



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:05 PM EDT

PDB ID : 6Q93 / pdb_00006q93
Title : MgADP-bound Fe protein of Vanadium nitrogenase from *Azotobacter vinelandii*
Authors : Rohde, M.; Gerhardt, S.; Einsle, O.
Deposited on : 2018-12-17
Resolution : 2.20 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:

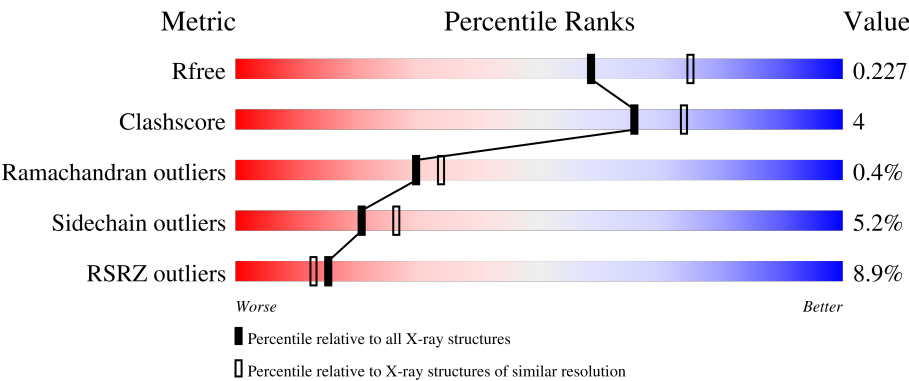
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	290	2% 85% 9% • 5%
1	B	290	39% 78% 14% • 6%
1	C	290	7% 85% 10% • • •
1	D	290	2% 84% 8% • 6%
1	E	290	7% 83% 11% • 5%

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Mol	Chain	Length	Quality of chain
1	F	290	4% 82% 10% 6%
1	G	290	3% 84% 9% 6%
1	H	290	5% 87% 12% ..

2 Entry composition

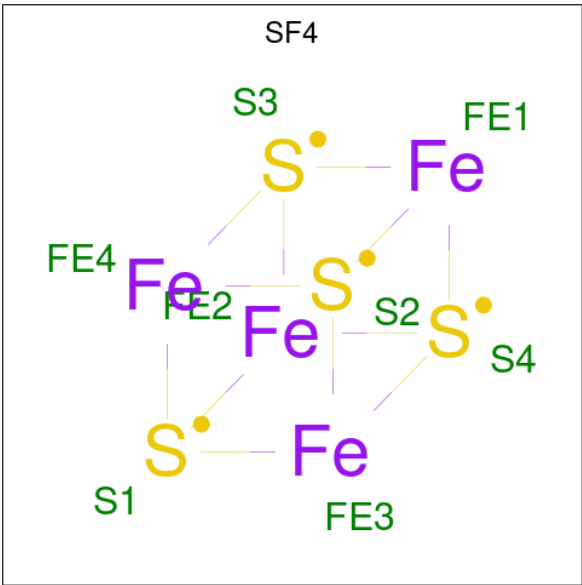
There are 5 unique types of molecules in this entry. The entry contains 17188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrogenase iron protein.

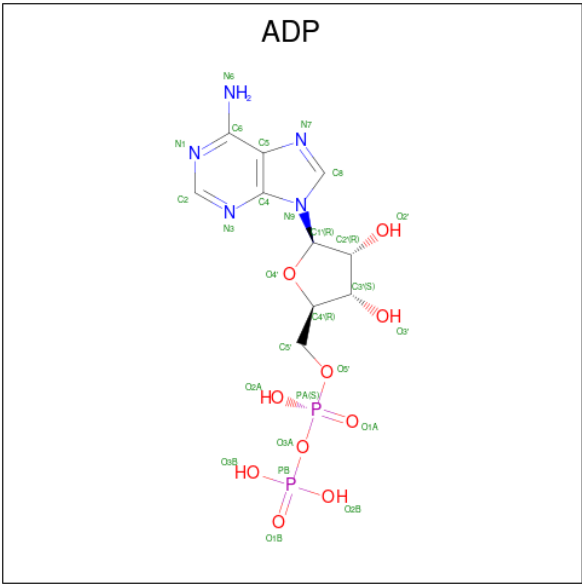
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2067	1295	352	400	20			
1	B	274	Total	C	N	O	S	0	0	0
			2043	1278	347	398	20			
1	C	284	Total	C	N	O	S	0	0	0
			2123	1328	361	414	20			
1	D	272	Total	C	N	O	S	0	0	0
			2029	1271	345	394	19			
1	E	275	Total	C	N	O	S	0	0	0
			2060	1290	351	399	20			
1	F	273	Total	C	N	O	S	0	0	0
			2043	1280	349	395	19			
1	G	272	Total	C	N	O	S	0	0	0
			2035	1274	348	394	19			
1	H	287	Total	C	N	O	S	0	0	0
			2141	1339	364	418	20			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	2	Total	Mg	0	0
			2	2		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	2	Total	Mg	0	0
			2	2		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	25	Total	O	0	0
			25	25		

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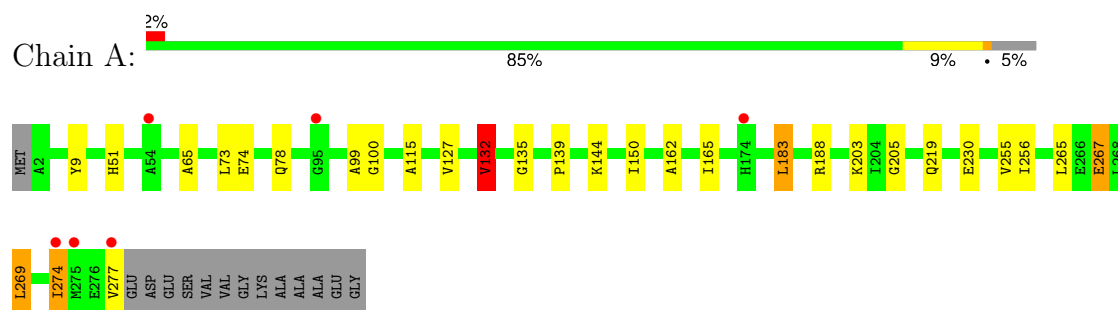
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	54	Total 54	O 54	0	0
5	D	37	Total 37	O 37	0	0
5	E	29	Total 29	O 29	0	0
5	F	81	Total 81	O 81	0	0
5	G	36	Total 36	O 36	0	0
5	H	53	Total 53	O 53	0	0

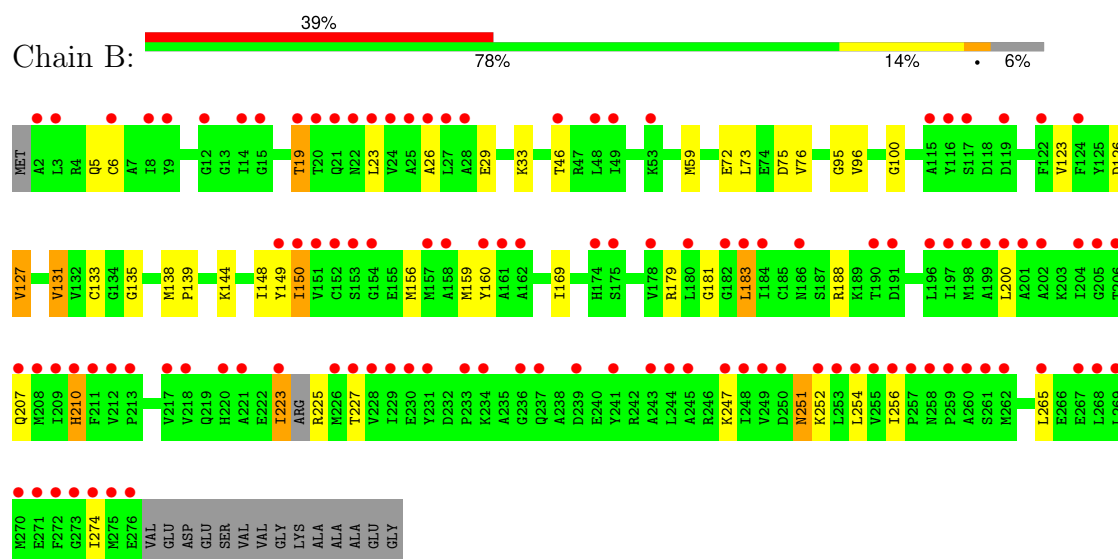
3 Residue-property plots [i](#)

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

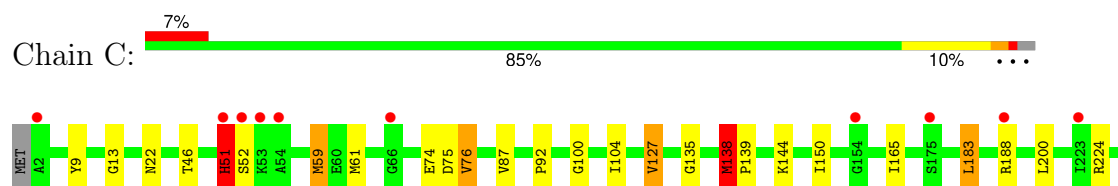
• Molecule 1: Nitrogenase iron protein

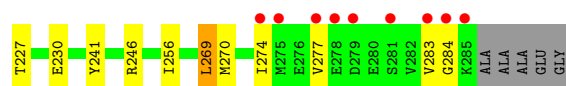


• Molecule 1: Nitrogenase iron protein

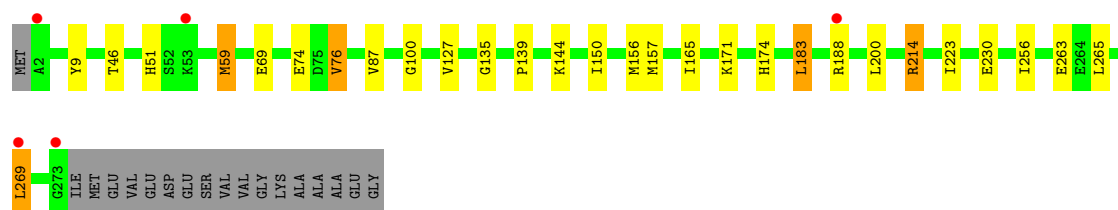
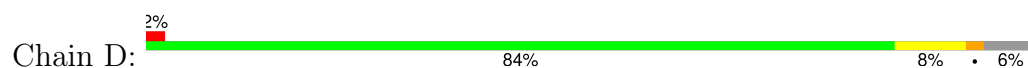


• Molecule 1: Nitrogenase iron protein

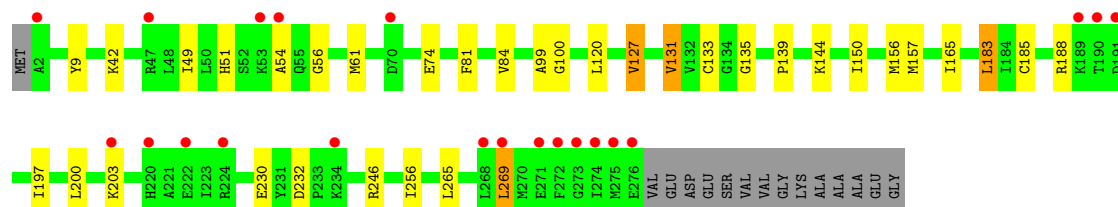
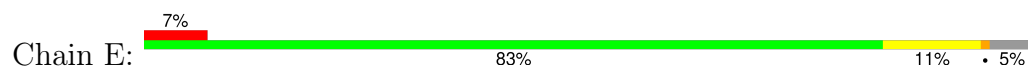




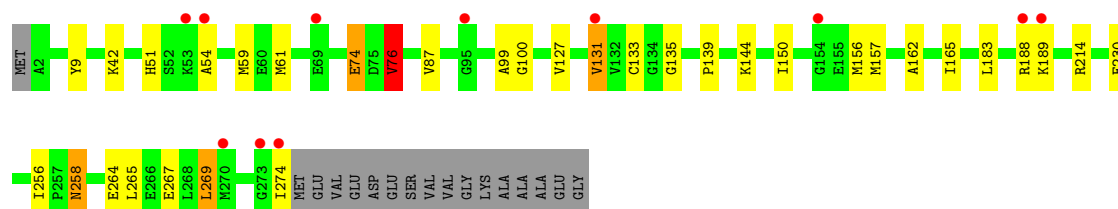
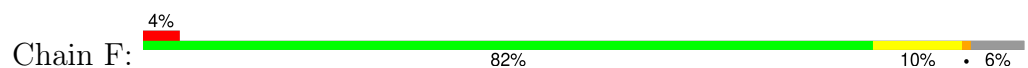
• Molecule 1: Nitrogenase iron protein



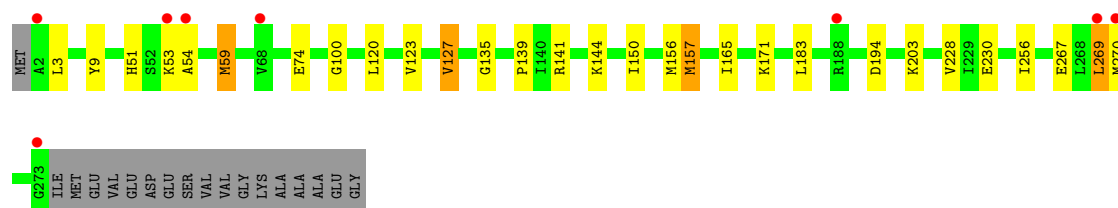
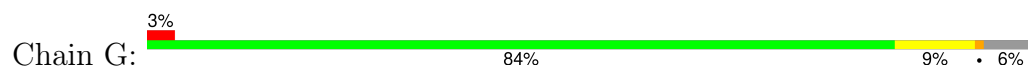
• Molecule 1: Nitrogenase iron protein



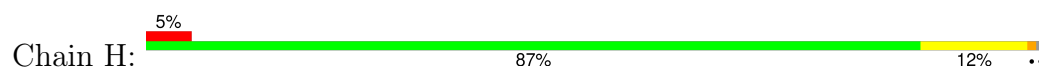
• Molecule 1: Nitrogenase iron protein

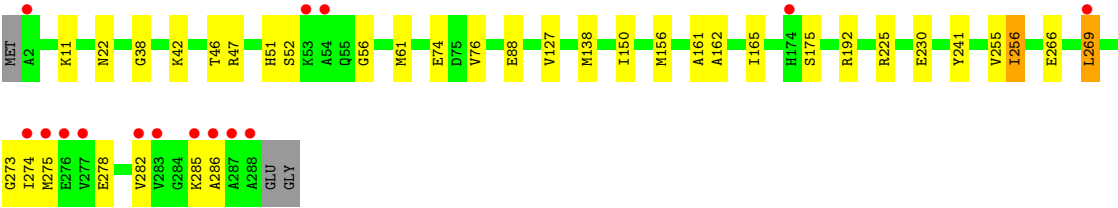


• Molecule 1: Nitrogenase iron protein



• Molecule 1: Nitrogenase iron protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	94.57Å 176.86Å 354.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.20 49.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.10-2.20) 99.9 (49.10-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.200 , 0.215 0.209 , 0.227	Depositor DCC
R_{free} test set	7601 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17188	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SF4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.83	0/2093	1.28	4/2819 (0.1%)
1	B	0.85	0/2067	1.37	11/2783 (0.4%)
1	C	0.85	1/2149 (0.0%)	1.29	7/2894 (0.2%)
1	D	0.79	0/2055	1.28	5/2769 (0.2%)
1	E	0.80	0/2086	1.31	3/2809 (0.1%)
1	F	0.80	0/2069	1.30	4/2787 (0.1%)
1	G	0.78	1/2061 (0.0%)	1.28	5/2776 (0.2%)
1	H	0.83	0/2167	1.31	4/2919 (0.1%)
All	All	0.82	2/16747 (0.0%)	1.30	43/22556 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	157	MET	SD-CE	-5.54	1.65	1.79
1	C	138	MET	SD-CE	-5.45	1.66	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	ILE	N-CA-C	-9.63	98.79	107.56
1	D	256	ILE	N-CA-C	-9.57	98.85	107.56
1	B	256	ILE	N-CA-C	-9.51	98.91	107.56
1	H	256	ILE	N-CA-C	-9.43	98.97	107.56
1	E	256	ILE	N-CA-C	-9.26	99.13	107.56
1	A	256	ILE	N-CA-C	-9.22	99.17	107.56
1	F	256	ILE	N-CA-C	-8.77	99.58	107.56
1	G	256	ILE	N-CA-C	-8.24	100.06	107.56
1	H	46	THR	CA-C-N	7.13	130.15	120.38
1	H	46	THR	C-N-CA	7.13	130.15	120.38
1	B	73	LEU	CA-C-N	6.82	129.73	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	LEU	C-N-CA	6.82	129.73	120.38
1	D	214	ARG	CB-CG-CD	6.65	126.59	111.30
1	A	267	GLU	CB-CG-CD	6.57	123.77	112.60
1	F	258	ASN	CA-CB-CG	6.43	119.03	112.60
1	G	127	VAL	N-CA-C	6.35	117.06	108.17
1	B	127	VAL	N-CA-C	5.89	117.07	108.58
1	E	127	VAL	N-CA-C	5.88	116.39	108.17
1	C	127	VAL	N-CA-C	5.80	116.29	108.17
1	B	19	THR	CA-C-N	5.75	128.78	120.79
1	B	19	THR	C-N-CA	5.75	128.78	120.79
1	F	127	VAL	N-CA-C	5.70	116.15	108.17
1	B	46	THR	CA-C-N	5.69	132.41	121.54
1	B	46	THR	C-N-CA	5.69	132.41	121.54
1	H	127	VAL	N-CA-C	5.63	116.06	108.17
1	D	127	VAL	N-CA-C	5.58	115.98	108.17
1	B	75	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	150	ILE	N-CA-C	5.50	115.91	107.77
1	F	76	VAL	N-CA-CB	-5.49	102.18	111.23
1	A	127	VAL	N-CA-C	5.46	115.81	108.17
1	A	132	VAL	CB-CA-C	5.28	117.72	111.59
1	B	126	ASP	CA-CB-CG	5.25	117.85	112.60
1	D	46	THR	CA-C-N	5.20	127.51	120.38
1	D	46	THR	C-N-CA	5.20	127.51	120.38
1	E	232	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	227	THR	N-CA-C	-5.11	103.66	110.55
1	C	51	HIS	CA-C-N	5.06	131.20	121.54
1	C	51	HIS	C-N-CA	5.06	131.20	121.54
1	G	194	ASP	CA-CB-CG	5.03	117.62	112.60
1	C	46	THR	CA-C-N	5.02	127.32	120.54
1	C	46	THR	C-N-CA	5.02	127.32	120.54
1	G	228	VAL	CA-C-N	5.01	127.60	120.53
1	G	228	VAL	C-N-CA	5.01	127.60	120.53

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	2067	0	2078	15	0
1	B	2043	0	2048	17	0
1	C	2123	0	2123	17	0
1	D	2029	0	2032	13	0
1	E	2060	0	2070	27	0
1	F	2043	0	2054	24	0
1	G	2035	0	2043	17	0
1	H	2141	0	2148	17	0
2	A	8	0	0	0	0
2	C	8	0	0	0	0
2	E	8	0	0	0	0
2	G	8	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	74	0	0	0	0
5	B	25	0	0	0	0
5	C	54	0	0	0	0
5	D	37	0	0	1	0
5	E	29	0	0	0	0
5	F	81	0	0	0	0
5	G	36	0	0	0	0
5	H	53	0	0	0	0
All	All	17188	0	16692	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (126) 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:157:MET:HA	1:E:157:MET:HE2	1.52	0.91
1:G:157:MET:HA	1:G:157:MET:HE2	1.52	0.91
1:B:207:GLN:HE22	1:B:251:ASN:HD21	1.22	0.87
1:E:49:ILE:HG21	1:E:84:VAL:HG23	1.57	0.86
1:F:157:MET:HA	1:F:157:MET:HE2	1.56	0.84
1:E:81:PHE:O	1:E:84:VAL:HG22	1.81	0.80
1:E:49:ILE:CG2	1:E:84:VAL:HG23	2.12	0.79
1:C:269:LEU:HD23	1:C:274:ILE:HB	1.68	0.73
1:E:49:ILE:CG2	1:E:84:VAL:CG2	2.67	0.72
1:B:156:MET:HE3	1:B:160:TYR:HB2	1.73	0.70
1:D:214:ARG:HD3	3:D:301:ADP:C2	2.25	0.70
1:F:74:GLU:HG3	1:G:141:ARG:HG2	1.71	0.70
1:E:49:ILE:HG21	1:E:84:VAL:CG2	2.21	0.69
1:F:61:MET:HE1	1:G:171:LYS:HE2	1.73	0.69
1:A:269:LEU:HD23	1:A:274:ILE:HB	1.74	0.69
1:C:270:MET:HE3	1:C:277:VAL:HA	1.76	0.68
1:G:100:GLY:O	1:G:135:GLY:HA3	1.96	0.66
1:C:51:HIS:CE1	1:C:230:GLU:OE1	2.51	0.64
1:A:51:HIS:HE1	1:A:230:GLU:OE1	1.80	0.63
1:E:157:MET:HE1	1:F:42:LYS:HD2	1.79	0.63
1:F:51:HIS:HE1	1:F:230:GLU:OE1	1.81	0.63
1:G:157:MET:HE3	1:H:42:LYS:HE3	1.82	0.61
1:D:51:HIS:HE1	1:D:230:GLU:OE1	1.84	0.61
1:E:51:HIS:HE1	1:E:230:GLU:OE2	1.84	0.61
1:E:157:MET:HE3	1:F:42:LYS:HE3	1.84	0.60
1:H:51:HIS:HE1	1:H:230:GLU:OE1	1.85	0.59
1:E:99:ALA:CB	1:F:131:VAL:HG22	2.33	0.59
1:E:42:LYS:HE3	1:F:157:MET:HE3	1.84	0.58
1:E:49:ILE:HG23	1:E:84:VAL:CG2	2.32	0.58
1:B:156:MET:CE	1:B:160:TYR:HB2	2.34	0.57
1:G:51:HIS:HE1	1:G:230:GLU:OE1	1.87	0.57
1:H:269:LEU:HD23	1:H:274:ILE:HB	1.87	0.57
1:C:51:HIS:HE1	1:C:230:GLU:OE1	1.89	0.55
1:F:189:LYS:HE2	1:F:214:ARG:HG2	1.89	0.55
1:B:156:MET:HA	1:B:159:MET:HE2	1.90	0.54
1:B:150:ILE:HB	1:B:183:LEU:HD12	1.91	0.53
1:C:224:ARG:NH2	1:H:51:HIS:HB3	2.24	0.53
1:A:9:TYR:HB3	1:A:165:ILE:HD13	1.91	0.52
1:E:157:MET:CE	1:F:42:LYS:HD2	2.38	0.52
1:A:65:ALA:HA	1:C:92:PRO:HB3	1.91	0.52
1:G:267:GLU:HA	1:G:270:MET:HE3	1.92	0.52
1:E:157:MET:CE	1:F:42:LYS:HE3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:LEU:HD11	1:G:123:VAL:HG23	1.92	0.52
1:G:157:MET:HE1	1:H:42:LYS:HD2	1.91	0.51
1:A:99:ALA:CB	1:B:131:VAL:HG22	2.41	0.51
1:B:131:VAL:HG13	1:B:133:CYS:SG	2.51	0.50
1:C:9:TYR:HB3	1:C:165:ILE:HD13	1.93	0.50
1:G:9:TYR:HB3	1:G:165:ILE:HD13	1.93	0.50
1:G:157:MET:HA	1:G:157:MET:CE	2.35	0.50
1:E:9:TYR:HB3	1:E:165:ILE:HD13	1.94	0.50
1:C:13:GLY:CA	1:D:157:MET:HG3	2.42	0.50
1:E:51:HIS:CE1	1:E:230:GLU:OE2	2.63	0.49
1:A:132:VAL:HG22	1:B:95:GLY:HA2	1.95	0.49
1:F:9:TYR:HB3	1:F:165:ILE:HD13	1.93	0.49
1:F:157:MET:HA	1:F:157:MET:CE	2.38	0.49
1:F:51:HIS:CE1	1:F:230:GLU:OE1	2.65	0.49
1:E:131:VAL:HG13	1:E:133:CYS:SG	2.52	0.48
1:B:139:PRO:HA	1:B:144:LYS:HB2	1.96	0.48
1:A:51:HIS:CE1	1:A:230:GLU:OE1	2.65	0.48
1:E:185:CYS:HB2	1:E:197:ILE:HG21	1.94	0.48
1:D:100:GLY:O	1:D:135:GLY:HA3	2.14	0.48
1:F:100:GLY:O	1:F:135:GLY:HA3	2.13	0.48
1:C:150:ILE:HB	1:C:183:LEU:HD12	1.96	0.48
1:H:51:HIS:CE1	1:H:230:GLU:OE1	2.67	0.48
1:B:210:HIS:CD2	1:B:247:LYS:HD3	2.48	0.48
1:B:5:GLN:HG2	1:B:123:VAL:HB	1.95	0.47
1:E:131:VAL:HG22	1:F:99:ALA:CB	2.45	0.47
1:H:266:GLU:HG2	1:H:275:MET:HE1	1.96	0.47
1:D:171:LYS:HE2	5:D:431:HOH:O	2.13	0.47
1:D:150:ILE:HB	1:D:183:LEU:HD12	1.96	0.47
1:B:19:THR:HG22	1:B:23:LEU:HD23	1.95	0.47
1:D:9:TYR:HB3	1:D:165:ILE:HD13	1.96	0.47
1:F:76:VAL:HG13	1:F:87:VAL:HG13	1.96	0.47
1:G:59:MET:HE3	1:G:59:MET:HB3	1.82	0.47
1:E:49:ILE:HD12	1:E:84:VAL:HG21	1.96	0.46
1:H:161:ALA:O	1:H:165:ILE:HG12	2.14	0.46
1:C:139:PRO:HA	1:C:144:LYS:HB2	1.98	0.46
1:A:100:GLY:O	1:A:135:GLY:HA3	2.16	0.46
1:B:148:ILE:HG21	1:B:169:ILE:HD11	1.98	0.46
1:F:264:GLU:HA	1:F:267:GLU:HG2	1.97	0.46
1:C:59:MET:HE3	1:C:59:MET:HB3	1.73	0.46
1:E:100:GLY:O	1:E:135:GLY:HA3	2.16	0.46
1:G:157:MET:CE	1:H:42:LYS:HD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD21	1:A:115:ALA:HB2	1.98	0.45
1:C:104:ILE:HG12	1:C:138:MET:HE3	1.97	0.45
1:G:156:MET:HE2	1:G:269:LEU:HD13	1.99	0.45
1:F:150:ILE:HG21	1:F:162:ALA:HA	1.97	0.45
1:D:76:VAL:HG13	1:D:87:VAL:HG13	1.99	0.45
1:F:156:MET:HE2	1:F:269:LEU:HD13	1.99	0.44
1:G:150:ILE:HB	1:G:183:LEU:HD23	2.00	0.44
1:E:139:PRO:HA	1:E:144:LYS:HB2	1.99	0.44
1:F:131:VAL:HG13	1:F:133:CYS:SG	2.58	0.44
1:H:255:VAL:HG22	1:H:256:ILE:O	2.18	0.44
1:B:100:GLY:O	1:B:135:GLY:HA3	2.18	0.44
1:H:192:ARG:HH21	1:H:273:GLY:HA3	1.83	0.43
1:E:56:GLY:HA3	1:E:61:MET:HE2	1.99	0.43
1:G:139:PRO:HA	1:G:144:LYS:HB2	1.99	0.43
1:B:149:TYR:CE1	1:B:181:GLY:HA3	2.54	0.43
1:C:61:MET:HE2	1:C:75:ASP:HB3	1.99	0.43
1:C:100:GLY:O	1:C:135:GLY:HA3	2.18	0.43
1:A:139:PRO:HA	1:A:144:LYS:HB2	2.01	0.43
1:E:150:ILE:HB	1:E:183:LEU:HD12	1.99	0.43
1:C:76:VAL:HG13	1:C:87:VAL:HG13	2.00	0.42
1:A:150:ILE:HB	1:A:183:LEU:HD12	1.99	0.42
1:D:156:MET:HE2	1:D:269:LEU:HD13	2.01	0.42
1:H:56:GLY:HA3	1:H:61:MET:HE3	2.01	0.42
1:H:156:MET:HE2	1:H:269:LEU:HD13	2.01	0.42
1:F:139:PRO:HA	1:F:144:LYS:HB2	2.00	0.42
1:H:47:ARG:HG3	1:H:52:SER:O	2.18	0.42
1:H:150:ILE:HG21	1:H:162:ALA:HA	2.01	0.42
1:E:156:MET:HE2	1:E:269:LEU:HD13	2.01	0.41
1:E:157:MET:HA	1:E:157:MET:CE	2.34	0.41
1:F:150:ILE:HB	1:F:183:LEU:HD23	2.02	0.41
1:C:13:GLY:HA3	1:D:157:MET:HG3	2.02	0.41
1:A:277:VAL:C	1:B:223:ILE:HD11	2.45	0.41
1:B:26:ALA:HA	1:B:29:GLU:HG2	2.02	0.41
1:G:51:HIS:CE1	1:G:230:GLU:OE1	2.71	0.41
1:A:205:GLY:O	1:A:255:VAL:HG21	2.21	0.40
1:E:99:ALA:HB2	1:F:131:VAL:HG22	2.01	0.40
1:H:22:ASN:HB3	1:H:241:TYR:CG	2.56	0.40
1:A:150:ILE:HG21	1:A:162:ALA:HA	2.04	0.40
1:C:22:ASN:HB3	1:C:241:TYR:CG	2.56	0.40
1:H:38:GLY:HA3	1:H:88:GLU:OE1	2.21	0.40
1:A:78:GLN:HG2	1:D:174:HIS:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:MET:HE3	1:D:59:MET:HB3	1.83	0.40
1:D:139:PRO:HA	1:D:144:LYS:HB2	2.02	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	274/290 (94%)	270 (98%)	4 (2%)	0	100	100
1	B	270/290 (93%)	263 (97%)	7 (3%)	0	100	100
1	C	282/290 (97%)	272 (96%)	6 (2%)	4 (1%)	9	7
1	D	270/290 (93%)	267 (99%)	3 (1%)	0	100	100
1	E	273/290 (94%)	270 (99%)	2 (1%)	1 (0%)	30	34
1	F	271/290 (93%)	267 (98%)	3 (1%)	1 (0%)	30	34
1	G	270/290 (93%)	267 (99%)	2 (1%)	1 (0%)	30	34
1	H	285/290 (98%)	277 (97%)	7 (2%)	1 (0%)	30	34
All	All	2195/2320 (95%)	2153 (98%)	34 (2%)	8 (0%)	30	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	286	ALA
1	C	52	SER
1	G	54	ALA
1	C	51	HIS
1	E	54	ALA
1	F	54	ALA
1	C	284	GLY
1	C	283	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/226 (96%)	207 (95%)	10 (5%)	24	32
1	B	214/226 (95%)	192 (90%)	22 (10%)	7	7
1	C	222/226 (98%)	212 (96%)	10 (4%)	24	33
1	D	212/226 (94%)	201 (95%)	11 (5%)	21	26
1	E	216/226 (96%)	205 (95%)	11 (5%)	21	27
1	F	214/226 (95%)	205 (96%)	9 (4%)	26	36
1	G	213/226 (94%)	206 (97%)	7 (3%)	33	45
1	H	224/226 (99%)	214 (96%)	10 (4%)	24	33
All	All	1732/1808 (96%)	1642 (95%)	90 (5%)	21	26

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

Mol	Chain	Res	Type
1	A	74	GLU
1	A	132	VAL
1	A	183	LEU
1	A	188	ARG
1	A	203	LYS
1	A	219	GLN
1	A	265	LEU
1	A	267	GLU
1	A	269	LEU
1	A	274	ILE
1	B	6	CYS
1	B	33	LYS
1	B	59	MET
1	B	72	GLU
1	B	76	VAL
1	B	96	VAL
1	B	127	VAL
1	B	131	VAL
1	B	138	MET

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Mol	Chain	Res	Type
1	B	179	ARG
1	B	183	LEU
1	B	188	ARG
1	B	200	LEU
1	B	210	HIS
1	B	223	ILE
1	B	225	ARG
1	B	227	THR
1	B	251	ASN
1	B	252	LYS
1	B	254	LEU
1	B	265	LEU
1	B	274	ILE
1	C	59	MET
1	C	74	GLU
1	C	76	VAL
1	C	127	VAL
1	C	138	MET
1	C	183	LEU
1	C	188	ARG
1	C	200	LEU
1	C	246	ARG
1	C	269	LEU
1	D	59	MET
1	D	69	GLU
1	D	74	GLU
1	D	76	VAL
1	D	183	LEU
1	D	188	ARG
1	D	200	LEU
1	D	223	ILE
1	D	263	GLU
1	D	265	LEU
1	D	269	LEU
1	E	74	GLU
1	E	120	LEU
1	E	127	VAL
1	E	131	VAL
1	E	183	LEU
1	E	188	ARG
1	E	200	LEU
1	E	203	LYS

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Mol	Chain	Res	Type
1	E	246	ARG
1	E	265	LEU
1	E	269	LEU
1	F	59	MET
1	F	74	GLU
1	F	76	VAL
1	F	131	VAL
1	F	188	ARG
1	F	258	ASN
1	F	265	LEU
1	F	269	LEU
1	F	274	ILE
1	G	53	LYS
1	G	59	MET
1	G	74	GLU
1	G	120	LEU
1	G	127	VAL
1	G	203	LYS
1	G	269	LEU
1	H	11	LYS
1	H	74	GLU
1	H	76	VAL
1	H	138	MET
1	H	175	SER
1	H	225	ARG
1	H	269	LEU
1	H	278	GLU
1	H	282	VAL
1	H	285	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	55	GLN
1	A	108	ASN
1	A	146	GLN
1	A	164	ASN
1	A	219	GLN
1	A	220	HIS
1	B	5	GLN
1	B	55	GLN

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Mol	Chain	Res	Type
1	B	78	GLN
1	B	108	ASN
1	B	146	GLN
1	B	164	ASN
1	B	210	HIS
1	B	219	GLN
1	B	251	ASN
1	C	51	HIS
1	C	108	ASN
1	C	146	GLN
1	C	164	ASN
1	C	216	ASN
1	C	219	GLN
1	D	51	HIS
1	D	108	ASN
1	D	146	GLN
1	D	164	ASN
1	D	219	GLN
1	E	51	HIS
1	E	55	GLN
1	E	78	GLN
1	E	146	GLN
1	E	164	ASN
1	E	174	HIS
1	E	216	ASN
1	E	219	GLN
1	F	51	HIS
1	F	55	GLN
1	F	108	ASN
1	F	146	GLN
1	F	219	GLN
1	F	220	HIS
1	G	51	HIS
1	G	78	GLN
1	G	108	ASN
1	G	146	GLN
1	G	164	ASN
1	G	207	GLN
1	H	5	GLN
1	H	51	HIS
1	H	55	GLN
1	H	78	GLN

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Mol	Chain	Res	Type
1	H	164	ASN
1	H	216	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 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	SF4	G	1001	1	0,12,12	-	-	-		
3	ADP	E	1002	4	28,29,29	0.38	0	43,45,45	0.47	0
3	ADP	D	301	4	28,29,29	0.41	0	43,45,45	0.49	0
3	ADP	F	301	4	28,29,29	0.42	0	43,45,45	0.51	0
3	ADP	G	1002	4	28,29,29	0.32	0	43,45,45	0.47	0
2	SF4	C	1001	1	0,12,12	-	-	-		
2	SF4	E	1001	1	0,12,12	-	-	-		
3	ADP	H	301	4	28,29,29	0.37	0	43,45,45	0.47	0
2	SF4	A	1001	1	0,12,12	-	-	-		
3	ADP	A	1002	4	28,29,29	0.44	0	43,45,45	0.52	0
3	ADP	B	301	4	28,29,29	0.41	0	43,45,45	0.44	0
3	ADP	C	1002	4	28,29,29	0.38	0	43,45,45	0.50	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	SF4	G	1001	1	-	-	0/6/5/5
3	ADP	E	1002	4	-	2/16/32/32	0/3/3/3
3	ADP	D	301	4	-	2/16/32/32	0/3/3/3
3	ADP	F	301	4	-	2/16/32/32	0/3/3/3
3	ADP	G	1002	4	-	2/16/32/32	0/3/3/3
2	SF4	A	1001	1	-	-	0/6/5/5
2	SF4	C	1001	1	-	-	0/6/5/5
2	SF4	E	1001	1	-	-	0/6/5/5
3	ADP	H	301	4	-	2/16/32/32	0/3/3/3
3	ADP	A	1002	4	-	2/16/32/32	0/3/3/3
3	ADP	B	301	4	-	2/16/32/32	0/3/3/3
3	ADP	C	1002	4	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

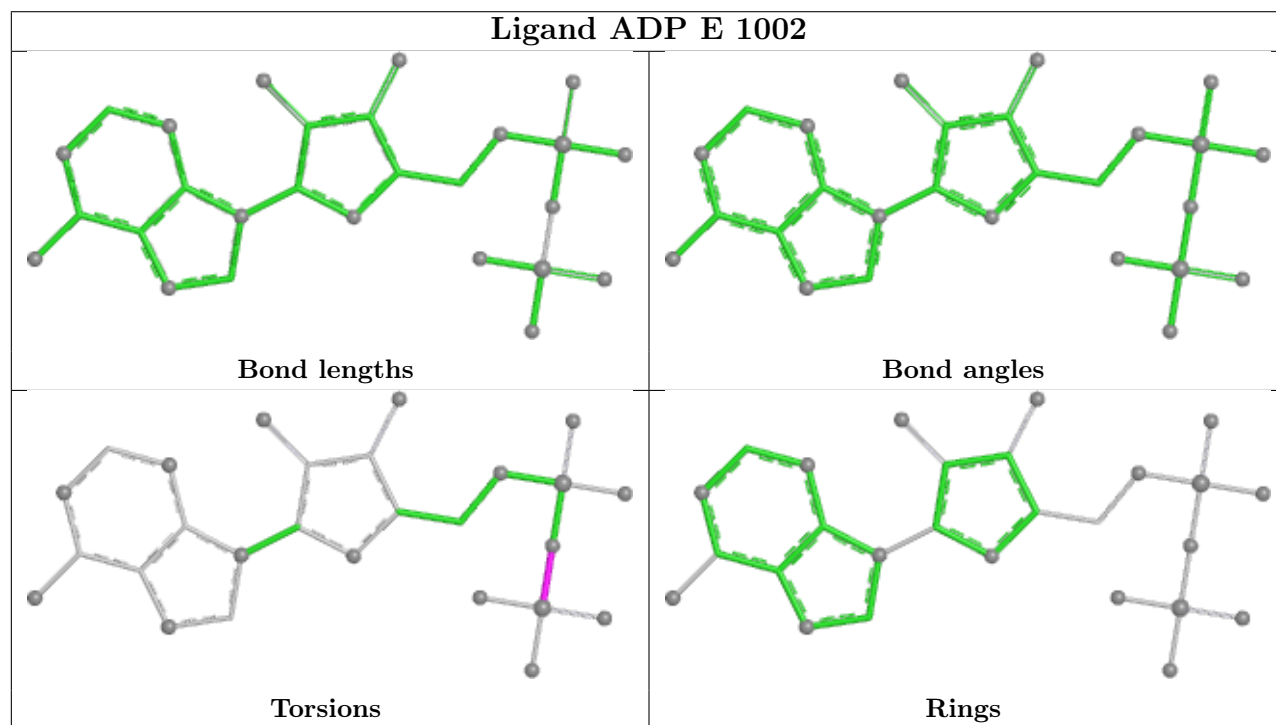
Mol	Chain	Res	Type	Atoms
3	A	1002	ADP	PA-O3A-PB-O2B
3	A	1002	ADP	PA-O3A-PB-O3B
3	B	301	ADP	PA-O3A-PB-O3B
3	C	1002	ADP	PA-O3A-PB-O3B
3	D	301	ADP	PA-O3A-PB-O2B
3	D	301	ADP	PA-O3A-PB-O3B
3	E	1002	ADP	PA-O3A-PB-O3B
3	F	301	ADP	PA-O3A-PB-O2B
3	F	301	ADP	PA-O3A-PB-O3B
3	G	1002	ADP	PA-O3A-PB-O2B
3	G	1002	ADP	PA-O3A-PB-O3B
3	H	301	ADP	PA-O3A-PB-O3B
3	E	1002	ADP	PA-O3A-PB-O1B
3	B	301	ADP	PA-O3A-PB-O1B
3	H	301	ADP	PA-O3A-PB-O1B
3	C	1002	ADP	PA-O3A-PB-O1B

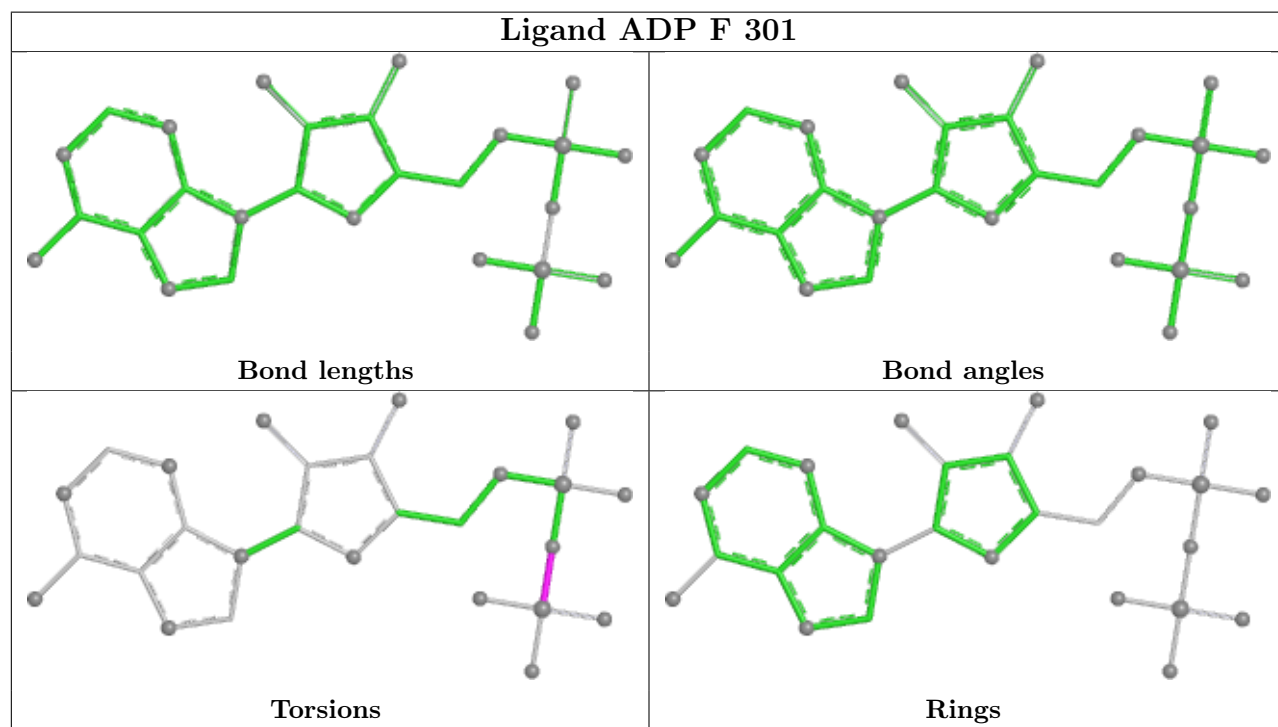
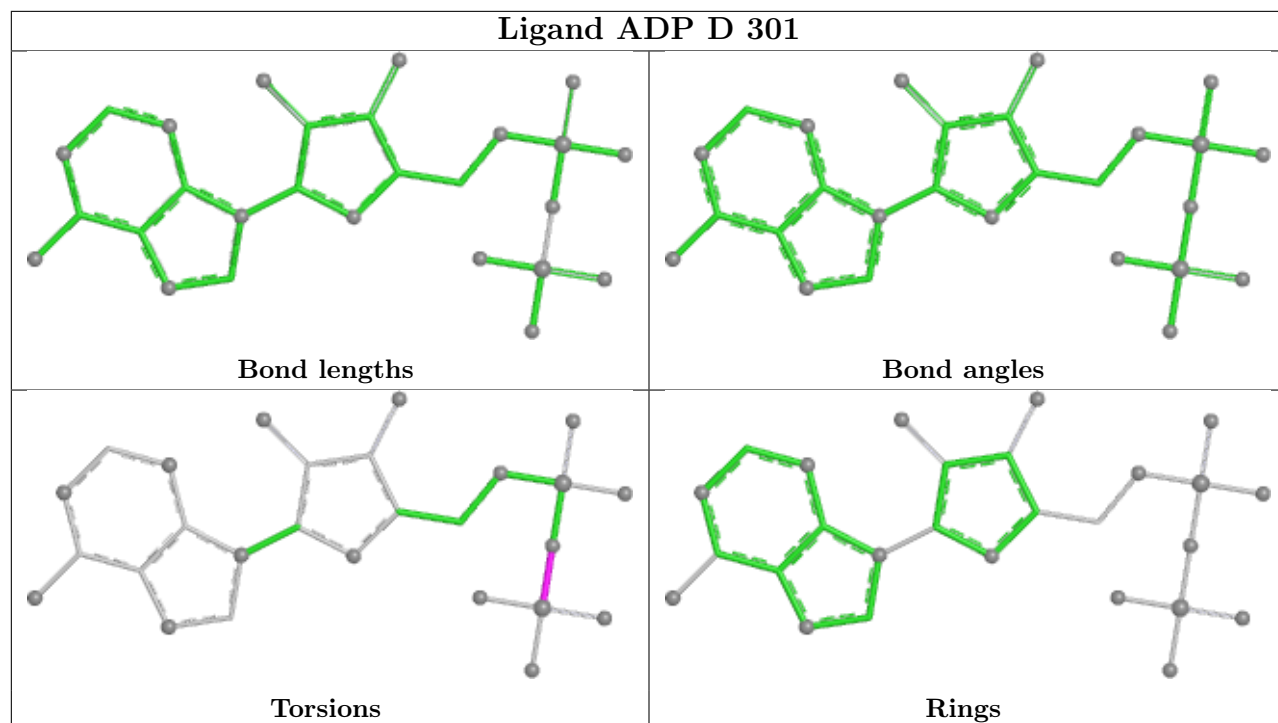
There are no ring outliers.

1 monomer is involved in 1 short contact:

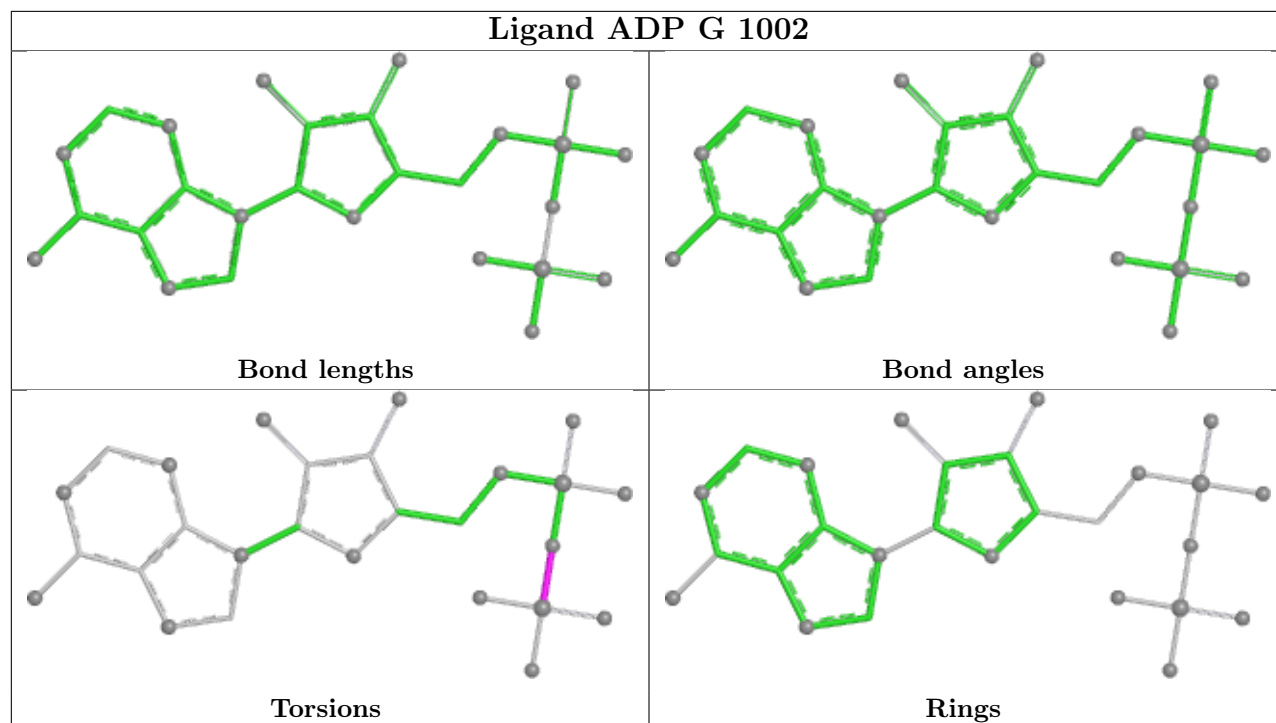
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	ADP	1	0

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.

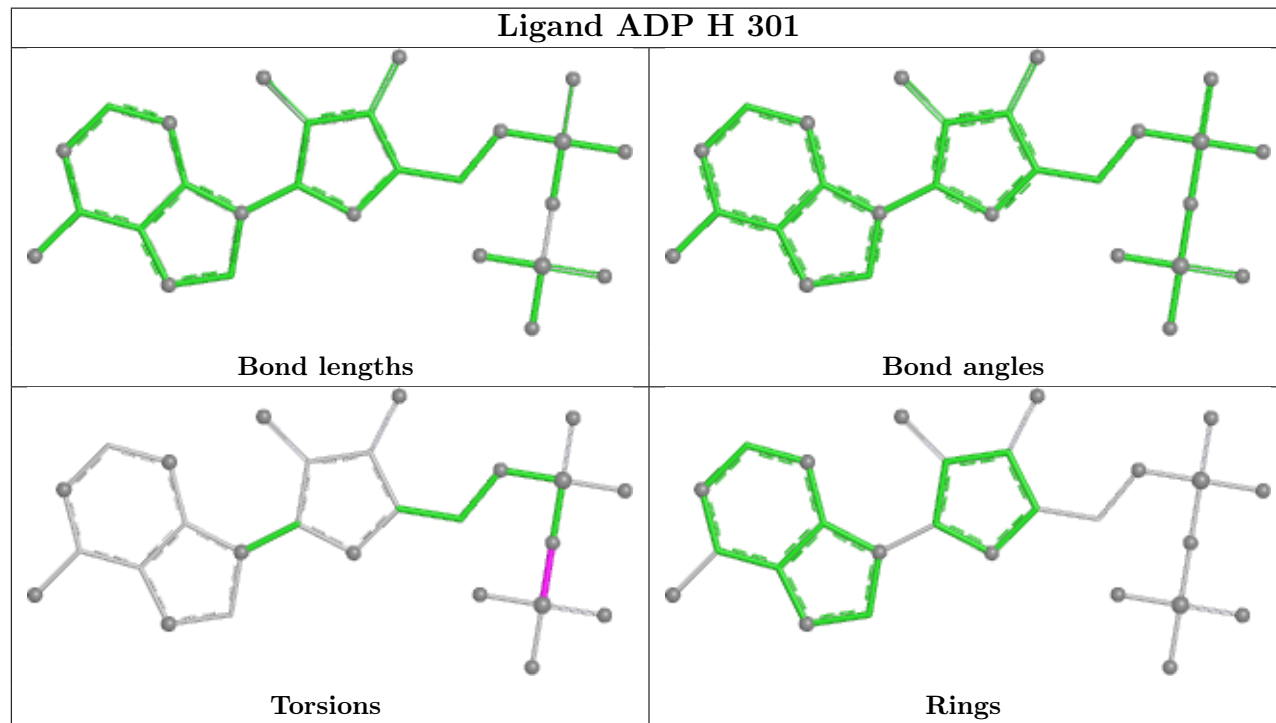


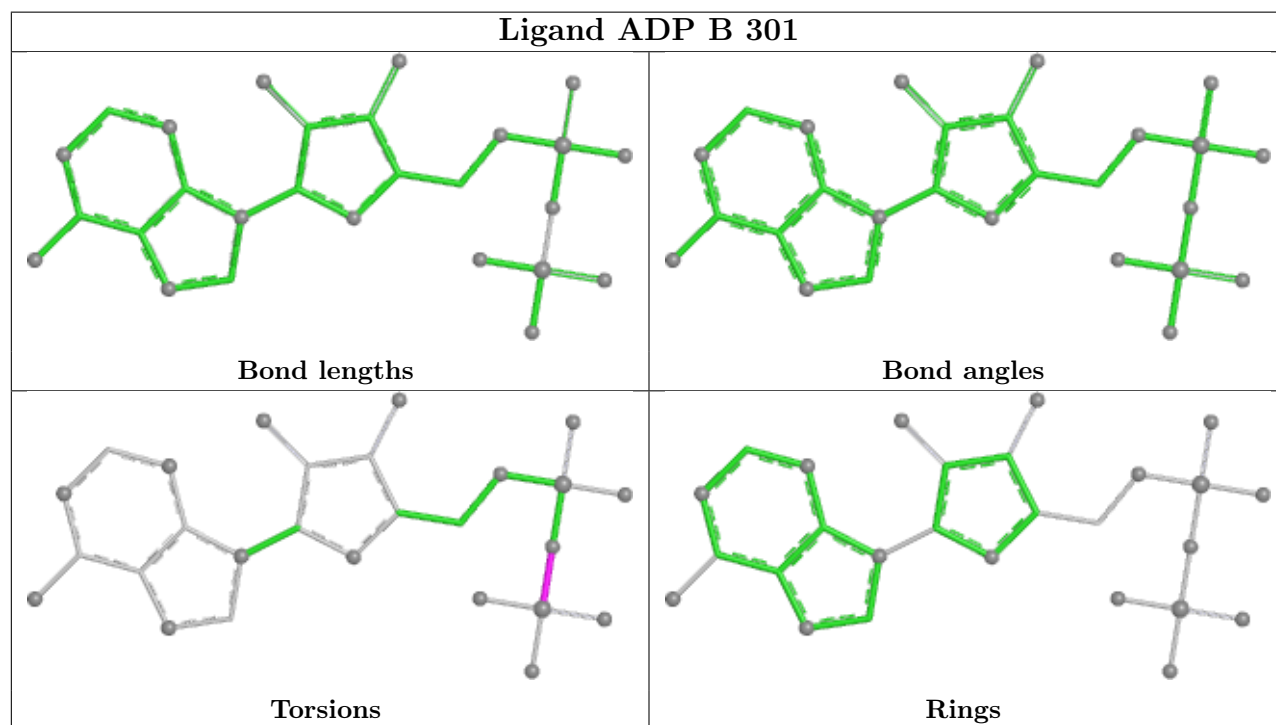
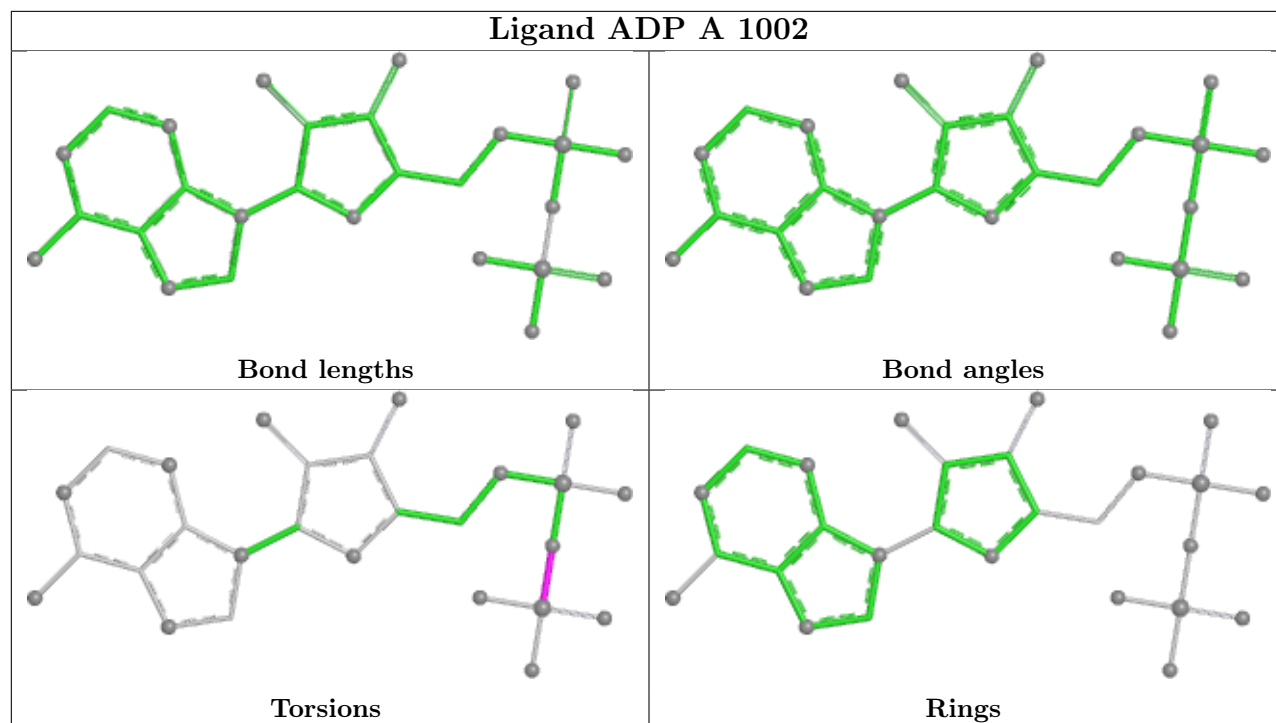


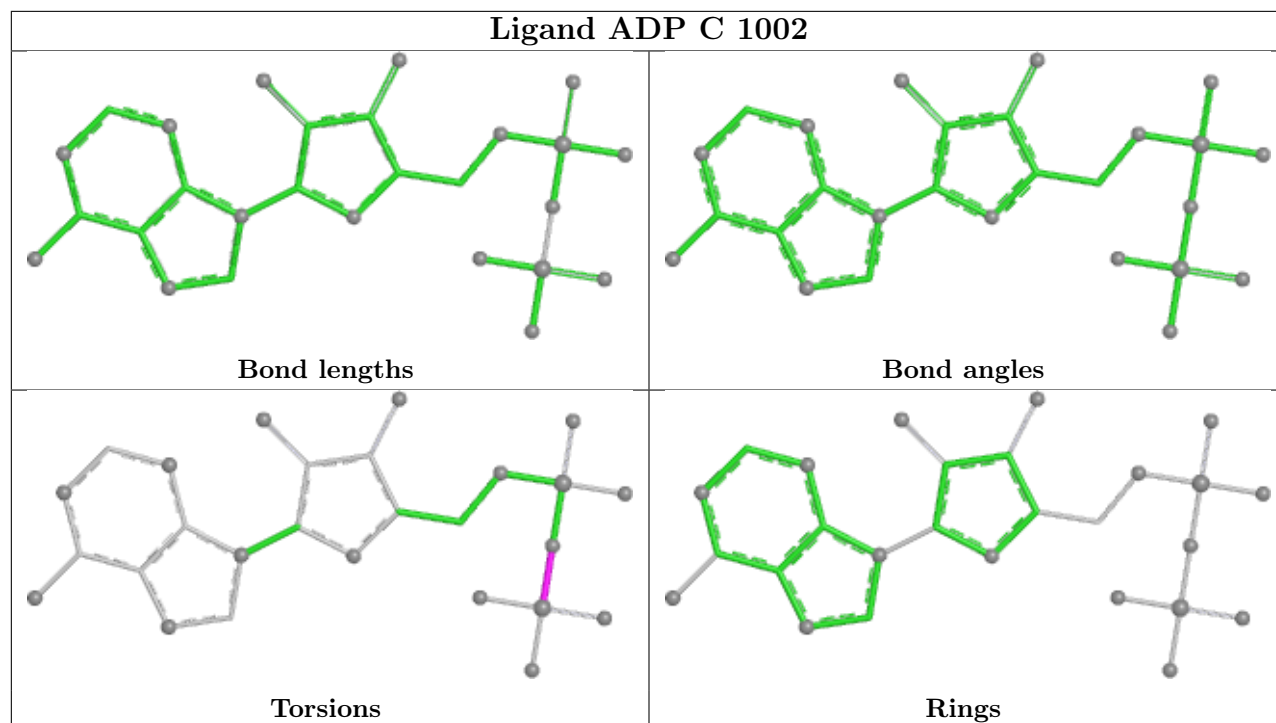
Ligand ADP G 1002



Ligand ADP H 301







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	276/290 (95%)	0.16	6 (2%) 62 59	35, 50, 87, 132	0
1	B	274/290 (94%)	1.73	112 (40%) 0 0	47, 86, 124, 144	0
1	C	284/290 (97%)	0.36	19 (6%) 24 21	38, 59, 108, 183	0
1	D	272/290 (93%)	0.32	5 (1%) 67 64	36, 64, 101, 118	0
1	E	275/290 (94%)	0.73	21 (7%) 20 17	44, 72, 103, 125	0
1	F	273/290 (94%)	0.18	11 (4%) 42 39	34, 53, 85, 125	0
1	G	272/290 (93%)	0.42	8 (2%) 53 50	39, 67, 100, 117	0
1	H	287/290 (98%)	0.28	15 (5%) 33 29	41, 63, 105, 172	0
All	All	2213/2320 (95%)	0.52	197 (8%) 15 13	34, 64, 108, 183	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	288	ALA	7.0
1	F	274	ILE	6.3
1	G	273	GLY	6.2
1	B	151	VAL	5.3
1	A	277	VAL	5.3
1	B	254	LEU	5.0
1	B	244	LEU	4.8
1	B	274	ILE	4.6
1	E	274	ILE	4.6
1	H	287	ALA	4.5
1	B	200	LEU	4.4
1	C	277	VAL	4.4
1	B	226	MET	4.4
1	C	283	VAL	4.3
1	B	26	ALA	4.3
1	D	273	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	285	LYS	4.3
1	B	245	ALA	4.2
1	C	281	SER	4.2
1	C	274	ILE	4.1
1	B	256	ILE	4.1
1	B	158	ALA	4.1
1	B	206	THR	4.1
1	B	184	ILE	4.0
1	B	229	ILE	3.9
1	B	217	VAL	3.9
1	B	24	VAL	3.8
1	F	54	ALA	3.7
1	B	183	LEU	3.6
1	B	2	ALA	3.6
1	B	241	TYR	3.6
1	B	209	ILE	3.6
1	B	270	MET	3.5
1	B	212	VAL	3.5
1	B	243	ALA	3.5
1	B	249	VAL	3.5
1	A	275	MET	3.5
1	C	223	ILE	3.5
1	H	277	VAL	3.4
1	B	205	GLY	3.4
1	B	48	LEU	3.4
1	B	204	ILE	3.4
1	B	208	MET	3.4
1	B	255	VAL	3.3
1	B	154	GLY	3.3
1	B	210	HIS	3.3
1	B	149	TYR	3.3
1	F	270	MET	3.2
1	E	269	LEU	3.2
1	B	8	ILE	3.2
1	E	276	GLU	3.2
1	E	2	ALA	3.2
1	D	269	LEU	3.2
1	B	152	CYS	3.1
1	C	284	GLY	3.1
1	B	257	PRO	3.1
1	B	197	ILE	3.1
1	B	180	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	253	LEU	3.1
1	B	231	TYR	3.0
1	B	250	ASP	3.0
1	A	274	ILE	3.0
1	B	202	ALA	3.0
1	G	269	LEU	3.0
1	B	49	ILE	3.0
1	C	2	ALA	2.9
1	B	196	LEU	2.9
1	B	248	ILE	2.9
1	B	117	SER	2.9
1	E	222	GLU	2.9
1	B	201	ALA	2.9
1	B	211	PHE	2.9
1	H	285	LYS	2.9
1	B	272	PHE	2.9
1	B	186	ASN	2.9
1	H	274	ILE	2.8
1	B	12	GLY	2.8
1	C	188	ARG	2.8
1	C	51	HIS	2.8
1	B	160	TYR	2.8
1	B	218	VAL	2.8
1	D	188	ARG	2.8
1	B	261	SER	2.8
1	A	54	ALA	2.8
1	B	122	PHE	2.8
1	E	224	ARG	2.8
1	D	53	LYS	2.7
1	C	175	SER	2.7
1	B	157	MET	2.7
1	B	3	LEU	2.7
1	B	9	TYR	2.7
1	B	207	GLN	2.7
1	B	228	VAL	2.7
1	B	275	MET	2.7
1	B	6	CYS	2.7
1	B	234	LYS	2.6
1	B	252	LYS	2.6
1	C	278	GLU	2.6
1	B	161	ALA	2.6
1	B	221	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	260	ALA	2.6
1	B	119	ASP	2.6
1	B	46	THR	2.6
1	B	182	GLY	2.6
1	B	236	GLY	2.6
1	B	268	LEU	2.6
1	B	269	LEU	2.6
1	H	275	MET	2.6
1	E	220	HIS	2.6
1	B	28	ALA	2.6
1	E	272	PHE	2.6
1	B	25	ALA	2.5
1	B	199	ALA	2.5
1	G	2	ALA	2.5
1	F	95	GLY	2.5
1	B	223	ILE	2.5
1	B	271	GLU	2.5
1	E	70	ASP	2.5
1	H	2	ALA	2.5
1	G	68	VAL	2.5
1	B	150	ILE	2.5
1	B	237	GLN	2.5
1	B	124	PHE	2.5
1	E	271	GLU	2.5
1	B	116	TYR	2.5
1	B	198	MET	2.5
1	B	262	MET	2.5
1	C	275	MET	2.5
1	B	174	HIS	2.5
1	A	95	GLY	2.5
1	E	54	ALA	2.4
1	E	190	THR	2.4
1	B	23	LEU	2.4
1	G	53	LYS	2.4
1	E	275	MET	2.4
1	G	270	MET	2.4
1	B	191	ASP	2.4
1	E	191	ASP	2.4
1	B	247	LYS	2.4
1	H	283	VAL	2.4
1	E	47	ARG	2.4
1	B	258	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	53	LYS	2.3
1	B	227	THR	2.3
1	B	178	VAL	2.3
1	H	282	VAL	2.3
1	B	259	PRO	2.3
1	B	190	THR	2.3
1	B	267	GLU	2.3
1	F	131	VAL	2.3
1	F	189	LYS	2.3
1	H	53	LYS	2.3
1	B	276	GLU	2.3
1	B	265	LEU	2.3
1	F	188	ARG	2.3
1	B	153	SER	2.3
1	C	52	SER	2.3
1	B	27	LEU	2.2
1	F	273	GLY	2.2
1	B	14	ILE	2.2
1	B	233	PRO	2.2
1	C	53	LYS	2.2
1	D	2	ALA	2.2
1	E	203	LYS	2.2
1	C	154	GLY	2.2
1	B	19	THR	2.2
1	B	22	ASN	2.2
1	B	53	LYS	2.2
1	B	239	ASP	2.1
1	H	276	GLU	2.1
1	A	174	HIS	2.1
1	B	220	HIS	2.1
1	H	174	HIS	2.1
1	B	273	GLY	2.1
1	C	66	GLY	2.1
1	G	54	ALA	2.1
1	G	188	ARG	2.1
1	B	230	GLU	2.1
1	C	279	ASP	2.1
1	E	273	GLY	2.1
1	F	154	GLY	2.1
1	E	268	LEU	2.1
1	B	15	GLY	2.1
1	B	115	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	234	LYS	2.1
1	H	54	ALA	2.1
1	B	20	THR	2.0
1	C	54	ALA	2.0
1	E	189	LYS	2.0
1	B	175	SER	2.0
1	F	69	GLU	2.0
1	B	162	ALA	2.0
1	H	286	ALA	2.0
1	B	21	GLN	2.0
1	H	269	LEU	2.0
1	B	213	PRO	2.0
1	E	53	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

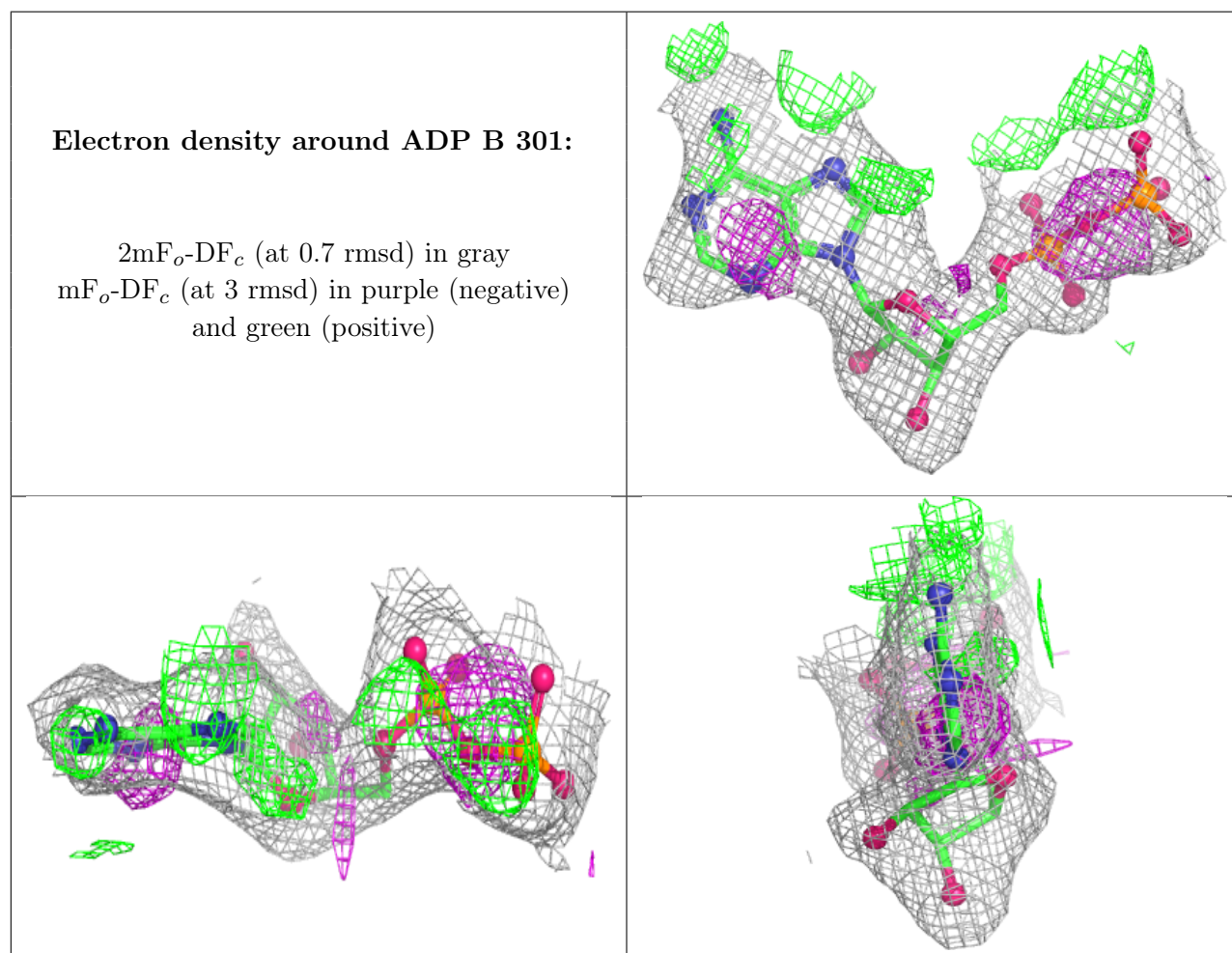
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	1004	1/1	0.72	0.34	94,94,94,94	0
3	ADP	B	301	27/27	0.85	0.12	67,79,87,89	0
4	MG	F	303	1/1	0.86	0.43	95,95,95,95	0
4	MG	E	1003	1/1	0.91	0.07	74,74,74,74	0
4	MG	B	302	1/1	0.92	0.11	87,87,87,87	0
3	ADP	E	1002	27/27	0.94	0.09	59,73,81,82	0
3	ADP	F	301	27/27	0.96	0.08	45,60,66,76	0
3	ADP	G	1002	27/27	0.96	0.07	51,69,77,78	0
3	ADP	D	301	27/27	0.96	0.07	51,65,74,76	0
3	ADP	A	1002	27/27	0.97	0.07	39,47,54,66	0

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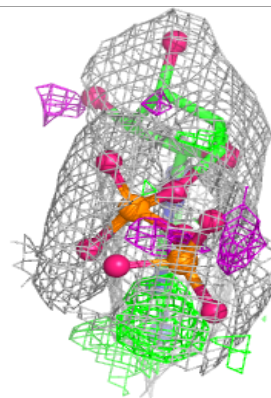
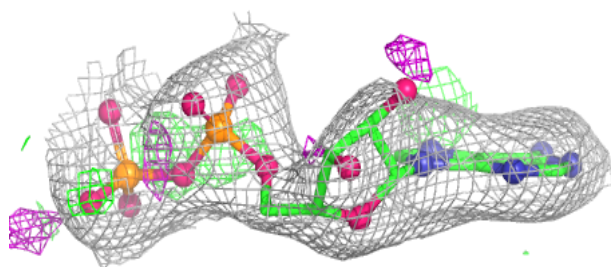
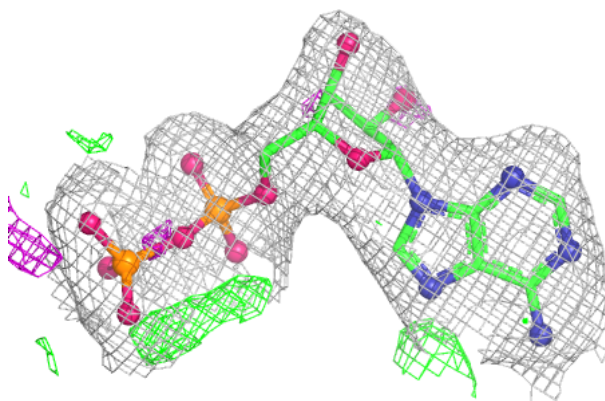
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	C	1002	27/27	0.98	0.05	40,47,52,53	0
3	ADP	H	301	27/27	0.98	0.05	36,47,56,56	0
4	MG	A	1003	1/1	0.99	0.03	42,42,42,42	0
2	SF4	A	1001	8/8	0.99	0.03	44,45,47,48	0
4	MG	C	1003	1/1	0.99	0.04	47,47,47,47	0
2	SF4	C	1001	8/8	0.99	0.03	43,44,44,45	0
4	MG	D	302	1/1	0.99	0.03	53,53,53,53	0
2	SF4	E	1001	8/8	0.99	0.03	45,47,48,49	0
4	MG	F	302	1/1	0.99	0.03	50,50,50,50	0
2	SF4	G	1001	8/8	0.99	0.03	44,46,48,48	0
4	MG	G	1003	1/1	0.99	0.04	53,53,53,53	0
4	MG	H	302	1/1	1.00	0.04	48,48,48,48	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.

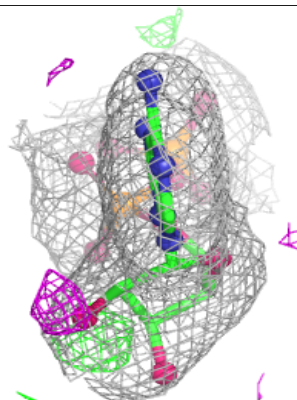
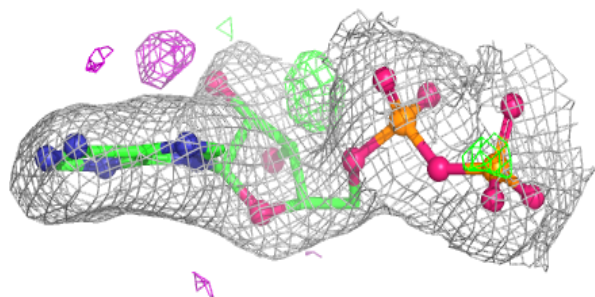
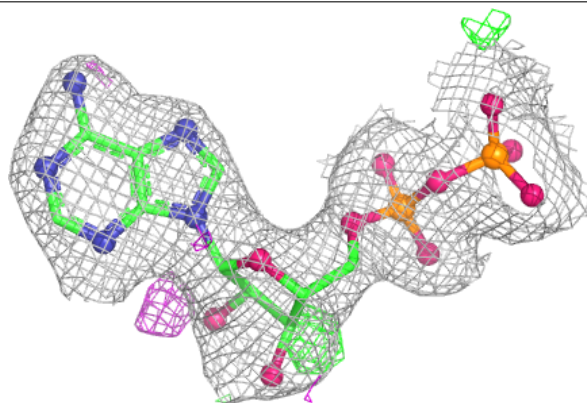


Electron density around ADP E 1002:

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

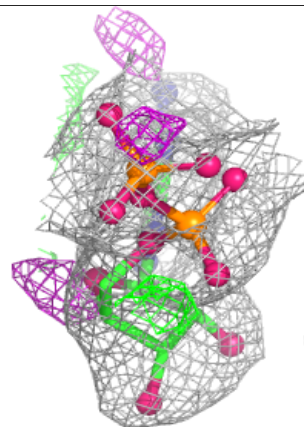
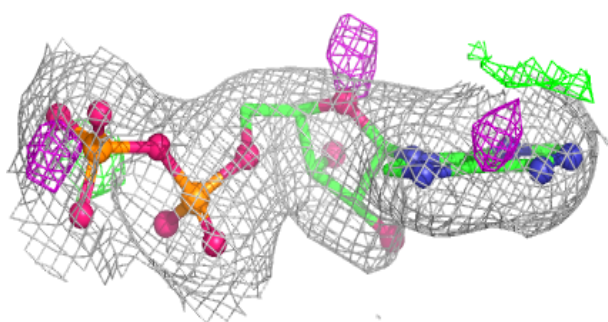
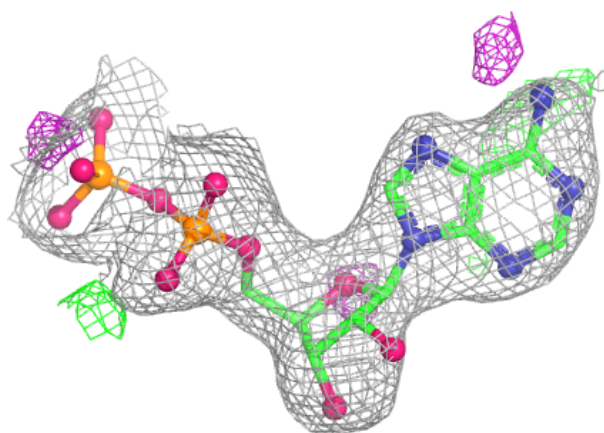
**Electron density around ADP F 301:**

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

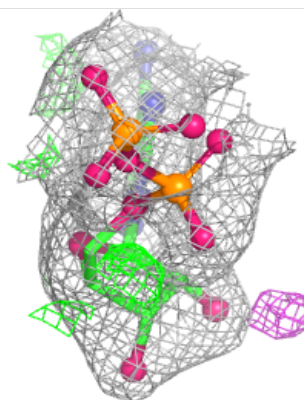
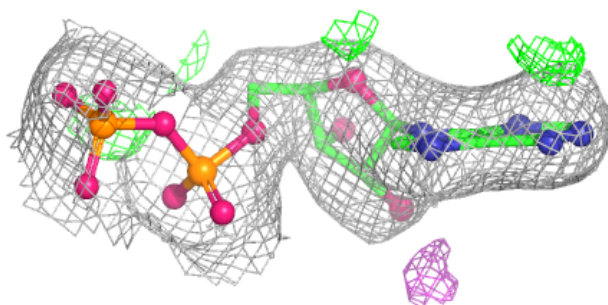
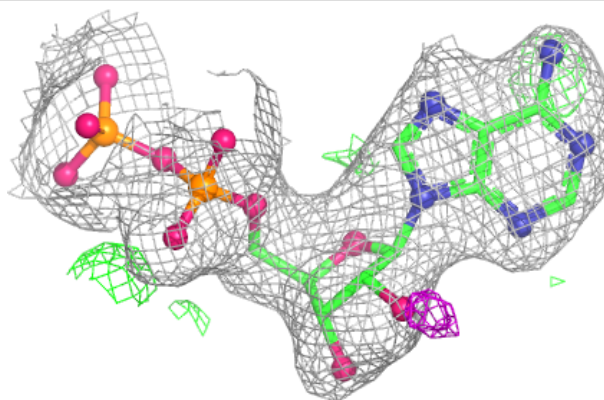


Electron density around ADP G 1002:

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

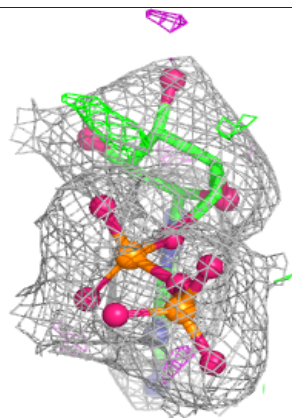
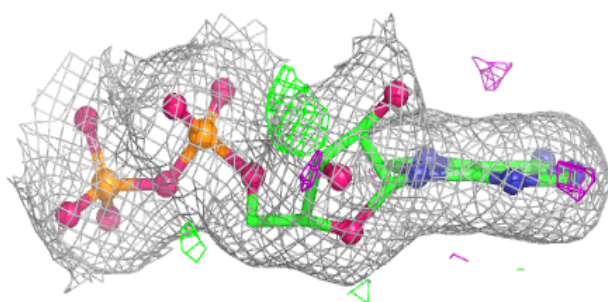
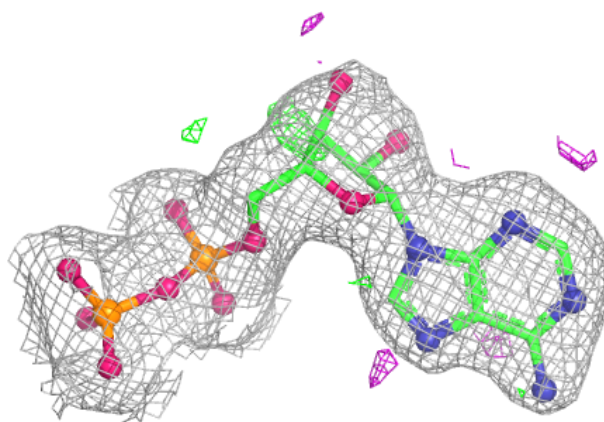
**Electron density around ADP D 301:**

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

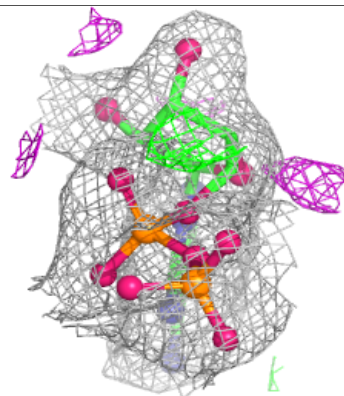
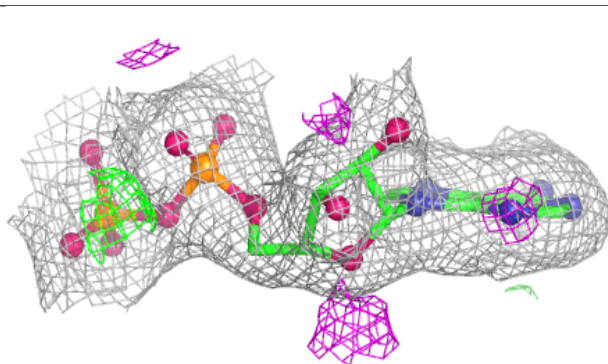
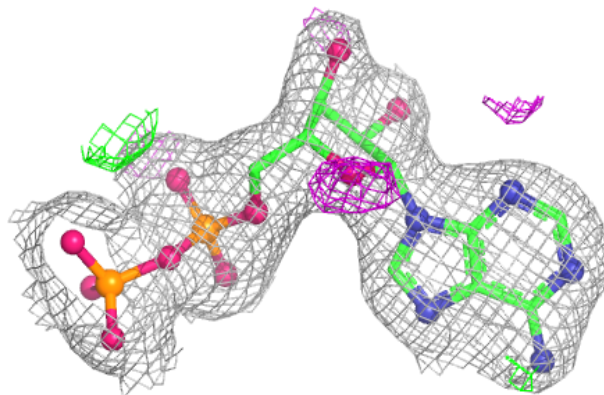


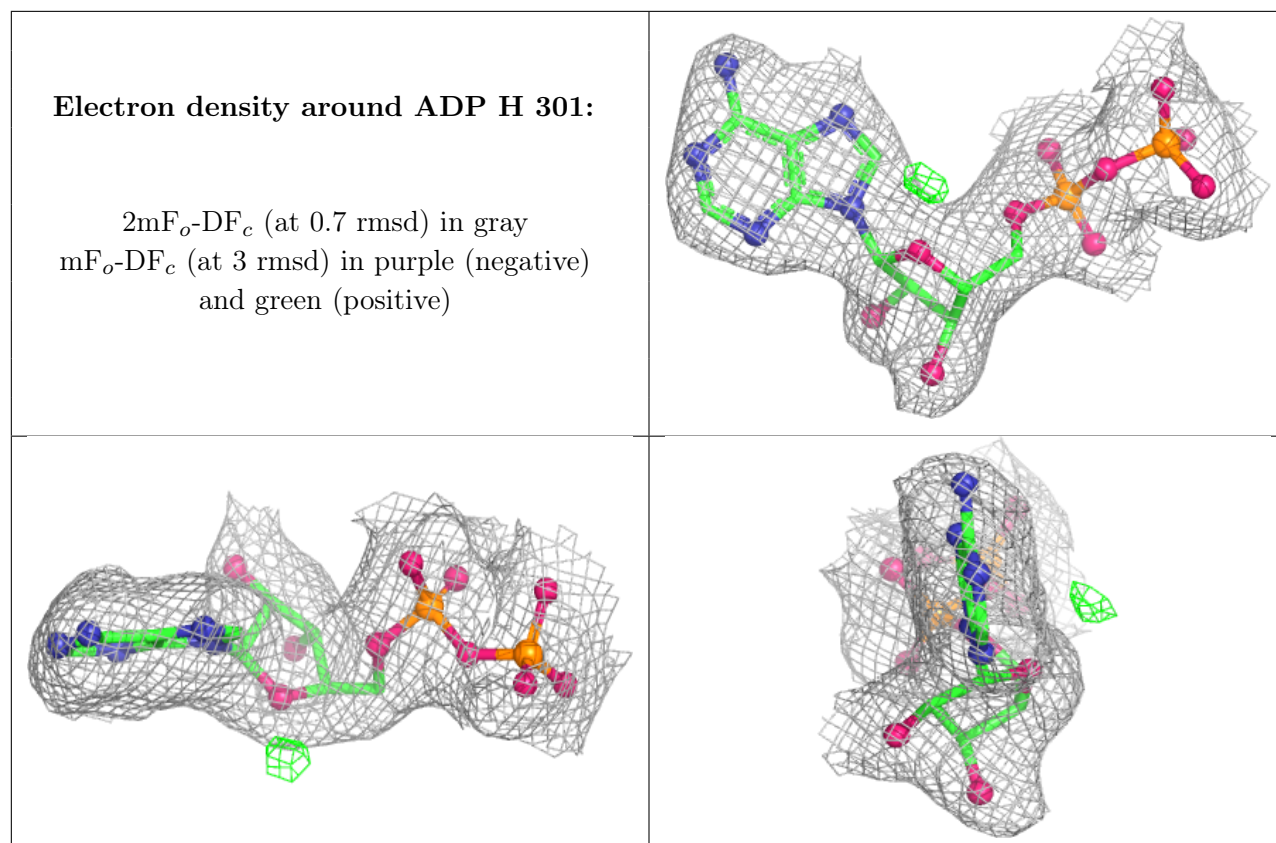
Electron density around ADP A 1002:

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

**Electron density around ADP C 1002:**

$2mF_o-DF_c$ (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.