



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:00 PM UTC

PDB ID : 2PUT / pdb_00002put
Title : The crystal structure of isomerase domain of glucosamine-6-phosphate synthase from *Candida albicans*
Authors : Raczynska, J.; Olchowoy, J.; Milewski, S.; Rypniewski, W.
Deposited on : 2007-05-09
Resolution : 1.90 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

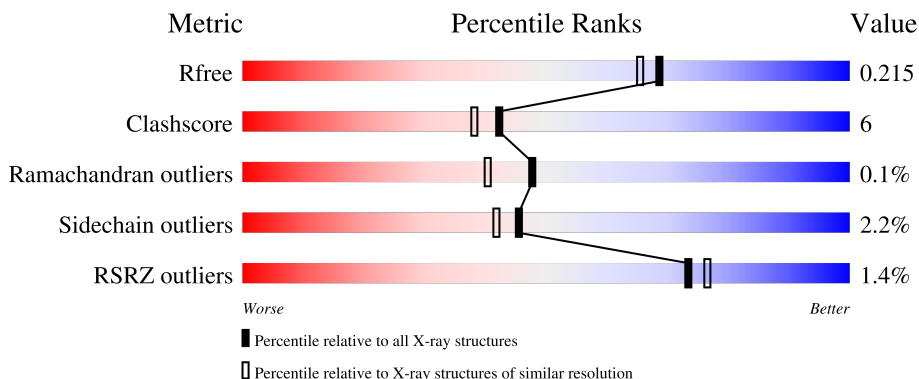
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



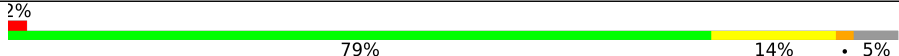
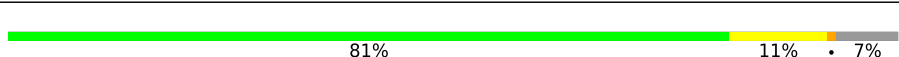
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	367	 80% 11% • 8%
1	B	367	 83% 12% • •
1	C	367	 79% 14% • 5%
1	D	367	 81% 11% • 7%

2 Entry composition [i](#)

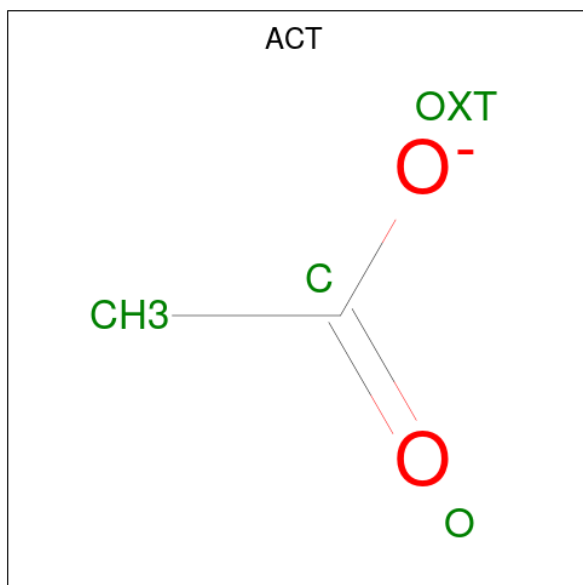
There are 6 unique types of molecules in this entry. The entry contains 11779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	Total 2642	C 1669	N 459	O 497	S 17	0	2	0
1	B	352	Total 2742	C 1730	N 476	O 519	S 17	0	2	0
1	C	350	Total 2745	C 1735	N 474	O 518	S 18	0	6	0
1	D	341	Total 2670	C 1685	N 462	O 506	S 17	0	4	0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

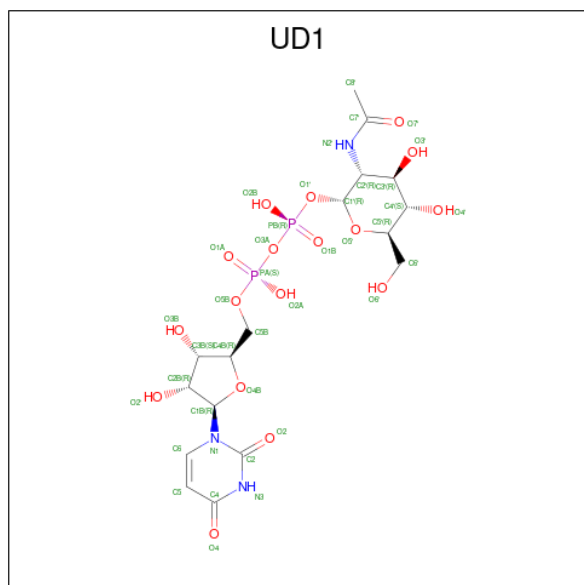


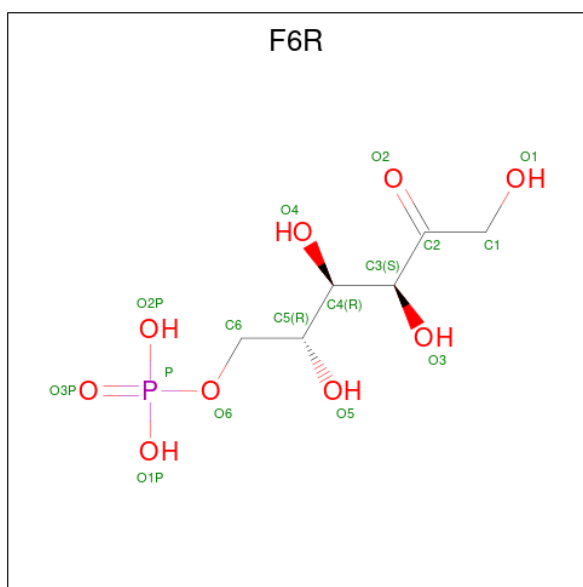
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	A	1	16	6	9	1	0	0
5	B	1	16	6	9	1	0	0
5	C	1	16	6	9	1	0	0
5	D	1	16	6	9	1	0	0

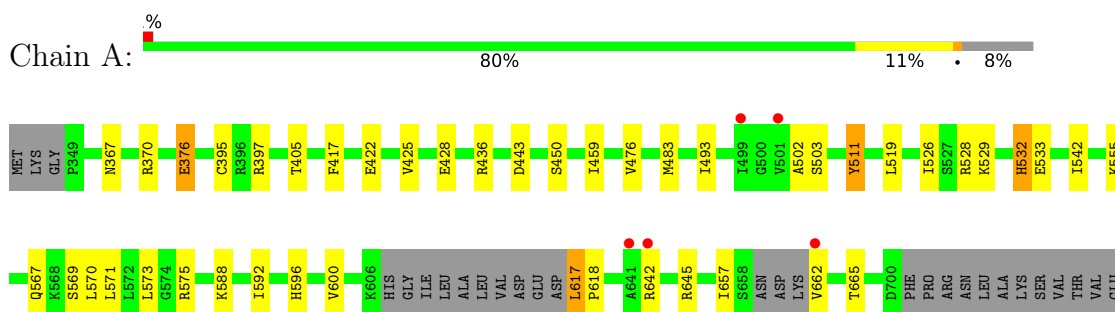
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	196	196	196	0	0
6	B	189	189	189	0	0
6	C	168	168	168	0	0
6	D	195	195	195	0	0

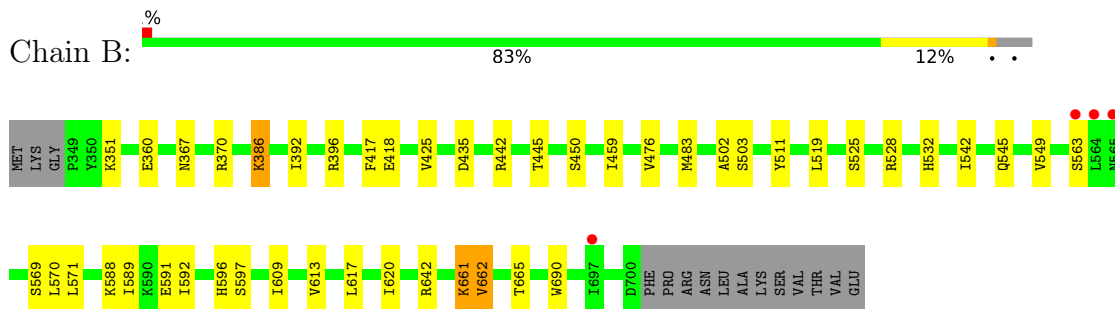
3 Residue-property plots [i](#)

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

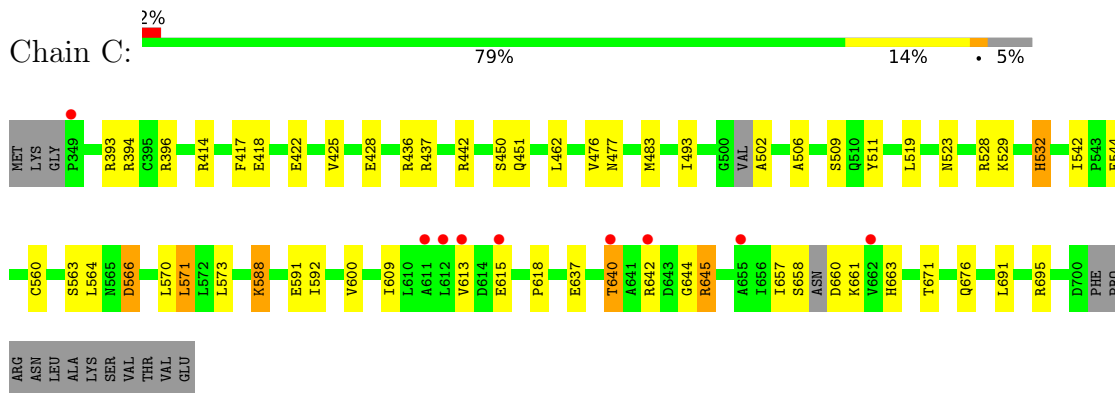
- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)




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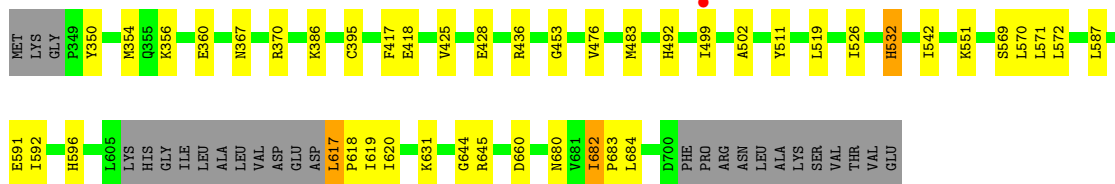


- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)



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Chain D:  81% 11% 7%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.03Å 118.19Å 100.03Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	19.94 – 1.90 19.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-1.90) 99.6 (19.94-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.171 , 0.215 0.171 , 0.215	Depositor DCC
R_{free} test set	2419 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11779	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: ACT, F6R, UD1, NA

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	1.00	1/2687 (0.0%)	1.02	1/3627 (0.0%)
1	B	0.99	2/2790 (0.1%)	1.01	1/3770 (0.0%)
1	C	0.98	1/2803 (0.0%)	0.98	1/3783 (0.0%)
1	D	0.98	2/2722 (0.1%)	1.01	2/3676 (0.1%)
All	All	0.99	6/11002 (0.1%)	1.01	5/14856 (0.0%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	542	ILE	CA-CB	12.02	1.60	1.54
1	B	542	ILE	CA-CB	11.73	1.60	1.54
1	A	542	ILE	CA-CB	7.75	1.58	1.54
1	D	542	ILE	CA-CB	6.56	1.58	1.53
1	D	645	ARG	N-CA	5.88	1.50	1.46
1	B	662	VAL	CA-C	5.32	1.59	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	VAL	N-CA-C	-14.74	87.28	108.36
1	D	644	GLY	N-CA-C	6.13	121.41	114.67
1	D	682	ILE	CB-CA-C	-5.63	106.63	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	TYR	N-CA-C	-5.44	105.25	111.07
1	C	644	GLY	N-CA-C	-5.24	105.91	111.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	661	LYS	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	2642	0	2702	35	0
1	B	2742	0	2798	32	0
1	C	2745	0	2812	44	0
1	D	2670	0	2725	33	0
2	A	4	0	3	0	0
2	C	4	0	3	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
4	A	39	0	25	1	0
4	B	39	0	25	0	0
4	C	39	0	25	1	0
4	D	39	0	25	1	0
5	A	16	0	11	1	0
5	B	16	0	11	1	0
5	C	16	0	11	1	0
5	D	16	0	11	1	0
6	A	196	0	0	4	0
6	B	189	0	0	4	0
6	C	168	0	0	6	0
6	D	195	0	0	7	0
All	All	11779	0	11187	139	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 (139) 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:459:ILE:HD13	1:B:483:MET:SD	1.92	1.10
1:C:502:ALA:HB3	1:C:592:ILE:HD11	1.34	1.08
1:B:386:LYS:HA	6:B:5565:HOH:O	1.54	1.07
1:C:502:ALA:CB	1:C:592:ILE:HD11	1.87	1.04
1:A:493:ILE:HD11	6:A:5691:HOH:O	1.71	0.90
1:C:451[B]:GLN:HE22	1:C:493:ILE:HD11	1.36	0.88
1:A:642:ARG:O	1:A:642:ARG:HG3	1.71	0.87
1:B:351:LYS:HE3	1:B:690:TRP:HH2	1.40	0.85
1:B:502:ALA:HB2	1:B:592:ILE:HD11	1.59	0.83
1:A:567:GLN:HG3	1:A:618:PRO:HG3	1.63	0.79
1:C:451[B]:GLN:NE2	1:C:493:ILE:HD11	2.02	0.74
1:C:428:GLU:OE1	1:C:436[A]:ARG:NH2	2.20	0.73
1:A:395:CYS:HB3	1:C:442[B]:ARG:NH1	2.04	0.72
1:B:351:LYS:HE3	1:B:690:TRP:CH2	2.25	0.72
1:B:591:GLU:OE1	5:B:5004:F6R:H1C1	1.90	0.71
1:A:570:LEU:HD13	1:A:618:PRO:HB2	1.74	0.70
1:C:591:GLU:OE1	5:C:5005:F6R:H1C1	1.92	0.69
1:A:526:ILE:HD13	1:D:526:ILE:HG12	1.75	0.69
1:A:376:GLU:H	1:A:376:GLU:CD	2.00	0.68
1:D:428:GLU:OE1	1:D:436[A]:ARG:NH2	2.25	0.68
1:D:350:TYR:HD2	1:D:356:LYS:HE3	1.58	0.68
1:B:665:THR:HG23	6:B:5418:HOH:O	1.93	0.68
1:B:502:ALA:CB	1:B:592:ILE:HD11	2.24	0.67
1:D:591[A]:GLU:OE1	5:D:5006:F6R:H1C1	1.95	0.67
1:B:571:LEU:HG	1:B:617:LEU:HD21	1.76	0.66
1:A:428:GLU:OE1	1:A:436[A]:ARG:NH2	2.26	0.64
1:D:631:LYS:HE2	6:D:5188:HOH:O	1.99	0.63
1:C:691:LEU:O	1:C:695:ARG:HD2	1.98	0.63
1:B:418:GLU:OE2	6:B:5682:HOH:O	2.15	0.63
1:C:451[B]:GLN:CD	1:C:477:ASN:HB2	2.23	0.62
1:A:502:ALA:HB2	1:A:592:ILE:HD11	1.80	0.62
1:A:645:ARG:HE	1:A:662:VAL:HG11	1.64	0.62
1:A:502:ALA:CB	1:A:592:ILE:HD11	2.31	0.60
1:A:367:ASN:OD1	1:A:370:ARG:NH2	2.34	0.60
1:A:596:HIS:CD2	1:B:609:ILE:HD12	2.36	0.60
1:D:660:ASP:O	6:D:5114:HOH:O	2.17	0.59
1:B:571:LEU:HD21	6:B:5738:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:CD1	1:A:483:MET:HG2	2.34	0.58
1:A:459:ILE:HD13	1:A:483:MET:HG2	1.87	0.57
1:C:451[B]:GLN:CD	1:C:506:ALA:HB1	2.30	0.57
1:D:502:ALA:HB2	1:D:592:ILE:HD11	1.87	0.56
1:D:386:LYS:HE2	6:D:5012:HOH:O	2.05	0.56
1:D:350:TYR:CD2	1:D:356:LYS:HE3	2.40	0.56
1:A:422:GLU:OE2	1:A:528:ARG:NH2	2.39	0.55
1:D:587:LEU:HD12	1:D:591[B]:GLU:HG3	1.87	0.55
1:C:566:ASP:OD1	1:C:566:ASP:N	2.36	0.55
1:B:525:SER:OG	1:B:528:ARG:HG2	2.07	0.54
1:C:502:ALA:HB2	1:C:592:ILE:HD11	1.84	0.54
1:A:571:LEU:HG	1:A:617:LEU:CD2	2.37	0.54
1:A:395:CYS:HB3	1:C:442[B]:ARG:HH12	1.68	0.53
1:C:637:GLU:HG3	6:C:5626:HOH:O	2.08	0.53
1:A:443:ASP:CG	6:A:5727:HOH:O	2.51	0.53
1:A:376:GLU:CD	1:A:376:GLU:N	2.67	0.53
1:B:459:ILE:CD1	1:B:483:MET:SD	2.83	0.53
1:C:502:ALA:CB	1:C:592:ILE:CD1	2.76	0.52
1:C:637:GLU:O	1:C:640:THR:HG22	2.08	0.52
1:B:613:VAL:O	1:B:642:ARG:NH2	2.43	0.52
1:C:544:GLU:HG3	6:C:5568:HOH:O	2.10	0.52
1:A:569:SER:OG	1:A:596:HIS:ND1	2.38	0.51
1:D:572:LEU:HD21	1:D:684:LEU:HD11	1.92	0.51
1:D:570:LEU:HD21	1:D:620:ILE:HD12	1.93	0.51
1:C:493:ILE:HD12	1:C:509[B]:SER:OG	2.10	0.51
1:A:571:LEU:HG	1:A:617:LEU:HD22	1.93	0.51
1:B:396:ARG:HD3	6:D:5077:HOH:O	2.11	0.51
1:A:526:ILE:CD1	1:D:526:ILE:HG12	2.40	0.50
1:C:609:ILE:O	1:C:613:VAL:HG13	2.11	0.50
1:B:417:PHE:HB3	1:B:425:VAL:HG21	1.93	0.50
1:C:417:PHE:HB3	1:C:425:VAL:HG21	1.94	0.49
1:C:462:LEU:HD22	1:C:483[A]:MET:CE	2.42	0.49
6:A:5727:HOH:O	1:C:394:ARG:HG2	2.13	0.49
1:B:525:SER:CB	1:B:528:ARG:HG2	2.42	0.49
1:C:483[B]:MET:HE1	6:C:5287:HOH:O	2.13	0.49
4:A:5002:UD1:H8'2	4:A:5002:UD1:H5'2	1.94	0.49
1:B:392:ILE:HG23	1:B:445:THR:HG21	1.95	0.49
1:A:575:ARG:HD3	1:B:435:ASP:OD2	2.13	0.48
4:C:5004:UD1:H8'2	4:C:5004:UD1:H5'2	1.95	0.48
4:D:5005:UD1:H8'2	4:D:5005:UD1:H5'2	1.95	0.48
1:B:503:SER:O	1:B:588:LYS:CE	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LEU:O	1:A:532:HIS:HE1	1.96	0.47
1:A:450:SER:O	1:A:476:VAL:HA	2.14	0.47
1:D:551:LYS:CE	6:D:5198:HOH:O	2.61	0.47
1:D:360:GLU:O	1:D:360:GLU:HG2	2.13	0.47
1:D:571:LEU:HG	1:D:617:LEU:HD11	1.97	0.46
1:D:569:SER:O	1:D:618:PRO:HD2	2.15	0.46
1:C:396:ARG:HD3	6:C:5164:HOH:O	2.14	0.46
1:B:545:GLN:O	1:B:549:VAL:HG23	2.16	0.46
1:A:529:LYS:O	1:A:533:GLU:HG3	2.16	0.46
1:B:459:ILE:HD11	1:B:483:MET:HG2	1.98	0.46
1:B:360:GLU:HG2	1:B:360:GLU:O	2.15	0.45
6:A:5727:HOH:O	1:C:394:ARG:CG	2.64	0.45
1:D:417:PHE:HB3	1:D:425:VAL:HG21	1.98	0.45
1:B:367:ASN:OD1	1:B:370:ARG:NH2	2.49	0.45
1:C:544:GLU:CG	6:C:5568:HOH:O	2.63	0.45
1:C:573:LEU:HD23	1:C:600:VAL:HB	1.97	0.45
1:D:453:GLY:O	1:D:483:MET:HG2	2.16	0.45
1:A:405:THR:OG1	5:A:5003:F6R:H1C2	2.16	0.45
1:A:417:PHE:HB3	1:A:425:VAL:HG21	1.98	0.45
1:C:658:SER:HB2	1:C:661:LYS:H	1.82	0.45
1:B:450:SER:O	1:B:476:VAL:HA	2.17	0.45
1:C:609:ILE:HD12	1:D:596:HIS:CD2	2.52	0.45
1:A:459:ILE:CD1	1:A:483:MET:CG	2.95	0.44
1:A:573:LEU:HD23	1:A:600:VAL:HB	1.98	0.44
1:D:502:ALA:CB	1:D:592:ILE:HD11	2.46	0.44
1:C:451[B]:GLN:CD	1:C:506:ALA:CB	2.90	0.44
1:B:569:SER:HA	1:B:596:HIS:O	2.18	0.44
1:B:519:LEU:O	1:B:532:HIS:HE1	2.01	0.43
1:C:645:ARG:O	1:C:645:ARG:HD3	2.18	0.43
1:D:367:ASN:OD1	1:D:370:ARG:CZ	2.66	0.43
1:D:682:ILE:HB	1:D:683:PRO:HD3	2.01	0.43
1:A:555:LYS:NZ	1:A:665:THR:O	2.46	0.43
1:C:450:SER:O	1:C:476[A]:VAL:HA	2.19	0.43
1:D:551:LYS:HE2	6:D:5198:HOH:O	2.18	0.43
1:C:393:ARG:NH2	1:C:523:ASN:OD1	2.51	0.43
1:C:422:GLU:OE2	1:C:528:ARG:NH2	2.50	0.43
1:C:560:CYS:HA	1:C:564:LEU:HB2	2.00	0.42
1:D:476:VAL:O	1:D:492:HIS:HA	2.19	0.42
1:C:414:ARG:O	1:C:418:GLU:HG3	2.19	0.42
1:D:519:LEU:O	1:D:532:HIS:HE1	2.02	0.42
1:A:569:SER:O	1:A:618:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:ILE:HG13	1:C:663:HIS:CE1	2.55	0.42
1:C:571:LEU:HD11	1:C:609:ILE:HD11	2.01	0.42
1:B:570:LEU:HD22	1:B:589:ILE:CD1	2.49	0.42
1:B:570:LEU:O	1:B:597:SER:HA	2.20	0.42
1:A:519:LEU:O	1:A:532:HIS:CE1	2.73	0.42
1:C:450:SER:O	1:C:476[B]:VAL:HA	2.20	0.41
1:C:519:LEU:O	1:C:532:HIS:HE1	2.04	0.41
1:C:570:LEU:HB2	1:C:618:PRO:HB2	2.01	0.41
1:D:519:LEU:O	1:D:532:HIS:CE1	2.74	0.41
1:D:569:SER:HB2	1:D:596:HIS:ND1	2.35	0.41
1:C:671:THR:CG2	1:C:676:GLN:HA	2.51	0.41
1:D:680:ASN:O	1:D:683:PRO:HD2	2.20	0.41
1:C:502:ALA:HB1	1:C:588:LYS:HE2	2.01	0.41
1:B:442[B]:ARG:NH2	1:D:395:CYS:HB3	2.35	0.41
1:D:418[A]:GLU:HG3	1:D:425:VAL:HB	2.01	0.41
1:B:570:LEU:HD21	1:B:620:ILE:HD12	2.04	0.40
1:D:354:MET:HE1	1:D:592:ILE:HG13	2.04	0.40
1:D:551:LYS:HE3	6:D:5198:HOH:O	2.21	0.40
1:A:503:SER:O	1:A:588:LYS:CE	2.69	0.40
1:C:529:LYS:NZ	6:C:5514:HOH:O	2.54	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	335/367 (91%)	331 (99%)	4 (1%)	0	100 100
1	B	352/367 (96%)	346 (98%)	5 (1%)	1 (0%)	36 29
1	C	350/367 (95%)	345 (99%)	5 (1%)	0	100 100
1	D	341/367 (93%)	339 (99%)	2 (1%)	0	100 100
All	All	1378/1468 (94%)	1361 (99%)	16 (1%)	1 (0%)	48 40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	LYS

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	297/319 (93%)	291 (98%)	6 (2%)	48	46
1	B	308/319 (97%)	304 (99%)	4 (1%)	61	61
1	C	310/319 (97%)	298 (96%)	12 (4%)	28	21
1	D	301/319 (94%)	296 (98%)	5 (2%)	53	52
All	All	1216/1276 (95%)	1189 (98%)	27 (2%)	45	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	GLU
1	A	397	ARG
1	A	511	TYR
1	A	532	HIS
1	A	617	LEU
1	A	657	ILE
1	B	511	TYR
1	B	563	SER
1	B	661	LYS
1	B	662	VAL
1	C	437	ARG
1	C	511	TYR
1	C	532	HIS
1	C	563	SER
1	C	566	ASP
1	C	571	LEU
1	C	588	LYS
1	C	615	GLU
1	C	640	THR

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Mol	Chain	Res	Type
1	C	642	ARG
1	C	645	ARG
1	C	660	ASP
1	D	499	ILE
1	D	511	TYR
1	D	532	HIS
1	D	617	LEU
1	D	619	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	510	GLN
1	B	545	GLN
1	B	638	GLN
1	C	510	GLN
1	C	545	GLN
1	D	545	GLN
1	D	567	GLN
1	D	638	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UD1	A	5002	3	40,41,41	1.01	5 (12%)	59,62,62	1.24	4 (6%)
5	F6R	C	5005	-	15,15,15	1.05	1 (6%)	16,21,21	0.96	1 (6%)
5	F6R	B	5004	-	15,15,15	0.76	0	16,21,21	1.48	3 (18%)
5	F6R	D	5006	-	15,15,15	1.23	2 (13%)	16,21,21	1.05	0
4	UD1	C	5004	3	40,41,41	1.25	6 (15%)	59,62,62	1.22	8 (13%)
2	ACT	A	713	-	3,3,3	0.93	0	3,3,3	1.41	0
2	ACT	C	713	-	3,3,3	0.98	0	3,3,3	1.26	0
4	UD1	D	5005	3	40,41,41	1.14	6 (15%)	59,62,62	1.41	6 (10%)
5	F6R	A	5003	-	15,15,15	0.91	0	16,21,21	1.25	3 (18%)
4	UD1	B	5003	3	40,41,41	1.09	5 (12%)	59,62,62	1.43	7 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UD1	A	5002	3	-	0/26/63/63	0/3/3/3
5	F6R	C	5005	-	-	0/20/20/20	-
5	F6R	B	5004	-	-	0/20/20/20	-
5	F6R	D	5006	-	-	0/20/20/20	-
4	UD1	C	5004	3	-	0/26/63/63	0/3/3/3
4	UD1	D	5005	3	-	1/26/63/63	0/3/3/3
5	F6R	A	5003	-	-	0/20/20/20	-
4	UD1	B	5003	3	-	2/26/63/63	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5004	UD1	PB-O3A	3.34	1.63	1.59
4	C	5004	UD1	C2-N3	-3.30	1.32	1.38
4	D	5005	UD1	C4-N3	-3.11	1.33	1.38
5	C	5005	F6R	P-O3P	3.02	1.59	1.50
4	C	5004	UD1	C4-N3	-2.79	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5002	UD1	C6-C5	2.76	1.41	1.35
4	D	5005	UD1	C2-N1	-2.67	1.34	1.38
5	D	5006	F6R	P-O3P	2.67	1.58	1.50
4	C	5004	UD1	C2-N1	-2.58	1.34	1.38
4	B	5003	UD1	O2-C2	2.38	1.27	1.23
4	B	5003	UD1	C6-C5	2.34	1.40	1.35
4	A	5002	UD1	C4-N3	-2.32	1.34	1.38
4	A	5002	UD1	C2-N1	-2.30	1.34	1.38
4	B	5003	UD1	PA-O3A	2.26	1.61	1.59
4	C	5004	UD1	C5-C4	-2.19	1.38	1.43
4	D	5005	UD1	PA-O3A	2.19	1.61	1.59
4	D	5005	UD1	O2-C2	2.18	1.26	1.23
4	A	5002	UD1	C5-C4	-2.18	1.39	1.43
4	B	5003	UD1	C4-N3	-2.16	1.34	1.38
4	D	5005	UD1	C2-N3	-2.15	1.34	1.38
4	A	5002	UD1	O2-C2	2.12	1.26	1.23
4	D	5005	UD1	C5-C4	-2.10	1.39	1.43
4	B	5003	UD1	PB-O3A	2.09	1.61	1.59
5	D	5006	F6R	P-O1P	-2.05	1.47	1.54
4	C	5004	UD1	PB-O2B	-2.01	1.46	1.55

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5005	UD1	C4-N3-C2	-4.81	120.64	126.61
4	B	5003	UD1	C4-N3-C2	-4.36	121.20	126.61
4	B	5003	UD1	C5-C4-N3	4.29	120.81	114.80
4	D	5005	UD1	N3-C2-N1	4.12	120.25	114.89
4	D	5005	UD1	C5-C4-N3	4.03	120.45	114.80
4	C	5004	UD1	C5-C4-N3	3.85	120.19	114.80
4	B	5003	UD1	N3-C2-N1	3.67	119.67	114.89
5	B	5004	F6R	O1P-P-O6	3.63	116.13	106.67
4	A	5002	UD1	C5-C4-N3	3.60	119.84	114.80
4	A	5002	UD1	C4-N3-C2	-3.36	122.45	126.61
4	A	5002	UD1	N3-C2-N1	3.35	119.26	114.89
4	B	5003	UD1	O4-C4-C5	-3.29	119.49	125.16
4	C	5004	UD1	C6-C5-C4	-2.85	115.89	119.53
4	C	5004	UD1	O4-C4-C5	-2.74	120.43	125.16
4	B	5003	UD1	O3A-PA-O1A	2.70	118.82	110.70
5	A	5003	F6R	O4-C4-C3	-2.62	104.58	109.29
4	C	5004	UD1	O3A-PA-O1A	2.59	118.51	110.70
5	B	5004	F6R	O3-C3-C4	-2.50	104.95	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5005	UD1	O4-C4-C5	-2.33	121.14	125.16
4	C	5004	UD1	O6'-C6'-C5'	-2.29	103.54	111.33
4	A	5002	UD1	O4-C4-C5	-2.28	121.23	125.16
4	B	5003	UD1	O5'-C5'-C4'	2.28	113.81	109.70
5	C	5005	F6R	O1-C1-C2	-2.22	106.85	112.73
4	C	5004	UD1	O1'-PB-O1B	-2.20	102.78	109.81
5	A	5003	F6R	O1P-P-O6	2.19	112.38	106.67
4	C	5004	UD1	C4-N3-C2	-2.13	123.97	126.61
5	A	5003	F6R	O4-C4-C5	2.11	113.73	108.93
5	B	5004	F6R	O1-C1-C2	-2.08	107.21	112.73
4	D	5005	UD1	O3B-C3B-C4B	-2.05	105.18	111.08
4	C	5004	UD1	N3-C2-N1	2.04	117.54	114.89
4	D	5005	UD1	O5'-C5'-C4'	2.03	113.37	109.70
4	B	5003	UD1	O2B-PB-O1'	2.00	114.85	106.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5003	UD1	C4'-C5'-C6'-O6'
4	B	5003	UD1	O5'-C5'-C6'-O6'
4	D	5005	UD1	C4'-C5'-C6'-O6'

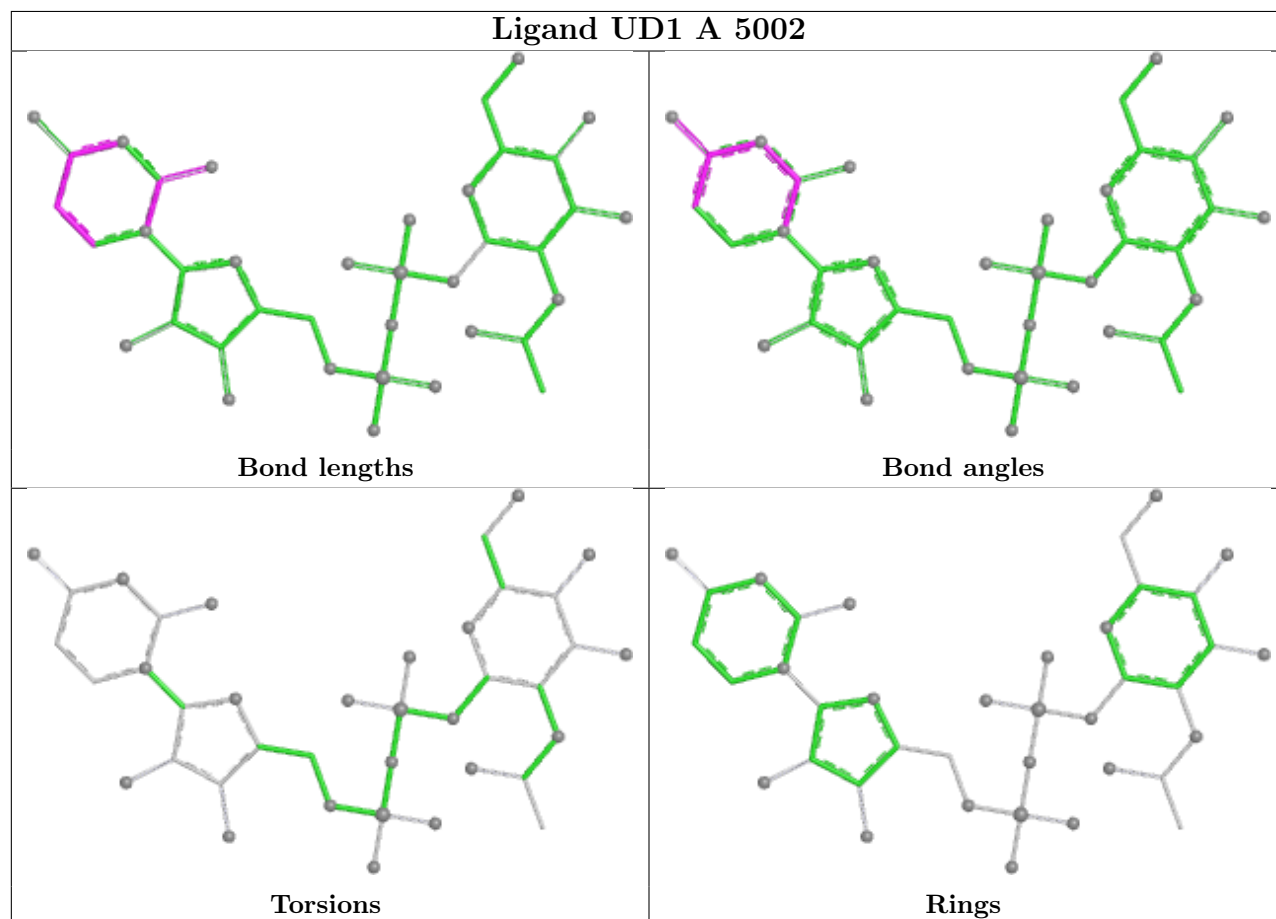
There are no ring outliers.

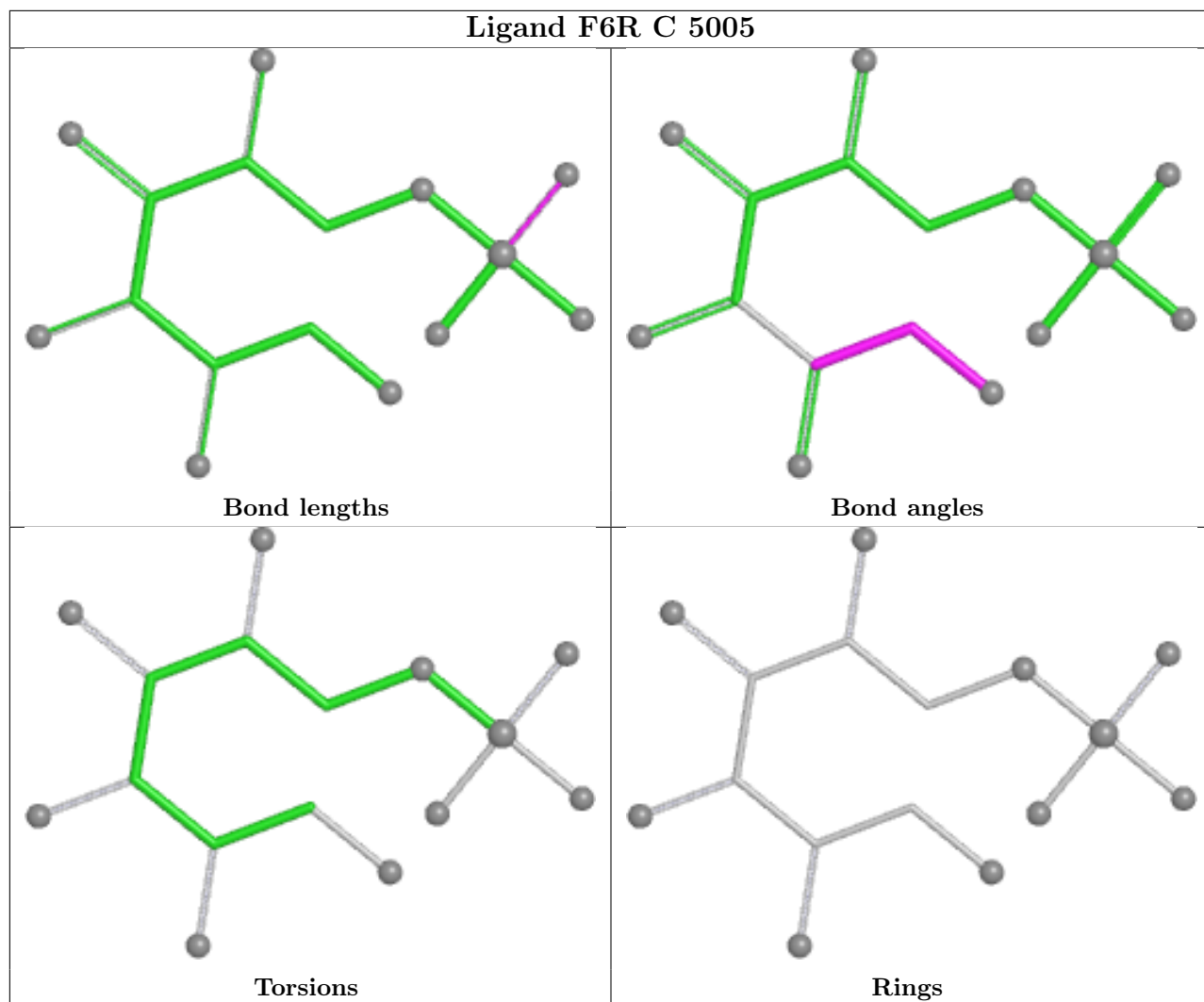
7 monomers are involved in 7 short contacts:

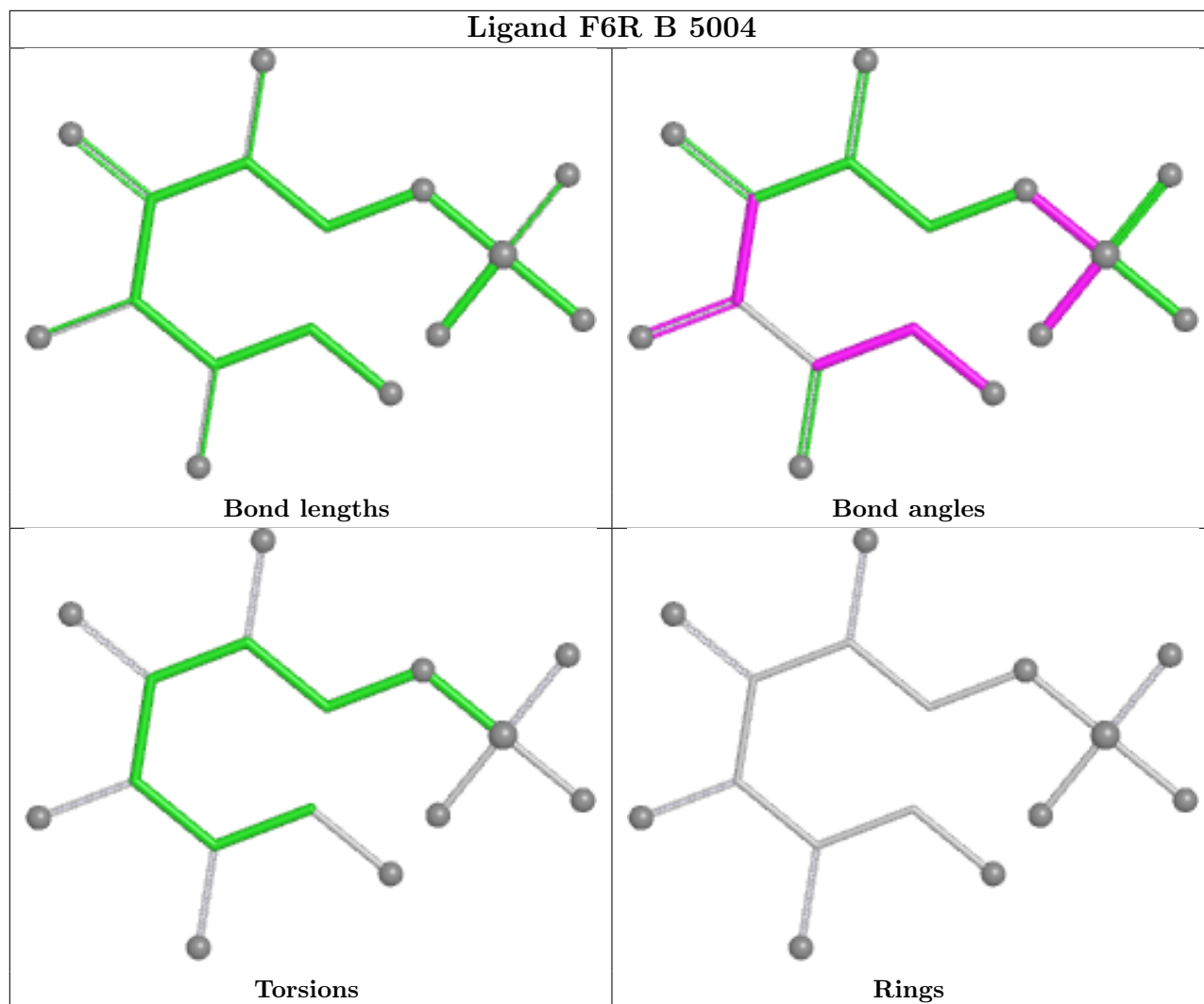
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5002	UD1	1	0
5	C	5005	F6R	1	0
5	B	5004	F6R	1	0
5	D	5006	F6R	1	0
4	C	5004	UD1	1	0
4	D	5005	UD1	1	0
5	A	5003	F6R	1	0

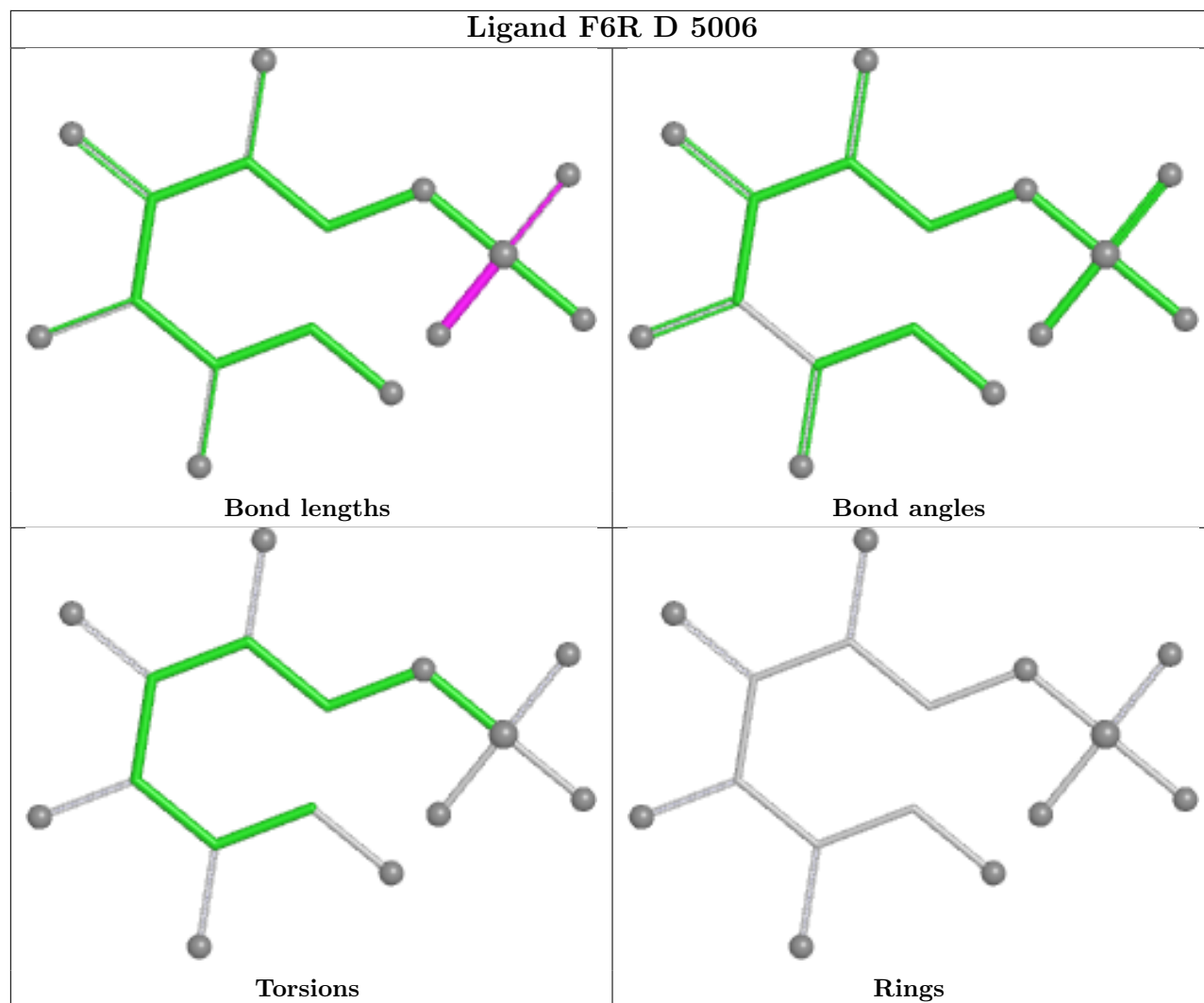
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

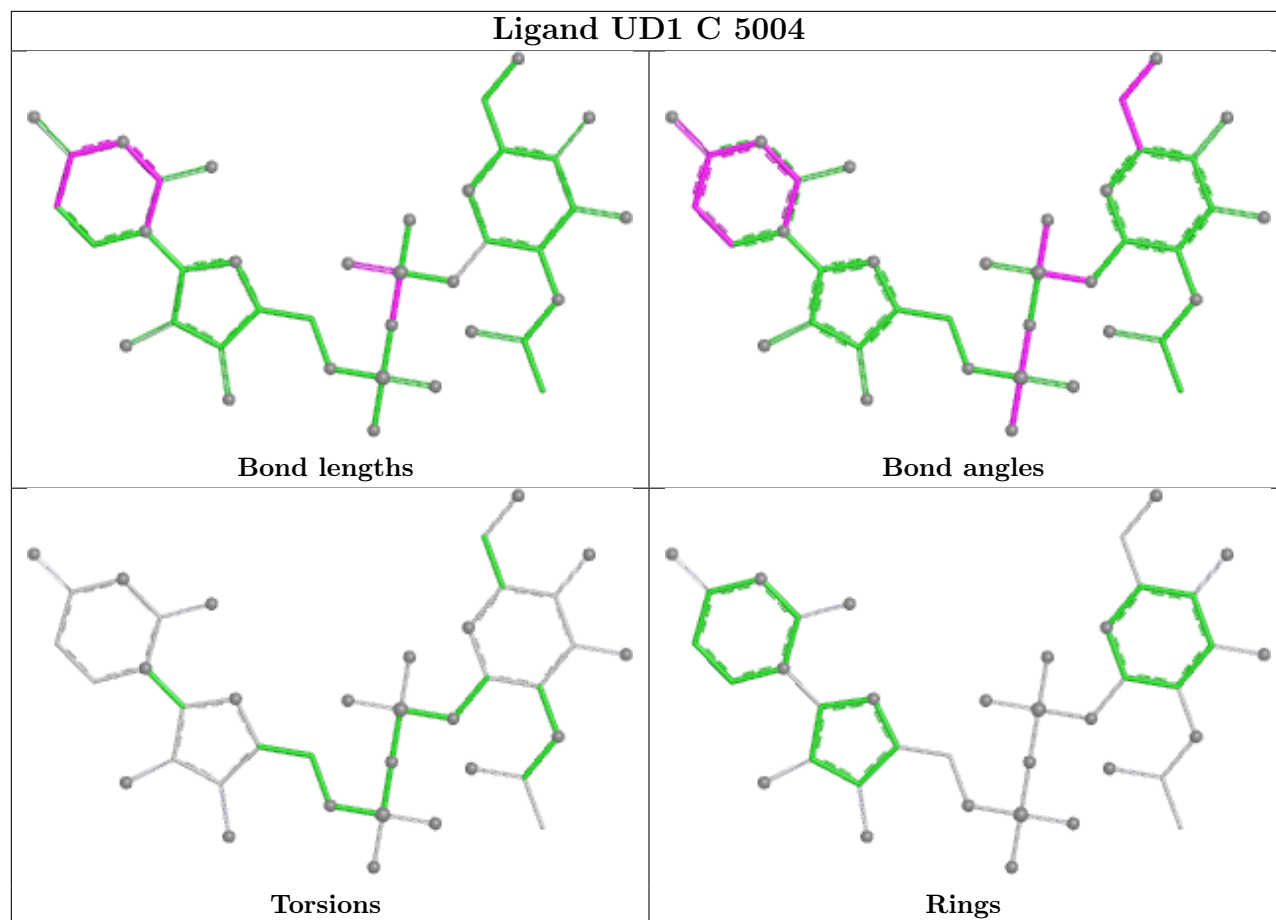
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

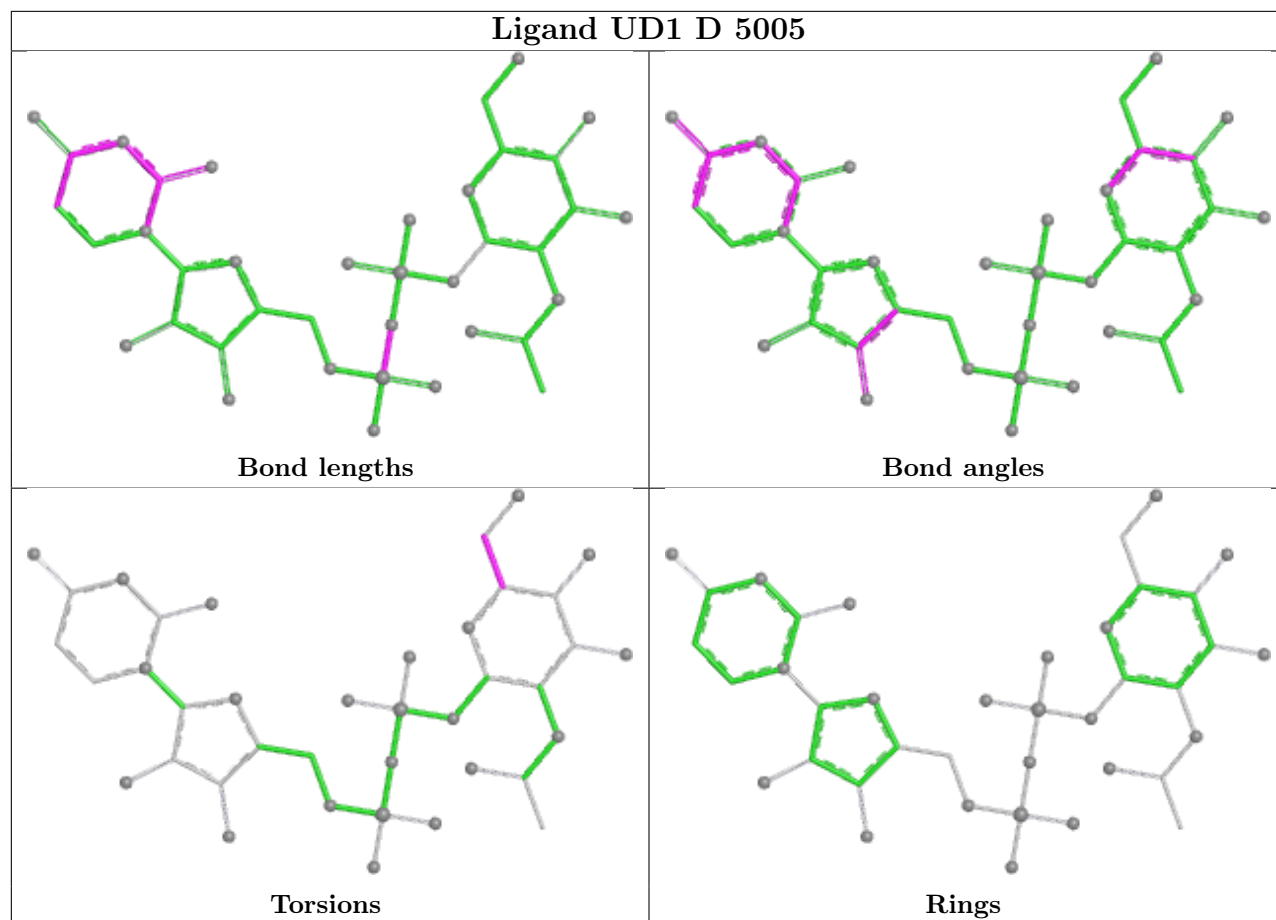


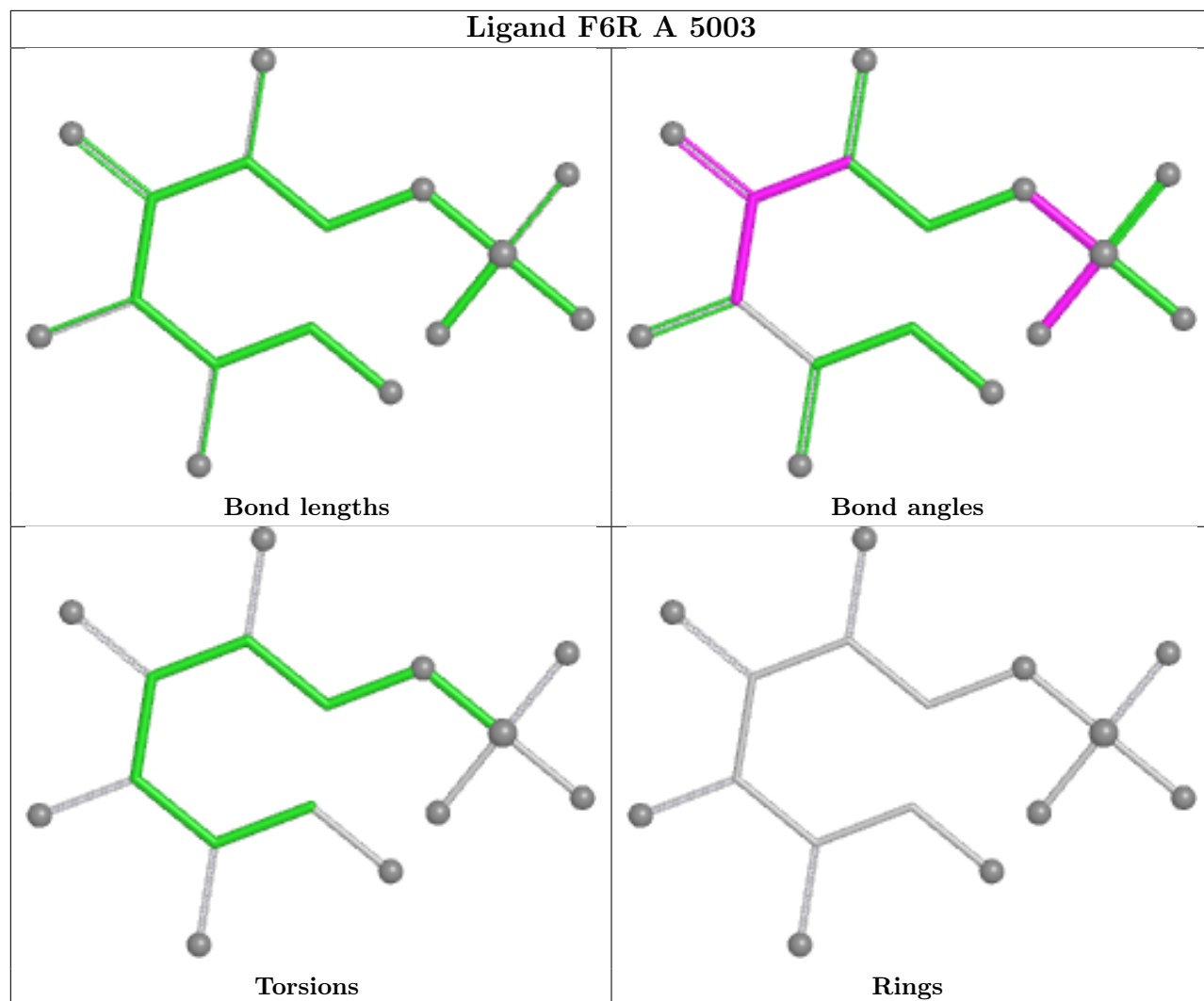


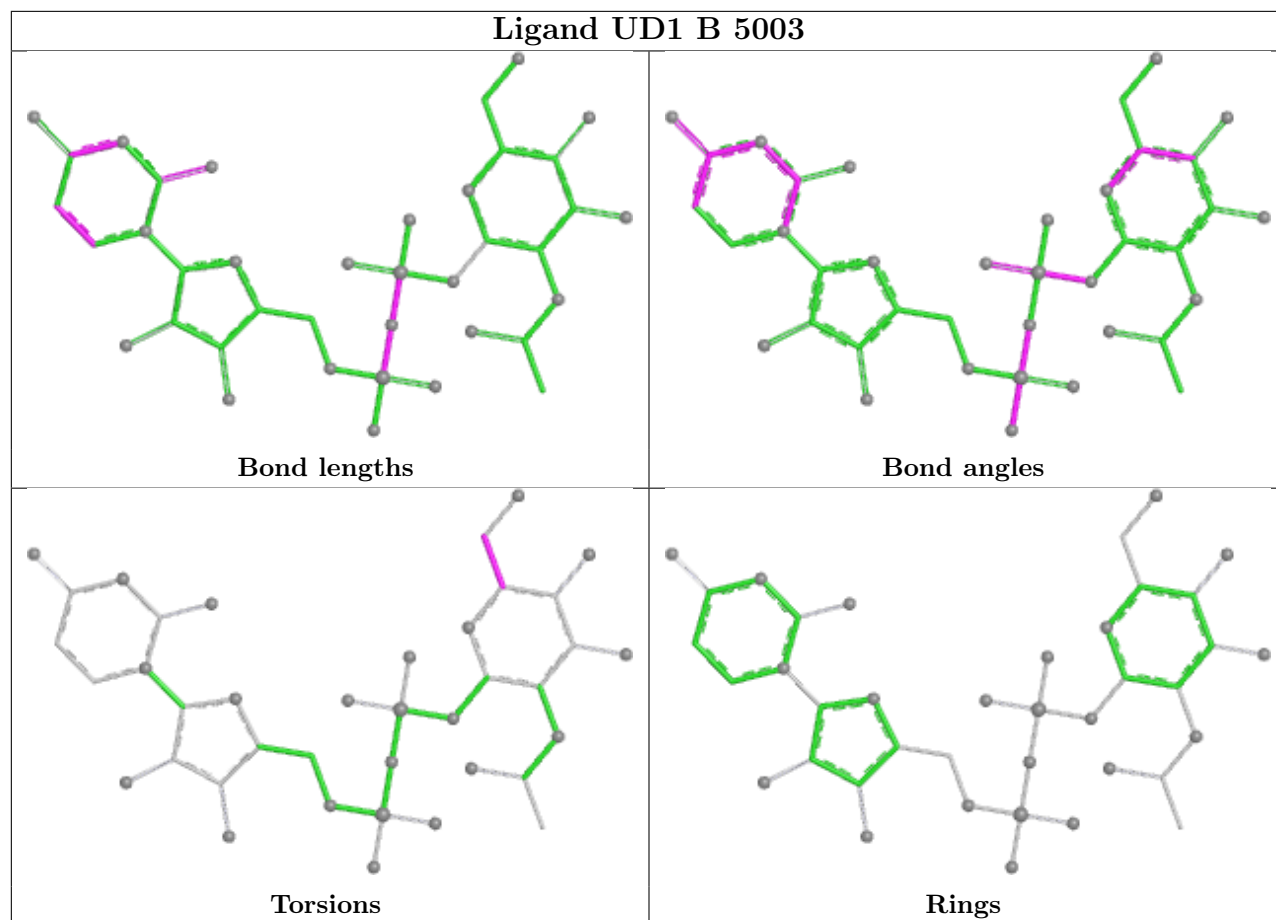












5.7 Other polymers [i](#)

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	339/367 (92%)	-0.31	5 (1%) 72 75	12, 22, 40, 53	2 (0%)
1	B	352/367 (95%)	-0.27	4 (1%) 78 80	11, 22, 46, 58	2 (0%)
1	C	350/367 (95%)	-0.18	9 (2%) 57 61	10, 24, 50, 63	6 (1%)
1	D	341/367 (92%)	-0.38	1 (0%) 90 91	9, 21, 37, 47	4 (1%)
All	All	1382/1468 (94%)	-0.29	19 (1%) 73 76	9, 22, 44, 63	14 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	641	ALA	3.8
1	C	662	VAL	3.4
1	C	611	ALA	3.3
1	C	655	ALA	3.0
1	C	640	THR	2.8
1	C	612	LEU	2.7
1	A	642	ARG	2.6
1	A	499	ILE	2.6
1	C	349	PRO	2.4
1	C	642	ARG	2.3
1	B	697	ILE	2.3
1	C	613	VAL	2.3
1	B	564	LEU	2.3
1	B	563	SER	2.2
1	B	565	ASN	2.2
1	D	499	ILE	2.2
1	A	501	VAL	2.2
1	C	615	GLU	2.1
1	A	662	VAL	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](#)

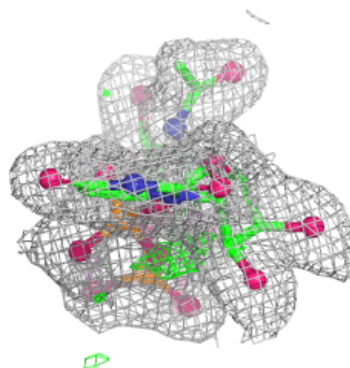
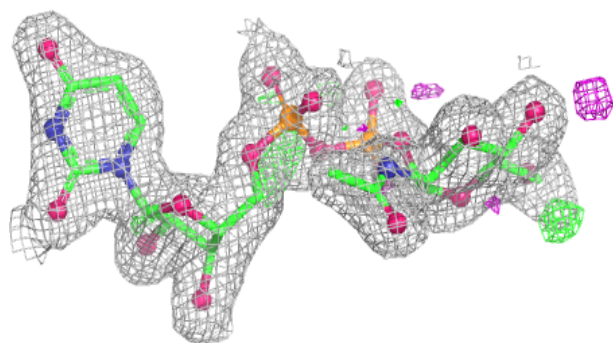
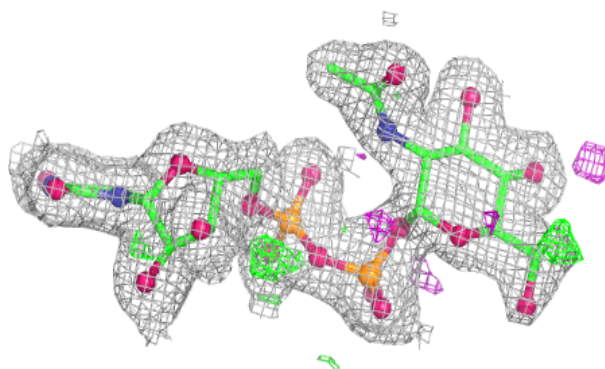
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	A	713	4/4	0.88	0.11	32,32,33,33	0
2	ACT	C	713	4/4	0.89	0.12	32,32,33,34	0
4	UD1	C	5004	39/39	0.96	0.07	14,23,28,37	0
4	UD1	B	5003	39/39	0.97	0.07	16,24,53,56	0
4	UD1	A	5002	39/39	0.97	0.06	18,24,45,50	0
4	UD1	D	5005	39/39	0.97	0.06	17,24,44,46	0
5	F6R	B	5004	16/16	0.97	0.07	15,22,36,36	0
5	F6R	C	5005	16/16	0.97	0.08	22,30,39,44	0
3	NA	A	5001	1/1	0.98	0.04	20,20,20,20	0
5	F6R	A	5003	16/16	0.98	0.05	17,22,30,30	0
3	NA	C	5003	1/1	0.98	0.03	20,20,20,20	0
3	NA	D	5004	1/1	0.98	0.07	23,23,23,23	0
5	F6R	D	5006	16/16	0.98	0.05	18,23,27,28	0
3	NA	B	5002	1/1	0.99	0.03	19,19,19,19	0

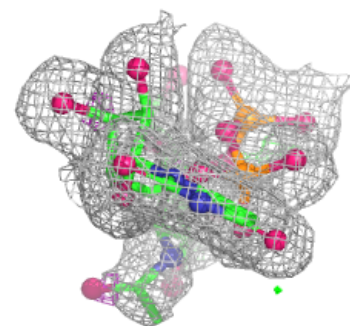
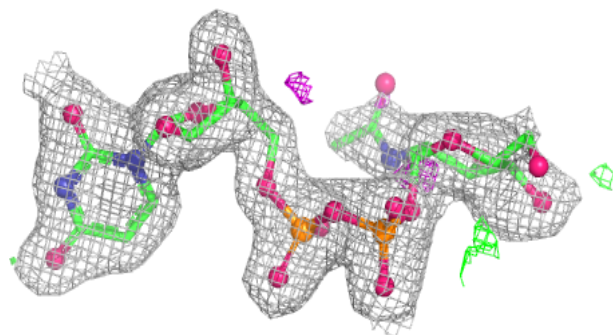
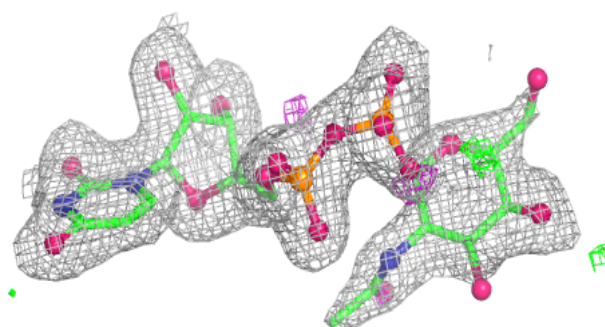
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UD1 C 5004:

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

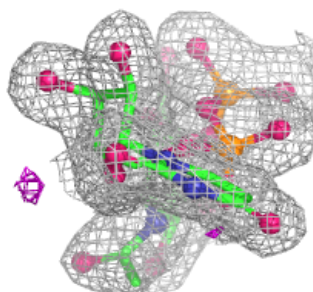
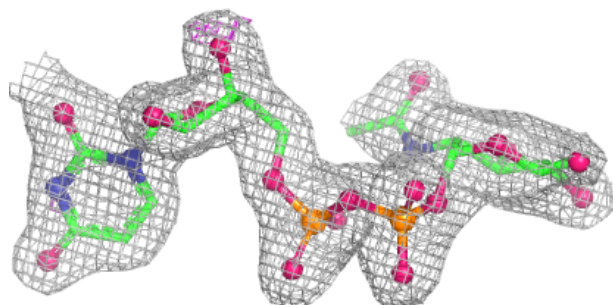
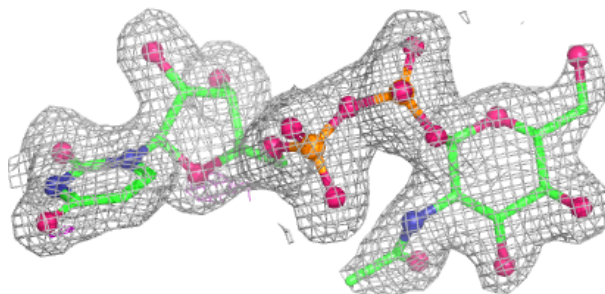
**Electron density around UD1 B 5003:**

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

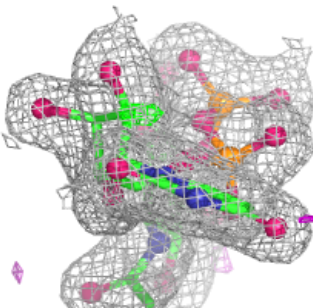
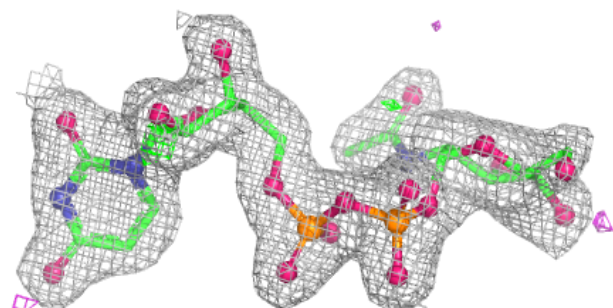
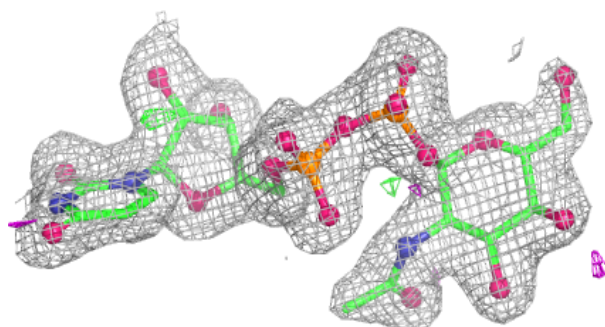


Electron density around UD1 A 5002:

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

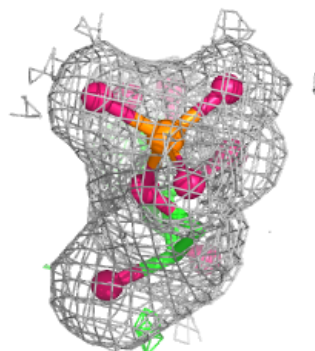
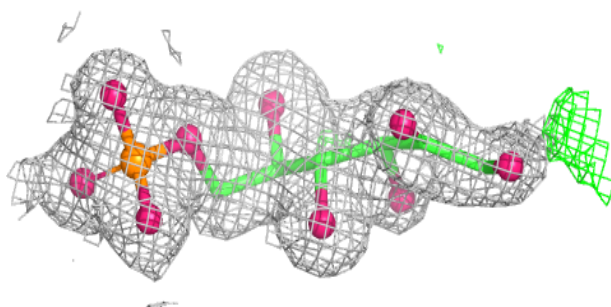
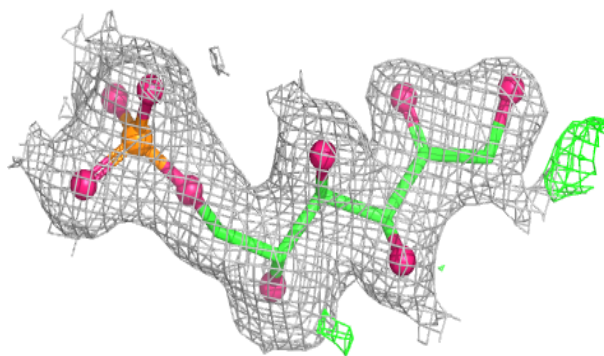
**Electron density around UD1 D 5005:**

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

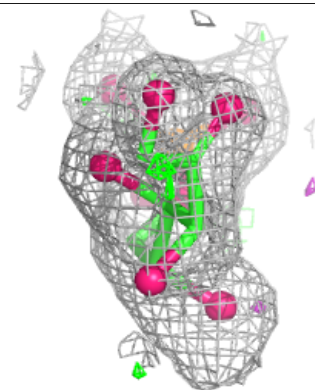
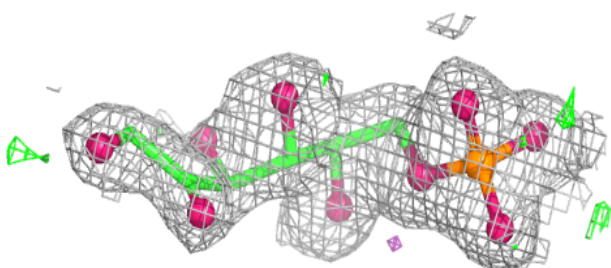
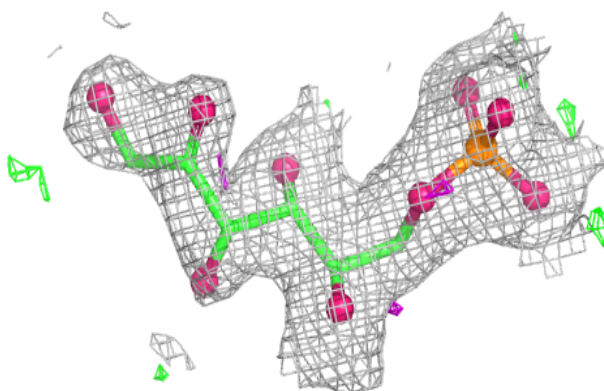


Electron density around F6R B 5004:

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

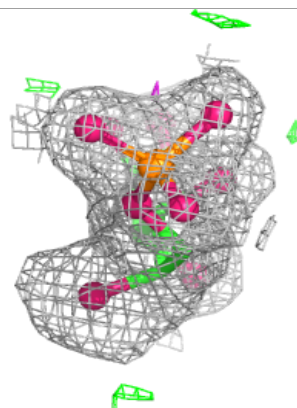
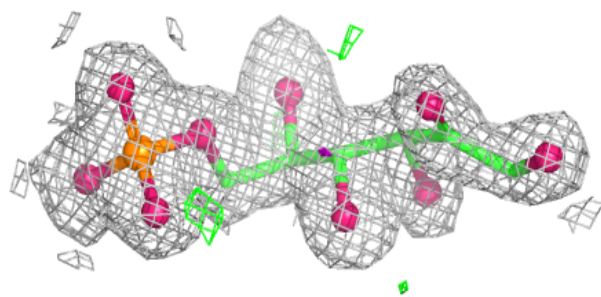
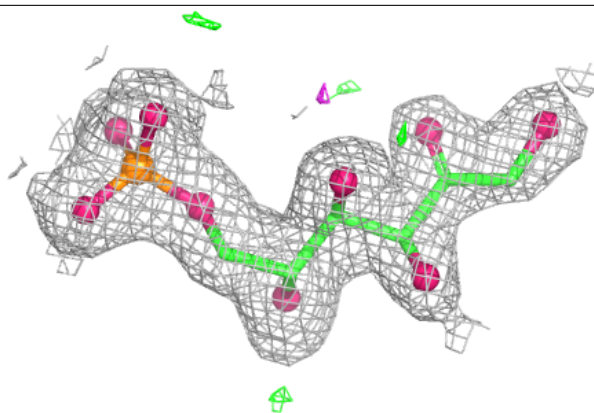
**Electron density around F6R C 5005:**

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

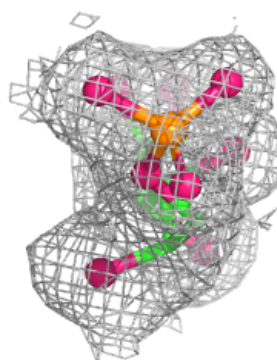
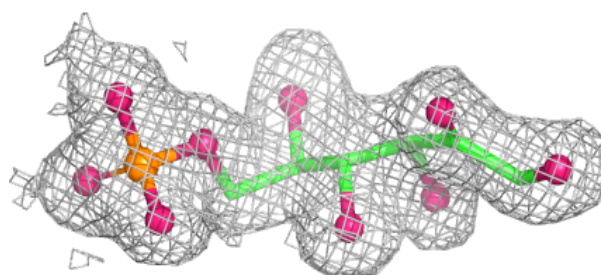
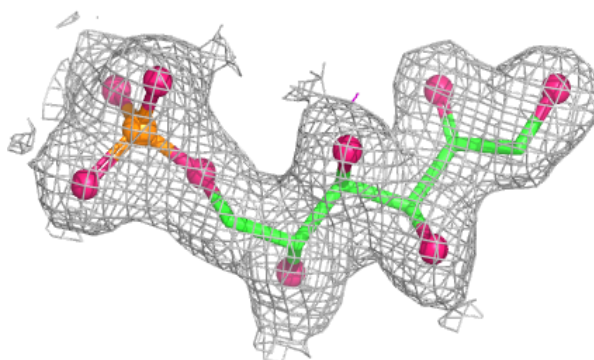


Electron density around F6R A 5003:

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

**Electron density around F6R D 5006:**

$2mF_o-DF_c$ (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.