



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 01:37 PM EDT

PDB ID : 8SAM
Title : Crystal structure of class III lanthipeptide synthetase LP-GS-ThurKC in complex with ATP
Authors : Hernandez Garcia, A.; Nair, S.K.
Deposited on : 2023-04-01
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

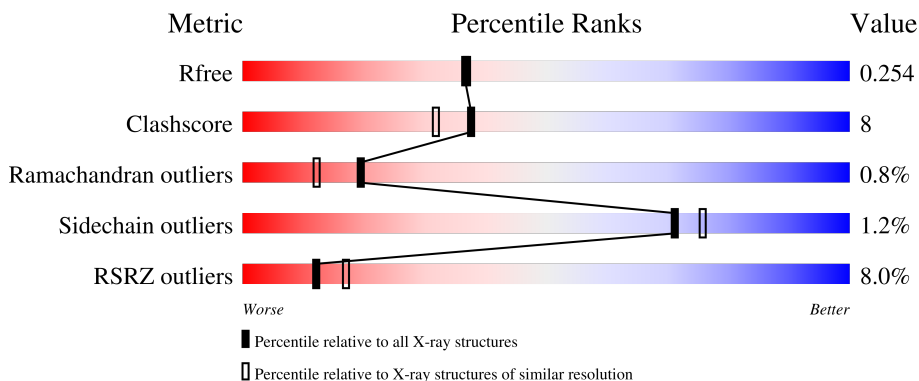
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	904	
1	B	904	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14329 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 Class III lanthipeptide, Class III lanthionine synthetase LanKC fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	859	6936	4453	1147	1313	23	0	0	0
1	B	858	6924	4445	1146	1310	23	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

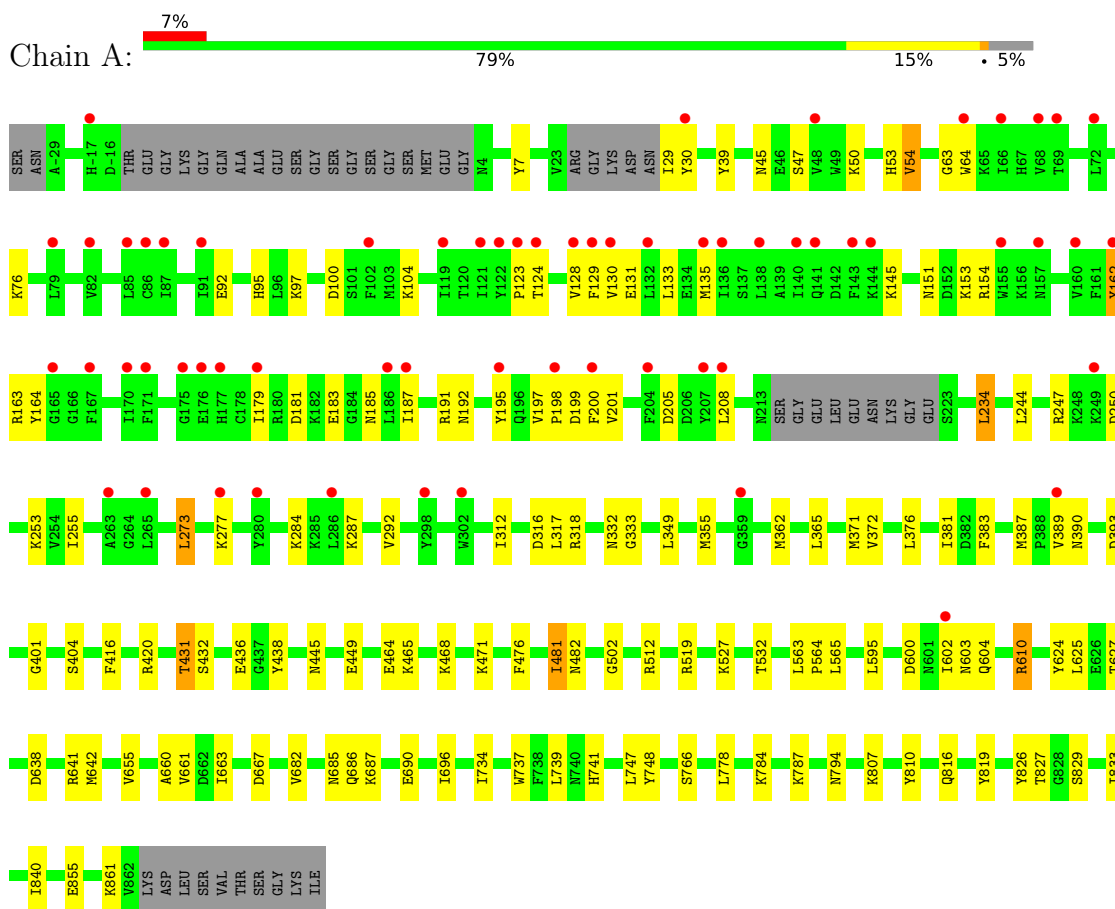
Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	SER	-	expression tag	UNP A0A7U1BAR4
A	-30	ASN	-	expression tag	UNP A0A7U1BAR4
A	-29	ALA	-	expression tag	UNP A0A7U1BAR4
A	-6	SER	-	linker	UNP A0A7U1BAR4
A	-5	GLY	-	linker	UNP A0A7U1BAR4
A	-4	SER	-	linker	UNP A0A7U1BAR4
A	-3	GLY	-	linker	UNP A0A7U1BAR4
A	-2	SER	-	linker	UNP A0A7U1BAR4
A	-1	GLY	-	linker	UNP A0A7U1BAR4
A	0	SER	-	linker	UNP A0A7U1BAR4
B	-31	SER	-	expression tag	UNP A0A7U1BAR4
B	-30	ASN	-	expression tag	UNP A0A7U1BAR4
B	-29	ALA	-	expression tag	UNP A0A7U1BAR4
B	-6	SER	-	linker	UNP A0A7U1BAR4
B	-5	GLY	-	linker	UNP A0A7U1BAR4
B	-4	SER	-	linker	UNP A0A7U1BAR4
B	-3	GLY	-	linker	UNP A0A7U1BAR4
B	-2	SER	-	linker	UNP A0A7U1BAR4
B	-1	GLY	-	linker	UNP A0A7U1BAR4
B	0	SER	-	linker	UNP A0A7U1BAR4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

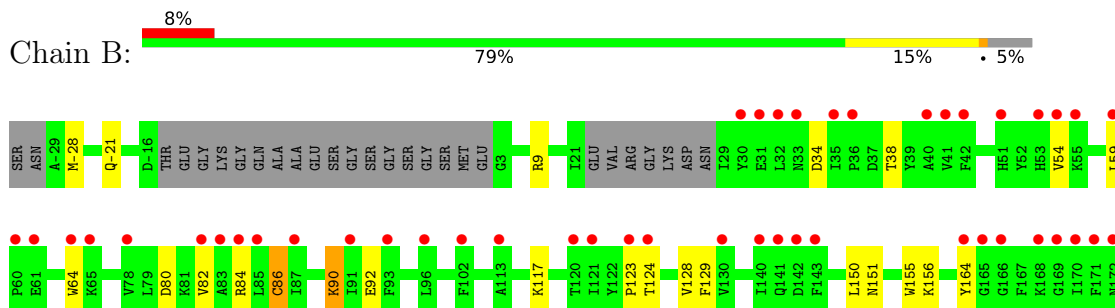
3 Residue-property plots

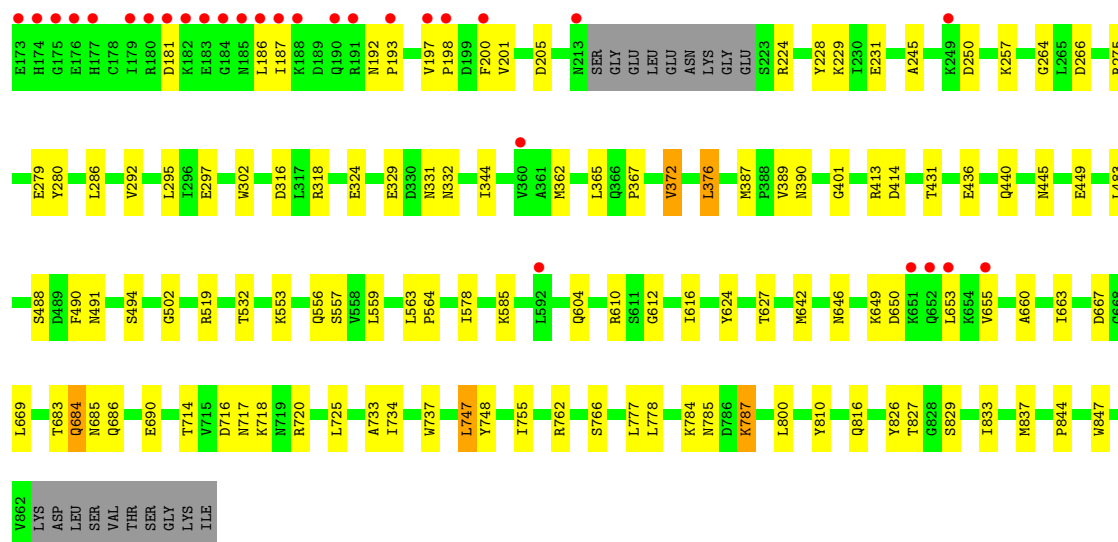
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Class III lanthipeptide, Class III lanthionine synthetase LanKC fusion



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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	54.02Å 228.66Å 84.59Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	49.01 – 2.15 49.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	86.4 (49.01-2.15) 86.4 (49.00-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.251 0.207 , 0.254	Depositor DCC
R_{free} test set	4665 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14329	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/7069	0.65	1/9537 (0.0%)
1	B	0.33	0/7057	0.65	0/9520
All	All	0.33	0/14126	0.65	1/19057 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	610	ARG	NE-CZ-NH2	-7.07	116.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	600	ASP	Peptide

5.2 Too-close contacts [i](#)

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	6936	0	6944	115	0
1	B	6924	0	6932	102	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	2	0
3	B	31	0	12	0	0
4	A	201	0	0	7	0
4	B	204	0	0	12	0
All	All	14329	0	13900	215	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 8.

All (215) 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:153:LYS:HB2	1:A:162:TYR:CE1	1.75	1.22
1:A:153:LYS:CB	1:A:162:TYR:HE1	1.69	1.03
1:A:794:ASN:HB3	4:A:1157:HOH:O	1.63	0.99
1:A:840:ILE:O	1:B:491:ASN:ND2	1.98	0.96
1:B:181:ASP:HB2	1:B:186:LEU:H	1.33	0.91
1:A:153:LYS:HB2	1:A:162:TYR:HE1	1.10	0.90
1:A:47:SER:O	1:A:97:LYS:NZ	2.08	0.87
1:B:286:LEU:HB3	1:B:292:VAL:HG21	1.56	0.85
1:B:228:TYR:HB3	4:B:1021:HOH:O	1.80	0.81
1:B:59:LEU:HD11	1:B:92:GLU:HB2	1.61	0.81
1:B:683:THR:O	1:B:683:THR:OG1	1.94	0.80
1:A:737:TRP:HE1	1:A:784:LYS:HE3	1.46	0.80
1:B:387:MET:CE	1:B:413:ARG:HH21	1.94	0.79
1:A:39:TYR:CE2	1:A:54:VAL:HG12	2.18	0.79
1:A:471:LYS:HE3	1:A:476:PHE:O	1.83	0.79
1:B:362:MET:O	1:B:414:ASP:OD1	2.01	0.78
1:B:245:ALA:HB1	4:B:1021:HOH:O	1.82	0.78
1:B:624:TYR:O	1:B:627:THR:O	2.02	0.78
1:B:387:MET:HE2	1:B:413:ARG:HH21	1.50	0.76
1:B:650:ASP:N	4:B:1001:HOH:O	2.21	0.73
1:A:603:ASN:OD1	1:A:642:MET:HG2	1.89	0.72
1:B:257:LYS:HE2	1:B:279:GLU:OE1	1.89	0.72
1:B:604:GLN:HG2	1:B:642:MET:HE1	1.72	0.71
1:A:130:VAL:HA	1:A:133:LEU:HD23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:HD21	1:A:465:LYS:HE2	1.72	0.71
1:A:54:VAL:HG13	1:A:92:GLU:HG3	1.74	0.70
1:A:153:LYS:HB2	1:A:162:TYR:CD1	2.27	0.69
1:A:624:TYR:O	1:A:627:THR:O	2.11	0.69
1:B:646:ASN:O	4:B:1001:HOH:O	2.08	0.69
1:A:431:THR:HG21	1:A:436:GLU:OE1	1.92	0.68
1:A:387:MET:CE	1:A:393:ASP:HB2	2.22	0.67
1:A:284:LYS:O	1:A:287:LYS:HG2	1.95	0.67
1:B:372:VAL:HG22	1:B:376:LEU:HA	1.77	0.67
1:A:247:ARG:HD3	4:A:1059:HOH:O	1.95	0.67
1:A:816:GLN:HG2	1:A:827:THR:HG21	1.77	0.66
1:B:684:GLN:N	4:B:1002:HOH:O	2.13	0.66
1:A:401:GLY:HA2	1:A:431:THR:O	1.96	0.65
1:B:716:ASP:OD2	1:B:720:ARG:HD3	1.96	0.65
1:A:179:ILE:HG13	1:A:187:ILE:HG23	1.77	0.65
1:A:595:LEU:O	4:A:1001:HOH:O	2.14	0.64
1:A:372:VAL:HG22	1:A:376:LEU:HA	1.80	0.64
1:B:816:GLN:HG2	1:B:827:THR:HG21	1.81	0.64
1:A:638:ASP:OD1	1:A:641:ARG:NH2	2.30	0.63
1:A:445:ASN:O	1:A:449:GLU:HG2	1.98	0.63
1:A:318:ARG:NH2	3:A:902:ATP:O3G	2.32	0.62
1:A:438:TYR:OH	1:A:807:LYS:NZ	2.33	0.62
1:B:181:ASP:HB2	1:B:186:LEU:N	2.11	0.62
1:A:563:LEU:HB3	1:A:564:PRO:HD3	1.80	0.62
1:B:389:VAL:O	1:B:390:ASN:HB2	2.00	0.62
1:B:197:VAL:HG21	1:B:205:ASP:OD2	2.01	0.61
1:A:151:ASN:HD21	1:A:191:ARG:HA	1.66	0.60
1:A:64:TRP:HB3	1:A:129:PHE:CE2	2.37	0.60
1:B:80:ASP:O	1:B:84:ARG:HB2	2.02	0.60
1:A:153:LYS:CB	1:A:162:TYR:CE1	2.54	0.60
1:A:387:MET:HE1	1:A:393:ASP:HB2	1.82	0.60
1:B:54:VAL:HG21	1:B:90:LYS:HG3	1.83	0.59
1:B:401:GLY:HA2	1:B:431:THR:O	2.01	0.59
1:A:50:LYS:HE2	1:A:95:HIS:CE1	2.38	0.59
1:B:329:GLU:HG2	1:B:762:ARG:NH2	2.17	0.59
1:A:355:MET:CE	1:A:383:PHE:HZ	2.16	0.58
1:B:734:ILE:HD11	1:B:778:LEU:HD13	1.85	0.58
1:B:286:LEU:CB	1:B:292:VAL:HG21	2.29	0.58
1:A:655:VAL:HG13	1:A:660:ALA:HB3	1.86	0.57
1:B:683:THR:C	1:B:685:ASN:H	2.07	0.57
1:A:389:VAL:O	1:A:390:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASP:HB3	1:B:275:ARG:HH21	1.69	0.56
1:B:387:MET:HE1	1:B:413:ARG:HH21	1.68	0.56
1:B:683:THR:HA	4:B:1002:HOH:O	2.06	0.56
1:A:387:MET:HE3	1:A:393:ASP:HB2	1.88	0.56
1:A:292:VAL:HG22	1:A:355:MET:HE2	1.88	0.55
1:A:787:LYS:HD3	1:A:787:LYS:C	2.26	0.55
1:B:372:VAL:HG21	1:B:376:LEU:HD13	1.87	0.55
1:A:284:LYS:HA	1:A:287:LYS:HD3	1.88	0.55
1:B:59:LEU:HD11	1:B:92:GLU:CB	2.35	0.55
1:A:197:VAL:HG21	1:A:205:ASP:OD2	2.07	0.55
1:A:734:ILE:HD11	1:A:778:LEU:HD13	1.89	0.55
1:A:312:ILE:HB	1:A:371:MET:HE3	1.89	0.54
1:B:229:LYS:N	4:B:1021:HOH:O	2.40	0.54
1:B:-28:MET:HB2	1:B:302:TRP:CD1	2.42	0.54
1:A:787:LYS:HE2	4:A:1185:HOH:O	2.06	0.54
1:A:661:VAL:CG1	1:A:663:ILE:HD12	2.38	0.54
1:B:124:THR:HG22	1:B:128:VAL:HG21	1.90	0.54
1:A:787:LYS:HD3	1:A:787:LYS:O	2.08	0.54
1:B:436:GLU:O	1:B:440:GLN:HB2	2.07	0.53
1:A:603:ASN:N	4:A:1012:HOH:O	2.41	0.53
1:A:292:VAL:HG22	1:A:355:MET:CE	2.39	0.53
1:B:445:ASN:HD21	1:B:483:LEU:HB3	1.74	0.53
1:B:683:THR:O	1:B:685:ASN:N	2.36	0.52
1:B:655:VAL:HG13	1:B:660:ALA:HB3	1.92	0.52
1:A:162:TYR:CE2	1:A:208:LEU:HD13	2.44	0.52
1:B:784:LYS:HG3	1:B:785:ASN:N	2.24	0.52
1:A:131:GLU:HB3	1:A:135:MET:HE2	1.92	0.51
1:A:481:ILE:HG22	1:A:482:ASN:N	2.26	0.51
1:A:610:ARG:HD2	1:A:667:ASP:OD1	2.10	0.51
1:B:787:LYS:HD2	1:B:787:LYS:N	2.26	0.51
1:B:280:TYR:CD1	1:B:295:LEU:HD11	2.46	0.51
1:A:30:TYR:HA	1:A:76:LYS:NZ	2.25	0.51
1:A:123:PRO:HB3	1:A:128:VAL:HG23	1.91	0.51
1:A:625:LEU:HD21	1:A:682:VAL:HG12	1.92	0.51
1:B:604:GLN:HG2	1:B:642:MET:CE	2.38	0.51
1:A:840:ILE:C	1:B:491:ASN:HD21	2.04	0.50
1:B:117:LYS:NZ	1:B:151:ASN:HD22	2.09	0.50
1:A:371:MET:HE2	1:A:381:ILE:HD13	1.93	0.50
1:B:324:GLU:OE2	4:B:1003:HOH:O	2.20	0.50
1:A:355:MET:HE1	1:A:383:PHE:HZ	1.77	0.50
1:B:488:SER:HG	1:B:490:PHE:HE1	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:TYR:CD2	1:A:827:THR:HG23	2.46	0.49
1:B:502:GLY:HA2	1:B:810:TYR:CD1	2.47	0.49
1:B:559:LEU:HD21	1:B:578:ILE:HG23	1.93	0.49
1:B:-28:MET:HB2	1:B:302:TRP:NE1	2.26	0.49
1:B:826:TYR:CD2	1:B:827:THR:HG23	2.47	0.49
1:A:153:LYS:HB3	1:A:162:TYR:HE1	1.66	0.49
1:B:82:VAL:O	1:B:86:CYS:HB2	2.13	0.49
1:B:653:LEU:HD21	1:B:669:LEU:HD21	1.94	0.48
1:A:164:TYR:CD1	1:A:198:PRO:HG2	2.48	0.48
1:A:131:GLU:HB3	1:A:135:MET:CE	2.44	0.48
1:A:244:LEU:HD11	1:A:253:LYS:HE3	1.95	0.48
1:A:29:ILE:HD12	1:A:29:ILE:N	2.29	0.48
1:B:491:ASN:HB2	4:B:1028:HOH:O	2.13	0.47
1:B:829:SER:O	1:B:833:ILE:HG13	2.14	0.47
1:B:686:GLN:O	1:B:690:GLU:HG3	2.14	0.47
1:B:733:ALA:HB2	1:B:755:ILE:HG21	1.97	0.47
1:A:661:VAL:HG12	1:A:663:ILE:HD12	1.96	0.47
1:B:280:TYR:CE1	1:B:295:LEU:HD11	2.49	0.47
1:A:151:ASN:ND2	1:A:192:ASN:H	2.13	0.47
1:B:344:ILE:HD11	1:B:376:LEU:HD12	1.97	0.47
1:A:686:GLN:O	1:A:690:GLU:HG3	2.15	0.47
1:B:686:GLN:NE2	4:B:1038:HOH:O	2.48	0.47
1:A:39:TYR:CZ	1:A:54:VAL:HG12	2.49	0.47
1:B:683:THR:CA	4:B:1002:HOH:O	2.63	0.47
1:B:192:ASN:HB3	1:B:193:PRO:HD2	1.97	0.46
1:B:123:PRO:HB3	1:B:128:VAL:HG23	1.96	0.46
1:B:372:VAL:CG2	1:B:376:LEU:HD13	2.45	0.46
1:B:747:LEU:HB3	1:B:748:TYR:CD2	2.50	0.46
1:A:181:ASP:HB3	1:A:183:GLU:H	1.81	0.46
1:A:603:ASN:OD1	1:A:603:ASN:O	2.34	0.46
1:A:696:ILE:HD12	1:A:739:LEU:HD22	1.98	0.46
1:B:329:GLU:HG2	1:B:762:ARG:HH21	1.79	0.46
1:B:387:MET:HE2	1:B:413:ARG:NH2	2.24	0.46
1:A:100:ASP:O	1:A:104:LYS:HG2	2.15	0.46
1:A:153:LYS:HG2	1:A:195:TYR:CD2	2.51	0.45
1:A:603:ASN:O	1:A:604:GLN:OE1	2.33	0.45
1:A:129:PHE:O	1:A:133:LEU:HD22	2.17	0.45
1:B:224:ARG:NH2	1:B:297:GLU:HB2	2.32	0.45
1:B:445:ASN:HD22	1:B:445:ASN:HA	1.61	0.45
1:A:371:MET:CE	1:A:381:ILE:HD13	2.46	0.45
1:A:30:TYR:HD1	1:A:76:LYS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:VAL:O	1:B:390:ASN:CB	2.63	0.45
1:A:355:MET:HE2	1:A:383:PHE:HZ	1.81	0.45
1:B:264:GLY:O	1:B:275:ARG:NH2	2.42	0.44
1:B:717:ASN:OD1	1:B:718:LYS:N	2.50	0.44
1:A:404:SER:HB2	1:A:416:PHE:CZ	2.53	0.44
1:B:445:ASN:O	1:B:449:GLU:HG2	2.18	0.44
1:A:464:GLU:O	1:A:468:LYS:HG2	2.18	0.43
1:B:200:PHE:CD1	1:B:201:VAL:HG13	2.53	0.43
1:A:355:MET:HE2	1:A:383:PHE:CZ	2.53	0.43
1:A:855:GLU:HG2	4:A:1152:HOH:O	2.17	0.43
1:B:663:ILE:HD12	1:B:714:THR:HB	2.00	0.43
1:A:741:HIS:CE1	1:A:861:LYS:HD2	2.54	0.43
1:B:64:TRP:HB3	1:B:129:PHE:CE1	2.54	0.43
1:B:164:TYR:CD1	1:B:198:PRO:HG2	2.53	0.43
1:B:318:ARG:HE	1:B:318:ARG:HB2	1.58	0.43
1:B:344:ILE:HD11	1:B:376:LEU:CD1	2.48	0.43
1:A:829:SER:O	1:A:833:ILE:HG13	2.18	0.43
1:B:519:ARG:HB2	1:B:532:THR:HG21	2.00	0.43
1:A:234:LEU:HD21	1:A:244:LEU:HB2	2.01	0.43
1:A:512:ARG:HG2	1:A:527:LYS:HG2	2.01	0.43
1:B:-21:GLN:HG3	1:B:150:LEU:HD22	2.01	0.43
1:B:610:ARG:HD2	1:B:667:ASP:OD1	2.18	0.43
1:B:553:LYS:HA	1:B:556:GLN:HG2	2.00	0.43
1:B:585:LYS:HB3	1:B:585:LYS:HE3	1.91	0.43
1:A:420:ARG:HE	1:A:431:THR:HG22	1.83	0.43
1:A:432:SER:HB3	1:A:819:TYR:HA	2.01	0.43
1:B:318:ARG:HG3	1:B:367:PRO:HB2	2.01	0.43
1:B:563:LEU:HB2	1:B:564:PRO:HD3	2.01	0.42
1:A:389:VAL:O	1:A:390:ASN:CB	2.66	0.42
1:A:747:LEU:HB3	1:A:748:TYR:CD2	2.54	0.42
1:B:9:ARG:NH1	4:B:1023:HOH:O	2.41	0.42
1:B:683:THR:C	1:B:685:ASN:N	2.72	0.42
1:A:371:MET:CE	1:A:381:ILE:HG21	2.49	0.42
1:A:685:ASN:OD1	1:A:687:LYS:HB2	2.19	0.42
1:A:200:PHE:CD2	1:A:201:VAL:HG13	2.54	0.42
1:B:316:ASP:OD1	1:B:318:ARG:HB2	2.20	0.42
1:B:777:LEU:HD11	1:B:800:LEU:HD13	2.00	0.42
1:A:153:LYS:HG2	1:A:195:TYR:CG	2.54	0.42
1:B:231:GLU:HA	1:B:231:GLU:OE2	2.20	0.42
1:A:318:ARG:HE	1:A:318:ARG:HB2	1.58	0.42
1:B:197:VAL:HG21	1:B:205:ASP:CG	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:HA	1:A:92:GLU:HG2	2.01	0.42
1:A:602:ILE:N	4:A:1012:HOH:O	2.53	0.42
1:B:155:TRP:CZ2	1:B:156:LYS:HE2	2.55	0.42
1:A:181:ASP:H	1:A:185:ASN:HA	1.85	0.42
1:A:387:MET:HE3	1:A:393:ASP:CB	2.49	0.42
1:B:833:ILE:O	1:B:837:MET:HG3	2.20	0.42
1:A:273:LEU:HD22	1:A:277:LYS:HG2	2.02	0.41
1:A:63:GLY:HA2	1:A:164:TYR:CE2	2.55	0.41
1:A:355:MET:CE	1:A:383:PHE:CZ	3.00	0.41
1:A:162:TYR:HE2	1:A:208:LEU:HD13	1.86	0.41
1:A:502:GLY:HA2	1:A:810:TYR:CD1	2.55	0.41
1:A:316:ASP:OD1	1:A:318:ARG:HB2	2.19	0.41
1:B:737:TRP:CD2	1:B:844:PRO:HG2	2.55	0.41
1:A:284:LYS:HA	1:A:287:LYS:HG2	2.03	0.41
1:A:124:THR:HG22	1:A:128:VAL:HG21	2.03	0.41
1:A:519:ARG:HB2	1:A:532:THR:HG21	2.03	0.41
1:A:7:TYR:OH	1:A:816:GLN:HG3	2.21	0.41
1:A:145:LYS:HD3	1:A:154:ARG:NH2	2.36	0.41
1:A:255:ILE:HG13	3:A:902:ATP:C6	2.56	0.41
1:B:612:GLY:O	1:B:616:ILE:HG13	2.21	0.40
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.97	0.40
1:A:30:TYR:HA	1:A:76:LYS:HZ3	1.87	0.40
1:B:725:LEU:HD11	1:B:847:TRP:CZ2	2.57	0.40
1:B:556:GLN:HG3	1:B:557:SER:N	2.37	0.40
1:A:163:ARG:HG2	1:A:164:TYR:N	2.36	0.40
1:B:491:ASN:HB3	1:B:494:SER:HB3	2.02	0.40
1:B:787:LYS:HD2	1:B:787:LYS:H	1.85	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	851/904 (94%)	801 (94%)	45 (5%)	5 (1%)	25 18
1	B	850/904 (94%)	811 (95%)	31 (4%)	8 (1%)	17 11
All	All	1701/1808 (94%)	1612 (95%)	76 (4%)	13 (1%)	19 12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	649	LYS
1	A	45	ASN
1	A	250	ASP
1	A	332	ASN
1	A	333	GLY
1	A	481	ILE
1	B	250	ASP
1	B	684	GLN
1	B	86	CYS
1	B	332	ASN
1	B	187	ILE
1	B	331	ASN
1	B	34	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	766/799 (96%)	756 (99%)	10 (1%)	69 74
1	B	764/799 (96%)	756 (99%)	8 (1%)	76 81
All	All	1530/1598 (96%)	1512 (99%)	18 (1%)	71 76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	162	TYR
1	A	199	ASP

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Mol	Chain	Res	Type
1	A	234	LEU
1	A	273	LEU
1	A	362	MET
1	A	365	LEU
1	A	431	THR
1	A	565	LEU
1	A	766	SER
1	B	38	THR
1	B	90	LYS
1	B	365	LEU
1	B	372	VAL
1	B	376	LEU
1	B	747	LEU
1	B	766	SER
1	B	787	LYS

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

Mol	Chain	Res	Type
1	A	151	ASN
1	A	357	ASN
1	B	8	HIS
1	B	151	ASN
1	B	357	ASN
1	B	369	ASN
1	B	445	ASN
1	B	601	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

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	B	901	2	26,33,33	0.65	0	31,52,52	0.81	1 (3%)
3	ATP	A	902	2	26,33,33	0.66	0	31,52,52	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	901	2	-	4/18/38/38	0/3/3/3
3	ATP	A	902	2	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	ATP	C5-C6-N6	2.40	123.99	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

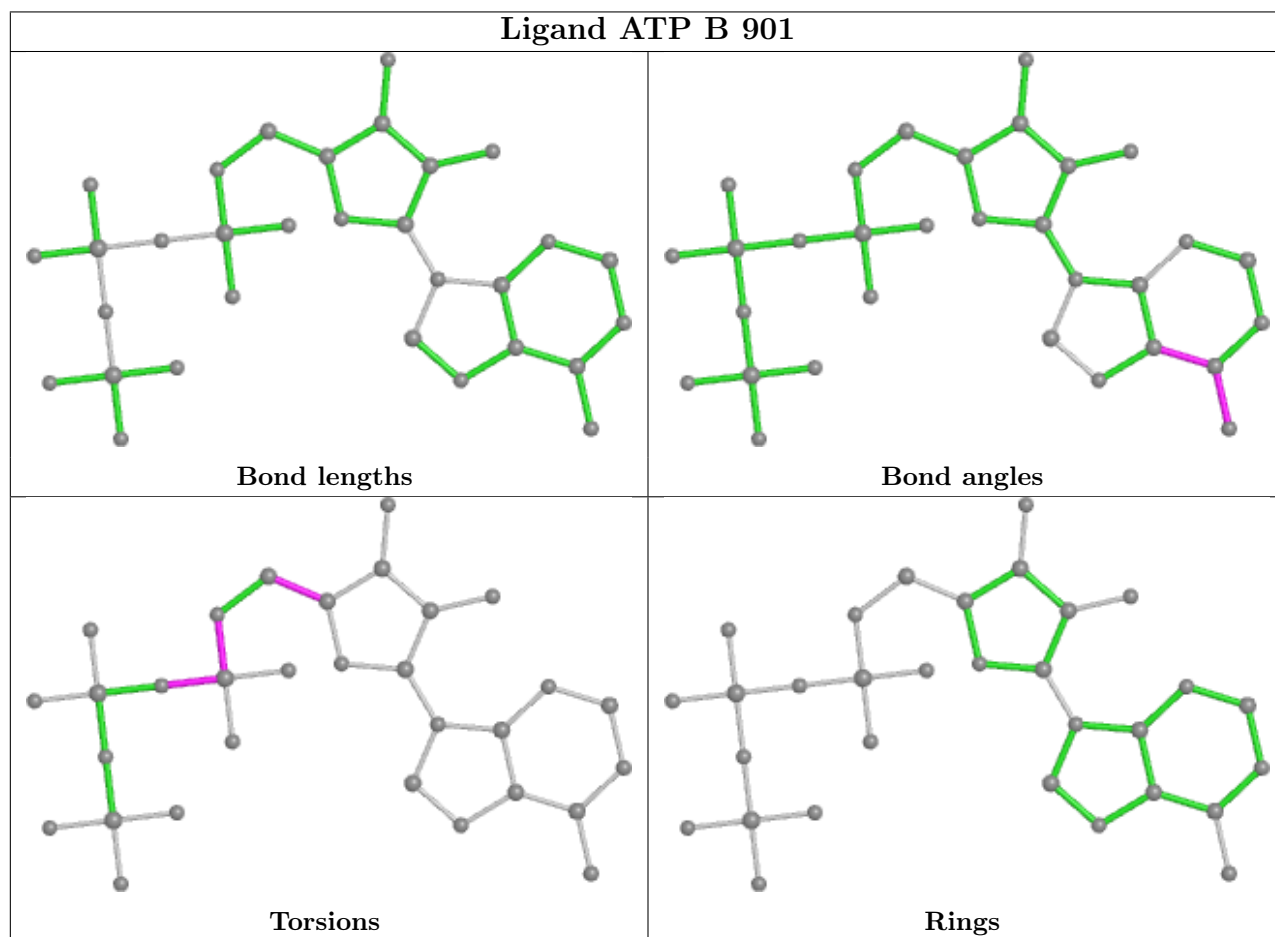
Mol	Chain	Res	Type	Atoms
3	B	901	ATP	PB-O3A-PA-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	C3'-C4'-C5'-O5'
3	A	902	ATP	PB-O3A-PA-O2A
3	B	901	ATP	C5'-O5'-PA-O1A

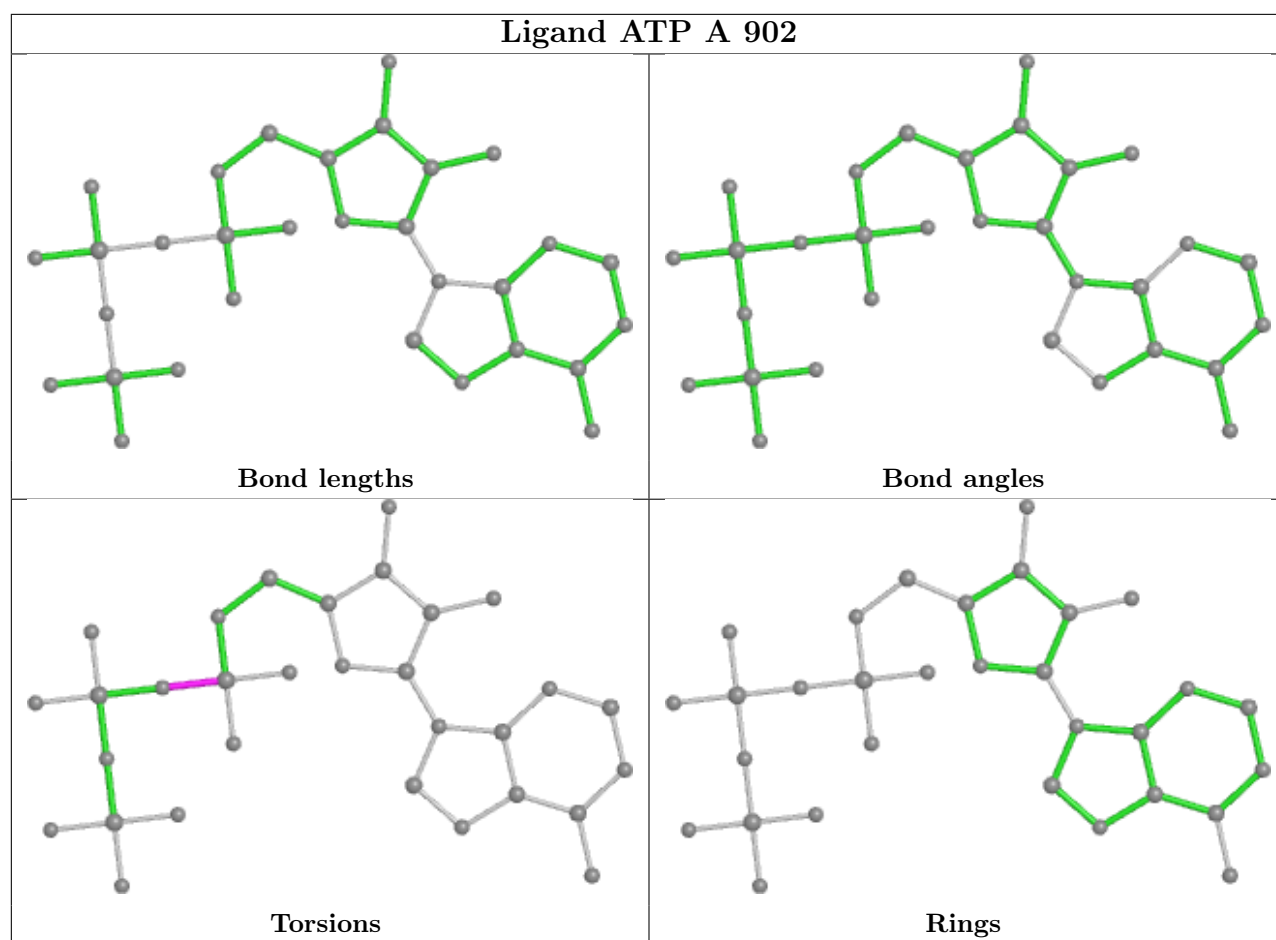
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	ATP	2	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	859/904 (95%)	0.53	62 (7%) 15 21	27, 55, 95, 154	0
1	B	858/904 (94%)	0.63	75 (8%) 10 14	28, 57, 114, 175	0
All	All	1717/1808 (94%)	0.58	137 (7%) 12 17	27, 56, 105, 175	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	LEU	15.7
1	B	187	ILE	12.4
1	B	174	HIS	10.5
1	B	171	PHE	7.4
1	B	653	LEU	7.3
1	B	35	ILE	6.7
1	B	170	ILE	6.7
1	B	655	VAL	6.6
1	B	164	TYR	6.6
1	B	175	GLY	6.4
1	B	82	VAL	6.3
1	B	32	LEU	5.9
1	B	165	GLY	5.8
1	B	182	LYS	5.7
1	B	83	ALA	5.4
1	A	171	PHE	5.3
1	B	188	LYS	5.2
1	B	179	ILE	5.1
1	B	197	VAL	5.0
1	B	185	ASN	5.0
1	B	96	LEU	4.9
1	B	249	LYS	4.9
1	A	140	ILE	4.8
1	B	173	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	181	ASP	4.8
1	B	36	PRO	4.5
1	A	249	LYS	4.4
1	A	208	LEU	4.2
1	B	184	GLY	4.1
1	A	129	PHE	4.1
1	B	140	ILE	4.1
1	B	652	GLN	4.1
1	B	168	LYS	4.1
1	B	113	ALA	4.1
1	B	93	PHE	4.1
1	B	85	LEU	4.0
1	B	177	HIS	4.0
1	A	175	GLY	3.9
1	A	162	TYR	3.9
1	B	180	ARG	3.9
1	A	302	TRP	3.9
1	B	193	PRO	3.8
1	A	155	TRP	3.8
1	B	651	LYS	3.8
1	A	187	ILE	3.8
1	B	172	ASN	3.8
1	A	136	ILE	3.7
1	B	143	PHE	3.7
1	B	30	TYR	3.7
1	A	298	TYR	3.6
1	A	91	ILE	3.6
1	A	207	TYR	3.5
1	B	59	LEU	3.5
1	A	170	ILE	3.5
1	A	121	ILE	3.5
1	A	195	TYR	3.4
1	A	143	PHE	3.4
1	B	60	PRO	3.3
1	B	40	ALA	3.3
1	A	602	ILE	3.3
1	A	138	LEU	3.3
1	B	42	PHE	3.2
1	B	53	HIS	3.2
1	A	64	TRP	3.2
1	B	33	ASN	3.2
1	A	-17	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	84	ARG	3.1
1	B	64	TRP	3.1
1	A	165	GLY	3.1
1	A	198	PRO	3.1
1	A	135	MET	3.1
1	B	55	LYS	3.0
1	A	167	PHE	3.0
1	B	61	GLU	3.0
1	B	191	ARG	3.0
1	B	130	VAL	3.0
1	B	200	PHE	3.0
1	B	78	VAL	2.9
1	B	213	ASN	2.9
1	B	31	GLU	2.9
1	A	144	LYS	2.9
1	B	176	GLU	2.9
1	A	204	PHE	2.8
1	B	102	PHE	2.8
1	A	123	PRO	2.8
1	B	169	GLY	2.7
1	A	176	GLU	2.7
1	A	141	GLN	2.7
1	A	186	LEU	2.7
1	B	54	VAL	2.7
1	B	198	PRO	2.7
1	A	69	THR	2.7
1	A	85	LEU	2.7
1	A	280	TYR	2.6
1	B	183	GLU	2.6
1	A	177	HIS	2.6
1	B	120	THR	2.6
1	A	277	LYS	2.6
1	A	72	LEU	2.6
1	A	160	VAL	2.5
1	A	66	ILE	2.5
1	A	82	VAL	2.5
1	A	389	VAL	2.5
1	B	87	ILE	2.5
1	B	51	HIS	2.5
1	A	179	ILE	2.5
1	A	263	ALA	2.5
1	B	190	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	359	GLY	2.4
1	A	122	TYR	2.4
1	B	141	GLN	2.4
1	B	123	PRO	2.4
1	A	132	LEU	2.3
1	B	41	VAL	2.3
1	B	166	GLY	2.3
1	A	87	ILE	2.3
1	A	119	ILE	2.3
1	B	124	THR	2.2
1	A	128	VAL	2.2
1	A	68	VAL	2.2
1	A	86	CYS	2.2
1	B	360	VAL	2.2
1	B	142	ASP	2.1
1	A	200	PHE	2.1
1	A	30	TYR	2.1
1	A	124	THR	2.1
1	A	48	VAL	2.1
1	B	121	ILE	2.1
1	A	79	LEU	2.1
1	A	265	LEU	2.1
1	A	130	VAL	2.1
1	A	157	ASN	2.1
1	A	102	PHE	2.1
1	B	65	LYS	2.1
1	A	286	LEU	2.0
1	B	91	ILE	2.0
1	B	592	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](#)

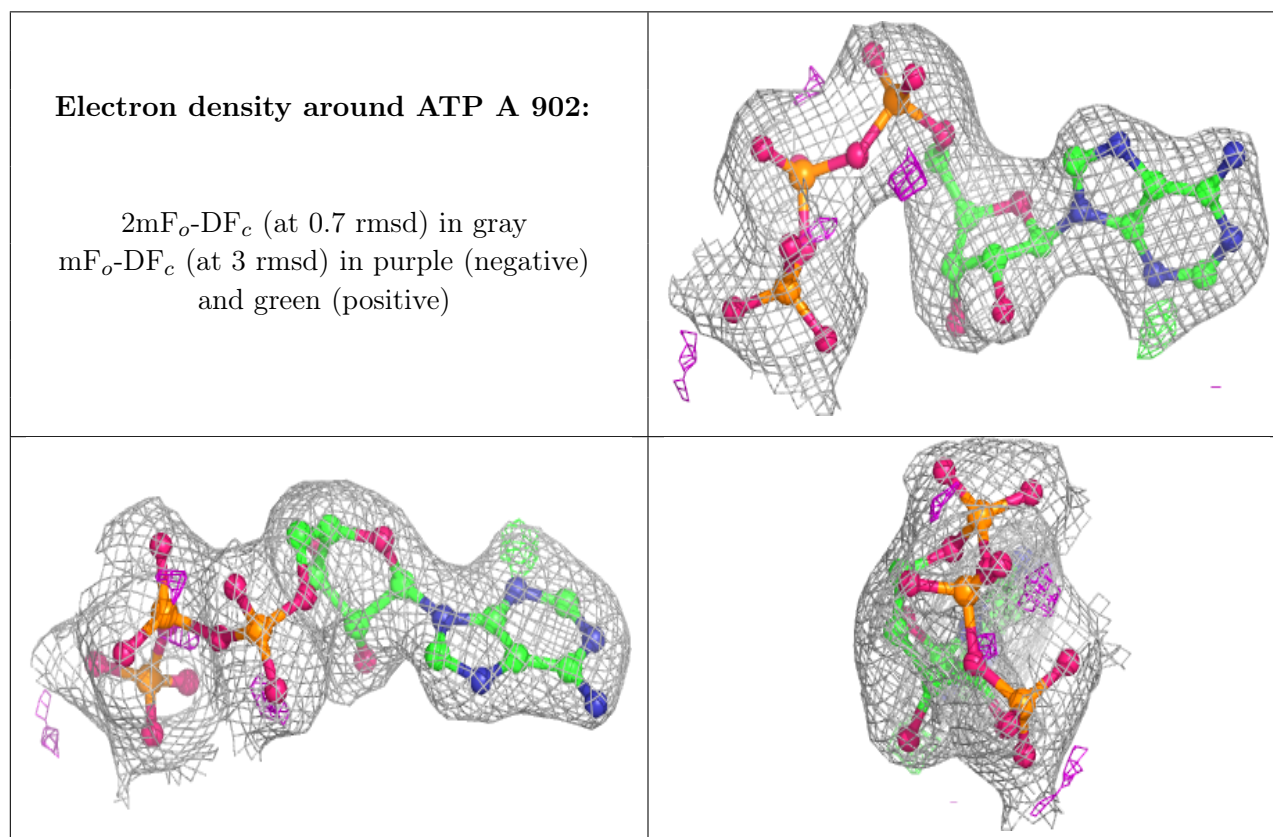
There are no monosaccharides in this entry.

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.

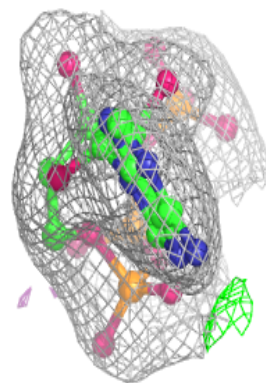
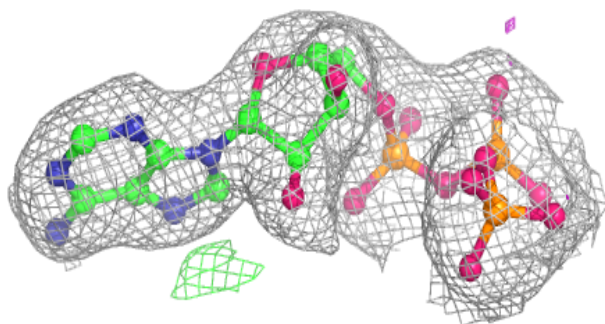
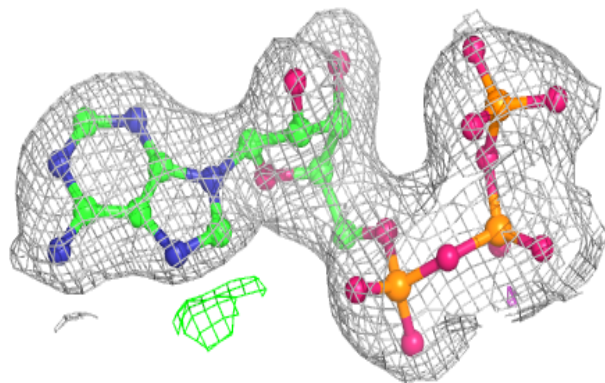
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ATP	A	902	31/31	0.95	0.09	57,67,84,89	0
3	ATP	B	901	31/31	0.96	0.10	57,69,85,90	0
2	CA	A	901	1/1	0.97	0.06	73,73,73,73	0
2	CA	B	902	1/1	0.98	0.06	67,67,67,67	0

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.



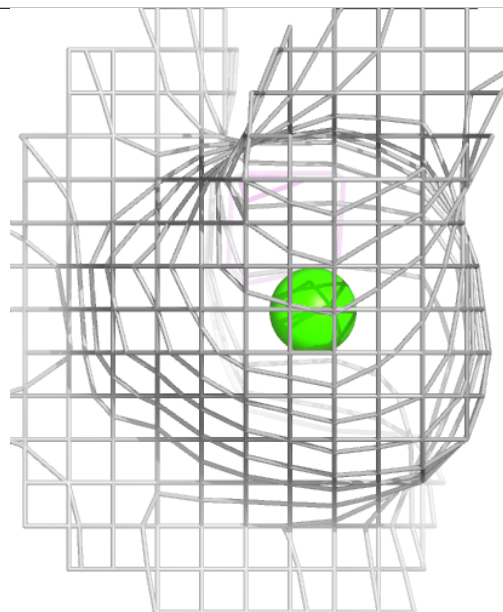
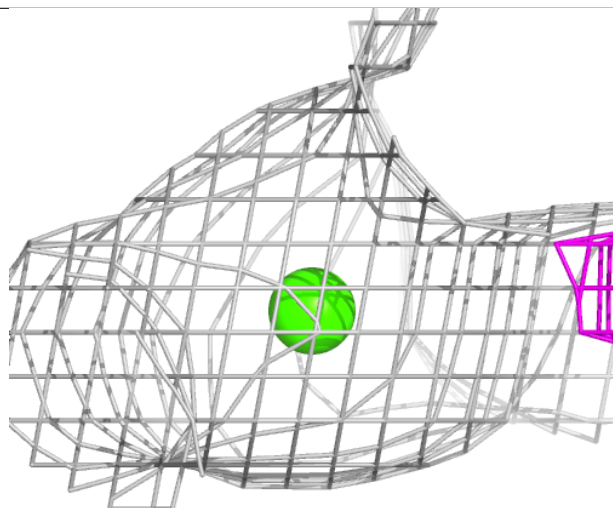
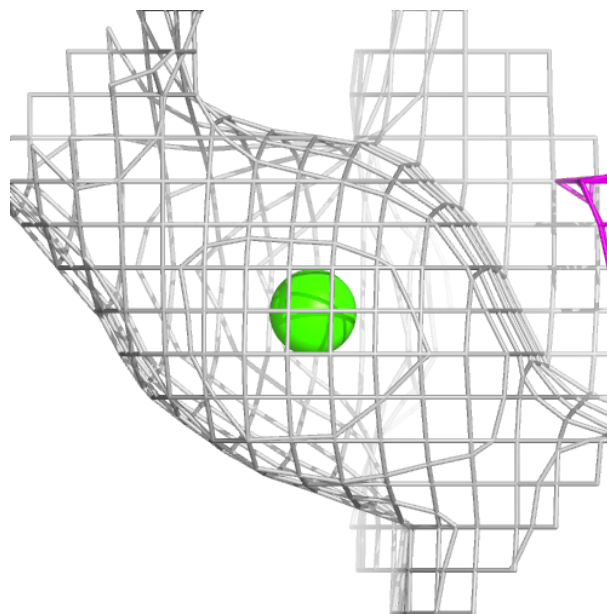
Electron density around ATP B 901:

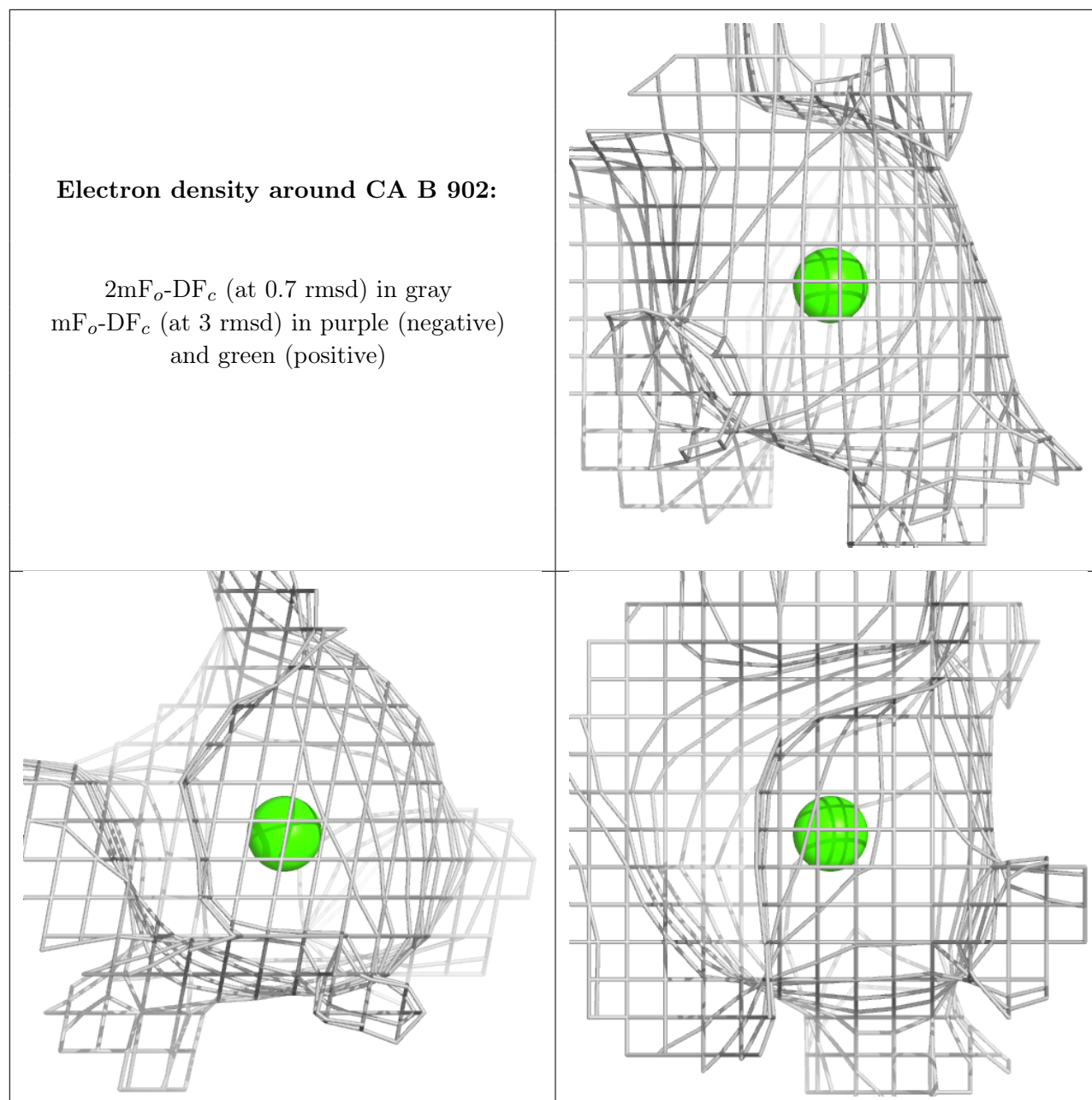
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA A 901:

$2mF_o-DF_c$ (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.