



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:13 AM UTC

PDB ID : 2Y0P / pdb_00002y0p
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis alpha-ketoglutarate decarboxylase in complex with the enamine-ThDP intermediate and acetyl-CoA
Authors : Wagner, T.; Bellinzoni, M.; Wehenkel, A.M.; O'Hare, H.M.; Alzari, P.M.
Deposited on : 2010-12-07
Resolution : 2.40 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

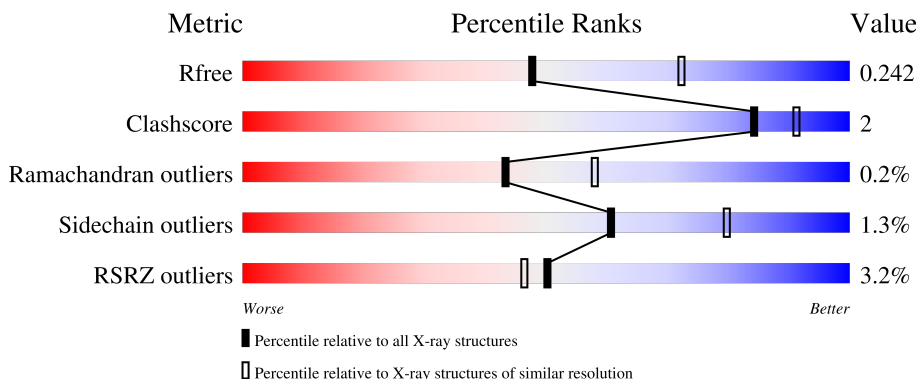
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

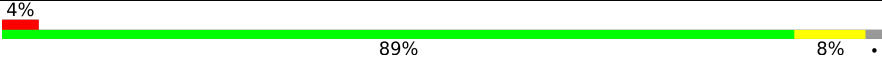
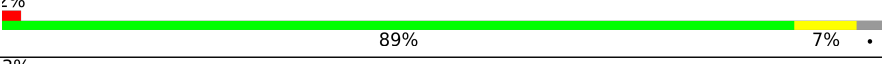
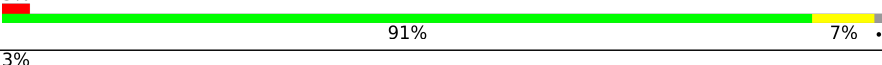
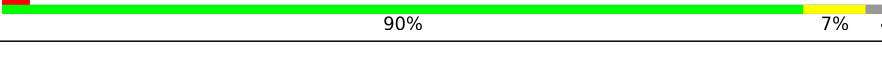
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	868	
1	B	868	
1	C	868	
1	D	868	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26809 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 2-OXOGLUTARATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	847	Total	C	N	O	S	0	0	0
			6518	4102	1151	1241	24			
1	B	839	Total	C	N	O	S	0	0	0
			6459	4065	1136	1234	24			
1	C	856	Total	C	N	O	S	0	0	0
			6577	4142	1157	1254	24			
1	D	837	Total	C	N	O	S	0	0	0
			6414	4043	1128	1219	24			

There are 4 discrepancies between the modelled and reference sequences:

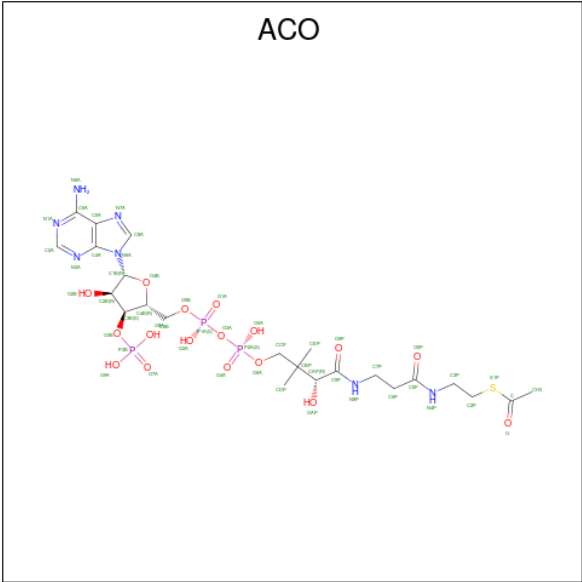
Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is (4E)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3-thiazol-2(3H)-ylidene}-4-hydroxybutanoic acid (CCD ID: TD7) (formula: C₁₆H₂₄N₄O₁₀P₂S).



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

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	D	1	Total	C	N	O	P		0	0
			38	16	5	14	3			

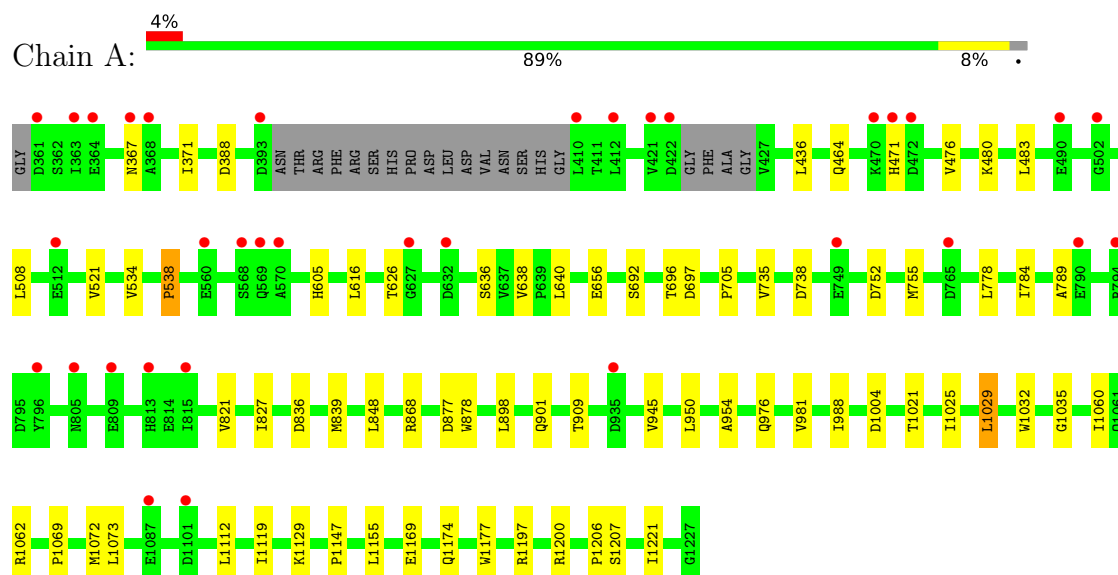
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	134	Total	O	0	0
			134	134		
5	B	143	Total	O	0	0
			143	143		
5	C	119	Total	O	0	0
			119	119		
5	D	118	Total	O	0	0
			118	118		

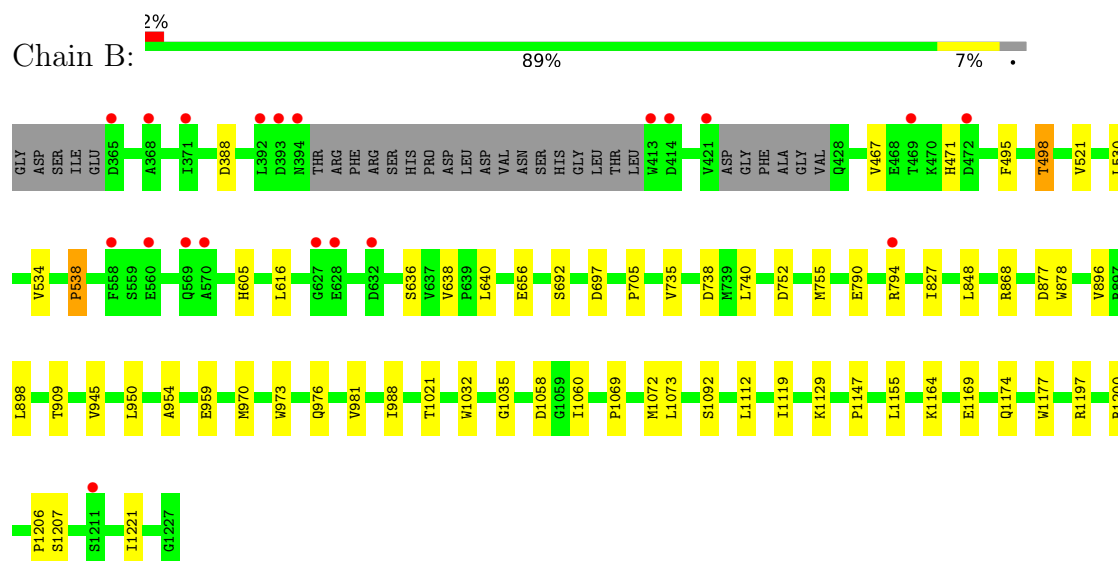
3 Residue-property plots [i](#)

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.

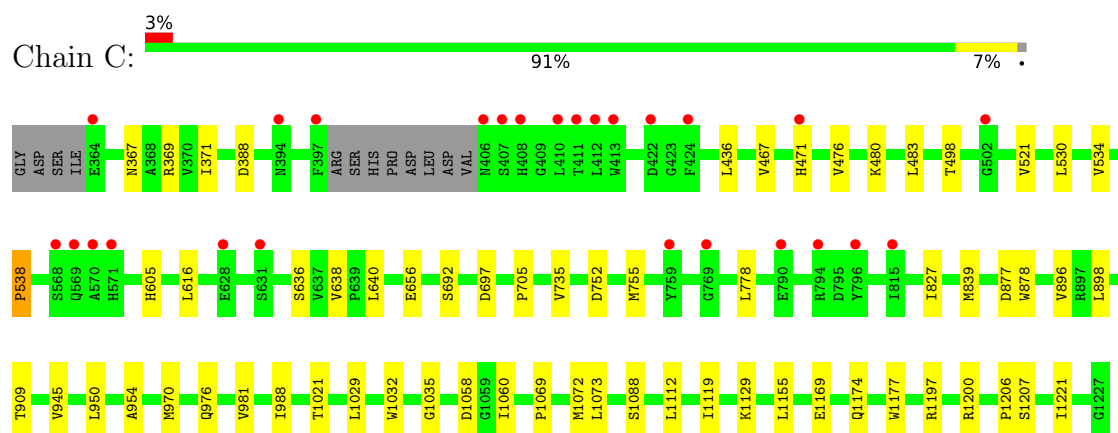
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



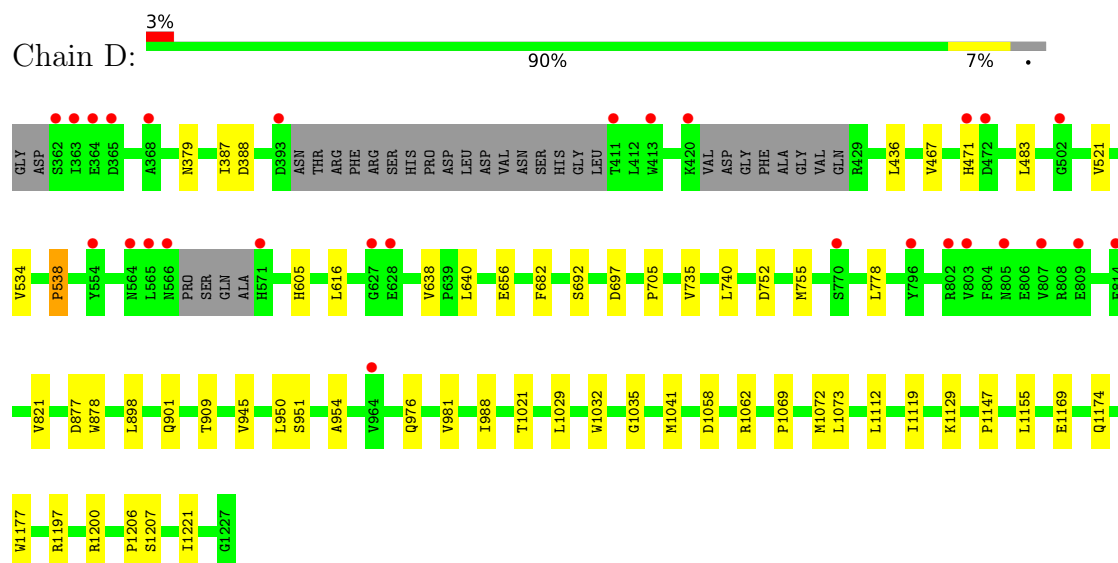
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.06Å 81.95Å 161.88Å 99.26° 97.09° 100.58°	Depositor
Resolution (Å)	35.14 – 2.40 35.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.8 (35.14-2.40) 95.8 (35.14-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.197 , 0.220 0.216 , 0.242	Depositor DCC
R_{free} test set	7517 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26809	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TD7, ACO, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	0/6650	1.24	7/9024 (0.1%)
1	B	0.75	0/6592	1.24	7/8949 (0.1%)
1	C	0.75	0/6713	1.24	4/9112 (0.0%)
1	D	0.74	0/6545	1.24	8/8885 (0.1%)
All	All	0.75	0/26500	1.24	26/35970 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	538	PRO	CA-C-N	6.12	128.98	120.29
1	D	538	PRO	C-N-CA	6.12	128.98	120.29
1	A	836	ASP	CA-CB-CG	5.91	118.51	112.60
1	D	388	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	388	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	388	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	379	ASN	CA-CB-CG	5.56	118.16	112.60
1	C	877	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	877	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	877	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	638	VAL	N-CA-C	5.33	113.74	107.77
1	C	638	VAL	N-CA-C	5.32	113.73	107.77
1	B	738	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	877	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	1058	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	538	PRO	CA-C-N	5.10	129.31	120.58
1	A	538	PRO	C-N-CA	5.10	129.31	120.58
1	D	638	VAL	N-CA-C	5.10	113.49	107.77
1	C	1058	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	1058	ASP	CA-CB-CG	5.06	117.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	VAL	N-CA-C	5.04	113.41	107.77
1	A	1004	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	682	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	538	PRO	CA-C-N	5.01	127.93	120.31
1	B	538	PRO	C-N-CA	5.01	127.93	120.31
1	C	388	ASP	CA-CB-CG	5.01	117.61	112.60

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	6518	0	6282	34	0
1	B	6459	0	6214	30	0
1	C	6577	0	6326	27	0
1	D	6414	0	6166	26	0
2	A	33	0	20	1	0
2	B	33	0	20	2	0
2	C	33	0	20	2	0
2	D	33	0	20	1	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
4	A	51	0	34	1	0
4	B	51	0	34	0	0
4	C	51	0	34	0	0
4	D	38	0	21	1	0
5	A	134	0	0	0	0
5	B	143	0	0	0	0
5	C	119	0	0	1	0
5	D	118	0	0	1	0
All	All	26809	0	25191	117	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 2.

All (117) 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:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.75	0.67
1:C:752:ASP:HB3	1:C:755:MET:HE2	1.81	0.63
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.81	0.63
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.81	0.62
1:D:752:ASP:HB3	1:D:755:MET:HE2	1.82	0.62
1:B:752:ASP:HB3	1:B:755:MET:HE2	1.82	0.61
1:C:827:ILE:HA	1:C:1060:ILE:HD11	1.82	0.60
2:A:2001:TD7:C11	2:A:2001:TD7:H4'1	2.15	0.59
1:B:848:LEU:HD12	1:B:868:ARG:HD3	1.84	0.59
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.83	0.59
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.84	0.59
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.85	0.59
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.85	0.59
2:C:2001:TD7:C11	2:C:2001:TD7:H4'1	2.16	0.59
2:D:2001:TD7:C11	2:D:2001:TD7:H4'1	2.15	0.58
2:B:2001:TD7:H4'1	2:B:2001:TD7:C11	2.16	0.58
1:A:1032:TRP:CZ2	1:A:1035:GLY:HA2	2.39	0.58
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.87	0.57
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	1.88	0.56
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	1.88	0.56
1:A:752:ASP:HB3	1:A:755:MET:HE2	1.87	0.55
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	1.88	0.55
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	1.89	0.54
1:A:839:MET:HE3	1:A:839:MET:HA	1.91	0.52
1:B:1032:TRP:CZ2	1:B:1035:GLY:HA2	2.44	0.52
1:D:705:PRO:HG2	1:D:735:VAL:HG13	1.91	0.52
1:A:705:PRO:HG2	1:A:735:VAL:HG13	1.91	0.51
1:C:534:VAL:HG11	1:C:616:LEU:HD23	1.92	0.51
1:B:705:PRO:HG2	1:B:735:VAL:HG13	1.92	0.51
1:C:705:PRO:HG2	1:C:735:VAL:HG13	1.93	0.51
1:D:534:VAL:HG11	1:D:616:LEU:HD23	1.94	0.50
1:A:534:VAL:HG11	1:A:616:LEU:HD23	1.93	0.50
1:D:483:LEU:HD22	1:D:778:LEU:HD12	1.94	0.50
1:D:1041:MET:HE1	5:D:2106:HOH:O	2.11	0.50
1:B:534:VAL:HG11	1:B:616:LEU:HD23	1.93	0.49
1:C:530:LEU:HD22	1:C:636:SER:HA	1.94	0.49
1:A:656:GLU:HB3	1:A:954:ALA:HB2	1.95	0.49
1:B:656:GLU:HB3	1:B:954:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:THR:HG21	1:A:1207:SER:HB3	1.95	0.48
1:D:1147:PRO:HA	4:D:2228:ACO:H143	1.96	0.48
1:C:656:GLU:HB3	1:C:954:ALA:HB2	1.94	0.48
1:D:1021:THR:HG21	1:D:1207:SER:HB3	1.95	0.48
1:A:909:THR:HG21	1:B:755:MET:HE1	1.96	0.47
1:B:1021:THR:HG21	1:B:1207:SER:HB3	1.96	0.47
1:D:898:LEU:O	1:D:945:VAL:HA	2.15	0.47
1:C:909:THR:HG21	1:D:755:MET:HE1	1.97	0.47
1:D:656:GLU:HB3	1:D:954:ALA:HB2	1.96	0.47
1:A:898:LEU:O	1:A:945:VAL:HA	2.15	0.47
1:C:1119:ILE:HD12	1:C:1169:GLU:HG2	1.96	0.47
1:B:1119:ILE:HD12	1:B:1169:GLU:HG2	1.97	0.47
1:C:1021:THR:HG21	1:C:1207:SER:HB3	1.96	0.46
1:A:626:THR:HG21	1:A:636:SER:OG	2.16	0.46
1:B:1200:ARG:HG3	1:B:1221:ILE:HD11	1.98	0.46
1:B:898:LEU:O	1:B:945:VAL:HA	2.16	0.46
1:B:790:GLU:O	1:B:794:ARG:HG2	2.15	0.46
1:C:755:MET:HE1	1:D:909:THR:HG21	1.98	0.46
1:A:755:MET:HE1	1:B:909:THR:HG21	1.96	0.46
1:D:1119:ILE:HD12	1:D:1169:GLU:HG2	1.98	0.46
1:A:1025:ILE:HG22	1:A:1029:LEU:HD22	1.98	0.46
1:C:898:LEU:O	1:C:945:VAL:HA	2.16	0.45
1:D:1200:ARG:HG3	1:D:1221:ILE:HD11	1.98	0.45
1:A:1119:ILE:HD12	1:A:1169:GLU:HG2	1.98	0.45
1:C:538:PRO:HD2	5:C:2012:HOH:O	2.17	0.45
1:C:1032:TRP:CZ2	1:C:1035:GLY:HA2	2.51	0.45
1:C:1174:GLN:OE1	1:C:1206:PRO:HA	2.17	0.45
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.46	0.45
1:A:483:LEU:HD22	1:A:778:LEU:HD12	1.99	0.44
1:A:1174:GLN:OE1	1:A:1206:PRO:HA	2.17	0.44
1:A:1069:PRO:CB	1:A:1072:MET:HB3	2.47	0.44
1:A:1200:ARG:HG3	1:A:1221:ILE:HD11	1.99	0.44
1:B:1174:GLN:OE1	1:B:1206:PRO:HA	2.17	0.44
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.18	0.44
1:A:784:ILE:HD12	1:A:789:ALA:HB2	1.99	0.44
1:A:821:VAL:O	1:A:1062:ARG:NH2	2.50	0.44
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.47	0.44
1:C:1200:ARG:HG3	1:C:1221:ILE:HD11	1.98	0.44
1:D:821:VAL:O	1:D:1062:ARG:NH2	2.51	0.44
1:D:1174:GLN:OE1	1:D:1206:PRO:HA	2.17	0.44
1:B:1069:PRO:CB	1:B:1072:MET:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1112:LEU:HB3	1:B:1164:LYS:HG2	2.00	0.43
1:A:878:TRP:HB3	1:A:1073:LEU:HD23	2.01	0.43
1:A:1147:PRO:HA	4:A:2228:ACO:H143	1.99	0.43
1:B:521:VAL:HG11	1:B:640:LEU:HD13	2.00	0.43
1:D:692:SER:HB2	1:D:697:ASP:OD2	2.18	0.43
1:A:508:LEU:O	1:A:508:LEU:HG	2.18	0.43
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.19	0.42
1:D:387:ILE:HD12	1:D:740:LEU:HD12	2.01	0.42
1:D:1032:TRP:CZ2	1:D:1035:GLY:HA2	2.54	0.42
1:A:827:ILE:HA	1:A:1060:ILE:HD11	2.01	0.42
1:A:476:VAL:HG12	1:A:480:LYS:HE3	2.01	0.42
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.55	0.42
2:C:2001:TD7:H6'	1:D:901:GLN:OE1	2.20	0.42
1:C:521:VAL:HG11	1:C:640:LEU:HD13	2.02	0.42
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.20	0.41
1:B:896:VAL:HG22	1:B:970:MET:HB3	2.02	0.41
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.55	0.41
1:A:901:GLN:OE1	2:B:2001:TD7:H6'	2.21	0.41
1:D:878:TRP:HB3	1:D:1073:LEU:HD23	2.03	0.41
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.56	0.41
1:B:1092:SER:HB2	1:B:1147:PRO:HG3	2.03	0.41
1:B:530:LEU:HD22	1:B:636:SER:HA	2.01	0.41
1:C:476:VAL:HG12	1:C:480:LYS:HE3	2.02	0.41
1:C:839:MET:HA	1:C:839:MET:HE3	2.03	0.41
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.02	0.41
1:A:521:VAL:HG11	1:A:640:LEU:HD13	2.03	0.41
1:C:878:TRP:HB3	1:C:1073:LEU:HD23	2.02	0.41
1:C:896:VAL:HG22	1:C:970:MET:HB3	2.03	0.41
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.56	0.40
1:B:959:GLU:HG3	1:B:973:TRP:HB2	2.03	0.40
1:B:827:ILE:HA	1:B:1060:ILE:HD11	2.02	0.40
1:C:483:LEU:HD22	1:C:778:LEU:HD12	2.02	0.40
1:A:1029:LEU:HD12	1:A:1029:LEU:HA	1.93	0.40
1:B:878:TRP:HB3	1:B:1073:LEU:HD23	2.02	0.40
1:A:848:LEU:HD12	1:A:868:ARG:HD2	2.04	0.40
1:B:495:PHE:O	1:B:498:THR:HG22	2.21	0.40
1:B:740:LEU:HD23	1:B:740:LEU:HA	1.99	0.40
1:D:521:VAL:HG11	1:D:640:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	841/868 (97%)	817 (97%)	22 (3%)	2 (0%)	43	58
1	B	833/868 (96%)	808 (97%)	23 (3%)	2 (0%)	43	58
1	C	852/868 (98%)	824 (97%)	26 (3%)	2 (0%)	43	58
1	D	829/868 (96%)	804 (97%)	23 (3%)	2 (0%)	43	58
All	All	3355/3472 (97%)	3253 (97%)	94 (3%)	8 (0%)	43	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	605	HIS
1	B	605	HIS
1	D	605	HIS
1	A	605	HIS
1	A	538	PRO
1	D	538	PRO
1	B	538	PRO
1	C	538	PRO

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	669/726 (92%)	660 (99%)	9 (1%)	61	80
1	B	665/726 (92%)	659 (99%)	6 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	674/726 (93%)	662 (98%)	12 (2%)	51	73
1	D	656/726 (90%)	648 (99%)	8 (1%)	63	81
All	All	2664/2904 (92%)	2629 (99%)	35 (1%)	61	80

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	371	ILE
1	A	436	LEU
1	A	464	GLN
1	A	471	HIS
1	A	950	LEU
1	A	976	GLN
1	A	1029	LEU
1	A	1129	LYS
1	B	467	VAL
1	B	471	HIS
1	B	498	THR
1	B	950	LEU
1	B	976	GLN
1	B	1129	LYS
1	C	367	ASN
1	C	369	ARG
1	C	371	ILE
1	C	436	LEU
1	C	467	VAL
1	C	471	HIS
1	C	498	THR
1	C	950	LEU
1	C	976	GLN
1	C	1029	LEU
1	C	1088	SER
1	C	1129	LYS
1	D	436	LEU
1	D	467	VAL
1	D	471	HIS
1	D	950	LEU
1	D	951	SER
1	D	976	GLN
1	D	1029	LEU

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Mol	Chain	Res	Type
1	D	1129	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	799	GLN
1	A	947	ASN
1	A	966	ASN
1	A	1016	GLN
1	A	1061	GLN
1	B	367	ASN
1	B	503	GLN
1	B	569	GLN
1	B	679	GLN
1	B	805	ASN
1	B	813	HIS
1	B	966	ASN
1	B	1030	GLN
1	B	1061	GLN
1	C	428	GLN
1	C	556	GLN
1	C	966	ASN
1	C	1061	GLN
1	D	679	GLN
1	D	966	ASN
1	D	1061	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

Of 12 ligands modelled in this entry, 4 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
4	ACO	D	2228	-	40,40,53	1.35	4 (10%)	55,63,79	1.65	10 (18%)
4	ACO	B	2228	-	51,53,53	1.54	6 (11%)	73,79,79	1.71	15 (20%)
4	ACO	C	2228	-	51,53,53	1.42	8 (15%)	73,79,79	1.82	12 (16%)
4	ACO	A	2228	-	51,53,53	1.37	7 (13%)	73,79,79	1.74	11 (15%)
2	TD7	D	2001	3	32,34,34	1.69	4 (12%)	40,50,50	1.66	12 (30%)
2	TD7	A	2001	3	32,34,34	1.68	4 (12%)	40,50,50	1.67	12 (30%)
2	TD7	B	2001	3	32,34,34	1.69	5 (15%)	40,50,50	1.63	11 (27%)
2	TD7	C	2001	3	32,34,34	1.70	4 (12%)	40,50,50	1.67	10 (25%)

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
4	ACO	D	2228	-	-	8/34/50/67	0/3/3/3
4	ACO	B	2228	-	-	12/51/67/67	0/3/3/3
4	ACO	C	2228	-	-	12/51/67/67	0/3/3/3
4	ACO	A	2228	-	-	10/51/67/67	0/3/3/3
2	TD7	D	2001	3	-	10/22/26/26	0/2/2/2
2	TD7	A	2001	3	-	10/22/26/26	0/2/2/2
2	TD7	B	2001	3	-	10/22/26/26	0/2/2/2
2	TD7	C	2001	3	-	10/22/26/26	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2228	ACO	P2A-O3A	5.22	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TD7	C2-N3	-4.73	1.30	1.39
2	A	2001	TD7	C2-N3	-4.70	1.30	1.39
2	D	2001	TD7	C2-N3	-4.58	1.30	1.39
2	B	2001	TD7	C2-N3	-4.55	1.30	1.39
4	C	2228	ACO	P3B-O7A	4.43	1.64	1.50
4	A	2228	ACO	P2A-O3A	4.10	1.63	1.59
2	B	2001	TD7	OL1-C11	4.07	1.43	1.32
2	C	2001	TD7	OL1-C11	4.07	1.43	1.32
4	B	2228	ACO	P3B-O7A	4.04	1.63	1.50
2	D	2001	TD7	OL1-C11	4.04	1.43	1.32
2	A	2001	TD7	C4-N3	-3.94	1.32	1.39
2	A	2001	TD7	OL1-C11	3.90	1.43	1.32
2	D	2001	TD7	C4-N3	-3.84	1.33	1.39
2	C	2001	TD7	C4-N3	-3.80	1.33	1.39
2	B	2001	TD7	C4-N3	-3.74	1.33	1.39
4	B	2228	ACO	P1A-O1A	3.73	1.63	1.50
4	A	2228	ACO	P3B-O7A	3.62	1.61	1.50
4	C	2228	ACO	P2A-O3A	3.48	1.63	1.59
2	C	2001	TD7	PB-O2B	3.45	1.61	1.50
2	A	2001	TD7	PB-O2B	3.41	1.61	1.50
4	A	2228	ACO	P1A-O1A	3.37	1.62	1.50
2	D	2001	TD7	PB-O2B	3.37	1.60	1.50
4	D	2228	ACO	P1A-O1A	3.31	1.62	1.50
2	B	2001	TD7	PB-O2B	3.28	1.60	1.50
4	D	2228	ACO	P3B-O7A	3.22	1.60	1.50
4	B	2228	ACO	C5A-C4A	3.20	1.44	1.39
4	D	2228	ACO	C5A-C4A	3.02	1.44	1.39
4	C	2228	ACO	P1A-O1A	2.98	1.61	1.50
4	B	2228	ACO	C5A-N7A	-2.59	1.34	1.39
4	B	2228	ACO	O4B-C1B	2.55	1.47	1.42
4	C	2228	ACO	P2A-O4A	2.50	1.59	1.50
4	C	2228	ACO	P3B-O8A	2.49	1.64	1.54
4	A	2228	ACO	C5A-C4A	2.45	1.43	1.39
4	A	2228	ACO	P1A-O3A	2.45	1.62	1.59
4	D	2228	ACO	P2A-O3A	2.40	1.62	1.59
4	C	2228	ACO	C5A-C4A	2.33	1.43	1.39
4	A	2228	ACO	P3B-O8A	2.13	1.62	1.54
4	C	2228	ACO	C2A-N1A	2.09	1.37	1.33
4	C	2228	ACO	CCP-CBP	2.08	1.56	1.52
2	B	2001	TD7	PA-O3A	2.06	1.61	1.59
4	A	2228	ACO	P2A-O4A	2.04	1.57	1.50

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2228	ACO	P3B-O3B-C3B	-5.88	107.74	123.43
4	C	2228	ACO	P3B-O3B-C3B	-5.25	109.41	123.43
4	C	2228	ACO	C5A-C4A-N3A	-4.90	119.97	126.72
4	A	2228	ACO	C5A-C4A-N3A	-4.87	120.01	126.72
4	C	2228	ACO	C5A-N7A-C8A	4.74	110.90	103.45
4	B	2228	ACO	P3B-O3B-C3B	-4.70	110.88	123.43
4	D	2228	ACO	C5A-C4A-N3A	-4.56	120.44	126.72
4	A	2228	ACO	N3A-C4A-N9A	4.44	134.72	127.17
4	C	2228	ACO	N3A-C4A-N9A	4.38	134.62	127.17
4	C	2228	ACO	N3A-C2A-N1A	-4.21	122.22	128.58
4	C	2228	ACO	C2P-C3P-N4P	-4.18	103.69	112.41
4	B	2228	ACO	C5A-C4A-N3A	-4.11	121.05	126.72
4	B	2228	ACO	N3A-C4A-N9A	4.11	134.16	127.17
2	A	2001	TD7	C4-C5-S1	-4.00	106.98	110.63
2	D	2001	TD7	C4-C5-S1	-3.95	107.03	110.63
4	D	2228	ACO	N3A-C4A-N9A	3.87	133.74	127.17
4	C	2228	ACO	N9A-C8A-N7A	-3.81	108.53	113.94
2	C	2001	TD7	C4-C5-S1	-3.76	107.21	110.63
4	A	2228	ACO	C5A-N7A-C8A	3.74	109.32	103.45
2	B	2001	TD7	C4-C5-S1	-3.67	107.29	110.63
4	D	2228	ACO	N3A-C2A-N1A	-3.67	123.03	128.58
4	C	2228	ACO	C4A-C5A-N7A	-3.56	106.51	110.58
4	D	2228	ACO	P3B-O3B-C3B	-3.50	114.07	123.43
4	B	2228	ACO	C2P-C3P-N4P	-3.50	105.10	112.41
4	A	2228	ACO	N3A-C2A-N1A	-3.40	123.44	128.58
4	C	2228	ACO	C2A-N3A-C4A	3.40	120.13	111.83
4	D	2228	ACO	C5A-N7A-C8A	3.38	108.76	103.45
4	B	2228	ACO	C5A-N7A-C8A	3.37	108.74	103.45
4	B	2228	ACO	N3A-C2A-N1A	-3.32	123.56	128.58
4	D	2228	ACO	O5A-P2A-O3A	3.26	116.08	107.27
2	C	2001	TD7	C6'-N1'-C2'	3.25	121.41	116.07
4	A	2228	ACO	C2A-N3A-C4A	3.22	119.70	111.83
4	D	2228	ACO	C4A-C5A-N7A	-3.21	106.92	110.58
4	B	2228	ACO	O5A-P2A-O3A	3.17	115.84	107.27
2	D	2001	TD7	C6'-N1'-C2'	3.15	121.24	116.07
4	B	2228	ACO	C6P-C7P-N8P	-3.06	105.49	112.00
4	A	2228	ACO	O5A-P2A-O3A	3.05	115.53	107.27
4	D	2228	ACO	C2A-N3A-C4A	3.03	119.23	111.83
2	B	2001	TD7	C6'-N1'-C2'	3.02	121.03	116.07
2	A	2001	TD7	C6'-N1'-C2'	3.02	121.03	116.07
4	C	2228	ACO	O5A-P2A-O3A	2.93	115.19	107.27
2	B	2001	TD7	CM4-C4-N3	2.89	126.50	122.27
4	A	2228	ACO	C4A-C5A-N7A	-2.87	107.30	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2228	ACO	N9A-C8A-N7A	-2.87	109.87	113.94
2	C	2001	TD7	CM2-C2'-N1'	2.80	120.19	117.20
2	C	2001	TD7	CM4-C4-N3	2.79	126.36	122.27
4	C	2228	ACO	C4A-N9A-C8A	2.78	108.66	105.74
2	D	2001	TD7	OL1-C11-CLB	2.73	121.39	114.08
2	D	2001	TD7	CM4-C4-N3	2.69	126.21	122.27
2	D	2001	TD7	CM2-C2'-N1'	2.69	120.06	117.20
2	A	2001	TD7	C5'-C6'-N1'	-2.68	119.47	123.83
4	B	2228	ACO	C7P-N8P-C9P	2.68	127.35	122.55
2	A	2001	TD7	CM4-C4-N3	2.67	126.18	122.27
2	C	2001	TD7	C5'-C6'-N1'	-2.67	119.49	123.83
4	A	2228	ACO	N9A-C8A-N7A	-2.66	110.16	113.94
2	B	2001	TD7	C5'-C6'-N1'	-2.62	119.56	123.83
2	C	2001	TD7	C7'-N3-C2	-2.61	122.91	126.13
4	A	2228	ACO	O6A-CCP-CBP	-2.57	106.42	110.55
2	B	2001	TD7	OL1-C11-CLB	2.55	120.91	114.08
2	B	2001	TD7	C7'-N3-C2	-2.55	122.98	126.13
2	D	2001	TD7	N1'-C2'-N3'	-2.54	121.30	125.53
2	C	2001	TD7	OL1-C11-CLB	2.52	120.82	114.08
4	B	2228	ACO	O6A-P2A-O4A	-2.48	99.09	108.94
2	B	2001	TD7	CM2-C2'-N1'	2.48	119.84	117.20
2	A	2001	TD7	C7'-N3-C2	-2.45	123.10	126.13
2	D	2001	TD7	C5'-C6'-N1'	-2.44	119.87	123.83
2	A	2001	TD7	OL1-C11-CLB	2.42	120.55	114.08
2	C	2001	TD7	N1'-C2'-N3'	-2.41	121.52	125.53
4	B	2228	ACO	C4A-N9A-C8A	2.37	108.23	105.74
2	A	2001	TD7	CM2-C2'-N1'	2.37	119.72	117.20
2	A	2001	TD7	CLB-C13-CLC	-2.34	107.47	113.67
4	B	2228	ACO	C2A-N3A-C4A	2.31	117.48	111.83
4	C	2228	ACO	C6P-C7P-N8P	-2.28	107.14	112.00
2	A	2001	TD7	N1'-C2'-N3'	-2.27	121.75	125.53
4	D	2228	ACO	N9A-C8A-N7A	-2.26	110.73	113.94
4	D	2228	ACO	O3A-P2A-O4A	-2.21	104.06	110.70
2	D	2001	TD7	C7'-N3-C2	-2.18	123.43	126.13
4	B	2228	ACO	O4B-C1B-N9A	2.18	112.27	108.09
2	C	2001	TD7	O3B-PB-O3A	2.17	111.90	104.64
2	A	2001	TD7	O3B-PB-O3A	2.16	111.88	104.64
2	C	2001	TD7	CLB-C13-CLC	-2.14	107.98	113.67
2	B	2001	TD7	N1'-C2'-N3'	-2.13	121.98	125.53
2	A	2001	TD7	C6-C5-S1	2.12	123.83	119.29
4	A	2228	ACO	C4A-N9A-C8A	2.11	107.96	105.74
2	B	2001	TD7	O3B-PB-O3A	2.07	111.58	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TD7	C6-C5-S1	2.06	123.71	119.29
2	D	2001	TD7	O3B-PB-O3A	2.06	111.53	104.64
2	D	2001	TD7	C7'-N3-C4	-2.06	122.38	124.98
4	B	2228	ACO	N6A-C6A-N1A	2.04	122.92	118.38
2	B	2001	TD7	CLB-C13-CLC	-2.03	108.28	113.67
2	D	2001	TD7	C5'-C7'-N3	-2.02	110.69	113.14
2	A	2001	TD7	C5'-C7'-N3	-2.02	110.70	113.14
2	D	2001	TD7	CLB-C13-CLC	-2.02	108.32	113.67

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2228	ACO	C5B-O5B-P1A-O1A
4	A	2228	ACO	C5B-O5B-P1A-O2A
4	A	2228	ACO	C5B-O5B-P1A-O3A
4	A	2228	ACO	S1P-C2P-C3P-N4P
4	A	2228	ACO	O-C-S1P-C2P
4	B	2228	ACO	C5B-O5B-P1A-O1A
4	B	2228	ACO	C5B-O5B-P1A-O2A
4	B	2228	ACO	C5B-O5B-P1A-O3A
4	B	2228	ACO	P2A-O3A-P1A-O5B
4	B	2228	ACO	S1P-C2P-C3P-N4P
4	C	2228	ACO	C5B-O5B-P1A-O1A
4	C	2228	ACO	C5B-O5B-P1A-O2A
4	C	2228	ACO	C5B-O5B-P1A-O3A
4	C	2228	ACO	OAP-CAP-CBP-CCP
4	C	2228	ACO	OAP-CAP-CBP-CDP
4	D	2228	ACO	C5B-O5B-P1A-O1A
4	D	2228	ACO	C5B-O5B-P1A-O2A
4	D	2228	ACO	C5B-O5B-P1A-O3A
4	A	2228	ACO	O4B-C4B-C5B-O5B
4	B	2228	ACO	O4B-C4B-C5B-O5B
4	C	2228	ACO	O4B-C4B-C5B-O5B
2	A	2001	TD7	CLC-C13-CLB-C11
2	B	2001	TD7	CLC-C13-CLB-C11
2	C	2001	TD7	CLC-C13-CLB-C11
2	D	2001	TD7	CLC-C13-CLB-C11
4	A	2228	ACO	C3B-C4B-C5B-O5B
4	A	2228	ACO	CH3-C-S1P-C2P
4	B	2228	ACO	O-C-S1P-C2P
4	B	2228	ACO	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	C	2228	ACO	C3B-C4B-C5B-O5B
4	A	2228	ACO	OAP-CAP-CBP-CDP
4	C	2228	ACO	OAP-CAP-CBP-CEP
4	B	2228	ACO	P1A-O3A-P2A-O4A
4	B	2228	ACO	CH3-C-S1P-C2P
2	A	2001	TD7	PA-O3A-PB-O2B
2	B	2001	TD7	PA-O3A-PB-O2B
2	C	2001	TD7	PA-O3A-PB-O2B
2	D	2001	TD7	PA-O3A-PB-O2B
2	A	2001	TD7	C5-C6-C7-O7
2	B	2001	TD7	C5-C6-C7-O7
2	C	2001	TD7	C5-C6-C7-O7
2	D	2001	TD7	C5-C6-C7-O7
4	D	2228	ACO	C3B-O3B-P3B-O7A
4	D	2228	ACO	O4B-C4B-C5B-O5B
2	A	2001	TD7	C7-O7-PA-O3A
2	A	2001	TD7	C7-O7-PA-O1A
2	A	2001	TD7	C7-O7-PA-O2A
2	B	2001	TD7	C7-O7-PA-O3A
2	B	2001	TD7	C7-O7-PA-O1A
2	B	2001	TD7	C7-O7-PA-O2A
2	C	2001	TD7	C7-O7-PA-O3A
2	C	2001	TD7	C7-O7-PA-O1A
2	C	2001	TD7	C7-O7-PA-O2A
2	D	2001	TD7	C7-O7-PA-O3A
2	D	2001	TD7	C7-O7-PA-O1A
2	D	2001	TD7	C7-O7-PA-O2A
4	A	2228	ACO	P1A-O3A-P2A-O5A
4	C	2228	ACO	P1A-O3A-P2A-O5A
4	D	2228	ACO	P1A-O3A-P2A-O5A
4	B	2228	ACO	C3B-O3B-P3B-O9A
4	C	2228	ACO	C3B-O3B-P3B-O9A
2	B	2001	TD7	CLB-C13-CLC-OL2
2	D	2001	TD7	CLB-C13-CLC-OL2
2	C	2001	TD7	CLB-C13-CLC-OL2
2	A	2001	TD7	CLB-C13-CLC-OL2
2	C	2001	TD7	CLB-C13-CLC-OL3
2	D	2001	TD7	CLB-C13-CLC-OL3
2	A	2001	TD7	CLB-C13-CLC-OL3
2	B	2001	TD7	CLB-C13-CLC-OL3
4	C	2228	ACO	O-C-S1P-C2P
4	C	2228	ACO	P1A-O3A-P2A-O4A

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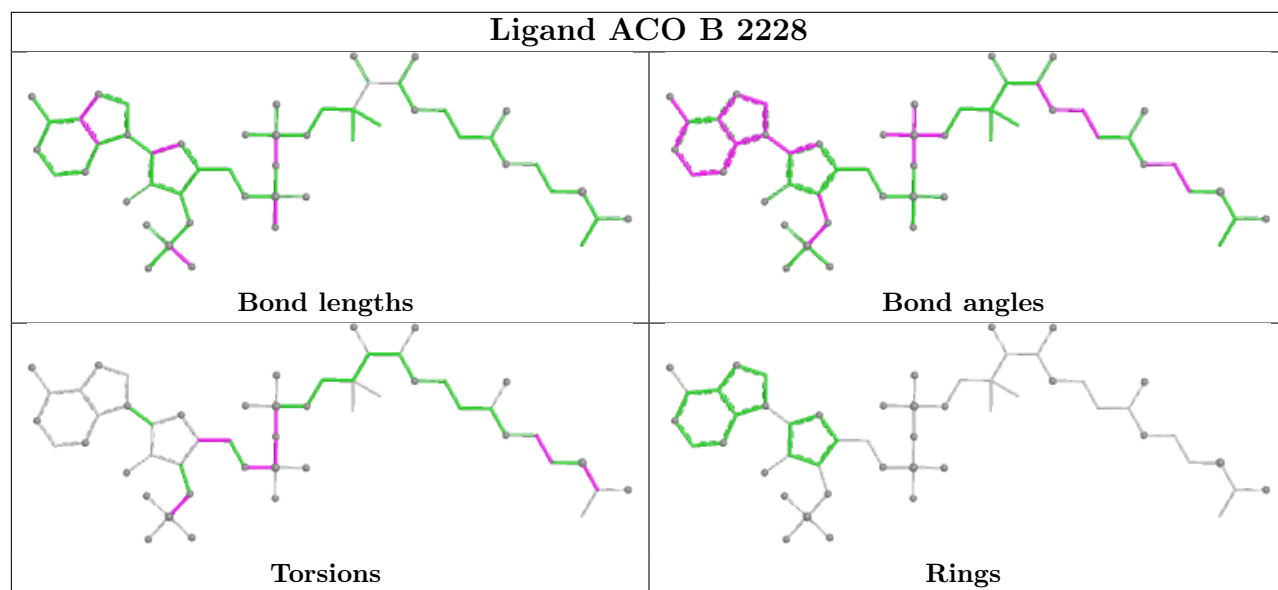
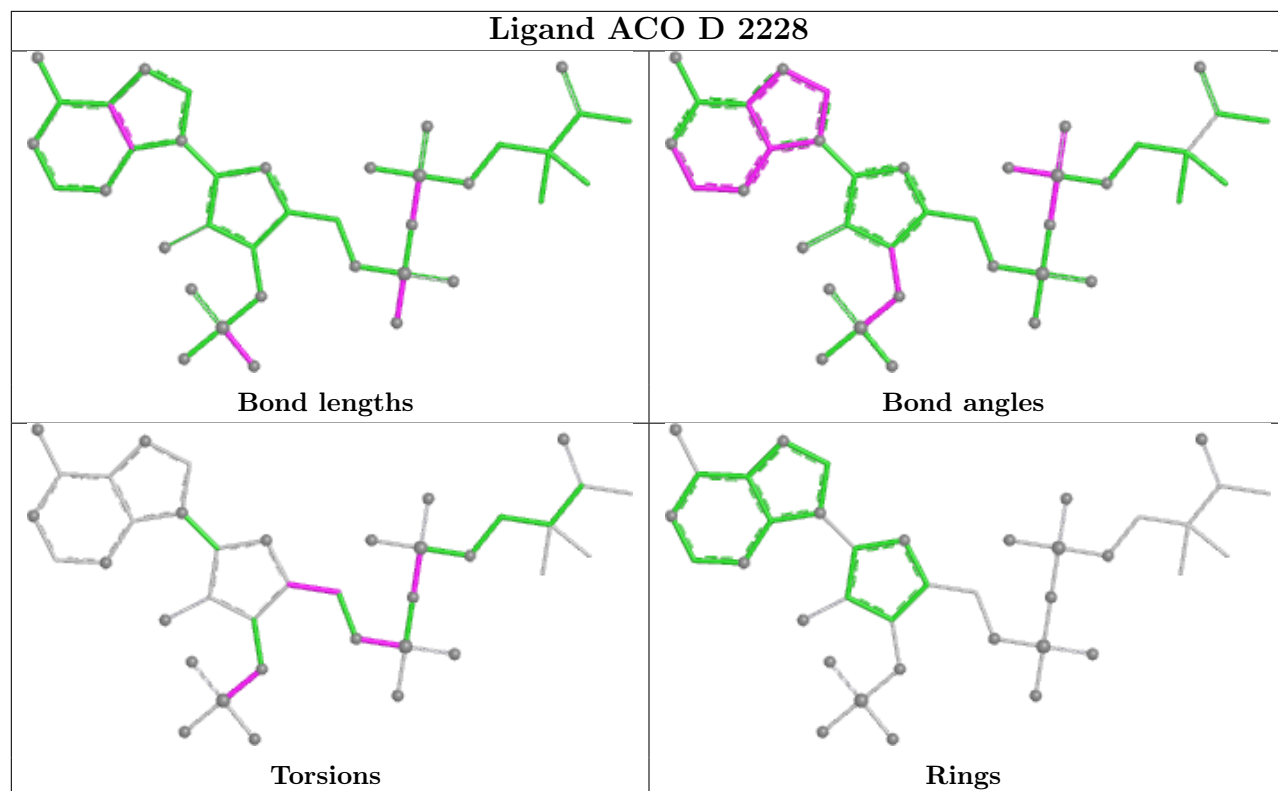
Mol	Chain	Res	Type	Atoms
4	D	2228	ACO	P1A-O3A-P2A-O4A
2	A	2001	TD7	C2-C11-CLB-C13
2	B	2001	TD7	C2-C11-CLB-C13
2	C	2001	TD7	C2-C11-CLB-C13
2	D	2001	TD7	C2-C11-CLB-C13
4	D	2228	ACO	C3B-C4B-C5B-O5B
2	D	2001	TD7	OL1-C11-CLB-C13
2	A	2001	TD7	OL1-C11-CLB-C13
4	B	2228	ACO	P1A-O3A-P2A-O5A
2	B	2001	TD7	OL1-C11-CLB-C13
2	C	2001	TD7	OL1-C11-CLB-C13

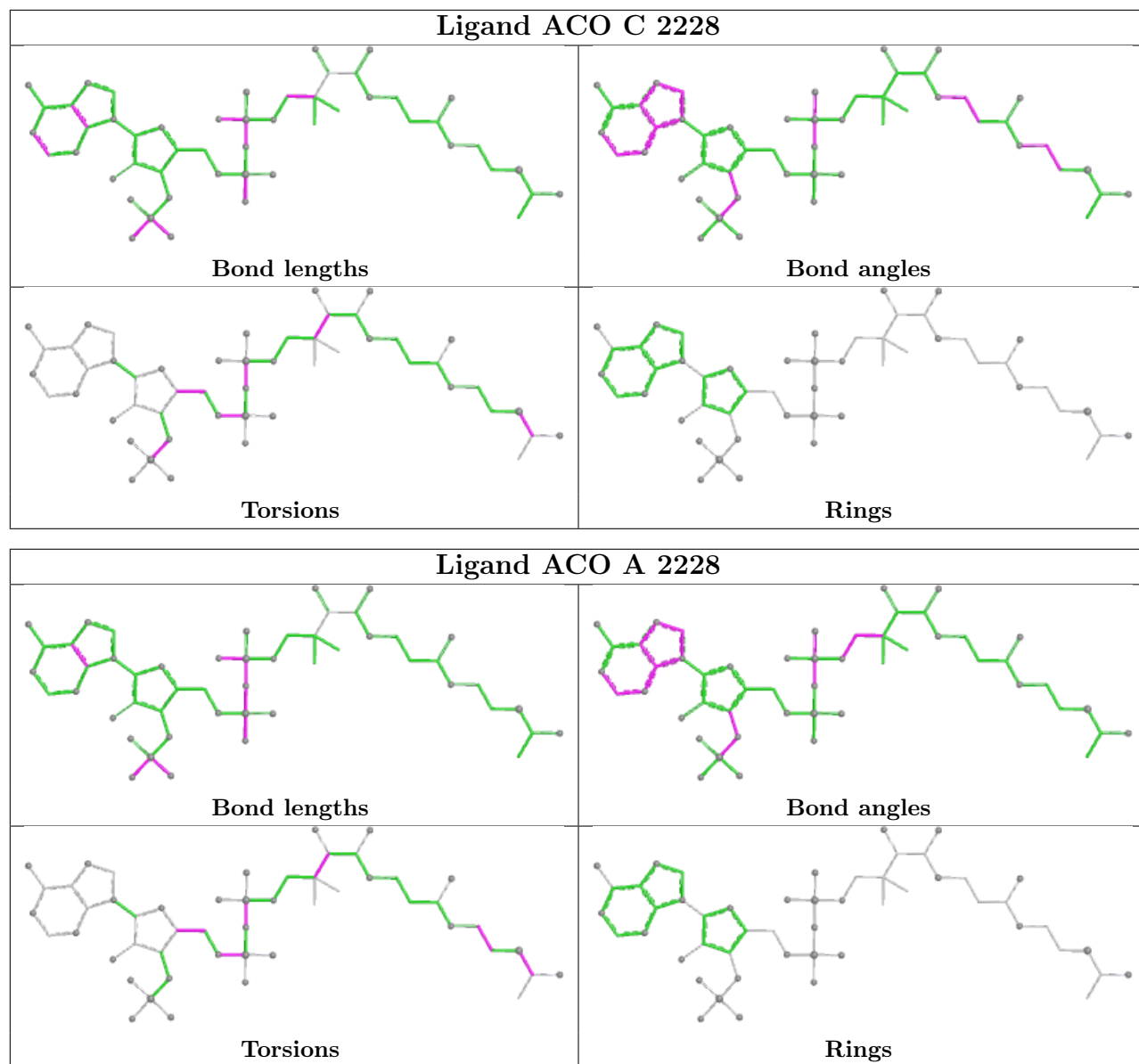
There are no ring outliers.

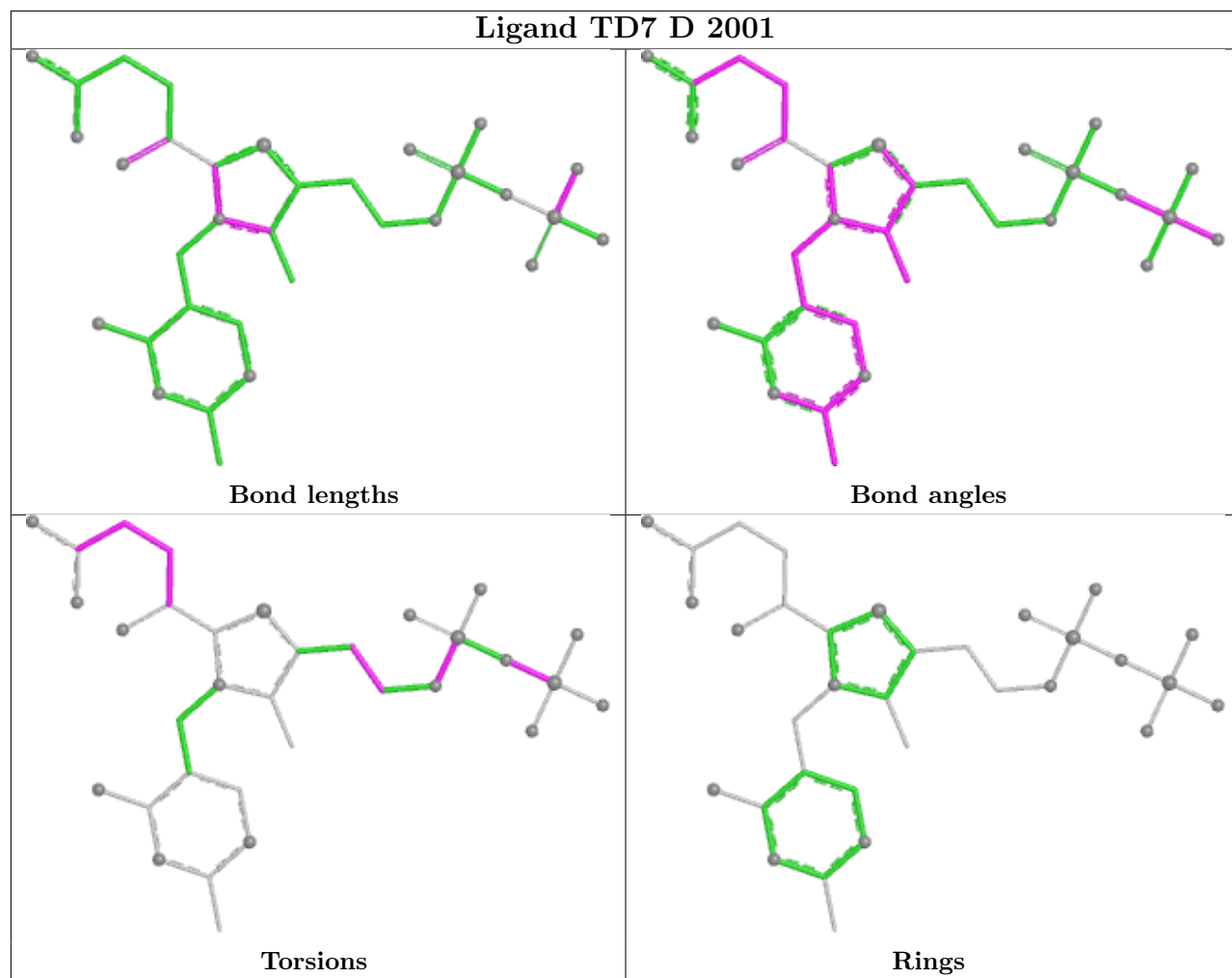
6 monomers are involved in 8 short contacts:

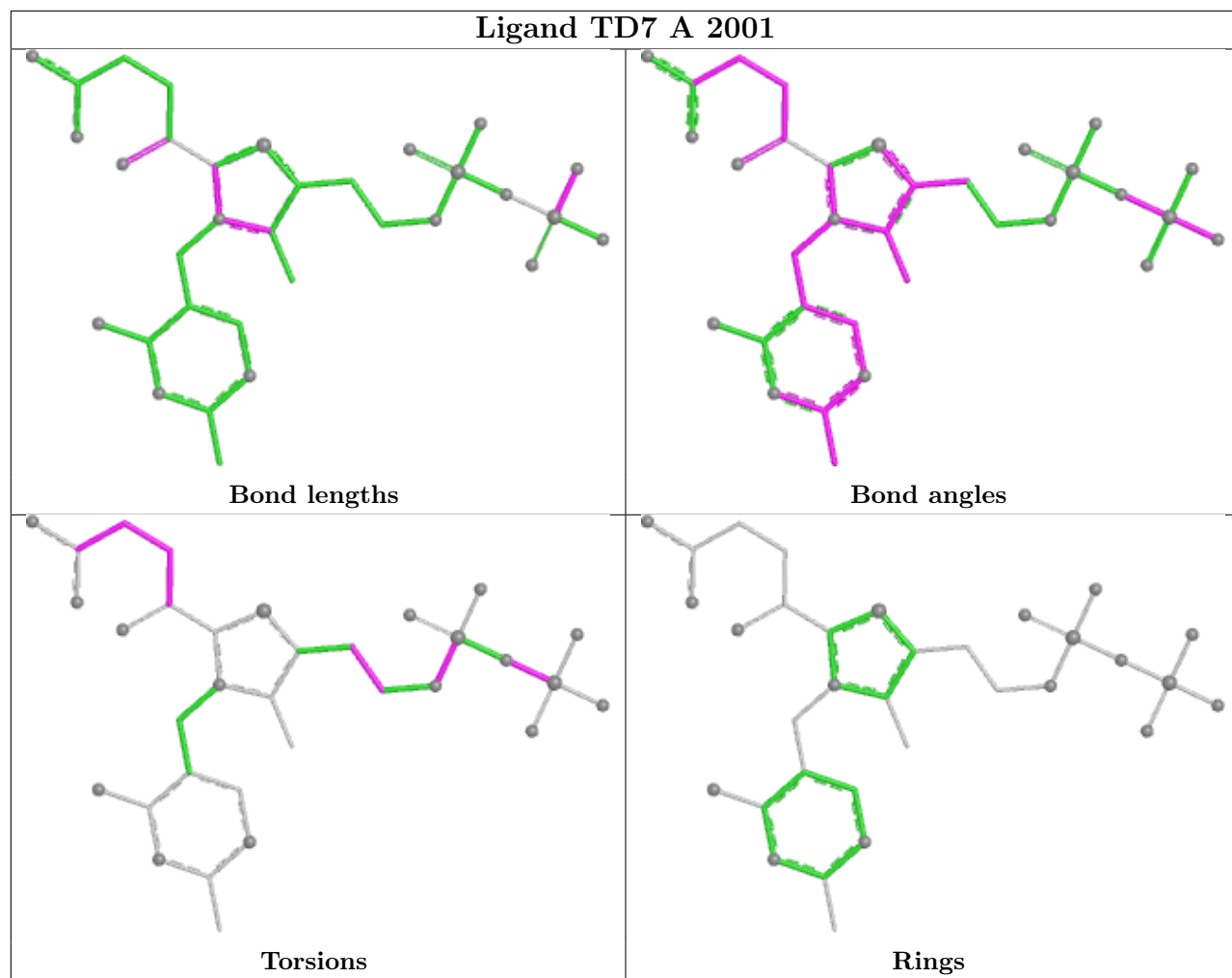
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2228	ACO	1	0
4	A	2228	ACO	1	0
2	D	2001	TD7	1	0
2	A	2001	TD7	1	0
2	B	2001	TD7	2	0
2	C	2001	TD7	2	0

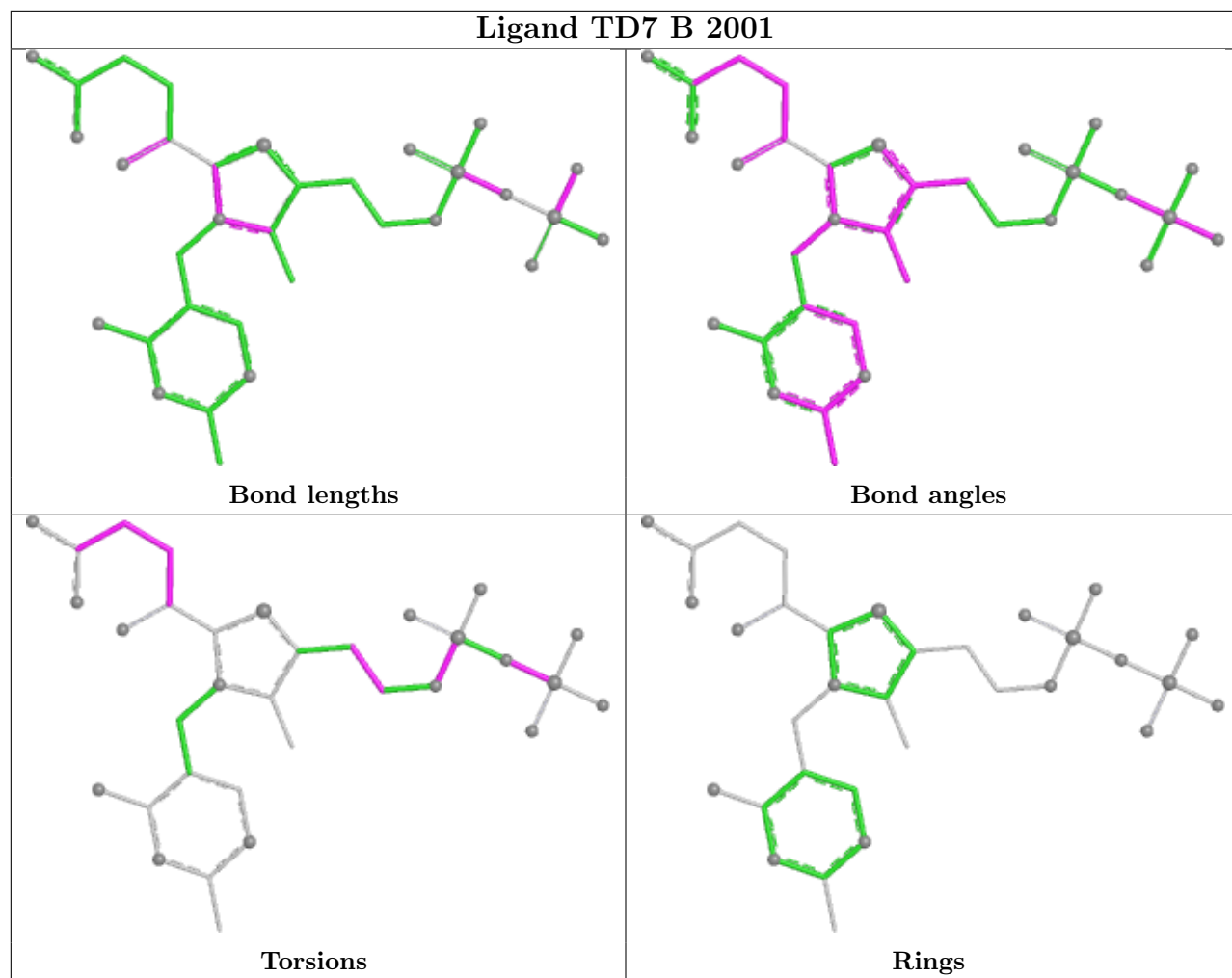
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

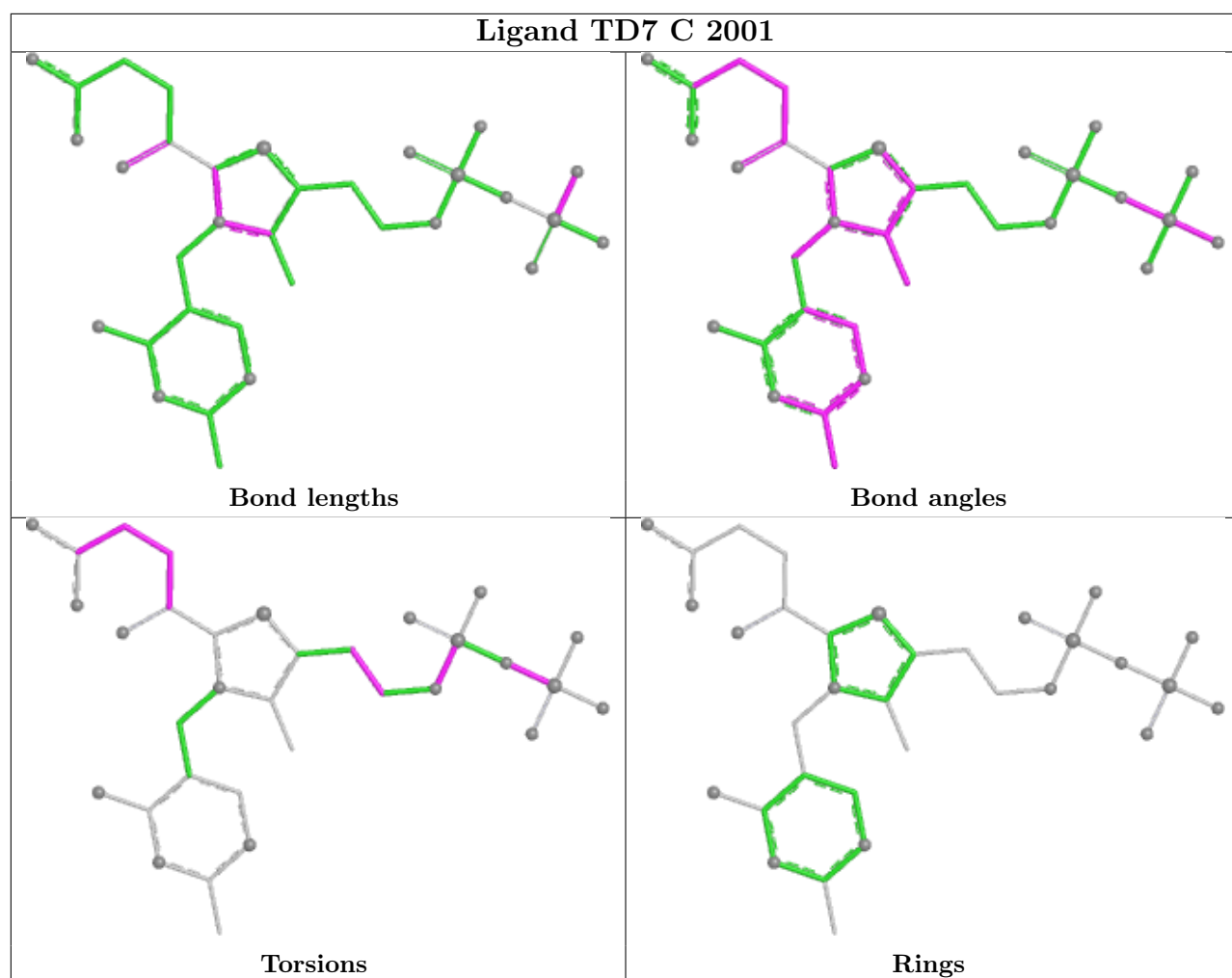












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	847/868 (97%)	0.31	34 (4%)	42	38	24, 41, 75, 106	0
1	B	839/868 (96%)	0.15	20 (2%)	59	55	22, 39, 66, 95	0
1	C	856/868 (98%)	0.29	26 (3%)	52	48	25, 43, 71, 101	0
1	D	837/868 (96%)	0.41	28 (3%)	49	45	27, 45, 73, 107	0
All	All	3379/3472 (97%)	0.29	108 (3%)	50	46	22, 42, 71, 107	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	566	ASN	5.6
1	A	393	ASP	5.6
1	D	502	GLY	5.0
1	A	502	GLY	4.4
1	A	568	SER	4.3
1	D	472	ASP	4.3
1	C	568	SER	4.0
1	B	394	ASN	3.9
1	D	363	ILE	3.9
1	C	397	PHE	3.8
1	B	472	ASP	3.7
1	C	502	GLY	3.7
1	D	796	TYR	3.6
1	B	421	VAL	3.6
1	C	407	SER	3.6
1	D	564	ASN	3.5
1	A	472	ASP	3.4
1	D	420	LYS	3.3
1	B	794	ARG	3.3
1	C	364	GLU	3.3
1	A	363	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	422	ASP	3.1
1	D	413	TRP	3.1
1	B	392	LEU	3.0
1	A	796	TYR	3.0
1	C	424	PHE	3.0
1	D	627	GLY	3.0
1	B	469	THR	3.0
1	C	406	ASN	3.0
1	B	413	TRP	2.9
1	A	361	ASP	2.9
1	A	560	GLU	2.9
1	C	631	SER	2.8
1	A	570	ALA	2.8
1	A	471	HIS	2.8
1	C	571	HIS	2.8
1	B	368	ALA	2.8
1	C	569	GLN	2.8
1	B	632	ASP	2.8
1	D	393	ASP	2.7
1	B	365	ASP	2.7
1	C	790	GLU	2.6
1	A	569	GLN	2.6
1	C	408	HIS	2.6
1	D	571	HIS	2.6
1	C	412	LEU	2.6
1	D	364	GLU	2.6
1	B	1211	SER	2.6
1	A	815	ILE	2.5
1	D	565	LEU	2.5
1	C	394	ASN	2.5
1	D	411	THR	2.5
1	C	796	TYR	2.5
1	A	809	GLU	2.5
1	C	794	ARG	2.4
1	D	803	VAL	2.4
1	B	560	GLU	2.4
1	B	371	ILE	2.4
1	A	421	VAL	2.4
1	B	569	GLN	2.4
1	A	813	HIS	2.4
1	C	471	HIS	2.4
1	D	471	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	628	GLU	2.4
1	D	554	TYR	2.4
1	D	809	GLU	2.3
1	A	765	ASP	2.3
1	D	814	GLU	2.3
1	C	413	TRP	2.3
1	A	364	GLU	2.3
1	C	769	GLY	2.3
1	A	632	ASP	2.3
1	A	790	GLU	2.3
1	A	367	ASN	2.2
1	C	759	TYR	2.3
1	D	805	ASN	2.2
1	C	815	ILE	2.2
1	A	490	GLU	2.2
1	A	749	GLU	2.2
1	B	558	PHE	2.2
1	A	805	ASN	2.2
1	B	393	ASP	2.2
1	D	365	ASP	2.2
1	D	628	GLU	2.2
1	D	807	VAL	2.2
1	B	570	ALA	2.2
1	C	411	THR	2.2
1	C	422	ASP	2.2
1	A	410	LEU	2.2
1	A	412	LEU	2.2
1	D	770	SER	2.2
1	A	470	LYS	2.2
1	A	368	ALA	2.1
1	B	414	ASP	2.1
1	D	964	VAL	2.1
1	D	368	ALA	2.1
1	D	362	SER	2.1
1	C	570	ALA	2.1
1	A	627	GLY	2.1
1	D	802	ARG	2.1
1	A	935	ASP	2.1
1	A	1101	ASP	2.1
1	C	410	LEU	2.0
1	A	512	GLU	2.0
1	A	1087	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	628	GLU	2.0
1	A	794	ARG	2.0
1	B	627	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

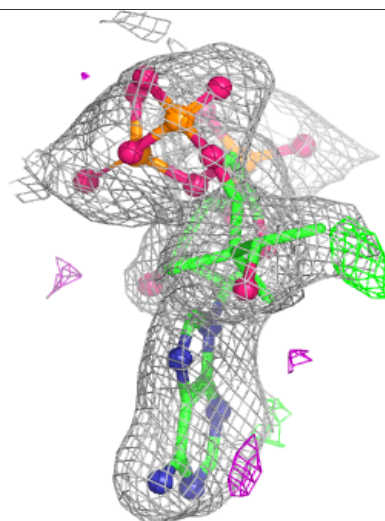
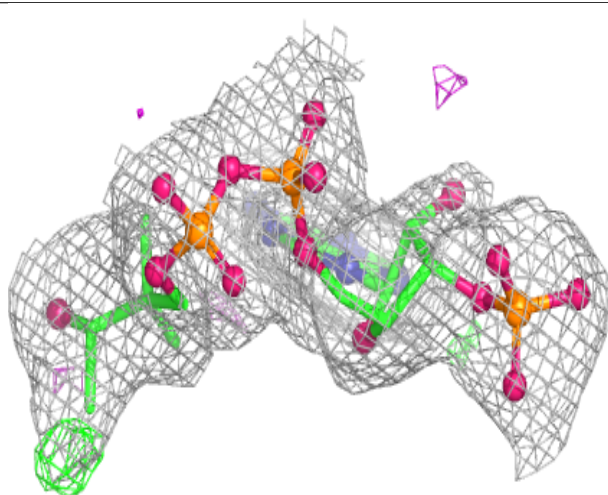
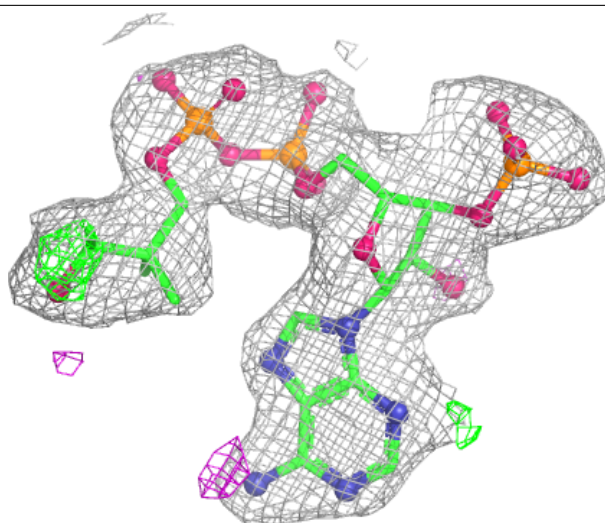
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACO	D	2228	38/51	0.90	0.09	43,57,63,65	0
4	ACO	C	2228	51/51	0.94	0.08	24,38,48,50	0
4	ACO	A	2228	51/51	0.94	0.09	37,50,63,66	0
4	ACO	B	2228	51/51	0.95	0.08	22,36,48,51	0
2	TD7	C	2001	33/33	0.97	0.08	17,29,68,190	0
2	TD7	D	2001	33/33	0.97	0.07	18,33,71,103	0
2	TD7	A	2001	33/33	0.97	0.09	15,29,115,173	0
2	TD7	B	2001	33/33	0.98	0.06	8,26,58,86	0
3	MG	A	2002	1/1	0.99	0.02	17,17,17,17	0
3	MG	C	2002	1/1	0.99	0.02	16,16,16,16	0
3	MG	B	2002	1/1	1.00	0.02	14,14,14,14	0
3	MG	D	2002	1/1	1.00	0.02	20,20,20,20	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.

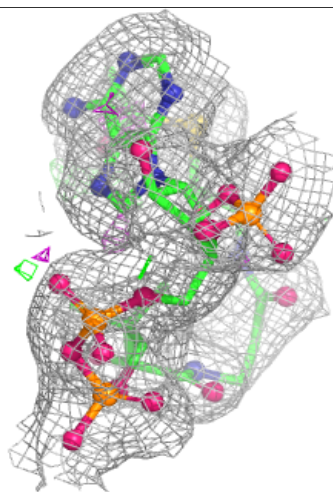
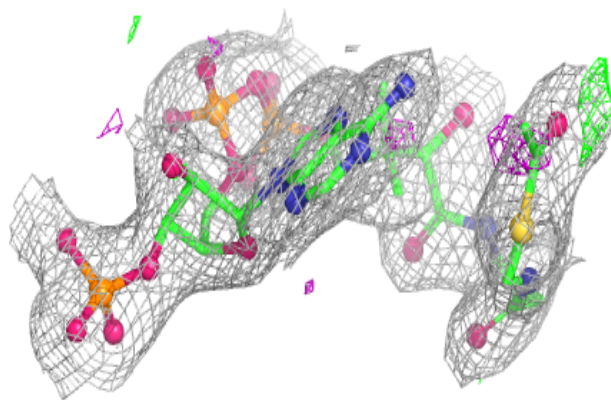
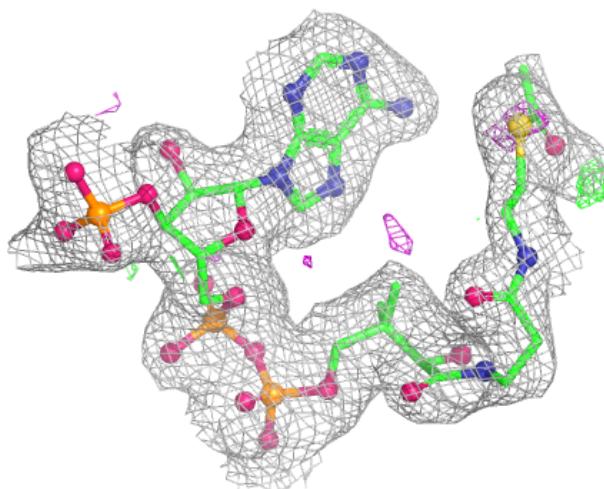
Electron density around ACO D 2228:

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



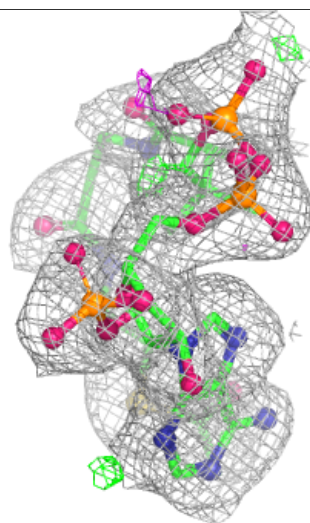
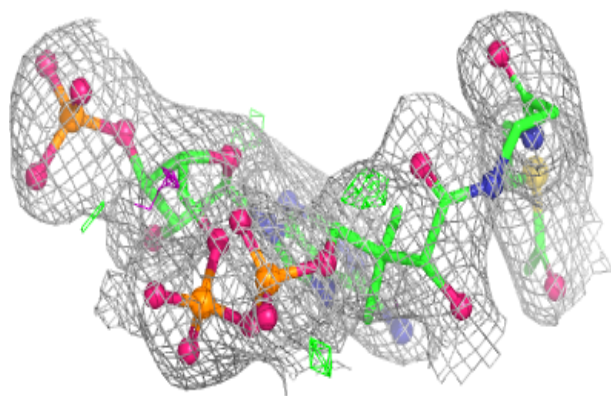
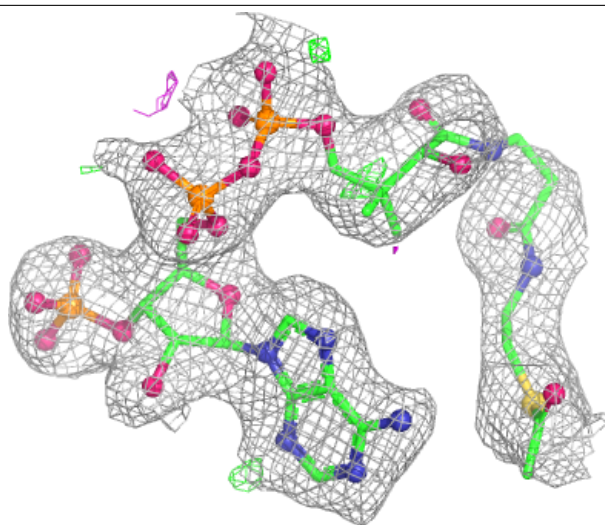
Electron density around ACO C 2228:

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



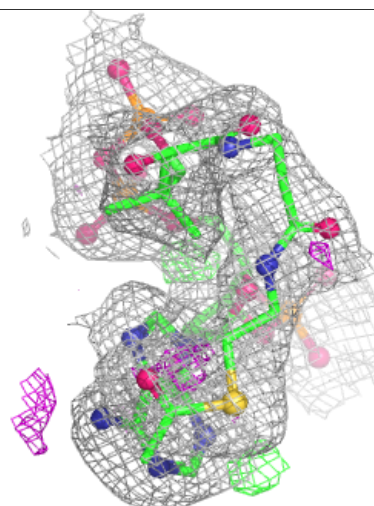
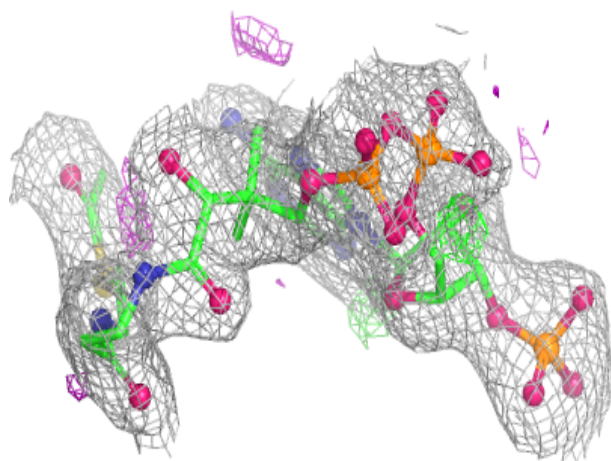
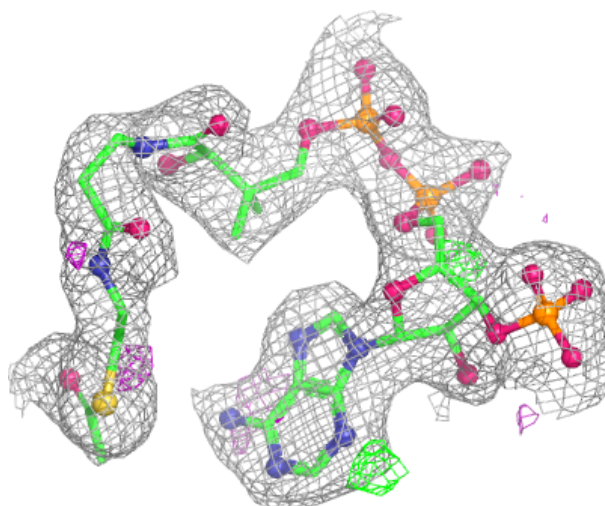
Electron density around ACO A 2228:

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



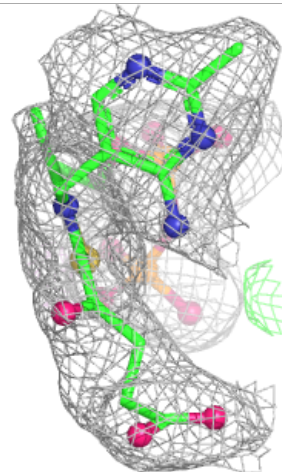
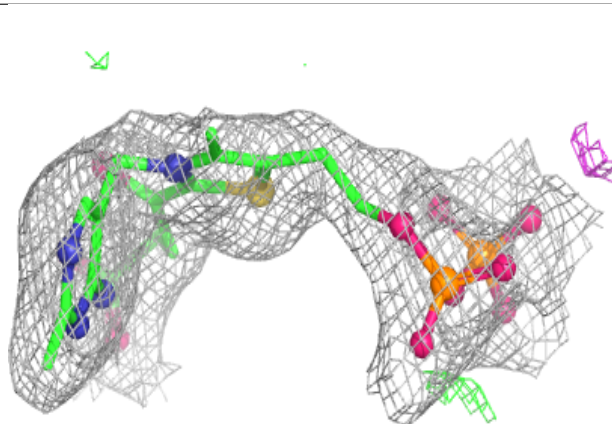
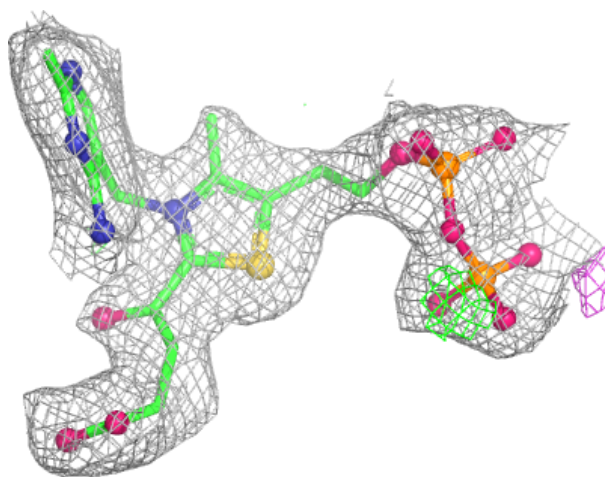
Electron density around ACO B 2228:

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



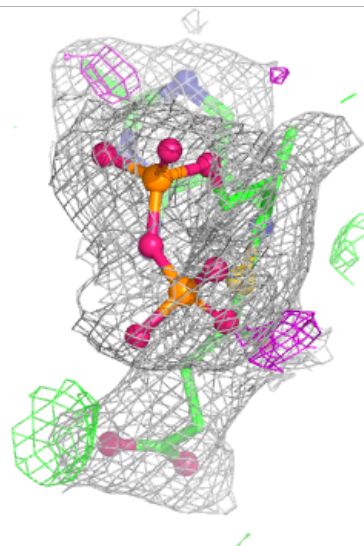
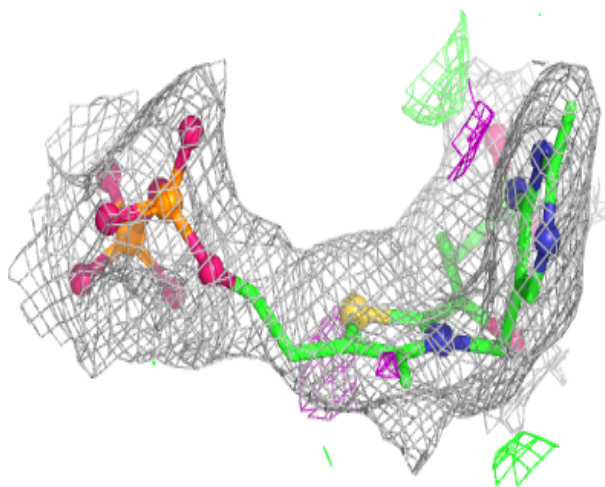
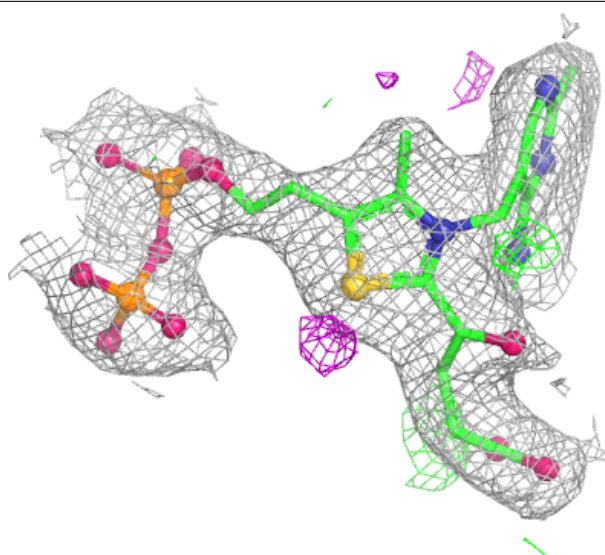
Electron density around TD7 C 2001:

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



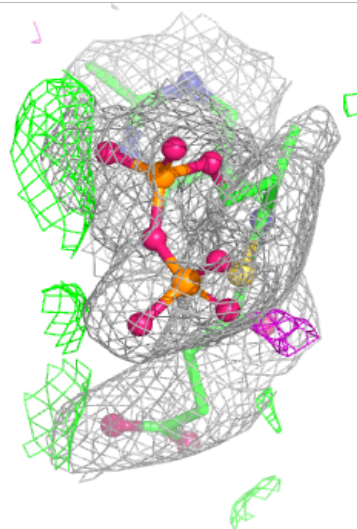
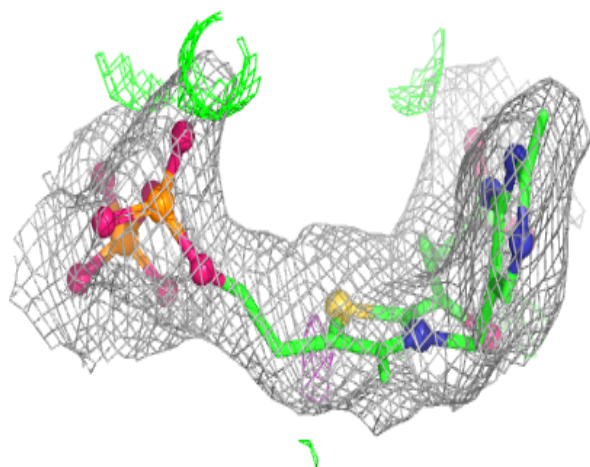
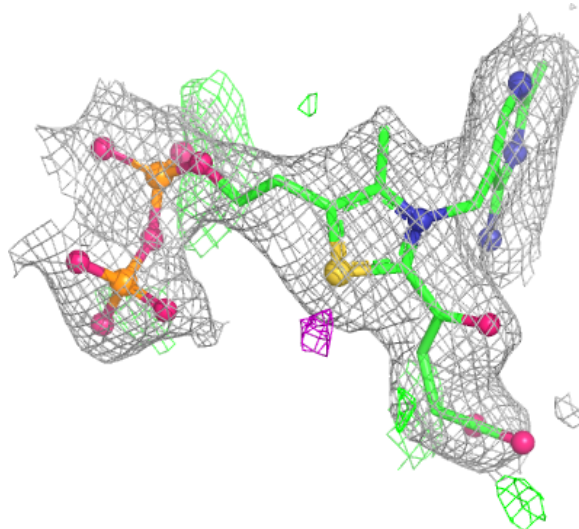
Electron density around TD7 D 2001:

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



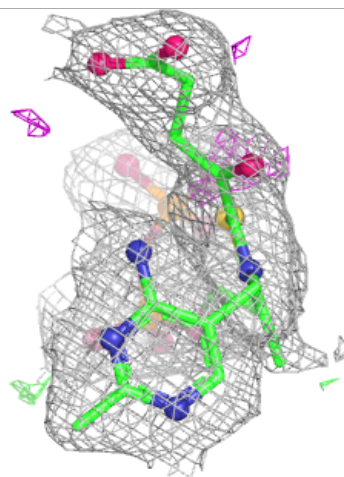
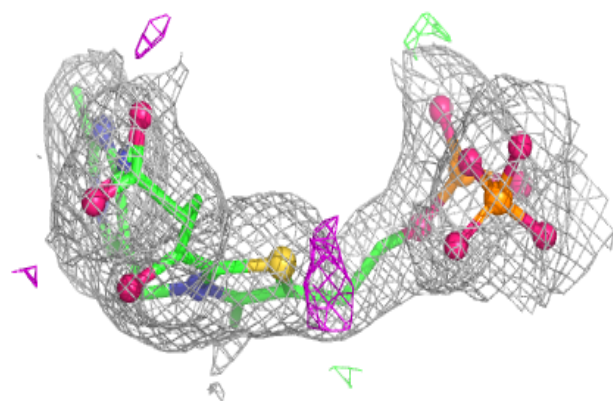
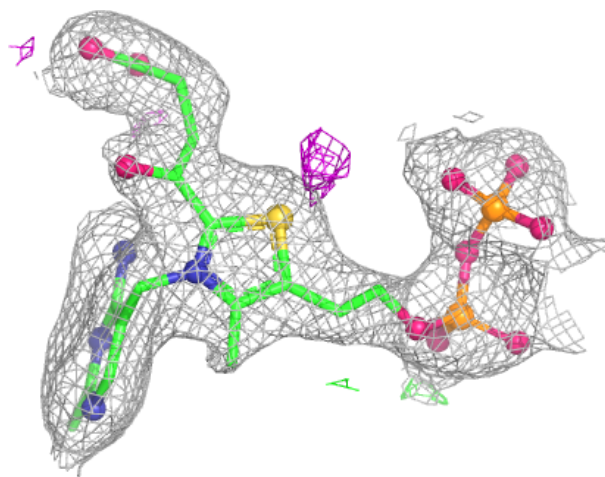
Electron density around TD7 A 2001:

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



Electron density around TD7 B 2001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.