



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:11 PM UTC

PDB ID : 8R7E / pdb_00008r7e
Title : MutSbeta bound to compound CHDI-00898647 in the canonical DNA-mismatch bound form
Authors : Thomsen, M.; Thieulin-Pardo, G.; Steinbacher, S.; Brace, G.; Tillack, K.; Johnson, P.; Ritzefeld, M.; Schaertl, S.; Frush, E.; Warfield, B.; Ballantyne, G.; Lee, J.-H.; Witte, D.; Finley, M.; Prasad, B.; Monteagudo, E.; Plotnikov, N.; Pacifici, R.; Maillard, M.; Wilkinson, H.; Iyer, R.; Dominguez, C.; Vogt, T.; Felsenfeld, D.; Haque, T.
Deposited on : 2023-11-24
Resolution : 2.78 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

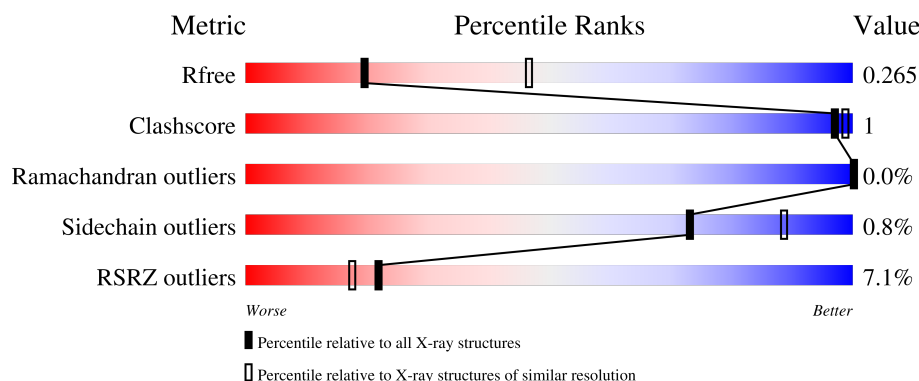
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	930	8% 87% 11%
1	E	930	5% 91% 6%
2	B	918	3% 86% 5% 8%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	F	918	11% 87% 10%
3	C	24	4% 88% 8%
3	G	24	88% 12%
4	D	24	83% 12%
4	H	24	4% 96%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28977 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	825	Total	C	N	O	S	373	1	0
			6570	4183	1114	1237	36			
1	E	875	Total	C	N	O	S	339	2	0
			6956	4423	1181	1316	36			

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	840	Total	C	N	O	S	177	0	0
			6721	4289	1148	1254	30			
2	F	827	Total	C	N	O	S	347	1	0
			6618	4220	1136	1232	30			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	GLY	-	expression tag	UNP P20585
B	218	PRO	-	expression tag	UNP P20585
F	217	GLY	-	expression tag	UNP P20585
F	218	PRO	-	expression tag	UNP P20585

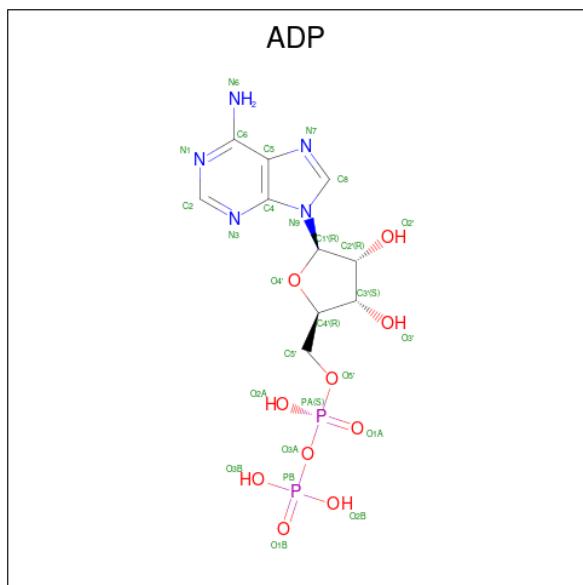
- Molecule 3 is a DNA chain called DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	P	0	0	0
			449	215	82	131	21			
3	G	21	Total	C	N	O	P	0	0	0
			432	205	80	126	21			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	23	Total	C	N	O	P	0	0	0
			469	224	88	135	22			
4	H	23	Total	C	N	O	P	0	0	0
			469	224	88	135	22			

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



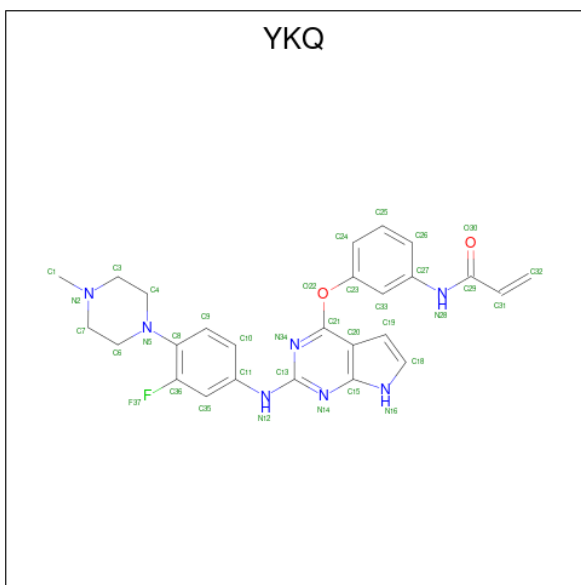


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

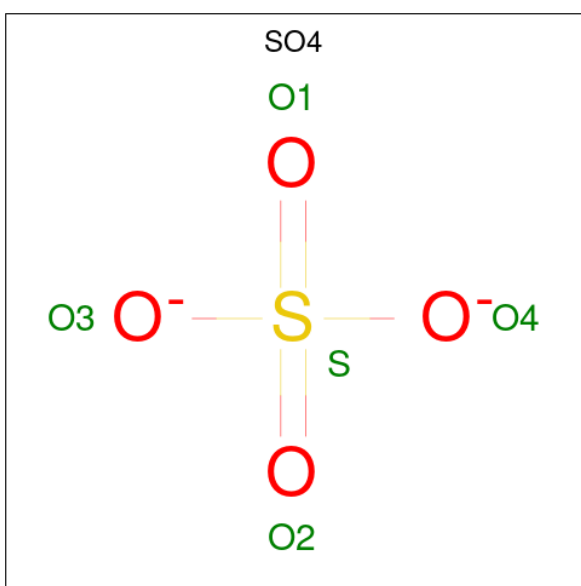
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	E	3	Total	Cl	0	0
			3	3		

- Molecule 8 is Abivertinib (CCD ID: YKQ) (formula: C₂₆H₂₆FN₇O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	F	N	O	0	0
			36	26	1	7	2		
8	F	1	Total	C	F	N	O	5	0
			36	26	1	7	2		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O S	0	0
			5 4 1			
9	B	1	Total	O S	0	0
			5 4 1			

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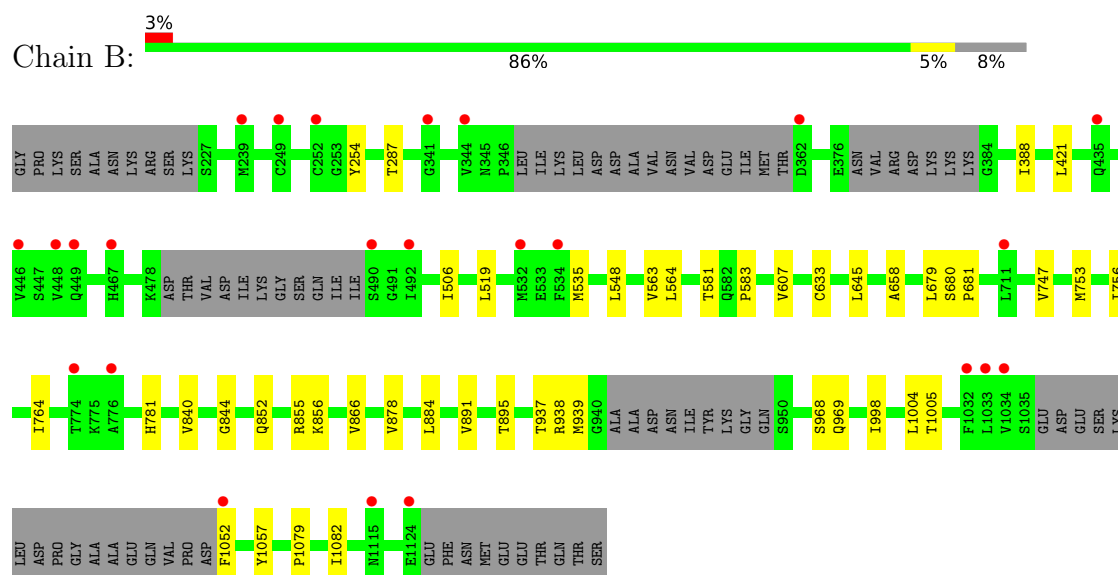
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		

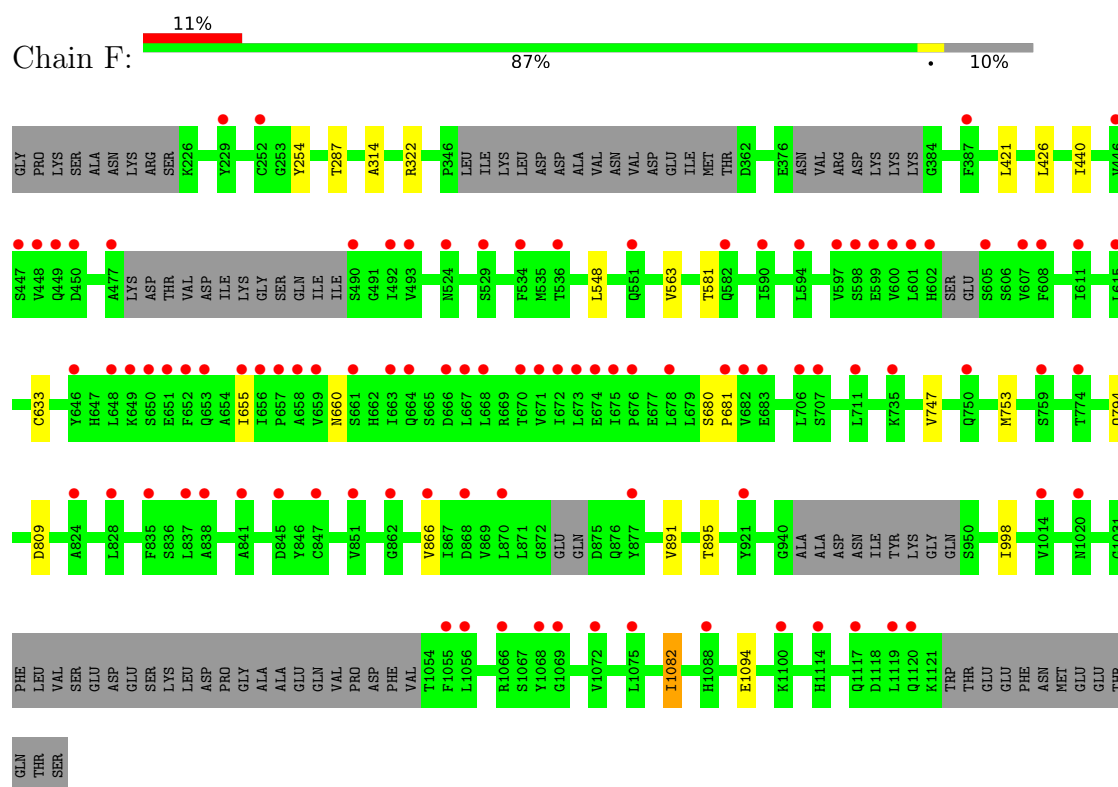
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	22	Total	O	0	0
			22	22		
10	B	27	Total	O	0	0
			27	27		
10	E	29	Total	O	0	0
			29	29		
10	F	34	Total	O	0	0
			34	34		
10	G	2	Total	O	0	0
			2	2		
10	H	3	Total	O	0	0
			3	3		

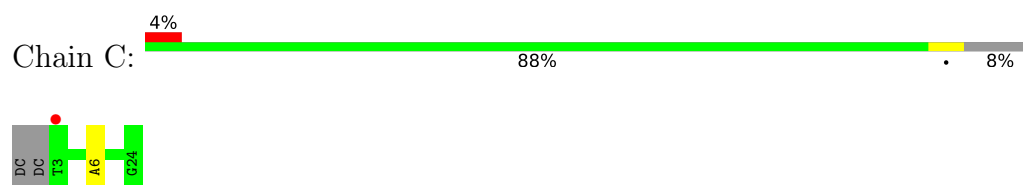
- Molecule 2: DNA mismatch repair protein Msh3



- Molecule 2: DNA mismatch repair protein Msh3

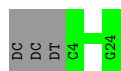


- Molecule 3: DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3')



- Molecule 3: DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3')

Chain G:  88% 12%



- Molecule 4: DNA (5'-D(*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3')

Chain D:  83% 12% .



- Molecule 4: DNA (5'-D(*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3')

Chain H:  4% 96% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.47Å 104.10Å 122.02Å 109.33° 91.81° 109.50°	Depositor
Resolution (Å)	113.66 – 2.78 113.66 – 2.78	Depositor EDS
% Data completeness (in resolution range)	72.8 (113.66-2.78) 72.8 (113.66-2.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.266 0.224 , 0.265	Depositor DCC
R_{free} test set	3915 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	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	0.92	EDS
Total number of atoms	28977	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% 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: CL, SO4, EDO, ADP, YKQ

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	1.04	0/6669	1.57	2/8975 (0.0%)
1	E	1.05	0/7066	1.59	2/9518 (0.0%)
2	B	1.04	0/6845	1.57	3/9240 (0.0%)
2	F	1.05	0/6737	1.57	4/9089 (0.0%)
3	C	0.31	0/503	0.71	0/775
3	G	0.32	0/484	0.73	0/745
4	D	0.33	0/526	0.73	0/810
4	H	0.32	0/526	0.69	0/810
All	All	1.01	0/29356	1.53	11/39962 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	655	ILE	CA-C-N	5.63	123.78	120.24
2	F	655	ILE	C-N-CA	5.63	123.78	120.24
2	B	388	ILE	CA-C-N	5.51	125.40	121.65
2	B	388	ILE	C-N-CA	5.51	125.40	121.65
1	E	650	PHE	CA-C-N	5.27	126.19	122.60
1	E	650	PHE	C-N-CA	5.27	126.19	122.60
2	F	1094	GLU	CA-C-N	5.24	125.76	119.94
2	F	1094	GLU	C-N-CA	5.24	125.76	119.94
2	B	844	GLY	CA-C-O	-5.06	118.74	122.23
1	A	879	GLN	CA-C-N	5.06	125.59	119.98
1	A	879	GLN	C-N-CA	5.06	125.59	119.98

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	6570	0	6637	5	0
1	E	6956	0	7010	12	0
2	B	6721	0	6816	25	0
2	F	6618	0	6720	9	0
3	C	449	0	250	1	0
3	G	432	0	237	0	0
4	D	469	0	260	2	0
4	H	469	0	260	0	0
5	A	27	0	12	0	0
5	E	27	0	12	0	0
6	A	4	0	6	0	0
6	B	8	0	12	0	0
6	E	4	0	6	0	0
6	F	4	0	6	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	E	3	0	0	0	0
8	B	36	0	0	0	0
8	F	36	0	0	0	0
9	B	15	0	0	0	0
9	F	10	0	0	0	0
10	A	22	0	0	0	0
10	B	27	0	0	0	0
10	E	29	0	0	2	0
10	F	34	0	0	0	0
10	G	2	0	0	0	0
10	H	3	0	0	0	0
All	All	28977	0	28244	51	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 1.

All (51) 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:E:183:GLN:HG3	10:E:1111:HOH:O	1.97	0.63
1:E:470:VAL:HG21	1:E:577:ILE:HD11	1.82	0.61
2:B:1079:PRO:HG2	2:B:1082:ILE:HD13	1.89	0.54
2:F:891:VAL:HG21	2:F:998:ILE:HG12	1.91	0.52
2:B:884:LEU:HB3	2:B:1004:LEU:HD22	1.92	0.51
1:A:769:TYR:CD1	2:B:1082:ILE:HD11	2.45	0.51
2:F:747:VAL:HB	2:F:753:MET:HE1	1.93	0.51
2:B:747:VAL:HB	2:B:753:MET:HE1	1.94	0.49
2:B:548:LEU:HD21	2:B:581:THR:HG23	1.95	0.49
1:A:525:VAL:HG23	1:A:551:PHE:CE1	2.47	0.48
2:B:563:VAL:HG21	2:B:866:VAL:HA	1.95	0.48
2:B:564:LEU:HA	2:B:840:VAL:HG21	1.94	0.48
1:E:89:VAL:HG11	1:E:131:PHE:CD2	2.50	0.47
1:E:769:TYR:CE2	1:E:773:LYS:HD2	2.50	0.47
1:A:685:ILE:HG23	1:A:695:VAL:HB	1.96	0.47
2:B:878:VAL:HG21	2:B:1057:TYR:HB2	1.97	0.46
2:F:548:LEU:HD11	2:F:581:THR:HG22	1.98	0.46
2:F:563:VAL:HG21	2:F:866:VAL:HA	1.97	0.46
1:E:264:GLN:HE21	1:E:264:GLN:HA	1.81	0.46
3:C:6:DA:C2	4:D:47:DA:C2	3.05	0.45
2:B:548:LEU:HD21	2:B:581:THR:CG2	2.47	0.45
2:B:852:GLN:HE22	2:B:856:LYS:HD3	1.82	0.45
2:B:891:VAL:HG21	2:B:998:ILE:HG12	1.99	0.44
2:B:891:VAL:HG22	2:B:1005:THR:HB	1.99	0.44
2:B:607:VAL:HG22	2:B:658:ALA:HB1	2.00	0.43
1:E:769:TYR:CD2	2:F:1082:ILE:HD11	2.53	0.43
2:B:855:ARG:HD2	2:B:1004:LEU:HG	2.01	0.42
2:B:937:THR:HB	2:B:939:MET:HE3	2.00	0.42
2:B:254:TYR:O	2:B:287:THR:HG23	2.18	0.42
2:B:764:ILE:HD12	2:B:764:ILE:N	2.34	0.42
2:B:535:MET:HE2	2:B:583:PRO:HB2	2.02	0.42
1:E:414:LEU:HD21	1:E:595:LEU:HD11	2.01	0.42
1:E:678:TYR:O	1:E:681:GLN:HG2	2.20	0.42
2:F:254:TYR:O	2:F:287:THR:HG23	2.20	0.42
1:E:167:ASP:O	1:E:171:ARG:N	2.53	0.41
2:B:756:ILE:HG12	2:B:764:ILE:HD11	2.01	0.41
2:B:756:ILE:CG1	2:B:764:ILE:HD11	2.50	0.41
2:F:314:ALA:HB1	2:F:794:GLN:HG3	2.02	0.41
2:F:680:SER:N	2:F:681:PRO:CD	2.84	0.41
2:B:855:ARG:NE	2:B:968:SER:O	2.54	0.41
1:E:639:HIS:HB3	1:E:642:VAL:HB	2.02	0.41
1:A:438:THR:HB	1:A:439:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:SER:N	2:B:681:PRO:CD	2.84	0.41
2:F:426:LEU:HD13	2:F:440:ILE:HD12	2.02	0.41
4:D:39:DC:H2'	4:D:40:DT:C6	2.56	0.41
1:A:301:LYS:HB2	1:A:707:CYS:HB3	2.02	0.40
2:B:645:LEU:HD22	2:B:679:LEU:HD22	2.03	0.40
1:E:590:GLU:HB3	1:E:591:PRO:HD3	2.03	0.40
2:B:506:ILE:HG22	2:B:519:LEU:HD11	2.02	0.40
2:B:855:ARG:HD3	2:B:969:GLN:HA	2.04	0.40
1:E:227:ARG:NH2	10:E:1106:HOH:O	2.53	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	800/930 (86%)	772 (96%)	28 (4%)	0	100	100
1	E	861/930 (93%)	833 (97%)	28 (3%)	0	100	100
2	B	828/918 (90%)	798 (96%)	30 (4%)	0	100	100
2	F	812/918 (88%)	783 (96%)	28 (3%)	1 (0%)	48	75
All	All	3301/3696 (89%)	3186 (96%)	114 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	322	ARG

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	725/804 (90%)	722 (100%)	3 (0%)	84	93
1	E	764/804 (95%)	755 (99%)	9 (1%)	63	84
2	B	750/818 (92%)	744 (99%)	6 (1%)	73	89
2	F	738/818 (90%)	732 (99%)	6 (1%)	73	89
All	All	2977/3244 (92%)	2953 (99%)	24 (1%)	73	89

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	GLN
1	A	631	ARG
1	A	648	ILE
2	B	421	LEU
2	B	633	CYS
2	B	781	HIS
2	B	895	THR
2	B	938	ARG
2	B	1052	PHE
1	E	231	ASP
1	E	264	GLN
1	E	377	GLN
1	E	425	GLU
1	E	648	ILE
1	E	799	ASN
1	E	810	THR
1	E	846	GLN
1	E	908	LEU
2	F	421	LEU
2	F	633	CYS
2	F	660	ASN
2	F	809	ASP
2	F	895	THR
2	F	1082	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	GLN
1	A	298	GLN
1	A	344	GLN
1	A	395	GLN
1	A	451	GLN
1	A	566	ASN
1	A	681	GLN
1	A	885	GLN
2	B	242	GLN
2	B	271	ASN
2	B	514	ASN
2	B	524	ASN
2	B	591	ASN
2	B	794	GLN
2	B	852	GLN
2	B	1020	ASN
2	B	1071	ASN
1	E	97	GLN
1	E	127	ASN
1	E	139	ASN
1	E	264	GLN
1	E	288	GLN
1	E	339	GLN
1	E	348	GLN
1	E	397	GLN
1	E	412	ASN
1	E	429	GLN
1	E	451	GLN
1	E	566	ASN
1	E	681	GLN
1	E	783	HIS
1	E	885	GLN
1	E	903	ASN
2	F	242	GLN
2	F	288	HIS
2	F	549	GLN
2	F	750	GLN
2	F	798	GLN
2	F	861	ASN
2	F	1020	ASN
2	F	1071	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	$\# Z > 2$
6	EDO	A	1002	-	3,3,3	0.11	0	2,2,2	0.25	0
9	SO4	B	1203	-	4,4,4	0.34	0	6,6,6	0.08	0
5	ADP	E	1001	-	28,29,29	0.43	0	43,45,45	0.50	0
9	SO4	B	1205	-	4,4,4	0.33	0	6,6,6	0.07	0
9	SO4	F	1203	-	4,4,4	0.35	0	6,6,6	0.06	0
6	EDO	E	1004	-	3,3,3	0.11	0	2,2,2	0.29	0
6	EDO	B	1207	-	3,3,3	0.09	0	2,2,2	0.15	0
6	EDO	F	1204	-	3,3,3	0.05	0	2,2,2	0.17	0
8	YKQ	B	1201	-	40,40,40	0.62	0	56,56,56	2.65	18 (32%)
9	SO4	F	1202	-	4,4,4	0.37	0	6,6,6	0.14	0
8	YKQ	F	1201	-	40,40,40	0.76	1 (2%)	56,56,56	2.84	19 (33%)
5	ADP	A	1001	-	28,29,29	0.54	0	43,45,45	0.46	0
9	SO4	B	1202	-	4,4,4	0.33	0	6,6,6	0.09	0
6	EDO	B	1204	-	3,3,3	0.11	0	2,2,2	0.30	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
6	EDO	A	1002	-	-	1/1/1/1	-
5	ADP	E	1001	-	-	1/16/32/32	0/3/3/3
6	EDO	E	1004	-	-	1/1/1/1	-
6	EDO	B	1207	-	-	0/1/1/1	-
6	EDO	F	1204	-	-	1/1/1/1	-
8	YKQ	B	1201	-	-	6/18/34/34	0/5/5/5
8	YKQ	F	1201	-	-	4/18/34/34	0/5/5/5
5	ADP	A	1001	-	-	2/16/32/32	0/3/3/3
6	EDO	B	1204	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1201	YKQ	C13-N12	2.15	1.41	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1201	YKQ	C20-C15-N14	-10.17	118.52	127.10
8	F	1201	YKQ	C20-C15-N14	-9.18	119.36	127.10
8	F	1201	YKQ	C31-C29-N28	9.14	120.04	113.84
8	F	1201	YKQ	C15-C20-C21	6.80	119.27	114.94
8	F	1201	YKQ	C21-C20-C19	-6.46	133.52	139.87
8	B	1201	YKQ	C15-C20-C21	6.35	118.99	114.94
8	B	1201	YKQ	C31-C29-N28	5.46	117.55	113.84
8	F	1201	YKQ	C20-C15-N16	-4.96	105.51	108.33
8	F	1201	YKQ	N16-C15-N14	4.78	135.13	127.45
8	B	1201	YKQ	F37-C36-C8	4.63	122.78	118.37
8	F	1201	YKQ	C13-N34-C21	4.61	123.31	115.38
8	B	1201	YKQ	C36-C8-N5	4.41	125.58	120.42
8	B	1201	YKQ	C13-N34-C21	4.32	122.81	115.38
8	B	1201	YKQ	C21-C20-C19	-4.21	135.73	139.87
8	B	1201	YKQ	O22-C21-C20	4.19	122.11	116.26
8	F	1201	YKQ	C15-N16-C18	4.13	110.49	108.11
8	B	1201	YKQ	C9-C8-N5	-4.09	116.01	122.42
8	B	1201	YKQ	N16-C15-N14	3.94	133.79	127.45
8	B	1201	YKQ	C35-C36-C8	-3.61	120.16	123.35
8	F	1201	YKQ	C35-C36-C8	-3.47	120.29	123.35
8	F	1201	YKQ	N34-C13-N14	-3.45	120.60	126.26
8	F	1201	YKQ	C11-N12-C13	-3.29	120.50	129.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1201	YKQ	C6-N5-C8	-3.24	108.48	116.19
8	F	1201	YKQ	C9-C8-N5	-3.08	117.60	122.42
8	B	1201	YKQ	N34-C13-N14	-3.03	121.29	126.26
8	F	1201	YKQ	O22-C21-N34	2.71	124.16	119.61
8	B	1201	YKQ	C11-C35-C36	2.62	121.01	118.82
8	B	1201	YKQ	C20-C21-N34	-2.59	117.18	122.39
8	F	1201	YKQ	O30-C29-C31	-2.56	118.87	122.70
8	F	1201	YKQ	C20-C21-N34	-2.52	117.33	122.39
8	B	1201	YKQ	C15-N16-C18	2.44	109.52	108.11
8	F	1201	YKQ	C36-C8-N5	2.42	123.25	120.42
8	F	1201	YKQ	F37-C36-C8	2.30	120.56	118.37
8	B	1201	YKQ	C15-C20-C19	-2.26	105.28	106.40
8	B	1201	YKQ	C27-N28-C29	-2.05	124.21	128.07
8	F	1201	YKQ	C32-C31-C29	-2.05	119.97	122.22
8	F	1201	YKQ	C23-O22-C21	2.01	122.62	118.27

There are no chirality outliers.

All (17) torsion outliers are listed below:

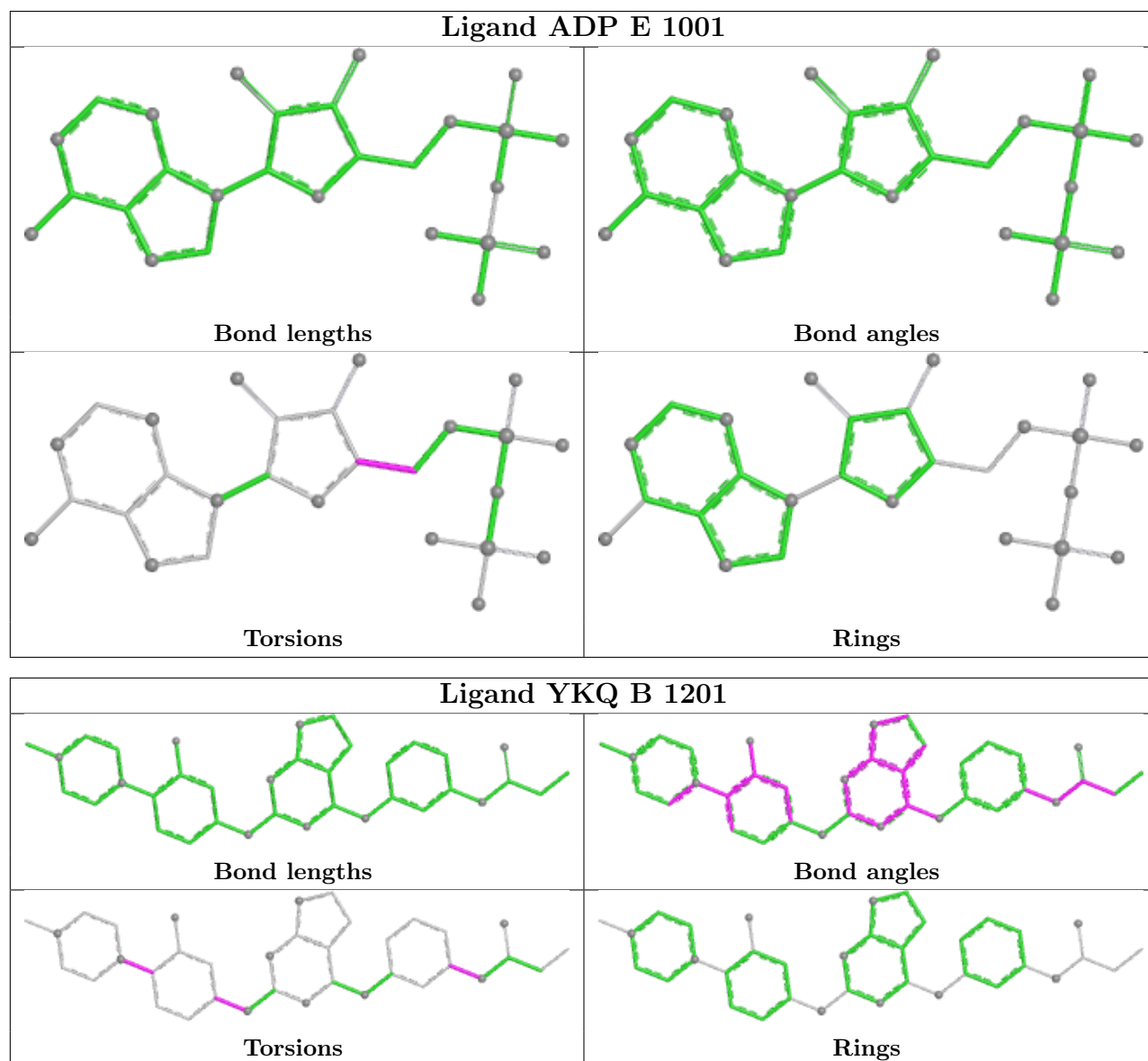
Mol	Chain	Res	Type	Atoms
8	B	1201	YKQ	C36-C8-N5-C6
8	B	1201	YKQ	C26-C27-N28-C29
8	B	1201	YKQ	C33-C27-N28-C29
5	E	1001	ADP	O4'-C4'-C5'-O5'
8	B	1201	YKQ	C35-C11-N12-C13
8	F	1201	YKQ	C33-C27-N28-C29
8	B	1201	YKQ	C10-C11-N12-C13
8	F	1201	YKQ	C35-C11-N12-C13
8	F	1201	YKQ	C26-C27-N28-C29
5	A	1001	ADP	PB-O3A-PA-O1A
5	A	1001	ADP	PB-O3A-PA-O2A
8	F	1201	YKQ	C10-C11-N12-C13
8	B	1201	YKQ	C9-C8-N5-C6
6	A	1002	EDO	O1-C1-C2-O2
6	B	1204	EDO	O1-C1-C2-O2
6	F	1204	EDO	O1-C1-C2-O2
6	E	1004	EDO	O1-C1-C2-O2

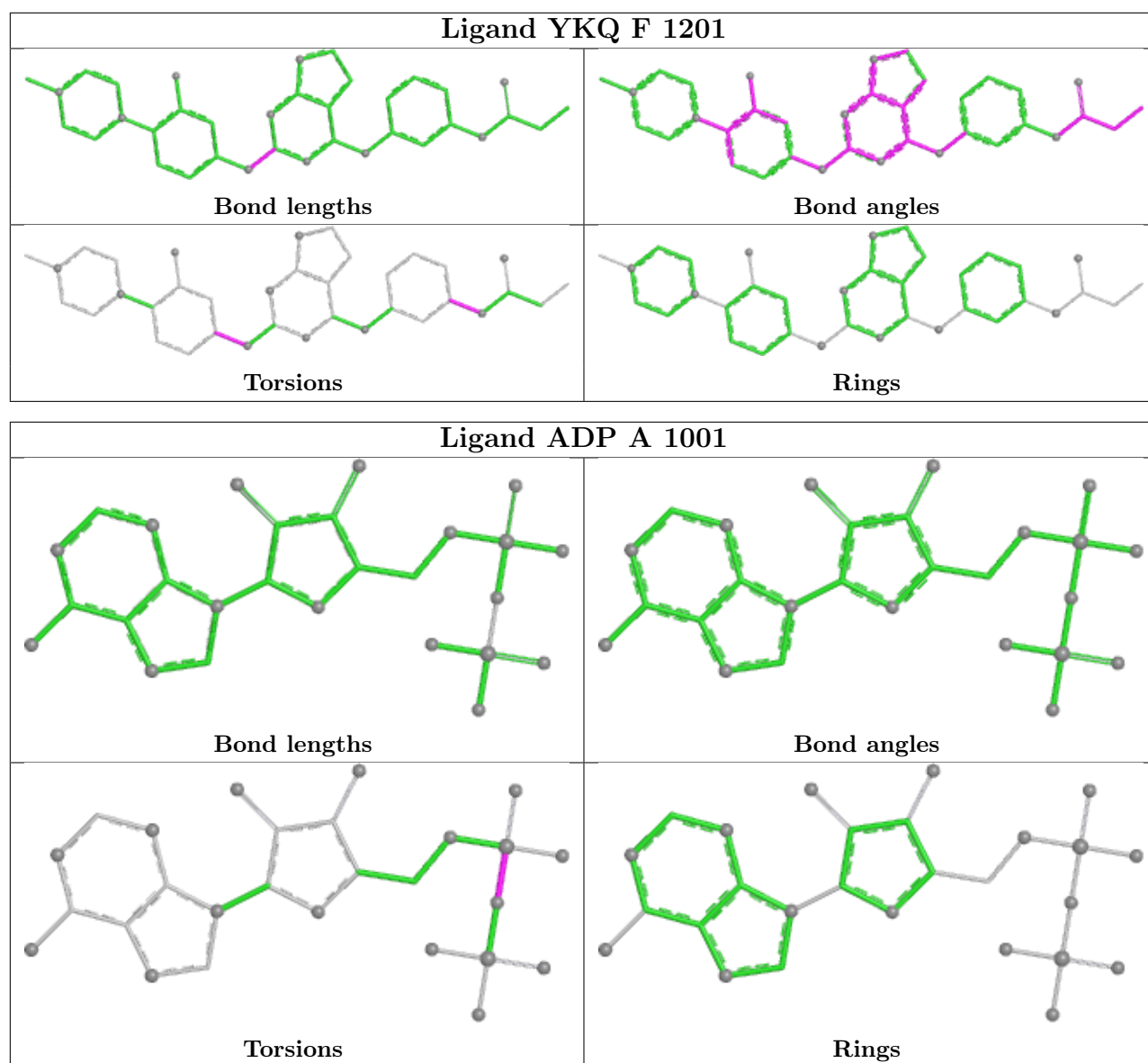
There are no ring outliers.

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	825/930 (88%)	0.64	72 (8%) 16 13	25, 64, 118, 168	124 (15%)
1	E	875/930 (94%)	0.50	51 (5%) 29 24	24, 59, 108, 138	123 (14%)
2	B	840/918 (91%)	0.25	24 (2%) 53 46	25, 54, 87, 139	67 (7%)
2	F	827/918 (90%)	0.75	97 (11%) 9 7	31, 64, 113, 159	132 (15%)
3	C	22/24 (91%)	0.39	1 (4%) 38 32	53, 97, 141, 145	0
3	G	21/24 (87%)	-0.02	0 100 100	41, 81, 130, 145	0
4	D	23/24 (95%)	0.16	0 100 100	47, 93, 136, 146	0
4	H	23/24 (95%)	0.11	1 (4%) 40 33	43, 70, 140, 161	0
All	All	3456/3792 (91%)	0.53	246 (7%) 22 17	24, 60, 111, 168	446 (12%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	490	SER	4.8
2	F	774	THR	4.7
2	F	1069	GLY	4.4
1	E	503	LEU	4.3
1	E	504	GLY	4.2
1	E	547	ASN	4.1
1	A	488	LEU	4.1
1	A	855	GLN	4.1
2	F	492	ILE	4.1
2	F	668	LEU	4.0
1	A	523	PHE	4.0
1	E	856	TYR	3.9
2	B	362	ASP	3.9
2	F	711	LEU	3.9
1	E	526	THR	3.9
1	E	517	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	514	ASP	3.7
2	F	682	VAL	3.7
2	F	655	ILE	3.7
2	F	675	ILE	3.6
1	A	522	TYR	3.6
2	F	1055	PHE	3.6
1	A	551	PHE	3.6
1	A	509	LYS	3.6
2	F	658	ALA	3.5
1	A	481	LEU	3.5
2	B	448	VAL	3.5
2	F	615	LEU	3.4
2	F	707	SER	3.4
2	B	490	SER	3.3
2	F	597	VAL	3.3
1	E	725	PHE	3.3
2	F	607	VAL	3.3
2	F	652	PHE	3.3
2	F	851	VAL	3.3
1	E	533	LEU	3.2
2	F	828	LEU	3.2
1	E	552	THR	3.2
1	A	463	VAL	3.2
1	E	492	MET	3.2
2	F	605	SER	3.2
2	F	671	VAL	3.2
1	A	581	ILE	3.1
2	B	1032	PHE	3.1
1	A	873	CYS	3.1
2	F	449	GLN	3.1
1	E	926	ILE	3.1
2	F	1072	VAL	3.0
1	A	559	LEU	3.0
1	E	929	ARG	3.0
2	F	1066	ARG	3.0
1	A	582	VAL	3.0
1	A	840	VAL	3.0
2	F	594	LEU	3.0
2	F	650	SER	3.0
1	A	465	ASN	3.0
2	F	646	TYR	3.0
2	F	657	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	3.0
1	A	648	ILE	3.0
1	E	828	ILE	3.0
1	A	578	VAL	3.0
2	F	678	LEU	3.0
1	A	562	GLU	3.0
1	E	507	PRO	2.9
1	A	133	ASP	2.9
1	A	492	MET	2.9
1	A	169	ILE	2.9
1	A	510	GLN	2.9
2	F	600	VAL	2.9
1	A	540	SER	2.9
2	F	666	ASP	2.9
1	A	70	ALA	2.9
2	F	598	SER	2.9
1	A	399	ALA	2.9
1	A	567	LYS	2.9
2	F	446	VAL	2.9
1	A	114	GLU	2.8
1	E	501	ARG	2.8
1	A	561	GLU	2.8
1	E	588	TYR	2.8
2	F	1014	VAL	2.8
1	A	756	THR	2.8
1	E	488	LEU	2.8
1	E	751	GLY	2.8
2	B	1033	LEU	2.8
2	F	1075	LEU	2.8
1	E	530	GLU	2.8
2	F	448	VAL	2.8
1	E	546	LYS	2.7
1	A	489	GLU	2.7
1	A	493	GLN	2.7
2	F	656	ILE	2.7
2	F	667	LEU	2.7
2	F	653	GLN	2.7
1	E	505	LEU	2.7
2	F	674	GLU	2.7
1	E	154	ALA	2.7
2	F	477	ALA	2.7
1	A	646	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	608	PHE	2.7
1	E	491	LYS	2.7
2	F	534	PHE	2.7
1	E	930	ILE	2.6
2	B	492	ILE	2.6
1	E	210	MET	2.6
2	B	532	MET	2.6
2	F	837	LEU	2.6
1	A	464	GLU	2.6
1	E	155	VAL	2.6
2	F	611	ILE	2.6
2	F	921	TYR	2.6
2	F	1088[A]	HIS	2.6
2	B	446	VAL	2.6
1	A	476	PRO	2.6
1	E	497	ILE	2.6
1	A	483	GLU	2.6
1	A	398	ALA	2.6
2	F	672	ILE	2.6
2	F	877	TYR	2.6
2	F	1056	LEU	2.5
1	A	874	TYR	2.5
2	B	344	VAL	2.5
2	F	493	VAL	2.5
1	A	896	PHE	2.5
1	A	554	SER	2.5
2	F	651	GLU	2.5
2	F	838	ALA	2.5
1	E	477	ASN	2.5
1	E	498	SER	2.5
2	F	601	LEU	2.5
1	A	207	ALA	2.5
1	A	289	PHE	2.5
1	E	869	ALA	2.5
1	A	486	ASN	2.5
1	E	534	ARG	2.5
2	F	529	SER	2.5
2	B	449	GLN	2.5
1	E	153	SER	2.4
2	F	602	HIS	2.4
2	F	845	ASP	2.4
2	F	229	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	207	ALA	2.4
1	A	752	ARG	2.4
1	E	478	LEU	2.4
2	F	663	ILE	2.4
2	F	1119	LEU	2.4
2	F	866	VAL	2.4
1	A	401	LEU	2.4
1	A	457	THR	2.4
2	F	661	SER	2.4
1	A	460	MET	2.4
2	F	750	GLN	2.4
1	A	511	ILE	2.4
2	B	711	LEU	2.4
2	F	590	ILE	2.4
2	B	467	HIS	2.4
2	B	1115	ASN	2.4
2	B	249	CYS	2.4
2	B	1034	VAL	2.4
1	E	484	ILE	2.3
2	F	447	SER	2.3
1	A	482	ARG	2.3
2	F	551	GLN	2.3
2	F	582	GLN	2.3
1	E	897	THR	2.3
2	F	524	ASN	2.3
1	A	474	PHE	2.3
1	E	481	LEU	2.3
1	E	559	LEU	2.3
2	F	824	ALA	2.3
2	B	774	THR	2.3
2	F	536	THR	2.3
1	A	871	LYS	2.3
1	A	872	LYS	2.3
1	A	507	PRO	2.3
2	F	664	GLN	2.3
1	A	470	VAL	2.3
1	A	913	ALA	2.3
4	H	27	DC	2.3
2	F	1068	TYR	2.3
2	F	835	PHE	2.3
1	E	14	ALA	2.2
1	E	299	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	759	SER	2.2
1	E	426	GLY	2.2
1	A	491	LYS	2.2
2	B	252	CYS	2.2
2	F	670	THR	2.2
1	E	515	SER	2.2
1	A	525	VAL	2.2
1	A	746	ILE	2.2
1	A	785[A]	HIS	2.2
1	E	867	GLU	2.2
2	F	599	GLU	2.2
1	E	543	ASP	2.2
2	F	450	ASP	2.2
1	A	425	GLU	2.2
1	A	526	THR	2.2
1	A	527	CYS	2.2
1	A	472	PRO	2.2
1	A	835	ASN	2.2
2	F	681	PRO	2.2
2	F	862	GLY	2.2
2	B	239	MET	2.2
2	F	387	PHE	2.2
2	B	776	ALA	2.1
1	E	16	GLU	2.1
2	B	1124	GLU	2.1
2	F	683	GLU	2.1
1	A	555	LYS	2.1
2	F	659	VAL	2.1
1	A	480	GLU	2.1
1	A	807	THR	2.1
1	E	495	THR	2.1
2	F	1120	GLN	2.1
1	A	469	LEU	2.1
2	F	673	LEU	2.1
2	F	706	LEU	2.1
2	B	341	GLY	2.1
1	E	145	ILE	2.1
2	F	1114	HIS	2.1
2	F	649	LYS	2.1
2	F	735	LYS	2.1
2	F	870	LEU	2.1
1	A	553	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	847	CYS	2.1
2	F	1020	ASN	2.1
2	B	1052	PHE	2.1
2	F	868	ASP	2.1
2	B	435	GLN	2.1
1	A	458	LEU	2.1
2	F	648	LEU	2.1
2	F	252	CYS	2.1
1	E	169	ILE	2.1
3	C	3	DT	2.0
2	F	1100	LYS	2.0
1	E	294[A]	PHE	2.0
1	E	396	ARG	2.0
2	B	534	PHE	2.0
2	F	841	ALA	2.0
1	A	585	SER	2.0
1	E	117	TRP	2.0
2	F	676	PRO	2.0
1	A	513	LEU	2.0
2	F	1117	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

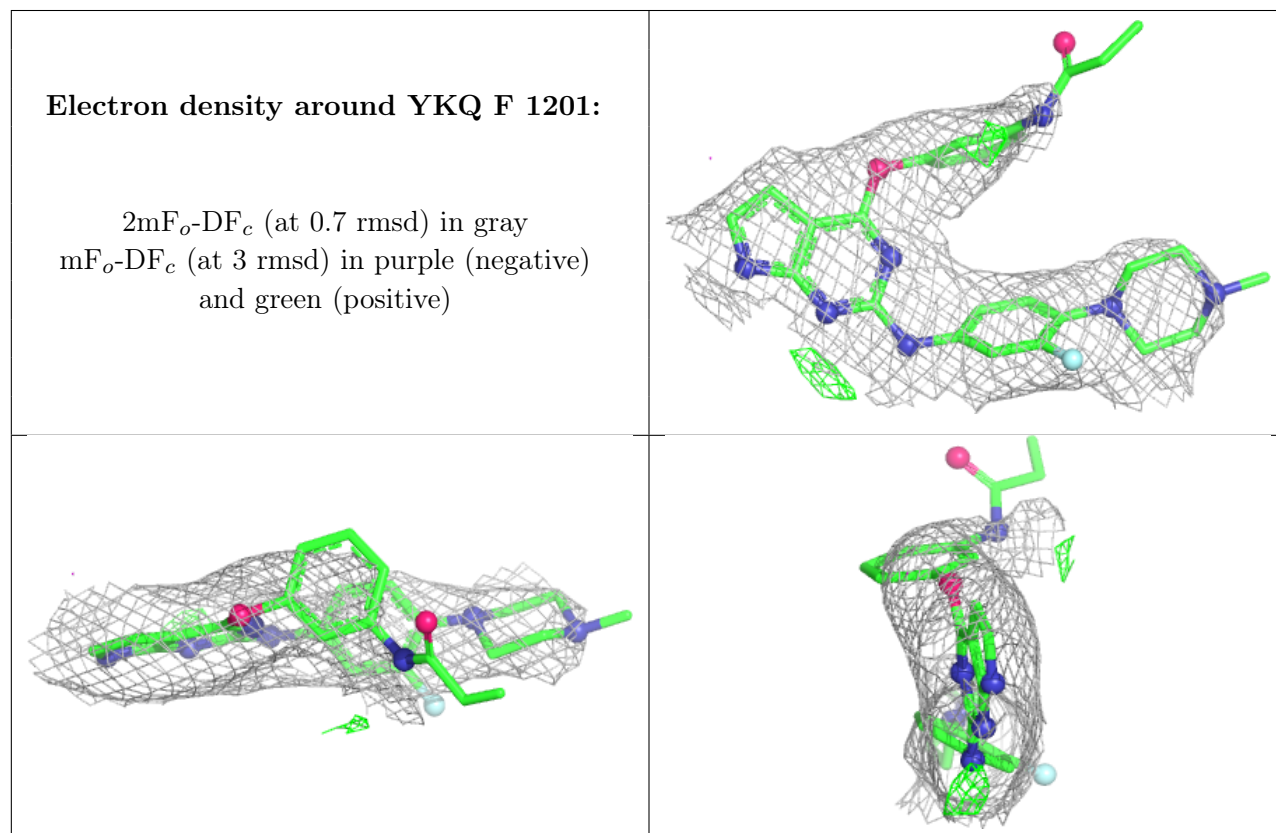
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SO4	F	1203	5/5	0.77	0.09	127,128,130,132	0
9	SO4	B	1203	5/5	0.81	0.09	110,111,112,112	0
9	SO4	F	1202	5/5	0.84	0.14	91,92,94,100	0

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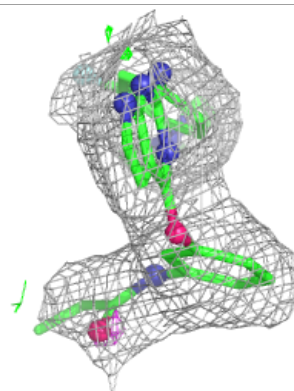
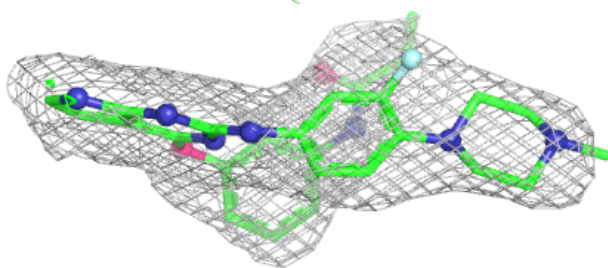
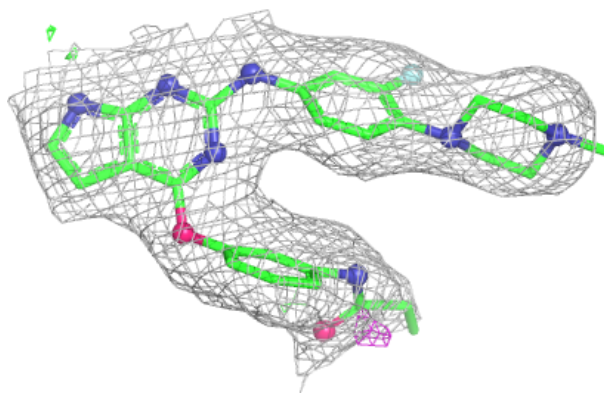
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	YKQ	F	1201	36/36	0.85	0.14	70,90,105,108	5
6	EDO	A	1002	4/4	0.87	0.21	66,69,70,70	0
7	CL	E	1002	1/1	0.90	0.09	74,74,74,74	0
9	SO4	B	1205	5/5	0.90	0.12	102,104,106,106	0
6	EDO	B	1204	4/4	0.91	0.10	46,47,47,47	0
6	EDO	E	1004	4/4	0.91	0.14	63,63,63,64	0
6	EDO	B	1207	4/4	0.93	0.14	56,57,57,59	0
7	CL	E	1005	1/1	0.93	0.06	78,78,78,78	0
8	YKQ	B	1201	36/36	0.93	0.10	45,57,75,77	0
5	ADP	E	1001	27/27	0.93	0.07	52,57,61,62	0
6	EDO	F	1204	4/4	0.94	0.12	44,45,46,48	0
9	SO4	B	1202	5/5	0.94	0.11	70,72,74,74	0
5	ADP	A	1001	27/27	0.94	0.07	43,48,56,59	0
7	CL	A	1003	1/1	0.96	0.05	57,57,57,57	0
7	CL	B	1206	1/1	0.97	0.05	63,63,63,63	0
7	CL	E	1003	1/1	0.97	0.05	76,76,76,76	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.

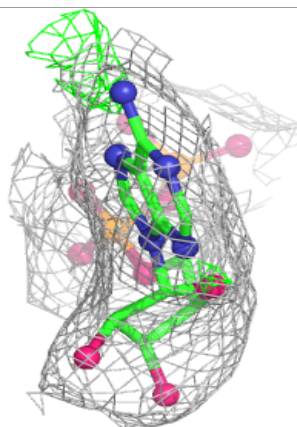
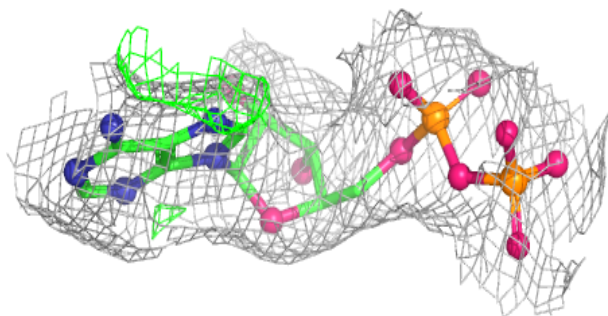
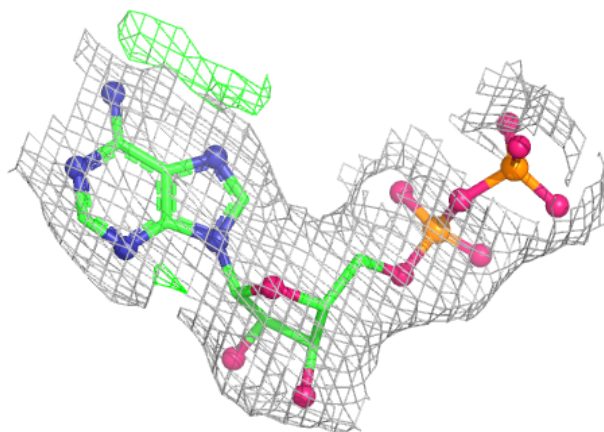


Electron density around YKQ B 1201:

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

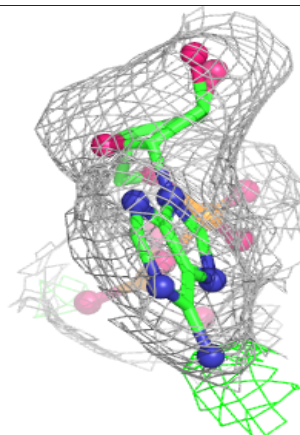
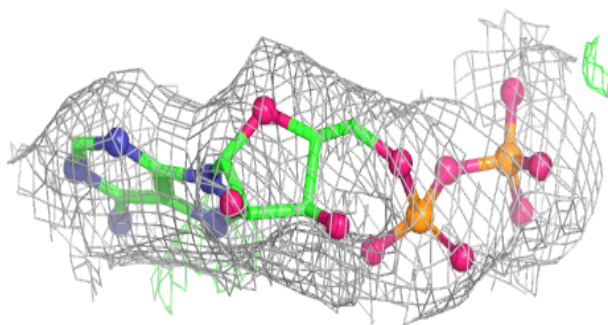
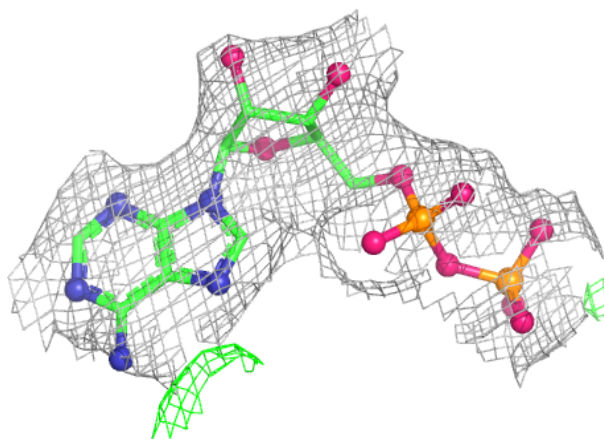
**Electron density around ADP E 1001:**

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



Electron density around ADP A 1001:

$2mF_o-DF_c$ (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.