



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:29 AM UTC

PDB ID : 4U0Z / pdb_00004u0z
Title : Eukaryotic Fic Domain containing protein with bound APCPP
Authors : Cole, A.R.; Bunney, T.D.; Katan, M.
Deposited on : 2014-07-14
Resolution : 2.95 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

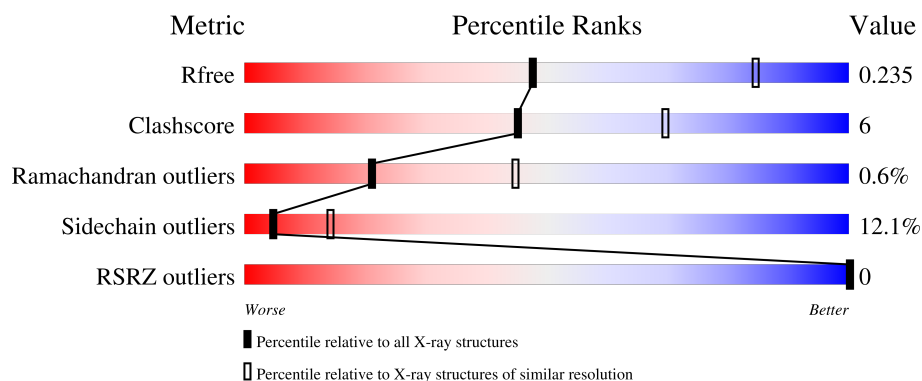
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

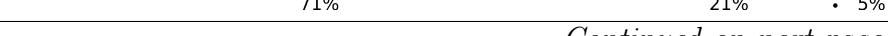
The reported resolution of this entry is 2.95 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	344	
1	B	344	
1	C	344	
1	D	344	
1	E	344	

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Mol	Chain	Length	Quality of chain
1	F	344	 72%19% • 6%
1	G	344	 72%20% • 6%
1	H	344	 69%21% • 8%

2 Entry composition

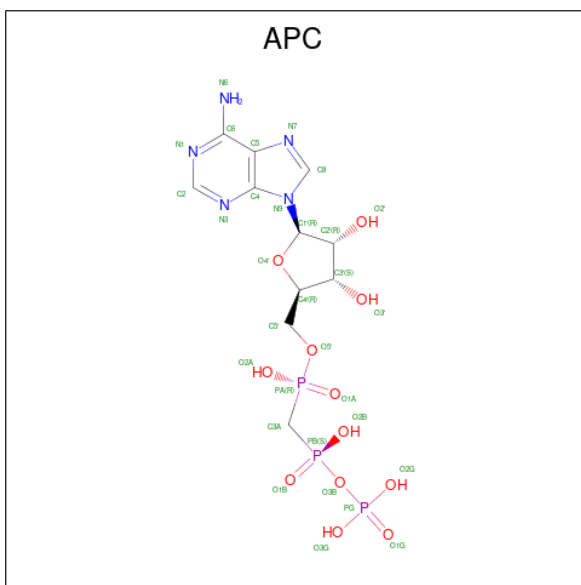
There are 4 unique types of molecules in this entry. The entry contains 21328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosine monophosphate-protein transferase FICD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2541	1622	438	472	9			
1	B	326	Total	C	N	O	S	0	0	0
			2528	1617	432	469	10			
1	C	329	Total	C	N	O	S	0	0	0
			2581	1649	444	476	12			
1	D	325	Total	C	N	O	S	0	0	0
			2528	1616	436	466	10			
1	E	327	Total	C	N	O	S	0	0	0
			2568	1640	441	476	11			
1	F	322	Total	C	N	O	S	0	0	0
			2502	1601	428	461	12			
1	G	322	Total	C	N	O	S	0	0	0
			2509	1607	428	462	12			
1	H	318	Total	C	N	O	S	0	0	0
			2499	1599	429	460	11			

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	B	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	C	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	D	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	E	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	F	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	G	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	H	1	Total 31	C 11	N 5	O 12	P 3	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

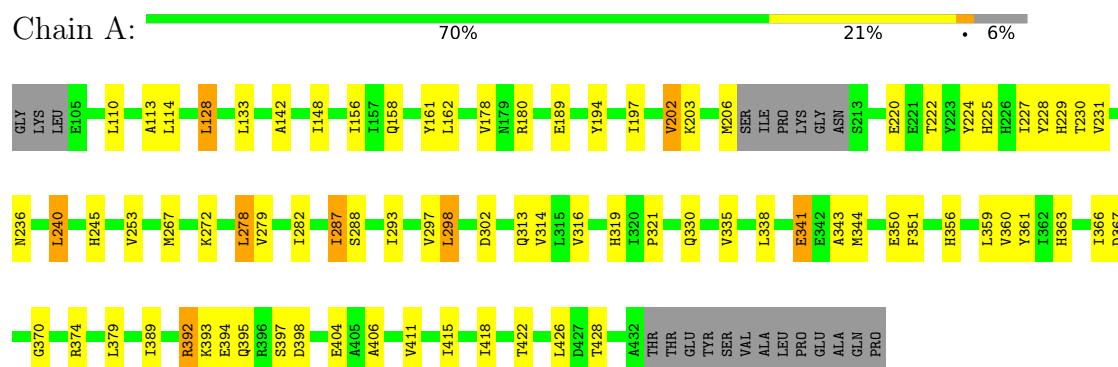
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total 96	O 96	0	0
4	B	101	Total 101	O 101	0	0
4	C	114	Total 114	O 114	0	0
4	D	86	Total 86	O 86	0	0
4	E	96	Total 96	O 96	0	0
4	F	96	Total 96	O 96	0	0
4	G	128	Total 128	O 128	0	0
4	H	99	Total 99	O 99	0	0

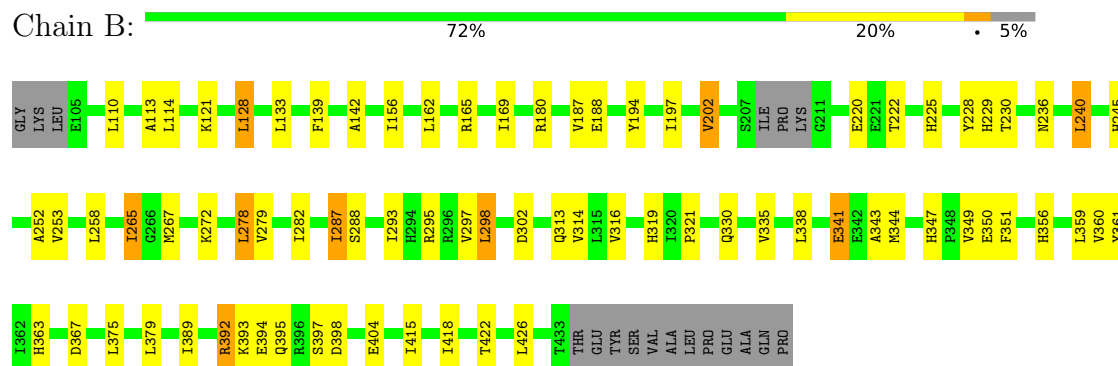
3 Residue-property plots

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

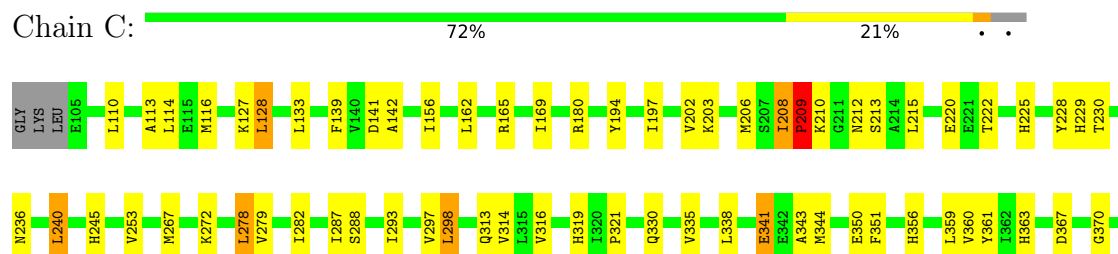
• Molecule 1: Adenosine monophosphate-protein transferase FICD



• Molecule 1: Adenosine monophosphate-protein transferase FICD



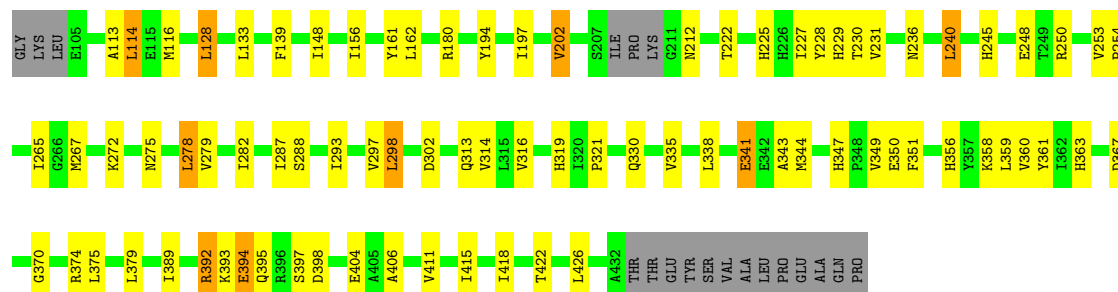
• Molecule 1: Adenosine monophosphate-protein transferase FICD





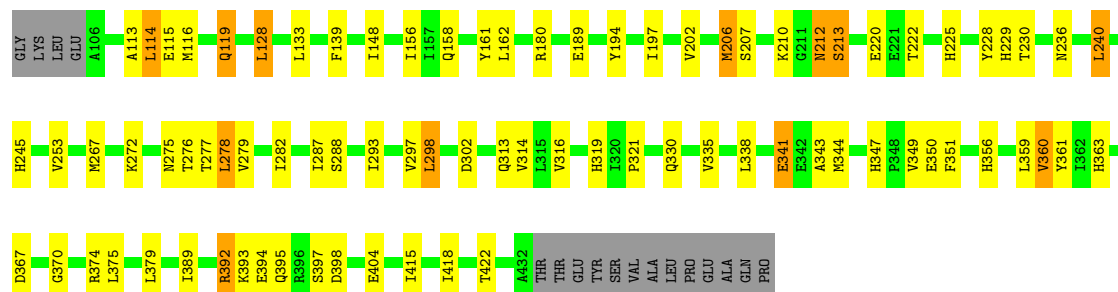
- Molecule 1: Adenosine monophosphate-protein transferase FICD

Chain D: 71% 21% 6%



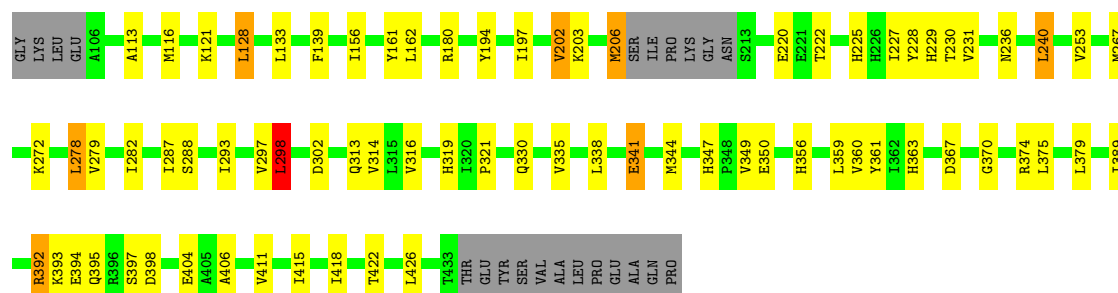
- Molecule 1: Adenosine monophosphate-protein transferase FICD

Chain E: 71% 21% 5%



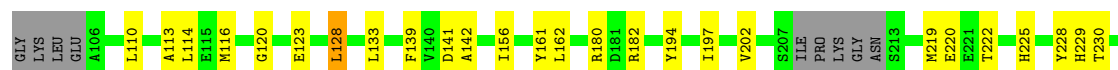
- Molecule 1: Adenosine monophosphate-protein transferase FICD

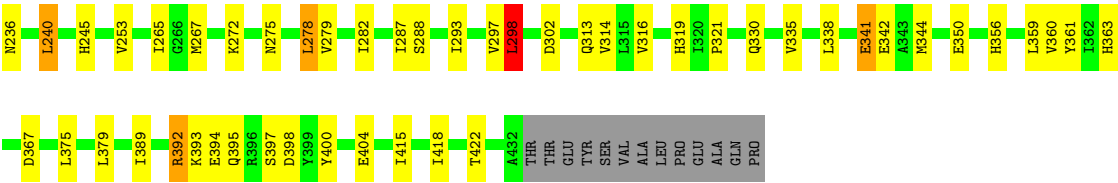
Chain F: 72% 19% 6%



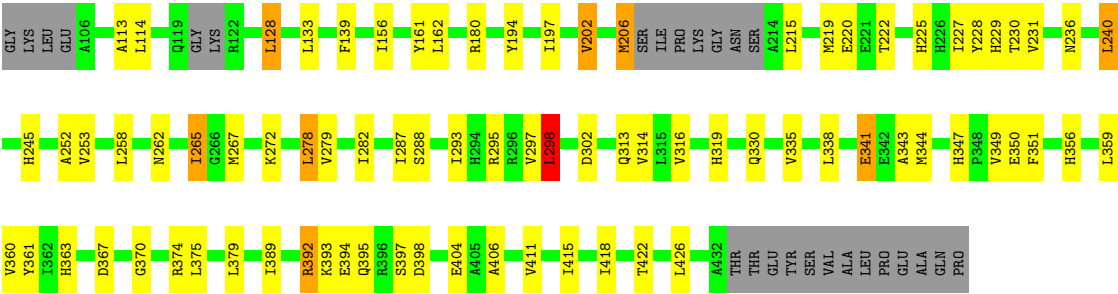
- Molecule 1: Adenosine monophosphate-protein transferase FICD

Chain G: 72% 20% 6%





• Molecule 1: Adenosine monophosphate-protein transferase FICD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.10Å 83.75Å 130.02Å 89.92° 89.57° 89.43°	Depositor
Resolution (Å)	43.34 – 2.95 43.34 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.0 (43.34-2.95) 94.9 (43.34-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.206 , 0.251 0.209 , 0.235	Depositor DCC
R_{free} test set	3307 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.417 for h,-k,-l 0.387 for -h,k,-l 0.387 for -h,-k,l	Xtriage
F_o , F_c correlation	0.96	EDS
Total number of atoms	21328	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5002e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.92	0/2596	1.50	12/3529 (0.3%)
1	B	0.87	0/2583	1.50	10/3514 (0.3%)
1	C	0.94	0/2638	1.53	12/3584 (0.3%)
1	D	0.88	0/2583	1.50	13/3512 (0.4%)
1	E	0.95	0/2625	1.51	15/3568 (0.4%)
1	F	0.88	0/2557	1.51	10/3477 (0.3%)
1	G	0.95	0/2564	1.51	15/3487 (0.4%)
1	H	0.88	0/2553	1.49	14/3468 (0.4%)
All	All	0.91	0/20699	1.51	101/28139 (0.4%)

There are no bond length outliers.

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	PRO	CA-C-N	8.07	136.95	121.54
1	C	209	PRO	C-N-CA	8.07	136.95	121.54
1	E	278	LEU	N-CA-C	7.78	120.89	111.40
1	H	278	LEU	N-CA-C	7.66	120.75	111.40
1	D	278	LEU	N-CA-C	7.66	120.74	111.40
1	A	278	LEU	N-CA-C	7.61	121.05	111.24
1	F	278	LEU	N-CA-C	7.60	120.67	111.40
1	B	278	LEU	N-CA-C	7.56	120.63	111.40
1	C	278	LEU	N-CA-C	7.56	120.62	111.40
1	G	278	LEU	N-CA-C	7.09	120.38	111.24
1	G	392	ARG	CA-C-N	6.46	129.26	120.54
1	G	392	ARG	C-N-CA	6.46	129.26	120.54
1	H	392	ARG	CA-C-N	6.36	129.13	120.54
1	H	392	ARG	C-N-CA	6.36	129.13	120.54
1	F	392	ARG	CA-C-N	6.22	128.93	120.54
1	F	392	ARG	C-N-CA	6.22	128.93	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	392	ARG	CA-C-N	6.12	128.76	120.38
1	E	392	ARG	C-N-CA	6.12	128.76	120.38
1	B	392	ARG	CA-C-N	6.06	128.72	120.54
1	B	392	ARG	C-N-CA	6.06	128.72	120.54
1	D	392	ARG	CA-C-N	5.92	128.53	120.54
1	D	392	ARG	C-N-CA	5.92	128.53	120.54
1	A	392	ARG	CA-C-N	5.86	128.45	120.54
1	A	392	ARG	C-N-CA	5.86	128.45	120.54
1	A	398	ASP	CA-C-N	5.83	128.09	120.28
1	A	398	ASP	C-N-CA	5.83	128.09	120.28
1	C	392	ARG	CA-C-N	5.82	128.40	120.54
1	C	392	ARG	C-N-CA	5.82	128.40	120.54
1	C	398	ASP	CA-C-N	5.82	128.08	120.28
1	C	398	ASP	C-N-CA	5.82	128.08	120.28
1	A	245	HIS	CA-C-N	5.66	127.90	120.60
1	A	245	HIS	C-N-CA	5.66	127.90	120.60
1	D	398	ASP	CA-C-N	5.64	127.83	120.28
1	D	398	ASP	C-N-CA	5.64	127.83	120.28
1	F	398	ASP	CA-C-N	5.62	127.82	120.28
1	F	398	ASP	C-N-CA	5.62	127.82	120.28
1	E	245	HIS	CA-C-N	5.54	127.75	120.60
1	E	245	HIS	C-N-CA	5.54	127.75	120.60
1	H	298	LEU	CA-C-N	5.50	126.08	119.98
1	H	298	LEU	C-N-CA	5.50	126.08	119.98
1	H	398	ASP	CA-C-N	5.48	127.62	120.28
1	H	398	ASP	C-N-CA	5.48	127.62	120.28
1	A	161	TYR	CA-C-N	5.46	127.54	120.44
1	A	161	TYR	C-N-CA	5.46	127.54	120.44
1	C	139	PHE	CA-CB-CG	5.46	119.26	113.80
1	G	298	LEU	CA-C-N	5.46	126.04	119.98
1	G	298	LEU	C-N-CA	5.46	126.04	119.98
1	B	398	ASP	CA-C-N	5.43	127.55	120.28
1	B	398	ASP	C-N-CA	5.43	127.55	120.28
1	E	115	GLU	CB-CG-CD	5.42	121.82	112.60
1	D	139	PHE	CA-CB-CG	5.41	119.21	113.80
1	E	189	GLU	CB-CG-CD	5.41	121.79	112.60
1	E	161	TYR	CA-C-N	5.40	127.46	120.44
1	E	161	TYR	C-N-CA	5.40	127.46	120.44
1	A	189	GLU	CB-CG-CD	5.39	121.76	112.60
1	G	275	ASN	N-CA-C	5.38	117.90	111.71
1	H	245	HIS	CA-C-N	5.37	127.53	120.60
1	H	245	HIS	C-N-CA	5.37	127.53	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	HIS	CA-C-N	5.35	127.50	120.60
1	D	245	HIS	C-N-CA	5.35	127.50	120.60
1	G	139	PHE	CA-CB-CG	5.35	119.15	113.80
1	E	398	ASP	CA-C-N	5.31	127.39	120.28
1	E	398	ASP	C-N-CA	5.31	127.39	120.28
1	H	161	TYR	CA-C-N	5.28	127.30	120.44
1	H	161	TYR	C-N-CA	5.28	127.30	120.44
1	G	161	TYR	CA-C-N	5.27	127.29	120.44
1	G	161	TYR	C-N-CA	5.27	127.29	120.44
1	E	139	PHE	CA-CB-CG	5.26	119.06	113.80
1	G	398	ASP	CA-C-N	5.26	127.32	120.28
1	G	398	ASP	C-N-CA	5.26	127.32	120.28
1	C	245	HIS	CA-C-N	5.24	127.36	120.60
1	C	245	HIS	C-N-CA	5.24	127.36	120.60
1	B	139	PHE	CA-CB-CG	5.22	119.02	113.80
1	B	245	HIS	CA-C-N	5.18	127.29	120.60
1	B	245	HIS	C-N-CA	5.18	127.29	120.60
1	G	245	HIS	CA-C-N	5.16	127.26	120.60
1	G	245	HIS	C-N-CA	5.16	127.26	120.60
1	H	139	PHE	CA-CB-CG	5.14	118.94	113.80
1	F	139	PHE	CA-CB-CG	5.12	118.92	113.80
1	D	161	TYR	CA-C-N	5.11	127.09	120.44
1	D	161	TYR	C-N-CA	5.11	127.09	120.44
1	E	275	ASN	N-CA-C	5.11	117.59	111.71
1	A	224	TYR	CA-C-N	5.10	127.06	120.44
1	A	224	TYR	C-N-CA	5.10	127.06	120.44
1	G	265	ILE	CA-C-N	5.09	125.59	119.94
1	G	265	ILE	C-N-CA	5.09	125.59	119.94
1	F	161	TYR	CA-C-N	5.09	127.06	120.44
1	F	161	TYR	C-N-CA	5.09	127.06	120.44
1	H	265	ILE	CA-C-N	5.06	125.55	119.94
1	H	265	ILE	C-N-CA	5.06	125.55	119.94
1	F	298	LEU	CA-C-N	5.05	125.59	119.98
1	F	298	LEU	C-N-CA	5.05	125.59	119.98
1	E	277	THR	CA-C-N	5.04	129.13	120.71
1	E	277	THR	C-N-CA	5.04	129.13	120.71
1	D	275	ASN	N-CA-C	5.04	117.51	111.71
1	D	265	ILE	CA-C-N	5.02	125.52	119.94
1	D	265	ILE	C-N-CA	5.02	125.52	119.94
1	B	265	ILE	CA-C-N	5.00	125.49	119.94
1	B	265	ILE	C-N-CA	5.00	125.49	119.94
1	C	298	LEU	CA-C-N	5.00	125.63	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	LEU	C-N-CA	5.00	125.63	120.03

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	2541	0	2457	30	0
1	B	2528	0	2412	31	0
1	C	2581	0	2503	31	0
1	D	2528	0	2419	37	0
1	E	2568	0	2476	30	0
1	F	2502	0	2383	26	0
1	G	2509	0	2407	29	0
1	H	2499	0	2403	32	0
2	A	31	0	14	0	0
2	B	31	0	14	0	0
2	C	31	0	14	0	0
2	D	31	0	14	0	0
2	E	31	0	14	1	0
2	F	31	0	14	0	0
2	G	31	0	14	1	0
2	H	31	0	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	96	0	0	6	0
4	B	101	0	0	3	0
4	C	114	0	0	3	0
4	D	86	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	96	0	0	3	0
4	F	96	0	0	0	0
4	G	128	0	0	3	0
4	H	99	0	0	1	0
All	All	21328	0	19572	237	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 6.

All (237) 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:C:209:PRO:HG3	1:C:212:ASN:HB2	1.53	0.90
1:G:141:ASP:HA	4:G:643:HOH:O	1.79	0.81
1:B:258:LEU:HD13	1:H:265:ILE:HD11	1.63	0.78
1:H:206:MET:SD	1:H:206:MET:C	2.75	0.70
1:E:158:GLN:HG3	4:E:626:HOH:O	1.91	0.70
1:G:342:GLU:OE2	4:G:661:HOH:O	2.13	0.67
1:B:265:ILE:HD11	1:H:258:LEU:HD13	1.77	0.66
1:D:148:ILE:HD11	4:D:683:HOH:O	1.95	0.66
1:C:141:ASP:HA	4:C:631:HOH:O	1.96	0.65
1:D:230:THR:HG21	1:D:267:MET:HE2	1.81	0.63
1:B:287:ILE:HG22	4:B:646:HOH:O	2.00	0.62
1:D:392:ARG:HH22	1:G:123:GLU:H	1.47	0.61
1:G:350:GLU:HG3	1:G:415:ILE:HD13	1.81	0.61
1:C:401:HIS:HD2	4:C:651:HOH:O	1.83	0.61
1:C:208:ILE:CB	1:C:209:PRO:HD3	2.31	0.61
1:D:248:GLU:HG3	4:D:614:HOH:O	2.00	0.61
1:D:114:LEU:HD11	4:D:683:HOH:O	2.01	0.60
1:E:148:ILE:HD11	4:E:627:HOH:O	2.01	0.60
1:D:392:ARG:HH22	1:G:123:GLU:N	1.99	0.60
1:B:230:THR:HG21	1:B:267:MET:HE2	1.84	0.59
1:C:350:GLU:HG3	1:C:415:ILE:HD13	1.83	0.59
1:F:206:MET:SD	1:F:206:MET:C	2.85	0.59
1:A:158:GLN:HG3	4:A:621:HOH:O	2.02	0.59
1:A:230:THR:HG21	1:A:267:MET:HE2	1.85	0.58
1:G:230:THR:HG21	1:G:267:MET:HE2	1.85	0.58
1:E:230:THR:HG21	1:E:267:MET:HE2	1.85	0.58
1:H:230:THR:HG21	1:H:267:MET:HE2	1.84	0.58
1:A:287:ILE:HG22	4:A:650:HOH:O	2.04	0.57
1:A:350:GLU:HG3	1:A:415:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:THR:HG21	1:F:267:MET:HE2	1.87	0.57
1:C:209:PRO:CG	1:C:212:ASN:HB2	2.31	0.56
1:F:350:GLU:HG3	1:F:415:ILE:HD13	1.87	0.56
1:C:230:THR:HG21	1:C:267:MET:HE2	1.87	0.56
1:E:350:GLU:HG3	1:E:415:ILE:HD13	1.87	0.56
1:F:203:LYS:O	1:F:206:MET:SD	2.63	0.56
1:A:229:HIS:CD2	1:A:393:LYS:H	2.24	0.56
1:B:350:GLU:HG3	1:B:415:ILE:HD13	1.86	0.56
1:C:229:HIS:CD2	1:C:393:LYS:H	2.24	0.56
1:C:229:HIS:HD2	1:C:393:LYS:H	1.53	0.55
1:A:229:HIS:HD2	1:A:393:LYS:H	1.53	0.55
1:B:188:GLU:HG3	4:B:667:HOH:O	2.07	0.55
1:B:229:HIS:HD2	1:B:393:LYS:H	1.54	0.55
1:D:229:HIS:CD2	1:D:393:LYS:H	2.25	0.55
1:D:254:PRO:HD2	4:D:650:HOH:O	2.07	0.55
1:B:229:HIS:CD2	1:B:393:LYS:H	2.25	0.54
1:G:229:HIS:HD2	1:G:393:LYS:H	1.55	0.54
1:F:229:HIS:HD2	1:F:393:LYS:H	1.56	0.54
1:F:418:ILE:O	1:F:422:THR:HG23	2.07	0.54
1:E:418:ILE:O	1:E:422:THR:HG23	2.08	0.54
1:H:222:THR:HA	1:H:225:HIS:HB3	1.90	0.54
1:H:350:GLU:HG3	1:H:415:ILE:HD13	1.89	0.54
1:A:222:THR:HA	1:A:225:HIS:HB3	1.90	0.54
1:D:222:THR:HA	1:D:225:HIS:HB3	1.90	0.53
1:D:350:GLU:HG3	1:D:415:ILE:HD13	1.89	0.53
1:E:222:THR:HA	1:E:225:HIS:HB3	1.91	0.53
1:F:222:THR:HA	1:F:225:HIS:HB3	1.91	0.53
1:G:229:HIS:CD2	1:G:393:LYS:H	2.26	0.53
1:D:418:ILE:O	1:D:422:THR:HG23	2.08	0.53
1:B:222:THR:HA	1:B:225:HIS:HB3	1.91	0.53
1:D:229:HIS:HD2	1:D:393:LYS:H	1.55	0.53
1:C:222:THR:HA	1:C:225:HIS:HB3	1.90	0.53
1:H:229:HIS:HD2	1:H:393:LYS:H	1.57	0.53
1:G:222:THR:HA	1:G:225:HIS:HB3	1.91	0.52
1:C:418:ILE:O	1:C:422:THR:HG23	2.09	0.52
1:H:418:ILE:O	1:H:422:THR:HG23	2.09	0.52
1:D:394:GLU:HG2	1:G:120:GLY:HA2	1.91	0.52
1:F:229:HIS:CD2	1:F:393:LYS:H	2.27	0.52
1:G:267:MET:HE1	1:G:375:LEU:HD21	1.91	0.52
1:H:229:HIS:CD2	1:H:393:LYS:H	2.27	0.52
1:G:418:ILE:O	1:G:422:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:ALA:HB2	1:G:128:LEU:HB3	1.92	0.52
1:G:319:HIS:HE1	1:G:361:TYR:O	1.94	0.51
1:D:358:LYS:NZ	4:D:622:HOH:O	2.44	0.51
1:B:418:ILE:O	1:B:422:THR:HG23	2.11	0.51
1:E:113:ALA:HB2	1:E:128:LEU:HB3	1.93	0.51
1:C:113:ALA:HB2	1:C:128:LEU:HB3	1.92	0.51
1:C:209:PRO:HG3	1:C:212:ASN:CB	2.34	0.50
1:H:113:ALA:HB2	1:H:128:LEU:HB3	1.94	0.50
1:E:335:VAL:HA	1:E:338:LEU:HD12	1.93	0.50
1:E:229:HIS:CD2	1:E:393:LYS:H	2.28	0.50
1:G:293:ILE:O	1:G:297:VAL:HG23	2.12	0.50
1:E:319:HIS:HE1	1:E:361:TYR:O	1.95	0.50
1:D:113:ALA:HB2	1:D:128:LEU:HB3	1.93	0.50
1:F:113:ALA:HB2	1:F:128:LEU:HB3	1.94	0.49
1:E:229:HIS:HD2	1:E:393:LYS:H	1.61	0.49
1:F:392:ARG:HB2	1:F:395:GLN:HG3	1.95	0.49
1:E:392:ARG:HB2	1:E:395:GLN:HG3	1.95	0.49
1:A:206:MET:C	4:A:680:HOH:O	2.55	0.49
1:B:293:ILE:O	1:B:297:VAL:HG23	2.13	0.49
1:E:228:TYR:HB2	1:E:240:LEU:HD23	1.95	0.49
1:H:335:VAL:HA	1:H:338:LEU:HD12	1.95	0.49
1:A:113:ALA:HB2	1:A:128:LEU:HB3	1.93	0.49
1:F:335:VAL:HA	1:F:338:LEU:HD12	1.95	0.49
1:G:313:GLN:HE21	1:G:314:VAL:H	1.60	0.49
1:G:392:ARG:HB2	1:G:395:GLN:HG3	1.95	0.49
1:B:113:ALA:HB2	1:B:128:LEU:HB3	1.94	0.48
1:A:335:VAL:HA	1:A:338:LEU:HD12	1.95	0.48
1:E:114:LEU:HD11	4:E:627:HOH:O	2.13	0.48
1:D:319:HIS:HE1	1:D:361:TYR:O	1.96	0.48
1:F:313:GLN:HE21	1:F:314:VAL:H	1.62	0.48
1:F:293:ILE:O	1:F:297:VAL:HG23	2.14	0.48
1:C:392:ARG:HB2	1:C:395:GLN:HG3	1.94	0.48
1:B:392:ARG:HB2	1:B:395:GLN:HG3	1.95	0.47
1:G:335:VAL:HA	1:G:338:LEU:HD12	1.96	0.47
1:B:295:ARG:NH2	1:H:295:ARG:NH2	2.62	0.47
1:B:319:HIS:HE1	1:B:361:TYR:O	1.97	0.47
1:D:228:TYR:HB2	1:D:240:LEU:HD23	1.97	0.47
1:H:319:HIS:HE1	1:H:361:TYR:O	1.97	0.47
1:A:228:TYR:HB2	1:A:240:LEU:HD23	1.97	0.47
1:D:370:GLY:O	1:D:374:ARG:HG3	2.14	0.47
1:F:319:HIS:HE1	1:F:361:TYR:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:HIS:HE1	1:A:361:TYR:O	1.96	0.47
1:C:127:LYS:HD2	4:C:610:HOH:O	2.13	0.47
1:C:293:ILE:O	1:C:297:VAL:HG23	2.15	0.47
1:H:262:ASN:ND2	4:H:646:HOH:O	2.43	0.47
1:H:313:GLN:HE21	1:H:314:VAL:H	1.63	0.47
1:E:313:GLN:HE21	1:E:314:VAL:H	1.63	0.46
1:B:228:TYR:HB2	1:B:240:LEU:HD23	1.97	0.46
1:C:228:TYR:HB2	1:C:240:LEU:HD23	1.97	0.46
1:B:335:VAL:HA	1:B:338:LEU:HD12	1.97	0.46
1:G:228:TYR:HB2	1:G:240:LEU:HD23	1.97	0.46
1:G:356:HIS:C	1:G:356:HIS:CD2	2.93	0.46
1:E:370:GLY:O	1:E:374:ARG:HG3	2.15	0.46
1:H:267:MET:HE1	1:H:375:LEU:HD21	1.97	0.46
1:A:418:ILE:O	1:A:422:THR:HG23	2.15	0.46
1:C:208:ILE:CB	1:C:209:PRO:CD	2.94	0.46
1:D:335:VAL:HA	1:D:338:LEU:HD12	1.97	0.46
1:H:228:TYR:HB2	1:H:240:LEU:HD23	1.98	0.46
1:A:313:GLN:HE21	1:A:314:VAL:H	1.62	0.46
1:C:319:HIS:HE1	1:C:361:TYR:O	1.98	0.46
1:D:293:ILE:O	1:D:297:VAL:HG23	2.16	0.46
1:A:293:ILE:O	1:A:297:VAL:HG23	2.16	0.46
1:E:293:ILE:O	1:E:297:VAL:HG23	2.17	0.45
1:F:341:GLU:HA	1:F:344:MET:HB3	1.99	0.45
1:B:341:GLU:HA	1:B:344:MET:HB3	1.99	0.45
1:F:356:HIS:C	1:F:356:HIS:CD2	2.94	0.45
1:A:341:GLU:HA	1:A:344:MET:HB3	1.98	0.45
1:A:178:VAL:HG23	4:A:692:HOH:O	2.16	0.45
1:A:370:GLY:O	1:A:374:ARG:HG3	2.16	0.45
1:D:392:ARG:HB2	1:D:395:GLN:HG3	1.97	0.45
1:A:343:ALA:HB1	1:A:351:PHE:CE1	2.52	0.45
1:C:335:VAL:HA	1:C:338:LEU:HD12	1.97	0.45
1:D:392:ARG:HH22	1:G:123:GLU:CB	2.30	0.45
1:F:314:VAL:O	1:F:321:PRO:HD2	2.16	0.45
1:G:341:GLU:HA	1:G:344:MET:HB3	1.99	0.45
1:B:298:LEU:HD13	1:B:302:ASP:HB3	1.98	0.45
1:C:341:GLU:HA	1:C:344:MET:HB3	1.99	0.45
1:F:228:TYR:HB2	1:F:240:LEU:HD23	1.99	0.45
1:B:252:ALA:HB1	1:H:252:ALA:HB1	1.98	0.45
1:B:313:GLN:HE21	1:B:314:VAL:H	1.64	0.45
1:B:314:VAL:O	1:B:321:PRO:HD2	2.17	0.44
1:B:187:VAL:HG13	4:B:667:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:MET:HE1	1:C:375:LEU:HD21	1.98	0.44
1:E:298:LEU:HD13	1:E:302:ASP:HB3	1.98	0.44
1:E:341:GLU:HA	1:E:344:MET:HB3	2.00	0.44
1:A:298:LEU:HD13	1:A:302:ASP:HB3	1.99	0.44
1:A:314:VAL:O	1:A:321:PRO:HD2	2.18	0.44
1:E:356:HIS:C	1:E:356:HIS:CD2	2.96	0.44
1:F:298:LEU:HD13	1:F:302:ASP:HB3	1.99	0.44
1:G:314:VAL:O	1:G:321:PRO:HD2	2.17	0.44
1:H:392:ARG:HB2	1:H:395:GLN:HG3	2.00	0.44
1:A:392:ARG:HB2	1:A:395:GLN:HG3	1.98	0.44
1:C:370:GLY:O	1:C:374:ARG:HG3	2.18	0.44
1:H:293:ILE:O	1:H:297:VAL:HG23	2.18	0.44
1:H:370:GLY:O	1:H:374:ARG:HG3	2.17	0.44
1:B:356:HIS:C	1:B:356:HIS:CD2	2.96	0.44
1:C:356:HIS:CD2	1:C:356:HIS:C	2.96	0.44
1:H:347:HIS:CD2	1:H:349:VAL:H	2.35	0.44
1:B:347:HIS:CD2	1:B:349:VAL:H	2.36	0.43
1:F:194:TYR:HA	1:F:197:ILE:HD12	1.99	0.43
1:E:347:HIS:CD2	1:E:349:VAL:H	2.35	0.43
1:H:341:GLU:HA	1:H:344:MET:HB3	2.00	0.43
1:D:298:LEU:HD13	1:D:302:ASP:HB3	1.99	0.43
1:G:400:TYR:CE1	2:G:501:APC:H8	2.53	0.43
1:H:298:LEU:HD13	1:H:302:ASP:HB3	1.99	0.43
1:H:356:HIS:CD2	1:H:356:HIS:C	2.96	0.43
1:A:194:TYR:HA	1:A:197:ILE:HD12	2.00	0.43
1:D:314:VAL:O	1:D:321:PRO:HD2	2.19	0.43
1:G:194:TYR:HA	1:G:197:ILE:HD12	1.99	0.43
1:H:215:LEU:O	1:H:219:MET:HG2	2.17	0.43
1:D:313:GLN:HE21	1:D:314:VAL:H	1.65	0.43
1:B:267:MET:HE1	1:B:375:LEU:HD21	1.99	0.43
1:E:360:VAL:HG13	2:E:501:APC:N3	2.33	0.43
1:D:356:HIS:C	1:D:356:HIS:CD2	2.97	0.43
1:D:267:MET:HE1	1:D:375:LEU:HD21	2.00	0.43
1:D:341:GLU:HA	1:D:344:MET:HB3	2.01	0.43
1:F:227:ILE:O	1:F:231:VAL:HG22	2.19	0.43
1:F:347:HIS:CD2	1:F:349:VAL:H	2.36	0.43
1:A:227:ILE:O	1:A:231:VAL:HG22	2.18	0.42
1:C:194:TYR:HA	1:C:197:ILE:HD12	2.00	0.42
1:D:343:ALA:HB1	1:D:351:PHE:CE1	2.54	0.42
1:E:119:GLN:HE21	1:E:119:GLN:HB3	1.71	0.42
1:E:267:MET:HE1	1:E:375:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:MET:HE1	1:F:375:LEU:HD21	2.01	0.42
1:H:194:TYR:HA	1:H:197:ILE:HD12	2.00	0.42
1:A:148:ILE:HD11	4:A:643:HOH:O	2.18	0.42
1:C:314:VAL:O	1:C:321:PRO:HD2	2.20	0.42
1:E:343:ALA:HB1	1:E:351:PHE:CE1	2.54	0.42
1:G:182:ARG:HG3	4:G:604:HOH:O	2.19	0.42
1:A:428:THR:HG23	4:A:604:HOH:O	2.19	0.42
1:C:343:ALA:HB1	1:C:351:PHE:CE1	2.55	0.42
1:C:110:LEU:HD13	1:C:142:ALA:HA	2.02	0.42
1:D:406:ALA:HB1	1:D:411:VAL:HG12	2.02	0.42
1:A:356:HIS:CD2	1:A:356:HIS:C	2.97	0.42
1:B:194:TYR:HA	1:B:197:ILE:HD12	2.01	0.41
1:A:202:VAL:HG23	1:A:426:LEU:HD21	2.02	0.41
1:E:194:TYR:HA	1:E:197:ILE:HD12	2.01	0.41
1:A:406:ALA:HB1	1:A:411:VAL:HG12	2.03	0.41
1:C:165:ARG:O	1:C:169:ILE:HG12	2.20	0.41
1:D:347:HIS:CD2	1:D:349:VAL:H	2.38	0.41
1:G:110:LEU:HD13	1:G:142:ALA:HA	2.02	0.41
1:B:343:ALA:HB1	1:B:351:PHE:CE1	2.56	0.41
1:D:392:ARG:HH22	1:G:123:GLU:CA	2.32	0.41
1:D:227:ILE:O	1:D:231:VAL:HG22	2.20	0.41
1:H:227:ILE:O	1:H:231:VAL:HG22	2.20	0.41
1:E:225:HIS:CE1	1:E:229:HIS:CE1	3.08	0.41
1:H:225:HIS:CE1	1:H:229:HIS:CE1	3.08	0.41
1:C:313:GLN:HE21	1:C:314:VAL:H	1.67	0.41
1:E:314:VAL:O	1:E:321:PRO:HD2	2.20	0.41
1:B:110:LEU:HD13	1:B:142:ALA:HA	2.03	0.41
1:B:202:VAL:HG23	1:B:426:LEU:HD21	2.02	0.41
1:D:225:HIS:CE1	1:D:229:HIS:CE1	3.09	0.41
1:A:110:LEU:HD13	1:A:142:ALA:HA	2.03	0.41
1:H:343:ALA:HB1	1:H:351:PHE:CE1	2.55	0.41
1:D:194:TYR:HA	1:D:197:ILE:HD12	2.02	0.40
1:E:206:MET:HE3	1:E:206:MET:HA	2.04	0.40
1:F:202:VAL:HG23	1:F:426:LEU:HD21	2.02	0.40
1:H:406:ALA:HB1	1:H:411:VAL:HG12	2.03	0.40
1:C:389:ILE:HG12	1:C:422:THR:HG22	2.03	0.40
1:D:250:ARG:HB2	4:D:621:HOH:O	2.20	0.40
1:F:406:ALA:HB1	1:F:411:VAL:HG12	2.03	0.40
1:G:298:LEU:HD13	1:G:302:ASP:HB3	2.02	0.40
1:B:165:ARG:O	1:B:169:ILE:HG12	2.21	0.40
1:D:202:VAL:HG23	1:D:426:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:ASN:HD22	1:E:213:SER:N	2.18	0.40
1:F:370:GLY:O	1:F:374:ARG:HG3	2.21	0.40
1:H:202:VAL:HG23	1:H:426:LEU:HD21	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	318/344 (92%)	310 (98%)	7 (2%)	1 (0%)	36	59
1	B	322/344 (94%)	313 (97%)	7 (2%)	2 (1%)	21	45
1	C	327/344 (95%)	315 (96%)	7 (2%)	5 (2%)	8	23
1	D	321/344 (93%)	311 (97%)	8 (2%)	2 (1%)	21	45
1	E	325/344 (94%)	315 (97%)	8 (2%)	2 (1%)	21	45
1	F	318/344 (92%)	312 (98%)	4 (1%)	2 (1%)	21	45
1	G	318/344 (92%)	311 (98%)	6 (2%)	1 (0%)	36	59
1	H	312/344 (91%)	307 (98%)	4 (1%)	1 (0%)	36	59
All	All	2561/2752 (93%)	2494 (97%)	51 (2%)	16 (1%)	21	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	208	ILE
1	C	209	PRO
1	C	210	LYS
1	C	213	SER
1	E	213	SER
1	D	212	ASN
1	F	121	LYS

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Mol	Chain	Res	Type
1	B	121	LYS
1	A	279	VAL
1	B	279	VAL
1	E	279	VAL
1	F	279	VAL
1	C	279	VAL
1	D	279	VAL
1	H	279	VAL
1	G	279	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	263/302 (87%)	232 (88%)	31 (12%)	5	15
1	B	255/302 (84%)	226 (89%)	29 (11%)	5	16
1	C	267/302 (88%)	234 (88%)	33 (12%)	4	13
1	D	255/302 (84%)	226 (89%)	29 (11%)	5	16
1	E	264/302 (87%)	228 (86%)	36 (14%)	3	11
1	F	251/302 (83%)	221 (88%)	30 (12%)	5	14
1	G	255/302 (84%)	224 (88%)	31 (12%)	5	14
1	H	255/302 (84%)	225 (88%)	30 (12%)	5	15
All	All	2065/2416 (86%)	1816 (88%)	249 (12%)	5	14

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	A	128	LEU
1	A	133	LEU
1	A	156	ILE
1	A	162	LEU
1	A	180	ARG

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Mol	Chain	Res	Type
1	A	202	VAL
1	A	203	LYS
1	A	220	GLU
1	A	236	ASN
1	A	240	LEU
1	A	253	VAL
1	A	272	LYS
1	A	278	LEU
1	A	282	ILE
1	A	287	ILE
1	A	288	SER
1	A	298	LEU
1	A	316	VAL
1	A	330	GLN
1	A	341	GLU
1	A	359	LEU
1	A	360	VAL
1	A	363	HIS
1	A	366	ILE
1	A	367	ASP
1	A	379	LEU
1	A	389	ILE
1	A	394	GLU
1	A	397	SER
1	A	404	GLU
1	B	114	LEU
1	B	128	LEU
1	B	133	LEU
1	B	156	ILE
1	B	162	LEU
1	B	180	ARG
1	B	202	VAL
1	B	220	GLU
1	B	236	ASN
1	B	240	LEU
1	B	253	VAL
1	B	272	LYS
1	B	278	LEU
1	B	282	ILE
1	B	287	ILE
1	B	288	SER
1	B	298	LEU

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Mol	Chain	Res	Type
1	B	316	VAL
1	B	330	GLN
1	B	341	GLU
1	B	359	LEU
1	B	360	VAL
1	B	363	HIS
1	B	367	ASP
1	B	379	LEU
1	B	389	ILE
1	B	394	GLU
1	B	397	SER
1	B	404	GLU
1	C	114	LEU
1	C	116	MET
1	C	128	LEU
1	C	133	LEU
1	C	156	ILE
1	C	162	LEU
1	C	180	ARG
1	C	202	VAL
1	C	203	LYS
1	C	206	MET
1	C	215	LEU
1	C	220	GLU
1	C	236	ASN
1	C	240	LEU
1	C	253	VAL
1	C	272	LYS
1	C	278	LEU
1	C	282	ILE
1	C	287	ILE
1	C	288	SER
1	C	298	LEU
1	C	316	VAL
1	C	330	GLN
1	C	341	GLU
1	C	359	LEU
1	C	360	VAL
1	C	363	HIS
1	C	367	ASP
1	C	379	LEU
1	C	389	ILE

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Mol	Chain	Res	Type
1	C	394	GLU
1	C	397	SER
1	C	404	GLU
1	D	114	LEU
1	D	116	MET
1	D	128	LEU
1	D	133	LEU
1	D	156	ILE
1	D	162	LEU
1	D	180	ARG
1	D	202	VAL
1	D	236	ASN
1	D	240	LEU
1	D	253	VAL
1	D	272	LYS
1	D	278	LEU
1	D	282	ILE
1	D	287	ILE
1	D	288	SER
1	D	298	LEU
1	D	316	VAL
1	D	330	GLN
1	D	341	GLU
1	D	359	LEU
1	D	360	VAL
1	D	363	HIS
1	D	367	ASP
1	D	379	LEU
1	D	389	ILE
1	D	394	GLU
1	D	397	SER
1	D	404	GLU
1	E	114	LEU
1	E	116	MET
1	E	119	GLN
1	E	128	LEU
1	E	133	LEU
1	E	156	ILE
1	E	162	LEU
1	E	180	ARG
1	E	202	VAL
1	E	206	MET

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Mol	Chain	Res	Type
1	E	207	SER
1	E	210	LYS
1	E	212	ASN
1	E	220	GLU
1	E	236	ASN
1	E	240	LEU
1	E	253	VAL
1	E	272	LYS
1	E	276	THR
1	E	278	LEU
1	E	282	ILE
1	E	287	ILE
1	E	288	SER
1	E	298	LEU
1	E	316	VAL
1	E	330	GLN
1	E	341	GLU
1	E	359	LEU
1	E	360	VAL
1	E	363	HIS
1	E	367	ASP
1	E	379	LEU
1	E	389	ILE
1	E	394	GLU
1	E	397	SER
1	E	404	GLU
1	F	116	MET
1	F	128	LEU
1	F	133	LEU
1	F	156	ILE
1	F	162	LEU
1	F	180	ARG
1	F	202	VAL
1	F	206	MET
1	F	220	GLU
1	F	236	ASN
1	F	240	LEU
1	F	253	VAL
1	F	272	LYS
1	F	278	LEU
1	F	282	ILE
1	F	287	ILE

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Mol	Chain	Res	Type
1	F	288	SER
1	F	298	LEU
1	F	316	VAL
1	F	330	GLN
1	F	341	GLU
1	F	359	LEU
1	F	360	VAL
1	F	363	HIS
1	F	367	ASP
1	F	379	LEU
1	F	389	ILE
1	F	394	GLU
1	F	397	SER
1	F	404	GLU
1	G	114	LEU
1	G	116	MET
1	G	128	LEU
1	G	133	LEU
1	G	156	ILE
1	G	162	LEU
1	G	180	ARG
1	G	202	VAL
1	G	219	MET
1	G	220	GLU
1	G	236	ASN
1	G	240	LEU
1	G	253	VAL
1	G	272	LYS
1	G	278	LEU
1	G	282	ILE
1	G	287	ILE
1	G	288	SER
1	G	298	LEU
1	G	316	VAL
1	G	330	GLN
1	G	341	GLU
1	G	359	LEU
1	G	360	VAL
1	G	363	HIS
1	G	367	ASP
1	G	379	LEU
1	G	389	ILE

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Mol	Chain	Res	Type
1	G	394	GLU
1	G	397	SER
1	G	404	GLU
1	H	114	LEU
1	H	128	LEU
1	H	133	LEU
1	H	156	ILE
1	H	162	LEU
1	H	180	ARG
1	H	202	VAL
1	H	206	MET
1	H	220	GLU
1	H	236	ASN
1	H	240	LEU
1	H	253	VAL
1	H	272	LYS
1	H	278	LEU
1	H	282	ILE
1	H	287	ILE
1	H	288	SER
1	H	298	LEU
1	H	316	VAL
1	H	330	GLN
1	H	341	GLU
1	H	359	LEU
1	H	360	VAL
1	H	363	HIS
1	H	367	ASP
1	H	379	LEU
1	H	389	ILE
1	H	394	GLU
1	H	397	SER
1	H	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	158	GLN
1	A	225	HIS
1	A	229	HIS
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	318	HIS
1	A	323	HIS
1	A	347	HIS
1	B	158	GLN
1	B	225	HIS
1	B	226	HIS
1	B	229	HIS
1	B	313	GLN
1	B	319	HIS
1	B	325	GLN
1	B	347	HIS
1	C	131	HIS
1	C	158	GLN
1	C	225	HIS
1	C	229	HIS
1	C	323	HIS
1	C	347	HIS
1	C	401	HIS
1	D	131	HIS
1	D	158	GLN
1	D	225	HIS
1	D	229	HIS
1	D	313	GLN
1	D	319	HIS
1	D	325	GLN
1	D	347	HIS
1	D	401	HIS
1	E	119	GLN
1	E	131	HIS
1	E	158	GLN
1	E	212	ASN
1	E	225	HIS
1	E	229	HIS
1	E	313	GLN
1	E	325	GLN
1	E	347	HIS
1	F	131	HIS
1	F	158	GLN
1	F	225	HIS
1	F	229	HIS
1	F	313	GLN
1	F	325	GLN

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Mol	Chain	Res	Type
1	F	347	HIS
1	G	131	HIS
1	G	158	GLN
1	G	192	GLN
1	G	225	HIS
1	G	229	HIS
1	G	313	GLN
1	G	325	GLN
1	G	347	HIS
1	H	131	HIS
1	H	158	GLN
1	H	225	HIS
1	H	229	HIS
1	H	313	GLN
1	H	325	GLN
1	H	347	HIS

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	APC	C	501	-	29,33,33	0.90	2 (6%)	44,52,52	1.27	3 (6%)
2	APC	B	501	-	29,33,33	0.78	2 (6%)	44,52,52	0.98	3 (6%)
2	APC	G	501	3	29,33,33	0.83	2 (6%)	44,52,52	1.27	3 (6%)
2	APC	H	501	-	29,33,33	0.88	3 (10%)	44,52,52	1.25	3 (6%)
2	APC	F	501	-	29,33,33	0.86	1 (3%)	44,52,52	1.01	4 (9%)
2	APC	D	501	-	29,33,33	0.83	2 (6%)	44,52,52	1.23	3 (6%)
2	APC	A	501	-	29,33,33	0.72	2 (6%)	44,52,52	1.02	4 (9%)
2	APC	E	501	3	29,33,33	0.84	2 (6%)	44,52,52	1.07	3 (6%)

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	APC	C	501	-	-	2/19/38/38	0/3/3/3
2	APC	B	501	-	-	3/19/38/38	0/3/3/3
2	APC	G	501	3	-	2/19/38/38	0/3/3/3
2	APC	H	501	-	-	2/19/38/38	0/3/3/3
2	APC	F	501	-	-	3/19/38/38	0/3/3/3
2	APC	D	501	-	-	2/19/38/38	0/3/3/3
2	APC	A	501	-	-	3/19/38/38	0/3/3/3
2	APC	E	501	3	-	3/19/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	APC	PG-O2G	-3.40	1.42	1.54
2	F	501	APC	PB-O3B	3.26	1.62	1.58
2	G	501	APC	PG-O2G	-2.77	1.44	1.54
2	D	501	APC	PG-O2G	-2.57	1.45	1.54
2	H	501	APC	PB-O3B	2.50	1.61	1.58
2	H	501	APC	PG-O2G	-2.50	1.45	1.54
2	E	501	APC	PB-O3B	2.39	1.61	1.58
2	G	501	APC	PA-O1A	2.33	1.57	1.51
2	E	501	APC	PB-O2B	-2.33	1.50	1.56
2	C	501	APC	PA-O1A	2.29	1.56	1.51
2	B	501	APC	PB-O3B	2.29	1.60	1.58
2	H	501	APC	PA-O1A	2.27	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	APC	PB-O1B	2.22	1.56	1.51
2	D	501	APC	PA-O1A	2.21	1.56	1.51
2	B	501	APC	PB-O2B	-2.12	1.51	1.56
2	A	501	APC	PB-O2B	-2.05	1.51	1.56

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	APC	O1B-PB-C3A	5.43	123.35	109.05
2	G	501	APC	O1B-PB-C3A	5.23	122.82	109.05
2	D	501	APC	O1B-PB-C3A	5.08	122.43	109.05
2	C	501	APC	O1B-PB-C3A	5.03	122.29	109.05
2	C	501	APC	O2G-PG-O3B	4.42	119.44	104.64
2	G	501	APC	O2G-PG-O3B	4.21	118.75	104.64
2	H	501	APC	O2G-PG-O3B	4.08	118.32	104.64
2	D	501	APC	O2G-PG-O3B	4.06	118.27	104.64
2	E	501	APC	O2B-PB-C3A	3.94	123.03	106.73
2	F	501	APC	O2B-PB-C3A	3.83	122.60	106.73
2	A	501	APC	O2B-PB-C3A	3.82	122.53	106.73
2	B	501	APC	O2B-PB-C3A	3.81	122.49	106.73
2	E	501	APC	O1B-PB-C3A	-3.44	99.99	109.05
2	A	501	APC	O1B-PB-C3A	-3.09	100.91	109.05
2	F	501	APC	O1B-PB-C3A	-3.01	101.11	109.05
2	B	501	APC	O1B-PB-C3A	-2.82	101.62	109.05
2	C	501	APC	O3G-PG-O3B	-2.50	96.24	104.64
2	E	501	APC	O3G-PG-O3B	-2.29	96.94	104.64
2	F	501	APC	O1A-PA-C3A	2.19	114.81	109.05
2	A	501	APC	O1A-PA-C3A	2.14	114.69	109.05
2	A	501	APC	O3G-PG-O3B	-2.14	97.46	104.64
2	F	501	APC	O3G-PG-O3B	-2.14	97.46	104.64
2	D	501	APC	O3G-PG-O3B	-2.13	97.48	104.64
2	B	501	APC	O1A-PA-C3A	2.08	114.52	109.05
2	H	501	APC	O3G-PG-O3B	-2.04	97.78	104.64
2	G	501	APC	O3G-PG-O3B	-2.03	97.82	104.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	APC	PB-C3A-PA-O2A
2	B	501	APC	PB-C3A-PA-O2A
2	E	501	APC	PB-C3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	F	501	APC	PB-C3A-PA-O2A
2	A	501	APC	PB-C3A-PA-O1A
2	B	501	APC	PB-C3A-PA-O1A
2	C	501	APC	PB-C3A-PA-O1A
2	D	501	APC	PB-C3A-PA-O1A
2	E	501	APC	PB-C3A-PA-O1A
2	F	501	APC	PB-C3A-PA-O1A
2	G	501	APC	PB-C3A-PA-O1A
2	H	501	APC	PB-C3A-PA-O1A
2	B	501	APC	C2'-C1'-N9-C8
2	C	501	APC	C2'-C1'-N9-C8
2	D	501	APC	C2'-C1'-N9-C8
2	E	501	APC	C2'-C1'-N9-C8
2	F	501	APC	C2'-C1'-N9-C8
2	H	501	APC	C2'-C1'-N9-C8
2	A	501	APC	C2'-C1'-N9-C8
2	G	501	APC	C2'-C1'-N9-C8

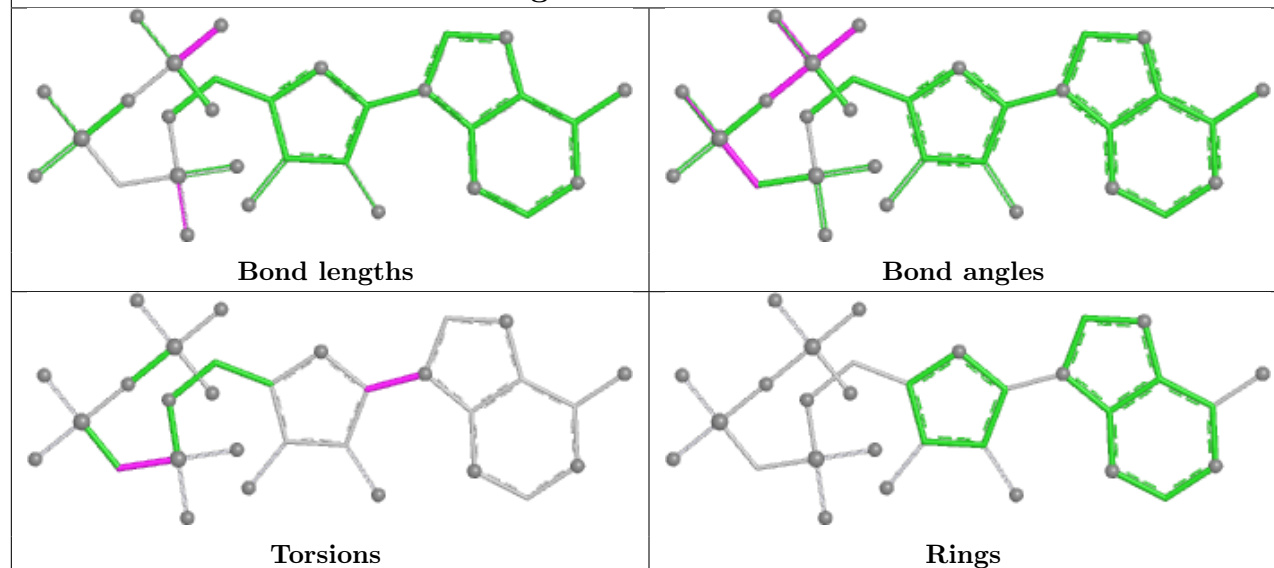
There are no ring outliers.

2 monomers are involved in 2 short contacts:

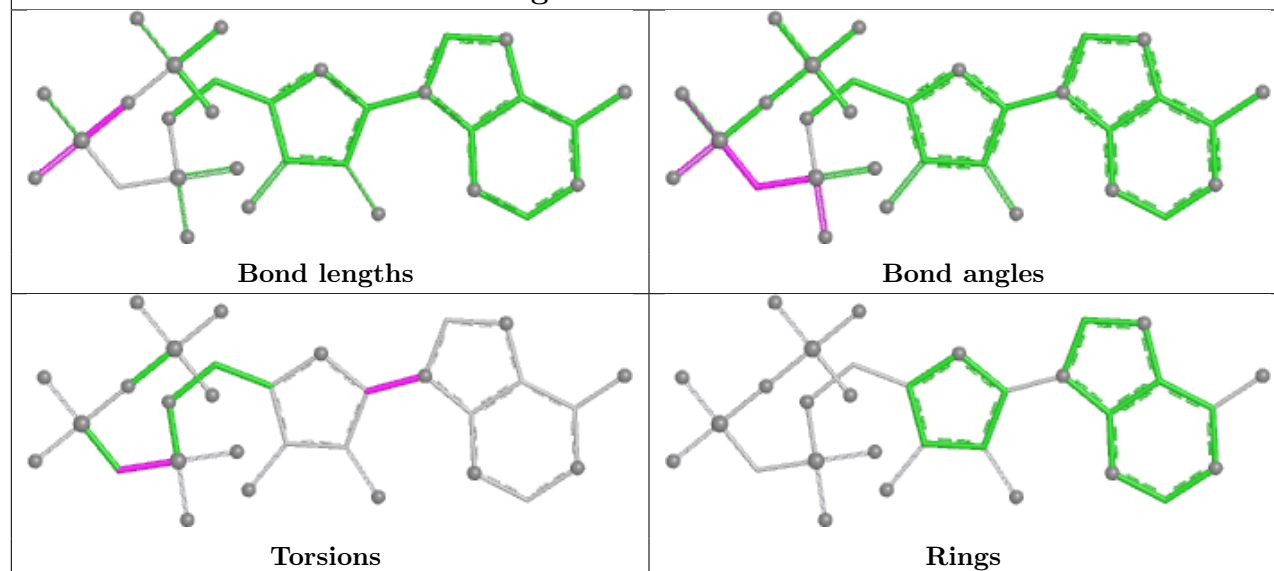
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	APC	1	0
2	E	501	APC	1	0

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.

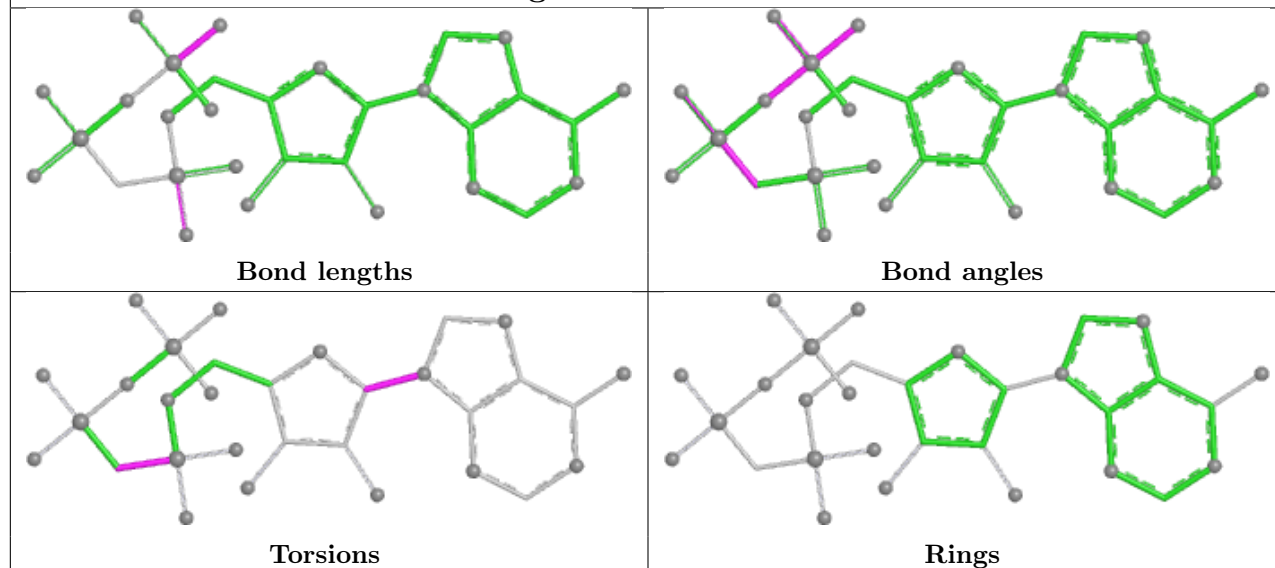
Ligand APC C 501



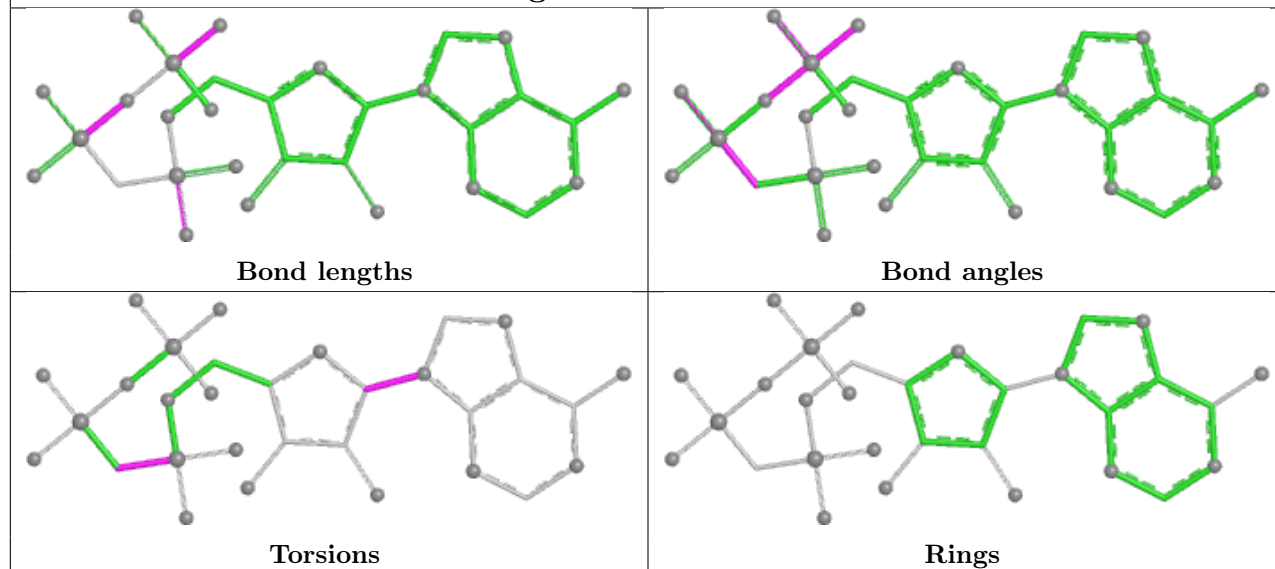
Ligand APC B 501



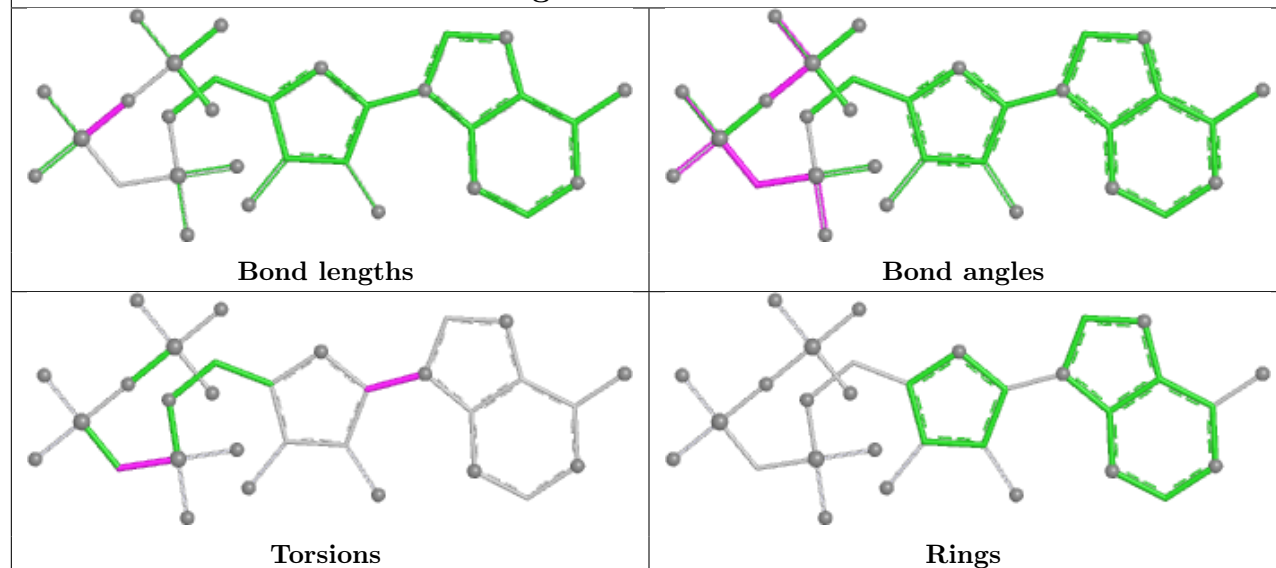
Ligand APC G 501



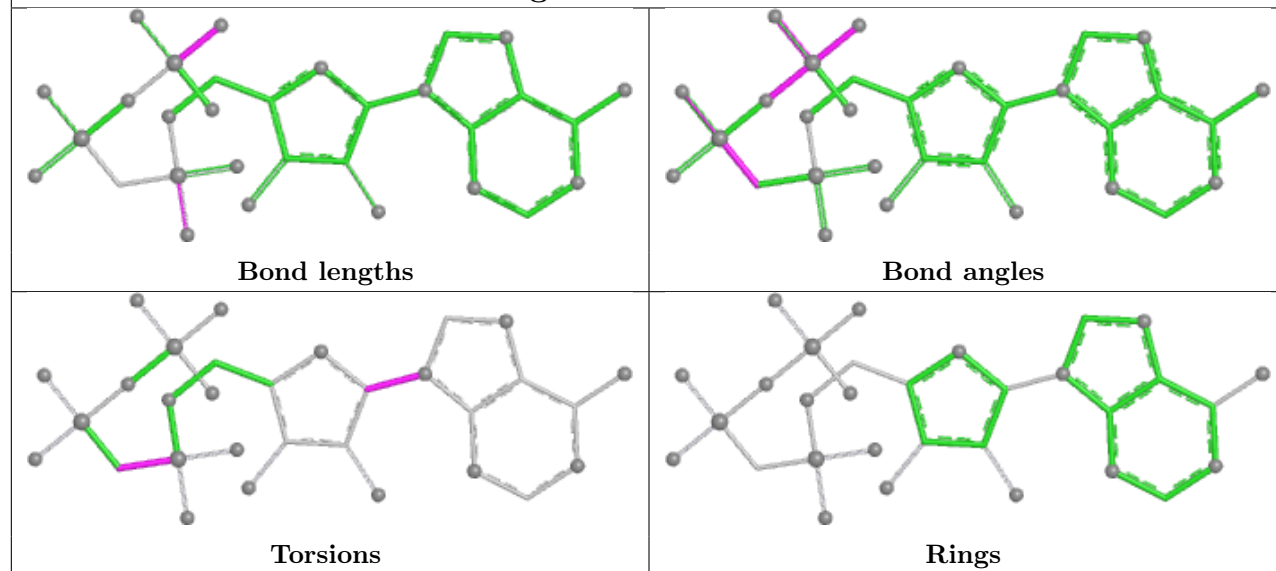
Ligand APC H 501

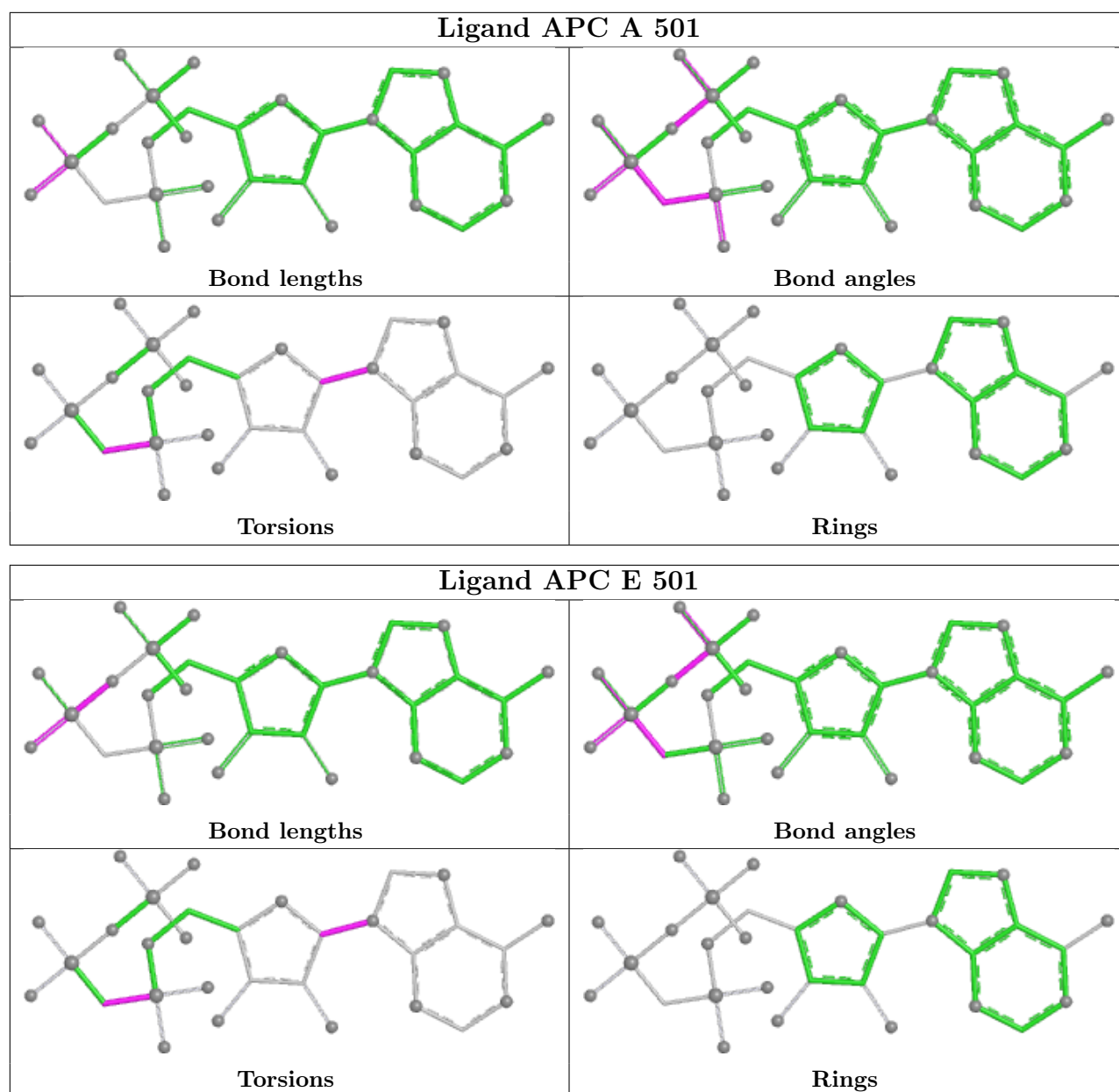


Ligand APC F 501



Ligand APC D 501





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	322/344 (93%)	-1.59	0 100 100	16, 48, 94, 121	0
1	B	326/344 (94%)	-1.51	0 100 100	38, 71, 116, 126	0
1	C	329/344 (95%)	-1.61	0 100 100	16, 47, 97, 118	0
1	D	325/344 (94%)	-1.51	0 100 100	40, 69, 111, 138	0
1	E	327/344 (95%)	-1.59	0 100 100	20, 46, 95, 114	0
1	F	322/344 (93%)	-1.47	0 100 100	42, 72, 120, 144	0
1	G	322/344 (93%)	-1.57	0 100 100	14, 49, 97, 112	0
1	H	318/344 (92%)	-1.50	0 100 100	40, 65, 109, 129	0
All	All	2591/2752 (94%)	-1.54	0 100 100	14, 60, 108, 144	0

There are no RSRZ outliers to report.

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](#)

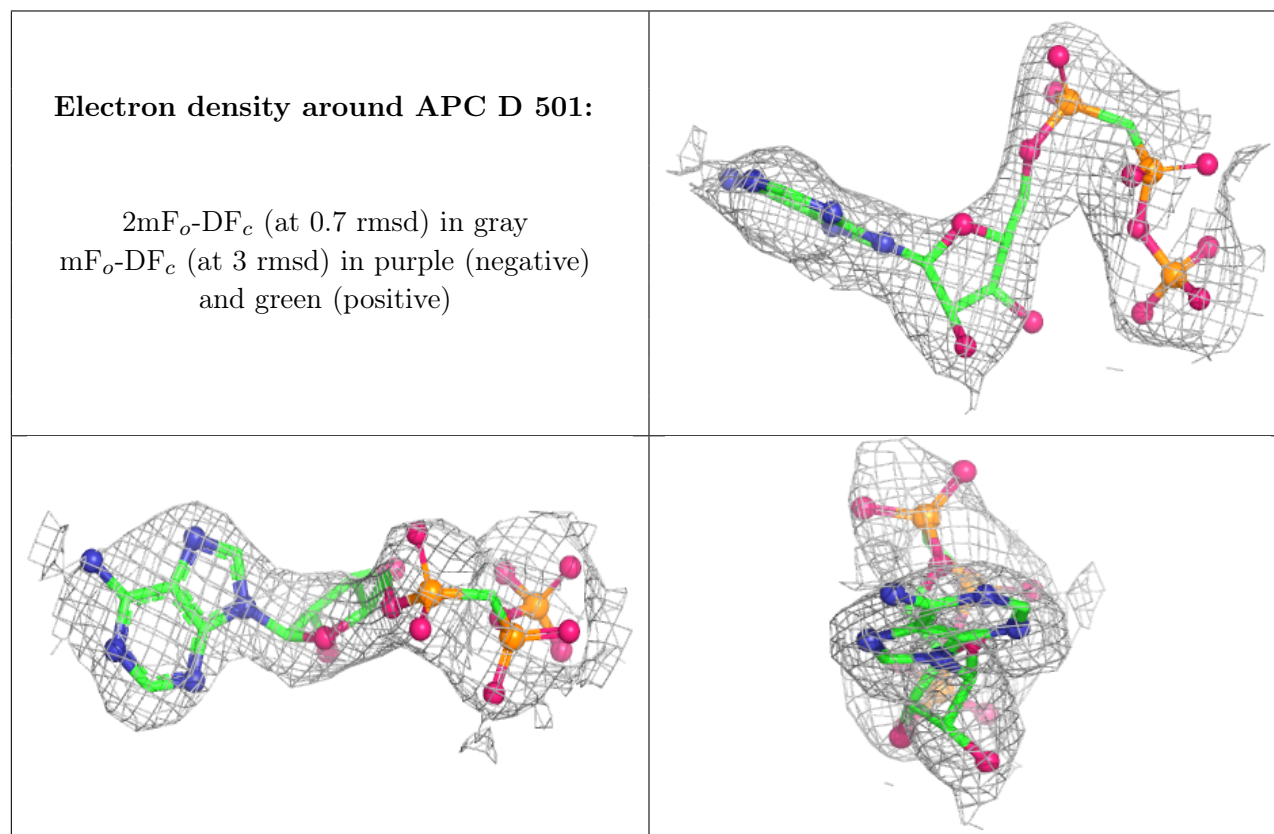
There are no oligosaccharides in this entry.

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.

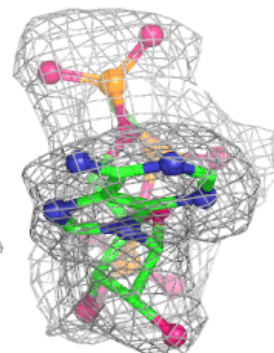
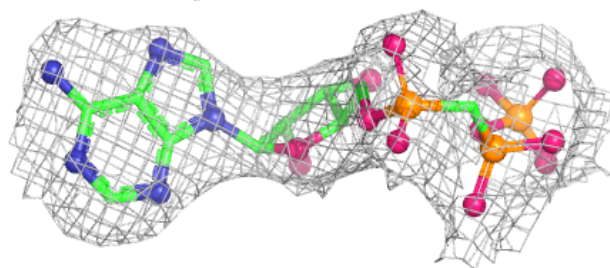
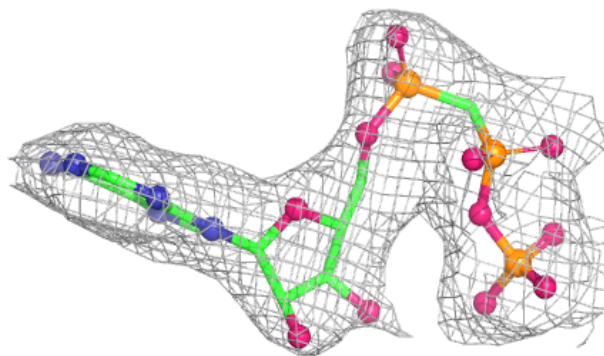
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	502	1/1	0.96	0.09	71,71,71,71	0
3	MG	D	502	1/1	0.98	0.04	86,86,86,86	0
3	MG	F	502	1/1	0.98	0.03	53,53,53,53	0
2	APC	D	501	31/31	0.99	0.04	79,92,96,97	0
2	APC	E	501	31/31	0.99	0.03	45,63,72,74	0
2	APC	F	501	31/31	0.99	0.03	62,82,94,95	0
2	APC	G	501	31/31	0.99	0.03	40,59,72,75	0
2	APC	H	501	31/31	0.99	0.04	80,92,95,97	0
2	APC	A	501	31/31	0.99	0.03	44,60,64,65	0
3	MG	B	502	1/1	0.99	0.04	52,52,52,52	0
2	APC	B	501	31/31	0.99	0.04	65,97,104,105	0
2	APC	C	501	31/31	0.99	0.03	33,55,63,66	0
3	MG	G	502	1/1	0.99	0.04	48,48,48,48	0
3	MG	H	502	1/1	0.99	0.03	64,64,64,64	0
3	MG	E	502	1/1	1.00	0.04	59,59,59,59	0
3	MG	C	502	1/1	1.00	0.03	32,32,32,32	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.

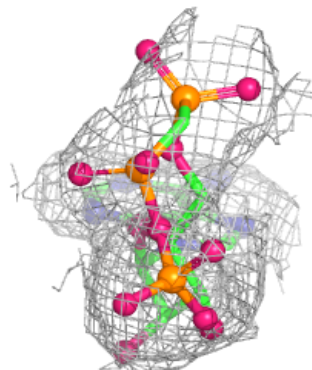
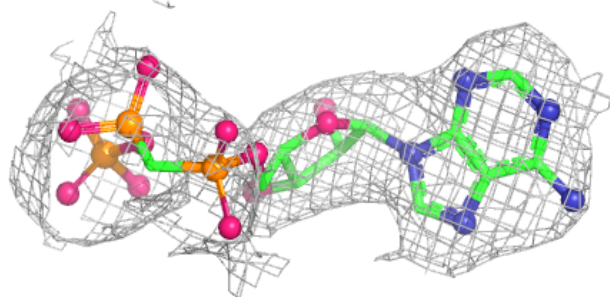
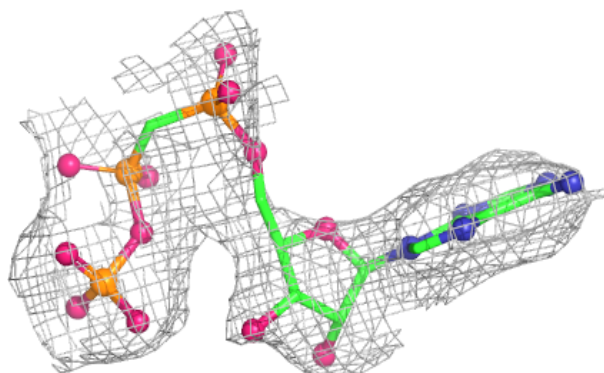


Electron density around APC E 501:

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

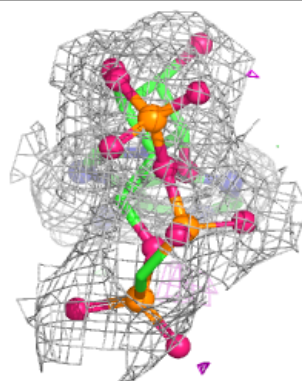
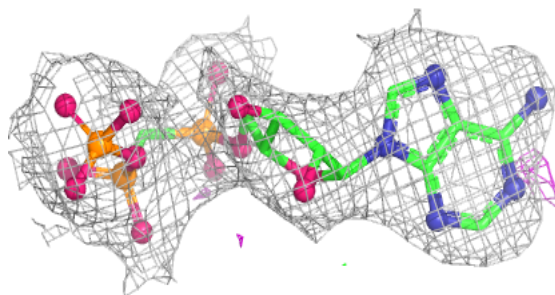
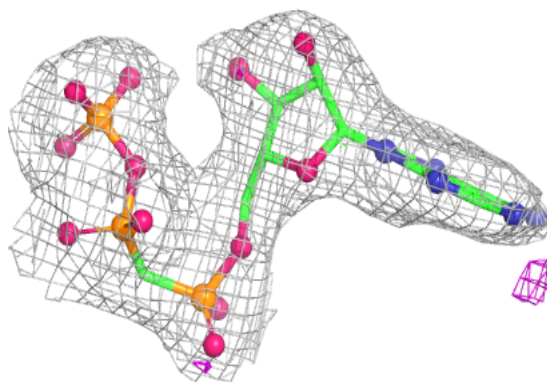
**Electron density around APC F 501:**

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

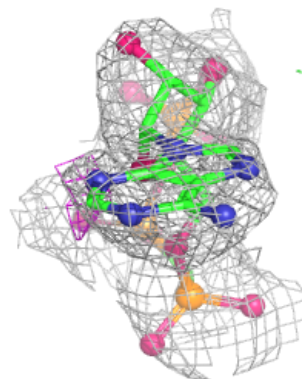
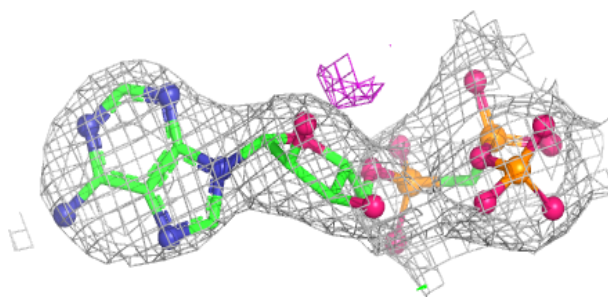
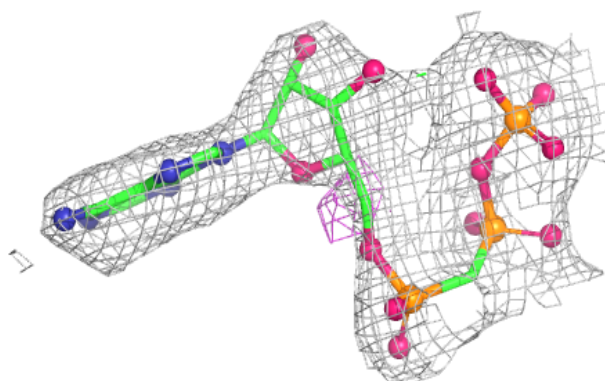


Electron density around APC G 501:

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

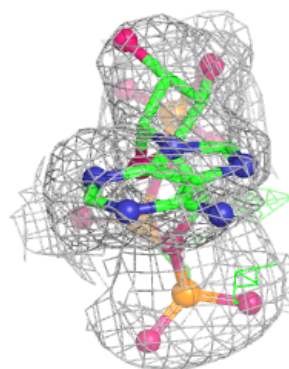
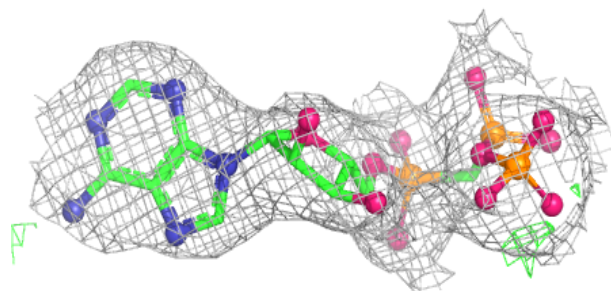
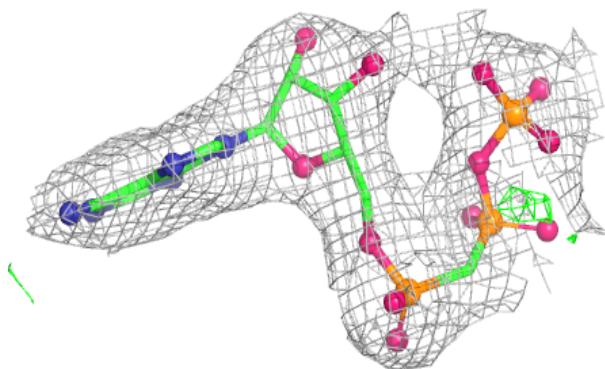
**Electron density around APC H 501:**

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

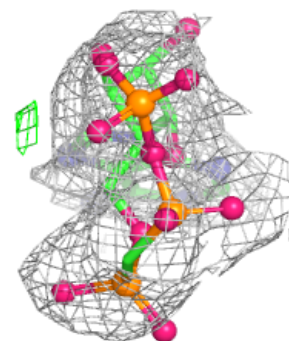
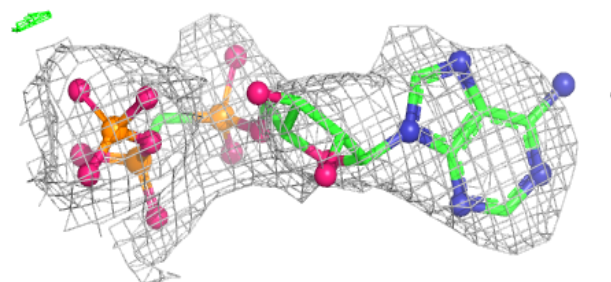
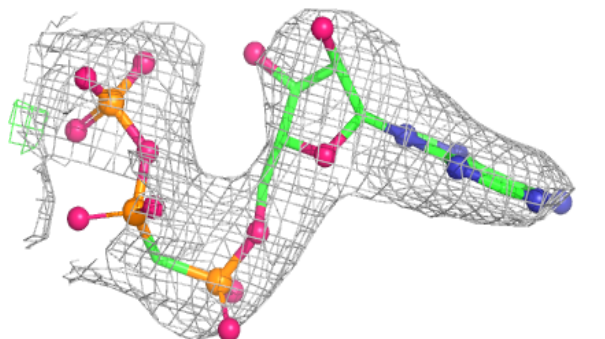


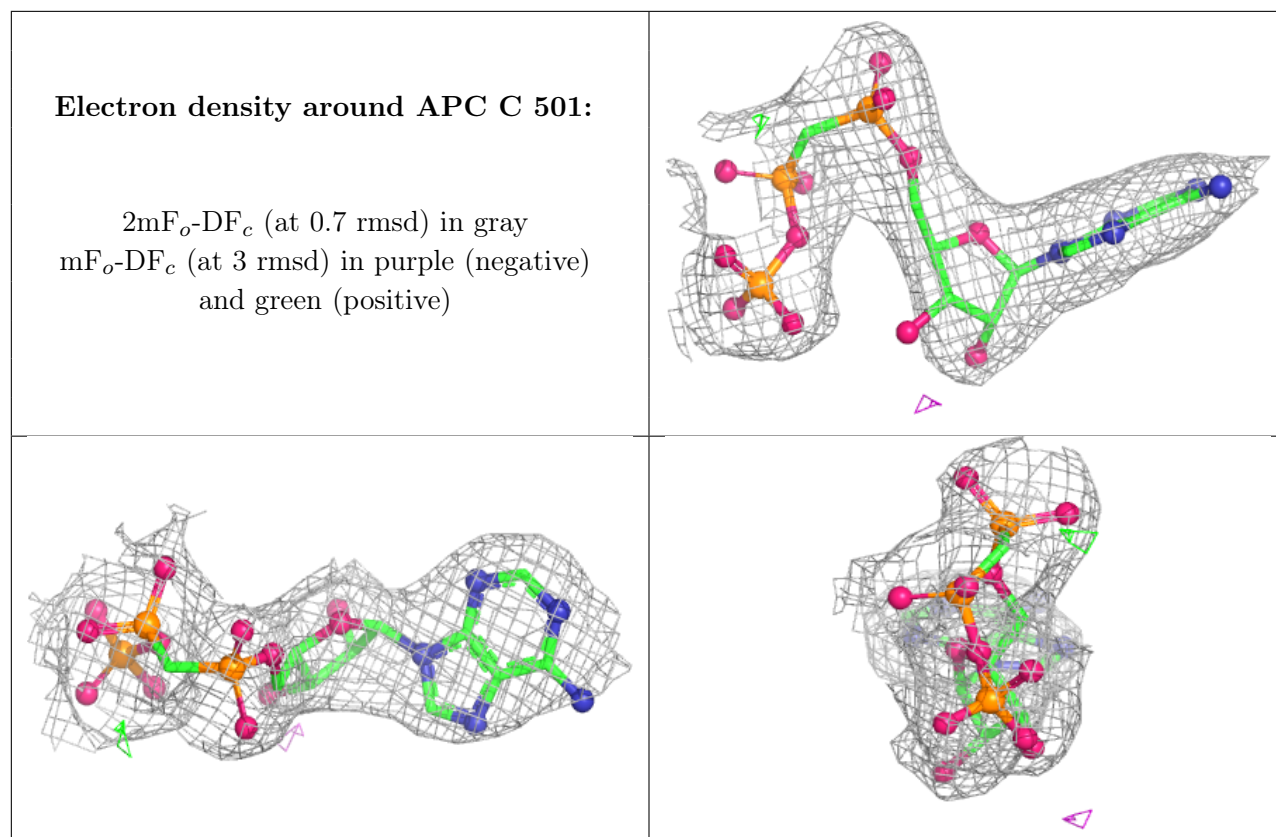
Electron density around APC A 501:

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

**Electron density around APC B 501:**

$2mF_o-DF_c$ (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.