



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:10 PM UTC

PDB ID : 7YNE / pdb_00007yne
Title : Crystal structure of fragmin domain-1 (1-160) in complex with G-form actin
Authors : Takeda, S.
Deposited on : 2022-07-30
Resolution : 2.70 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:

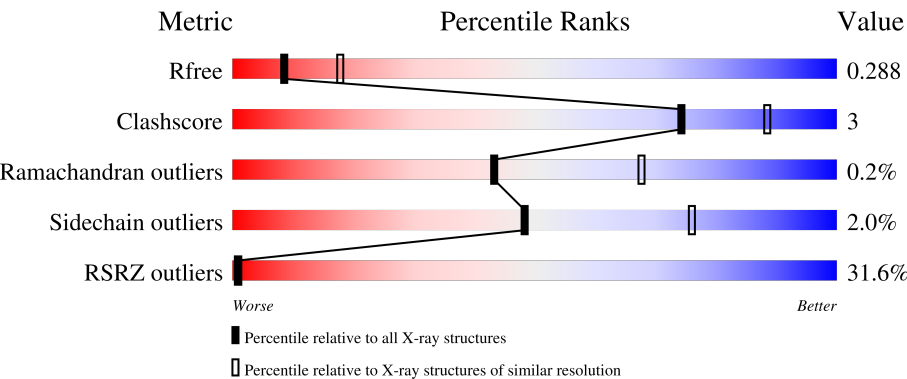
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	377	6% 81% 13% 6%
1	C	377	8% 80% 11% 8%
1	E	377	57% 80% 10% 9%
1	G	377	54% 81% 6% 12%
2	B	162	% 85% 14%

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Mol	Chain	Length	Quality of chain
2	D	162	3%86%14%
2	F	162	46%79%19%
2	H	162	31%83%16%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14719 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2704	1719	444	522	19			
1	C	347	Total	C	N	O	S	0	1	0
			2688	1709	445	515	19			
1	E	342	Total	C	N	O	S	0	0	0
			2387	1510	392	467	18			
1	G	332	Total	C	N	O	S	0	0	0
			2313	1459	385	456	13			

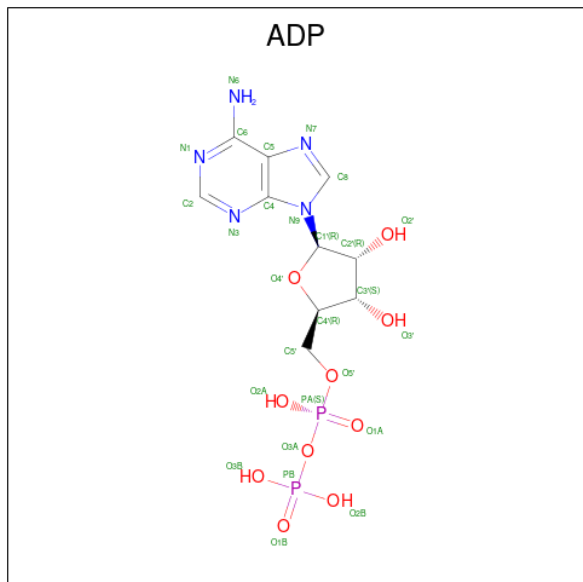
- Molecule 2 is a protein called Actin-binding protein fragmin P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	140	Total	C	N	O	0	0	0
			1120	722	186	212			
2	D	140	Total	C	N	O	0	0	0
			1087	702	178	207			
2	F	132	Total	C	N	O	0	0	0
			979	630	159	190			
2	H	136	Total	C	N	O	0	0	0
			1027	661	169	197			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q94707
B	0	PRO	-	expression tag	UNP Q94707
D	-1	GLY	-	expression tag	UNP Q94707
D	0	PRO	-	expression tag	UNP Q94707
F	-1	GLY	-	expression tag	UNP Q94707
F	0	PRO	-	expression tag	UNP Q94707
H	-1	GLY	-	expression tag	UNP Q94707
H	0	PRO	-	expression tag	UNP Q94707

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	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	E	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		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		
4	H	2	Total	Ca	0	0
			2	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	P	0	0
			5	4	1		

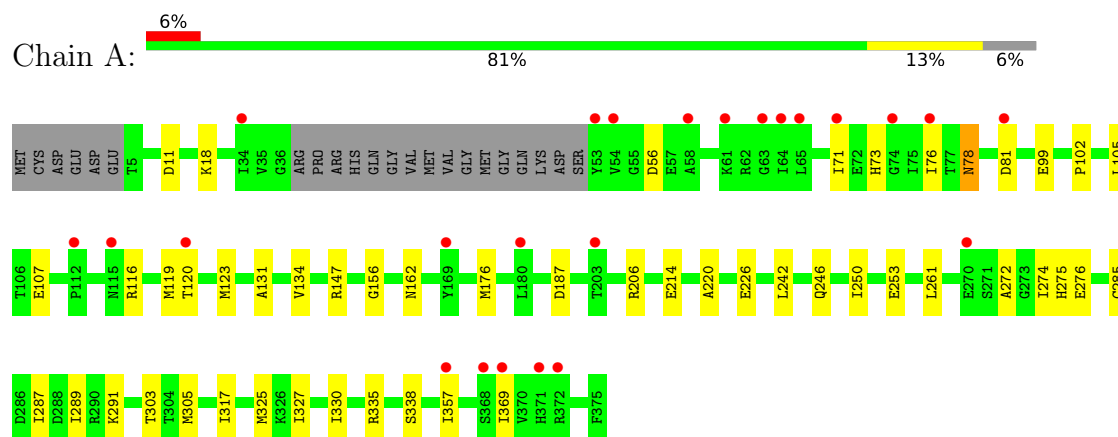
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	69	Total O 69 69	0	0
9	B	70	Total O 70 70	0	0
9	C	84	Total O 84 84	0	0
9	D	37	Total O 37 37	0	0
9	E	2	Total O 2 2	0	0
9	F	2	Total O 2 2	0	0
9	G	3	Total O 3 3	0	0

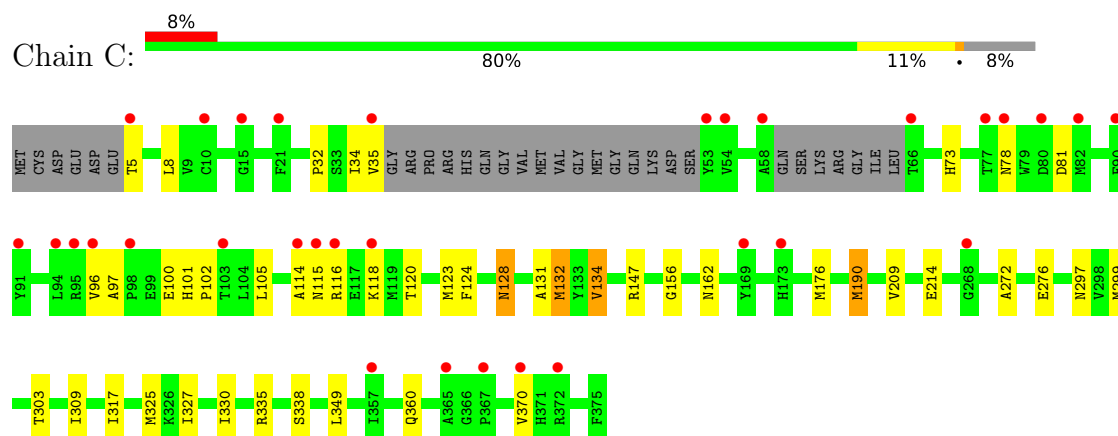
3 Residue-property plots [i](#)

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.

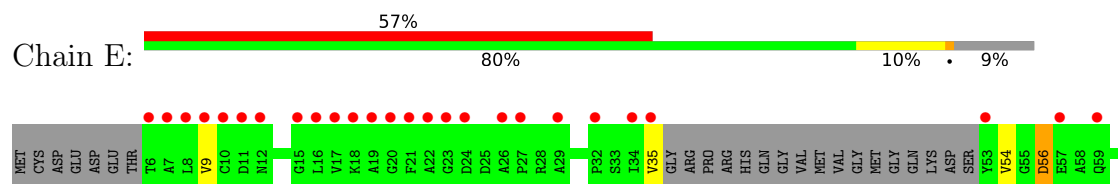
- Molecule 1: Actin, alpha skeletal muscle

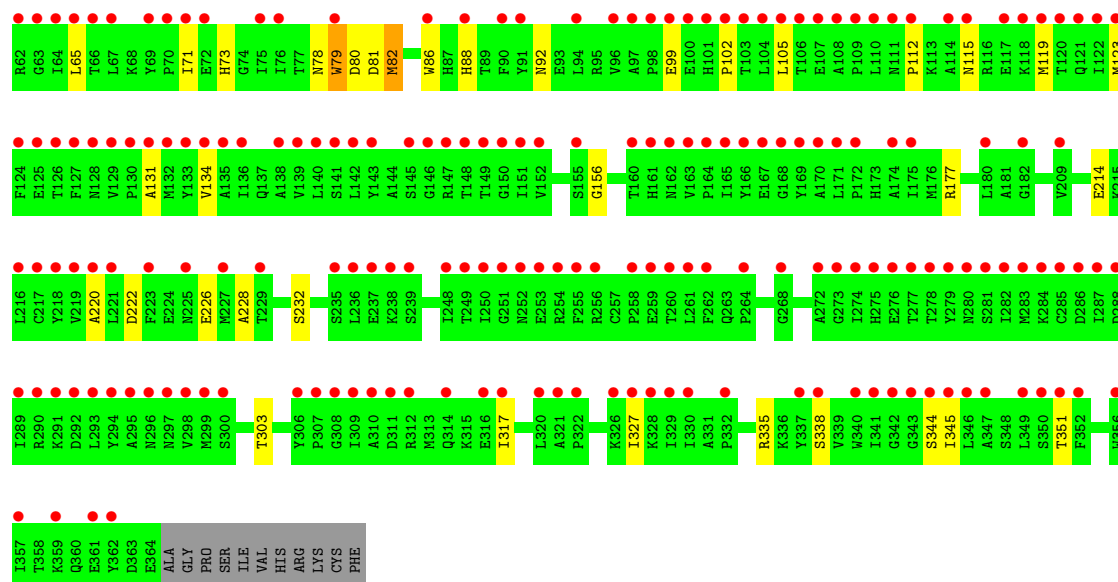


- Molecule 1: Actin, alpha skeletal muscle



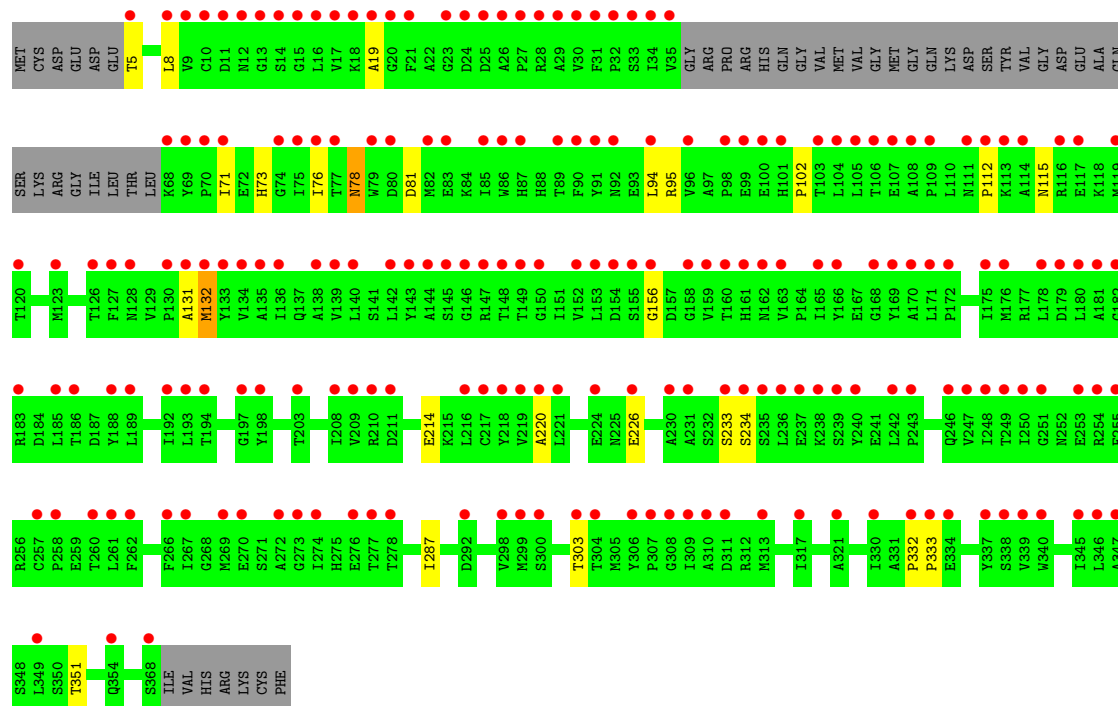
- Molecule 1: Actin, alpha skeletal muscle





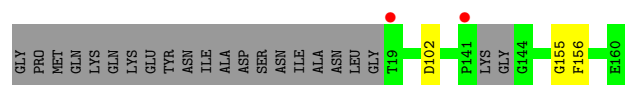
• Molecule 1: Actin, alpha skeletal muscle

Chain G: 54% 81% 6% 12%

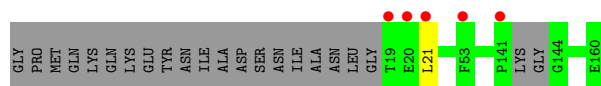
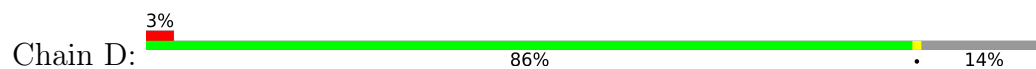


• Molecule 2: Actin-binding protein fragmin P

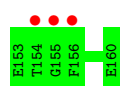
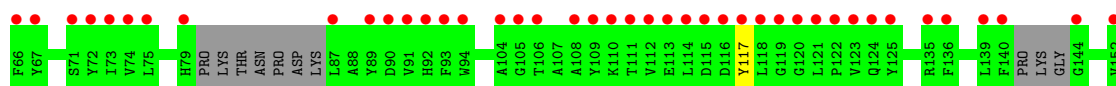
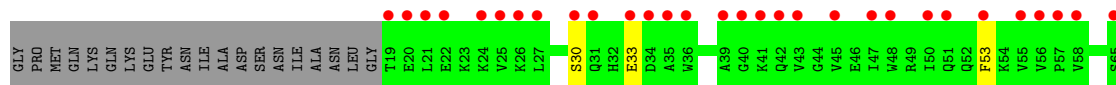
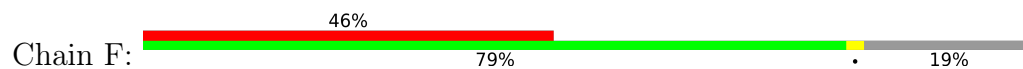
Chain B: 85% 14% 1%



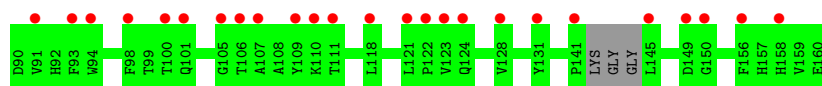
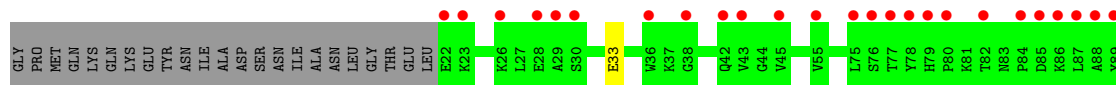
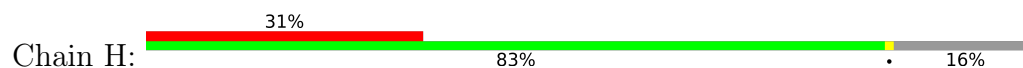
- Molecule 2: Actin-binding protein fragmin P



- Molecule 2: Actin-binding protein fragmin P



- Molecule 2: Actin-binding protein fragmin P



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.90Å 98.00Å 420.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.70 49.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.21-2.70) 99.9 (49.21-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.273 , 0.308 (Not available) , 0.288	Depositor DCC
R_{free} test set	3296 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14719	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ADP, CA, EDO, PO4, ACT, HIC

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	0.08	0/2749	0.22	0/3738
1	C	0.09	0/2736	0.25	0/3714
1	E	0.08	0/2423	0.24	0/3322
1	G	0.08	0/2350	0.22	0/3226
2	B	0.08	0/1152	0.26	0/1562
2	D	0.08	0/1119	0.24	0/1525
2	F	0.07	0/1006	0.21	0/1374
2	H	0.07	0/1059	0.22	0/1447
All	All	0.08	0/14594	0.24	0/19908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2704	0	2615	27	0
1	C	2688	0	2623	23	0
1	E	2387	0	2129	21	0
1	G	2313	0	2032	15	0
2	B	1120	0	1061	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1087	0	994	0	0
2	F	979	0	839	3	0
2	H	1027	0	892	1	0
3	A	27	0	12	1	0
3	C	27	0	12	1	0
3	E	27	0	12	1	0
3	G	27	0	12	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	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	2	0	0	0	0
5	A	4	0	3	0	0
5	B	8	0	6	0	0
5	D	4	0	3	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	4	0	6	0	0
8	D	5	0	0	0	0
9	A	69	0	0	0	0
9	B	70	0	0	0	0
9	C	84	0	0	0	0
9	D	37	0	0	0	0
9	E	2	0	0	0	0
9	F	2	0	0	0	0
9	G	3	0	0	0	0
All	All	14719	0	13251	87	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 3.

All (87) 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:220:ALA:HB1	1:E:226:GLU:HG3	1.45	0.96
1:E:56:ASP:N	1:E:56:ASP:OD1	2.20	0.75
1:C:78:ASN:ND2	1:C:81:ASP:OD1	2.23	0.72
1:E:79:TRP:O	1:E:81:ASP:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:TRP:O	1:E:82:MET:N	2.22	0.68
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.76	0.68
1:E:35:VAL:HG11	1:E:81:ASP:HB3	1.76	0.68
1:C:190:MET:HG3	1:C:209:VAL:HG21	1.78	0.65
1:E:92:ASN:O	1:G:95:ARG:NH2	2.29	0.65
1:A:78:ASN:OD1	1:A:78:ASN:N	2.30	0.64
1:C:317:ILE:HG22	1:C:327:ILE:HD13	1.79	0.63
1:G:112:PRO:HD2	1:G:115:ASN:HD21	1.62	0.63
1:E:222:ASP:O	1:E:226:GLU:HG2	1.99	0.62
1:A:187:ASP:OD1	1:A:206:ARG:NH1	2.33	0.62
1:A:317:ILE:HG22	1:A:327:ILE:HD13	1.83	0.60
1:E:317:ILE:HG22	1:E:327:ILE:HD13	1.82	0.60
1:C:156:GLY:O	1:C:303:THR:OG1	2.21	0.59
1:G:220:ALA:HB1	1:G:226:GLU:HG3	1.85	0.59
1:G:78:ASN:N	1:G:78:ASN:OD1	2.36	0.58
1:E:112:PRO:HD2	1:E:115:ASN:HD21	1.70	0.57
1:A:105:LEU:HD11	1:A:123:MET:HE3	1.87	0.56
1:A:156:GLY:O	1:A:303:THR:OG1	2.22	0.56
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.39	0.56
1:E:156:GLY:O	1:E:303:THR:OG1	2.24	0.55
1:A:357:ILE:HD13	1:A:369:ILE:HG23	1.88	0.54
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.89	0.53
1:G:156:GLY:O	1:G:303:THR:OG1	2.26	0.53
1:E:351:THR:HG21	2:F:33:GLU:HB2	1.89	0.53
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.32	0.52
1:G:351:THR:HG21	2:H:33:GLU:HB2	1.90	0.52
1:E:102:PRO:HB3	1:E:131:ALA:HB3	1.92	0.51
1:C:120:THR:HG21	1:C:370:VAL:HB	1.92	0.51
1:C:128:ASN:O	1:C:128:ASN:CG	2.54	0.51
1:A:272:ALA:HB1	1:A:276:GLU:HB2	1.92	0.51
1:E:71:ILE:HD11	1:E:82:MET:HE2	1.93	0.50
1:E:214:GLU:HG2	3:E:401:ADP:C4	2.47	0.50
1:A:71:ILE:HG12	1:A:76:ILE:HG12	1.92	0.50
1:E:335:ARG:HA	1:E:338:SER:HB3	1.94	0.49
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.94	0.49
1:C:8:LEU:HD21	1:C:96:VAL:HG21	1.95	0.49
1:A:11:ASP:HB3	1:A:18:LYS:HB2	1.95	0.48
1:G:78:ASN:ND2	1:G:81:ASP:OD2	2.46	0.48
1:A:275:HIS:CE1	1:A:276:GLU:HG3	2.49	0.48
1:C:105:LEU:HD11	1:C:123:MET:HE3	1.95	0.48
1:A:261:LEU:HB3	1:A:274:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:HG2	1:A:325:MET:HE1	1.97	0.47
1:C:8:LEU:HD13	1:C:101:HIS:HB3	1.96	0.47
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.97	0.47
1:C:325:MET:HE3	1:C:325:MET:HA	1.97	0.46
1:E:86:TRP:CH2	1:E:119:MET:HG3	2.50	0.46
1:C:35:VAL:HG11	1:C:81:ASP:HB3	1.97	0.46
1:C:272:ALA:HB1	1:C:276:GLU:HB2	1.98	0.46
1:A:325:MET:HA	1:A:325:MET:HE3	1.98	0.45
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.98	0.45
1:G:19:ALA:HB1	1:G:94:LEU:HD11	1.98	0.45
1:C:100:GLU:HG3	1:C:101:HIS:CD2	2.52	0.44
1:A:76:ILE:HD12	1:A:119:MET:HE2	1.98	0.44
1:E:88:HIS:HA	1:E:92:ASN:HD22	1.82	0.44
1:C:32:PRO:HB2	1:C:34:ILE:HG12	1.99	0.44
1:C:116[A]:ARG:HH21	1:C:134:VAL:HG22	1.82	0.44
1:G:214:GLU:HG2	3:G:401:ADP:C4	2.53	0.44
1:C:124:PHE:CE2	1:C:132:MET:HG2	2.53	0.43
1:C:299:MET:HE1	1:C:309:ILE:HG23	2.00	0.43
1:G:71:ILE:HG12	1:G:76:ILE:HG12	2.00	0.43
1:A:214:GLU:HG2	3:A:401:ADP:C4	2.53	0.43
1:C:214:GLU:HG2	3:C:401:ADP:C4	2.53	0.43
1:E:105:LEU:HD11	1:E:123:MET:HE3	2.00	0.43
1:G:287:ILE:H	1:G:287:ILE:HD12	1.84	0.43
1:A:305:MET:HA	1:A:335:ARG:HH21	1.85	0.42
2:F:30:SER:HB2	2:F:117:TYR:HB2	2.02	0.42
1:A:147:ARG:NH2	1:A:330:ILE:HG12	2.34	0.42
2:B:102:ASP:OD2	2:B:155:GLY:N	2.53	0.42
1:C:335:ARG:HA	1:C:338:SER:HB3	2.02	0.41
1:E:345:ILE:HG23	2:F:53:PHE:HE1	1.85	0.41
1:A:335:ARG:HA	1:A:338:SER:HB3	2.02	0.41
1:A:102:PRO:HB3	1:A:131:ALA:HB3	2.02	0.41
1:A:242:LEU:HD12	1:A:246:GLN:HB3	2.02	0.41
1:G:233:SER:OG	1:G:234:SER:N	2.53	0.41
1:A:287:ILE:HD12	1:A:287:ILE:H	1.86	0.41
1:E:9:VAL:HG21	1:E:344:SER:HA	2.02	0.41
1:E:228:ALA:O	1:E:232:SER:OG	2.30	0.41
1:G:132:MET:HE3	1:G:132:MET:HB2	1.93	0.41
1:A:162:ASN:HB2	1:A:176:MET:HB2	2.02	0.41
1:A:250:ILE:HG13	1:A:253:GLU:HB2	2.03	0.40
1:G:332:PRO:HA	1:G:333:PRO:HD3	1.96	0.40
1:C:147:ARG:NH2	1:C:330:ILE:HG12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ALA:O	1:C:118:LYS:HG2	2.22	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	350/377 (93%)	341 (97%)	9 (3%)	0	100	100
1	C	341/377 (90%)	332 (97%)	8 (2%)	1 (0%)	36	60
1	E	337/377 (89%)	327 (97%)	8 (2%)	2 (1%)	21	44
1	G	327/377 (87%)	321 (98%)	6 (2%)	0	100	100
2	B	136/162 (84%)	135 (99%)	1 (1%)	0	100	100
2	D	136/162 (84%)	133 (98%)	3 (2%)	0	100	100
2	F	126/162 (78%)	125 (99%)	1 (1%)	0	100	100
2	H	132/162 (82%)	130 (98%)	2 (2%)	0	100	100
All	All	1885/2156 (87%)	1844 (98%)	38 (2%)	3 (0%)	43	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	80	ASP
1	C	97	ALA
1	E	79	TRP

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	284/319 (89%)	279 (98%)	5 (2%)	51	78
1	C	286/319 (90%)	277 (97%)	9 (3%)	35	65
1	E	220/319 (69%)	212 (96%)	8 (4%)	31	60
1	G	210/319 (66%)	206 (98%)	4 (2%)	50	77
2	B	116/135 (86%)	115 (99%)	1 (1%)	70	87
2	D	108/135 (80%)	107 (99%)	1 (1%)	70	87
2	F	89/135 (66%)	89 (100%)	0	100	100
2	H	96/135 (71%)	96 (100%)	0	100	100
All	All	1409/1816 (78%)	1381 (98%)	28 (2%)	48	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	78	ASN
1	A	99	GLU
1	A	120	THR
1	A	134	VAL
2	B	156	PHE
1	C	5	THR
1	C	115	ASN
1	C	128	ASN
1	C	132	MET
1	C	134	VAL
1	C	190	MET
1	C	297	ASN
1	C	349	LEU
1	C	360	GLN
2	D	21	LEU
1	E	54	VAL
1	E	56	ASP
1	E	65	LEU
1	E	78	ASN
1	E	82	MET
1	E	99	GLU
1	E	134	VAL
1	E	177	ARG

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Mol	Chain	Res	Type
1	G	5	THR
1	G	8	LEU
1	G	78	ASN
1	G	132	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	297	ASN
2	B	42	GLN
1	C	88	HIS
1	E	78	ASN
1	E	88	HIS
1	E	92	ASN
1	E	162	ASN
2	F	52	GLN
1	G	88	HIS
1	G	297	ASN
2	H	32	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	HIC	G	73	1	10,11,12	1.55	1 (10%)	9,14,16	1.28	1 (11%)
1	HIC	A	73	1	10,11,12	1.53	1 (10%)	9,14,16	1.31	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	C	73	1	10,11,12	1.55	1 (10%)	9,14,16	1.28	1 (11%)
1	HIC	E	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.26	1 (11%)

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
1	HIC	G	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	73	1	-	3/5/6/8	0/1/1/1
1	HIC	C	73	1	-	2/5/6/8	0/1/1/1
1	HIC	E	73	1	-	3/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	HIC	CD2-CG	3.16	1.41	1.36
1	E	73	HIC	CD2-CG	3.13	1.41	1.36
1	A	73	HIC	CD2-CG	3.11	1.41	1.36
1	G	73	HIC	CD2-CG	3.11	1.41	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-3.28	111.41	112.66
1	G	73	HIC	NE2-CE1-ND1	-3.17	111.45	112.66
1	C	73	HIC	NE2-CE1-ND1	-3.17	111.45	112.66
1	E	73	HIC	NE2-CE1-ND1	-3.08	111.48	112.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	O-C-CA-CB
1	E	73	HIC	O-C-CA-CB
1	A	73	HIC	CA-CB-CG-ND1
1	C	73	HIC	CA-CB-CG-ND1
1	E	73	HIC	CA-CB-CG-ND1
1	G	73	HIC	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
1	A	73	HIC	CA-CB-CG-CD2
1	C	73	HIC	CA-CB-CG-CD2
1	E	73	HIC	CA-CB-CG-CD2
1	G	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	G	401	4	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
3	ADP	E	401	4	28,29,29	1.43	4 (14%)	43,45,45	1.84	8 (18%)
5	ACT	B	203	-	3,3,3	1.36	0	3,3,3	1.52	0
3	ADP	C	401	4	28,29,29	1.40	4 (14%)	43,45,45	1.79	9 (20%)
8	PO4	D	204	-	4,4,4	0.99	0	6,6,6	0.44	0
5	ACT	D	203	-	3,3,3	1.36	0	3,3,3	1.48	0
5	ACT	B	204	-	3,3,3	1.26	0	3,3,3	1.56	0
3	ADP	A	401	4	28,29,29	1.40	4 (14%)	43,45,45	1.82	9 (20%)
5	ACT	A	403	-	3,3,3	1.40	1 (33%)	3,3,3	1.36	0
7	EDO	A	405	-	3,3,3	0.43	0	2,2,2	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	G	401	4	-	0/16/32/32	0/3/3/3
3	ADP	E	401	4	-	0/16/32/32	0/3/3/3
3	ADP	C	401	4	-	0/16/32/32	0/3/3/3
3	ADP	A	401	4	-	0/16/32/32	0/3/3/3
7	EDO	A	405	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	ADP	C5-C4	4.81	1.47	1.39
3	G	401	ADP	C5-C4	4.73	1.47	1.39
3	C	401	ADP	C5-C4	4.70	1.47	1.39
3	A	401	ADP	C5-C4	4.65	1.47	1.39
3	E	401	ADP	C5-C6	2.78	1.48	1.41
3	G	401	ADP	C5-C6	2.76	1.48	1.41
3	A	401	ADP	C5-C6	2.72	1.48	1.41
3	C	401	ADP	C5-C6	2.72	1.48	1.41
3	G	401	ADP	C8-N7	2.44	1.36	1.31
3	C	401	ADP	C8-N7	2.44	1.36	1.31
3	E	401	ADP	C8-N7	2.41	1.36	1.31
3	A	401	ADP	C8-N7	2.36	1.36	1.31
3	E	401	ADP	C5-N7	-2.30	1.34	1.39
3	G	401	ADP	C5-N7	-2.23	1.35	1.39
3	A	401	ADP	C5-N7	-2.23	1.35	1.39
3	C	401	ADP	C5-N7	-2.21	1.35	1.39
5	A	403	ACT	CH3-C	2.04	1.57	1.49

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	ADP	C5-C4-N3	-5.98	118.48	126.72
3	G	401	ADP	C5-C4-N3	-5.83	118.69	126.72
3	A	401	ADP	C5-C4-N3	-5.76	118.78	126.72
3	C	401	ADP	C5-C4-N3	-5.67	118.91	126.72
3	E	401	ADP	N3-C4-N9	4.71	135.18	127.17
3	G	401	ADP	N3-C4-N9	4.57	134.94	127.17
3	A	401	ADP	N3-C4-N9	4.53	134.88	127.17
3	C	401	ADP	N3-C4-N9	4.45	134.73	127.17
3	E	401	ADP	C2-N3-C4	3.76	121.02	111.83
3	G	401	ADP	C2-N3-C4	3.71	120.90	111.83
3	C	401	ADP	C2-N3-C4	3.69	120.85	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C2-N3-C4	3.68	120.81	111.83
3	A	401	ADP	C4-C5-N7	-3.55	106.53	110.58
3	G	401	ADP	C4-C5-N7	-3.55	106.53	110.58
3	E	401	ADP	C4-C5-N7	-3.50	106.58	110.58
3	C	401	ADP	C4-C5-N7	-3.45	106.64	110.58
3	C	401	ADP	N3-C2-N1	-3.33	123.53	128.58
3	A	401	ADP	N3-C2-N1	-3.26	123.65	128.58
3	G	401	ADP	N3-C2-N1	-3.23	123.69	128.58
3	E	401	ADP	N3-C2-N1	-3.20	123.74	128.58
3	A	401	ADP	C4-N9-C8	2.73	108.60	105.74
3	G	401	ADP	C4-N9-C8	2.68	108.55	105.74
3	C	401	ADP	C4-N9-C8	2.64	108.51	105.74
3	A	401	ADP	C5-N7-C8	2.63	107.58	103.45
3	G	401	ADP	C5-N7-C8	2.60	107.53	103.45
3	E	401	ADP	C4-N9-C8	2.59	108.46	105.74
3	E	401	ADP	C5-N7-C8	2.59	107.52	103.45
3	C	401	ADP	C5-N7-C8	2.52	107.41	103.45
3	C	401	ADP	C6-C5-N7	2.18	136.30	132.09
3	G	401	ADP	C6-C5-N7	2.14	136.22	132.09
3	A	401	ADP	C6-C5-N7	2.13	136.20	132.09
3	A	401	ADP	N9-C8-N7	-2.10	110.95	113.94
3	E	401	ADP	C6-C5-N7	2.08	136.09	132.09
3	G	401	ADP	N9-C8-N7	-2.06	111.02	113.94
3	C	401	ADP	N9-C8-N7	-2.01	111.08	113.94

There are no chirality outliers.

There are no torsion outliers.

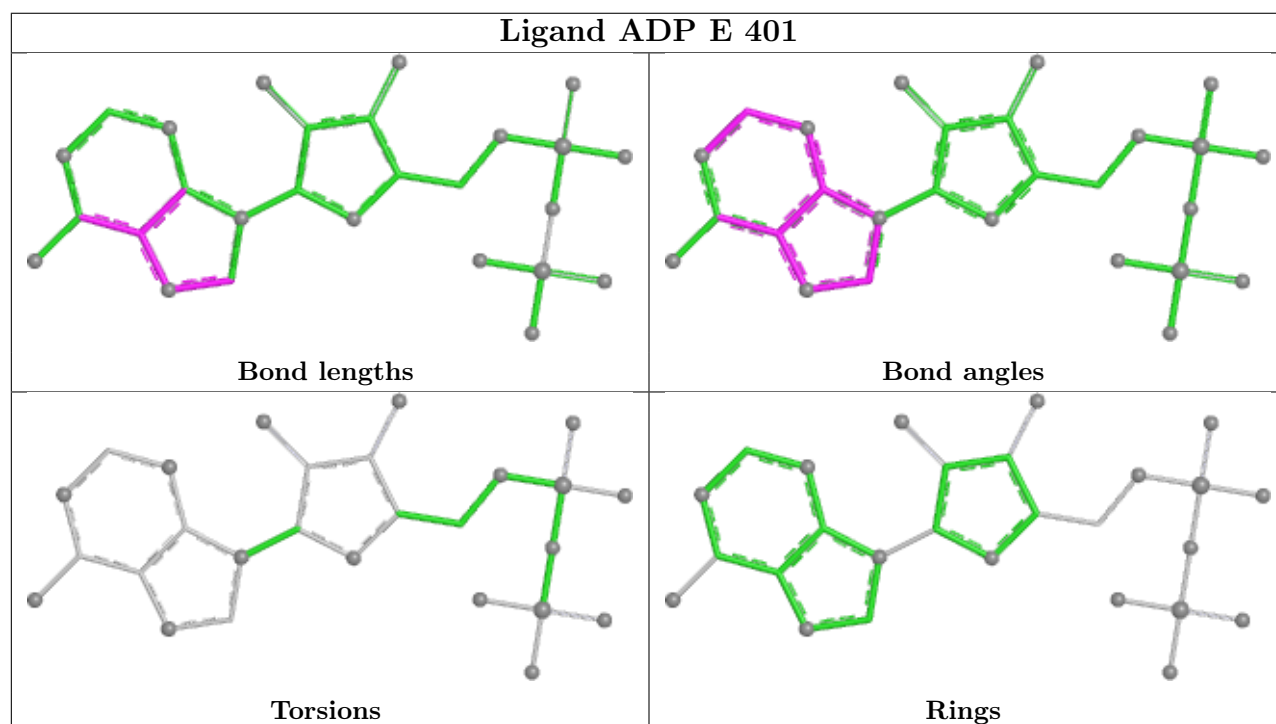
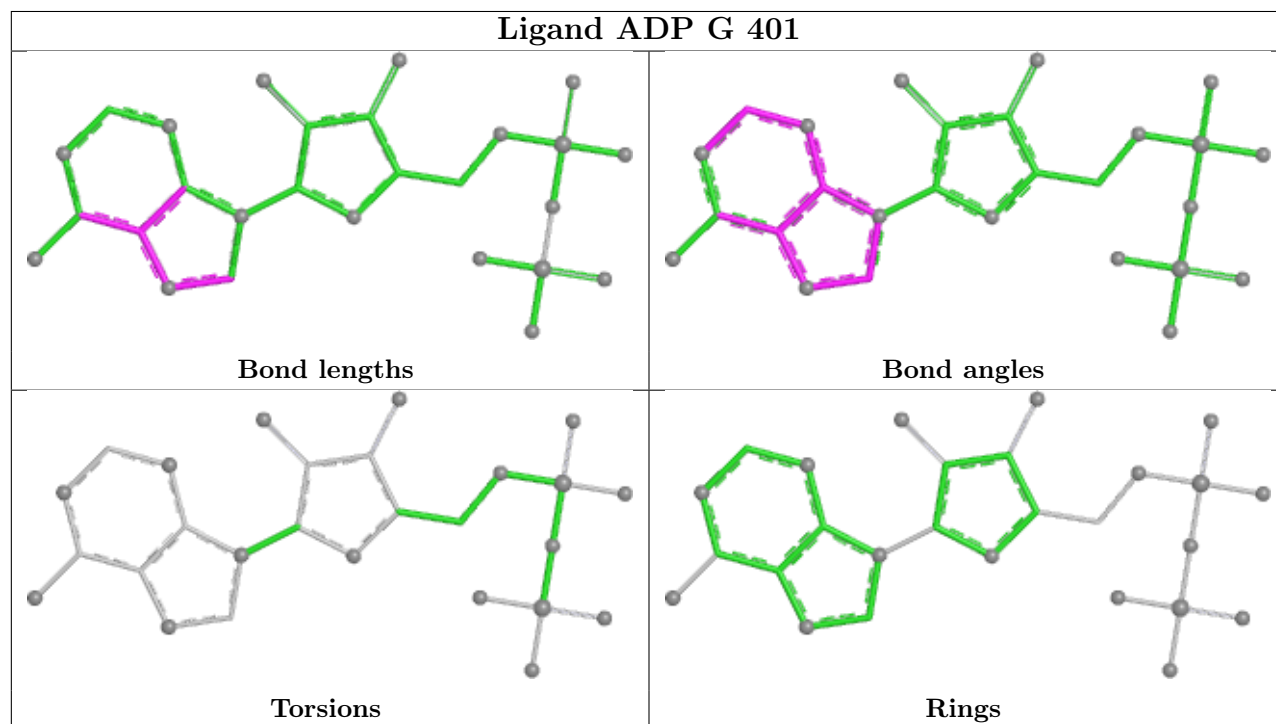
There are no ring outliers.

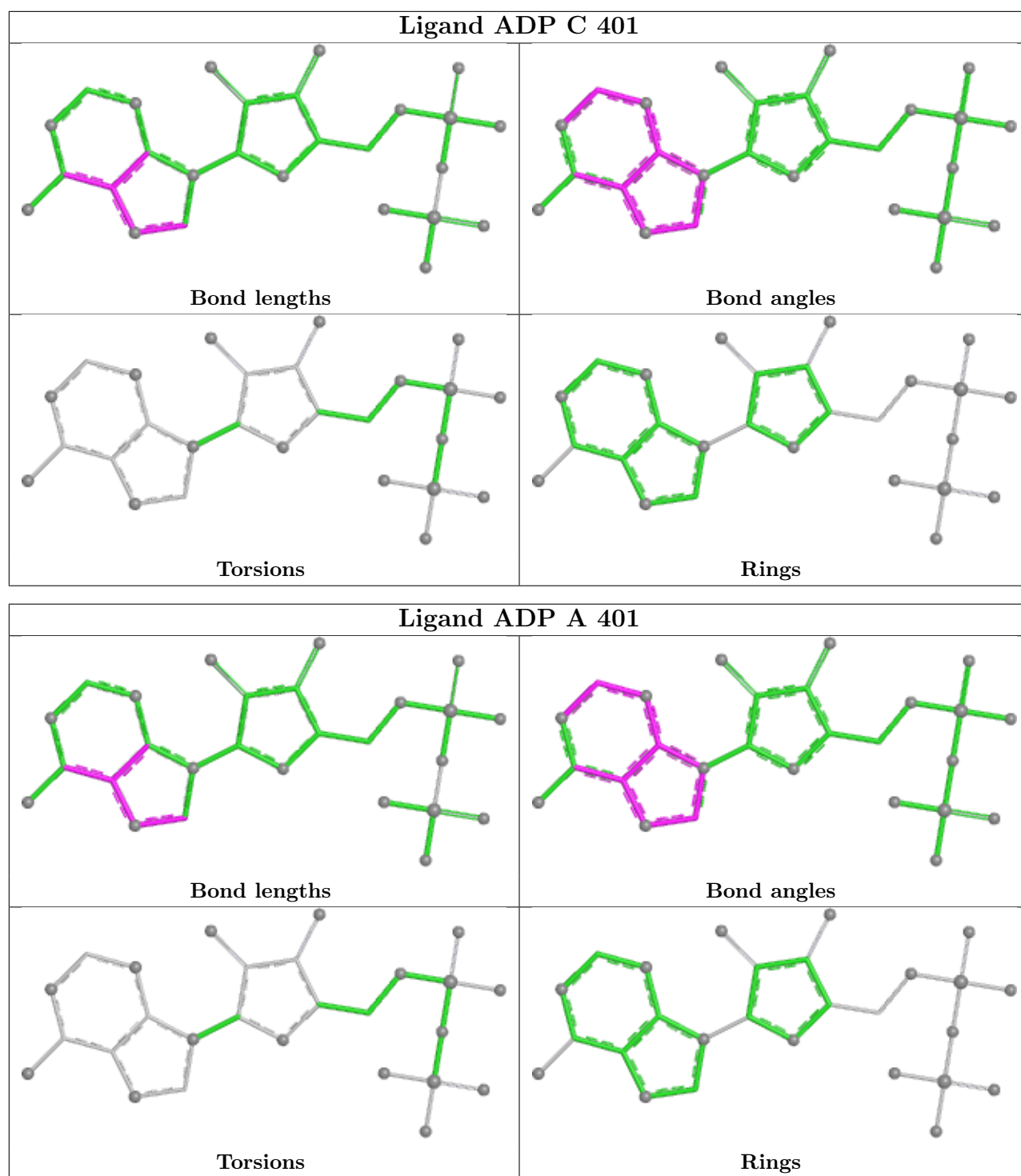
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	ADP	1	0
3	E	401	ADP	1	0
3	C	401	ADP	1	0
3	A	401	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	354/377 (93%)	0.49	24 (6%) 23 20	27, 58, 110, 148	0
1	C	346/377 (91%)	0.60	32 (9%) 14 12	28, 53, 109, 171	1 (0%)
1	E	341/377 (90%)	2.53	214 (62%) 0 0	60, 109, 167, 233	0
1	G	331/377 (87%)	2.46	204 (61%) 0 0	100, 127, 168, 226	0
2	B	140/162 (86%)	-0.17	2 (1%) 73 72	25, 34, 70, 94	0
2	D	140/162 (86%)	0.33	5 (3%) 46 42	36, 53, 91, 106	0
2	F	132/162 (81%)	2.29	75 (56%) 0 0	89, 125, 155, 223	0
2	H	136/162 (83%)	1.78	50 (36%) 1 0	82, 113, 173, 350	0
All	All	1920/2156 (89%)	1.37	606 (31%) 1 1	25, 91, 155, 350	1 (0%)

All (606) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	154	ASP	8.1
1	G	138	ALA	7.7
1	G	248	ILE	7.0
2	F	73	ILE	6.8
1	E	166	TYR	6.7
1	G	33	SER	6.5
2	F	74	VAL	6.3
1	E	275	HIS	6.2
1	G	261	LEU	6.1
1	E	220	ALA	6.1
1	E	102	PRO	6.0
1	E	165	ILE	6.0
1	E	262	PHE	5.8
1	E	251	GLY	5.5
1	E	341	ILE	5.5
1	E	250	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	236	LEU	5.5
1	E	330	ILE	5.4
1	E	344	SER	5.4
1	E	357	ILE	5.3
1	E	65	LEU	5.2
1	G	198	TYR	5.2
1	E	34	ILE	5.2
2	F	75	LEU	5.1
1	E	298	VAL	5.1
1	G	89	THR	5.1
2	F	114	LEU	5.1
2	F	36	TRP	5.0
1	E	362	TYR	5.0
1	E	138	ALA	5.0
1	G	155	SER	5.0
1	E	322	PRO	5.0
1	E	63	GLY	5.0
1	G	90	PHE	5.0
1	G	260	THR	4.9
1	G	94	LEU	4.9
1	E	29	ALA	4.9
1	G	172	PRO	4.8
1	G	156	GLY	4.8
1	G	243	PRO	4.8
1	G	221	LEU	4.8
1	E	174	ALA	4.7
2	F	58	VAL	4.7
1	E	19	ALA	4.7
1	E	103	THR	4.7
1	E	297	ASN	4.7
1	E	346	LEU	4.6
1	E	168	GLY	4.6
1	E	311	ASP	4.6
1	E	218	TYR	4.6
1	G	100	GLU	4.5
1	E	10	CYS	4.5
1	G	14	SER	4.5
1	E	293	LEU	4.5
1	G	142	LEU	4.5
1	E	170	ALA	4.4
1	E	143	TYR	4.4
2	H	89	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	90	PHE	4.4
1	E	124	PHE	4.4
2	H	22	GLU	4.4
1	E	12	ASN	4.4
2	F	105	GLY	4.4
1	G	10	CYS	4.4
1	G	163	VAL	4.4
1	E	274	ILE	4.4
1	G	96	VAL	4.4
2	F	140	PHE	4.3
1	E	105	LEU	4.3
1	G	313	MET	4.2
2	H	106	THR	4.2
1	E	169	TYR	4.2
1	E	349	LEU	4.2
1	G	12	ASN	4.2
1	E	98	PRO	4.2
1	E	294	TYR	4.2
1	E	164	PRO	4.2
1	G	303	THR	4.2
2	F	91	VAL	4.2
1	G	180	LEU	4.2
1	E	342	GLY	4.1
1	E	35	VAL	4.1
1	E	96	VAL	4.1
1	E	160	THR	4.1
1	E	261	LEU	4.1
1	E	120	THR	4.1
1	G	159	VAL	4.1
2	H	84	PRO	4.1
1	G	188	TYR	4.1
2	F	117	TYR	4.1
2	H	85	ASP	4.1
1	E	131	ALA	4.1
1	G	309	ILE	4.1
1	E	100	GLU	4.0
1	E	107	GLU	4.0
1	E	347	ALA	4.0
1	E	289	ILE	4.0
1	E	94	LEU	4.0
1	G	80	ASP	4.0
1	E	282	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	171	LEU	3.9
1	G	189	LEU	3.9
2	F	45	VAL	3.9
1	E	238	LYS	3.9
1	C	80	ASP	3.9
1	G	240	TYR	3.9
1	G	77	THR	3.9
1	G	171	LEU	3.9
1	E	272	ALA	3.9
1	G	158	GLY	3.9
1	A	65	LEU	3.8
1	C	53	TYR	3.8
2	F	110	LYS	3.8
1	E	20	GLY	3.8
1	E	273	GLY	3.8
1	E	356	TRP	3.8
1	G	219	VAL	3.8
1	E	285	CYS	3.8
1	G	149	THR	3.8
1	E	172	PRO	3.8
1	E	314	GLN	3.7
1	G	74	GLY	3.7
1	G	236	LEU	3.7
1	G	250	ILE	3.7
1	E	239	SER	3.7
2	F	120	GLY	3.7
1	E	163	VAL	3.7
1	G	262	PHE	3.7
1	E	119	MET	3.7
1	E	110	LEU	3.7
1	G	103	THR	3.7
1	C	116[A]	ARG	3.6
1	C	114	ALA	3.6
1	E	276	GLU	3.6
2	F	104	ALA	3.6
2	H	88	ALA	3.6
1	E	217	CYS	3.6
1	G	145	SER	3.6
1	G	299	MET	3.6
1	E	27	PRO	3.6
2	F	25	VAL	3.6
2	F	31	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	91	VAL	3.6
1	E	329	ILE	3.5
1	E	288	ASP	3.5
1	E	150	GLY	3.5
2	F	48	TRP	3.5
1	E	109	PRO	3.5
1	E	9	VAL	3.5
2	F	65	SER	3.5
2	F	79	HIS	3.5
1	G	311	ASP	3.5
1	G	23	GLY	3.5
1	E	338	SER	3.5
2	F	135	ARG	3.5
1	G	231	ALA	3.5
1	G	32	PRO	3.5
1	E	296	ASN	3.5
1	E	139	VAL	3.5
1	C	372	ARG	3.5
1	E	312	ARG	3.5
1	G	274	ILE	3.4
1	G	306	TYR	3.4
1	E	72	GLU	3.4
2	F	113	GLU	3.4
1	G	119	MET	3.4
1	C	115	ASN	3.4
2	F	39	ALA	3.4
1	E	67	LEU	3.4
1	E	235	SER	3.4
1	G	105	LEU	3.4
1	E	152	VAL	3.4
1	G	139	VAL	3.4
1	G	339	VAL	3.4
2	H	79	HIS	3.4
2	H	124	GLN	3.4
1	E	127	PHE	3.4
2	H	123	VAL	3.4
1	G	86	TRP	3.3
1	E	316	GLU	3.3
1	G	217	CYS	3.3
1	E	134	VAL	3.3
1	G	31	PHE	3.3
2	F	53	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	116	ASP	3.3
1	G	35	VAL	3.3
2	H	45	VAL	3.3
1	G	71	ILE	3.3
1	G	91	TYR	3.3
1	E	104	LEU	3.3
1	E	290	ARG	3.3
1	E	255	PHE	3.3
1	G	17	VAL	3.3
1	G	238	LYS	3.3
1	E	8	LEU	3.3
1	E	306	TYR	3.3
1	G	69	TYR	3.3
1	G	269	MET	3.3
1	A	270	GLU	3.3
1	C	94	LEU	3.3
1	G	107	GLU	3.3
1	E	132	MET	3.3
1	G	15	GLY	3.3
1	A	71	ILE	3.3
1	E	317	ILE	3.3
1	G	317	ILE	3.3
1	E	16	LEU	3.2
2	D	21	LEU	3.2
2	H	122	PRO	3.2
1	G	220	ALA	3.2
1	C	21	PHE	3.2
1	G	76	ILE	3.2
2	H	128	VAL	3.2
1	E	64	ILE	3.2
1	G	85	ILE	3.2
2	F	55	VAL	3.2
2	F	112	VAL	3.2
1	G	140	LEU	3.2
1	G	153	LEU	3.2
1	G	194	THR	3.2
1	G	246	GLN	3.2
1	E	114	ALA	3.2
2	F	125	TYR	3.2
2	H	78	TYR	3.2
1	E	151	ILE	3.2
2	H	55	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	221	LEU	3.2
1	G	333	PRO	3.2
1	A	64	ILE	3.2
1	G	34	ILE	3.2
1	G	345	ILE	3.2
1	E	299	MET	3.1
1	G	68	LYS	3.1
1	C	103	THR	3.1
1	E	7	ALA	3.1
1	E	295	ALA	3.1
1	G	300	SER	3.1
2	F	154	THR	3.1
1	G	146	GLY	3.1
1	E	18	LYS	3.1
2	F	92	HIS	3.1
1	C	5	THR	3.1
2	D	19	THR	3.1
1	G	20	GLY	3.1
1	G	182	GLY	3.1
1	G	308	GLY	3.1
1	G	175	ILE	3.1
1	E	253	GLU	3.1
1	E	126	THR	3.1
1	E	146	GLY	3.1
1	E	149	THR	3.1
1	G	13	GLY	3.1
2	F	26	LYS	3.1
1	E	258	PRO	3.0
1	G	70	PRO	3.0
2	F	42	GLN	3.0
2	F	47	ILE	3.0
1	G	181	ALA	3.0
2	F	109	TYR	3.0
1	C	66	THR	3.0
1	E	249	THR	3.0
2	H	150	GLY	3.0
1	G	131	ALA	3.0
1	G	79	TRP	3.0
1	E	237	GLU	3.0
1	E	53	TYR	3.0
1	G	337	TYR	3.0
2	F	72	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	148	THR	3.0
1	G	192	ILE	3.0
1	G	197	GLY	3.0
1	E	21	PHE	3.0
1	E	219	VAL	3.0
1	G	16	LEU	3.0
2	F	30	SER	3.0
1	E	260	THR	3.0
1	G	272	ALA	3.0
2	H	156	PHE	3.0
1	G	178	LEU	2.9
2	F	118	LEU	2.9
1	E	111	ASN	2.9
1	E	345	ILE	2.9
1	E	15	GLY	2.9
1	E	352	PHE	2.9
1	G	235	SER	2.9
1	G	239	SER	2.9
1	E	128	ASN	2.9
1	G	136	ILE	2.9
1	G	249	THR	2.9
1	E	129	VAL	2.9
1	G	134	VAL	2.9
2	F	66	PHE	2.9
2	H	121	LEU	2.9
1	G	99	GLU	2.9
1	G	334	GLU	2.9
1	C	78	ASN	2.9
2	F	50	ILE	2.9
1	E	23	GLY	2.9
2	H	29	ALA	2.9
1	A	61	LYS	2.9
1	E	223	PHE	2.9
1	G	9	VAL	2.9
1	G	152	VAL	2.9
2	F	156	PHE	2.9
1	G	111	ASN	2.9
1	A	76	ILE	2.9
2	F	67	TYR	2.9
1	G	26	ALA	2.9
1	G	346	LEU	2.9
2	H	107	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	161	HIS	2.9
1	E	300	SER	2.8
2	F	90	ASP	2.8
1	E	277	THR	2.8
1	G	278	THR	2.8
1	E	259	GLU	2.8
1	G	27	PRO	2.8
1	G	258	PRO	2.8
1	E	145	SER	2.8
1	G	267	ILE	2.8
1	C	169	TYR	2.8
1	E	91	TYR	2.8
2	F	21	LEU	2.8
1	C	96	VAL	2.8
1	G	209	VAL	2.8
2	H	43	VAL	2.8
1	G	123	MET	2.8
1	G	128	ASN	2.8
1	E	180	LEU	2.8
2	H	75	LEU	2.8
1	G	144	ALA	2.8
2	H	77	THR	2.8
1	C	90	PHE	2.8
1	E	337	TYR	2.8
1	C	367	PRO	2.8
2	H	76	SER	2.8
1	E	140	LEU	2.8
1	E	343	GLY	2.8
2	F	139	LEU	2.8
2	F	144	GLY	2.8
1	E	361	GLU	2.8
2	H	82	THR	2.8
2	F	136	PHE	2.8
2	F	41	LYS	2.7
1	E	71	ILE	2.7
1	E	287	ILE	2.7
2	H	87	LEU	2.7
1	E	6	THR	2.7
1	G	83	GLU	2.7
1	G	230	ALA	2.7
1	E	121	GLN	2.7
1	E	161	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	247	VAL	2.7
2	F	93	PHE	2.7
1	G	98	PRO	2.7
1	G	307	PRO	2.7
1	A	180	LEU	2.7
2	F	87	LEU	2.7
1	A	54	VAL	2.7
1	E	112	PRO	2.7
1	E	130	PRO	2.7
2	H	141	PRO	2.7
1	E	327	ILE	2.7
1	A	63	GLY	2.7
1	G	120	THR	2.7
1	E	11	ASP	2.7
1	E	70	PRO	2.7
1	G	332	PRO	2.7
1	G	133	TYR	2.6
1	G	169	TYR	2.6
2	F	89	TYR	2.6
2	H	109	TYR	2.6
1	E	350	SER	2.6
1	G	21	PHE	2.6
1	G	347	ALA	2.6
1	G	106	THR	2.6
1	G	127	PHE	2.6
1	G	218	TYR	2.6
1	G	185	LEU	2.6
1	G	234	SER	2.6
1	G	298	VAL	2.6
1	G	338	SER	2.6
2	F	152	VAL	2.6
1	E	32	PRO	2.6
1	G	126	THR	2.6
1	E	123	MET	2.6
1	E	133	TYR	2.6
1	E	147	ARG	2.6
1	E	117	GLU	2.6
1	E	26	ALA	2.6
1	G	130	PRO	2.6
1	E	86	TRP	2.6
1	E	106	THR	2.6
1	G	147	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	308	GLY	2.6
1	C	35	VAL	2.6
1	G	112	PRO	2.6
2	F	123	VAL	2.6
1	A	369	ILE	2.5
2	F	27	LEU	2.5
1	E	256	ARG	2.5
1	A	74	GLY	2.5
1	A	58	ALA	2.5
1	G	266	PHE	2.5
2	F	111	THR	2.5
1	G	132	MET	2.5
1	G	340	TRP	2.5
1	E	328	LYS	2.5
1	G	104	LEU	2.5
1	G	113	LYS	2.5
1	G	216	LEU	2.5
1	A	169	TYR	2.5
1	E	264	PRO	2.5
2	F	57	PRO	2.5
1	E	97	ALA	2.5
1	G	108	ALA	2.5
2	F	51	GLN	2.5
1	E	122	ILE	2.5
2	H	26	LYS	2.5
1	G	28	ARG	2.5
1	G	210	ARG	2.5
1	G	242	LEU	2.5
2	F	20	GLU	2.5
1	C	91	TYR	2.5
1	G	251	GLY	2.5
1	C	98	PRO	2.5
1	E	66	THR	2.5
1	G	162	ASN	2.5
1	C	173	HIS	2.5
1	E	167	GLU	2.5
1	G	143	TYR	2.5
1	G	273	GLY	2.5
1	E	227	MET	2.5
1	G	30	VAL	2.5
2	B	19	THR	2.4
1	E	142	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	309	ILE	2.4
1	G	8	LEU	2.4
1	G	211	ASP	2.4
1	E	332	PRO	2.4
2	F	56	VAL	2.4
1	E	278	THR	2.4
1	G	203	THR	2.4
1	G	75	ILE	2.4
2	F	115	ASP	2.4
2	H	80	PRO	2.4
1	E	326	LYS	2.4
1	E	17	VAL	2.4
1	C	95	ARG	2.4
1	C	365	ALA	2.4
1	E	108	ALA	2.4
2	H	93	PHE	2.4
1	E	175	ILE	2.4
1	E	162	ASN	2.4
1	G	176	MET	2.4
1	E	307	PRO	2.4
2	B	141	PRO	2.4
1	C	54	VAL	2.4
1	E	279	TYR	2.4
1	G	114	ALA	2.4
1	G	330	ILE	2.4
1	E	286	ASP	2.4
1	E	118	LYS	2.4
1	G	168	GLY	2.4
1	E	254	ARG	2.4
1	G	183	ARG	2.4
2	F	43	VAL	2.4
1	G	310	ALA	2.4
1	G	193	LEU	2.3
1	C	357	ILE	2.3
1	E	76	ILE	2.3
1	G	208	ILE	2.3
1	A	203	THR	2.3
1	A	371	HIS	2.3
1	E	225	ASN	2.3
1	E	281	SER	2.3
1	E	291	LYS	2.3
1	G	292	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	101	GLN	2.3
2	H	105	GLY	2.3
1	G	349	LEU	2.3
2	F	108	ALA	2.3
1	E	136	ILE	2.3
1	G	270	GLU	2.3
2	D	20	GLU	2.3
1	G	11	ASP	2.3
1	G	25	ASP	2.3
1	E	69	TYR	2.3
1	G	186	THR	2.3
2	F	19	THR	2.3
1	C	118	LYS	2.3
1	E	284	LYS	2.3
1	E	24	ASP	2.3
1	E	292	ASP	2.3
1	A	372	ARG	2.3
1	G	116	ARG	2.3
2	F	119	GLY	2.3
1	E	209	VAL	2.3
1	C	58	ALA	2.3
1	E	310	ALA	2.3
1	G	18	LYS	2.3
2	F	22	GLU	2.3
1	E	280	ASN	2.3
1	E	62	ARG	2.3
2	F	34	ASP	2.3
1	E	182	GLY	2.3
1	G	321	ALA	2.2
1	E	148	THR	2.2
1	E	229	THR	2.2
1	A	115	ASN	2.2
2	H	30	SER	2.2
1	C	268	GLY	2.2
2	F	40	GLY	2.2
1	E	79	TRP	2.2
1	E	216	LEU	2.2
1	G	29	ALA	2.2
1	G	165	ILE	2.2
2	H	23	LYS	2.2
1	E	252	ASN	2.2
1	E	59	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	24	ASP	2.2
2	F	121	LEU	2.2
2	H	145	LEU	2.2
1	E	359	LYS	2.2
2	H	86	LYS	2.2
2	D	53	PHE	2.2
2	H	98	PHE	2.2
1	G	5	THR	2.2
1	G	253	GLU	2.2
2	F	122	PRO	2.2
1	E	141	SER	2.2
1	C	370	VAL	2.2
1	E	340	TRP	2.2
1	G	170	ALA	2.2
2	F	35	ALA	2.2
1	G	226	GLU	2.2
1	E	115	ASN	2.2
1	A	368	SER	2.2
1	E	101	HIS	2.2
2	H	158	HIS	2.2
1	G	255	PHE	2.2
1	E	22	ALA	2.1
1	E	135	ALA	2.1
1	E	321	ALA	2.1
1	G	135	ALA	2.1
2	F	94	TRP	2.1
2	H	94	TRP	2.1
1	E	125	GLU	2.1
1	G	224	GLU	2.1
1	G	237	GLU	2.1
2	H	100	THR	2.1
2	H	42	GLN	2.1
1	E	320	LEU	2.1
2	H	118	LEU	2.1
1	E	268	GLY	2.1
1	E	99	GLU	2.1
1	A	120	THR	2.1
1	E	351	THR	2.1
1	G	160	THR	2.1
1	G	277	THR	2.1
1	C	10	CYS	2.1
1	G	257	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	166	TYR	2.1
2	F	155	GLY	2.1
1	A	81	ASP	2.1
1	E	248	ILE	2.1
1	G	368	SER	2.1
2	F	33	GLU	2.1
2	H	110	LYS	2.1
1	A	112	PRO	2.1
1	G	109	PRO	2.1
2	D	141	PRO	2.1
1	G	82	MET	2.1
1	A	53	TYR	2.1
1	G	101	HIS	2.1
2	H	131	TYR	2.1
1	A	357	ILE	2.1
1	G	179	ASP	2.1
2	H	149	ASP	2.1
1	E	155	SER	2.1
2	F	24	LYS	2.1
2	F	124	GLN	2.1
1	E	88	HIS	2.1
1	G	150	GLY	2.1
1	E	75	ILE	2.1
1	G	19	ALA	2.0
1	G	276	GLU	2.0
2	H	28	GLU	2.0
2	H	36	TRP	2.0
1	C	77	THR	2.0
1	G	304	THR	2.0
2	H	111	THR	2.0
1	C	82	MET	2.0
1	G	87	HIS	2.0
1	G	92	ASN	2.0
2	H	38	GLY	2.0
1	E	57	GLU	2.0
1	G	117	GLU	2.0
1	G	233	SER	2.0
2	F	71	SER	2.0
1	E	283	MET	2.0
2	F	106	THR	2.0
1	G	354	GLN	2.0
1	A	34	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	15	GLY	2.0
1	G	254	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HIC	G	73	11/12	0.49	0.24	161,168,176,176	0
1	HIC	E	73	11/12	0.66	0.17	105,109,117,119	0
1	HIC	C	73	11/12	0.84	0.21	80,90,101,104	0
1	HIC	A	73	11/12	0.86	0.14	68,71,92,112	0

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.

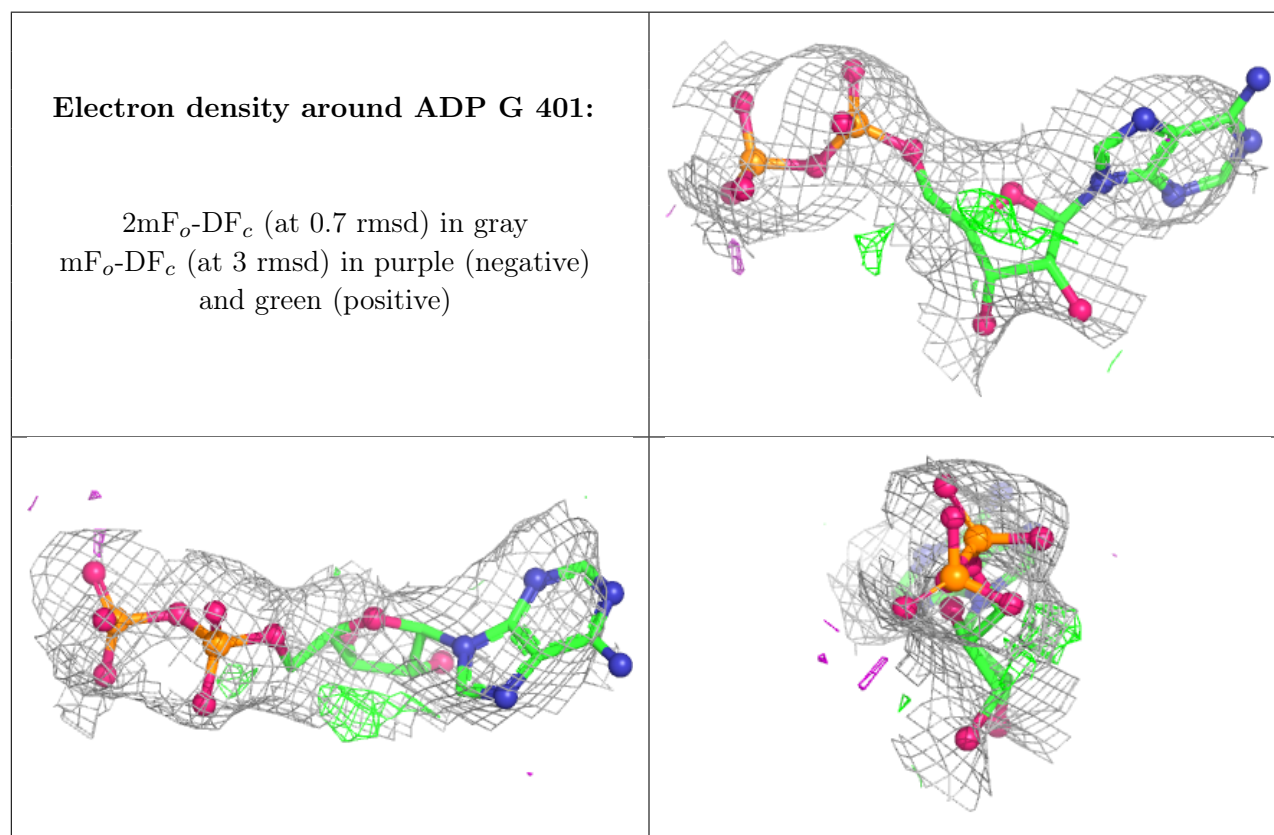
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	403	4/4	0.59	0.20	54,70,74,77	0
6	NA	C	403	1/1	0.70	0.15	79,79,79,79	0
6	NA	A	404	1/1	0.73	0.12	51,51,51,51	0
3	ADP	G	401	27/27	0.77	0.16	92,102,124,137	0
4	CA	F	400	1/1	0.83	0.08	121,121,121,121	0
4	CA	G	402	1/1	0.84	0.14	119,119,119,119	0
8	PO4	D	204	5/5	0.84	0.19	89,92,111,119	0
4	CA	H	400	1/1	0.86	0.14	137,137,137,137	0
7	EDO	A	405	4/4	0.87	0.14	34,51,52,53	0
3	ADP	E	401	27/27	0.89	0.12	62,74,84,95	0
5	ACT	D	203	4/4	0.91	0.14	45,47,48,60	0
4	CA	E	402	1/1	0.92	0.10	81,81,81,81	0

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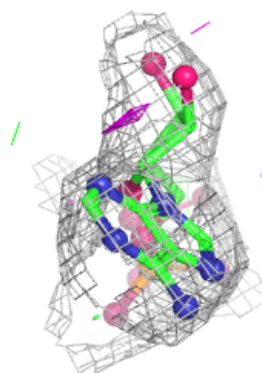
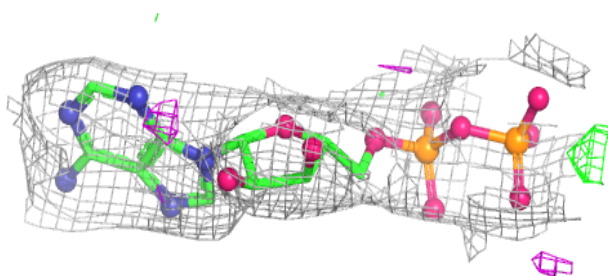
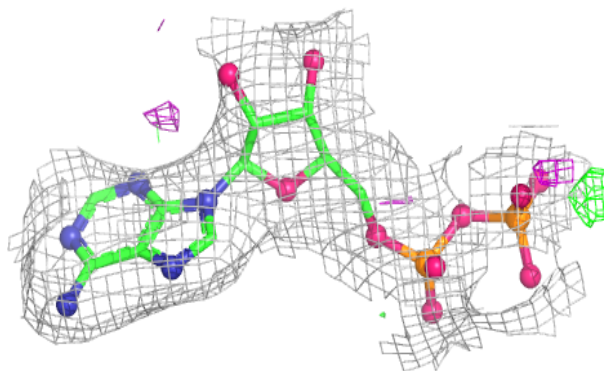
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	A	402	1/1	0.92	0.10	59,59,59,59	0
5	ACT	B	204	4/4	0.94	0.12	29,39,40,41	0
4	CA	C	402	1/1	0.94	0.07	58,58,58,58	0
4	CA	F	401	1/1	0.95	0.06	101,101,101,101	0
3	ADP	A	401	27/27	0.95	0.08	32,41,47,52	0
4	CA	H	401	1/1	0.96	0.13	95,95,95,95	0
3	ADP	C	401	27/27	0.96	0.06	29,36,45,53	0
4	CA	B	201	1/1	0.97	0.09	48,48,48,48	0
5	ACT	B	203	4/4	0.97	0.05	23,32,33,38	0
4	CA	B	202	1/1	0.99	0.04	32,32,32,32	0
4	CA	D	202	1/1	0.99	0.02	49,49,49,49	0
4	CA	D	201	1/1	1.00	0.01	44,44,44,44	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.

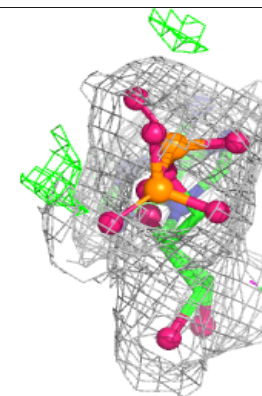
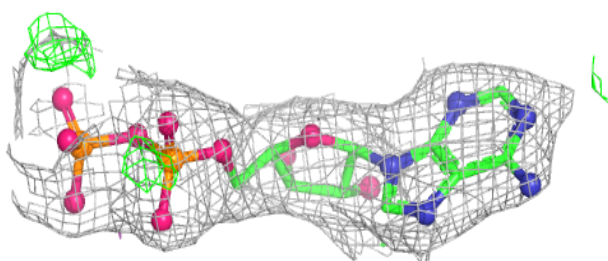
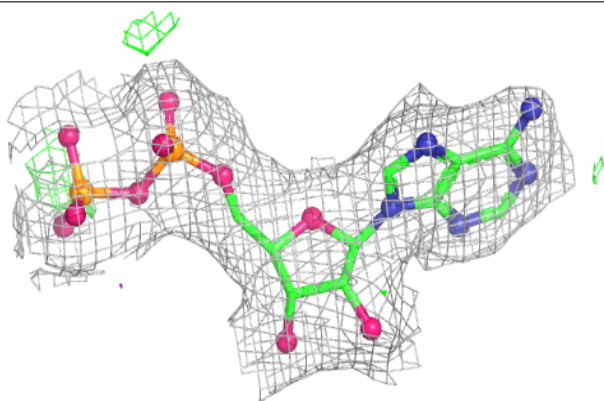


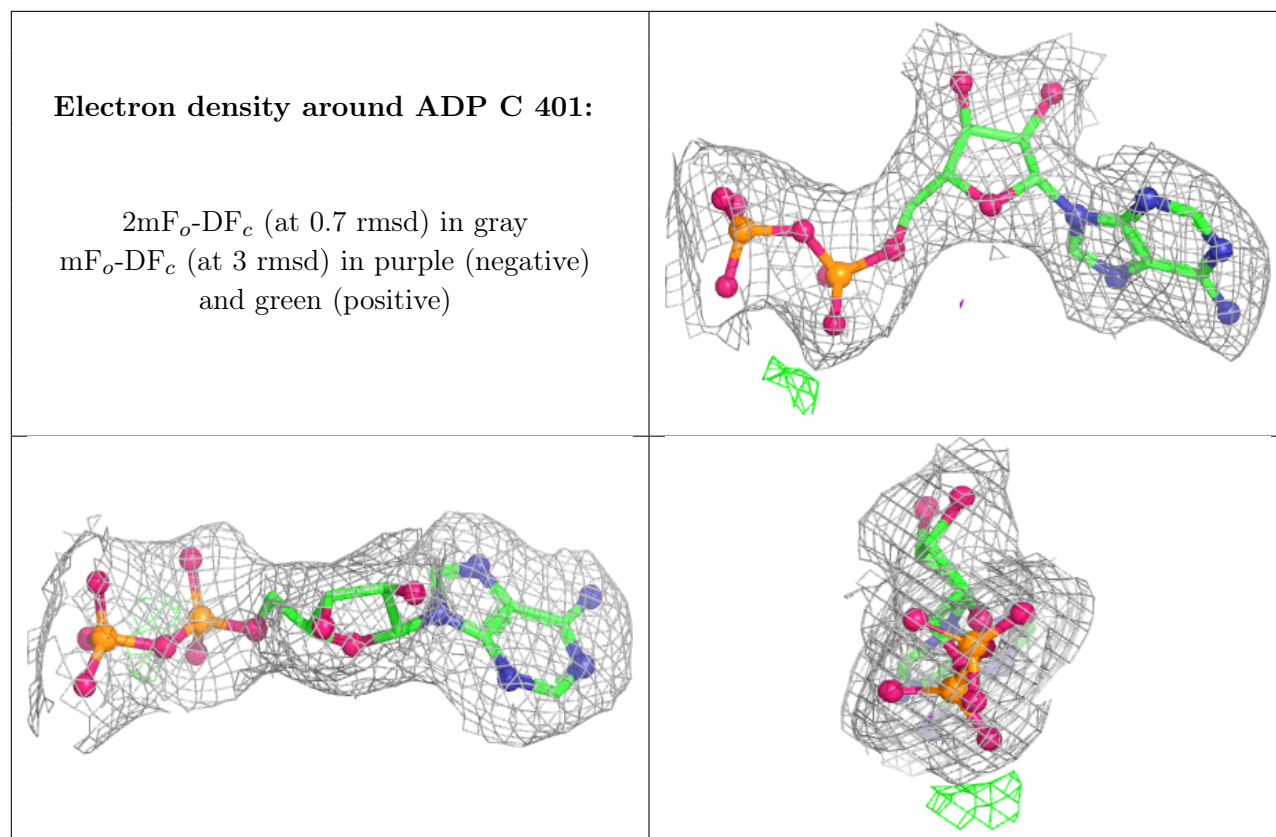
Electron density around ADP E 401:

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

**Electron density around ADP A 401:**

$2mF_o - DF_c$ (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.