



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:06 PM EDT

PDB ID : 6YCZ / pdb_00006ycz
Title : Plasmodium falciparum Myosin A delta-Nter, Post-Rigor state
Authors : Moussaoui, D.; Robblee, J.P.; Auguin, D.; Krementsova, E.B.; Robert-Paganin, J.; Trybus, K.M.; Houdusse, A.
Deposited on : 2020-03-19
Resolution : 3.27 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

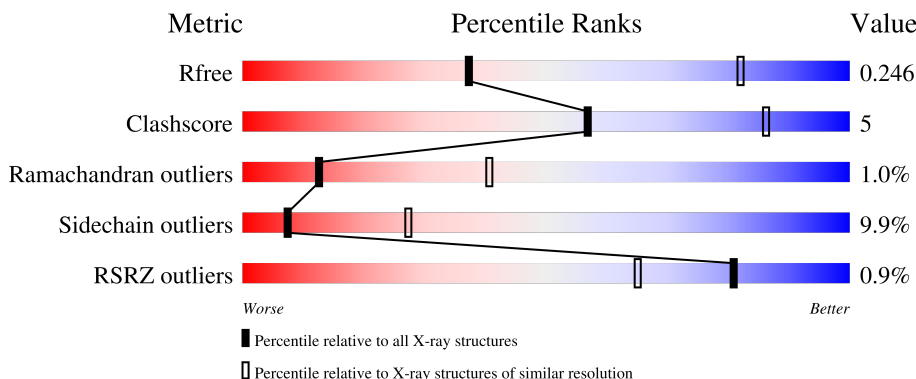
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

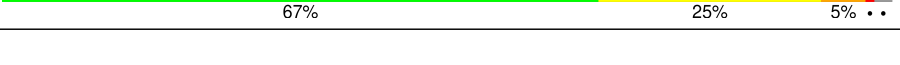
The reported resolution of this entry is 3.27 Å.

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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	818	
2	B	204	
3	C	134	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8556 atoms, of which 12 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 Myosin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	795	6361	4053	1080	1195	33	0	6	0

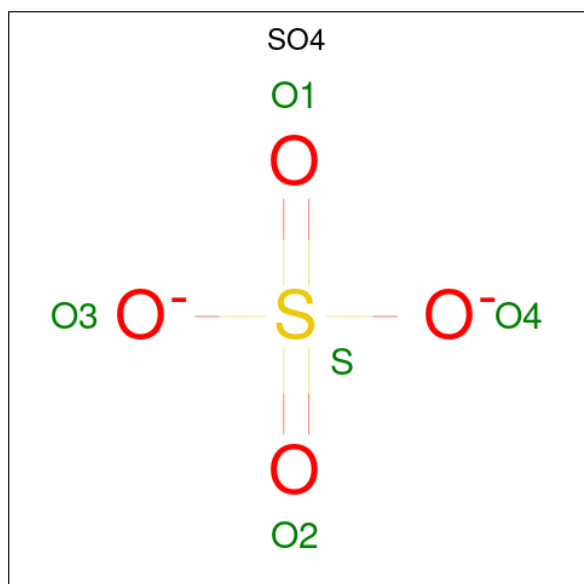
- Molecule 2 is a protein called Myosin A tail domain interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	131	1051	661	167	218	5	0	0	0

- Molecule 3 is a protein called Uncharacterized protein.

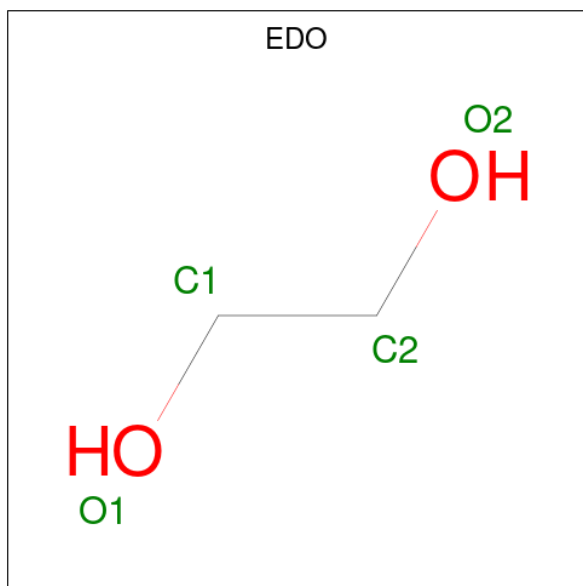
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	131	1077	687	175	209	6	0	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

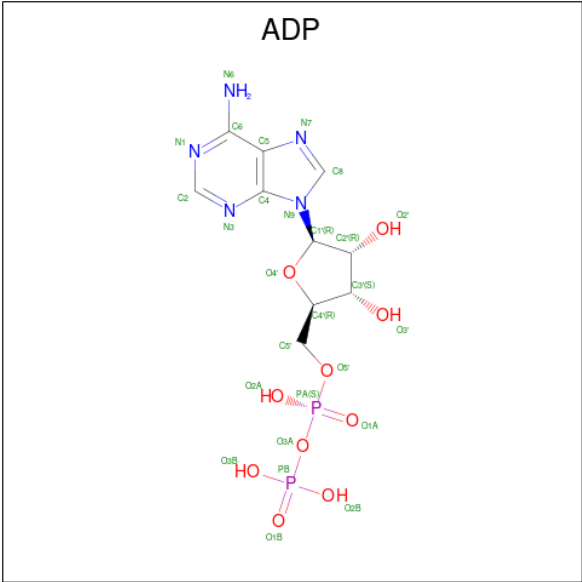


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

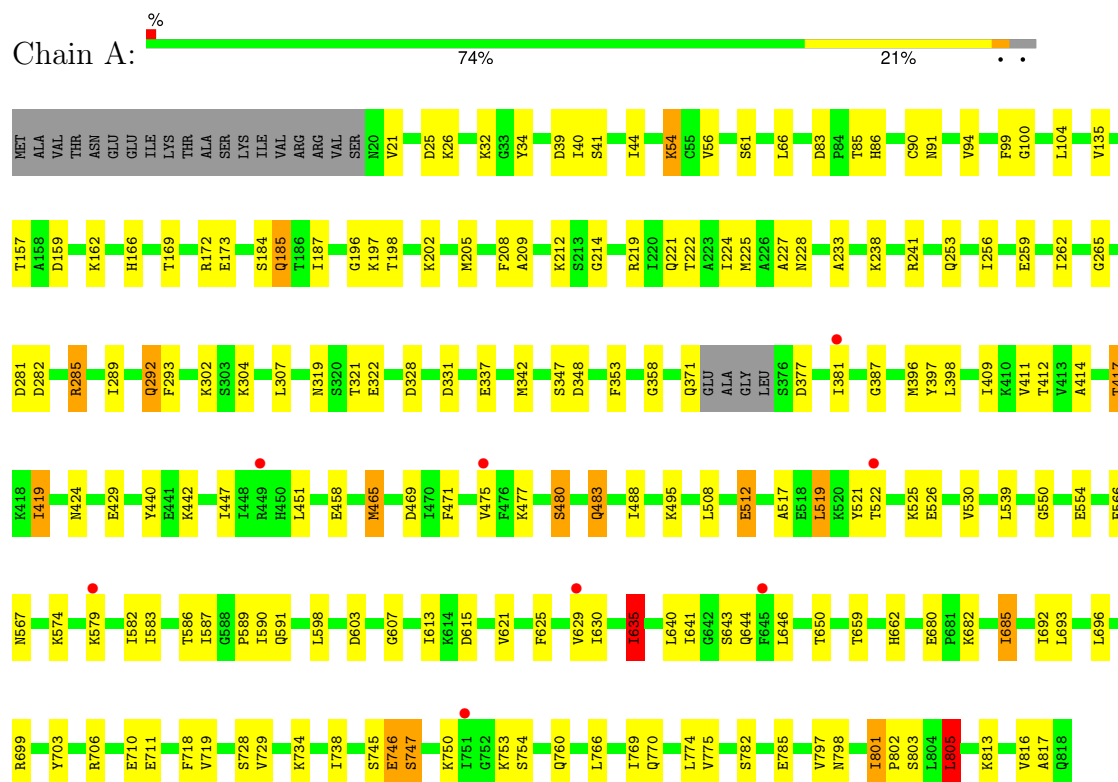
- Molecule 8 is water.

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

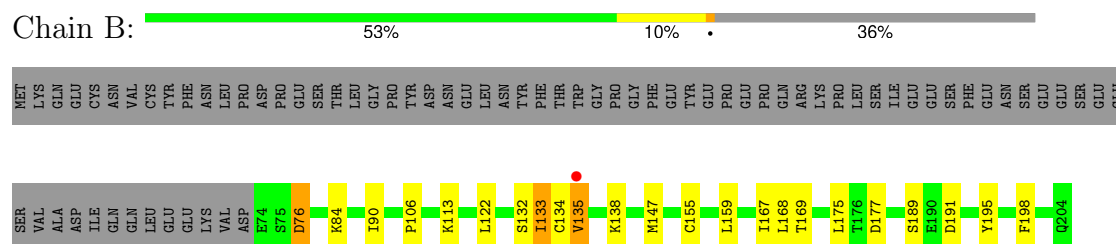
3 Residue-property plots [i](#)

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: Myosin-A

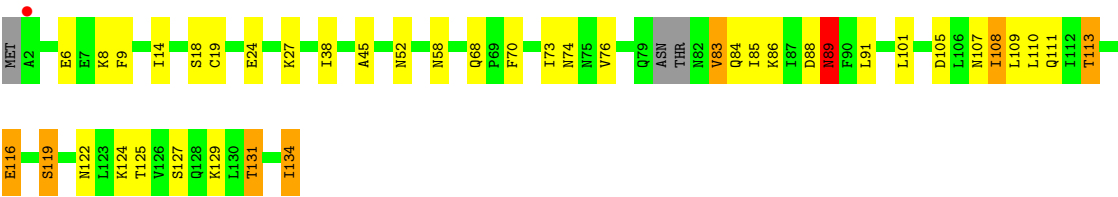


• Molecule 2: Myosin A tail domain interacting protein



• Molecule 3: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.08Å 114.43Å 170.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 3.27 48.30 – 3.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.30-3.27) 99.9 (48.30-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.179 , 0.227 0.193 , 0.246	Depositor DCC
R_{free} test set	1399 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 88.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8556	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, EDO, MG, SO4

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	0.88	0/6474	1.43	55/8729 (0.6%)
2	B	0.82	0/1068	1.46	4/1440 (0.3%)
3	C	0.87	1/1096 (0.1%)	1.54	14/1476 (0.9%)
All	All	0.88	1/8638 (0.0%)	1.45	73/11645 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	83	VAL	CA-C	5.17	1.59	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	293	PHE	CA-CB-CG	7.51	121.31	113.80
1	A	25	ASP	CA-CB-CG	6.82	119.42	112.60
2	B	191	ASP	CA-CB-CG	6.80	119.40	112.60
3	C	24	GLU	CB-CG-CD	6.56	123.75	112.60
1	A	521	TYR	CA-C-N	6.49	130.99	121.31
1	A	521	TYR	C-N-CA	6.49	130.99	121.31
3	C	127	SER	CA-C-N	6.46	128.83	120.44
3	C	127	SER	C-N-CA	6.46	128.83	120.44
1	A	719	VAL	N-CA-C	-6.38	104.30	110.42
1	A	353	PHE	CA-CB-CG	-6.21	107.59	113.80
1	A	643	SER	CA-C-N	6.06	128.69	120.38
1	A	643	SER	C-N-CA	6.06	128.69	120.38
3	C	89	ASN	CA-C-N	5.98	128.22	120.44
3	C	89	ASN	C-N-CA	5.98	128.22	120.44
1	A	100	GLY	N-CA-C	5.88	121.95	114.66
1	A	214	GLY	N-CA-C	5.75	118.38	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	567	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	292	GLN	CA-C-N	5.66	127.79	120.44
1	A	292	GLN	C-N-CA	5.66	127.79	120.44
1	A	703	TYR	CA-C-N	5.63	128.29	120.29
1	A	703	TYR	C-N-CA	5.63	128.29	120.29
2	B	76	ASP	CA-C-N	5.61	127.63	120.56
2	B	76	ASP	C-N-CA	5.61	127.63	120.56
1	A	411	VAL	CA-C-N	5.60	129.21	120.75
1	A	411	VAL	C-N-CA	5.60	129.21	120.75
3	C	8	LYS	CA-C-N	5.55	128.00	120.44
3	C	8	LYS	C-N-CA	5.55	128.00	120.44
3	C	116	GLU	CA-C-O	5.52	121.14	117.94
3	C	105	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	685	ILE	CA-C-N	5.49	128.08	120.29
1	A	685	ILE	C-N-CA	5.49	128.08	120.29
1	A	281	ASP	CA-C-N	-5.46	112.72	122.07
1	A	281	ASP	C-N-CA	-5.46	112.72	122.07
1	A	417	THR	N-CA-C	5.41	117.51	110.53
1	A	319	ASN	CA-C-N	5.38	128.03	120.28
1	A	319	ASN	C-N-CA	5.38	128.03	120.28
1	A	285	ARG	CB-CG-CD	-5.33	99.05	111.30
1	A	554	GLU	CA-C-N	5.33	127.42	120.28
1	A	554	GLU	C-N-CA	5.33	127.42	120.28
1	A	172	ARG	CA-C-N	5.30	127.70	120.54
1	A	172	ARG	C-N-CA	5.30	127.70	120.54
1	A	409	ILE	CA-C-N	5.30	129.45	122.30
1	A	409	ILE	C-N-CA	5.30	129.45	122.30
1	A	805	LEU	CA-C-N	5.30	127.64	120.44
1	A	805	LEU	C-N-CA	5.30	127.64	120.44
3	C	9	PHE	CA-CB-CG	5.29	119.09	113.80
3	C	58	ASN	CA-C-N	5.28	127.30	120.44
3	C	58	ASN	C-N-CA	5.28	127.30	120.44
1	A	83	ASP	CA-CB-CG	5.27	117.87	112.60
2	B	189	SER	N-CA-C	-5.22	106.59	113.12
3	C	108	ILE	CA-C-N	5.16	127.45	120.38
3	C	108	ILE	C-N-CA	5.16	127.45	120.38
1	A	447	ILE	CA-C-N	5.15	127.05	120.56
1	A	447	ILE	C-N-CA	5.15	127.05	120.56
1	A	322	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	775	VAL	CA-C-N	5.13	127.67	120.28
1	A	775	VAL	C-N-CA	5.13	127.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	SER	CA-C-N	5.13	127.22	120.60
1	A	782	SER	C-N-CA	5.13	127.22	120.60
1	A	746	GLU	CA-C-N	5.13	130.11	121.14
1	A	746	GLU	C-N-CA	5.13	130.11	121.14
1	A	387	GLY	CA-C-N	5.08	127.05	120.70
1	A	387	GLY	C-N-CA	5.08	127.05	120.70
1	A	465	MET	CA-C-N	5.06	125.71	120.60
1	A	465	MET	C-N-CA	5.06	125.71	120.60
1	A	710	GLU	CA-C-N	5.05	127.31	120.65
1	A	710	GLU	C-N-CA	5.05	127.31	120.65
1	A	711	GLU	CA-C-N	5.04	127.28	120.38
1	A	711	GLU	C-N-CA	5.04	127.28	120.38
1	A	750	LYS	CA-C-N	5.03	126.90	120.56
1	A	750	LYS	C-N-CA	5.03	126.90	120.56

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	6361	0	6457	61	0
2	B	1051	0	1005	9	0
3	C	1077	0	1057	12	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	4	6	6	0	0
5	C	4	6	6	0	0
6	A	1	0	0	0	0
7	A	27	0	12	2	0
8	A	4	0	0	0	0
All	All	8544	12	8543	78	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 (78) 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)
3:C:68:GLN:HE22	3:C:76:VAL:H	1.41	0.68
2:B:168:LEU:HB3	2:B:175:LEU:HD12	1.77	0.66
1:A:233:ALA:HB1	1:A:289[B]:ILE:HG23	1.79	0.64
1:A:766:LEU:HA	1:A:769:ILE:HD12	1.81	0.62
1:A:414:ALA:HB3	1:A:419:ILE:HD13	1.81	0.62
3:C:91:LEU:HD21	3:C:110:LEU:HD11	1.82	0.61
1:A:209:ALA:HB2	1:A:225:MET:HE3	1.82	0.61
2:B:113:LYS:HD2	2:B:133:ILE:HG21	1.84	0.60
1:A:798:ASN:HA	1:A:801:ILE:HD12	1.85	0.59
1:A:197:LYS:HE3	7:A:905:ADP:O2B	2.04	0.58
1:A:785:GLU:HA	3:C:101:LEU:HD11	1.86	0.57
1:A:159:ASP:O	1:A:162:LYS:HG2	2.05	0.57
1:A:729:VAL:HG13	1:A:734:LYS:HG3	1.87	0.57
1:A:718:PHE:H	1:A:770:GLN:HE21	1.54	0.56
1:A:342:MET:HE3	1:A:451:LEU:HB2	1.88	0.55
1:A:61[A]:SER:OG	1:A:66:LEU:HA	2.06	0.55
1:A:212:LYS:HD2	1:A:259:GLU:HG2	1.90	0.54
1:A:238:LYS:HB3	1:A:285:ARG:HB2	1.90	0.53
1:A:488:ILE:HD13	1:A:539:LEU:HD11	1.91	0.53
1:A:221:GLN:HG3	1:A:262:ILE:HB	1.91	0.52
1:A:54:LYS:HD2	1:A:90:CYS:SG	2.50	0.51
3:C:70:PHE:HD2	3:C:131:THR:HG23	1.74	0.51
1:A:39[B]:ASP:OD1	1:A:86:HIS:HD2	1.94	0.50
1:A:41:SER:HB3	1:A:44:ILE:HD12	1.94	0.50
1:A:397:TYR:HB2	1:A:621:VAL:HG21	1.93	0.50
1:A:205:MET:HB3	1:A:225:MET:HE1	1.94	0.50
1:A:289[B]:ILE:HD11	1:A:440:TYR:OH	2.13	0.49
1:A:358:GLY:HA3	1:A:396:MET:HG3	1.94	0.48
1:A:582:ILE:HD12	1:A:591:GLN:HB2	1.95	0.48
2:B:167:ILE:HG13	3:C:19:CYS:SG	2.54	0.48
1:A:603:ASP:O	1:A:641:ILE:HD11	2.14	0.48
1:A:32:LYS:HD3	3:C:45:ALA:HA	1.96	0.47
1:A:166:HIS:O	1:A:169:THR:HB	2.14	0.47
1:A:693:LEU:HA	1:A:696:LEU:HD12	1.95	0.47
1:A:582:ILE:HB	1:A:591:GLN:HG3	1.97	0.47
1:A:197:LYS:HB3	1:A:469:ASP:OD1	2.16	0.45
1:A:185:GLN:HG3	1:A:662:HIS:CE1	2.51	0.45
1:A:424:ASN:ND2	1:A:424:ASN:H	2.15	0.45
1:A:185:GLN:HE21	1:A:662:HIS:HE1	1.64	0.45
3:C:14:ILE:HB	3:C:19:CYS:HA	1.98	0.45
2:B:106:PRO:HB3	2:B:134:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:PHE:HB3	3:C:73:ILE:HD12	1.99	0.44
1:A:396:MET:HB3	1:A:398:LEU:HD12	1.99	0.44
1:A:398:LEU:HD21	1:A:613:ILE:HG12	2.00	0.44
2:B:169:THR:HG21	2:B:177:ASP:HA	1.99	0.44
1:A:184:SER:HB3	1:A:659:THR:HG22	1.98	0.44
1:A:302:LYS:HA	1:A:307:LEU:HD12	2.00	0.44
1:A:635:ILE:HD13	1:A:640:LEU:HD21	2.00	0.43
1:A:745:SER:C	1:A:747:SER:H	2.27	0.43
1:A:512:GLU:HG3	1:A:753:LYS:H	1.84	0.43
1:A:253:GLN:O	1:A:265:GLY:HA2	2.19	0.43
1:A:797:VAL:HG13	2:B:147:MET:HE1	2.00	0.43
1:A:39[B]:ASP:OD1	1:A:86:HIS:CD2	2.72	0.43
1:A:196:GLY:HA2	7:A:905:ADP:O2A	2.19	0.43
2:B:195:TYR:HA	2:B:198:PHE:HB3	2.01	0.42
3:C:122:ASN:OD1	3:C:124:LYS:HB2	2.18	0.42
1:A:99:PHE:CE1	1:A:104:LEU:HB2	2.54	0.42
1:A:208:PHE:HB3	1:A:256:ILE:HG12	2.01	0.42
2:B:84:LYS:HB2	2:B:90:ILE:HD11	2.01	0.42
1:A:292:GLN:HA	1:A:328:ASP:HB3	2.01	0.42
1:A:208:PHE:CZ	1:A:465:MET:HE3	2.54	0.42
1:A:99:PHE:CD1	1:A:104:LEU:HB2	2.54	0.42
1:A:802:PRO:HA	1:A:805:LEU:HD12	2.01	0.42
1:A:517:ALA:C	1:A:519:LEU:H	2.28	0.42
2:B:132:SER:O	2:B:135:VAL:HG12	2.20	0.42
1:A:682:LYS:HA	1:A:685:ILE:HD12	2.01	0.42
1:A:135:VAL:HG22	1:A:692:ILE:HG12	2.02	0.41
1:A:198:THR:O	1:A:202:LYS:HG3	2.20	0.41
1:A:224:ILE:O	1:A:227:ALA:HB3	2.21	0.41
1:A:442:LYS:HG3	1:A:625:PHE:CE2	2.55	0.41
1:A:285:ARG:HH22	1:A:328:ASP:CG	2.29	0.41
1:A:587:ILE:HD11	1:A:590:ILE:HD11	2.03	0.41
3:C:131:THR:HA	3:C:134:ILE:HD12	2.03	0.40
1:A:582:ILE:HD11	1:A:589:PRO:HB2	2.02	0.40
3:C:86:LYS:HB2	3:C:89:ASN:HB2	2.03	0.40
1:A:233:ALA:O	1:A:289[B]:ILE:HG13	2.22	0.40
1:A:480:SER:H	1:A:483:GLN:HG2	1.86	0.40
3:C:113:THR:HA	3:C:129:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	797/818 (97%)	741 (93%)	49 (6%)	7 (1%)	14	43
2	B	129/204 (63%)	122 (95%)	7 (5%)	0	100	100
3	C	127/134 (95%)	118 (93%)	6 (5%)	3 (2%)	4	24
All	All	1053/1156 (91%)	981 (93%)	62 (6%)	10 (1%)	12	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	GLY
1	A	321	THR
1	A	635	ILE
1	A	817	ALA
3	C	83	VAL
3	C	119	SER
1	A	21	VAL
3	C	113	THR
1	A	34	TYR
1	A	550	GLY

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	713/726 (98%)	644 (90%)	69 (10%)	8	28
2	B	117/186 (63%)	110 (94%)	7 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	123/126 (98%)	104 (85%)	19 (15%)	2	13
All	All	953/1038 (92%)	858 (90%)	95 (10%)	7	27

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	40	ILE
1	A	54	LYS
1	A	56	VAL
1	A	85	THR
1	A	91	ASN
1	A	94	VAL
1	A	157	THR
1	A	173	GLU
1	A	185	GLN
1	A	187	ILE
1	A	219	ARG
1	A	222	THR
1	A	228	ASN
1	A	241	ARG
1	A	282	ASP
1	A	304	LYS
1	A	337	GLU
1	A	347	SER
1	A	371	GLN
1	A	377	ASP
1	A	381[A]	ILE
1	A	381[B]	ILE
1	A	412	THR
1	A	417	THR
1	A	419	ILE
1	A	429	GLU
1	A	458	GLU
1	A	471	PHE
1	A	475	VAL
1	A	477	LYS
1	A	480	SER
1	A	483	GLN
1	A	495	LYS
1	A	508	LEU
1	A	512	GLU

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Mol	Chain	Res	Type
1	A	519	LEU
1	A	522	THR
1	A	525	LYS
1	A	526	GLU
1	A	530	VAL
1	A	566	GLU
1	A	574	LYS
1	A	579	LYS
1	A	583	ILE
1	A	586	THR
1	A	598	LEU
1	A	615	ASP
1	A	629	VAL
1	A	630	ILE
1	A	635	ILE
1	A	644	GLN
1	A	646	LEU
1	A	650	THR
1	A	680	GLU
1	A	699	ARG
1	A	706	ARG
1	A	728	SER
1	A	738	ILE
1	A	746	GLU
1	A	747	SER
1	A	754	SER
1	A	760	GLN
1	A	774	LEU
1	A	801	ILE
1	A	803	SER
1	A	805	LEU
1	A	813	LYS
1	A	816	VAL
2	B	76	ASP
2	B	122	LEU
2	B	133	ILE
2	B	135	VAL
2	B	138	LYS
2	B	155	CYS
2	B	159	LEU
3	C	6	GLU
3	C	18	SER

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Mol	Chain	Res	Type
3	C	27	LYS
3	C	38	ILE
3	C	52	ASN
3	C	74	ASN
3	C	84	GLN
3	C	85	ILE
3	C	88	ASP
3	C	89	ASN
3	C	107	ASN
3	C	108	ILE
3	C	109	LEU
3	C	111	GLN
3	C	116	GLU
3	C	119	SER
3	C	125	THR
3	C	131	THR
3	C	134	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	59	GLN
1	A	86	HIS
1	A	185	GLN
1	A	258	HIS
1	A	283	ASN
1	A	424	ASN
1	A	580	ASN
1	A	584	GLN
1	A	585	HIS
1	A	654	ASN
1	A	672	ASN
1	A	686	GLN
1	A	737	ASN
1	A	770	GLN
1	A	779	ASN
1	A	795	GLN
1	A	810	HIS
1	A	818	GLN
2	B	94	ASN
3	C	33	ASN

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Mol	Chain	Res	Type
3	C	49	ASN
3	C	65	ASN
3	C	68	GLN
3	C	75	ASN
3	C	128	GLN

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
7	ADP	A	905	6	28,29,29	0.61	1 (3%)	43,45,45	0.56	0
4	SO4	A	902	-	4,4,4	0.49	0	6,6,6	0.45	0
4	SO4	B	301	-	4,4,4	0.36	0	6,6,6	0.22	0
5	EDO	C	201	-	3,3,3	0.48	0	2,2,2	0.52	0
5	EDO	A	903	-	3,3,3	0.75	0	2,2,2	0.07	0
4	SO4	A	901	-	4,4,4	0.26	0	6,6,6	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
7	ADP	A	905	6	-	0/16/32/32	0/3/3/3
5	EDO	C	201	-	-	0/1/1/1	-
5	EDO	A	903	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	905	ADP	PB-O3B	-2.63	1.45	1.54

There are no bond angle outliers.

There are no chirality outliers.

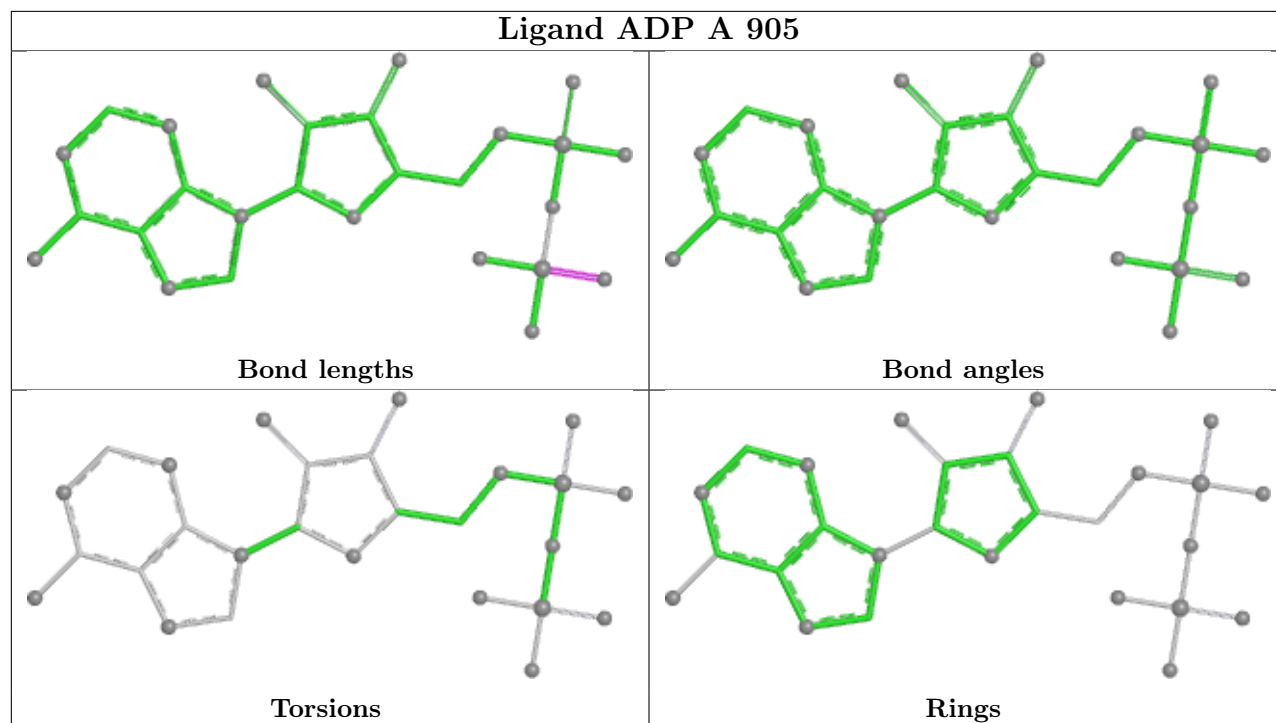
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	905	ADP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	795/818 (97%)	-0.13	8 (1%) 79 63	30, 82, 143, 174	6 (0%)
2	B	131/204 (64%)	-0.04	1 (0%) 82 68	69, 106, 154, 164	0
3	C	131/134 (97%)	0.04	1 (0%) 82 68	60, 93, 145, 174	0
All	All	1057/1156 (91%)	-0.10	10 (0%) 81 65	30, 86, 145, 174	6 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381[A]	ILE	3.8
3	C	2	ALA	3.2
1	A	629	VAL	2.3
1	A	522	THR	2.3
1	A	475	VAL	2.3
2	B	135	VAL	2.2
1	A	751	ILE	2.2
1	A	579	LYS	2.1
1	A	645	PHE	2.1
1	A	449[A]	ARG	2.1

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

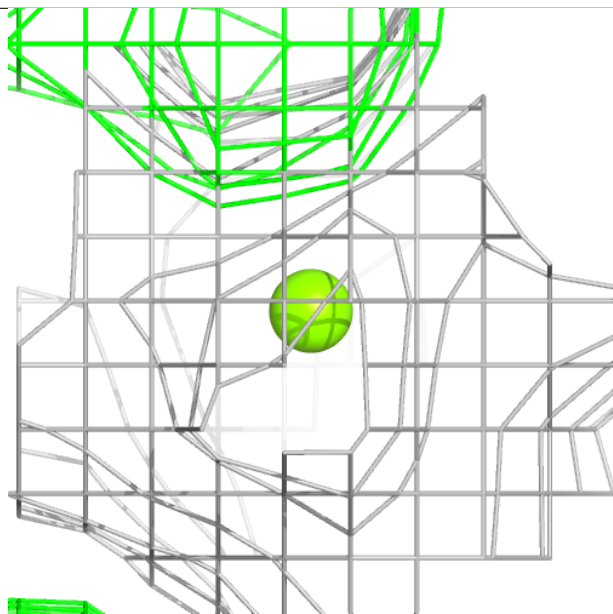
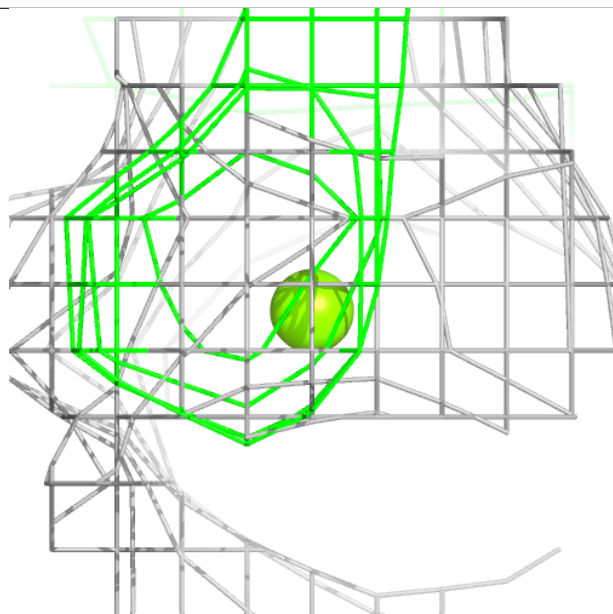
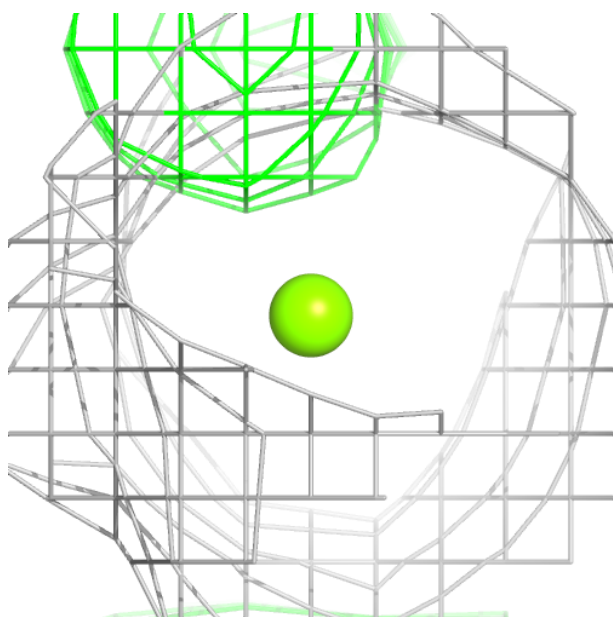
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	C	201	4/4	0.72	0.19	90,91,93,93	0
5	EDO	A	903	4/4	0.73	0.21	85,87,91,91	0
4	SO4	A	901	5/5	0.91	0.09	96,97,98,98	0
4	SO4	A	902	5/5	0.95	0.06	88,89,91,94	0
4	SO4	B	301	5/5	0.95	0.07	103,104,105,105	0
6	MG	A	904	1/1	0.97	0.09	52,52,52,52	0
7	ADP	A	905	27/27	0.97	0.07	58,64,69,71	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.

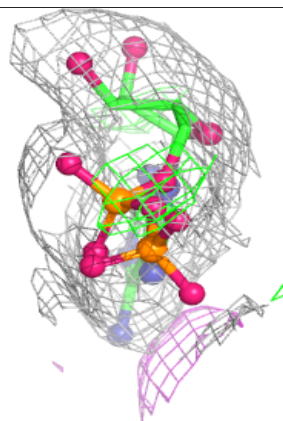
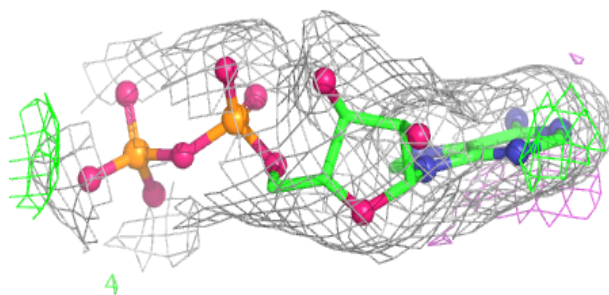
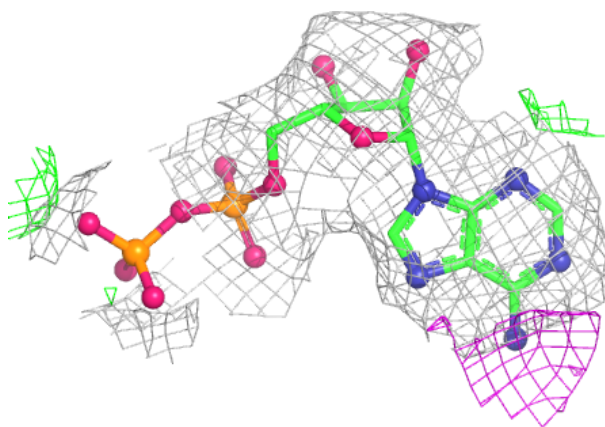
Electron density around MG A 904:

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



Electron density around ADP A 905:

$2mF_o-DF_c$ (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.