



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:30 PM UTC

PDB ID : 4BEB / pdb_00004beb
Title : MUTANT (K220E) 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 : 2013-03-07
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

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

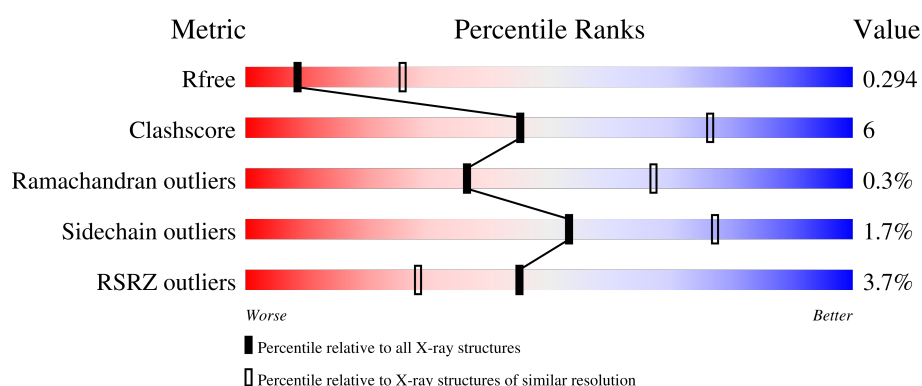
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 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	1038	 2% 67% 13% • 19%
1	B	1038	 4% 67% 14% • 19%
1	C	1038	 3% 69% 11% • 19%
1	D	1038	 4% 67% 12% • 20%

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

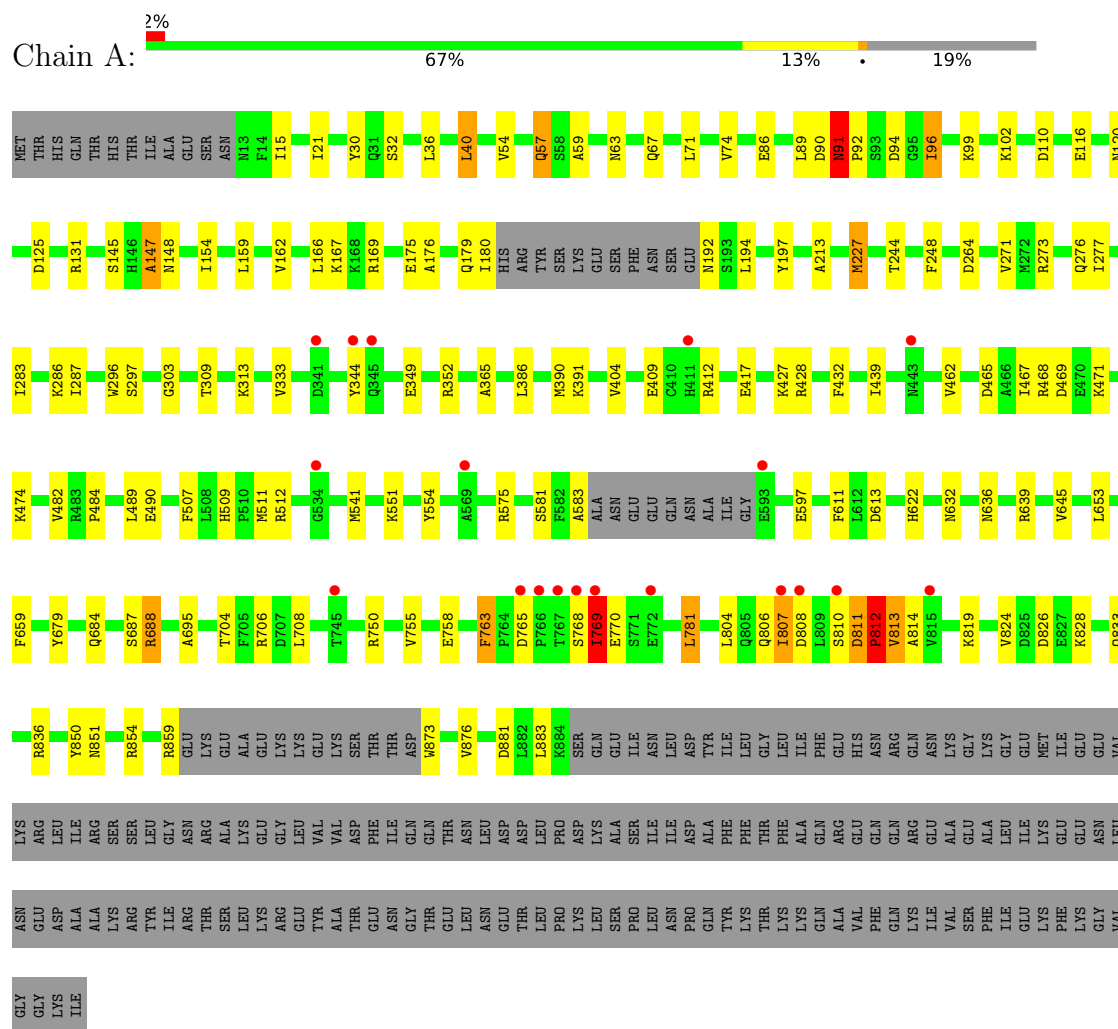


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

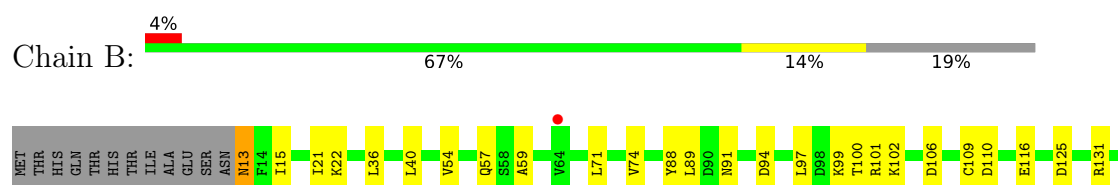
3 Residue-property plots [i](#)

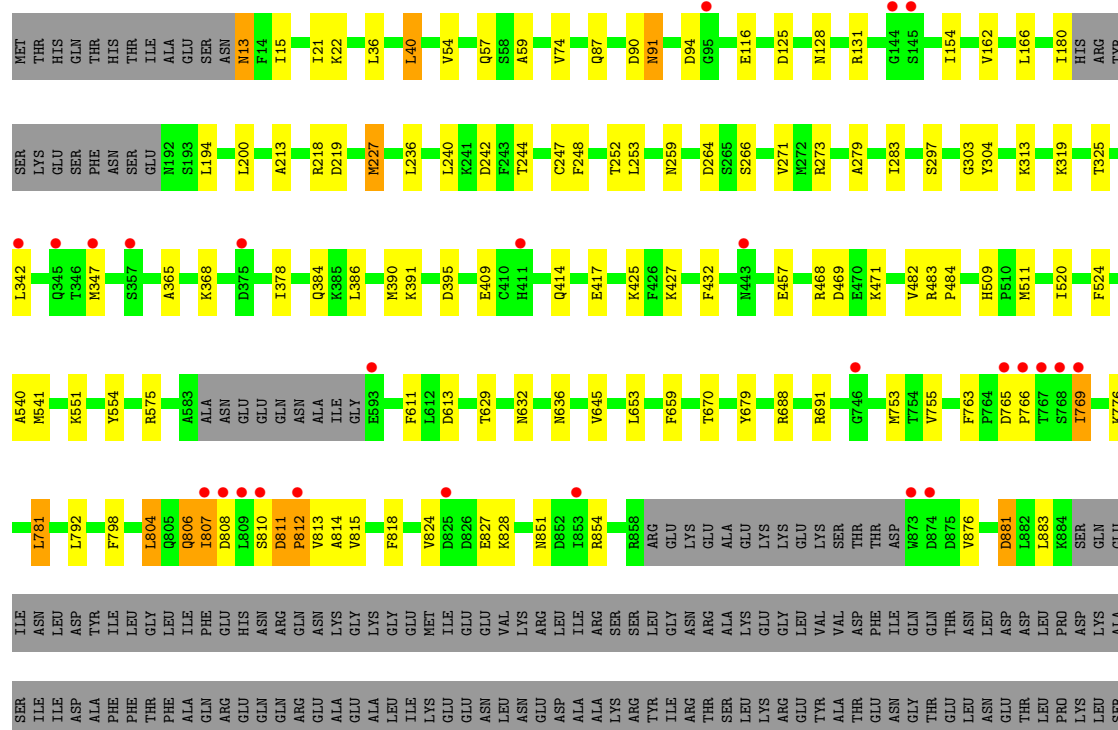
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: TYPE I RESTRICTION ENZYME HSDR



• Molecule 1: TYPE I RESTRICTION ENZYME HSDR





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

● Molecule 1: TYPE I RESTRICTION ENZYME HSDR



GLY VAL GLY GLY ILE	ASN	LEU	ASN	GLY	ASP	ALA	ALA	LYS	ARG	TYR	ILE	ARG	THR	SER	LEU	LYS	LYS	ARG	GLY	TYR	ALA	VAL	ASP	THR	GLY	ASN	THR	GLN	THR	ASN	LEU	ASN	GLY	THR	LYS	VAL	THR	GLN	THR	ILE	ALA	GLU	SER	ASN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.11Å 123.11Å 160.11Å 90.00° 111.48° 90.00°	Depositor
Resolution (Å)	19.89 – 2.99 19.89 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.89-2.99) 98.0 (19.89-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.255 , 0.296 0.255 , 0.294	Depositor DCC
R_{free} test set	970 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	1.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

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: 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	A	0.32	0/6954	0.85	18/9383 (0.2%)
1	B	0.30	0/6979	0.84	17/9418 (0.2%)
1	C	0.32	0/6933	0.83	13/9355 (0.1%)
1	D	0.30	0/6901	0.79	5/9309 (0.1%)
All	All	0.31	0/27767	0.83	53/37465 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	811	ASP	CA-C-N	12.86	134.64	121.65
1	C	811	ASP	C-N-CA	12.86	134.64	121.65
1	B	811	ASP	CA-C-N	11.87	134.67	119.84
1	B	811	ASP	C-N-CA	11.87	134.67	119.84
1	A	811	ASP	CA-C-N	11.49	134.20	119.84
1	A	811	ASP	C-N-CA	11.49	134.20	119.84
1	A	763	PHE	CA-C-N	-9.59	107.86	119.84
1	A	763	PHE	C-N-CA	-9.59	107.86	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	812	PRO	CA-C-O	-9.56	114.02	121.38
1	B	395	ASP	N-CA-C	7.71	121.50	112.72
1	A	91	ASN	CA-C-N	7.45	127.47	119.28
1	A	91	ASN	C-N-CA	7.45	127.47	119.28
1	B	216	THR	N-CA-C	-7.25	98.42	109.95
1	B	807	ILE	CA-C-N	6.86	134.05	121.70
1	B	807	ILE	C-N-CA	6.86	134.05	121.70
1	D	769	ILE	N-CA-C	-6.83	98.63	108.53
1	A	813	VAL	N-CA-C	6.75	129.89	111.00
1	A	807	ILE	CA-C-N	6.72	133.79	121.70
1	A	807	ILE	C-N-CA	6.72	133.79	121.70
1	C	90	ASP	N-CA-C	6.64	120.70	112.59
1	A	812	PRO	CA-C-N	6.55	133.50	121.70
1	A	812	PRO	C-N-CA	6.55	133.50	121.70
1	D	807	ILE	CA-C-N	6.42	133.26	121.70
1	D	807	ILE	C-N-CA	6.42	133.26	121.70
1	B	813	VAL	N-CA-C	6.42	128.98	111.00
1	B	812	PRO	CA-C-N	6.33	133.09	121.70
1	B	812	PRO	C-N-CA	6.33	133.09	121.70
1	B	572	LYS	CA-C-N	6.06	126.03	120.03
1	B	572	LYS	C-N-CA	6.06	126.03	120.03
1	C	807	ILE	CA-C-N	6.02	132.54	121.70
1	C	807	ILE	C-N-CA	6.02	132.54	121.70
1	C	812	PRO	N-CA-C	5.99	123.01	113.12
1	C	769	ILE	N-CA-C	5.87	116.62	107.28
1	C	679	TYR	CB-CA-C	-5.78	109.89	116.54
1	D	509	HIS	CA-C-N	5.77	125.90	119.32
1	D	509	HIS	C-N-CA	5.77	125.90	119.32
1	B	220	GLU	CB-CA-C	-5.77	109.94	116.63
1	B	148	ASN	CA-C-N	5.64	131.85	121.70
1	B	148	ASN	C-N-CA	5.64	131.85	121.70
1	A	90	ASP	N-CA-C	5.61	120.11	112.88
1	A	812	PRO	N-CA-C	5.59	123.98	112.47
1	C	763	PHE	N-CA-C	5.57	118.22	108.75
1	C	425	LYS	N-CA-C	5.55	118.51	111.69
1	B	812	PRO	N-CA-C	5.43	123.65	112.47
1	B	396	LEU	CA-C-N	5.28	124.91	119.05
1	B	396	LEU	C-N-CA	5.28	124.91	119.05
1	A	679	TYR	CB-CA-C	-5.27	110.47	116.54
1	C	679	TYR	N-CA-C	5.27	116.33	108.31
1	A	145	SER	N-CA-C	5.26	116.88	108.41
1	A	769	ILE	N-CA-C	-5.22	100.86	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	769	ILE	CB-CA-C	-5.17	104.26	110.99
1	A	32	SER	N-CA-C	5.02	117.00	110.53
1	A	679	TYR	N-CA-C	5.01	115.92	108.31

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	89	0
1	B	6846	0	6672	83	0
1	C	6802	0	6636	73	0
1	D	6772	0	6607	78	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	12	0	0
All	All	27369	0	26623	317	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 (317) 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:313:LYS:NZ	1:C:409:GLU:OE2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:386:LEU:HG	1:B:390:MET:HE2	1.81	0.61
1:C:541:MET:HE2	1:C:653:LEU:HD23	1.82	0.61
1:D:386:LEU:HG	1:D:390:MET:HE2	1.82	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:342:LEU:HB3	1:C:347:MET:HE2	1.83	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:386:LEU:HG	1:A:390:MET:HE2	1.85	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:541:MET:HE2	1:B:653:LEU:HD23	1.86	0.56
1:C:218:ARG:HA	1:C:219:ASP:C	2.30	0.56
1:B:812:PRO:HA	1:B:814:ALA:H	1.70	0.56
1:C:386:LEU:HG	1:C:390:MET:HE2	1.88	0.55
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
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:A:541:MET:HE2	1:A:653:LEU:HD23	1.92	0.52
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:259:ASN:O	1:C:319:LYS:NZ	2.32	0.52
1:C:812:PRO:HA	1:C:815:VAL:H	1.75	0.52
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:C:753:MET:HE2	1:C:753:MET:HA	1.93	0.51
1:A:490:GLU:HB3	1:A:706:ARG:HA	1.93	0.51
1:B:750:ARG:HH21	1:B:784:GLU:CD	2.19	0.50
1:D:859:ARG:H	1:D:859:ARG:NH1	2.04	0.50
1:C:613:ASP:OD1	1:C:629:THR:OG1	2.13	0.50
1:C:91:ASN:OD1	1:C:91:ASN:N	2.36	0.50
1:C:391:LYS:HD3	1:C:417:GLU:OE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:824:VAL:HG13	1:C:828:LYS:HB3	1.94	0.49
1:A:96:ILE:HD12	1:A:96:ILE:H	1.77	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: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:B:753:MET:HA	1:B:753:MET:HE2	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:695:ALA:HB3	1:B:881:ASP:HB2	1.95	0.48
1:B:772:GLU:HG2	1:B:873:TRP:HE1	1.79	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
1:A:86:GLU:O	1:A:91:ASN:HB3	2.14	0.47
1:B:91:ASN:HB2	1:B:94:ASP:CG	2.39	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:91:ASN:HA	1:A:92:PRO:HD3	1.70	0.47
1:A:125:ASP:OD2	1:A:131:ARG:NH1	2.47	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:B:833:GLN:O	1:B:836:ARG:NH2	2.48	0.47
1:D:770:GLU:O	1:D:775:LYS:NZ	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: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:D:264:ASP:HB2	1:D:349:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:342:LEU:HD13	1:D:347:MET:HE2	1.97	0.46
1:A:91:ASN:O	1:A:94:ASP:HB2	2.15	0.46
1:A:175:GLU:O	1:A:179:GLN:HG3	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:D:582:PHE:H	1:D:604:MET:HG2	1.80	0.46
1:B:807:ILE:HD13	1:B:807:ILE:HA	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:D:628:SER:OG	1:D:630:ASP:OD1	2.33	0.45
1:A:71:LEU:O	1:A:131:ARG:NH2	2.47	0.45
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.75	0.45
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:322:ARG:O	1:B:325:THR:OG1	2.33	0.45
1:B:325:THR:HG21	1:B:378:ILE:HB	1.98	0.45
1:C:319:LYS:HA	1:C:319:LYS:HD2	1.76	0.45
1:A:750:ARG:NH1	1:A:758:GLU:OE1	2.50	0.45
1:B:541:MET:HE1	1:B:659:PHE:HB3	1.99	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:A:541:MET:HE1	1:A:659:PHE:HB3	1.99	0.45
1:D:304:TYR:CZ	1:D:457:GLU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:A:575:ARG:HA	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:342:LEU:HB3	1:B:347:MET:HE2	2.00	0.43
1:B:683:MET:HG3	1:B:719:PHE:CD2	2.52	0.43
1:D:194:LEU:HD23	1:D:194:LEU:HA	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:OD1	1:B:13:ASN:N	2.49	0.43
1:B:88:TYR:CZ	1:B:109:CYS:HB2	2.53	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: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:57:GLN:CD	1:A:192:ASN:HB3	2.43	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
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: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:HE2	1:D:368:LYS:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:LEU:HD12	1:A:166:LEU:HD21	2.01	0.42
1:A:167:LYS:HE3	1:A:176:ALA:HB1	2.01	0.42
1:A:811:ASP:C	1:A:814:ALA:H	2.28	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:H	1:D:859:ARG:HD3	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:C:541:MET:HE1	1:C:659:PHE:HB3	2.01	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: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
1:C:427:LYS:HA	1:C:427:LYS:HD3	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: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:A:89:LEU:HD11	1:A:159:LEU:HD21	2.01	0.41
1:A:819:LYS:NZ	1:A:826:ASP:OD1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:A:194:LEU:HA	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:21:ILE:H	1:D:21:ILE:HG12	1.64	0.41
1:D:171:VAL:O	1:D:205:ASN:ND2	2.40	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:297:SER:OG	1:A:427:LYS:O	2.26	0.41
1:A:391:LYS:HD3	1:A:417:GLU:OE2	2.21	0.41
1:A:412:ARG:HG2	1:A:439:ILE:HD11	2.03	0.41
1:A:482:VAL:O	1:A:484:PRO:HD3	2.21	0.41
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.92	0.41
1:C:482:VAL:HG23	1:C:483:ARG:HG3	2.03	0.41
1:B:471:LYS:HA	1:B:471:LYS:HD3	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:HD2	1:D:575:ARG:HA	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
1:C:15:ILE:HB	1:C:252:THR:HG23	2.03	0.40
1:C:304:TYR:CZ	1:C:457:GLU:HB2	2.56	0.40
1:C:368:LYS:HE2	1:C:368:LYS:HB3	1.84	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

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	831/1038 (80%)	793 (95%)	36 (4%)	2 (0%)	43	73
1	B	834/1038 (80%)	800 (96%)	32 (4%)	2 (0%)	43	73
1	C	830/1038 (80%)	796 (96%)	33 (4%)	1 (0%)	48	78
1	D	821/1038 (79%)	782 (95%)	35 (4%)	4 (0%)	24	58
All	All	3316/4152 (80%)	3171 (96%)	136 (4%)	9 (0%)	36	67

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
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%)	723 (98%)	14 (2%)	50	75
1	B	741/927 (80%)	728 (98%)	13 (2%)	51	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	736/927 (79%)	722 (98%)	14 (2%)	50	75
1	D	733/927 (79%)	723 (99%)	10 (1%)	59	80
All	All	2947/3708 (80%)	2896 (98%)	51 (2%)	53	77

All (51) 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	180	ILE
1	A	227	MET
1	A	309	THR
1	A	489	LEU
1	A	613	ASP
1	A	688	ARG
1	A	781	LEU
1	A	804	LEU
1	B	13	ASN
1	B	21	ILE
1	B	40	LEU
1	B	57	GLN
1	B	74	VAL
1	B	110	ASP
1	B	180	ILE
1	B	215	THR
1	B	326	GLU
1	B	489	LEU
1	B	610	GLU
1	B	804	LEU
1	B	883	LEU
1	C	13	ASN
1	C	21	ILE
1	C	40	LEU
1	C	74	VAL
1	C	91	ASN
1	C	180	ILE
1	C	227	MET

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Mol	Chain	Res	Type
1	C	236	LEU
1	C	688	ARG
1	C	781	LEU
1	C	804	LEU
1	C	827	GLU
1	C	881	ASP
1	C	883	LEU
1	D	21	ILE
1	D	180	ILE
1	D	215	THR
1	D	227	MET
1	D	239	ASP
1	D	753	MET
1	D	781	LEU
1	D	804	LEU
1	D	828	LYS
1	D	859	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	46	ASN
1	A	163	GLN
1	A	251	HIS
1	A	363	ASN
1	A	485	GLN
1	A	622	HIS
1	A	822	HIS
1	B	13	ASN
1	B	42	GLN
1	B	363	ASN
1	B	402	GLN
1	B	822	HIS
1	C	13	ASN
1	C	179	GLN
1	C	228	ASN
1	C	363	ASN
1	C	401	GLN
1	C	402	GLN
1	C	790	ASN
1	D	42	GLN

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Mol	Chain	Res	Type
1	D	57	GLN
1	D	87	GLN
1	D	163	GLN
1	D	363	ASN
1	D	387	ASN
1	D	414	GLN
1	D	518	GLN
1	D	522	ASN
1	D	726	ASN
1	D	833	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	1886	2	32,33,33	1.44	6 (18%)	48,52,52	1.72	10 (20%)
3	ATP	D	1886	2	32,33,33	1.44	5 (15%)	48,52,52	1.72	9 (18%)
3	ATP	B	1886	2	32,33,33	1.52	7 (21%)	48,52,52	1.73	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	C	1886	2	32,33,33	1.39	5 (15%)	48,52,52	1.76	8 (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	A	1886	2	-	3/22/38/38	0/3/3/3
3	ATP	D	1886	2	-	1/22/38/38	0/3/3/3
3	ATP	B	1886	2	-	1/22/38/38	0/3/3/3
3	ATP	C	1886	2	-	1/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1886	ATP	C5-C4	4.80	1.47	1.39
3	D	1886	ATP	C5-C4	4.73	1.47	1.39
3	A	1886	ATP	C5-C4	4.63	1.47	1.39
3	C	1886	ATP	C5-C4	4.59	1.47	1.39
3	D	1886	ATP	C5-C6	2.83	1.48	1.41
3	B	1886	ATP	C5-C6	2.82	1.48	1.41
3	B	1886	ATP	PB-O3B	2.69	1.62	1.59
3	C	1886	ATP	C5-C6	2.65	1.48	1.41
3	A	1886	ATP	C5-C6	2.61	1.48	1.41
3	D	1886	ATP	PB-O3B	2.60	1.62	1.59
3	A	1886	ATP	PB-O3B	2.56	1.62	1.59
3	B	1886	ATP	PA-O3A	2.46	1.62	1.59
3	B	1886	ATP	PB-O3A	2.37	1.62	1.59
3	D	1886	ATP	C8-N7	2.34	1.36	1.31
3	C	1886	ATP	C5-N7	-2.34	1.34	1.39
3	A	1886	ATP	C5-N7	-2.32	1.34	1.39
3	A	1886	ATP	C8-N7	2.30	1.36	1.31
3	B	1886	ATP	C8-N7	2.26	1.36	1.31
3	C	1886	ATP	C8-N7	2.23	1.36	1.31
3	B	1886	ATP	C5-N7	-2.16	1.35	1.39
3	D	1886	ATP	C5-N7	-2.12	1.35	1.39
3	C	1886	ATP	PB-O3B	2.07	1.61	1.59
3	A	1886	ATP	PA-O3A	2.06	1.61	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1886	ATP	C5-C4-N3	-5.72	118.84	126.72
3	C	1886	ATP	C5-C4-N3	-5.64	118.95	126.72
3	D	1886	ATP	C5-C4-N3	-5.56	119.06	126.72
3	A	1886	ATP	C5-C4-N3	-5.55	119.08	126.72
3	B	1886	ATP	N3-C4-N9	4.63	135.05	127.17
3	C	1886	ATP	N3-C4-N9	4.55	134.91	127.17
3	A	1886	ATP	N3-C4-N9	4.47	134.78	127.17
3	D	1886	ATP	N3-C4-N9	4.39	134.63	127.17
3	B	1886	ATP	C2-N3-C4	3.61	120.65	111.83
3	B	1886	ATP	C4-C5-N7	-3.56	106.51	110.58
3	D	1886	ATP	C2-N3-C4	3.56	120.53	111.83
3	A	1886	ATP	C2-N3-C4	3.55	120.50	111.83
3	D	1886	ATP	C4-C5-N7	-3.54	106.53	110.58
3	C	1886	ATP	C2-N3-C4	3.54	120.48	111.83
3	C	1886	ATP	C4-C5-N7	-3.45	106.63	110.58
3	A	1886	ATP	C4-C5-N7	-3.39	106.71	110.58
3	A	1886	ATP	N3-C2-N1	-3.26	123.65	128.58
3	B	1886	ATP	N3-C2-N1	-3.16	123.79	128.58
3	D	1886	ATP	N3-C2-N1	-3.14	123.83	128.58
3	C	1886	ATP	N3-C2-N1	-3.14	123.83	128.58
3	C	1886	ATP	C4-N9-C8	2.90	108.79	105.74
3	B	1886	ATP	C4-N9-C8	2.89	108.77	105.74
3	A	1886	ATP	C4-N9-C8	2.85	108.73	105.74
3	D	1886	ATP	C4-N9-C8	2.81	108.69	105.74
3	B	1886	ATP	C5-N7-C8	2.64	107.59	103.45
3	C	1886	ATP	C5-N7-C8	2.62	107.56	103.45
3	D	1886	ATP	C5-N7-C8	2.55	107.45	103.45
3	A	1886	ATP	C5-N7-C8	2.54	107.44	103.45
3	D	1886	ATP	C6-C5-N7	2.16	136.26	132.09
3	C	1886	ATP	N9-C8-N7	-2.16	110.87	113.94
3	B	1886	ATP	C6-C5-N7	2.13	136.20	132.09
3	A	1886	ATP	N9-C8-N7	-2.09	110.97	113.94
3	D	1886	ATP	N9-C8-N7	-2.06	111.01	113.94
3	B	1886	ATP	N9-C8-N7	-2.05	111.02	113.94
3	A	1886	ATP	C2-N1-C6	2.04	122.09	118.73
3	A	1886	ATP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (6) 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

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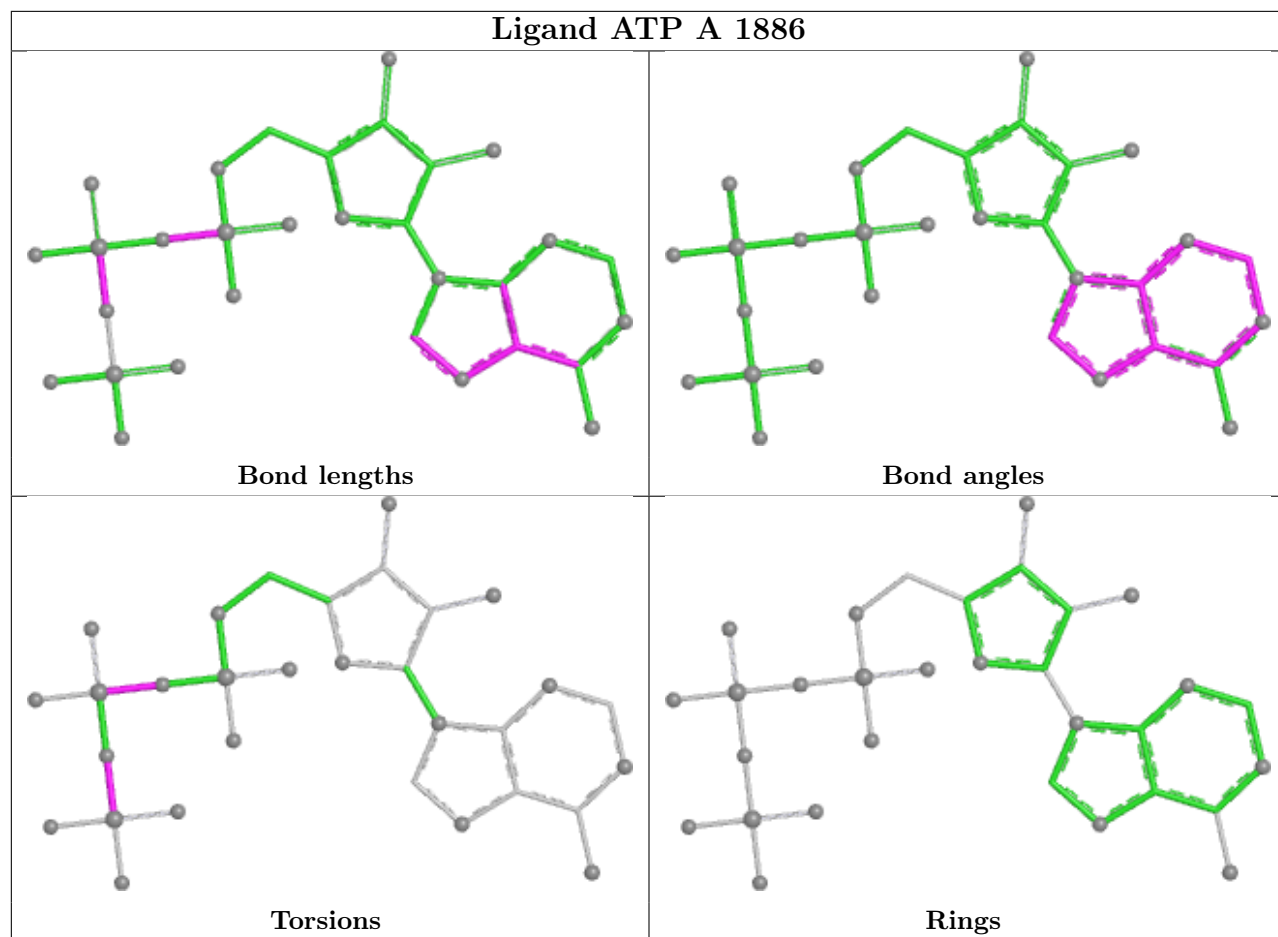
Mol	Chain	Res	Type	Atoms
3	A	1886	ATP	PB-O3B-PG-O2G
3	A	1886	ATP	PA-O3A-PB-O2B
3	B	1886	ATP	PG-O3B-PB-O1B
3	C	1886	ATP	PA-O3A-PB-O2B

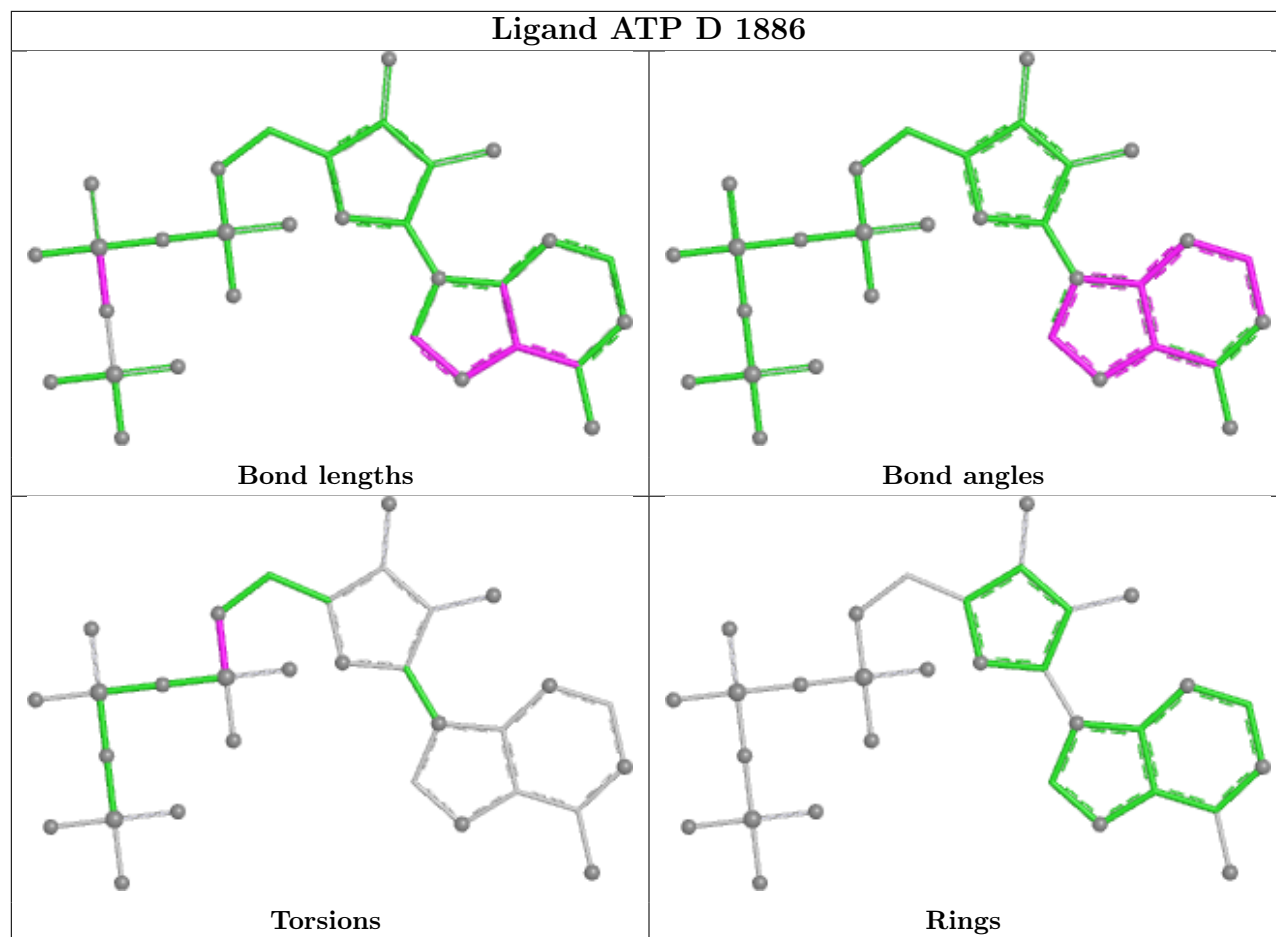
There are no ring outliers.

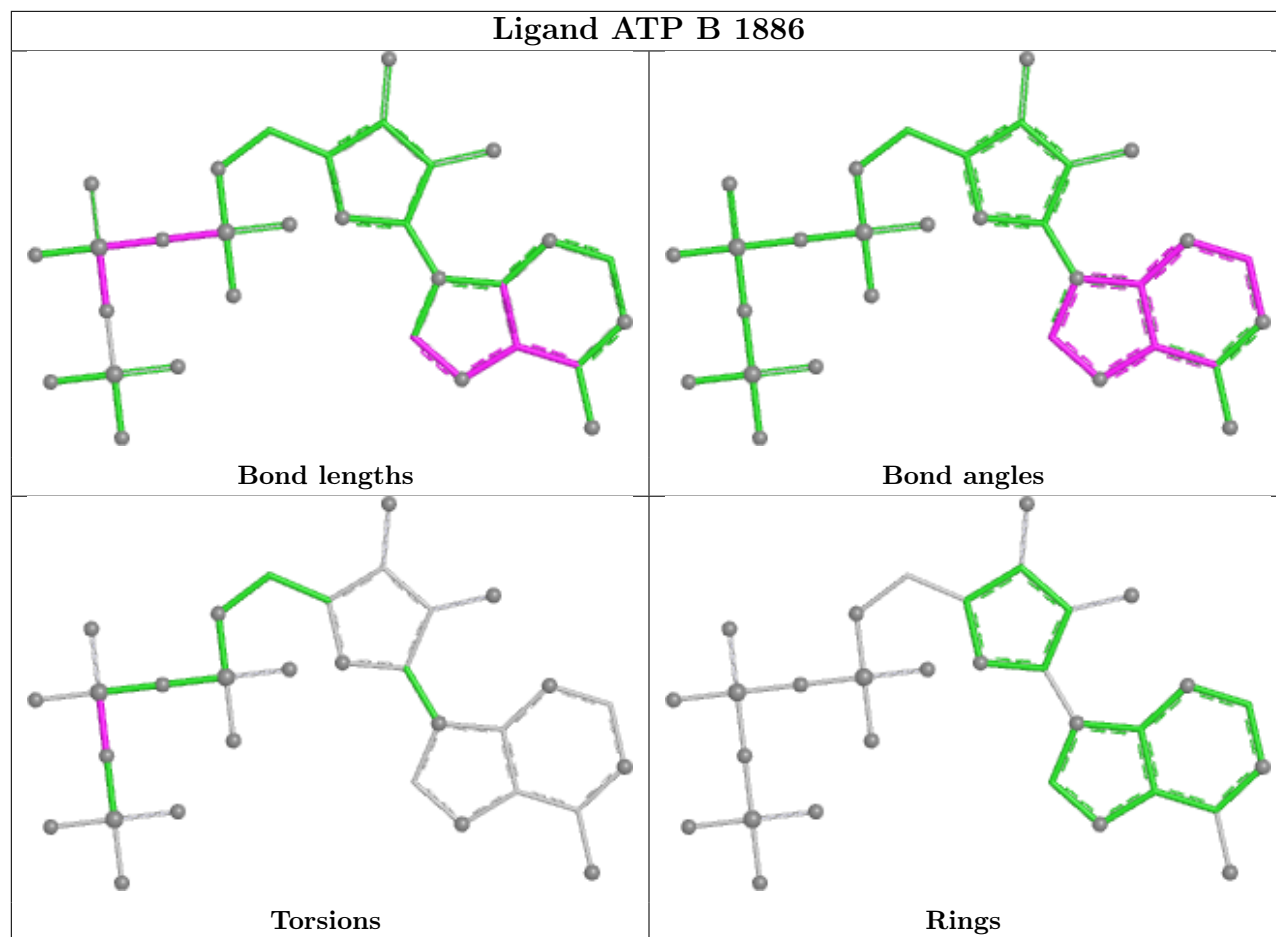
1 monomer is involved in 1 short contact:

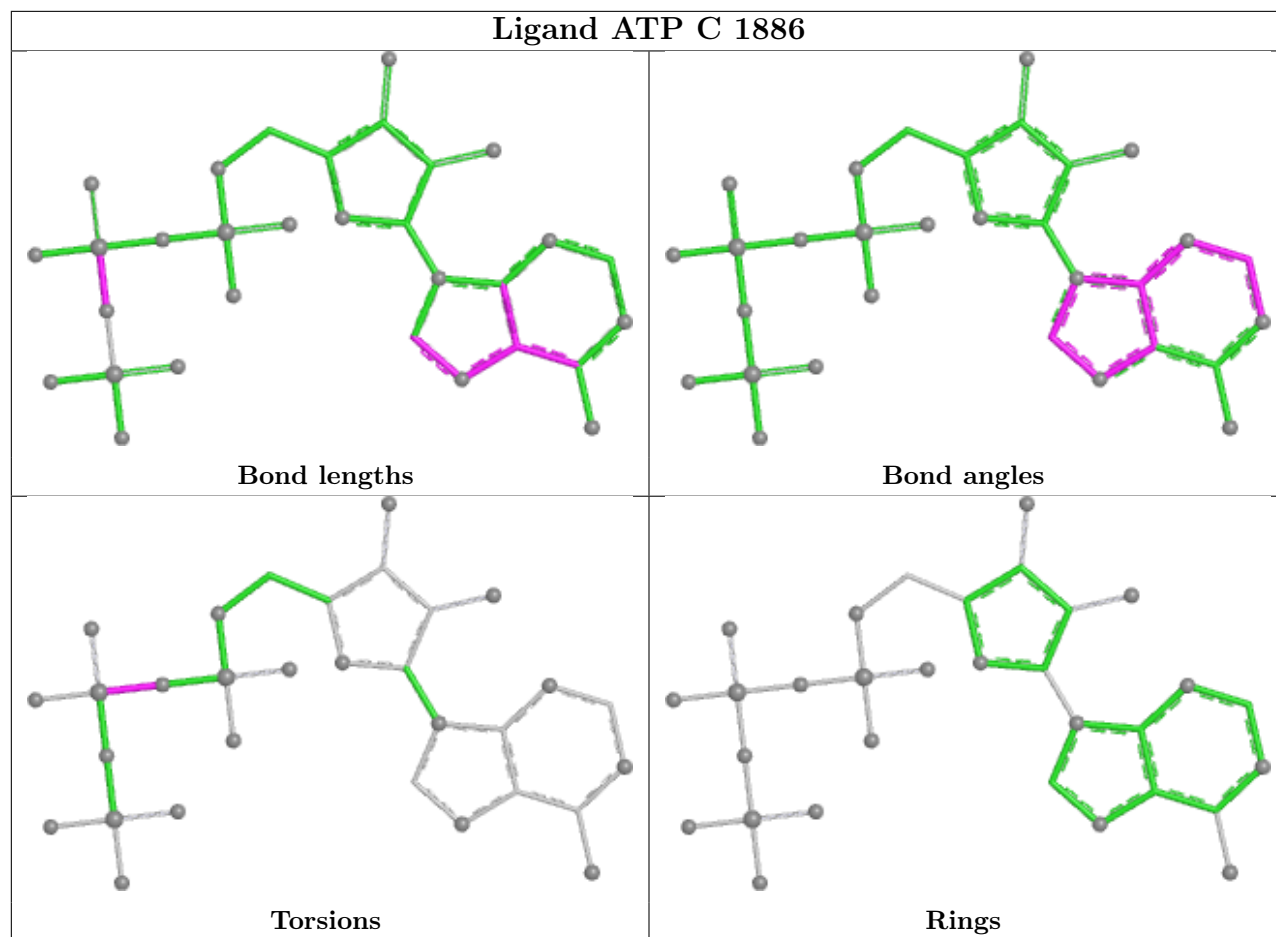
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1886	ATP	1	0

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, 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	839/1038 (80%)	0.19	19 (2%) 61 42	20, 42, 79, 109	0
1	B	842/1038 (81%)	0.51	41 (4%) 35 21	38, 58, 86, 114	0
1	C	838/1038 (80%)	0.20	26 (3%) 51 34	21, 42, 79, 105	0
1	D	833/1038 (80%)	0.58	39 (4%) 36 22	41, 62, 91, 117	0
All	All	3352/4152 (80%)	0.37	125 (3%) 45 28	20, 54, 85, 117	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	767	THR	5.0
1	D	767	THR	4.8
1	A	766	PRO	4.5
1	A	767	THR	4.4
1	D	583	ALA	4.2
1	C	342	LEU	4.2
1	D	535	SER	4.0
1	B	769	ILE	3.9
1	C	769	ILE	3.9
1	A	534	GLY	3.8
1	A	768	SER	3.8
1	A	769	ILE	3.7
1	B	810	SER	3.7
1	C	807	ILE	3.7
1	B	766	PRO	3.6
1	C	812	PRO	3.4
1	D	745	THR	3.4
1	B	768	SER	3.3
1	D	871	THR	3.3
1	A	815	VAL	3.3
1	B	343	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	746	GLY	3.2
1	D	768	SER	3.2
1	C	766	PRO	3.2
1	B	812	PRO	3.2
1	D	533	PRO	3.2
1	D	343	ASP	3.1
1	D	746	GLY	3.1
1	D	216	THR	3.1
1	B	813	VAL	3.0
1	D	357	SER	3.0
1	B	807	ILE	3.0
1	C	767	THR	3.0
1	D	532	PHE	3.0
1	D	723	ASN	3.0
1	B	815	VAL	3.0
1	D	822	HIS	3.0
1	D	769	ILE	2.9
1	A	765	ASP	2.9
1	D	766	PRO	2.9
1	D	764	PRO	2.9
1	C	144	GLY	2.8
1	C	808	ASP	2.8
1	D	265	SER	2.8
1	C	809	LEU	2.8
1	D	807	ILE	2.8
1	D	221	ASN	2.8
1	C	345	GLN	2.7
1	C	746	GLY	2.7
1	C	768	SER	2.7
1	B	142	GLN	2.7
1	C	375	ASP	2.6
1	B	170	GLY	2.6
1	C	810	SER	2.6
1	C	765	ASP	2.6
1	D	811	ASP	2.6
1	D	884	LYS	2.5
1	B	482	VAL	2.5
1	D	810	SER	2.5
1	A	569	ALA	2.5
1	C	874	ASP	2.5
1	A	772	GLU	2.5
1	B	770	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	216	THR	2.5
1	B	423	LYS	2.5
1	B	144	GLY	2.5
1	C	443	ASN	2.5
1	A	808	ASP	2.4
1	B	808	ASP	2.4
1	B	180	ILE	2.4
1	A	810	SER	2.4
1	A	807	ILE	2.4
1	D	341	ASP	2.4
1	A	745	THR	2.4
1	A	345	GLN	2.3
1	A	344	TYR	2.3
1	C	411	HIS	2.3
1	B	765	ASP	2.3
1	C	825	ASP	2.3
1	B	593	GLU	2.3
1	A	411	HIS	2.3
1	C	357	SER	2.3
1	C	873	TRP	2.3
1	B	344	TYR	2.3
1	B	760	GLU	2.3
1	B	814	ALA	2.3
1	B	481	ASP	2.2
1	B	145	SER	2.2
1	C	145	SER	2.2
1	A	593	GLU	2.2
1	B	684	GLN	2.2
1	D	179	GLN	2.2
1	D	224	ASP	2.2
1	B	64	VAL	2.2
1	D	570	THR	2.2
1	D	880	VAL	2.2
1	D	345	GLN	2.1
1	B	811	ASP	2.1
1	D	765	ASP	2.1
1	D	774	GLU	2.1
1	D	26	THR	2.1
1	B	342	LEU	2.1
1	B	772	GLU	2.1
1	D	631	SER	2.1
1	B	627	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	744	ALA	2.1
1	D	392	ALA	2.1
1	C	593	GLU	2.1
1	B	236	LEU	2.1
1	D	353	PHE	2.1
1	A	341	ASP	2.1
1	B	871	THR	2.1
1	B	357	SER	2.0
1	D	347	MET	2.0
1	C	95	GLY	2.0
1	B	176	ALA	2.0
1	B	293	ALA	2.0
1	D	356	ASP	2.0
1	D	747	GLU	2.0
1	D	638	TYR	2.0
1	C	347	MET	2.0
1	A	443	ASN	2.0
1	B	148	ASN	2.0
1	C	853	ILE	2.0
1	B	356	ASP	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.

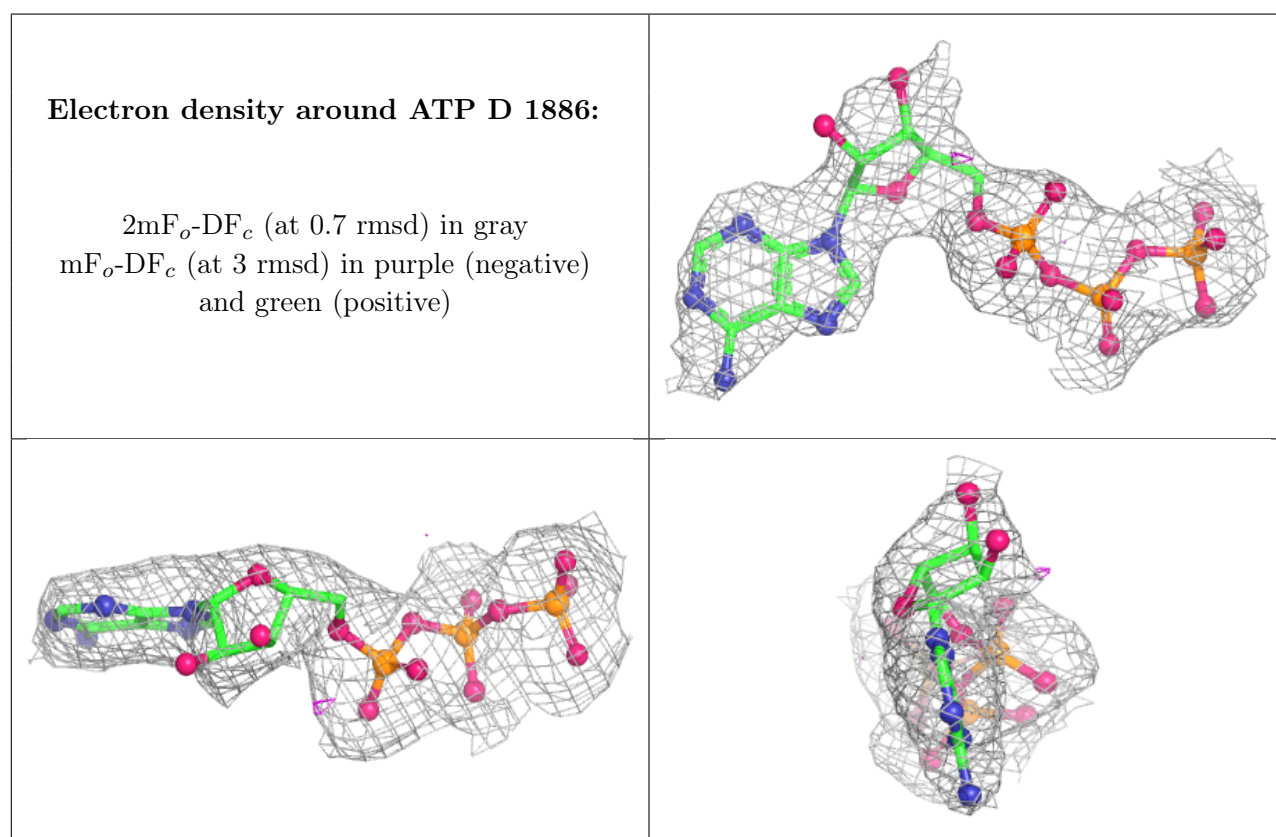
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	1885	1/1	0.79	0.19	52,52,52,52	0
2	MG	A	1885	1/1	0.88	0.15	45,45,45,45	0
2	MG	D	1885	1/1	0.91	0.25	67,67,67,67	0

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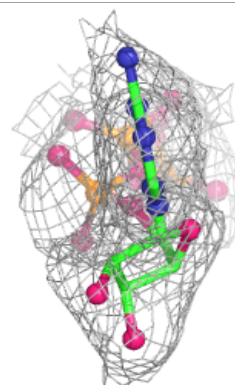
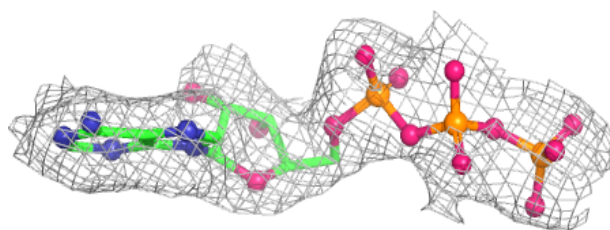
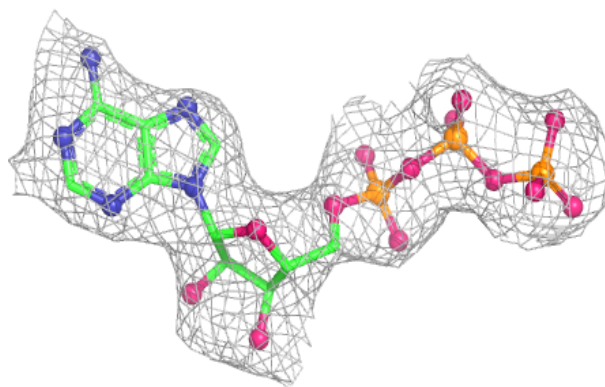
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	1885	1/1	0.93	0.07	37,37,37,37	0
3	ATP	D	1886	31/31	0.93	0.09	45,51,60,62	0
3	ATP	B	1886	31/31	0.94	0.07	42,50,57,61	0
3	ATP	A	1886	31/31	0.96	0.07	27,34,43,51	0
3	ATP	C	1886	31/31	0.97	0.07	21,29,39,40	0

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.

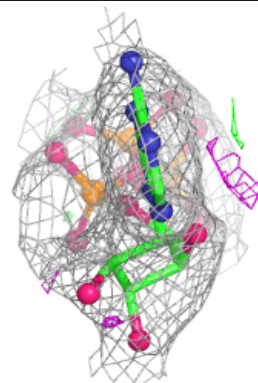
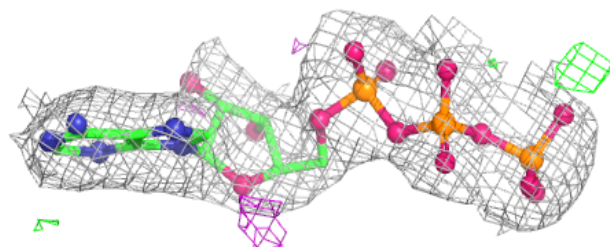
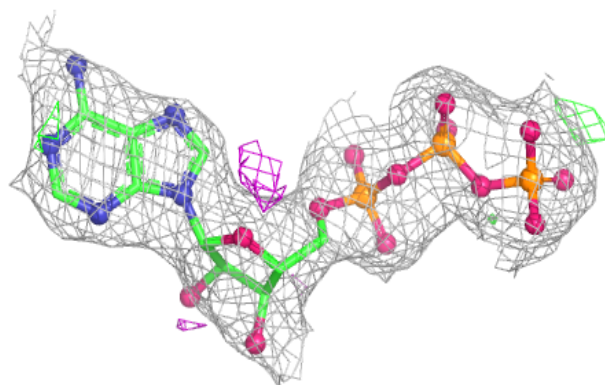


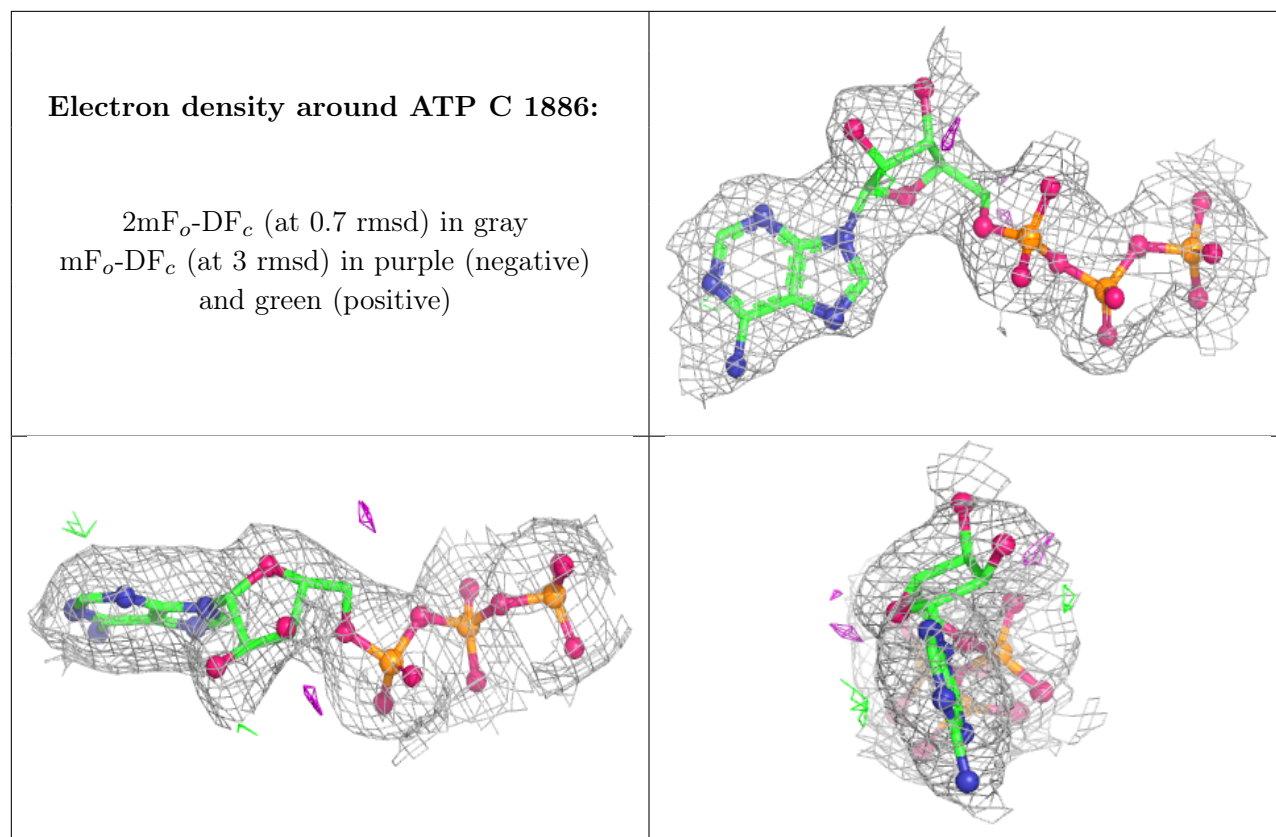
Electron density around ATP B 1886:

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

**Electron density around ATP 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 [i](#)

There are no such residues in this entry.