



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:07 PM UTC

PDB ID : 2AA3 / pdb_00002aa3
Title : Crystal structure of Plasmodium vivax lactate dehydrogenase complex with APADH
Authors : Chaikuad, A.; Fairweather, V.; Conners, R.; Joseph-Horne, T.; Turgut-Balik, D.; Brady, R.L.
Deposited on : 2005-07-13
Resolution : 2.05 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

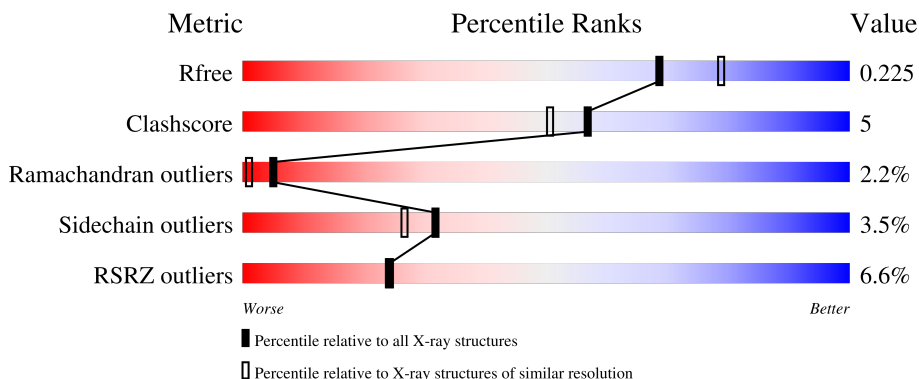
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	321	 3% 86% 9% . .
1	B	321	 5% 82% 14% . .
1	C	321	 6% 86% 10% . .
1	D	321	 11% 80% 16% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AP0	A	1401	X	-	-	-
3	AP0	B	1407	X	-	-	-
3	AP0	C	1405	X	-	-	-
3	AP0	D	1403	X	-	-	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10302 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2408	1540	403	451	14	106	1	0
1	B	315	2398	1534	400	450	14	34	1	0
1	C	318	2433	1557	409	453	14	118	2	0
1	D	315	2398	1534	400	450	14	125	1	0

There are 24 discrepancies between the modelled and reference sequences:

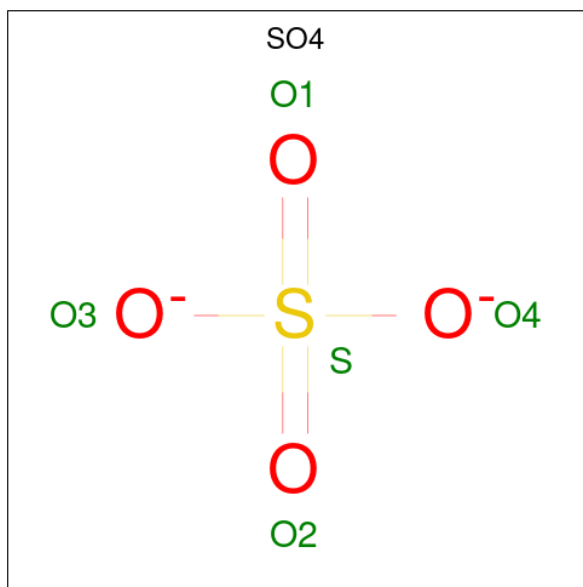
Chain	Residue	Modelled	Actual	Comment	Reference
A	330	HIS	-	expression tag	GB 66967948
A	331	HIS	-	expression tag	GB 66967948
A	332	HIS	-	expression tag	GB 66967948
A	333	HIS	-	expression tag	GB 66967948
A	334	HIS	-	expression tag	GB 66967948
A	335	HIS	-	expression tag	GB 66967948
B	330	HIS	-	expression tag	GB 66967948
B	331	HIS	-	expression tag	GB 66967948
B	332	HIS	-	expression tag	GB 66967948
B	333	HIS	-	expression tag	GB 66967948
B	334	HIS	-	expression tag	GB 66967948
B	335	HIS	-	expression tag	GB 66967948
C	330	HIS	-	expression tag	GB 66967948
C	331	HIS	-	expression tag	GB 66967948
C	332	HIS	-	expression tag	GB 66967948
C	333	HIS	-	expression tag	GB 66967948
C	334	HIS	-	expression tag	GB 66967948
C	335	HIS	-	expression tag	GB 66967948
D	330	HIS	-	expression tag	GB 66967948
D	331	HIS	-	expression tag	GB 66967948
D	332	HIS	-	expression tag	GB 66967948

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Chain	Residue	Modelled	Actual	Comment	Reference
D	333	HIS	-	expression tag	GB 66967948
D	334	HIS	-	expression tag	GB 66967948
D	335	HIS	-	expression tag	GB 66967948

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



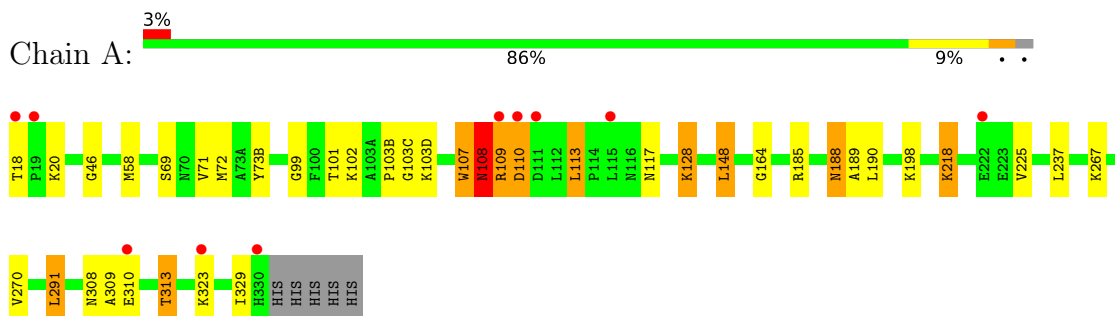
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETYL PYRIDINE ADENINE DINUCLEOTIDE, REDUCED (CCD ID: AP0) (formula: C₂₂H₃₀N₆O₁₄P₂).

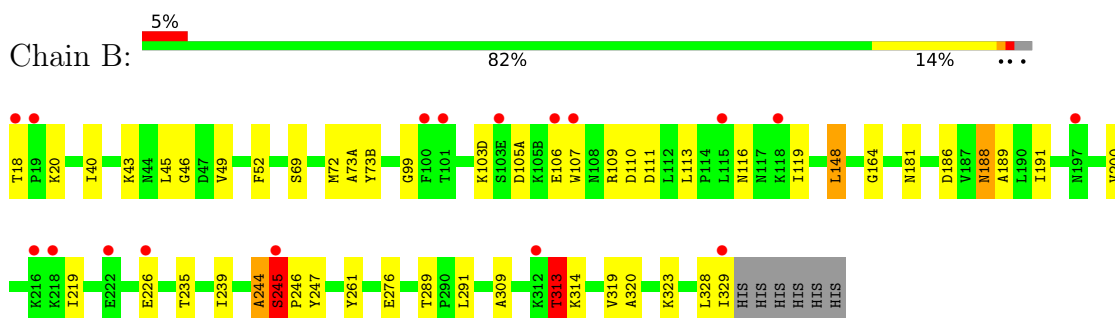
3 Residue-property plots [i](#)

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.

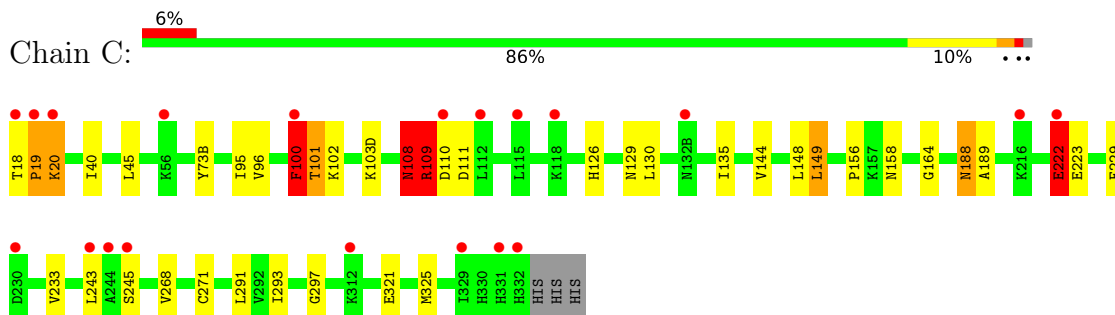
- Molecule 1: L-lactate dehydrogenase



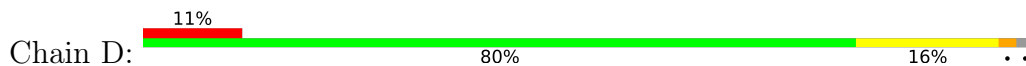
- Molecule 1: L-lactate dehydrogenase

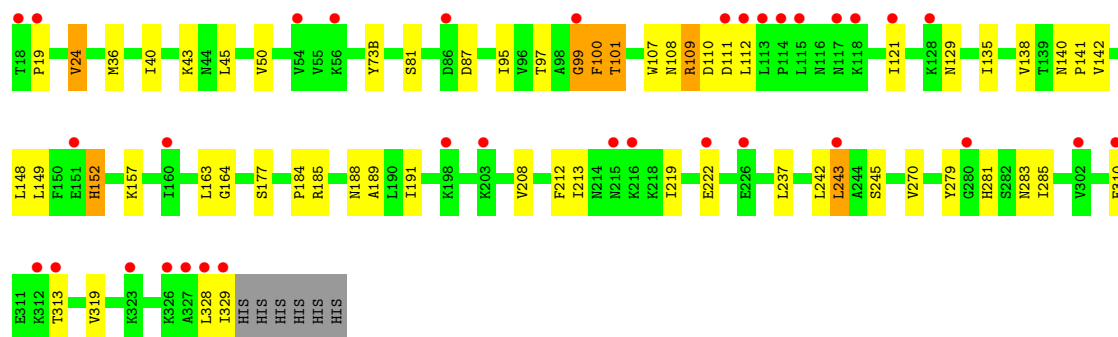


- Molecule 1: L-lactate dehydrogenase



- Molecule 1: L-lactate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.48Å 128.45Å 130.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.67 – 2.05 91.64 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.3 (91.67-2.05) 98.4 (91.64-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.04Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.226 0.191 , 0.225	Depositor DCC
R_{free} test set	4276 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: SO4, AP0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.25	8/2448 (0.3%)	1.06	10/3315 (0.3%)
1	B	1.21	7/2437 (0.3%)	1.18	11/3300 (0.3%)
1	C	1.21	10/2478 (0.4%)	1.15	11/3356 (0.3%)
1	D	1.11	6/2437 (0.2%)	1.06	4/3300 (0.1%)
All	All	1.20	31/9800 (0.3%)	1.11	36/13271 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	2	1
1	D	1	2
All	All	3	6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	LYS	CE-NZ	12.65	1.87	1.49
1	A	128	LYS	CE-NZ	11.87	1.84	1.49
1	B	107	TRP	CA-CB	9.15	1.69	1.53
1	D	100	PHE	CA-C	8.94	1.64	1.52
1	C	222	GLU	CD-OE1	8.62	1.41	1.25
1	D	100	PHE	N-CA	8.43	1.57	1.46
1	A	108	ASN	C-N	8.42	1.45	1.33
1	C	109	ARG	C-N	7.92	1.44	1.33
1	C	110	ASP	CA-CB	7.85	1.66	1.53
1	C	222	GLU	CD-OE2	7.46	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	GLU	CD-OE1	7.25	1.39	1.25
1	B	219	ILE	CA-CB	6.73	1.62	1.55
1	A	218	LYS	CD-CE	6.62	1.72	1.52
1	B	313	THR	CA-CB	6.61	1.64	1.53
1	B	226	GLU	CD-OE2	6.44	1.37	1.25
1	A	99	GLY	C-N	6.41	1.42	1.33
1	C	100	PHE	C-N	-6.22	1.25	1.33
1	D	24	VAL	CA-CB	6.21	1.61	1.54
1	B	105(A)	ASP	CA-CB	-6.11	1.43	1.53
1	C	96	VAL	CA-CB	6.07	1.61	1.53
1	A	323	LYS	CD-CE	6.03	1.70	1.52
1	C	144	VAL	CA-CB	5.89	1.61	1.54
1	B	247	TYR	C-O	-5.61	1.17	1.24
1	C	95	ILE	CA-CB	5.37	1.60	1.54
1	D	222	GLU	CD-OE2	5.34	1.35	1.25
1	C	40	ILE	CA-CB	5.34	1.60	1.54
1	D	135	ILE	CA-CB	5.30	1.60	1.54
1	C	268	VAL	CA-CB	5.28	1.60	1.54
1	A	270	VAL	CA-CB	5.15	1.60	1.54
1	D	95	ILE	CA-CB	5.14	1.60	1.54
1	A	71	VAL	CA-CB	5.11	1.60	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	PHE	O-C-N	17.47	145.82	122.59
1	B	106	GLU	CA-CB-CG	16.56	147.21	114.10
1	B	107	TRP	CB-CA-C	-15.30	90.97	109.80
1	B	106	GLU	CB-CG-CD	12.16	133.28	112.60
1	C	110	ASP	O-C-N	-10.42	108.74	122.59
1	C	100	PHE	CA-C-N	-10.11	102.23	121.54
1	C	100	PHE	C-N-CA	-10.11	102.23	121.54
1	D	100	PHE	N-CA-C	9.70	131.46	110.80
1	C	110	ASP	CA-CB-CG	-8.35	104.25	112.60
1	C	110	ASP	CB-CA-C	-7.78	94.95	110.42
1	A	99	GLY	O-C-N	7.72	132.73	123.55
1	A	218	LYS	CD-CE-NZ	-7.15	89.02	111.90
1	B	235	THR	N-CA-C	6.07	117.56	111.07
1	B	244	ALA	N-CA-C	-6.04	97.94	110.80
1	A	108	ASN	O-C-N	6.00	130.57	122.59
1	B	107	TRP	N-CA-CB	-5.99	99.97	109.19
1	B	276	GLU	CA-C-N	-5.96	116.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	GLU	C-N-CA	-5.96	116.98	123.30
1	C	110	ASP	N-CA-CB	-5.89	100.53	110.49
1	A	225	VAL	N-CA-C	-5.79	105.09	110.53
1	B	289	THR	CA-C-N	-5.75	113.84	119.76
1	B	289	THR	C-N-CA	-5.75	113.84	119.76
1	C	297	GLY	N-CA-C	-5.62	105.37	111.21
1	A	109	ARG	CA-C-N	5.51	131.61	121.70
1	A	109	ARG	C-N-CA	5.51	131.61	121.70
1	C	245	SER	CA-C-N	5.46	125.46	119.89
1	C	245	SER	C-N-CA	5.46	125.46	119.89
1	C	45	LEU	N-CA-C	5.35	118.97	112.23
1	B	245	SER	N-CA-C	5.21	121.31	109.81
1	D	152	HIS	N-CA-C	5.19	118.78	112.23
1	D	245	SER	CA-C-N	-5.19	112.83	120.46
1	D	245	SER	C-N-CA	-5.19	112.83	120.46
1	A	291	LEU	CA-CB-CG	5.19	134.47	116.30
1	A	113	LEU	CA-C-N	-5.07	113.81	119.19
1	A	113	LEU	C-N-CA	-5.07	113.81	119.19
1	A	323	LYS	CG-CD-CE	-5.02	99.75	111.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	101	THR	CB,CA
1	D	110	ASP	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TRP	Peptide
1	A	108	ASN	Peptide
1	B	244	ALA	Peptide
1	C	108	ASN	Peptide
1	D	99	GLY	Mainchain,Peptide

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	2408	0	2505	20	0
1	B	2398	0	2498	27	0
1	C	2433	0	2530	31	0
1	D	2398	0	2497	25	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
4	A	149	0	0	1	0
4	B	121	0	0	1	0
4	C	121	0	0	2	0
4	D	88	0	0	0	0
All	All	10302	0	10134	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (88) 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:B:239:ILE:HG22	1:B:245:SER:H	1.24	1.03
1:B:319:VAL:HG12	1:B:323:LYS:HE2	1.47	0.94
1:C:291:LEU:HD11	1:C:293:ILE:HD11	1.51	0.92
1:C:291:LEU:CD1	1:C:293:ILE:HD11	2.04	0.86
1:C:73(B)[B]:TYR:CD2	1:D:73(B)[B]:TYR:CD2	2.65	0.84
1:C:73(B)[B]:TYR:CE2	1:D:73(B)[B]:TYR:CD2	2.67	0.82
1:C:73(B)[B]:TYR:CD2	1:D:73(B)[B]:TYR:CE2	2.68	0.81
1:C:126:HIS:HE1	4:C:1511:HOH:O	1.67	0.76
1:A:69:SER:HA	1:A:72:MET:HE2	1.71	0.72
1:A:218:LYS:CD	1:A:218:LYS:NZ	2.52	0.72
1:A:20:LYS:HE3	1:A:46:GLY:HA2	1.72	0.71
1:C:291:LEU:CD1	1:C:293:ILE:CD1	2.68	0.70
1:B:320:ALA:HA	1:B:323:LYS:HE3	1.73	0.70
1:C:73(B)[B]:TYR:CE2	1:D:73(B)[B]:TYR:HD2	2.09	0.69
1:B:99:GLY:HA2	1:B:119:ILE:HD13	1.74	0.69
1:C:73(B)[B]:TYR:HD2	1:D:73(B)[B]:TYR:CE2	2.14	0.65
1:B:69:SER:HA	1:B:72:MET:HE2	1.80	0.63
1:A:58:MET:HG2	1:C:243[B]:LEU:HD22	1.81	0.63
1:C:129:ASN:OD1	1:C:130:LEU:HG	2.01	0.61
1:A:128:LYS:NZ	1:A:128:LYS:CD	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HD21	1:B:329:ILE:HD13	1.83	0.59
1:A:109:ARG:HB2	1:A:110:ASP:CA	2.33	0.58
1:A:309:ALA:O	1:A:313:THR:HG23	2.03	0.58
1:D:121:ILE:HG12	1:D:152:HIS:CE1	2.38	0.58
1:B:110:ASP:HA	1:B:113:LEU:HD23	1.87	0.56
1:B:239:ILE:CG2	1:B:245:SER:H	2.09	0.56
1:D:188:ASN:HD22	1:D:189:ALA:H	1.53	0.55
1:B:20:LYS:HE3	1:B:46:GLY:HA2	1.88	0.54
1:C:321:GLU:HG3	1:C:325:MET:HE2	1.90	0.54
1:B:239:ILE:HG22	1:B:245:SER:N	2.08	0.53
1:A:308:ASN:OD1	1:A:310:GLU:HG2	2.09	0.52
1:A:18:THR:HG21	4:A:1534:HOH:O	2.09	0.51
1:C:291:LEU:HD13	1:C:293:ILE:CD1	2.39	0.51
1:D:142:VAL:HG11	1:D:163:LEU:O	2.10	0.51
1:B:261:TYR:O	1:C:18:THR:HG23	2.12	0.50
1:C:188:ASN:HD22	1:C:189:ALA:H	1.59	0.50
1:B:188:ASN:HD22	1:B:189:ALA:H	1.61	0.49
1:D:24:VAL:HG22	1:D:50:VAL:HB	1.95	0.48
1:B:103(D):LYS:CE	1:B:111:ASP:OD2	2.61	0.48
1:C:222:GLU:HG2	1:C:223:GLU:N	2.27	0.48
1:D:242:LEU:O	1:D:243:LEU:HB2	2.13	0.48
1:C:19:PRO:O	1:C:20:LYS:O	2.32	0.48
1:B:73(A):ALA:O	1:B:73(B)[B]:TYR:HB2	2.14	0.47
1:D:138:VAL:O	3:D:1403:AP0:H2	2.14	0.47
1:A:73(B)[B]:TYR:CD1	1:B:73(B)[B]:TYR:CD2	3.03	0.46
1:C:156:PRO:HB2	1:C:158:ASN:OD1	2.15	0.46
1:B:116:ASN:HA	1:B:119:ILE:HD12	1.98	0.46
1:B:245:SER:HA	1:B:246:PRO:HD2	1.75	0.46
1:D:36:MET:O	1:D:40:ILE:HG13	2.16	0.46
1:A:188:ASN:HD22	1:A:189:ALA:H	1.63	0.46
1:D:310:GLU:O	1:D:313:THR:HG22	2.16	0.45
1:A:58:MET:HG2	1:C:243[B]:LEU:CD2	2.47	0.45
1:A:185:ARG:HD2	1:C:73(B)[B]:TYR:HD1	1.82	0.45
1:B:73(B)[B]:TYR:HE1	1:D:185:ARG:CZ	2.29	0.44
1:A:73(B)[B]:TYR:HD1	1:B:73(B)[B]:TYR:CE2	2.35	0.44
1:C:100:PHE:N	1:C:100:PHE:CD2	2.85	0.44
1:C:126:HIS:HD2	4:C:1508:HOH:O	1.99	0.44
1:D:279:TYR:O	1:D:281:HIS:CD2	2.71	0.44
1:C:229:PHE:O	1:C:233:VAL:HG23	2.17	0.44
1:D:208:VAL:HB	1:D:212:PHE:CE1	2.53	0.43
1:D:213:ILE:HA	1:D:219:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PHE:N	1:C:100:PHE:HD2	2.16	0.43
1:C:271:CYS:HB2	1:C:291:LEU:HD21	2.00	0.43
1:D:285:ILE:HG12	1:D:319:VAL:HG13	2.01	0.43
1:B:111:ASP:HB2	4:B:1476:HOH:O	2.19	0.43
1:C:291:LEU:HD12	1:C:291:LEU:C	2.44	0.42
1:D:43:LYS:HB2	1:D:45:LEU:HG	2.01	0.42
1:D:97:THR:HG22	1:D:138:VAL:HB	2.02	0.42
1:A:185:ARG:HD2	1:C:73(B)[B]:TYR:CD1	2.54	0.42
1:B:40:ILE:HG21	1:B:49:VAL:HG22	2.02	0.42
1:A:73(B)[B]:TYR:CD1	1:B:73(B)[B]:TYR:CE2	3.07	0.42
1:B:191:ILE:HA	1:B:200:VAL:O	2.20	0.42
1:D:81:SER:OG	1:D:87:ASP:OD2	2.24	0.42
1:B:309:ALA:O	1:B:313:THR:HG23	2.20	0.41
1:D:140:ASN:HA	1:D:141:PRO:C	2.45	0.41
1:B:43:LYS:HB2	1:B:45:LEU:HG	2.02	0.41
1:D:177:SER:CB	1:D:184:PRO:HA	2.50	0.41
1:D:191:ILE:O	1:D:270:VAL:HG11	2.21	0.41
1:C:73(B)[B]:TYR:HE2	1:D:73(B)[B]:TYR:HD2	1.63	0.41
1:A:113:LEU:HB3	1:A:329:ILE:HD11	2.03	0.41
1:A:267:LYS:HA	1:B:186:ASP:OD2	2.21	0.41
1:C:135:ILE:HG21	1:C:149:LEU:HD13	2.03	0.41
1:C:291:LEU:HD13	1:C:293:ILE:HD13	2.02	0.41
3:D:1403:AP0:H2	3:D:1403:AP0:H81	1.83	0.41
1:A:117:ASN:ND2	1:A:148:LEU:HG	2.35	0.40
1:B:52:PHE:CE2	3:B:1407:AP0:H111	2.56	0.40
1:C:243[B]:LEU:HD12	1:C:243[B]:LEU:HA	1.77	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	315/321 (98%)	296 (94%)	11 (4%)	8 (2%)	4 0
1	B	314/321 (98%)	302 (96%)	10 (3%)	2 (1%)	21 13
1	C	318/321 (99%)	294 (92%)	17 (5%)	7 (2%)	5 1
1	D	314/321 (98%)	291 (93%)	12 (4%)	11 (4%)	3 0
All	All	1261/1284 (98%)	1183 (94%)	50 (4%)	28 (2%)	5 1

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	103(C)	GLY
1	A	108	ASN
1	B	245	SER
1	C	20	LYS
1	C	101	THR
1	C	103(D)	LYS
1	C	109	ARG
1	D	19	PRO
1	D	100	PHE
1	D	111	ASP
1	D	112	LEU
1	D	328	LEU
1	A	103(D)	LYS
1	A	110	ASP
1	C	108	ASN
1	D	101	THR
1	D	107	TRP
1	D	108	ASN
1	D	99	GLY
1	D	109	ARG
1	D	164	GLY
1	A	164	GLY
1	C	164	GLY
1	A	103(B)	PRO
1	A	101	THR
1	B	164	GLY
1	C	19	PRO

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	269/273 (98%)	261 (97%)	8 (3%)	36	32
1	B	268/273 (98%)	258 (96%)	10 (4%)	30	25
1	C	272/273 (100%)	263 (97%)	9 (3%)	33	28
1	D	268/273 (98%)	257 (96%)	11 (4%)	27	21
All	All	1077/1092 (99%)	1039 (96%)	38 (4%)	32	27

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	TRP
1	A	148	LEU
1	A	188	ASN
1	A	190	LEU
1	A	198	LYS
1	A	237	LEU
1	A	291	LEU
1	A	313	THR
1	B	18	THR
1	B	109	ARG
1	B	148	LEU
1	B	181	ASN
1	B	188	ASN
1	B	245	SER
1	B	291	LEU
1	B	313	THR
1	B	314	LYS
1	B	328	LEU
1	C	100	PHE
1	C	102	LYS
1	C	108	ASN
1	C	109	ARG
1	C	111	ASP
1	C	148	LEU

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Mol	Chain	Res	Type
1	C	149	LEU
1	C	188	ASN
1	C	222	GLU
1	D	101	THR
1	D	109	ARG
1	D	110	ASP
1	D	129	ASN
1	D	148	LEU
1	D	149	LEU
1	D	157	LYS
1	D	237	LEU
1	D	243	LEU
1	D	283	ASN
1	D	329	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	117	ASN
1	A	132(B)	ASN
1	A	152	HIS
1	A	178	GLN
1	A	188	ASN
1	A	234	ASN
1	A	306	GLN
1	B	42	GLN
1	B	140	ASN
1	B	152	HIS
1	B	178	GLN
1	B	188	ASN
1	B	234	ASN
1	C	126	HIS
1	C	140	ASN
1	C	152	HIS
1	C	188	ASN
1	C	210(B)	GLN
1	C	214	ASN
1	C	234	ASN
1	C	332	HIS
1	D	117	ASN
1	D	132(B)	ASN

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Mol	Chain	Res	Type
1	D	188	ASN
1	D	234	ASN
1	D	306	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands 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
3	AP0	D	1403	-	47,48,48	2.25	9 (19%)	65,73,73	2.29	21 (32%)
3	AP0	C	1405	-	47,48,48	2.07	11 (23%)	65,73,73	2.22	21 (32%)
2	SO4	C	1002	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	A	1001	-	4,4,4	0.26	0	6,6,6	0.45	0
3	AP0	B	1407	-	47,48,48	2.26	11 (23%)	65,73,73	2.19	16 (24%)
3	AP0	A	1401	-	47,48,48	2.20	10 (21%)	65,73,73	2.55	21 (32%)

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	AP0	C	1405	-	2/2/13/16	4/30/72/72	0/5/5/5
3	AP0	A	1401	-	2/2/13/16	5/30/72/72	0/5/5/5
3	AP0	D	1403	-	2/2/13/16	3/30/72/72	0/5/5/5
3	AP0	B	1407	-	2/2/13/16	3/30/72/72	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1403	AP0	C8N-C7N	-7.86	1.34	1.50
3	B	1407	AP0	PN-O3	7.28	1.67	1.59
3	B	1407	AP0	C8N-C7N	-7.24	1.36	1.50
3	C	1405	AP0	C8N-C7N	-6.60	1.37	1.50
3	D	1403	AP0	C2D-C1D	-6.24	1.33	1.53
3	A	1401	AP0	C2D-C1D	-6.08	1.34	1.53
3	A	1401	AP0	C8N-C7N	-5.68	1.39	1.50
3	D	1403	AP0	C4N-C3N	-5.54	1.39	1.50
3	C	1405	AP0	C2D-C1D	-5.49	1.36	1.53
3	D	1403	AP0	PN-O3	5.28	1.65	1.59
3	A	1401	AP0	PN-O3	5.26	1.65	1.59
3	B	1407	AP0	C2D-C1D	-5.17	1.37	1.53
3	C	1405	AP0	C4N-C3N	-5.16	1.40	1.50
3	A	1401	AP0	O2D-C2D	-5.11	1.30	1.43
3	A	1401	AP0	C4N-C3N	-4.77	1.41	1.50
3	B	1407	AP0	C4N-C3N	-4.61	1.41	1.50
3	C	1405	AP0	PA-O3	4.33	1.64	1.59
3	A	1401	AP0	C4N-C5N	-4.33	1.37	1.49
3	B	1407	AP0	PA-O3	3.88	1.63	1.59
3	D	1403	AP0	O2D-C2D	-3.80	1.33	1.43
3	C	1405	AP0	O2D-C2D	-3.78	1.33	1.43
3	D	1403	AP0	C1D-N1N	-3.46	1.36	1.46
3	C	1405	AP0	C4N-C5N	-3.18	1.40	1.49
3	D	1403	AP0	C4N-C5N	-3.07	1.41	1.49
3	A	1401	AP0	C6N-C5N	3.04	1.42	1.33
3	C	1405	AP0	PN-O3	3.02	1.62	1.59
3	B	1407	AP0	C4N-C5N	-2.87	1.41	1.49
3	B	1407	AP0	O2D-C2D	-2.76	1.36	1.43
3	C	1405	AP0	C1D-N1N	-2.67	1.39	1.46
3	A	1401	AP0	C1D-N1N	-2.65	1.39	1.46
3	B	1407	AP0	C1D-N1N	-2.64	1.39	1.46
3	D	1403	AP0	C8A-N7A	2.61	1.36	1.31
3	B	1407	AP0	C6N-C5N	2.59	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	AP0	C8A-N7A	2.58	1.36	1.31
3	D	1403	AP0	C6N-C5N	2.43	1.40	1.33
3	B	1407	AP0	C8A-N7A	2.32	1.36	1.31
3	C	1405	AP0	C4A-N9A	-2.27	1.33	1.37
3	B	1407	AP0	C7N-C3N	2.25	1.52	1.48
3	A	1401	AP0	C4A-N9A	-2.05	1.33	1.37
3	C	1405	AP0	C5A-N7A	-2.05	1.35	1.39
3	C	1405	AP0	C8A-N7A	2.01	1.35	1.31

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401	AP0	C2D-C1D-N1N	7.89	132.71	113.31
3	A	1401	AP0	O7N-C7N-C3N	-7.53	112.62	119.67
3	B	1407	AP0	C2D-C1D-N1N	7.43	131.57	113.31
3	C	1405	AP0	C2D-C1D-N1N	7.39	131.48	113.31
3	D	1403	AP0	O4D-C1D-N1N	6.72	120.90	108.08
3	A	1401	AP0	C3D-C2D-C1D	6.70	114.13	101.46
3	D	1403	AP0	C2D-C1D-N1N	5.79	127.54	113.31
3	A	1401	AP0	O2D-C2D-C1D	5.63	129.49	110.10
3	C	1405	AP0	O2D-C2D-C1D	5.62	129.45	110.10
3	C	1405	AP0	C3D-C2D-C1D	5.43	111.74	101.46
3	B	1407	AP0	C5A-C4A-N3A	-5.29	119.43	126.72
3	D	1403	AP0	C3D-C2D-C1D	5.23	111.36	101.46
3	D	1403	AP0	C5A-C4A-N3A	-5.14	119.64	126.72
3	A	1401	AP0	O4D-C1D-N1N	5.03	117.68	108.08
3	B	1407	AP0	O2D-C2D-C1D	5.03	127.42	110.10
3	C	1405	AP0	O4D-C1D-N1N	4.85	117.34	108.08
3	A	1401	AP0	N1A-C2A-N3A	-4.80	121.31	128.58
3	B	1407	AP0	O4D-C1D-N1N	4.71	117.07	108.08
3	D	1403	AP0	O2D-C2D-C1D	4.66	126.16	110.10
3	C	1405	AP0	C5A-C4A-N3A	-4.63	120.34	126.72
3	A	1401	AP0	O3D-C3D-C2D	-4.61	97.05	111.82
3	D	1403	AP0	N1A-C2A-N3A	-4.59	121.63	128.58
3	C	1405	AP0	N1A-C2A-N3A	-4.54	121.72	128.58
3	B	1407	AP0	C3D-C2D-C1D	4.37	109.73	101.46
3	A	1401	AP0	C5A-C4A-N3A	-4.22	120.91	126.72
3	B	1407	AP0	N1A-C2A-N3A	-4.07	122.42	128.58
3	B	1407	AP0	N3A-C4A-N9A	3.97	133.92	127.17
3	A	1401	AP0	N9A-C8A-N7A	-3.80	108.54	113.94
3	D	1403	AP0	N9A-C8A-N7A	-3.75	108.62	113.94
3	B	1407	AP0	N9A-C8A-N7A	-3.66	108.75	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1403	AP0	C2A-N3A-C4A	3.56	120.53	111.83
3	D	1403	AP0	C4A-C5A-N7A	-3.33	106.78	110.58
3	D	1403	AP0	O2D-C2D-C3D	3.33	122.48	111.82
3	B	1407	AP0	O2D-C2D-C3D	3.32	122.47	111.82
3	D	1403	AP0	O4B-C1B-N9A	3.32	114.46	108.09
3	B	1407	AP0	O3D-C3D-C2D	-3.27	101.34	111.82
3	C	1405	AP0	C2A-N3A-C4A	3.24	119.75	111.83
3	C	1405	AP0	N9A-C8A-N7A	-3.17	109.44	113.94
3	A	1401	AP0	C4A-C5A-N7A	-3.15	106.98	110.58
3	D	1403	AP0	O3D-C3D-C2D	-3.05	102.04	111.82
3	B	1407	AP0	C2A-N3A-C4A	3.04	119.27	111.83
3	D	1403	AP0	C5A-N7A-C8A	3.02	108.20	103.45
3	B	1407	AP0	C4A-N9A-C8A	3.01	108.90	105.74
3	A	1401	AP0	C5A-N7A-C8A	2.93	108.06	103.45
3	B	1407	AP0	C5A-N7A-C8A	2.92	108.05	103.45
3	C	1405	AP0	N3A-C4A-N9A	2.90	132.10	127.17
3	D	1403	AP0	N3A-C4A-N9A	2.87	132.04	127.17
3	C	1405	AP0	O3D-C3D-C2D	-2.77	102.94	111.82
3	A	1401	AP0	C4A-N9A-C1B	-2.76	120.17	126.63
3	D	1403	AP0	O7N-C7N-C3N	-2.72	117.12	119.67
3	A	1401	AP0	C2A-N1A-C6A	2.71	123.18	118.73
3	D	1403	AP0	C6N-N1N-C2N	2.71	122.22	119.32
3	D	1403	AP0	C3N-C2N-N1N	-2.70	119.23	123.20
3	A	1401	AP0	O2N-PN-O1N	2.66	124.80	112.44
3	B	1407	AP0	O4B-C1B-N9A	2.64	113.16	108.09
3	A	1401	AP0	C2A-N3A-C4A	2.61	118.20	111.83
3	B	1407	AP0	C4A-C5A-N7A	-2.57	107.64	110.58
3	A	1401	AP0	C3N-C2N-N1N	-2.53	119.49	123.20
3	D	1403	AP0	O2N-PN-O1N	2.53	124.21	112.44
3	C	1405	AP0	C3N-C2N-N1N	-2.53	119.49	123.20
3	A	1401	AP0	C4A-N9A-C8A	2.51	108.38	105.74
3	A	1401	AP0	C8N-C7N-C3N	2.50	123.45	120.22
3	C	1405	AP0	C1D-N1N-C6N	-2.49	115.50	120.77
3	C	1405	AP0	O7N-C7N-C3N	-2.42	117.40	119.67
3	C	1405	AP0	O4B-C1B-C2B	-2.32	101.65	106.62
3	A	1401	AP0	N3A-C4A-N9A	2.30	131.08	127.17
3	D	1403	AP0	C5A-C4A-N9A	2.29	108.31	105.81
3	C	1405	AP0	C5A-N7A-C8A	2.27	107.01	103.45
3	C	1405	AP0	C4A-C5A-N7A	-2.25	108.01	110.58
3	D	1403	AP0	C4A-N9A-C8A	2.24	108.09	105.74
3	D	1403	AP0	C1D-N1N-C6N	-2.21	116.10	120.77
3	C	1405	AP0	O4B-C1B-N9A	2.19	112.29	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1405	AP0	O2D-C2D-C3D	2.17	118.76	111.82
3	A	1401	AP0	O4B-C1B-N9A	2.16	112.25	108.09
3	C	1405	AP0	O2N-PN-O1N	2.16	122.50	112.44
3	C	1405	AP0	C4A-N9A-C8A	2.11	107.95	105.74
3	B	1407	AP0	O4D-C1D-C2D	2.05	111.01	106.62
3	C	1405	AP0	C6N-N1N-C2N	2.03	121.49	119.32
3	A	1401	AP0	C5A-C4A-N9A	2.01	108.00	105.81

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1401	AP0	C2D
3	A	1401	AP0	C1D
3	B	1407	AP0	C2D
3	B	1407	AP0	C1D
3	C	1405	AP0	C2D
3	C	1405	AP0	C1D
3	D	1403	AP0	C2D
3	D	1403	AP0	C1D

All (15) torsion outliers are listed below:

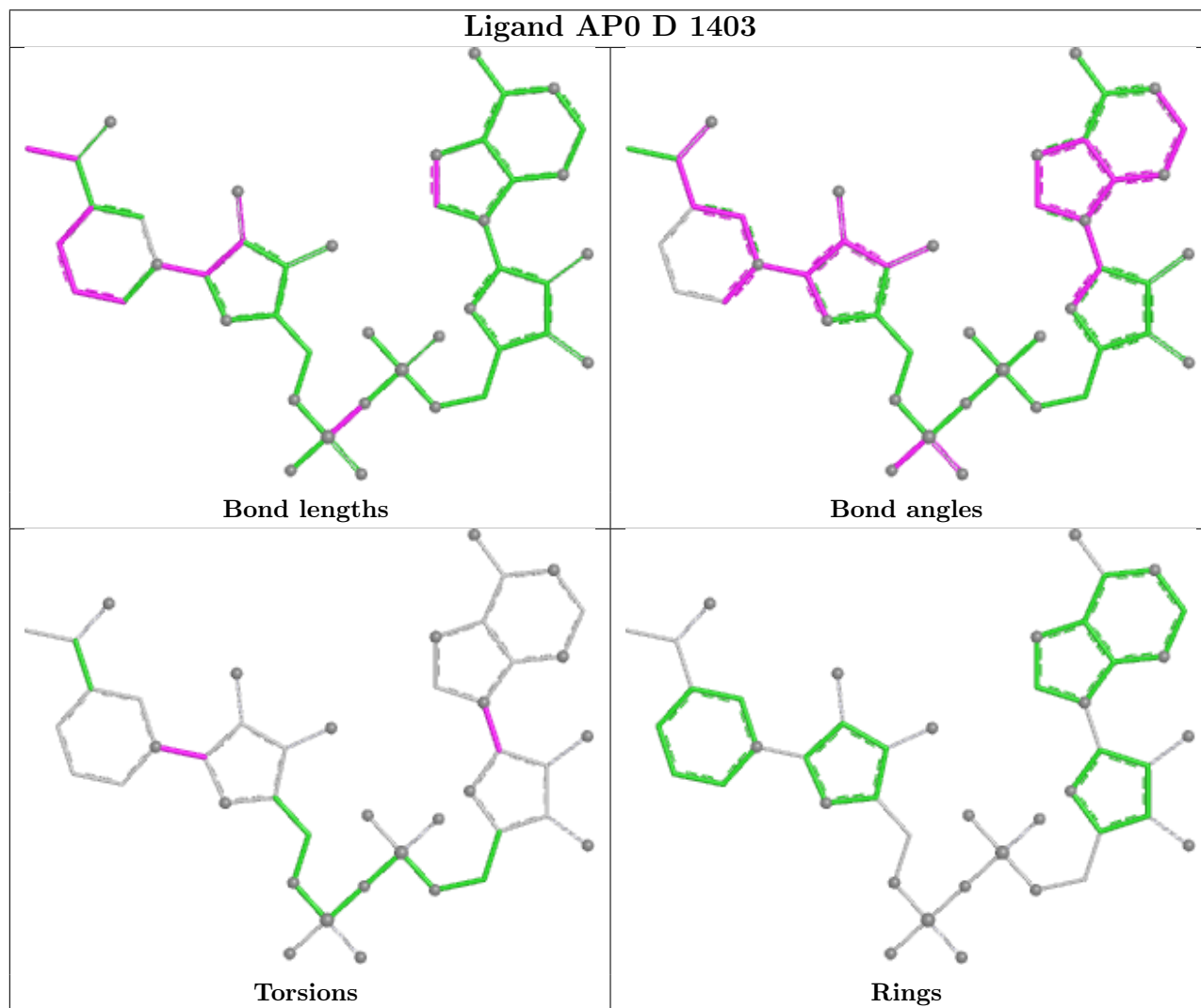
Mol	Chain	Res	Type	Atoms
3	C	1405	AP0	O4D-C1D-N1N-C6N
3	D	1403	AP0	O4D-C1D-N1N-C6N
3	A	1401	AP0	C2B-C1B-N9A-C8A
3	C	1405	AP0	C2B-C1B-N9A-C8A
3	A	1401	AP0	O4D-C1D-N1N-C2N
3	D	1403	AP0	O4D-C1D-N1N-C2N
3	A	1401	AP0	O4D-C1D-N1N-C6N
3	B	1407	AP0	O4D-C1D-N1N-C6N
3	C	1405	AP0	O4D-C1D-N1N-C2N
3	B	1407	AP0	O4D-C1D-N1N-C2N
3	A	1401	AP0	O4B-C1B-N9A-C8A
3	C	1405	AP0	O4B-C1B-N9A-C8A
3	A	1401	AP0	O4B-C4B-C5B-O5B
3	D	1403	AP0	C2B-C1B-N9A-C8A
3	B	1407	AP0	C2B-C1B-N9A-C8A

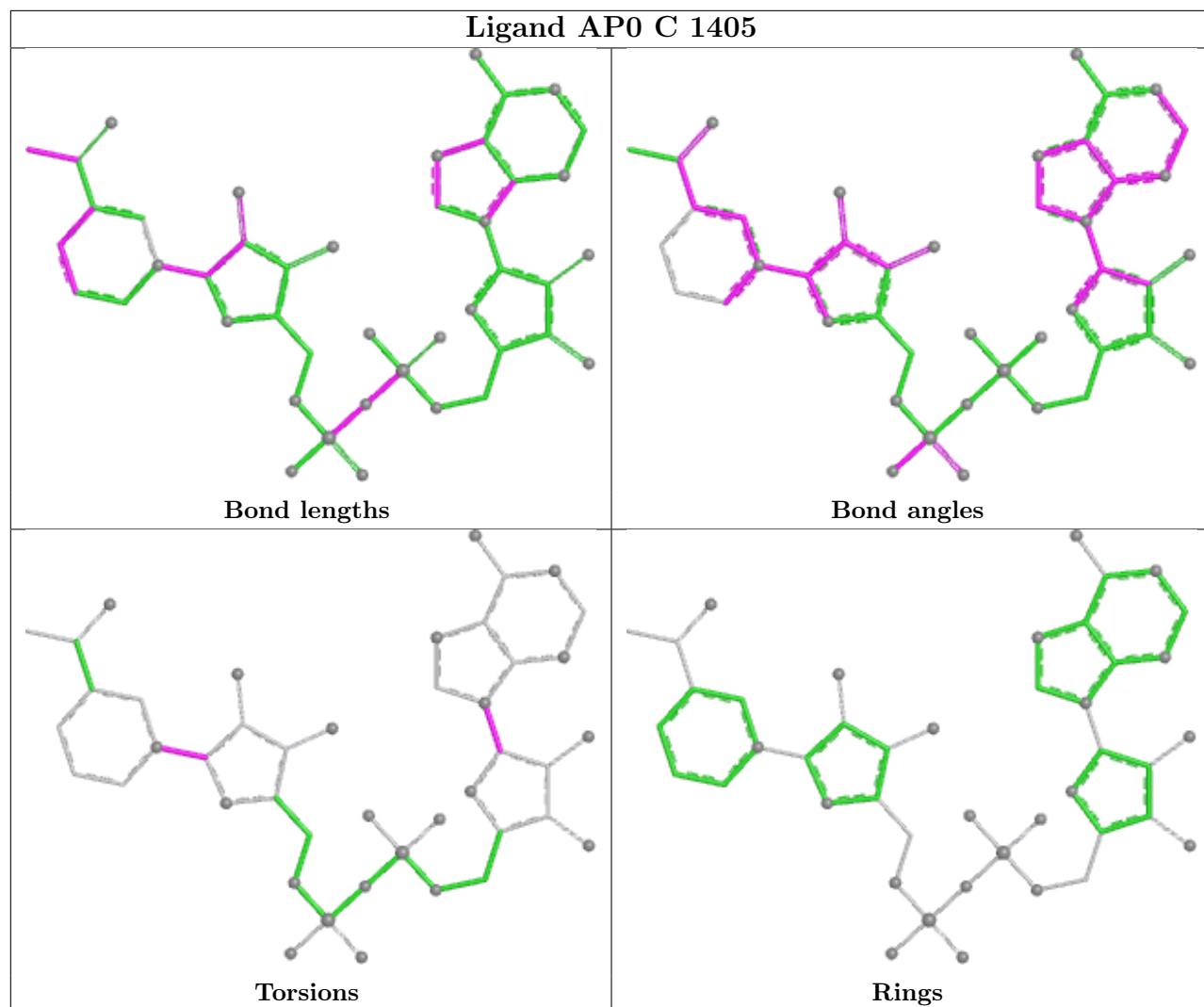
There are no ring outliers.

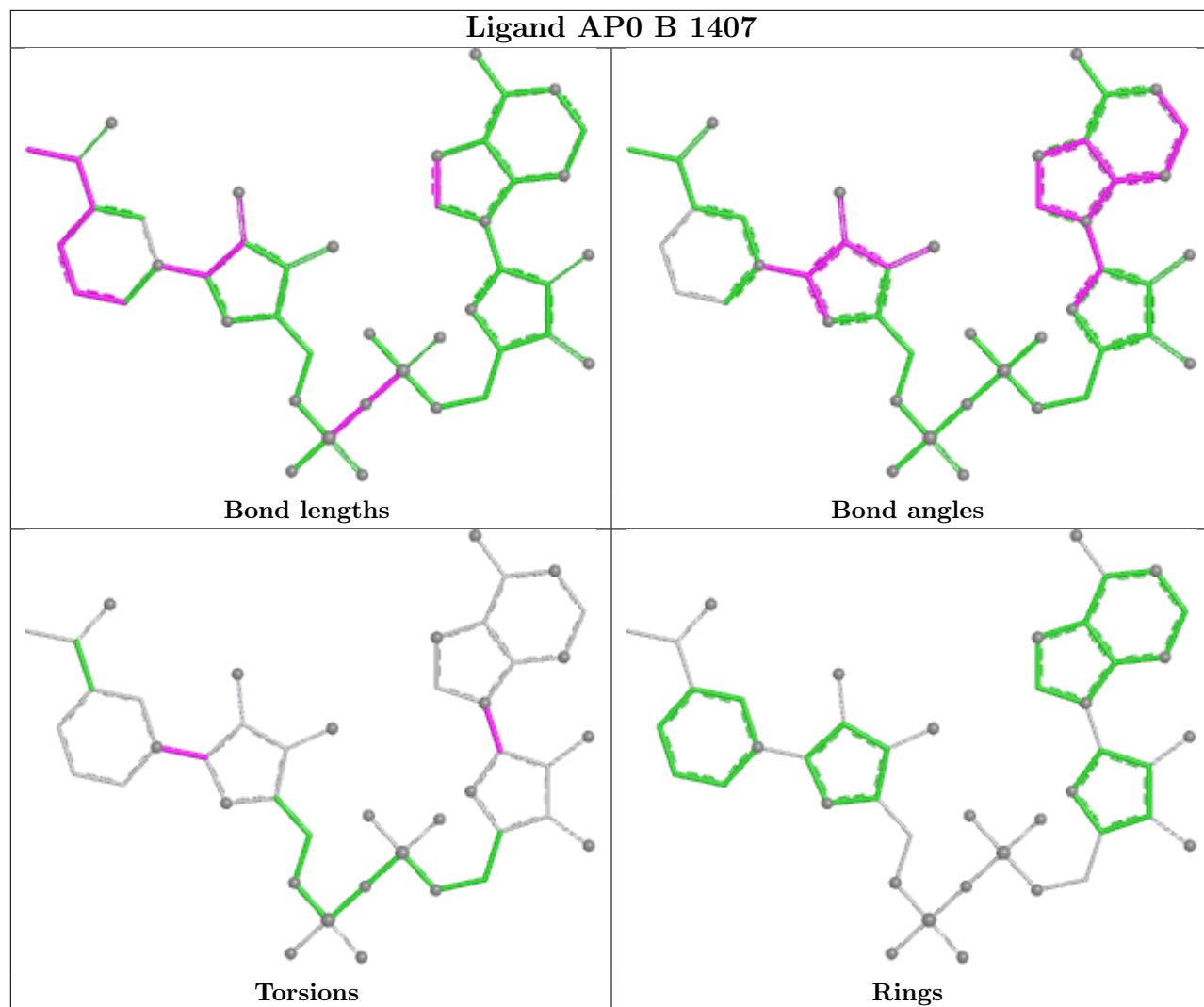
2 monomers are involved in 3 short contacts:

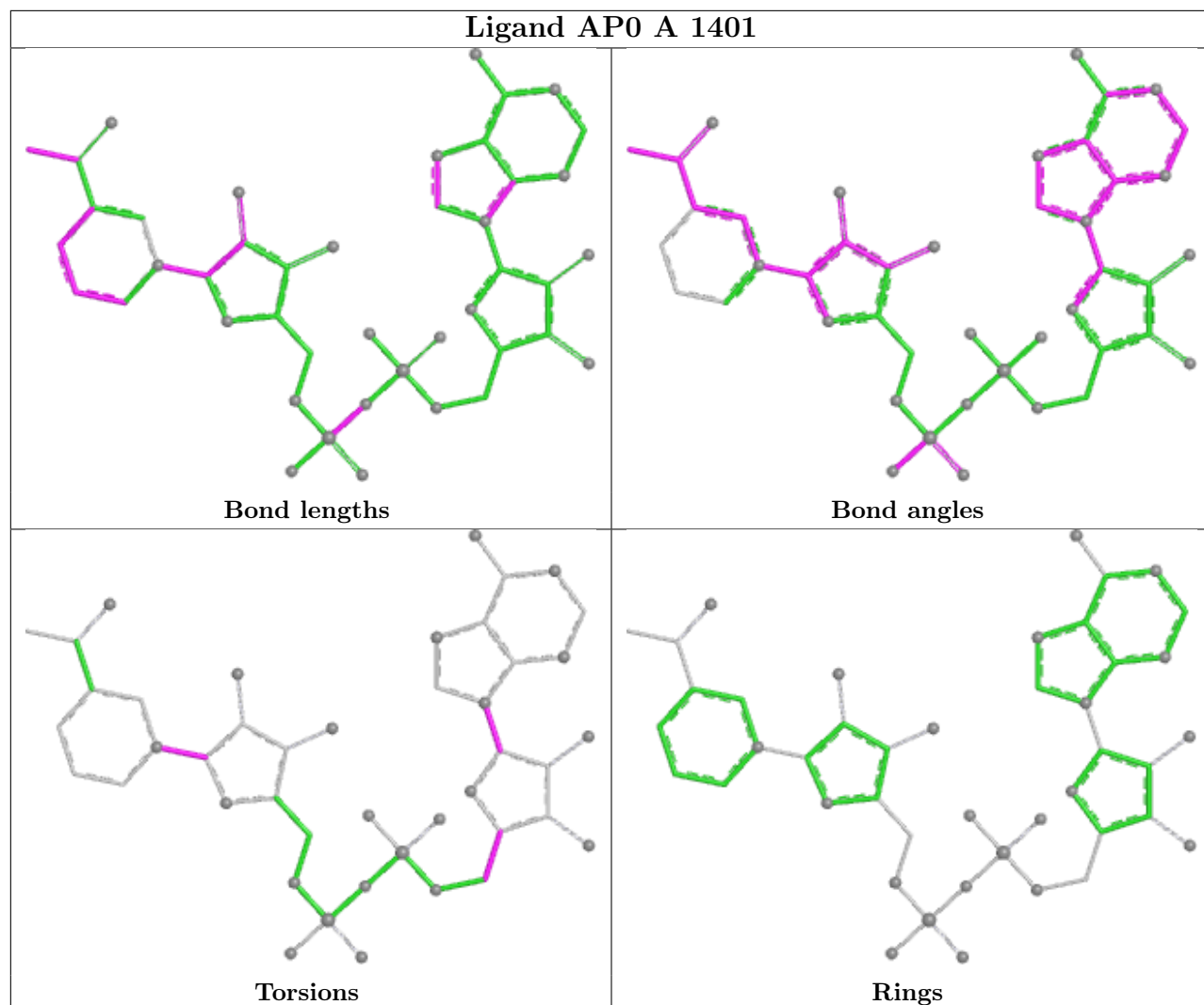
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1403	AP0	2	0
3	B	1407	AP0	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/321 (94%)	-0.31	10 (3%) 49 49	7, 16, 28, 43	20 (6%)
1	B	315/321 (98%)	-0.13	17 (5%) 31 31	7, 18, 31, 40	33 (10%)
1	C	304/321 (94%)	-0.11	20 (6%) 24 24	4, 19, 29, 42	38 (12%)
1	D	300/321 (93%)	0.56	34 (11%) 10 9	2, 22, 38, 49	41 (13%)
All	All	1222/1284 (95%)	0.00	81 (6%) 24 24	2, 19, 34, 49	132 (10%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	LEU	22.5
1	D	111	ASP	17.7
1	D	18	THR	10.4
1	D	118	LYS	8.3
1	D	326	LYS	8.1
1	A	109	ARG	7.7
1	B	19	PRO	6.9
1	D	328	LEU	6.5
1	D	128	LYS	6.5
1	A	18	THR	6.4
1	C	216	LYS	6.4
1	B	18	THR	6.3
1	C	18	THR	6.1
1	C	110	ASP	6.0
1	D	323	LYS	5.8
1	A	19	PRO	5.8
1	C	19	PRO	5.7
1	D	215	ASN	5.6
1	D	329	ILE	5.6
1	D	310	GLU	5.5
1	D	312	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	216	LYS	5.3
1	D	19	PRO	5.2
1	D	327	ALA	5.1
1	D	113	LEU	4.9
1	C	222	GLU	4.8
1	D	115	LEU	4.6
1	D	198	LYS	4.5
1	D	216	LYS	4.5
1	C	100	PHE	4.3
1	B	115	LEU	4.1
1	C	332	HIS	4.0
1	A	115	LEU	3.9
1	A	330	HIS	3.8
1	B	312	LYS	3.7
1	C	329	ILE	3.7
1	D	86	ASP	3.6
1	C	244	ALA	3.5
1	C	115	LEU	3.5
1	D	114	PRO	3.3
1	A	111	ASP	3.2
1	B	103(E)	SER	3.2
1	B	222	GLU	3.2
1	D	203	LYS	3.2
1	B	197	ASN	3.2
1	C	312	LYS	3.1
1	D	280	GLY	3.1
1	D	222	GLU	3.1
1	C	243[A]	LEU	3.0
1	C	112	LEU	2.9
1	B	118	LYS	2.9
1	C	132(B)	ASN	2.9
1	D	151	GLU	2.8
1	A	310	GLU	2.7
1	D	313	THR	2.7
1	B	226	GLU	2.6
1	B	106	GLU	2.6
1	C	56	LYS	2.6
1	A	110	ASP	2.6
1	C	331	HIS	2.5
1	C	118	LYS	2.5
1	C	245	SER	2.4
1	D	117	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	329	ILE	2.3
1	D	56	LYS	2.3
1	B	245	SER	2.3
1	B	100	PHE	2.3
1	B	107	TRP	2.3
1	B	101	THR	2.2
1	D	54	VAL	2.2
1	D	302	VAL	2.2
1	C	230	ASP	2.2
1	A	323	LYS	2.2
1	D	99	GLY	2.2
1	D	226	GLU	2.2
1	B	218	LYS	2.2
1	C	20	LYS	2.1
1	D	243	LEU	2.1
1	A	222	GLU	2.1
1	D	160	ILE	2.1
1	D	121	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

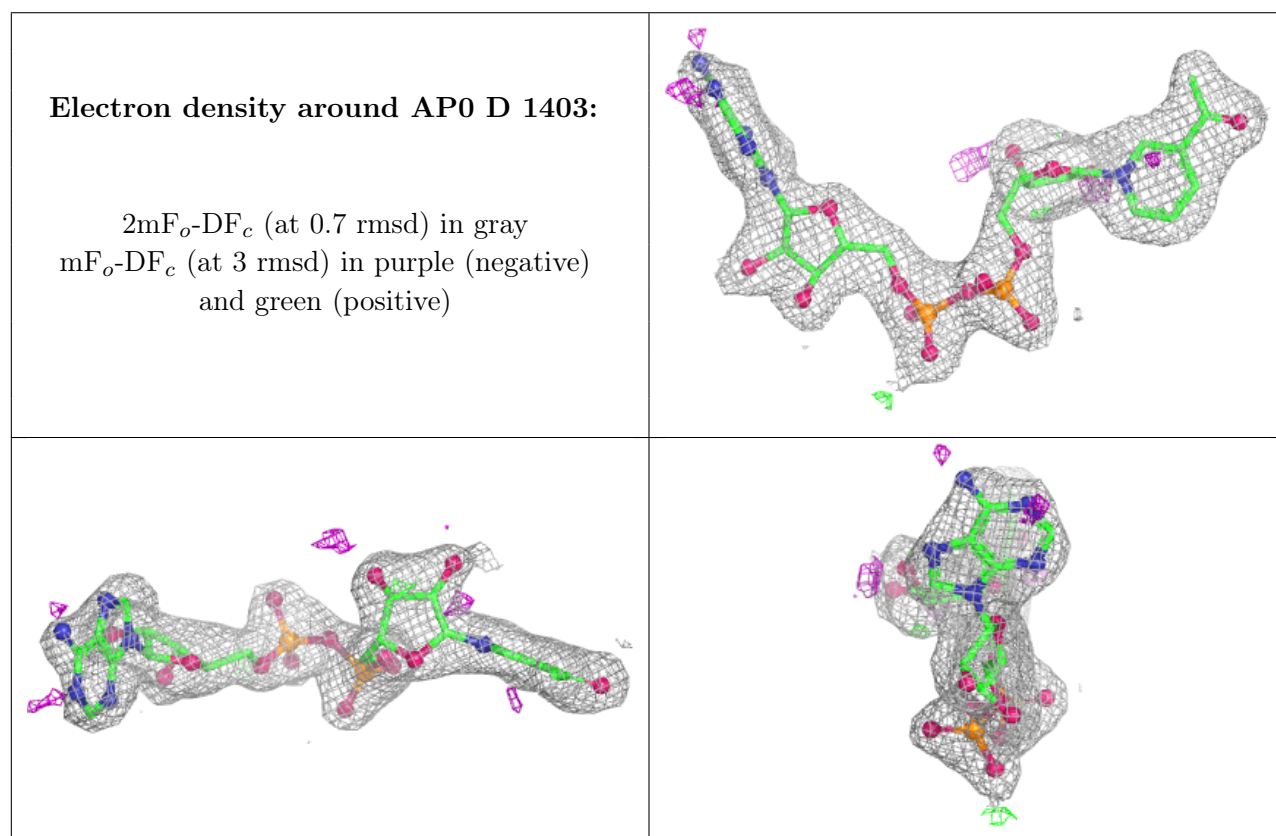
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	C	1002	5/5	0.84	0.14	35,38,39,40	5
2	SO4	A	1001	5/5	0.91	0.13	29,29,31,32	5
3	AP0	D	1403	44/44	0.94	0.09	24,31,38,39	0
3	AP0	C	1405	44/44	0.96	0.07	14,22,28,33	0
3	AP0	B	1407	44/44	0.96	0.07	17,23,34,36	0

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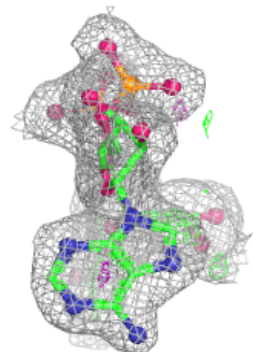
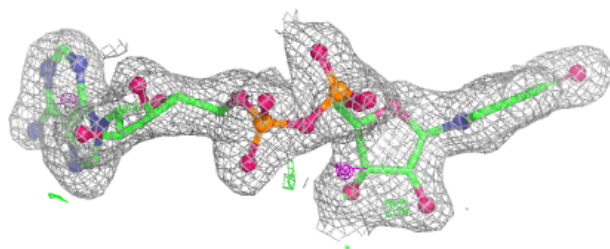
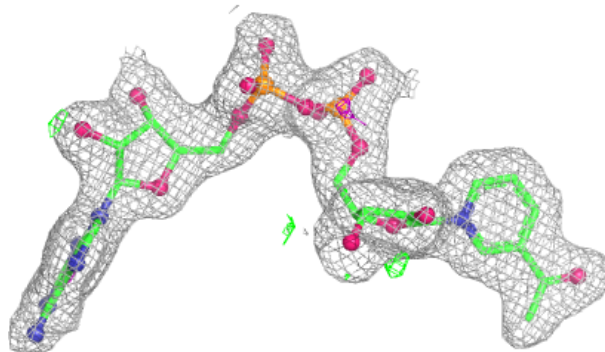
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AP0	A	1401	44/44	0.97	0.06	14,19,27,28	0

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.

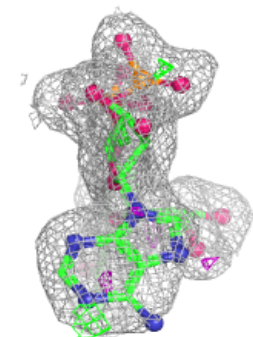
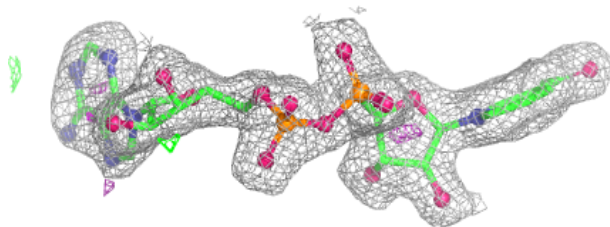
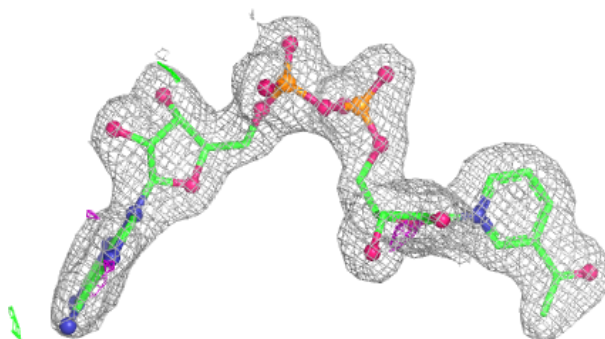


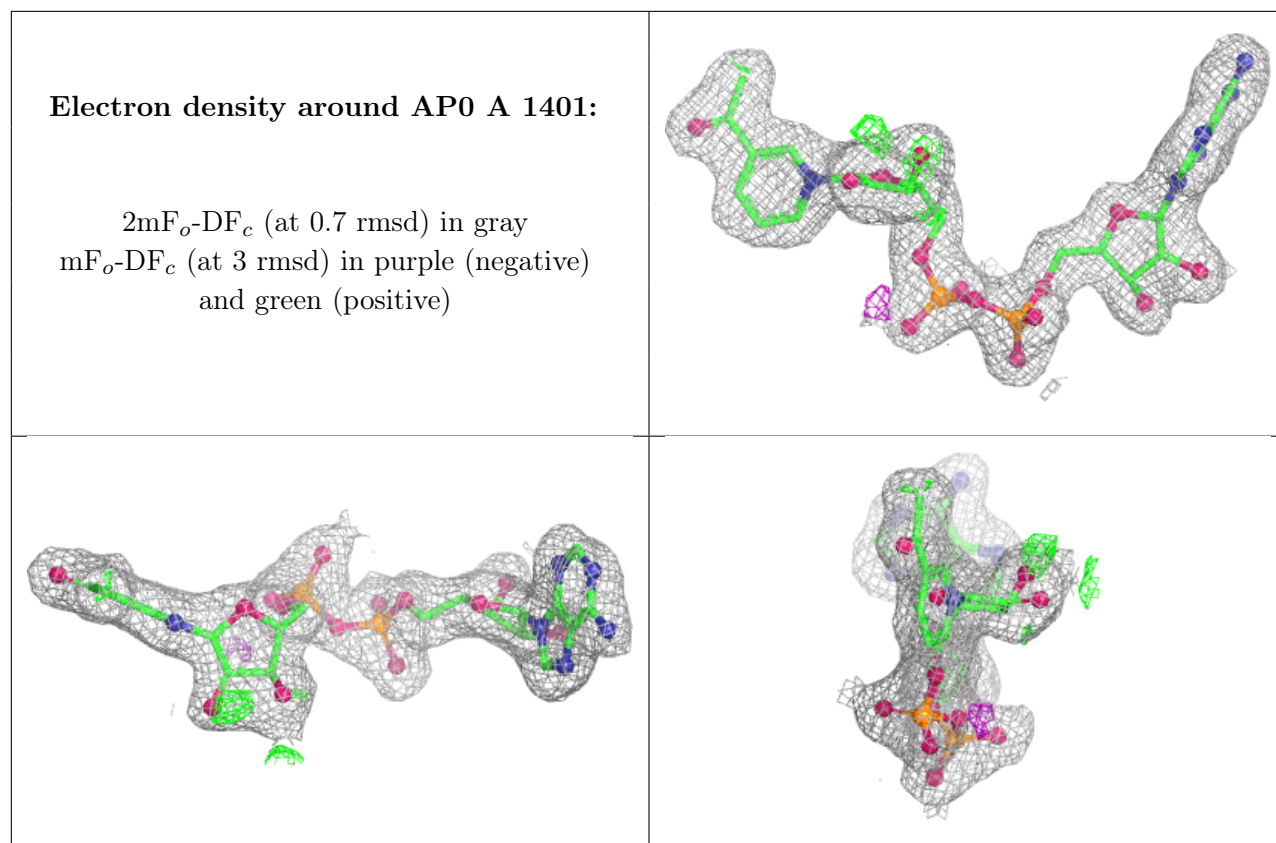
Electron density around AP0 C 1405:

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

**Electron density around AP0 B 1407:**

$2mF_o-DF_c$ (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.