



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:51 PM BST

PDB ID : 4BEC
Title : MUTANT (K220A) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP
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Deposited on : 2013-03-07
Resolution : 2.84 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 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 : 2.13.1
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) : 2.13.1

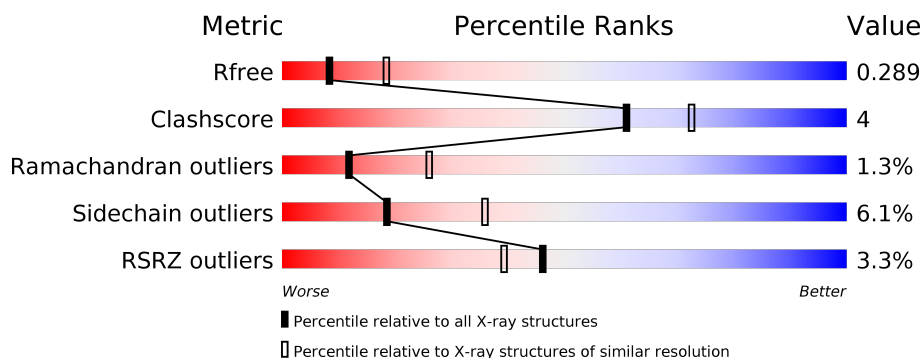
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 ≥ 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>3%</div> <div> <div></div> <div>68%</div> <div>12%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	1038	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>18%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13761 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	845	Total	C	N	O	S	0	0	0
			6836	4348	1152	1320	16			
1	B	846	Total	C	N	O	S	0	0	0
			6853	4361	1161	1315	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	ALA	LYS	engineered mutation	UNP Q304R3
B	220	ALA	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		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

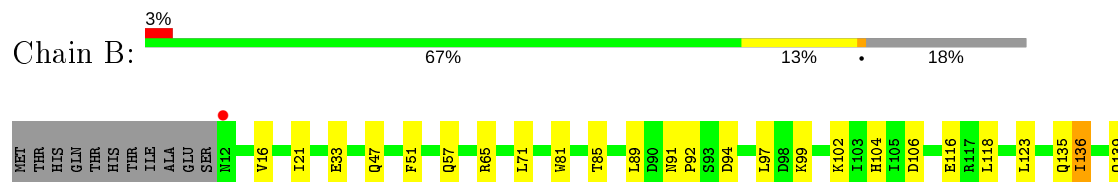


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	4	Total O 4 4	0	0

- 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, α , β , γ	86.33 Å 124.49 Å 128.76 Å 90.00° 108.31° 90.00°	Depositor
Resolution (Å)	18.86 – 2.84 18.86 – 2.84	Depositor EDS
% Data completeness (in resolution range)	97.5 (18.86-2.84) 97.9 (18.86-2.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.83 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.234 , 0.280 0.240 , 0.289	Depositor DCC
R_{free} test set	3022 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13761	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: 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	0.53	0/6970	0.67	2/9413 (0.0%)
1	B	0.48	0/6988	0.65	0/9432
All	All	0.51	0/13958	0.66	2/18845 (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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	191	GLU	C-N-CA	-5.33	108.37	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	TYR	Peptide
1	A	807	ILE	Peptide
1	B	183	TYR	Peptide
1	B	807	ILE	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	6836	0	6633	55	0
1	B	6853	0	6663	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
All	All	13761	0	13320	121	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 (121) 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:213:ALA:HB2	1:A:271:VAL:HG23	1.59	0.82
1:B:534:GLY:HA2	1:B:535:SER:HB3	1.62	0.81
1:B:532:PHE:HB3	1:B:533:PRO:CD	2.15	0.77
1:B:824:VAL:HG13	1:B:828:LYS:HB3	1.69	0.74
1:B:532:PHE:HB3	1:B:533:PRO:HD3	1.70	0.73
1:A:179:GLN:O	1:A:183:TYR:CB	2.37	0.72
1:A:824:VAL:HG13	1:A:828:LYS:HB3	1.70	0.72
1:B:184:SER:O	1:B:186:GLU:N	2.23	0.72
1:A:591:ILE:N	1:A:592:GLY:HA2	2.07	0.69
1:A:57:GLN:HE22	1:A:193:SER:HB3	1.57	0.69
1:A:184:SER:O	1:A:186:GLU:N	2.24	0.68
1:B:213:ALA:HB2	1:B:271:VAL:HG23	1.74	0.68
1:B:179:GLN:O	1:B:183:TYR:CB	2.41	0.68
1:B:216:THR:OG1	1:B:217:LYS:N	2.26	0.68
1:B:97:LEU:HD21	1:B:267:GLN:HB3	1.75	0.68
1:A:139:GLN:NE2	1:A:149:ARG:O	2.28	0.67
1:B:139:GLN:NE2	1:B:149:ARG:O	2.28	0.67
1:A:343:ASP:H	1:A:346:THR:HG22	1.61	0.66
1:A:154:ILE:HB	1:A:162:VAL:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:OG1	1:A:217:LYS:N	2.28	0.62
1:A:97:LEU:HD21	1:A:267:GLN:HB3	1.84	0.60
1:B:343:ASP:H	1:B:346:THR:HG22	1.67	0.60
1:A:591:ILE:HB	1:A:593:GLU:H	1.66	0.59
1:B:534:GLY:CA	1:B:535:SER:HB3	2.33	0.57
1:B:57:GLN:HE22	1:B:193:SER:HB3	1.70	0.57
1:A:684:GLN:O	1:A:688:ARG:NH1	2.39	0.56
1:B:526:GLN:HA	1:B:531:THR:CG2	2.36	0.55
1:A:200:LEU:HD13	1:A:271:VAL:HG21	1.88	0.55
1:B:673:VAL:HB	1:B:704:THR:HG22	1.88	0.55
1:A:174:ARG:NH2	1:A:879:GLU:OE1	2.40	0.55
1:A:687:SER:O	1:A:690:ASN:ND2	2.40	0.54
1:A:204:SER:HB2	1:A:209:THR:HG23	1.89	0.54
1:A:47:GLN:NE2	1:A:249:GLN:OE1	2.40	0.54
1:A:99:LYS:HD2	1:A:197:TYR:CZ	2.43	0.54
1:B:581:SER:OG	1:B:598:THR:O	2.15	0.54
1:B:530:ARG:HD3	1:B:536:LYS:O	2.08	0.53
1:B:175:GLU:O	1:B:179:GLN:HG2	2.10	0.52
1:A:175:GLU:O	1:A:179:GLN:HG2	2.09	0.52
1:A:673:VAL:HB	1:A:704:THR:HG22	1.92	0.52
1:B:313:LYS:NZ	1:B:409:GLU:OE2	2.40	0.51
1:B:463:ILE:O	1:B:467:ILE:HG12	2.10	0.51
1:A:676:ASN:OD1	1:A:706:ARG:NH1	2.44	0.51
1:B:47:GLN:NE2	1:B:249:GLN:OE1	2.44	0.50
1:B:247:CYS:HA	1:B:252:THR:HG21	1.94	0.50
1:A:619:TYR:OH	1:A:644:ARG:HD2	2.10	0.49
1:B:568:SER:HG	1:B:570:THR:HG1	1.59	0.49
1:B:583:ALA:HA	1:B:597:GLU:HA	1.94	0.49
1:B:544:VAL:HG22	1:B:655:VAL:O	2.13	0.49
1:B:174:ARG:NH2	1:B:879:GLU:OE1	2.46	0.49
1:B:619:TYR:OH	1:B:644:ARG:HD2	2.13	0.49
1:B:755:VAL:HG13	1:B:781:LEU:HD22	1.95	0.49
1:B:686:PHE:CZ	1:B:702:ILE:HG21	2.48	0.49
1:B:104:HIS:NE2	1:B:199:GLN:OE1	2.39	0.48
1:B:224:ASP:N	1:B:224:ASP:OD1	2.46	0.48
1:A:128:ASN:ND2	1:A:131:ARG:HG3	2.29	0.48
1:A:527:LYS:HE3	1:A:703:VAL:HG21	1.95	0.48
1:B:219:ASP:O	1:B:220:ALA:HB3	2.14	0.48
1:A:116:GLU:HB3	1:B:365:ALA:HB3	1.96	0.48
1:A:224:ASP:N	1:A:224:ASP:OD1	2.45	0.48
1:A:686:PHE:CZ	1:A:702:ILE:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:GLN:O	1:B:688:ARG:NH1	2.47	0.48
1:A:759:LEU:HD23	1:A:781:LEU:HD13	1.95	0.48
1:A:16:VAL:O	1:A:282:ARG:NH2	2.47	0.47
1:B:581:SER:OG	1:B:581:SER:O	2.31	0.47
1:A:463:ILE:O	1:A:467:ILE:HG12	2.14	0.47
1:B:99:LYS:HD2	1:B:197:TYR:CZ	2.48	0.47
1:B:94:ASP:OD2	1:B:102:LYS:NZ	2.46	0.47
1:A:758:GLU:HB3	1:A:781:LEU:HD11	1.96	0.47
1:B:200:LEU:HD13	1:B:271:VAL:HG21	1.97	0.47
1:B:544:VAL:HA	1:B:674:ASP:O	2.15	0.47
1:B:33:GLU:HG3	1:B:150:TYR:CD1	2.50	0.46
1:B:280:THR:HG23	1:B:320:ALA:HB2	1.98	0.46
1:A:65:ARG:HG3	1:A:81:TRP:CD2	2.51	0.46
1:A:390:MET:O	1:A:425:LYS:NZ	2.47	0.46
1:A:831:GLU:O	1:A:834:THR:OG1	2.25	0.45
1:B:16:VAL:O	1:B:282:ARG:NH2	2.49	0.45
1:B:57:GLN:NE2	1:B:193:SER:HB3	2.32	0.45
1:B:879:GLU:O	1:B:883:LEU:HB2	2.17	0.45
1:A:544:VAL:HG22	1:A:655:VAL:O	2.17	0.45
1:A:219:ASP:O	1:A:220:ALA:HB3	2.16	0.44
1:A:57:GLN:NE2	1:A:193:SER:HB3	2.29	0.44
1:B:176:ALA:O	1:B:179:GLN:HB2	2.18	0.44
1:B:687:SER:O	1:B:690:ASN:ND2	2.51	0.44
1:B:234:ASN:O	1:B:468:ARG:NH2	2.50	0.44
1:B:33:GLU:HG3	1:B:150:TYR:CE1	2.53	0.43
1:A:879:GLU:O	1:A:883:LEU:HB2	2.19	0.43
1:B:759:LEU:HD23	1:B:781:LEU:HD13	1.99	0.43
1:B:65:ARG:HG3	1:B:81:TRP:CD2	2.54	0.43
1:B:637:TYR:O	1:B:641:LEU:HB2	2.19	0.42
1:B:838:PRO:HB2	1:B:843:ILE:HD11	2.01	0.42
1:A:679:TYR:CD1	1:A:718:LEU:HD12	2.54	0.42
1:B:204:SER:HB2	1:B:209:THR:HG23	2.00	0.42
1:A:544:VAL:HA	1:A:674:ASP:O	2.19	0.42
1:A:735:GLU:O	1:A:739:GLY:N	2.52	0.42
1:B:343:ASP:O	1:B:347:MET:HG3	2.20	0.42
1:B:337:VAL:HG12	1:B:408:ASP:HB3	2.01	0.42
1:B:336:VAL:HA	1:B:381:THR:O	2.20	0.42
1:A:176:ALA:O	1:A:179:GLN:HB2	2.20	0.42
1:A:369:ARG:NH2	1:B:116:GLU:O	2.53	0.42
1:A:482:VAL:O	1:A:484:PRO:HD3	2.20	0.42
1:A:264:ASP:HB2	1:A:349:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:TYR:O	1:A:641:LEU:HB2	2.20	0.41
1:A:832:LEU:HD23	1:A:835:ILE:HD12	2.02	0.41
1:B:302:GLY:HA3	1:B:431:GLN:O	2.20	0.41
1:B:339:ARG:NH1	1:B:360:GLY:O	2.53	0.41
1:B:704:THR:HG21	1:B:708:LEU:HD12	2.01	0.41
1:A:530:ARG:NH2	1:A:651:ASP:OD1	2.49	0.41
1:B:123:LEU:HD22	1:B:159:LEU:HD11	2.03	0.41
1:B:85:THR:HA	1:B:89:LEU:HB3	2.03	0.41
1:A:44:LEU:HD13	1:A:136:ILE:HG21	2.02	0.41
1:B:660:LEU:HD23	1:B:660:LEU:HA	1.93	0.41
1:B:91:ASN:HA	1:B:92:PRO:HD3	1.94	0.41
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.94	0.40
1:A:336:VAL:HA	1:A:381:THR:O	2.21	0.40
1:A:474:LYS:HB3	1:A:728:VAL:O	2.21	0.40
1:B:304:TYR:CZ	1:B:457:GLU:HB2	2.56	0.40
1:A:337:VAL:O	1:A:382:THR:HA	2.22	0.40
1:B:162:VAL:HG22	1:B:200:LEU:HB3	2.02	0.40
1:B:51:PHE:HA	1:B:136:ILE:HG12	2.03	0.40
1:A:337:VAL:HG12	1:A:408:ASP:HB3	2.03	0.40
1:B:641:LEU:HD11	1:B:653:LEU:HD13	2.03	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	837/1038 (81%)	787 (94%)	40 (5%)	10 (1%)	13	28
1	B	838/1038 (81%)	782 (93%)	45 (5%)	11 (1%)	12	26
All	All	1675/2076 (81%)	1569 (94%)	85 (5%)	21 (1%)	12	26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	184	SER
1	A	185	LYS
1	A	810	SER
1	B	179	GLN
1	B	185	LYS
1	A	183	TYR
1	A	582	PHE
1	B	183	TYR
1	B	184	SER
1	B	807	ILE
1	A	187	SER
1	A	807	ILE
1	B	187	SER
1	B	533	PRO
1	B	535	SER
1	B	808	ASP
1	B	809	LEU
1	A	220	ALA
1	B	220	ALA
1	A	769	ILE

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	739/926 (80%)	692 (94%)	47 (6%)	17	34
1	B	739/926 (80%)	696 (94%)	43 (6%)	20	38
All	All	1478/1852 (80%)	1388 (94%)	90 (6%)	18	36

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	65	ARG
1	A	71	LEU

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Mol	Chain	Res	Type
1	A	106	ASP
1	A	118	LEU
1	A	136	ILE
1	A	163	GLN
1	A	169	ARG
1	A	215	THR
1	A	224	ASP
1	A	236	LEU
1	A	240	LEU
1	A	253	LEU
1	A	282	ARG
1	A	336	VAL
1	A	371	LEU
1	A	377	LYS
1	A	410	CYS
1	A	411	HIS
1	A	422	LEU
1	A	424	LYS
1	A	481	ASP
1	A	507	PHE
1	A	531	THR
1	A	532	PHE
1	A	575	ARG
1	A	629	THR
1	A	641	LEU
1	A	652	LEU
1	A	655	VAL
1	A	688	ARG
1	A	690	ASN
1	A	698	THR
1	A	709	GLU
1	A	718	LEU
1	A	725	LYS
1	A	753	MET
1	A	765	ASP
1	A	780	LYS
1	A	781	LEU
1	A	789	GLU
1	A	804	LEU
1	A	805	GLN
1	A	836	ARG
1	A	840	ASP

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Mol	Chain	Res	Type
1	A	880	VAL
1	A	883	LEU
1	B	21	ILE
1	B	71	LEU
1	B	106	ASP
1	B	118	LEU
1	B	135	GLN
1	B	136	ILE
1	B	163	GLN
1	B	169	ARG
1	B	215	THR
1	B	224	ASP
1	B	236	LEU
1	B	240	LEU
1	B	253	LEU
1	B	282	ARG
1	B	289	SER
1	B	308	THR
1	B	309	THR
1	B	336	VAL
1	B	371	LEU
1	B	372	ASP
1	B	374	ASP
1	B	377	LYS
1	B	442	GLU
1	B	481	ASP
1	B	507	PHE
1	B	575	ARG
1	B	629	THR
1	B	652	LEU
1	B	655	VAL
1	B	668	LEU
1	B	688	ARG
1	B	690	ASN
1	B	698	THR
1	B	709	GLU
1	B	718	LEU
1	B	753	MET
1	B	765	ASP
1	B	781	LEU
1	B	804	LEU
1	B	805	GLN

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Mol	Chain	Res	Type
1	B	836	ARG
1	B	859	ARG
1	B	883	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	139	GLN
1	A	690	ASN
1	B	57	GLN
1	B	139	GLN
1	B	228	ASN
1	B	690	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1887	2	26,33,33	1.14	2 (7%)	31,52,52	1.67	9 (29%)
3	ATP	B	1887	2	26,33,33	1.06	2 (7%)	31,52,52	1.62	7 (22%)

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	1887	2	-	0/18/38/38	0/3/3/3
3	ATP	B	1887	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	A	1887	ATP	C5-C4	2.80	1.48	1.40
3	A	1887	ATP	C2'-C1'	-2.72	1.49	1.53
3	B	1887	ATP	C5-C4	2.67	1.48	1.40
3	B	1887	ATP	C2'-C1'	-2.40	1.50	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1887	ATP	N3-C2-N1	-3.38	123.40	128.68
3	A	1887	ATP	N3-C2-N1	-3.15	123.75	128.68
3	B	1887	ATP	C3'-C2'-C1'	3.10	105.65	100.98
3	B	1887	ATP	PB-O3B-PG	-2.91	122.83	132.83
3	A	1887	ATP	O2G-PG-O1G	2.82	121.72	110.68
3	A	1887	ATP	PB-O3B-PG	-2.76	123.35	132.83
3	A	1887	ATP	PA-O3A-PB	-2.69	123.61	132.83
3	B	1887	ATP	PA-O3A-PB	-2.54	124.09	132.83
3	A	1887	ATP	C3'-C2'-C1'	2.47	104.70	100.98
3	A	1887	ATP	C4-C5-N7	-2.42	106.88	109.40
3	A	1887	ATP	O5'-PA-O1A	-2.40	99.68	109.07
3	A	1887	ATP	O2B-PB-O1B	2.32	123.69	112.24
3	A	1887	ATP	C2-N1-C6	2.14	122.42	118.75
3	B	1887	ATP	N6-C6-N1	2.12	122.97	118.57
3	B	1887	ATP	C2-N1-C6	2.08	122.32	118.75
3	B	1887	ATP	O4'-C1'-C2'	-2.01	103.98	106.93

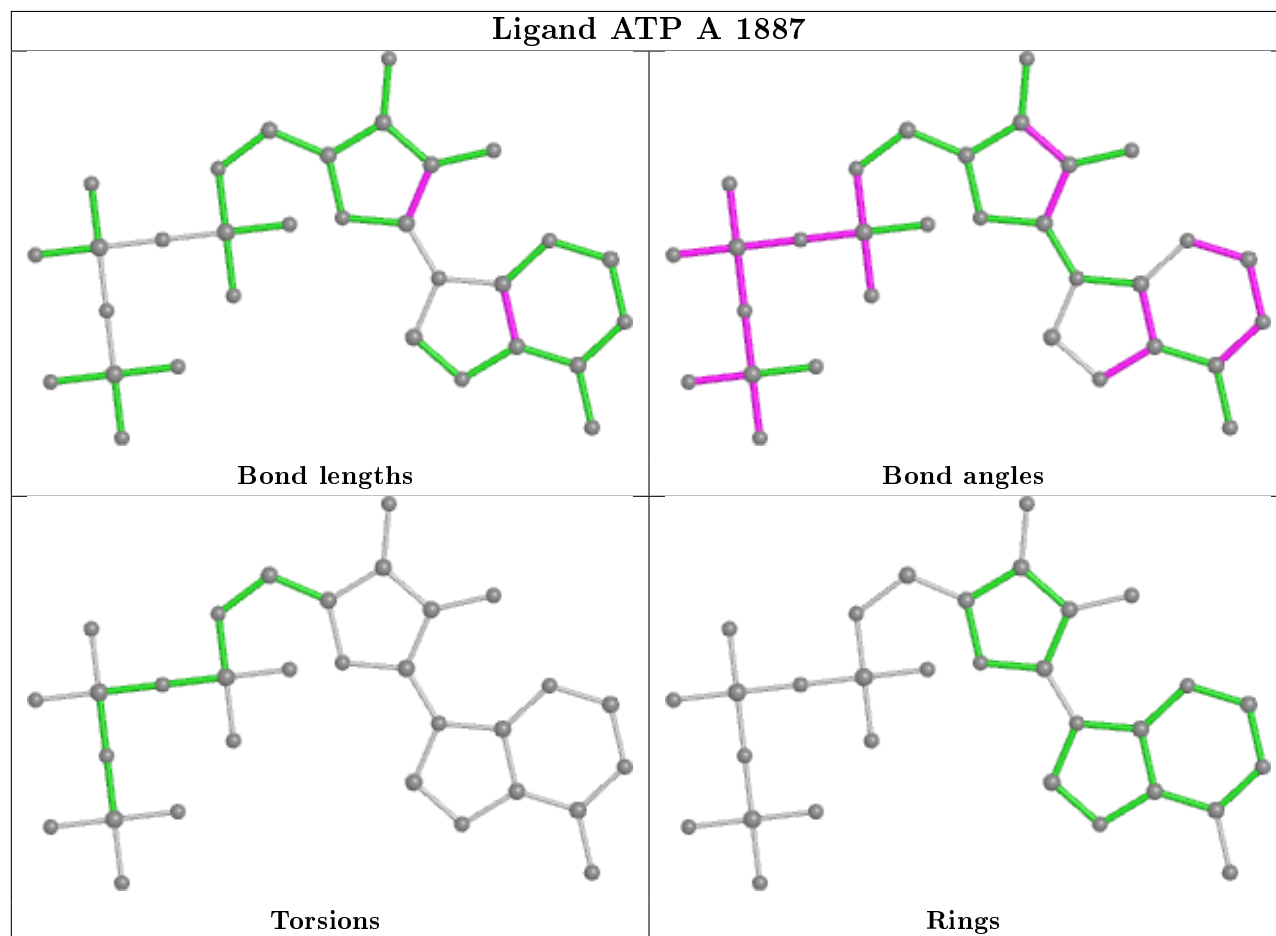
There are no chirality outliers.

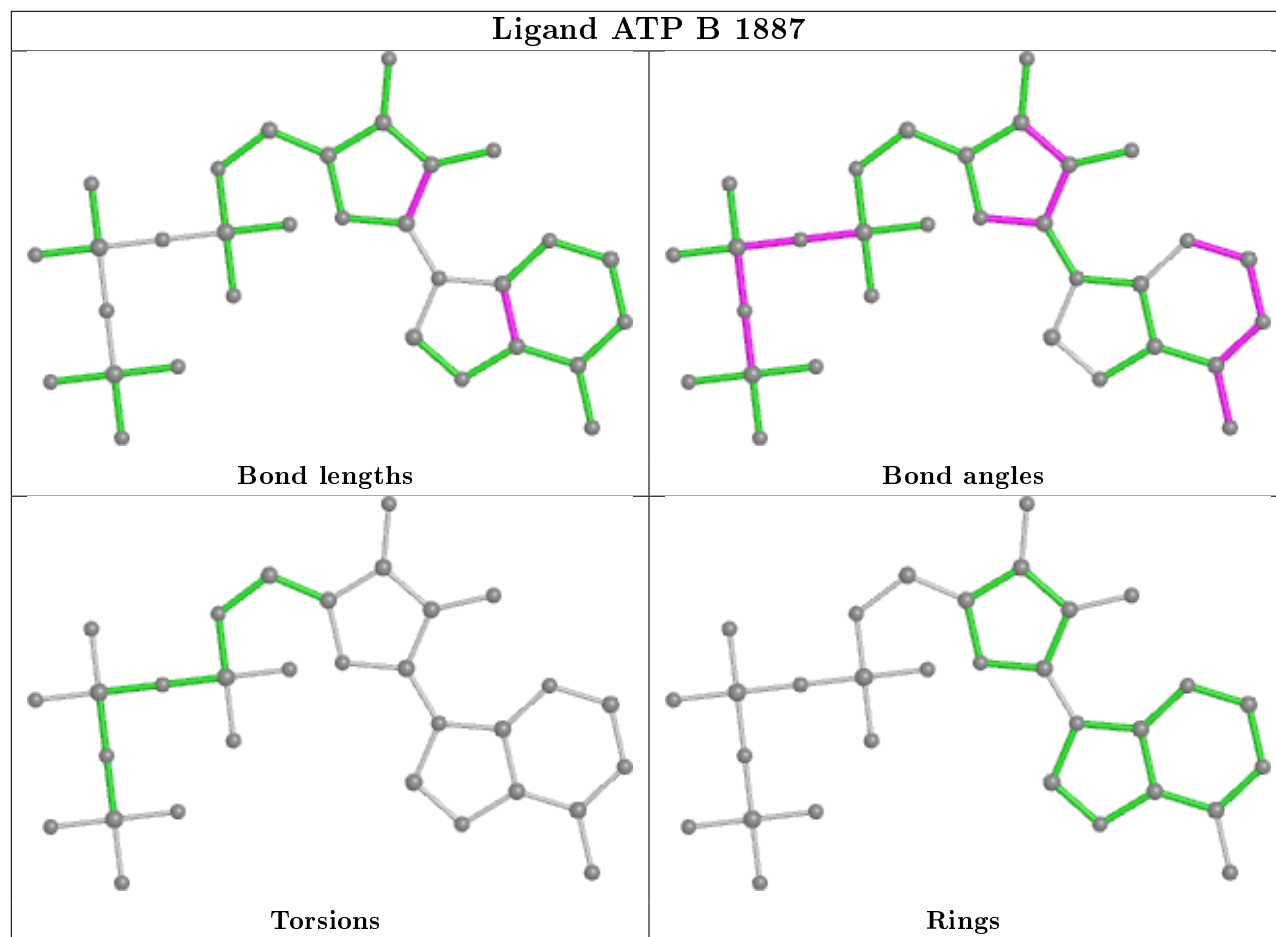
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	845/1038 (81%)	-0.16	30 (3%) 42 35	12, 47, 92, 140	0
1	B	846/1038 (81%)	-0.11	26 (3%) 49 42	20, 51, 94, 137	0
All	All	1691/2076 (81%)	-0.13	56 (3%) 46 39	12, 49, 93, 140	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	SER	7.0
1	B	768	SER	5.7
1	A	768	SER	5.3
1	B	184	SER	4.6
1	B	190	SER	4.3
1	B	745	THR	4.3
1	B	767	THR	4.2
1	A	534	GLY	4.1
1	B	183	TYR	3.9
1	B	810	SER	3.8
1	A	745	THR	3.8
1	A	186	GLU	3.8
1	A	183	TYR	3.6
1	A	810	SER	3.6
1	B	848	SER	3.5
1	A	767	THR	3.5
1	B	811	ASP	3.2
1	B	140	PHE	3.2
1	B	813	VAL	3.2
1	A	187	SER	3.2
1	B	374	ASP	3.2
1	B	841	ARG	3.1
1	A	813	VAL	3.1
1	A	185	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	189	ASN	2.9
1	A	532	PHE	2.9
1	A	848	SER	2.9
1	B	186	GLU	2.9
1	B	533	PRO	2.8
1	A	533	PRO	2.8
1	B	185	LYS	2.7
1	A	809	LEU	2.7
1	A	826	ASP	2.7
1	A	190	SER	2.7
1	A	844	GLN	2.7
1	A	827	GLU	2.6
1	A	812	PRO	2.6
1	B	855	ASP	2.6
1	B	187	SER	2.5
1	A	188	PHE	2.4
1	B	808	ASP	2.3
1	A	593	GLU	2.3
1	B	499	SER	2.3
1	A	604	MET	2.3
1	A	744	ALA	2.3
1	A	811	ASP	2.2
1	B	447	SER	2.2
1	A	583	ALA	2.2
1	B	300	GLU	2.2
1	B	844	GLN	2.2
1	A	820	ALA	2.2
1	B	534	GLY	2.1
1	A	219	ASP	2.1
1	A	836	ARG	2.0
1	B	12	ASN	2.0
1	A	445	LEU	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](#)

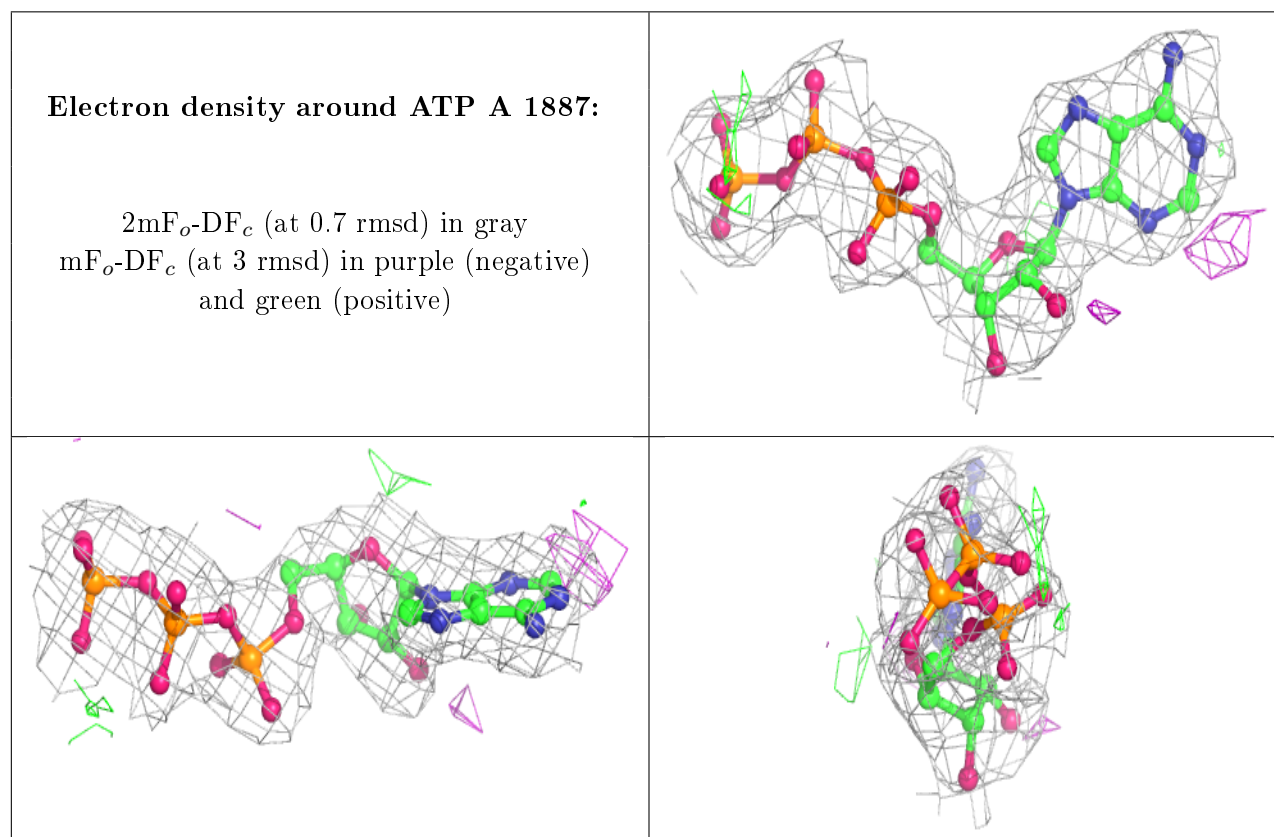
There are no monosaccharides in this entry.

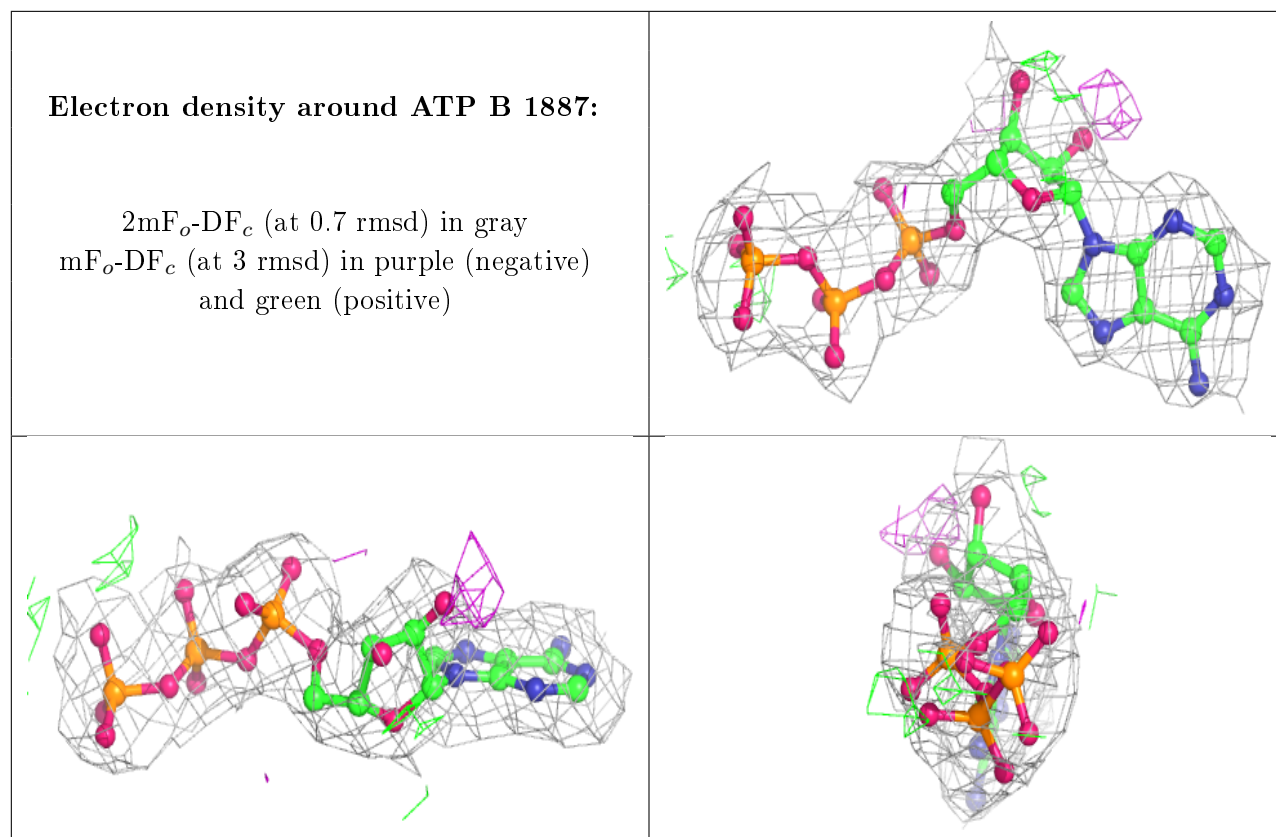
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	MG	B	1886	1/1	0.60	0.23	47,47,47,47	0
2	MG	A	1886	1/1	0.70	0.17	50,50,50,50	0
3	ATP	A	1887	31/31	0.98	0.09	21,28,34,36	0
3	ATP	B	1887	31/31	0.98	0.09	23,34,43,44	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.