:TYR:HB3	1:B:611:PHE:HZ	1.66	0.60
1:A:755:VAL:HG13	1:A:781:LEU:HD22	1.83	0.60
1:B:297:SER:OG	1:B:427:LYS:O	2.14	0.60
1:B:854:ARG:NH2	1:B:858:ARG:HH22	2.00	0.60
1:A:554:TYR:HB3	1:A:611:PHE:HZ	1.67	0.60
1:B:204:SER:HB2	1:B:209:THR:HG23	1.84	0.60
1:D:213:ALA:HB2	1:D:271:VAL:HG23	1.83	0.59
1:D:755:VAL:HG13	1:D:781:LEU:HD22	1.84	0.59
1:D:741:THR:HA	1:D:748:ALA:HA	1.82	0.59
1:C:645:VAL:HG21	1:C:653:LEU:HD22	1.83	0.59
1:D:344:TYR:HA	1:D:639:ARG:CZ	2.33	0.59
1:D:541:MET:HG3	1:D:668:LEU:HD11	1.85	0.59
1:D:347:MET:HB2	1:D:639:ARG:NH2	2.17	0.59
1:A:851:ASN:OD1	1:A:854:ARG:NH1	2.35	0.58
1:A:91:ASN:OD1	1:A:91:ASN:N	2.34	0.58
1:C:244:THR:HA	1:C:248:PHE:HB2	1.86	0.57
1:A:763:PHE:HD1	1:A:768:SER:HB3	1.70	0.57
1:D:297:SER:OG	1:D:427:LYS:O	2.16	0.57
1:A:811:ASP:O	1:A:814:ALA:N	2.37	0.57
1:A:581:SER:HB3	1:A:597:GLU:HB3	1.87	0.56
1:D:117:ARG:NH1	1:D:119:GLU:OE2	2.38	0.56
1:B:854:ARG:HH21	1:B:858:ARG:HH22	1.52	0.56
1:B:812:PRO:HA	1:B:814:ALA:H	1.70	0.56
1:C:811:ASP:O	1:C:814:ALA:N	2.34	0.55
1:A:349:GLU:OE2	1:A:352:ARG:NH2	2.30	0.55
1:B:22:LYS:HG3	1:B:242:ASP:OD2	2.06	0.55
1:B:344:TYR:HD1	1:B:639:ARG:HG2	1.70	0.55
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.36	0.55
1:C:776:LYS:HG2	1:C:876:VAL:HG11	1.89	0.55
1:C:154:ILE:HB	1:C:162:VAL:HB	1.89	0.54
1:B:645:VAL:HG21	1:B:653:LEU:HD22	1.89	0.54
1:B:811:ASP:O	1:B:814:ALA:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:THR:HA	1:B:248:PHE:HB2	1.89	0.54
1:A:873:TRP:HE3	1:A:876:VAL:HG21	1.73	0.53
1:C:54:VAL:HG13	1:C:59:ALA:HB3	1.90	0.53
1:C:554:TYR:HB3	1:C:611:PHE:HZ	1.72	0.53
1:B:745:THR:O	1:B:747:GLU:HB2	2.09	0.53
1:D:769:ILE:CG2	1:D:770:GLU:HA	2.38	0.53
1:B:54:VAL:HG13	1:B:59:ALA:HB3	1.91	0.53
1:B:213:ALA:HB2	1:B:271:VAL:HG23	1.91	0.53
1:C:227:MET:HG2	1:C:273:ARG:HG2	1.89	0.53
1:B:162:VAL:HG22	1:B:200:LEU:HB3	1.92	0.52
1:B:462:VAL:HG23	1:B:465:ASP:H	1.73	0.52
1:C:812:PRO:HA	1:C:815:VAL:H	1.75	0.52
1:C:218:ARG:HA	1:C:219:ASP:C	2.30	0.51
1:D:462:VAL:HG23	1:D:465:ASP:H	1.75	0.51
1:D:482:VAL:HG23	1:D:483:ARG:HG3	1.93	0.51
1:C:806:GLN:CB	1:C:807:ILE:HA	2.41	0.51
1:A:490:GLU:HB3	1:A:706:ARG:HA	1.93	0.51
1:D:859:ARG:H	1:D:859:ARG:NH1	2.04	0.50
1:C:91:ASN:N	1:C:91:ASN:OD1	2.36	0.50
1:C:391:LYS:HD3	1:C:417:GLU:OE2	2.11	0.49
1:C:824:VAL:HG13	1:C:828:LYS:HB3	1.94	0.49
1:A:462:VAL:HG23	1:A:465:ASP:H	1.76	0.49
1:A:645:VAL:HG21	1:A:653:LEU:HD22	1.94	0.49
1:A:96:ILE:H	1:A:96:ILE:HD12	1.77	0.49
1:A:695:ALA:HB3	1:A:881:ASP:HB2	1.94	0.49
1:A:812:PRO:HA	1:A:814:ALA:H	1.78	0.49
1:D:804:LEU:HD23	1:D:818:PHE:CE2	2.47	0.49
1:B:154:ILE:HB	1:B:162:VAL:HB	1.94	0.49
1:A:147:ALA:HB1	1:A:148:ASN:CA	2.33	0.49
1:D:204:SER:HB2	1:D:209:THR:HG23	1.95	0.49
1:D:465:ASP:OD1	1:D:468:ARG:NH1	2.44	0.48
1:D:765:ASP:HB2	1:D:766:PRO:HA	1.94	0.48
1:A:303:GLY:O	1:A:432:PHE:HA	2.13	0.48
1:B:772:GLU:HG2	1:B:873:TRP:HE1	1.79	0.48
1:B:695:ALA:HB3	1:B:881:ASP:HB2	1.95	0.48
1:B:355:PRO:HD2	1:B:370:ASN:HD21	1.79	0.48
1:C:384:GLN:HG3	1:C:414:GLN:HG3	1.96	0.48
1:B:71:LEU:O	1:B:131:ARG:NH2	2.41	0.48
1:B:873:TRP:HE3	1:B:876:VAL:HG21	1.78	0.48
1:D:36:LEU:HB3	1:D:166:LEU:HD22	1.95	0.48
1:D:554:TYR:HB3	1:D:611:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:O	1:A:91:ASN:HB3	2.14	0.47
1:A:244:THR:HA	1:A:248:PHE:HB2	1.96	0.47
1:D:814:ALA:HA	1:D:817:LYS:HB3	1.94	0.47
1:A:125:ASP:OD2	1:A:131:ARG:NH1	2.47	0.47
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.70	0.47
1:C:162:VAL:HG22	1:C:200:LEU:HB3	1.96	0.47
1:D:384:GLN:HG3	1:D:414:GLN:HG3	1.96	0.47
1:B:772:GLU:HG3	1:B:856:TRP:HH2	1.78	0.47
1:D:770:GLU:O	1:D:775:LYS:NZ	2.48	0.47
1:B:833:GLN:O	1:B:836:ARG:NH2	2.48	0.47
1:B:36:LEU:HB3	1:B:166:LEU:HD22	1.96	0.47
1:C:13:ASN:N	1:C:13:ASN:HD22	2.11	0.47
1:D:313:LYS:NZ	1:D:409:GLU:OE2	2.48	0.47
1:D:806:GLN:CB	1:D:807:ILE:HA	2.45	0.46
1:A:36:LEU:HB3	1:A:166:LEU:HD22	1.97	0.46
1:D:264:ASP:HB2	1:D:349:GLU:OE1	2.15	0.46
1:D:15:ILE:HD11	1:D:277:ILE:HG21	1.96	0.46
1:D:89:LEU:HD11	1:D:159:LEU:HD21	1.97	0.46
1:A:63:ASN:O	1:A:67:GLN:HG2	2.15	0.46
1:C:297:SER:OG	1:C:427:LYS:O	2.21	0.46
1:D:303:GLY:O	1:D:432:PHE:HA	2.15	0.46
1:A:175:GLU:O	1:A:179:GLN:HG3	2.15	0.46
1:A:91:ASN:O	1:A:94:ASP:HB2	2.15	0.46
1:C:264:ASP:OD1	1:C:266:SER:OG	2.24	0.46
1:D:509:HIS:CE1	1:D:511:MET:HB2	2.51	0.46
1:A:807:ILE:HD13	1:A:807:ILE:HA	1.88	0.46
1:B:750:ARG:HH21	1:B:784:GLU:CD	2.19	0.46
1:D:582:PHE:H	1:D:604:MET:HG2	1.80	0.46
1:B:807:ILE:HA	1:B:807:ILE:HD13	1.90	0.46
1:D:298:LYS:HB2	1:D:300:GLU:HG2	1.97	0.46
1:A:57:GLN:HE21	1:A:57:GLN:HA	1.81	0.46
1:B:384:GLN:HG3	1:B:414:GLN:HG3	1.98	0.46
1:C:575:ARG:HD2	1:C:575:ARG:HA	1.71	0.46
1:C:792:LEU:HB3	1:C:798:PHE:CG	2.51	0.46
1:A:824:VAL:HG13	1:A:828:LYS:HB3	1.97	0.46
1:D:402:GLN:NE2	1:D:430:TYR:OH	2.47	0.46
1:B:393:GLU:HB3	1:B:396:LEU:HG	1.98	0.45
1:D:40:LEU:HD12	1:D:166:LEU:HD21	1.96	0.45
1:D:265:SER:HB3	1:D:352:ARG:HE	1.81	0.45
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.75	0.45
1:A:71:LEU:O	1:A:131:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ILE:HG22	1:A:770:GLU:HA	1.98	0.45
1:C:691:ARG:HH22	3:C:1886:ATP:PG	2.40	0.45
1:D:256:VAL:HA	1:D:260:TYR:HB2	1.97	0.45
1:A:344:TYR:HD2	1:A:639:ARG:HG2	1.82	0.45
1:C:128:ASN:ND2	1:C:131:ARG:HG3	2.32	0.45
1:D:36:LEU:HD11	1:D:206:GLY:HA3	1.98	0.45
1:D:63:ASN:O	1:D:67:GLN:HG2	2.17	0.45
1:D:88:TYR:O	1:D:102:LYS:HE2	2.16	0.45
1:B:325:THR:HG21	1:B:378:ILE:HB	1.98	0.45
1:C:319:LYS:HD2	1:C:319:LYS:HA	1.76	0.45
1:A:750:ARG:NH1	1:A:758:GLU:OE1	2.50	0.45
1:B:851:ASN:HA	1:B:854:ARG:NH1	2.32	0.45
1:C:22:LYS:HG3	1:C:242:ASP:OD2	2.16	0.45
1:D:304:TYR:CZ	1:D:457:GLU:HB2	2.52	0.45
1:A:468:ARG:HD2	1:A:469:ASP:OD1	2.17	0.44
1:D:113:PHE:HE1	1:D:119:GLU:HB2	1.83	0.44
1:A:36:LEU:O	1:A:40:LEU:HB2	2.17	0.44
1:B:575:ARG:HD2	1:B:575:ARG:HA	1.71	0.44
1:C:162:VAL:HG21	1:C:253:LEU:HD11	2.00	0.44
1:D:873:TRP:HE3	1:D:876:VAL:HG21	1.82	0.44
1:A:296:TRP:NE1	1:A:428:ARG:HG2	2.32	0.44
1:A:471:LYS:HA	1:A:471:LYS:HD3	1.81	0.44
1:C:509:HIS:CE1	1:C:511:MET:HB2	2.52	0.44
1:D:102:LYS:HA	1:D:106:ASP:HB2	2.00	0.44
1:A:575:ARG:HA	1:A:575:ARG:HD2	1.74	0.44
1:D:40:LEU:HD11	1:D:164:ILE:HG21	1.99	0.44
1:B:99:LYS:HD2	1:B:197:TYR:CE2	2.53	0.43
1:B:683:MET:HG3	1:B:719:PHE:CD2	2.52	0.43
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.91	0.43
1:D:683:MET:HG3	1:D:719:PHE:CD2	2.53	0.43
1:B:811:ASP:HA	1:B:812:PRO:HD3	1.76	0.43
1:B:13:ASN:N	1:B:13:ASN:OD1	2.49	0.43
1:B:229:TRP:CD1	1:B:247:CYS:HB2	2.54	0.43
1:B:304:TYR:CZ	1:B:457:GLU:HB2	2.53	0.43
1:B:88:TYR:CZ	1:B:109:CYS:HB2	2.53	0.43
1:C:40:LEU:HG	1:C:240:LEU:HD21	2.01	0.43
1:C:471:LYS:HA	1:C:471:LYS:HD3	1.88	0.43
1:B:427:LYS:HD3	1:B:427:LYS:HA	1.74	0.43
1:C:325:THR:HG21	1:C:378:ILE:HB	1.99	0.43
1:A:833:GLN:O	1:A:836:ARG:NH2	2.52	0.43
1:B:509:HIS:HA	1:B:510:PRO:HD3	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:ARG:NH2	1:B:777:ASP:HB3	2.34	0.43
1:D:18:ASP:HA	1:D:232:SER:OG	2.19	0.43
1:B:264:ASP:HB2	1:B:349:GLU:OE1	2.19	0.43
1:B:91:ASN:HB2	1:B:94:ASP:CG	2.39	0.43
1:C:303:GLY:O	1:C:432:PHE:HA	2.18	0.43
1:D:391:LYS:HD3	1:D:417:GLU:OE2	2.19	0.43
1:B:873:TRP:O	1:B:876:VAL:HG22	2.19	0.43
1:C:395:ASP:HB3	1:D:836:ARG:HB2	2.01	0.43
1:C:247:CYS:HA	1:C:252:THR:HG21	2.01	0.43
1:D:368:LYS:HB3	1:D:368:LYS:HE2	1.92	0.43
1:B:256:VAL:HA	1:B:260:TYR:HB2	2.00	0.42
1:D:855:ASP:O	1:D:858:ARG:NH1	2.52	0.42
1:A:227:MET:HG2	1:A:273:ARG:HG2	2.01	0.42
1:B:100:THR:HG23	1:B:199:GLN:OE1	2.19	0.42
1:B:368:LYS:HE2	1:B:368:LYS:HB3	1.77	0.42
1:D:873:TRP:O	1:D:876:VAL:HG22	2.20	0.42
1:A:15:ILE:HD11	1:A:277:ILE:HG21	2.01	0.42
1:A:167:LYS:HE3	1:A:176:ALA:HB1	2.01	0.42
1:A:40:LEU:HD12	1:A:166:LEU:HD21	2.01	0.42
1:D:280:THR:HG21	1:D:323:LEU:HD12	2.01	0.42
1:D:745:THR:O	1:D:747:GLU:N	2.52	0.42
1:A:575:ARG:HE	1:A:622:HIS:CG	2.38	0.42
1:A:684:GLN:O	1:A:688:ARG:NE	2.50	0.42
1:D:859:ARG:HD3	1:D:859:ARG:H	1.84	0.42
1:A:687:SER:HB2	1:A:688:ARG:HH21	1.84	0.42
1:A:704:THR:HG21	1:A:708:LEU:HD12	2.01	0.42
1:C:279:ALA:O	1:C:283:ILE:HG13	2.20	0.42
1:D:262:VAL:HG21	1:D:315:LEU:HD11	2.01	0.42
1:A:99:LYS:HD2	1:A:197:TYR:CE2	2.55	0.42
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.84	0.42
1:A:551:LYS:HA	1:A:611:PHE:CZ	2.55	0.42
1:A:850:TYR:CD2	1:A:883:LEU:HD11	2.54	0.42
1:B:337:VAL:O	1:B:382:THR:HA	2.20	0.42
1:B:303:GLY:O	1:B:432:PHE:HA	2.20	0.42
1:B:88:TYR:O	1:B:102:LYS:NZ	2.46	0.42
1:C:36:LEU:HB3	1:C:166:LEU:HD22	2.02	0.42
1:C:765:ASP:HB2	1:C:766:PRO:HA	2.01	0.42
1:C:36:LEU:O	1:C:40:LEU:HB2	2.20	0.41
1:C:755:VAL:HG13	1:C:781:LEU:HD22	2.01	0.41
1:A:467:ILE:HD13	1:A:474:LYS:HG2	2.02	0.41
1:B:490:GLU:HB3	1:B:706:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:LYS:HD3	1:C:427:LYS:HA	1.76	0.41
1:C:551:LYS:HG2	1:C:611:PHE:CG	2.55	0.41
1:A:509:HIS:CE1	1:A:511:MET:HB2	2.55	0.41
1:D:792:LEU:HB3	1:D:798:PHE:CG	2.55	0.41
1:A:507:PHE:O	1:A:512:ARG:NH1	2.49	0.41
1:D:772:GLU:OE2	1:D:873:TRP:NE1	2.42	0.41
1:A:89:LEU:HD11	1:A:159:LEU:HD21	2.01	0.41
1:A:30:TYR:HD2	1:A:169:ARG:HD3	1.85	0.41
1:A:54:VAL:HG13	1:A:59:ALA:HB3	2.01	0.41
1:B:102:LYS:HA	1:B:106:ASP:HB2	2.03	0.41
1:C:468:ARG:HD2	1:C:469:ASP:OD1	2.20	0.41
1:C:482:VAL:O	1:C:484:PRO:HD3	2.20	0.41
1:A:264:ASP:HB2	1:A:349:GLU:OE1	2.20	0.41
1:B:200:LEU:HD13	1:B:271:VAL:HG21	2.03	0.41
1:B:482:VAL:HG23	1:B:483:ARG:HG3	2.01	0.41
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.86	0.41
1:A:333:VAL:HG22	1:A:404:VAL:HB	2.02	0.41
1:B:516:ILE:HG23	1:B:705:PHE:CE1	2.56	0.41
1:D:171:VAL:O	1:D:205:ASN:ND2	2.40	0.41
1:D:21:ILE:H	1:D:21:ILE:HG12	1.64	0.41
1:A:273:ARG:N	1:A:276:GLN:OE1	2.49	0.41
1:A:283:ILE:O	1:A:287:ILE:HG13	2.20	0.41
1:A:412:ARG:HG2	1:A:439:ILE:HD11	2.03	0.41
1:A:391:LYS:HD3	1:A:417:GLU:OE2	2.21	0.41
1:A:482:VAL:O	1:A:484:PRO:HD3	2.21	0.41
1:C:482:VAL:HG23	1:C:483:ARG:HG3	2.03	0.41
1:A:297:SER:OG	1:A:427:LYS:O	2.26	0.41
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.92	0.41
1:B:471:LYS:HD3	1:B:471:LYS:HA	1.84	0.41
1:C:91:ASN:O	1:C:94:ASP:HB2	2.21	0.41
1:D:334:PHE:HZ	1:D:371:LEU:HD21	1.86	0.41
1:C:804:LEU:HD23	1:C:818:PHE:CE2	2.56	0.40
1:D:471:LYS:HD3	1:D:471:LYS:HA	1.83	0.40
1:D:575:ARG:HA	1:D:575:ARG:HD2	1.77	0.40
1:A:859:ARG:H	1:A:859:ARG:HG3	1.63	0.40
1:C:520:ILE:O	1:C:524:PHE:HB2	2.21	0.40
1:C:540:ALA:HB2	1:C:670:THR:HB	2.02	0.40
1:A:769:ILE:CG2	1:A:770:GLU:HA	2.52	0.40
1:B:281:GLU:OE2	1:B:282:ARG:NH1	2.50	0.40
1:A:873:TRP:CE3	1:A:876:VAL:HG21	2.55	0.40
1:B:262:VAL:HG22	1:B:319:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ILE:HB	1:C:252:THR:HG23	2.03	0.40
1:C:368:LYS:HE2	1:C:368:LYS:HB3	1.84	0.40
1:C:304:TYR:CZ	1:C:457:GLU:HB2	2.56	0.40
1:D:581:SER:HB2	1:D:634:PHE:CZ	2.56	0.40
1:B:15:ILE:HD11	1:B:277:ILE:HG21	2.03	0.40
1:B:482:VAL:O	1:B:484:PRO:HD3	2.21	0.40
1:B:532:PHE:CG	1:B:533:PRO:HD2	2.57	0.40
1:B:855:ASP:HA	1:B:858:ARG:HH11	1.86	0.40
1:D:99:LYS:HD2	1:D:197:TYR:CE2	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	A	831/1038 (80%)	793 (95%)	36 (4%)	2 (0%)	47	80
1	B	834/1038 (80%)	800 (96%)	32 (4%)	2 (0%)	47	80
1	C	830/1038 (80%)	796 (96%)	33 (4%)	1 (0%)	51	83
1	D	821/1038 (79%)	782 (95%)	35 (4%)	4 (0%)	29	66
All	All	3316/4152 (80%)	3171 (96%)	136 (4%)	9 (0%)	41	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	746	GLY
1	D	813	VAL
1	A	765	ASP
1	C	813	VAL
1	B	813	VAL
1	D	744	ALA

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Mol	Chain	Res	Type
1	A	813	VAL
1	B	765	ASP
1	D	532	PHE

### 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	737/927 (80%)	724 (98%)	13 (2%)	59	83
1	B	741/927 (80%)	727 (98%)	14 (2%)	57	82
1	C	736/927 (79%)	722 (98%)	14 (2%)	57	82
1	D	733/927 (79%)	725 (99%)	8 (1%)	73	90
All	All	2947/3708 (80%)	2898 (98%)	49 (2%)	60	84

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	40	LEU
1	A	57	GLN
1	A	74	VAL
1	A	91	ASN
1	A	96	ILE
1	A	309	THR
1	A	489	LEU
1	A	507	PHE
1	A	613	ASP
1	A	688	ARG
1	A	781	LEU
1	A	826	ASP
1	B	13	ASN
1	B	21	ILE
1	B	40	LEU
1	B	57	GLN
1	B	74	VAL

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Mol	Chain	Res	Type
1	B	110	ASP
1	B	215	THR
1	B	326	GLU
1	B	489	LEU
1	B	610	GLU
1	B	613	ASP
1	B	771	SER
1	B	781	LEU
1	B	804	LEU
1	C	13	ASN
1	C	21	ILE
1	C	40	LEU
1	C	74	VAL
1	C	91	ASN
1	C	227	MET
1	C	236	LEU
1	C	507	PHE
1	C	688	ARG
1	C	771	SER
1	C	781	LEU
1	C	827	GLU
1	C	881	ASP
1	C	883	LEU
1	D	21	ILE
1	D	215	THR
1	D	239	ASP
1	D	507	PHE
1	D	753	MET
1	D	781	LEU
1	D	828	LYS
1	D	859	ARG

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

Mol	Chain	Res	Type
1	C	57	GLN
1	D	57	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	ATP	B	1886	2	26,33,33	0.95	1 (3%)	31,52,52	1.34	5 (16%)
3	ATP	D	1886	2	26,33,33	0.93	1 (3%)	31,52,52	1.44	5 (16%)
3	ATP	A	1886	2	26,33,33	0.91	1 (3%)	31,52,52	1.36	3 (9%)
3	ATP	C	1886	2	26,33,33	0.91	1 (3%)	31,52,52	1.41	5 (16%)

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	ATP	B	1886	2	-	0/18/38/38	0/3/3/3
3	ATP	D	1886	2	-	3/18/38/38	0/3/3/3
3	ATP	A	1886	2	-	2/18/38/38	0/3/3/3
3	ATP	C	1886	2	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1886	ATP	C5-C4	2.54	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1886	ATP	C5-C4	2.49	1.47	1.40
3	A	1886	ATP	C5-C4	2.43	1.47	1.40
3	C	1886	ATP	C5-C4	2.39	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1886	ATP	N3-C2-N1	-3.22	123.65	128.68
3	B	1886	ATP	N3-C2-N1	-3.12	123.79	128.68
3	D	1886	ATP	N3-C2-N1	-3.11	123.83	128.68
3	C	1886	ATP	N3-C2-N1	-3.10	123.83	128.68
3	D	1886	ATP	PA-O3A-PB	-3.08	122.25	132.83
3	B	1886	ATP	C4-C5-N7	-2.77	106.51	109.40
3	D	1886	ATP	C4-C5-N7	-2.75	106.53	109.40
3	C	1886	ATP	C4-C5-N7	-2.66	106.63	109.40
3	C	1886	ATP	PA-O3A-PB	-2.63	123.81	132.83
3	A	1886	ATP	C4-C5-N7	-2.58	106.71	109.40
3	A	1886	ATP	PA-O3A-PB	-2.57	124.01	132.83
3	D	1886	ATP	C3'-C2'-C1'	2.48	104.71	100.98
3	B	1886	ATP	PA-O3A-PB	-2.34	124.78	132.83
3	C	1886	ATP	C3'-C2'-C1'	2.21	104.31	100.98
3	D	1886	ATP	PB-O3B-PG	-2.20	125.28	132.83
3	C	1886	ATP	PB-O3B-PG	-2.20	125.29	132.83
3	B	1886	ATP	C3'-C2'-C1'	2.08	104.11	100.98
3	B	1886	ATP	PB-O3B-PG	-2.03	125.87	132.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

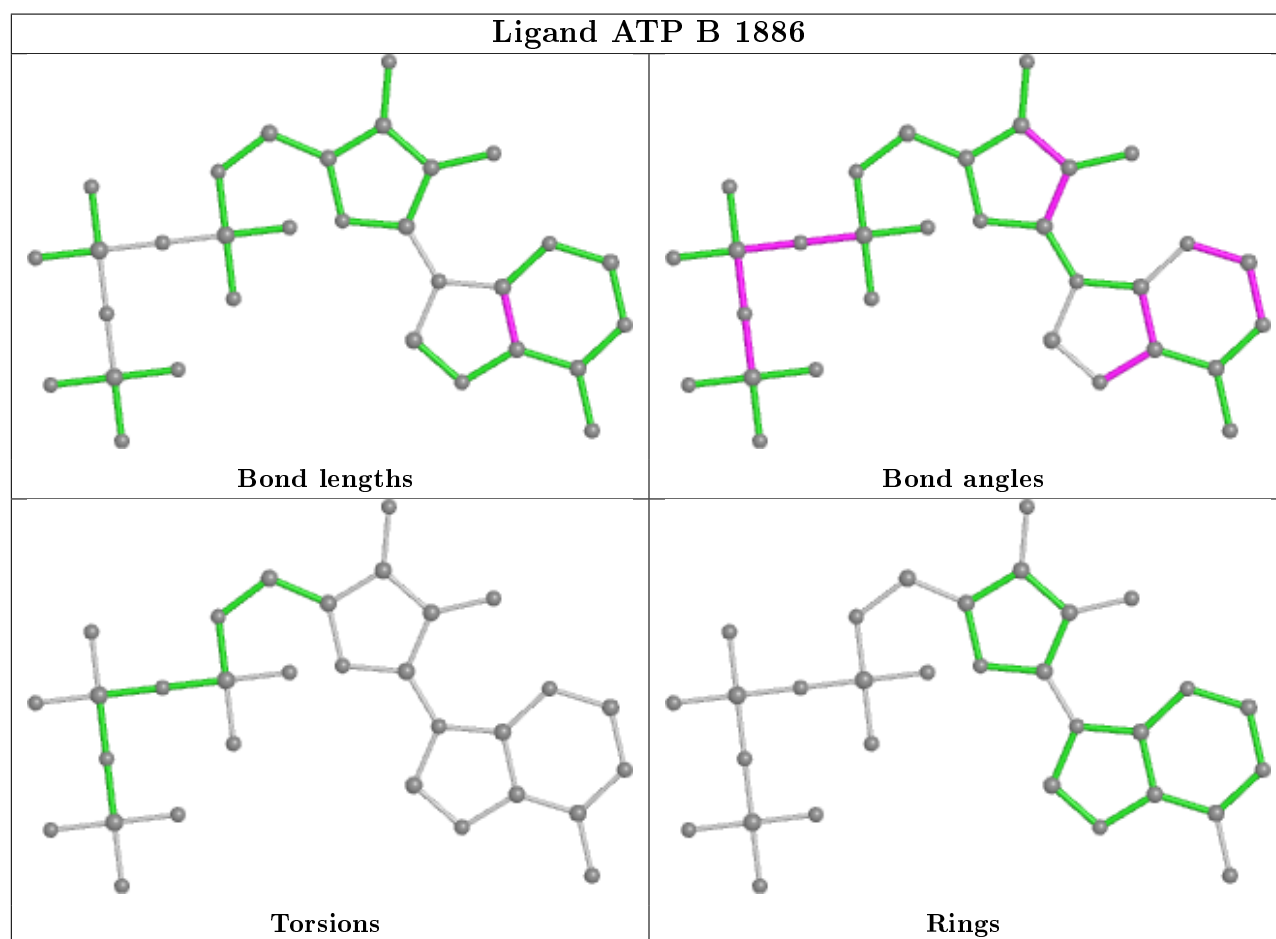
Mol	Chain	Res	Type	Atoms
3	D	1886	ATP	C5'-O5'-PA-O2A
3	A	1886	ATP	PB-O3B-PG-O1G
3	A	1886	ATP	PB-O3B-PG-O2G
3	D	1886	ATP	C5'-O5'-PA-O3A
3	D	1886	ATP	C5'-O5'-PA-O1A

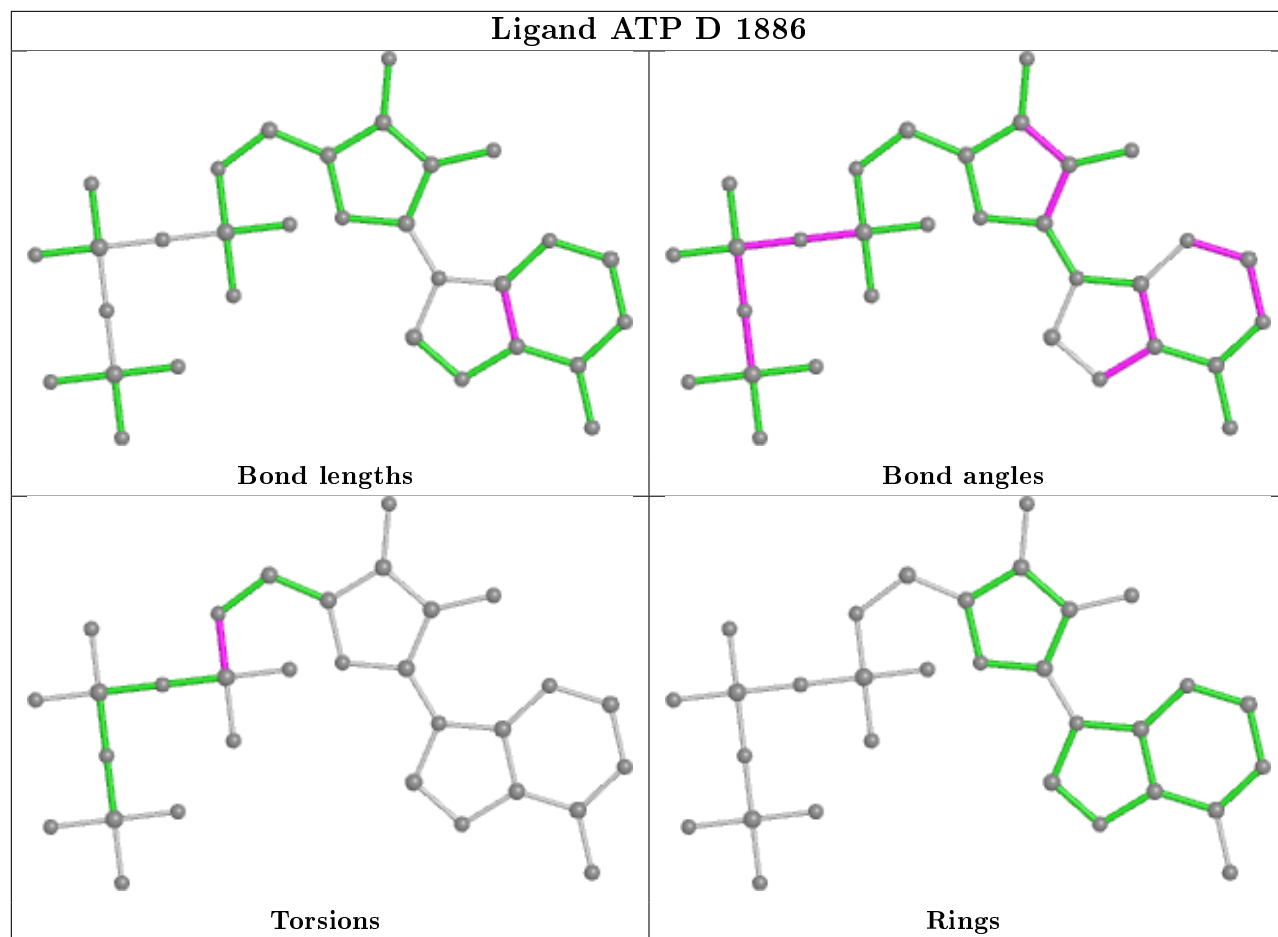
There are no ring outliers.

1 monomer is involved in 1 short contact:

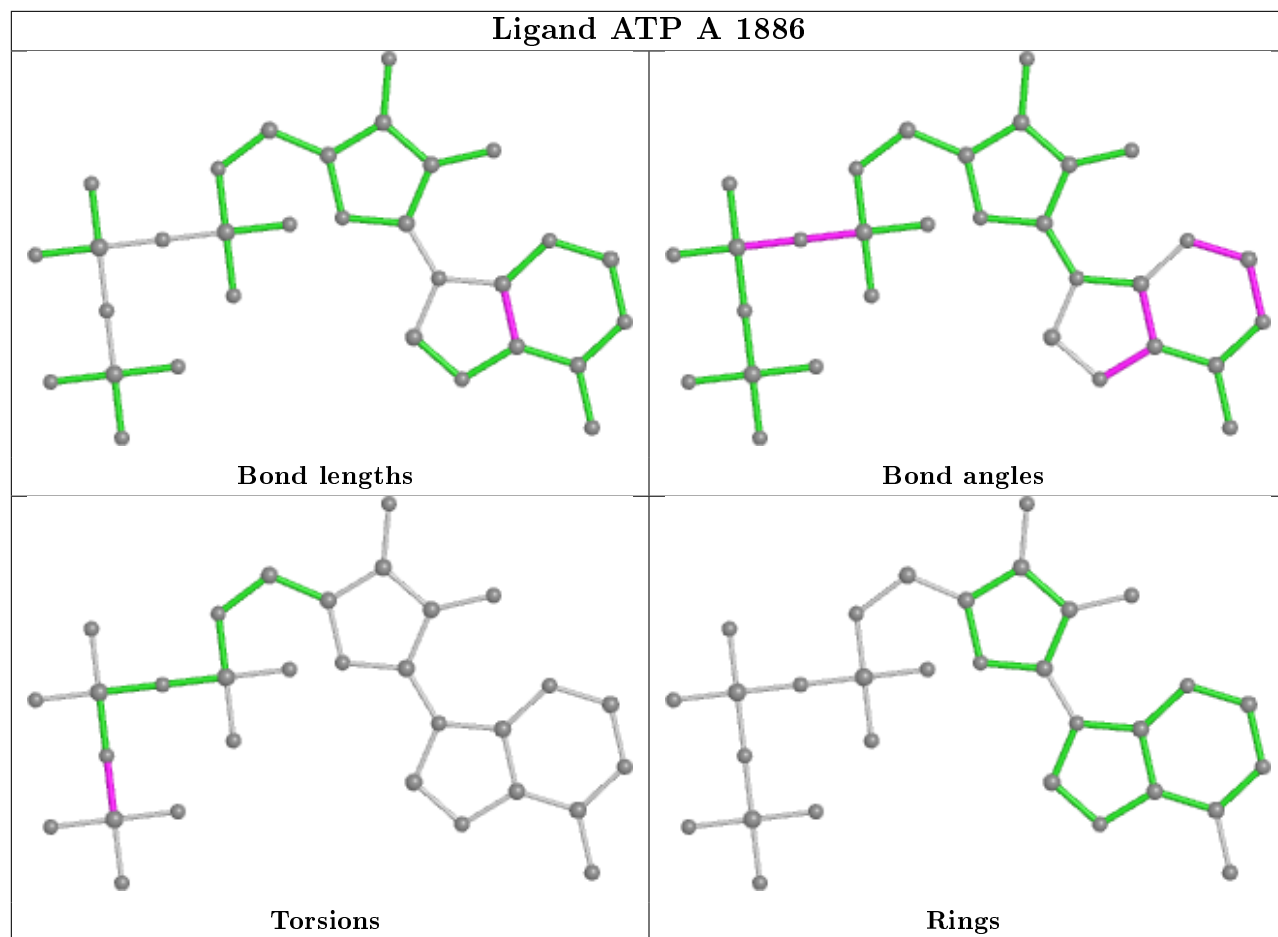
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1886	ATP	1	0

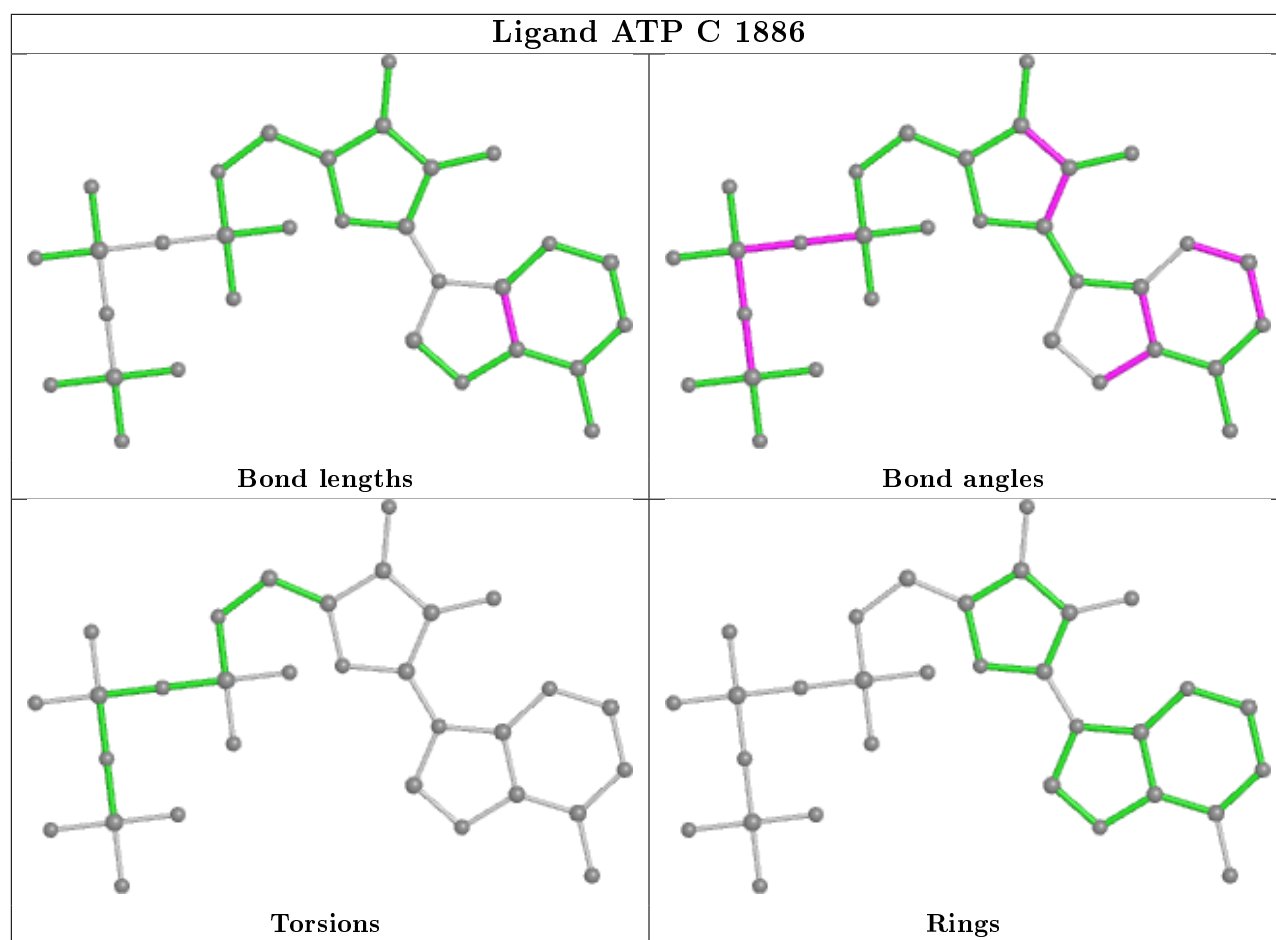
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	839/1038 (80%)	0.01	42 (5%) 28 17	20, 42, 79, 109	0
1	B	842/1038 (81%)	0.26	57 (6%) 17 9	38, 58, 86, 115	0
1	C	838/1038 (80%)	0.02	39 (4%) 31 18	21, 42, 79, 105	0
1	D	833/1038 (80%)	0.33	50 (6%) 21 12	41, 62, 91, 117	0
All	All	3352/4152 (80%)	0.15	188 (5%) 24 13	20, 54, 85, 117	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	767	THR	10.0
1	C	145	SER	8.5
1	A	767	THR	8.0
1	C	767	THR	6.2
1	D	583	ALA	6.1
1	D	767	THR	5.8
1	D	535	SER	5.6
1	B	146	HIS	5.5
1	B	810	SER	5.2
1	D	26	THR	5.1
1	B	744	ALA	4.9
1	A	146	HIS	4.8
1	D	745	THR	4.8
1	B	768	SER	4.8
1	B	148	ASN	4.7
1	B	147	ALA	4.7
1	C	146	HIS	4.6
1	B	219	ASP	4.6
1	D	810	SER	4.6
1	B	145	SER	4.5
1	C	375	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	375	ASP	4.4
1	D	533	PRO	4.4
1	B	446	GLY	4.3
1	A	809	LEU	4.2
1	A	859	ARG	4.2
1	D	532	PHE	4.2
1	C	810	SER	4.2
1	A	218	ARG	4.2
1	A	570	THR	4.2
1	C	745	THR	4.1
1	C	532	PHE	4.0
1	A	534	GLY	3.9
1	B	144	GLY	3.9
1	A	816	GLU	3.7
1	C	768	SER	3.6
1	D	219	ASP	3.6
1	B	26	THR	3.5
1	B	743	ALA	3.5
1	A	768	SER	3.5
1	A	145	SER	3.4
1	D	768	SER	3.4
1	C	219	ASP	3.4
1	D	493	THR	3.4
1	B	770	GLU	3.4
1	A	745	THR	3.4
1	A	219	ASP	3.4
1	D	292	THR	3.4
1	D	624	LYS	3.3
1	B	215	THR	3.3
1	B	217	LYS	3.3
1	A	810	SER	3.3
1	A	569	ALA	3.3
1	D	536	LYS	3.2
1	A	624	LYS	3.2
1	B	746	GLY	3.1
1	B	218	ARG	3.1
1	B	858	ARG	3.1
1	D	570	THR	3.1
1	C	807	ILE	3.1
1	B	533	PRO	3.1
1	D	216	THR	3.0
1	C	217	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	723	ASN	3.0
1	D	218	ARG	3.0
1	D	822	HIS	3.0
1	A	766	PRO	3.0
1	D	617	ARG	2.9
1	C	841	ARG	2.9
1	C	569	ALA	2.9
1	A	533	PRO	2.9
1	B	374	ASP	2.9
1	D	531	THR	2.9
1	B	807	ILE	2.9
1	C	220	GLU	2.9
1	B	628	SER	2.9
1	C	746	GLY	2.9
1	D	29	SER	2.8
1	C	533	PRO	2.8
1	D	840	ASP	2.8
1	D	632	ASN	2.8
1	B	809	LEU	2.8
1	B	356	ASP	2.8
1	B	722	LYS	2.8
1	C	772	GLU	2.8
1	C	812	PRO	2.7
1	D	482	VAL	2.7
1	B	808	ASP	2.7
1	D	179	GLN	2.7
1	D	770	GLU	2.7
1	A	743	ALA	2.6
1	B	500	ALA	2.6
1	B	569	ALA	2.6
1	A	411	HIS	2.6
1	B	170	GLY	2.6
1	B	511	MET	2.6
1	C	446	GLY	2.6
1	D	747	GLU	2.6
1	D	140	PHE	2.6
1	B	747	GLU	2.5
1	C	567	LYS	2.5
1	A	631	SER	2.5
1	B	748	ALA	2.5
1	A	499	SER	2.5
1	D	571	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	340	LYS	2.5
1	A	345	GLN	2.5
1	B	87	GLN	2.5
1	C	299	PRO	2.5
1	B	92	PRO	2.5
1	D	356	ASP	2.5
1	D	809	LEU	2.5
1	A	374	ASP	2.4
1	A	446	GLY	2.4
1	C	142	GLN	2.4
1	D	351	GLN	2.4
1	A	147	ALA	2.4
1	A	744	ALA	2.4
1	B	772	GLU	2.4
1	A	808	ASP	2.4
1	C	855	ASP	2.4
1	A	841	ARG	2.4
1	C	744	ALA	2.4
1	A	220	GLU	2.4
1	D	562	GLU	2.4
1	A	807	ILE	2.4
1	C	143	ALA	2.3
1	C	499	SER	2.3
1	C	147	ALA	2.3
1	B	443	ASN	2.3
1	C	593	GLU	2.3
1	A	344	TYR	2.3
1	B	375	ASP	2.3
1	B	534	GLY	2.3
1	D	722	LYS	2.3
1	B	806	GLN	2.3
1	B	445	LEU	2.3
1	C	218	ARG	2.3
1	C	411	HIS	2.3
1	D	28	ASP	2.3
1	D	236	LEU	2.3
1	A	844	GLN	2.3
1	B	447	SER	2.3
1	A	772	GLU	2.3
1	C	342	LEU	2.3
1	B	567	LYS	2.3
1	A	617	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	144	GLY	2.2
1	A	812	PRO	2.2
1	D	812	PRO	2.2
1	C	813	VAL	2.2
1	D	841	ARG	2.2
1	B	423	LYS	2.2
1	C	352	ARG	2.2
1	C	583	ALA	2.2
1	B	593	GLU	2.2
1	D	348	LYS	2.2
1	D	534	GLY	2.2
1	C	809	LEU	2.2
1	B	841	ARG	2.2
1	B	344	TYR	2.2
1	D	217	LYS	2.2
1	B	236	LEU	2.2
1	A	115	ASP	2.1
1	B	749	LYS	2.1
1	B	115	ASP	2.1
1	C	443	ASN	2.1
1	B	631	SER	2.1
1	C	445	LEU	2.1
1	C	808	ASP	2.1
1	D	631	SER	2.1
1	A	445	LEU	2.1
1	C	570	THR	2.1
1	D	769	ILE	2.1
1	B	456	ARG	2.1
1	A	723	ASN	2.1
1	B	420	LYS	2.1
1	A	375	ASP	2.0
1	D	265	SER	2.0
1	B	293	ALA	2.0
1	B	827	GLU	2.0
1	D	496	LYS	2.0
1	D	807	ILE	2.0
1	B	141	GLU	2.0
1	D	442	GLU	2.0
1	B	859	ARG	2.0
1	A	765	ASP	2.0
1	A	217	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

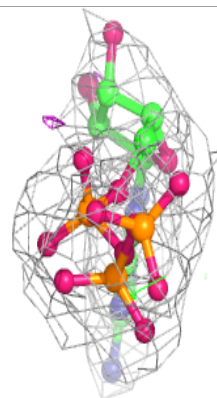
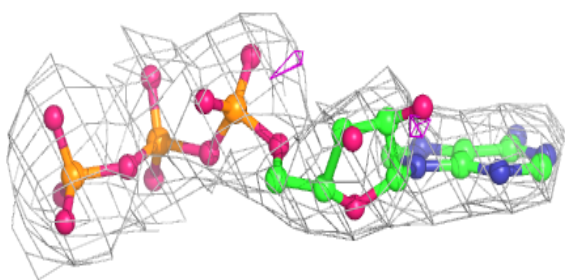
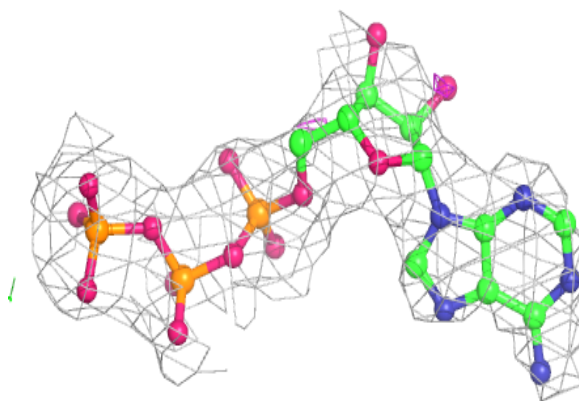
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	1885	1/1	0.80	0.22	52,52,52,52	0
2	MG	D	1885	1/1	0.89	0.26	67,67,67,67	0
2	MG	C	1885	1/1	0.91	0.16	37,37,37,37	0
2	MG	A	1885	1/1	0.92	0.20	45,45,45,45	0
3	ATP	D	1886	31/31	0.95	0.14	45,51,60,62	0
3	ATP	B	1886	31/31	0.96	0.12	42,50,57,61	0
3	ATP	C	1886	31/31	0.97	0.13	21,29,39,40	0
3	ATP	A	1886	31/31	0.97	0.12	27,34,43,51	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.

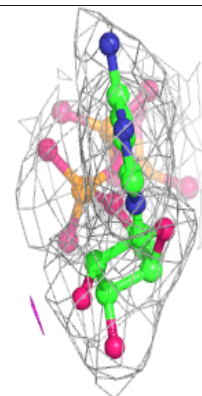
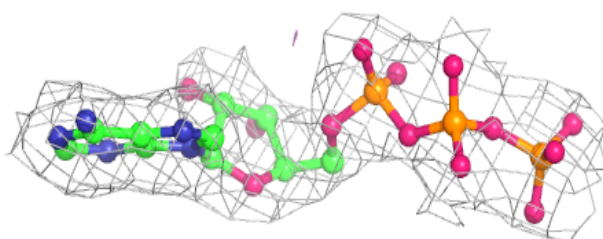
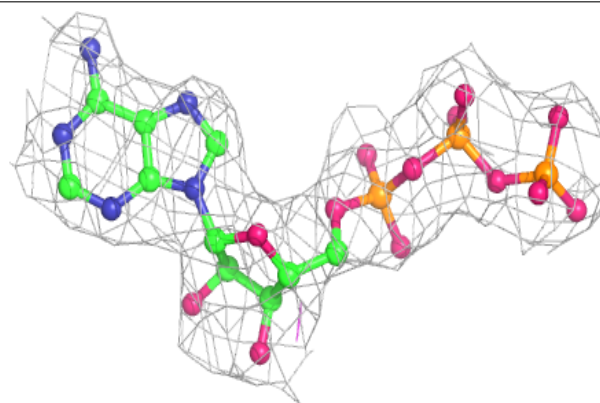


**Electron density around ATP D 1886:**

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

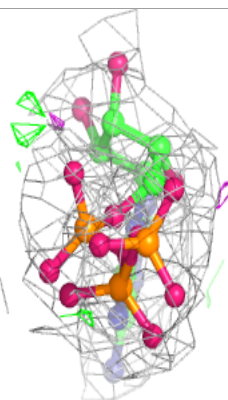
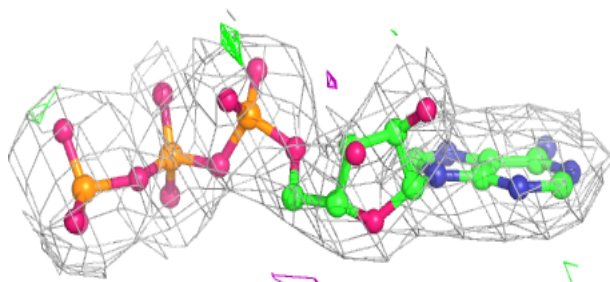
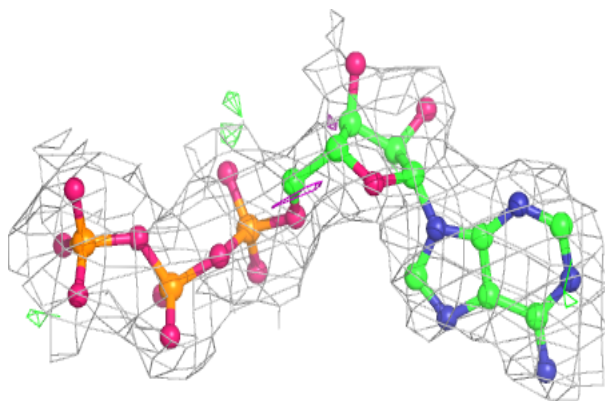
**Electron density around ATP B 1886:**

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

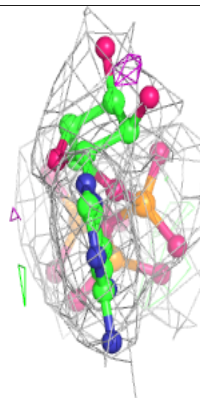
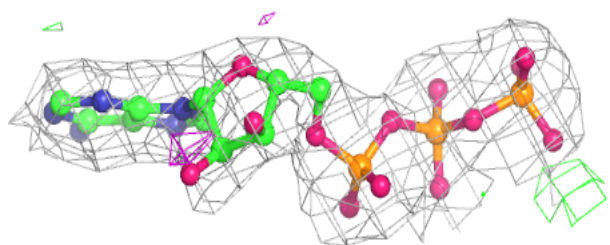
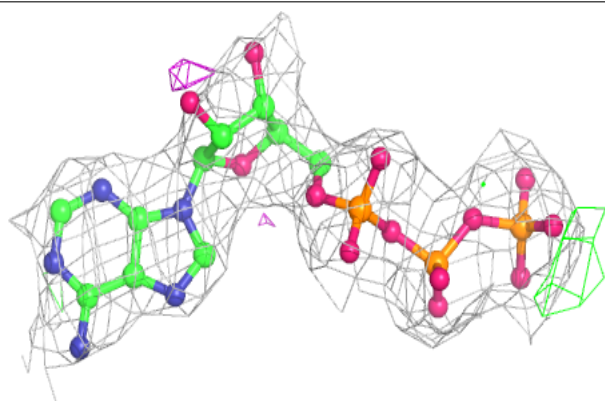


**Electron density around ATP C 1886:**

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

**Electron density around ATP A 1886:**

$2mF_o-DF_c$  (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.