



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 01:09 pm BST

PDB ID : 28ZT / pdb_000028zt
Title : Crystal structure of human DHX9 in complex with ATX-968 and ADP
Authors : Knopp, A.; Le Bihan, Y.-V.; van Montfort, R.L.M.
Deposited on : 2026-03-03
Resolution : 3.40 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

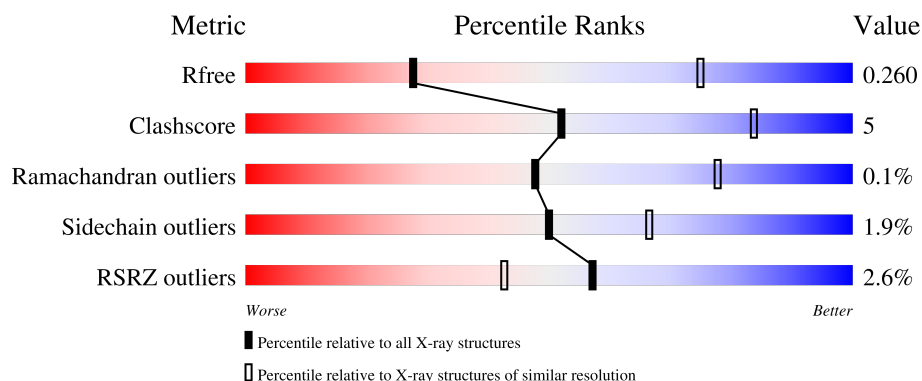
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1010	2% 73% 12% 14%
1	B	1010	2% 73% 11% 15%
1	C	1010	0% 74% 11% 15%
1	D	1010	3% 71% 6% 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24736 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 ATP-dependent RNA helicase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	864	Total	C	N	O	S	0	1	0
			6484	4154	1088	1203	39			
1	B	858	Total	C	N	O	S	0	0	1
			6253	4014	1047	1154	38			
1	C	860	Total	C	N	O	S	0	0	1
			6405	4116	1069	1181	39			
1	D	783	Total	C	N	O	S	0	0	0
			5362	3411	896	1031	24			

There are 36 discrepancies between the modelled and reference sequences:

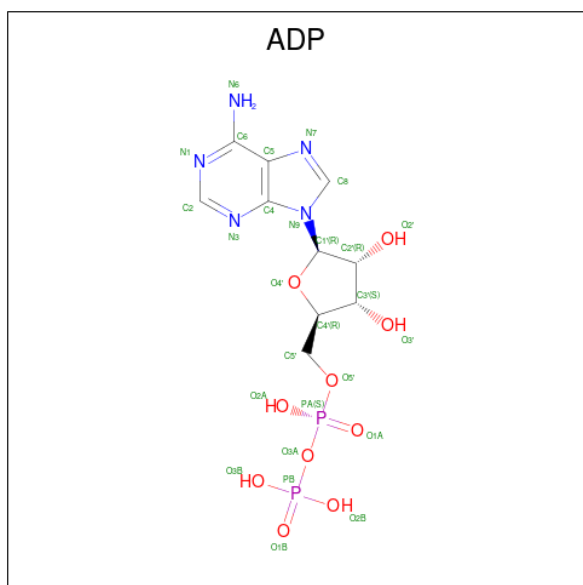
Chain	Residue	Modelled	Actual	Comment	Reference
A	149	MET	-	initiating methionine	UNP Q08211
A	1151	ASP	-	expression tag	UNP Q08211
A	1152	TYR	-	expression tag	UNP Q08211
A	1153	LYS	-	expression tag	UNP Q08211
A	1154	ASP	-	expression tag	UNP Q08211
A	1155	ASP	-	expression tag	UNP Q08211
A	1156	ASP	-	expression tag	UNP Q08211
A	1157	ASP	-	expression tag	UNP Q08211
A	1158	LYS	-	expression tag	UNP Q08211
B	149	MET	-	initiating methionine	UNP Q08211
B	1151	ASP	-	expression tag	UNP Q08211
B	1152	TYR	-	expression tag	UNP Q08211
B	1153	LYS	-	expression tag	UNP Q08211
B	1154	ASP	-	expression tag	UNP Q08211
B	1155	ASP	-	expression tag	UNP Q08211
B	1156	ASP	-	expression tag	UNP Q08211
B	1157	ASP	-	expression tag	UNP Q08211
B	1158	LYS	-	expression tag	UNP Q08211
C	149	MET	-	initiating methionine	UNP Q08211
C	1151	ASP	-	expression tag	UNP Q08211
C	1152	TYR	-	expression tag	UNP Q08211

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1153	LYS	-	expression tag	UNP Q08211
C	1154	ASP	-	expression tag	UNP Q08211
C	1155	ASP	-	expression tag	UNP Q08211
C	1156	ASP	-	expression tag	UNP Q08211
C	1157	ASP	-	expression tag	UNP Q08211
C	1158	LYS	-	expression tag	UNP Q08211
D	149	MET	-	initiating methionine	UNP Q08211
D	1151	ASP	-	expression tag	UNP Q08211
D	1152	TYR	-	expression tag	UNP Q08211
D	1153	LYS	-	expression tag	UNP Q08211
D	1154	ASP	-	expression tag	UNP Q08211
D	1155	ASP	-	expression tag	UNP Q08211
D	1156	ASP	-	expression tag	UNP Q08211
D	1157	ASP	-	expression tag	UNP Q08211
D	1158	LYS	-	expression tag	UNP Q08211

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

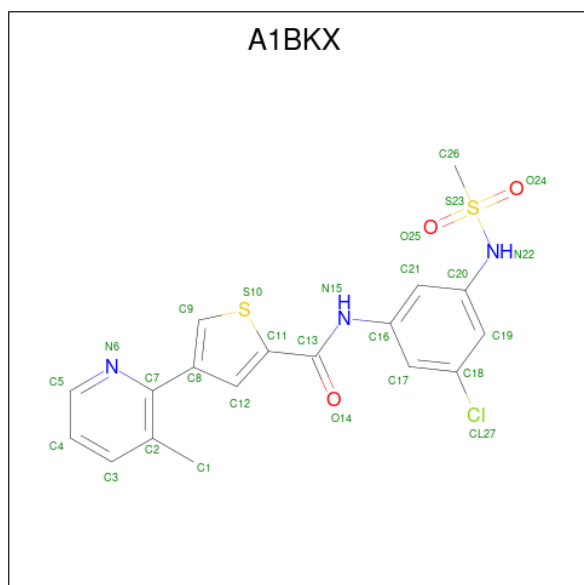


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is (4M)-N-[3-chloro-5-(methanesulfonamido)phenyl]-4-(3-methylpyridin-2-yl)thiophene-2-carboxamide (CCD ID: A1BKX) (formula: C₁₈H₁₆ClN₃O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	
			27	18	1	3	3	2	0
4	B	1	Total	C	Cl	N	O	S	
			27	18	1	3	3	2	0
4	C	1	Total	C	Cl	N	O	S	
			26	17	1	3	3	2	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		

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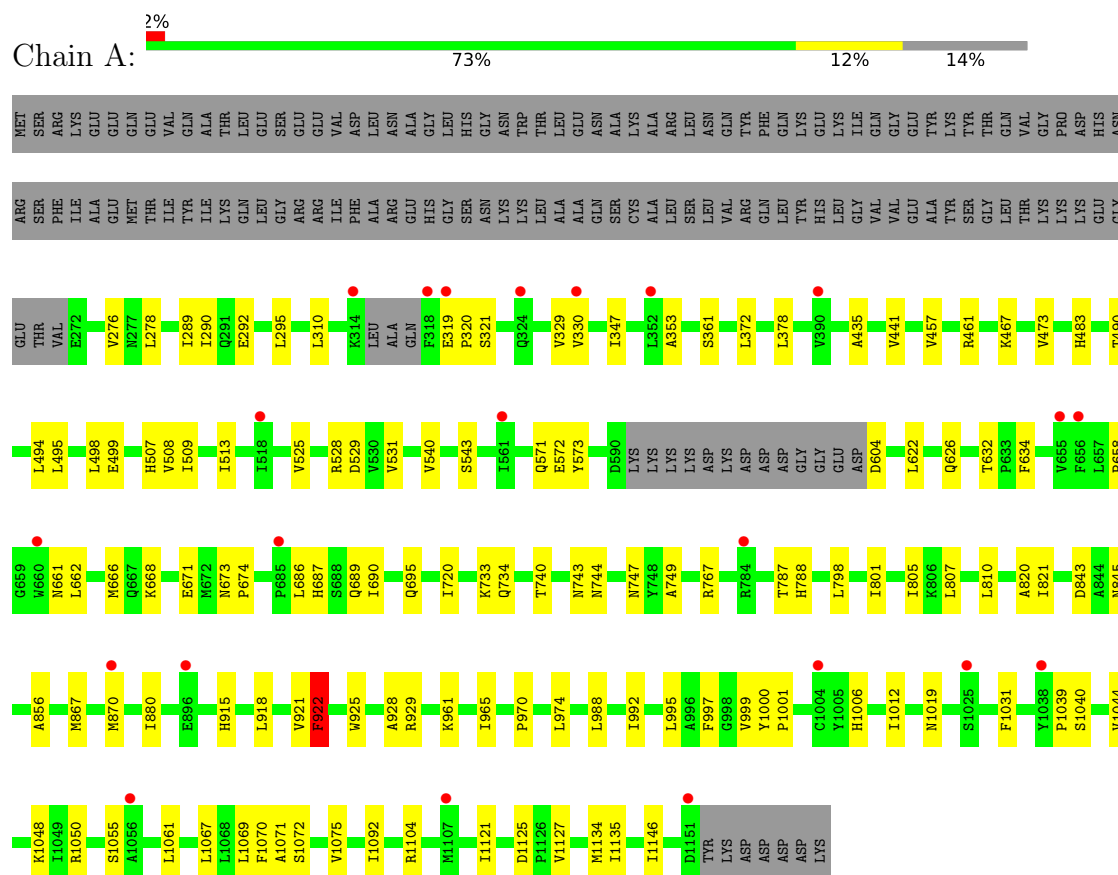
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	10	Total 10	O 10	0	0
5	C	8	Total 8	O 8	0	0
5	D	4	Total 4	O 4	0	0

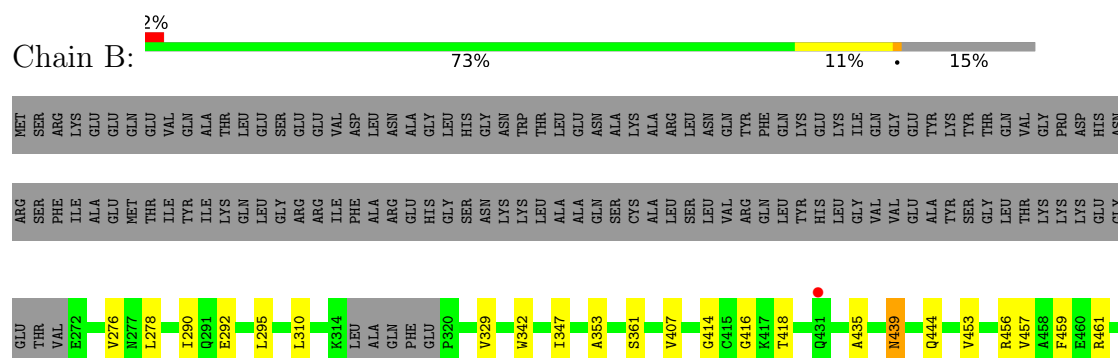
3 Residue-property plots

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.

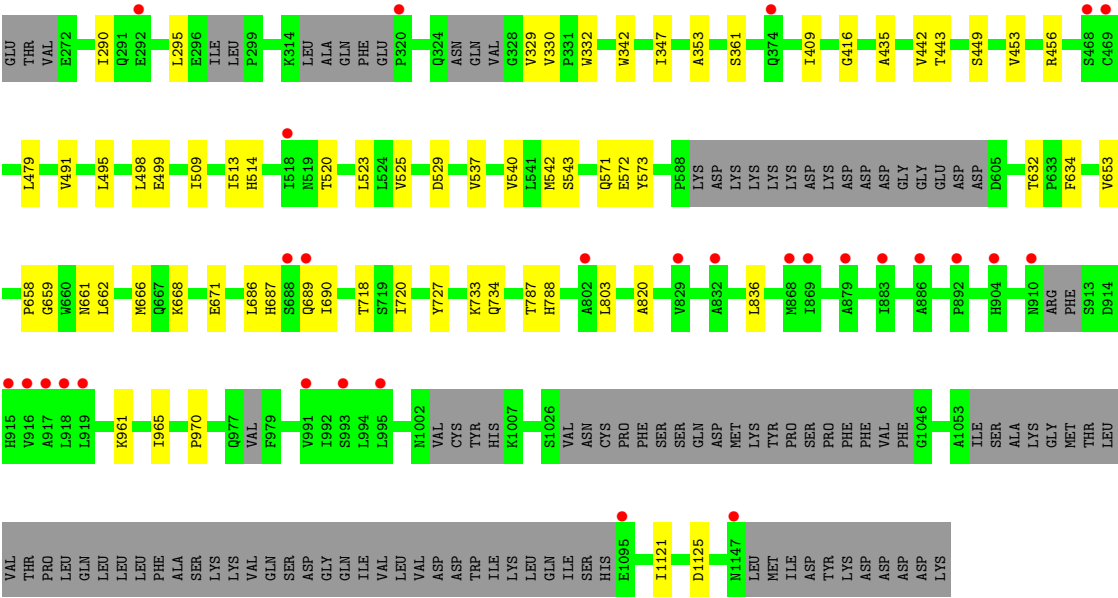
• Molecule 1: ATP-dependent RNA helicase A



• Molecule 1: ATP-dependent RNA helicase A







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.61Å 166.97Å 293.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.40 49.73 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.73-3.40) 99.9 (49.73-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.235 , 0.258 0.240 , 0.260	Depositor DCC
R_{free} test set	4130 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	130.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 108.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24736	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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, A1BKX, ADP

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	0.66	1/6627 (0.0%)	1.06	6/9041 (0.1%)
1	B	0.66	0/6388	1.07	8/8735 (0.1%)
1	C	0.64	0/6549	1.06	8/8943 (0.1%)
1	D	0.62	0/5461	1.04	2/7493 (0.0%)
All	All	0.65	1/25025 (0.0%)	1.06	24/34212 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	LYS	CA-C	5.47	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	747	ASN	CA-CB-CG	7.63	120.23	112.60
1	C	521	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	922	PHE	CA-CB-CG	-6.10	107.70	113.80
1	C	906	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	632	THR	CB-CA-C	5.69	116.31	109.31
1	C	370	TYR	N-CA-C	-5.62	105.21	112.68
1	D	632	THR	CB-CA-C	5.60	116.20	109.31
1	C	972	ASP	CA-CB-CG	5.56	118.16	112.60
1	D	659	GLY	N-CA-C	5.55	117.22	111.95
1	B	632	THR	CB-CA-C	5.43	115.99	109.31
1	B	513	ILE	CA-C-N	5.42	128.54	120.31
1	B	513	ILE	C-N-CA	5.42	128.54	120.31
1	A	843	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	906	ASN	CA-CB-CG	5.33	117.93	112.60
1	C	632	THR	CB-CA-C	5.32	115.85	109.31
1	A	928	ALA	CA-C-N	5.26	127.32	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	928	ALA	C-N-CA	5.26	127.32	120.28
1	C	659	GLY	N-CA-C	5.25	118.83	112.48
1	B	659	GLY	CA-C-N	5.14	127.17	120.28
1	B	659	GLY	C-N-CA	5.14	127.17	120.28
1	B	605	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	1125	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	1125	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	798	LEU	N-CA-C	5.00	119.03	113.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6484	0	6143	74	0
1	B	6253	0	5786	72	0
1	C	6405	0	6008	55	0
1	D	5362	0	4607	35	0
2	A	27	0	12	0	0
2	B	27	0	12	4	0
2	C	27	0	12	1	0
2	D	27	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	27	0	0	1	0
4	B	27	0	0	1	0
4	C	26	0	0	0	0
5	A	18	0	0	0	0
5	B	10	0	0	0	0
5	C	8	0	0	0	0
5	D	4	0	0	0	0
All	All	24736	0	22592	240	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 5.

All (240) 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:B:687:HIS:CD2	1:B:690:ILE:HG23	1.96	0.99
1:B:347:ILE:HG22	1:B:353:ALA:HB2	1.50	0.90
1:B:347:ILE:HG22	1:B:353:ALA:CB	2.03	0.88
1:B:743:ASN:O	1:B:743:ASN:ND2	2.11	0.84
1:C:740:THR:HB	1:C:743:ASN:HB3	1.58	0.83
1:B:687:HIS:HD2	1:B:690:ILE:HG23	1.42	0.82
1:C:347:ILE:HG22	1:C:353:ALA:HB2	1.63	0.80
1:A:740:THR:HB	1:A:743:ASN:HB2	1.67	0.77
1:A:915:HIS:CD2	1:A:995:LEU:HD11	2.21	0.76
1:D:347:ILE:HG22	1:D:353:ALA:HB2	1.69	0.72
1:C:347:ILE:HG22	1:C:353:ALA:CB	2.19	0.71
1:D:347:ILE:HG22	1:D:353:ALA:CB	2.20	0.71
1:C:740:THR:HB	1:C:743:ASN:CB	2.20	0.71
1:A:918:LEU:O	1:A:921:VAL:HG22	1.90	0.70
1:B:513:ILE:HG12	1:B:543:SER:HB2	1.73	0.70
1:A:347:ILE:HG22	1:A:353:ALA:HB2	1.71	0.70
1:A:321:SER:HB3	1:A:845:ASN:ND2	2.10	0.67
1:C:512:GLU:OE2	1:C:514:HIS:HE1	1.78	0.67
1:C:660:TRP:HB2	1:C:687:HIS:CD2	2.30	0.66
1:A:867:MET:HE3	1:A:880:ILE:HG23	1.78	0.65
1:B:550:MET:HG2	1:B:821:ILE:HD11	1.77	0.65
1:A:997:PHE:HB2	1:A:1070:PHE:HB3	1.80	0.63
1:C:550:MET:HG2	1:C:821:ILE:HD11	1.80	0.63
1:B:874:PHE:O	1:B:1136:ARG:NH1	2.31	0.63
1:B:997:PHE:HB2	1:B:1070:PHE:HB3	1.81	0.62
1:A:801:ILE:O	1:A:805:ILE:HG13	2.01	0.61
1:A:457:VAL:O	1:A:461:ARG:HG3	2.00	0.61
1:A:921:VAL:HG23	1:A:922:PHE:N	2.16	0.61
1:C:997:PHE:HB2	1:C:1070:PHE:HB3	1.82	0.60
1:D:416:GLY:HA2	2:D:1301:ADP:H5'1	1.83	0.60
1:C:787:THR:HG22	1:C:788:HIS:CD2	2.37	0.60
1:A:361:SER:HA	1:A:435:ALA:HB3	1.84	0.60
1:A:441:VAL:HG13	1:A:441:VAL:O	2.01	0.60
1:A:744:ASN:O	1:A:744:ASN:ND2	2.35	0.59
1:A:747:ASN:HB2	1:A:1048:LYS:O	2.01	0.59
1:B:787:THR:HG22	1:B:788:HIS:CD2	2.37	0.59
1:C:658:PRO:HD2	1:C:662:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:HIS:HB3	1:C:690:ILE:HG23	1.84	0.58
1:B:361:SER:HA	1:B:435:ALA:HB3	1.87	0.57
1:A:441:VAL:HG13	1:A:508:VAL:HA	1.86	0.57
1:D:513:ILE:HG12	1:D:543:SER:HB2	1.86	0.57
1:A:787:THR:HG22	1:A:788:HIS:CD2	2.39	0.57
1:B:414:GLY:N	2:B:1301:ADP:O1B	2.26	0.57
1:B:747:ASN:HB2	1:B:1048:LYS:O	2.05	0.56
1:D:787:THR:HG22	1:D:788:HIS:CD2	2.40	0.55
1:D:361:SER:HA	1:D:435:ALA:HB3	1.87	0.55
1:B:807:LEU:HD22	1:B:856:ALA:HB1	1.88	0.55
1:C:361:SER:HA	1:C:435:ALA:HB3	1.87	0.55
1:C:807:LEU:HD22	1:C:856:ALA:HB1	1.88	0.55
1:B:290:ILE:HG23	1:B:295:LEU:HB2	1.89	0.55
1:B:1006:HIS:HA	1:B:1012:ILE:HG22	1.88	0.55
1:C:290:ILE:HG23	1:C:295:LEU:HB2	1.89	0.55
1:A:441:VAL:HG11	1:A:508:VAL:HG22	1.89	0.55
1:B:861:GLU:CD	1:B:862:PRO:HD2	2.32	0.55
2:B:1301:ADP:O2A	2:B:1301:ADP:O2B	2.24	0.55
1:C:330:VAL:HG11	1:C:498:LEU:HD22	1.87	0.55
1:A:347:ILE:HG22	1:A:353:ALA:CB	2.38	0.54
1:A:330:VAL:HG11	1:A:498:LEU:HD22	1.88	0.54
1:A:441:VAL:HG12	1:A:507:HIS:O	2.07	0.54
1:D:290:ILE:HG23	1:D:295:LEU:HB2	1.89	0.54
1:A:1006:HIS:HA	1:A:1012:ILE:HG22	1.89	0.54
1:B:347:ILE:CG2	1:B:353:ALA:HB2	2.31	0.54
1:B:1072:SER:OG	1:B:1104:ARG:NH2	2.41	0.54
1:C:1072:SER:OG	1:C:1104:ARG:NH2	2.41	0.53
1:A:1072:SER:OG	1:A:1104:ARG:NH2	2.42	0.53
4:B:1303:A1BXX:C9	4:B:1303:A1BXX:C1	2.87	0.53
1:A:289:ILE:HG21	1:A:1134:MET:HG2	1.91	0.53
1:A:658:PRO:HG3	1:A:733:LYS:HB2	1.91	0.53
1:C:512:GLU:OE2	1:C:514:HIS:CE1	2.61	0.52
1:A:290:ILE:HG23	1:A:295:LEU:HB2	1.90	0.52
1:C:1006:HIS:HA	1:C:1012:ILE:HG22	1.90	0.52
1:A:690:ILE:CG1	1:A:695:GLN:HG3	2.40	0.52
1:A:747:ASN:CB	1:A:1048:LYS:O	2.57	0.52
1:A:925:TRP:O	1:A:929:ARG:HB2	2.10	0.52
1:A:915:HIS:CG	1:A:995:LEU:HD21	2.45	0.51
1:A:961:LYS:HG2	1:A:974:LEU:HB3	1.92	0.51
1:A:744:ASN:C	1:A:744:ASN:HD22	2.18	0.51
1:D:330:VAL:HG11	1:D:498:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HA	1:B:498:LEU:HD12	1.93	0.51
1:C:908:ALA:HB2	1:C:1027:VAL:HG11	1.93	0.51
1:C:1000:TYR:CD1	1:C:1001:PRO:HA	2.46	0.51
1:A:1000:TYR:CD1	1:A:1001:PRO:HA	2.46	0.51
1:C:1034:GLN:H	1:C:1034:GLN:CD	2.18	0.51
1:A:441:VAL:CG1	1:A:508:VAL:HA	2.41	0.50
1:B:444:GLN:NE2	1:B:511:ASP:HB3	2.26	0.50
1:D:970:PRO:HD2	1:D:1121:ILE:HD11	1.94	0.50
1:A:805:ILE:HA	1:A:810:LEU:HD12	1.94	0.50
1:B:658:PRO:HG3	1:B:733:LYS:HB2	1.93	0.50
1:B:1000:TYR:CD1	1:B:1001:PRO:HA	2.47	0.50
1:A:970:PRO:HD2	1:A:1121:ILE:HD11	1.93	0.49
1:A:749:ALA:HB2	1:A:1050:ARG:HB3	1.94	0.49
1:B:514:HIS:CE1	1:B:544:ALA:HB2	2.48	0.49
1:B:740:THR:HG22	1:B:743:ASN:H	1.78	0.49
1:D:686:LEU:HD21	1:D:720:ILE:HD11	1.95	0.48
1:B:525:VAL:HG22	1:B:820:ALA:HA	1.95	0.48
1:C:970:PRO:HD2	1:C:1121:ILE:HD11	1.94	0.48
1:A:441:VAL:CG1	1:A:508:VAL:HG22	2.43	0.48
1:C:935:ALA:HA	1:C:938:ARG:HG2	1.96	0.48
1:B:407:VAL:HG22	1:B:559:PRO:HG2	1.95	0.48
1:C:512:GLU:HB3	1:C:515:GLU:HG3	1.96	0.48
1:C:686:LEU:HD21	1:C:720:ILE:HD11	1.96	0.48
1:D:342:TRP:HB3	1:D:479:LEU:HD22	1.95	0.48
1:B:721:THR:HB	2:B:1301:ADP:H3'	1.95	0.48
1:B:851:LEU:HD13	1:B:1115:THR:HG21	1.96	0.47
1:B:444:GLN:HE22	1:B:511:ASP:HB3	1.78	0.47
1:B:686:LEU:HD21	1:B:720:ILE:HD11	1.96	0.47
1:B:471:TYR:HA	1:B:488:PHE:O	2.14	0.47
1:A:1040:SER:HB3	1:A:1061:LEU:HD21	1.96	0.47
1:B:658:PRO:HD2	1:B:662:LEU:HD12	1.97	0.47
1:C:988:LEU:O	1:C:992:ILE:HG12	2.15	0.47
1:A:999:VAL:CG2	1:A:1044:VAL:HB	2.45	0.47
1:B:739:PHE:CZ	1:B:741:ALA:HA	2.49	0.47
1:B:867:MET:HE3	1:B:880:ILE:HG23	1.95	0.47
4:A:1303:A1BKX:C9	4:A:1303:A1BKX:C1	2.93	0.47
1:B:988:LEU:O	1:B:992:ILE:HG12	2.15	0.47
1:C:457:VAL:O	1:C:461:ARG:HG3	2.15	0.46
1:A:921:VAL:CG2	1:A:922:PHE:N	2.78	0.46
1:D:658:PRO:HD2	1:D:662:LEU:HD12	1.97	0.46
1:A:687:HIS:CD2	1:A:689:GLN:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:LEU:O	1:A:992:ILE:HG12	2.15	0.46
1:B:908:ALA:HB2	1:B:1027:VAL:HG11	1.98	0.46
1:D:658:PRO:HG3	1:D:733:LYS:HB2	1.96	0.46
1:A:525:VAL:HG22	1:A:820:ALA:HA	1.97	0.46
1:B:1069:LEU:HD21	1:B:1135:ILE:HG23	1.97	0.46
1:D:509:ILE:HG12	1:D:540:VAL:HB	1.97	0.46
1:D:514:HIS:NE2	1:D:718:THR:HB	2.31	0.46
1:B:444:GLN:HE22	1:B:511:ASP:CB	2.28	0.46
1:B:739:PHE:HA	1:B:746:THR:HA	1.98	0.46
1:C:658:PRO:HG3	1:C:733:LYS:HB2	1.98	0.46
1:A:668:LYS:HA	1:A:671:GLU:HG2	1.98	0.46
1:A:686:LEU:HD21	1:A:720:ILE:HD11	1.96	0.46
1:C:1040:SER:HB3	1:C:1061:LEU:HD21	1.96	0.46
1:A:310:LEU:HD12	1:A:1075:VAL:HG12	1.98	0.46
1:A:658:PRO:HD2	1:A:662:LEU:HD12	1.97	0.46
1:B:278:LEU:HD11	1:B:1092:ILE:HD11	1.98	0.46
1:C:495:LEU:HA	1:C:498:LEU:HD12	1.96	0.46
1:D:525:VAL:HG22	1:D:820:ALA:HA	1.98	0.46
1:C:1069:LEU:HD21	1:C:1135:ILE:HG23	1.97	0.45
1:D:442:VAL:HG22	1:D:509:ILE:HB	1.97	0.45
1:D:803:LEU:HD21	1:D:836:LEU:HD22	1.98	0.45
1:C:310:LEU:HD12	1:C:1075:VAL:HG12	1.98	0.45
1:C:525:VAL:HG22	1:C:820:ALA:HA	1.97	0.45
1:B:416:GLY:HA2	2:B:1301:ADP:H5'1	1.98	0.45
1:B:1040:SER:HB3	1:B:1061:LEU:HD21	1.97	0.45
1:C:509:ILE:HG12	1:C:540:VAL:HB	1.98	0.45
1:B:310:LEU:HD12	1:B:1075:VAL:HG12	1.98	0.45
1:D:668:LYS:HA	1:D:671:GLU:HG2	1.97	0.45
1:A:495:LEU:HA	1:A:498:LEU:HD12	1.99	0.45
1:A:1069:LEU:HD21	1:A:1135:ILE:HG23	1.99	0.45
1:B:739:PHE:O	1:B:739:PHE:CD1	2.70	0.45
1:B:457:VAL:O	1:B:461:ARG:HG3	2.17	0.45
1:B:418:THR:CG2	1:B:453:VAL:HG21	2.47	0.45
1:A:473:VAL:HG12	1:A:490:THR:HG23	1.99	0.45
1:C:278:LEU:HD11	1:C:1092:ILE:HD11	1.98	0.44
1:A:622:LEU:HG	1:A:626:GLN:HE21	1.82	0.44
1:D:653:VAL:HG22	1:D:727:TYR:HB2	1.99	0.44
1:A:278:LEU:HD11	1:A:1092:ILE:HD11	1.98	0.44
1:A:329:VAL:HG22	1:A:529:ASP:HB3	1.99	0.44
1:D:409:ILE:HB	1:D:542:MET:HG2	1.99	0.44
1:D:456:ARG:NH1	2:D:1301:ADP:C2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:VAL:HG21	1:D:520:THR:OG1	2.18	0.44
1:A:495:LEU:HD23	1:A:498:LEU:HD12	1.99	0.44
1:B:509:ILE:HG12	1:B:540:VAL:HB	1.99	0.44
1:C:721:THR:HB	2:C:1301:ADP:H3'	2.00	0.44
1:C:999:VAL:CG2	1:C:1044:VAL:HB	2.48	0.44
1:D:687:HIS:CD2	1:D:689:GLN:H	2.36	0.44
1:B:276:VAL:HB	1:B:1092:ILE:HG13	2.00	0.44
1:C:1039:PRO:HB2	1:C:1146:ILE:HG23	2.00	0.44
1:D:443:THR:HB	1:D:491:VAL:HG22	2.00	0.44
1:B:347:ILE:CG2	1:B:353:ALA:CB	2.88	0.44
1:B:970:PRO:HD2	1:B:1121:ILE:HD11	2.00	0.44
1:D:329:VAL:HG22	1:D:529:ASP:HB3	1.99	0.43
1:A:319:GLU:HA	1:A:320:PRO:HD3	1.86	0.43
1:A:509:ILE:HG12	1:A:540:VAL:HB	2.00	0.43
1:B:439:ASN:HD22	1:B:439:ASN:HA	1.72	0.43
1:B:700:ASP:HA	1:B:701:PRO:HD3	1.92	0.43
1:A:372:LEU:HA	1:A:378:LEU:HD23	2.00	0.43
1:B:528:ARG:O	1:B:531:VAL:HG12	2.18	0.43
1:B:418:THR:HG21	1:B:453:VAL:HG21	1.99	0.43
1:A:321:SER:HB3	1:A:845:ASN:HD21	1.83	0.43
1:B:745:MET:SD	1:B:1002:ASN:OD1	2.77	0.43
1:C:329:VAL:HG22	1:C:529:ASP:HB3	2.00	0.43
1:B:570:VAL:HB	1:B:762:LYS:HE2	2.01	0.43
1:B:875:TYR:HA	1:B:973:CYS:HB2	2.01	0.43
1:A:571:GLN:HG2	1:A:573:TYR:CZ	2.54	0.42
1:A:1039:PRO:HB2	1:A:1146:ILE:HG23	2.00	0.42
1:B:513:ILE:CG1	1:B:543:SER:HB2	2.45	0.42
1:A:687:HIS:HB3	1:A:690:ILE:HG23	2.01	0.42
1:A:961:LYS:O	1:A:965:ILE:HG12	2.19	0.42
1:B:999:VAL:CG2	1:B:1044:VAL:HB	2.49	0.42
1:A:807:LEU:HD22	1:A:856:ALA:HB1	2.02	0.42
1:B:329:VAL:HG22	1:B:529:ASP:HB3	2.01	0.42
1:B:471:TYR:HE1	1:B:476:GLU:HG2	1.84	0.42
1:B:870:MET:HE1	1:B:1070:PHE:CE1	2.54	0.42
1:B:961:LYS:O	1:B:965:ILE:HG12	2.19	0.42
1:C:401:ILE:HA	1:C:407:VAL:HG21	2.02	0.42
1:B:456:ARG:NH1	1:B:459:PHE:CE2	2.88	0.42
1:C:375:ASP:O	1:C:379:GLN:HG3	2.19	0.42
1:B:653:VAL:HG22	1:B:727:TYR:HB2	2.02	0.42
1:D:961:LYS:O	1:D:965:ILE:HG12	2.19	0.42
1:D:495:LEU:HA	1:D:498:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:HB	1:A:1092:ILE:HG13	2.02	0.42
1:A:528:ARG:O	1:A:531:VAL:HG12	2.20	0.42
1:A:870:MET:HE1	1:A:1070:PHE:CE1	2.55	0.42
1:C:608:CYS:SG	1:C:784:ARG:HD3	2.60	0.42
1:A:292:GLU:HG2	1:A:1127:VAL:HG23	2.02	0.41
1:A:1067:LEU:HA	1:A:1071:ALA:HB3	2.02	0.41
1:C:276:VAL:HB	1:C:1092:ILE:HG13	2.02	0.41
1:B:342:TRP:CH2	1:B:487:MET:HB3	2.55	0.41
1:C:870:MET:HE1	1:C:1070:PHE:CE1	2.55	0.41
1:C:961:LYS:O	1:C:965:ILE:HG12	2.20	0.41
1:C:1067:LEU:HA	1:C:1071:ALA:HB3	2.02	0.41
1:B:739:PHE:CE2	1:B:741:ALA:HA	2.55	0.41
1:C:440:ILE:HG12	1:C:507:HIS:HB2	2.02	0.41
1:D:687:HIS:HB3	1:D:690:ILE:HG23	2.03	0.41
1:C:375:ASP:HB3	1:C:378:LEU:HB3	2.03	0.41
1:D:491:VAL:HG13	1:D:523:LEU:HD22	2.02	0.41
1:A:749:ALA:CB	1:A:1050:ARG:HB3	2.50	0.41
1:C:700:ASP:HA	1:C:701:PRO:HD3	1.91	0.41
1:D:571:GLN:HG2	1:D:573:TYR:CZ	2.56	0.41
1:A:634:PHE:HD1	1:A:666:MET:SD	2.44	0.41
1:C:456:ARG:NH1	1:C:459:PHE:CE2	2.89	0.41
1:D:332:TRP:CE2	1:D:537:VAL:HG23	2.55	0.41
2:D:1301:ADP:O2B	2:D:1301:ADP:O2A	2.38	0.41
1:A:513:ILE:HG13	1:A:543:SER:HB2	2.03	0.41
1:B:292:GLU:HG2	1:B:1127:VAL:HG23	2.03	0.41
1:C:441:VAL:HG12	1:C:505:ILE:HG21	2.03	0.41
1:C:805:ILE:HG21	1:C:813:ILE:HA	2.04	0.41
1:D:332:TRP:NE1	1:D:537:VAL:HG23	2.36	0.41
1:D:634:PHE:HD1	1:D:666:MET:SD	2.44	0.41
1:A:743:ASN:N	1:A:743:ASN:HD22	2.19	0.40
1:B:734:GLN:HE21	1:B:734:GLN:HB3	1.67	0.40
1:A:673:ASN:HA	1:A:674:PRO:HD3	1.96	0.40
1:C:292:GLU:HG2	1:C:1127:VAL:HG23	2.03	0.40
1:D:449:SER:O	1:D:453:VAL:HG23	2.21	0.40
1:B:550:MET:HE2	1:B:550:MET:HB3	1.97	0.40
1:B:634:PHE:HD1	1:B:666:MET:SD	2.44	0.40
1:C:571:GLN:HG2	1:C:573:TYR:CZ	2.56	0.40
1:A:494:LEU:O	1:A:498:LEU:HG	2.22	0.40
1:C:679:HIS:CD2	1:C:679:HIS:H	2.39	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	859/1010 (85%)	821 (96%)	37 (4%)	1 (0%)	48	78
1	B	850/1010 (84%)	813 (96%)	36 (4%)	1 (0%)	48	78
1	C	854/1010 (85%)	818 (96%)	36 (4%)	0	100	100
1	D	763/1010 (76%)	733 (96%)	30 (4%)	0	100	100
All	All	3326/4040 (82%)	3185 (96%)	139 (4%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	PHE
1	B	1031	PHE

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	647/888 (73%)	635 (98%)	12 (2%)	50	66
1	B	590/888 (66%)	579 (98%)	11 (2%)	50	66
1	C	625/888 (70%)	609 (97%)	16 (3%)	40	61
1	D	441/888 (50%)	436 (99%)	5 (1%)	65	74
All	All	2303/3552 (65%)	2259 (98%)	44 (2%)	50	66

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	HIS
1	A	499	GLU
1	A	572	GLU
1	A	604	ASP
1	A	661	ASN
1	A	734	GLN
1	A	767	ARG
1	A	821	ILE
1	A	922	PHE
1	A	1019	ASN
1	A	1055	SER
1	A	1125	ASP
1	B	439	ASN
1	B	483	HIS
1	B	499	GLU
1	B	572	GLU
1	B	642	LYS
1	B	661	ASN
1	B	734	GLN
1	B	739	PHE
1	B	821	ILE
1	B	1055	SER
1	B	1125	ASP
1	C	483	HIS
1	C	499	GLU
1	C	553	GLU
1	C	572	GLU
1	C	644	ILE
1	C	661	ASN
1	C	734	GLN
1	C	744	ASN
1	C	747	ASN
1	C	769	ARG
1	C	821	ILE
1	C	922	PHE
1	C	927	ASP
1	C	972	ASP
1	C	1055	SER
1	C	1125	ASP
1	D	499	GLU
1	D	572	GLU
1	D	661	ASN
1	D	734	GLN

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Mol	Chain	Res	Type
1	D	1125	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	338	ASN
1	A	340	ASN
1	A	346	ASN
1	A	404	ASN
1	A	439	ASN
1	A	483	HIS
1	A	626	GLN
1	A	679	HIS
1	A	743	ASN
1	A	744	ASN
1	A	747	ASN
1	A	760	GLN
1	A	946	ASN
1	B	338	ASN
1	B	340	ASN
1	B	404	ASN
1	B	439	ASN
1	B	444	GLN
1	B	483	HIS
1	B	679	HIS
1	B	687	HIS
1	B	734	GLN
1	B	743	ASN
1	B	757	ASN
1	B	760	GLN
1	B	799	HIS
1	B	946	ASN
1	C	338	ASN
1	C	340	ASN
1	C	404	ASN
1	C	483	HIS
1	C	514	HIS
1	C	679	HIS
1	C	744	ASN
1	C	760	GLN
1	C	845	ASN

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Mol	Chain	Res	Type
1	C	946	ASN
1	D	338	ASN
1	D	340	ASN
1	D	346	ASN
1	D	404	ASN
1	D	687	HIS
1	D	734	GLN
1	D	747	ASN
1	D	757	ASN
1	D	946	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
2	ADP	D	1301	3	27,29,29	0.35	0	42,45,45	0.57	0
4	A1BXX	A	1303	-	29,29,29	0.34	0	39,42,42	0.30	0
2	ADP	C	1301	3	27,29,29	0.36	0	42,45,45	0.54	0
2	ADP	A	1301	3	27,29,29	0.26	0	42,45,45	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1BKX	C	1303	-	28,28,29	0.40	0	37,40,42	0.59	0
2	ADP	B	1301	3	27,29,29	0.54	0	42,45,45	0.53	1 (2%)
4	A1BKX	B	1303	-	29,29,29	0.42	1 (3%)	39,42,42	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	D	1301	3	-	6/16/32/32	0/3/3/3
4	A1BKX	A	1303	-	-	2/17/17/17	0/3/3/3
2	ADP	C	1301	3	-	5/16/32/32	0/3/3/3
2	ADP	A	1301	3	-	5/16/32/32	0/3/3/3
4	A1BKX	C	1303	-	-	2/17/17/17	0/3/3/3
2	ADP	B	1301	3	-	4/16/32/32	0/3/3/3
4	A1BKX	B	1303	-	-	2/17/17/17	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1303	A1BKX	C7-C2	2.10	1.42	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	ADP	PA-O3A-PB	-2.03	125.86	132.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ADP	PA-O3A-PB-O2B
2	A	1301	ADP	PA-O3A-PB-O3B
2	B	1301	ADP	PA-O3A-PB-O2B
2	C	1301	ADP	PA-O3A-PB-O2B
2	D	1301	ADP	PA-O3A-PB-O2B
2	D	1301	ADP	O4'-C4'-C5'-O5'
2	D	1301	ADP	C3'-C4'-C5'-O5'

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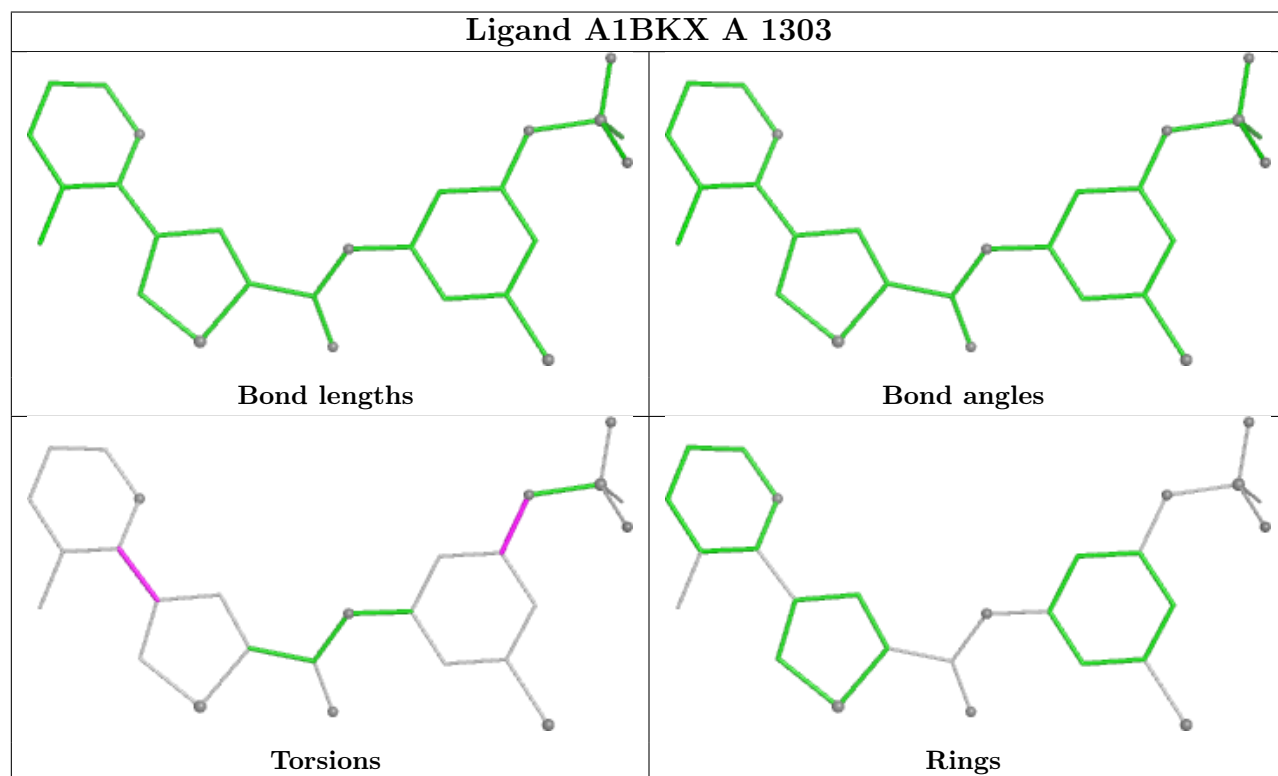
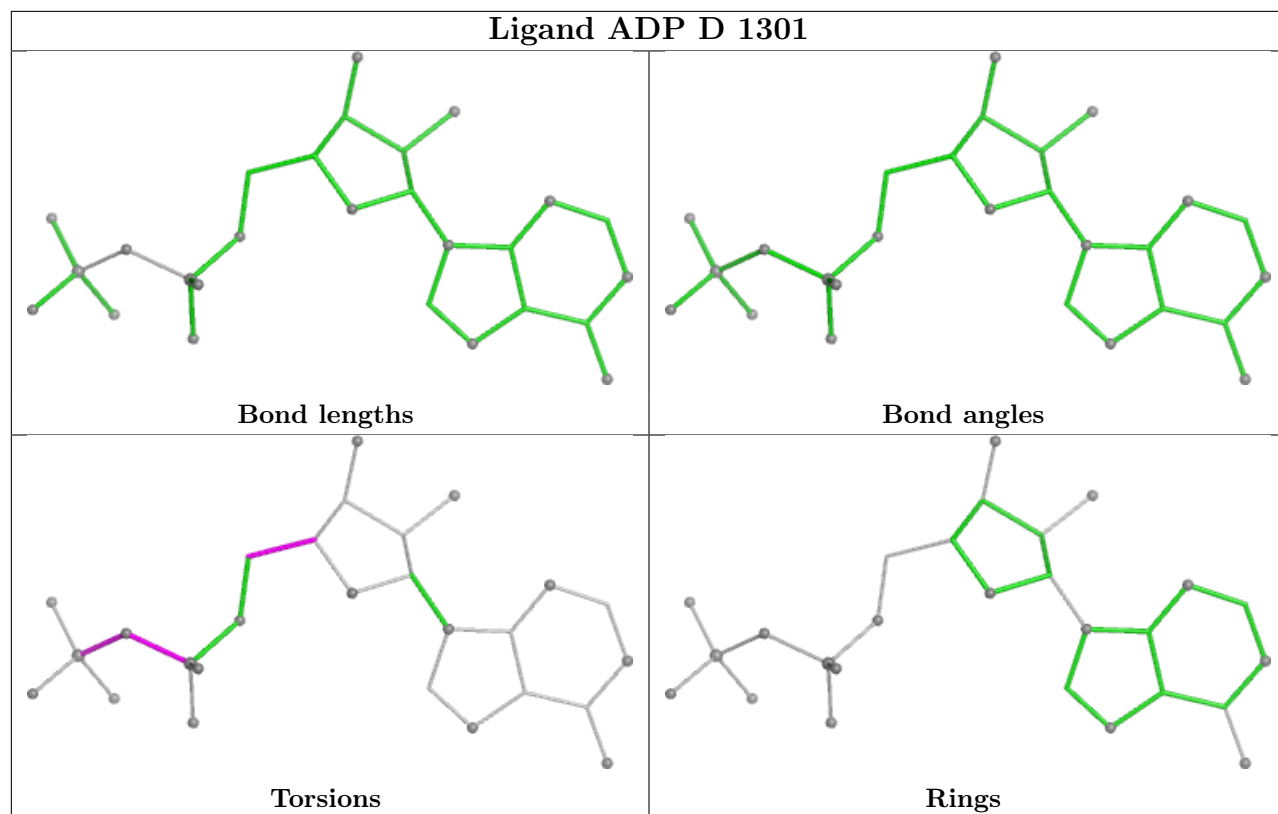
Mol	Chain	Res	Type	Atoms
2	D	1301	ADP	PA-O3A-PB-O1B
2	B	1301	ADP	PB-O3A-PA-O1A
2	A	1301	ADP	C5'-O5'-PA-O3A
2	A	1301	ADP	C5'-O5'-PA-O2A
2	D	1301	ADP	PB-O3A-PA-O2A
2	C	1301	ADP	PA-O3A-PB-O1B
4	B	1303	A1BKK	C19-C20-N22-S23
4	C	1303	A1BKK	C19-C20-N22-S23
4	A	1303	A1BKK	C19-C20-N22-S23
2	C	1301	ADP	PB-O3A-PA-O1A
2	D	1301	ADP	PB-O3A-PA-O1A
2	C	1301	ADP	O4'-C4'-C5'-O5'
4	B	1303	A1BKK	C21-C20-N22-S23
2	B	1301	ADP	PA-O3A-PB-O1B
4	C	1303	A1BKK	C21-C20-N22-S23
2	B	1301	ADP	PB-O3A-PA-O2A
2	C	1301	ADP	PB-O3A-PA-O2A
2	A	1301	ADP	C5'-O5'-PA-O1A
4	A	1303	A1BKK	C2-C7-C8-C12

There are no ring outliers.

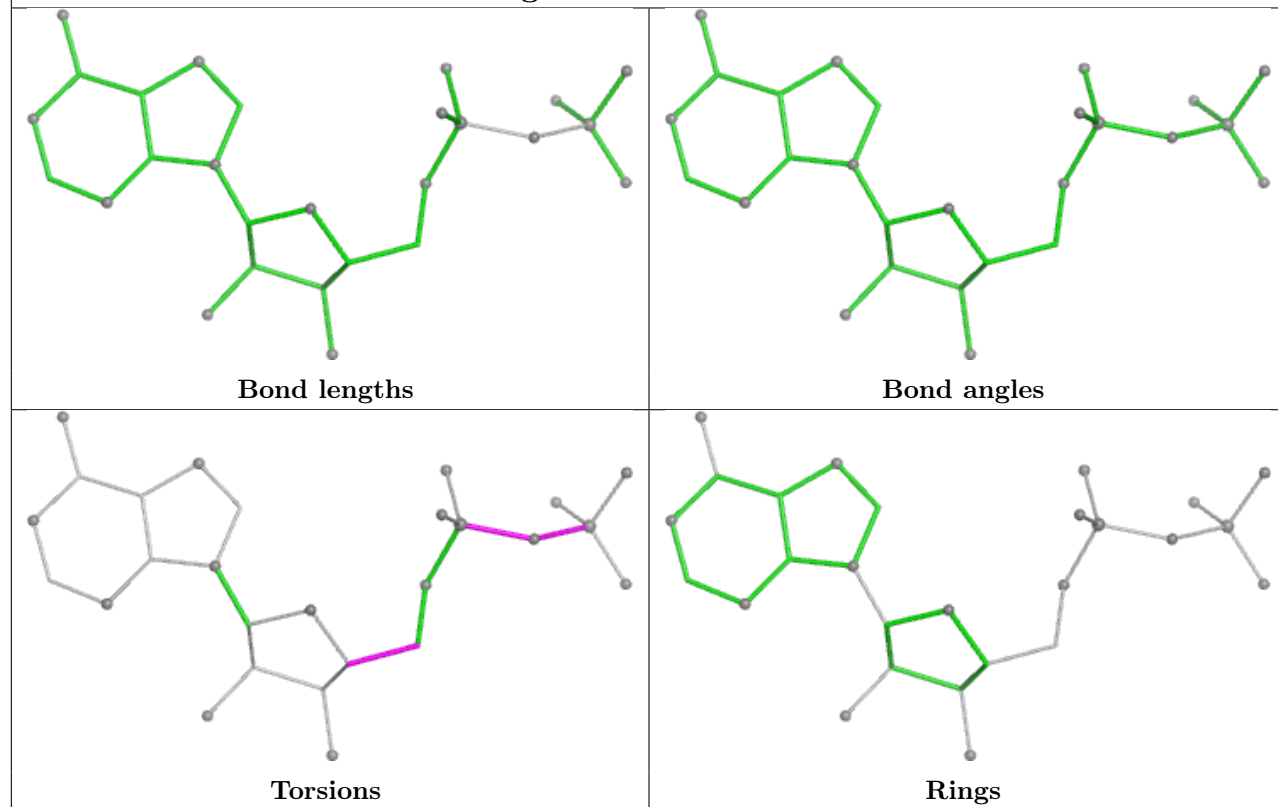
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1301	ADP	3	0
4	A	1303	A1BKK	1	0
2	C	1301	ADP	1	0
2	B	1301	ADP	4	0
4	B	1303	A1BKK	1	0

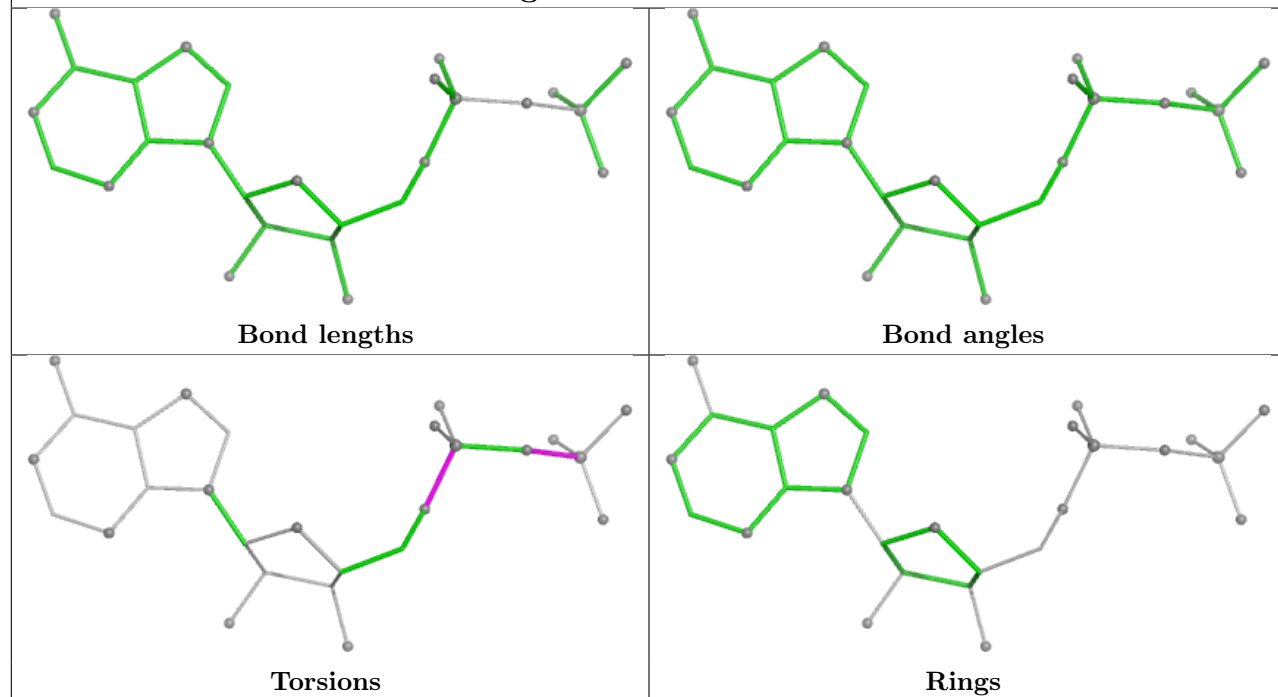
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



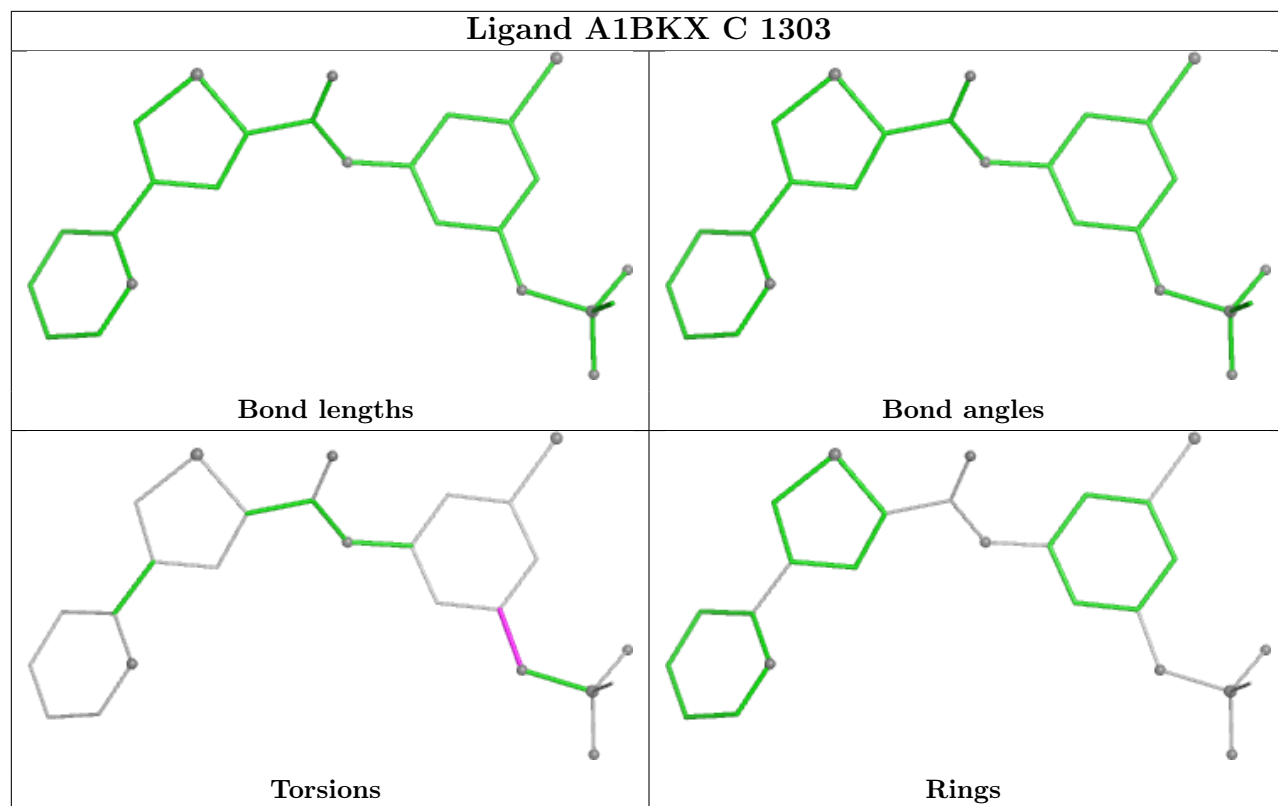
Ligand ADP C 1301



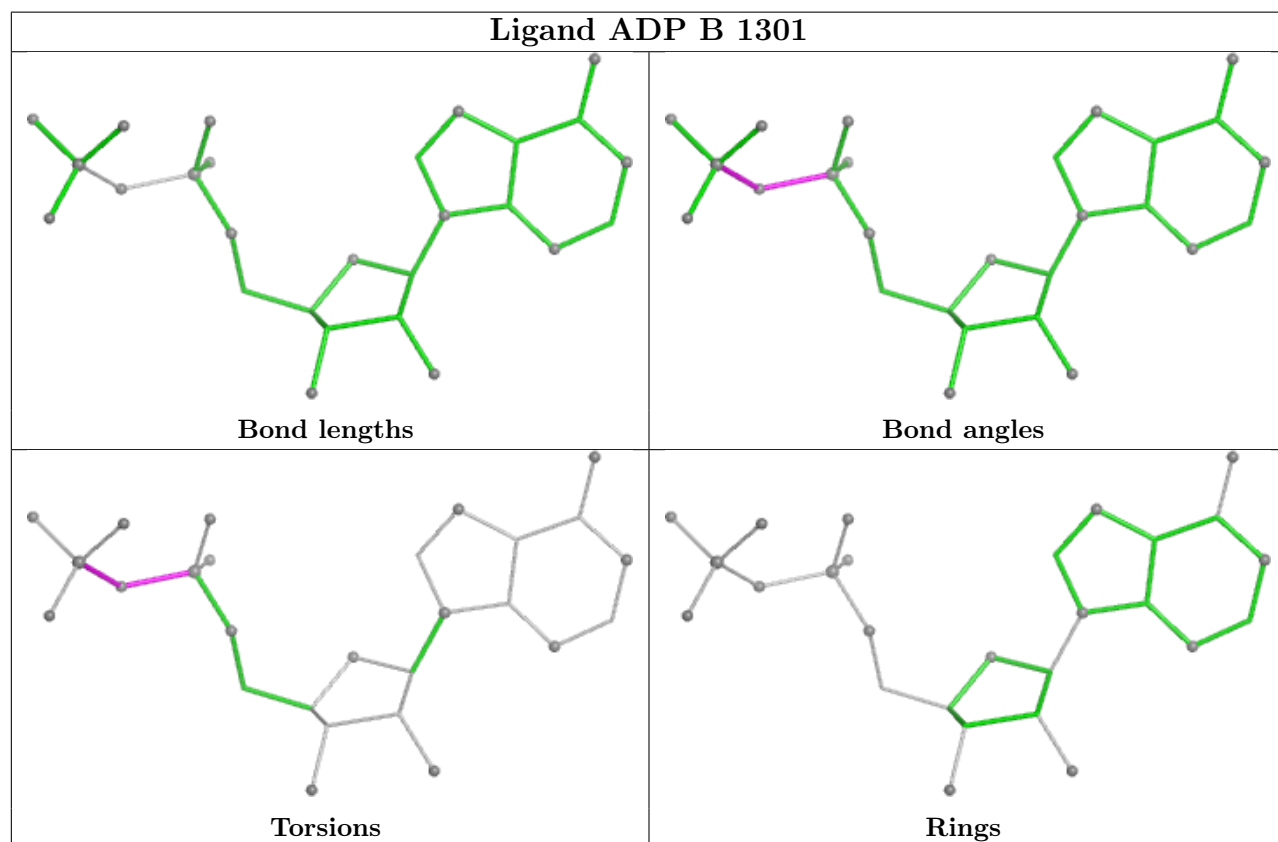
Ligand ADP A 1301

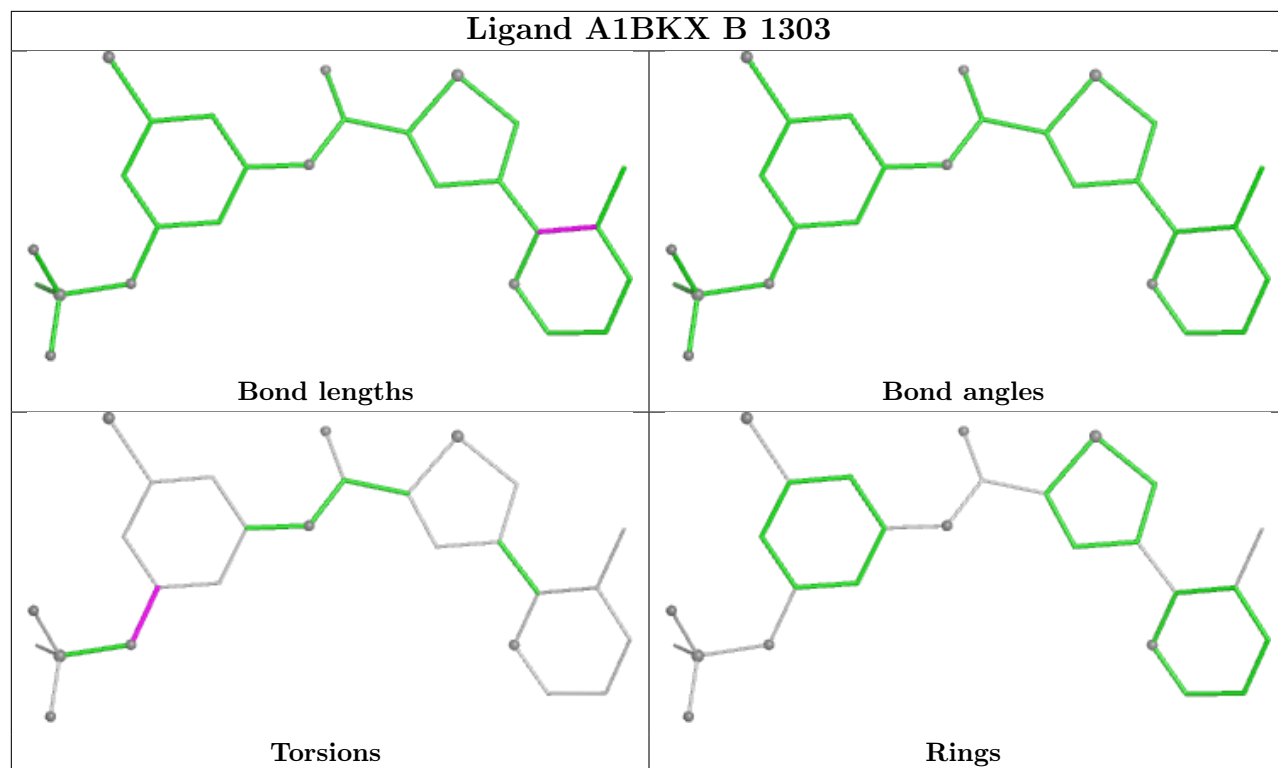


Ligand A1BKX C 1303



Ligand ADP B 1301





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	864/1010 (85%)	0.00	22 (2%) 58 43	61, 127, 180, 218	1 (0%)
1	B	858/1010 (84%)	0.09	22 (2%) 57 42	87, 144, 201, 241	0
1	C	860/1010 (85%)	-0.09	13 (1%) 72 57	105, 139, 202, 230	0
1	D	783/1010 (77%)	0.16	29 (3%) 45 32	125, 187, 265, 286	0
All	All	3365/4040 (83%)	0.04	86 (2%) 57 42	61, 144, 233, 286	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	879	ALA	5.4
1	B	889	PHE	5.4
1	D	916	VAL	5.2
1	C	896	GLU	4.8
1	D	910	ASN	4.5
1	D	886	ALA	4.4
1	B	873	ILE	4.2
1	D	918	LEU	4.1
1	B	893	PHE	4.1
1	D	915	HIS	3.9
1	A	1038	TYR	3.9
1	B	888	CYS	3.7
1	D	688	SER	3.7
1	C	441	VAL	3.7
1	B	475	PHE	3.5
1	D	917	ALA	3.3
1	A	896	GLU	3.0
1	A	1025	SER	3.0
1	D	1147	ASN	3.0
1	D	469	CYS	3.0
1	B	1137	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	869	ILE	2.9
1	A	330	VAL	2.9
1	D	993	SER	2.9
1	D	892	PRO	2.8
1	B	1138	ILE	2.8
1	C	314	LYS	2.8
1	D	991	VAL	2.8
1	C	772	PHE	2.7
1	C	319	GLU	2.7
1	A	685	PRO	2.6
1	C	369	MET	2.6
1	D	802	ALA	2.6
1	A	655	VAL	2.5
1	B	841	ALA	2.5
1	C	311	ASN	2.5
1	C	283	GLU	2.5
1	A	784[A]	ARG	2.5
1	C	748	TYR	2.5
1	A	1056	ALA	2.4
1	B	1128	ASN	2.4
1	A	1004	CYS	2.4
1	B	882	THR	2.4
1	B	903	ILE	2.4
1	A	319	GLU	2.4
1	C	440	ILE	2.4
1	B	431	GLN	2.4
1	D	374	GLN	2.4
1	B	1054	ILE	2.3
1	B	947	MET	2.3
1	A	390	VAL	2.3
1	B	867	MET	2.3
1	D	868	MET	2.3
1	B	922	PHE	2.3
1	D	468	SER	2.3
1	D	829	VAL	2.3
1	A	660	TRP	2.3
1	A	314	LYS	2.3
1	C	733	LYS	2.3
1	A	318	PHE	2.3
1	C	656	PHE	2.3
1	A	324	GLN	2.3
1	D	689	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1047	GLU	2.2
1	B	736	VAL	2.2
1	D	320	PRO	2.2
1	D	919	LEU	2.2
1	C	1025	SER	2.2
1	D	1095	GLU	2.2
1	A	1107	MET	2.2
1	A	656	PHE	2.2
1	B	993	SER	2.2
1	D	883	ILE	2.2
1	A	1151	ASP	2.2
1	A	352	LEU	2.1
1	A	870	MET	2.1
1	D	832	ALA	2.1
1	D	292	GLU	2.1
1	B	737	LYS	2.0
1	A	561	ILE	2.0
1	B	945	LEU	2.0
1	A	518	ILE	2.0
1	B	660	TRP	2.0
1	D	904	HIS	2.0
1	D	995	LEU	2.0
1	D	518	ILE	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](#)

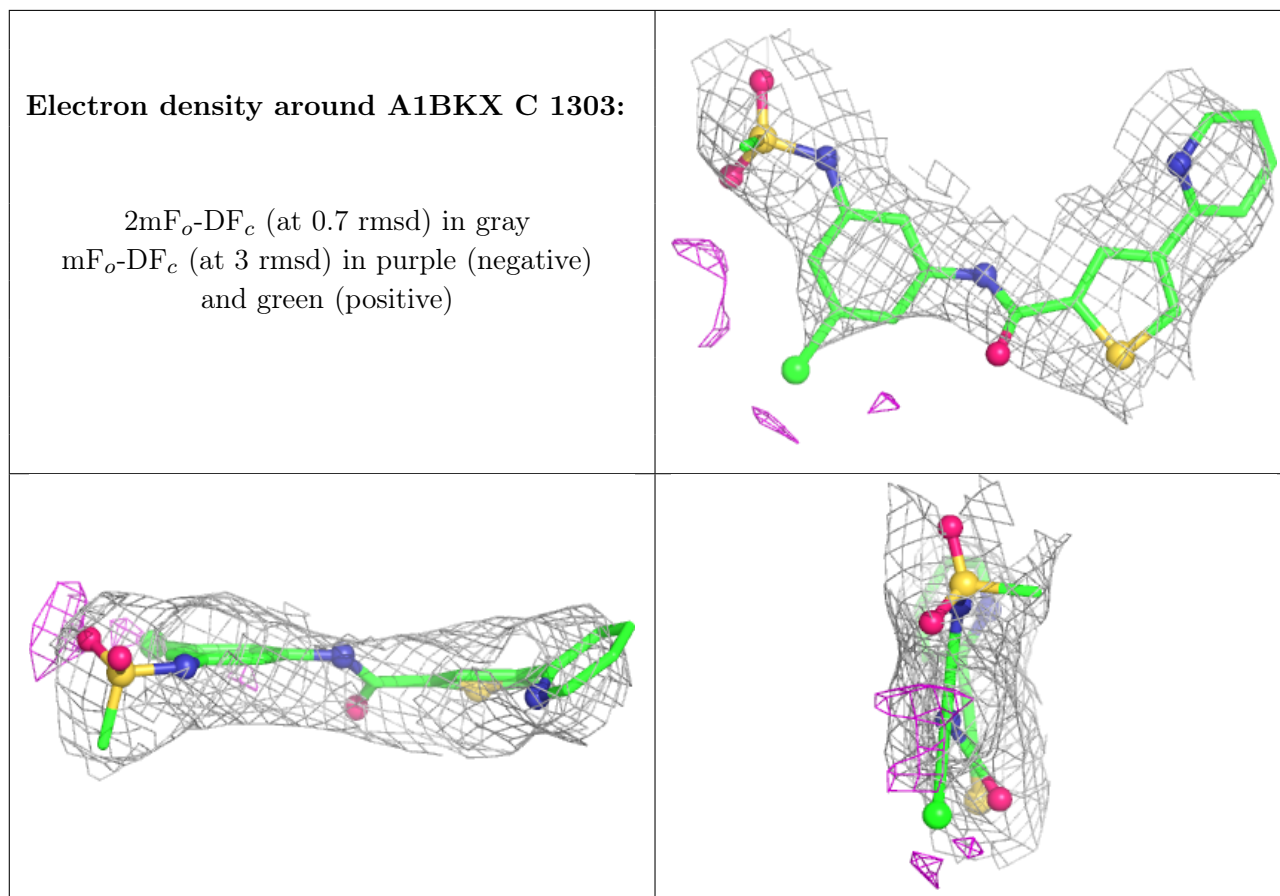
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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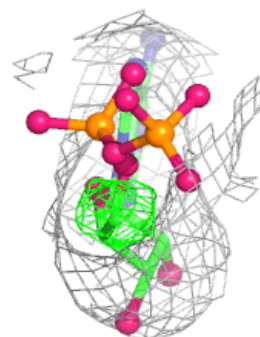
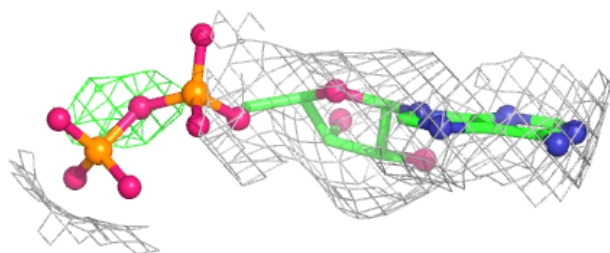
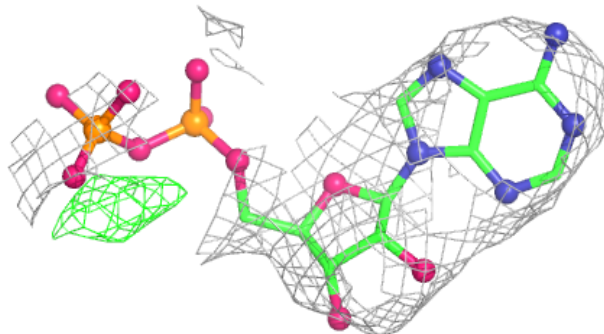
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	1302	1/1	0.91	0.20	83,83,83,83	0
4	A1BKX	C	1303	26/27	0.91	0.10	160,161,162,162	0
3	MG	C	1302	1/1	0.92	0.15	78,78,78,78	0
2	ADP	D	1301	27/27	0.92	0.07	175,177,179,179	0
2	ADP	B	1301	27/27	0.94	0.08	108,112,114,114	0
2	ADP	A	1301	27/27	0.94	0.07	131,134,135,135	0
4	A1BKX	B	1303	27/27	0.94	0.09	130,133,136,136	0
3	MG	A	1302	1/1	0.94	0.14	66,66,66,66	0
2	ADP	C	1301	27/27	0.95	0.08	125,129,130,130	0
4	A1BKX	A	1303	27/27	0.95	0.09	144,145,146,146	0
3	MG	D	1302	1/1	0.96	0.06	112,112,112,112	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.

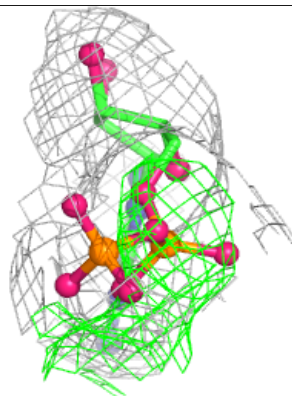
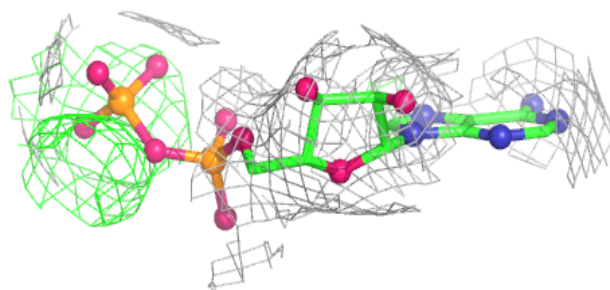
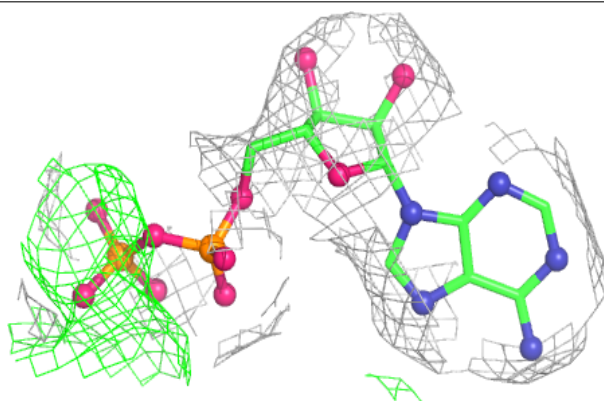


Electron density around ADP D 1301:

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

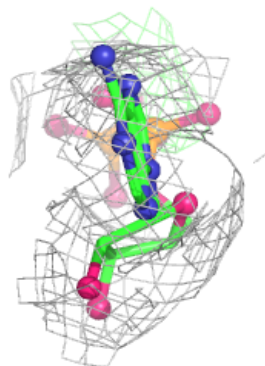
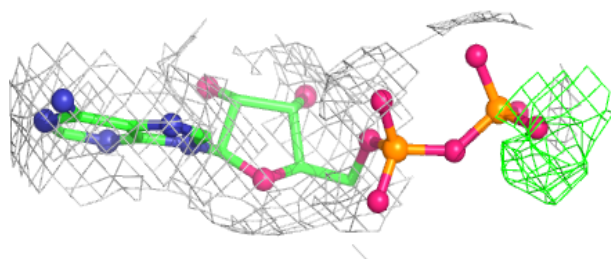
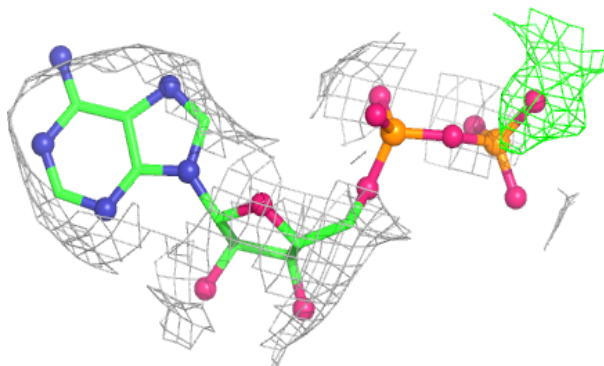
**Electron density around ADP B 1301:**

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

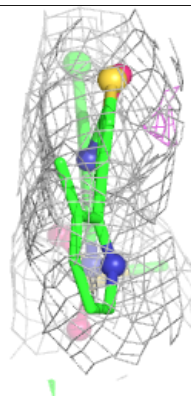
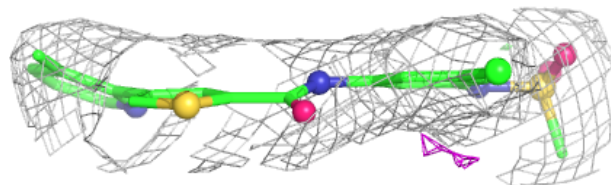
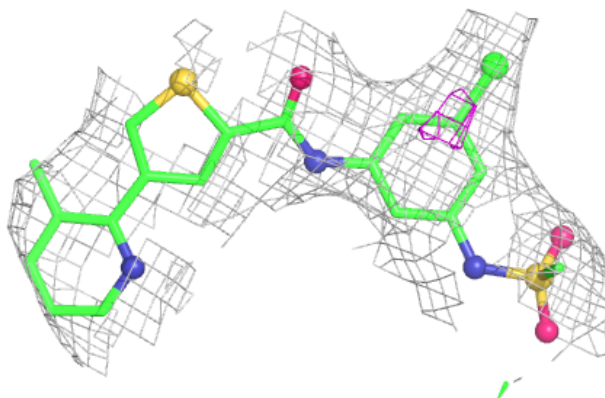


Electron density around ADP A 1301:

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

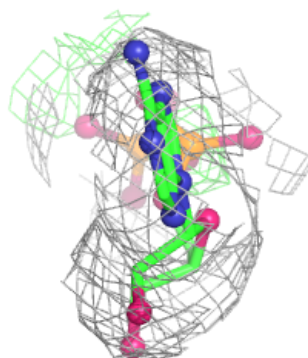
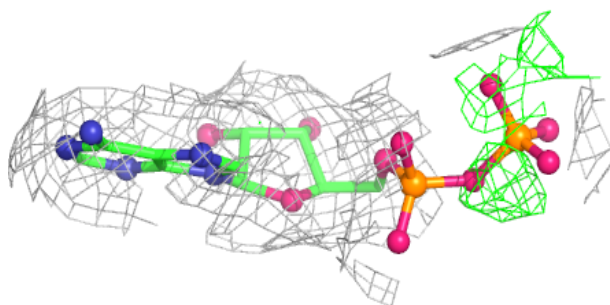
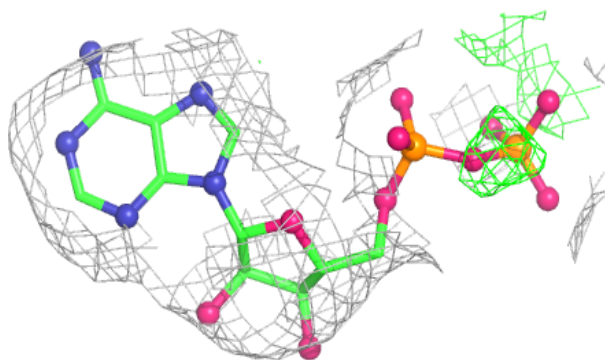
**Electron density around A1BKX B 1303:**

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

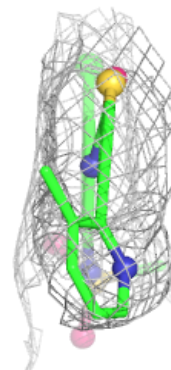
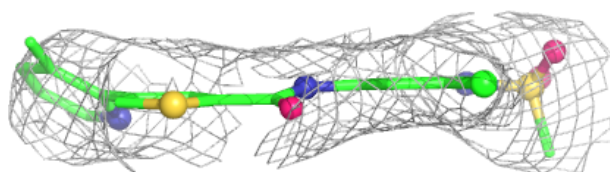
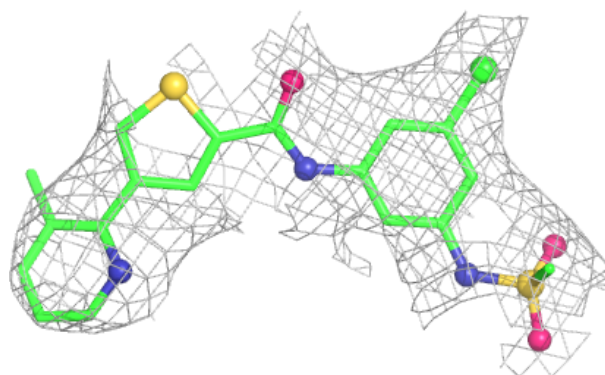


Electron density around ADP C 1301:

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

**Electron density around A1BKX A 1303:**

$2mF_o-DF_c$ (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.