



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:27 PM UTC

PDB ID : 8FM0 / pdb_00008fm0
Title : HIV-1 gp120 complex with CJF-III-214
Authors : Gong, Z.; Hendrickson, W.A.
Deposited on : 2022-12-22
Resolution : 2.08 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

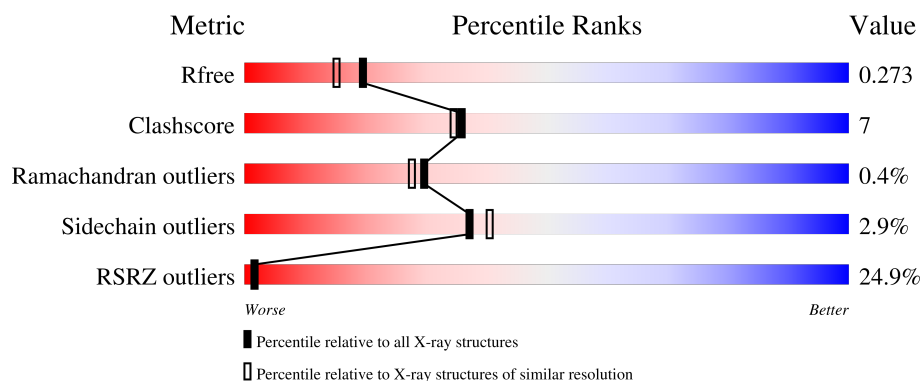
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	358	
1	B	358	
1	C	358	
1	D	358	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11208 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	A	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	C	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	D	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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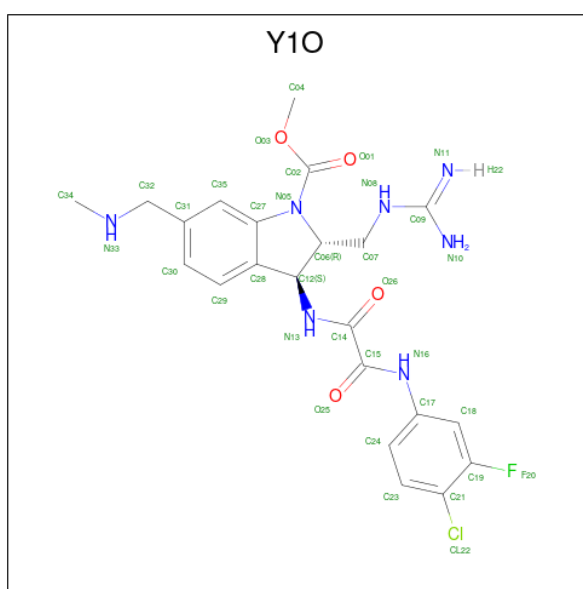
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is methyl (2R,3S)-2-(carbamimidamidomethyl)-3-[2-(4-chloro-3-fluoroanilino)(oxo)acetamido]-6-[(methylamino)methyl]-2,3-dihydro-1H-indole-1-carboxylate (CCD ID: Y1O) (formula: C₂₂H₂₅ClFN₇O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	F	N	O	0	0
			35	22	1	1	7	4		
3	A	1	Total	C	Cl	F	N	O	0	0
			35	22	1	1	7	4		
3	C	1	Total	C	Cl	F	N	O	0	0
			35	22	1	1	7	4		
3	D	1	Total	C	Cl	F	N	O	0	0
			35	22	1	1	7	4		

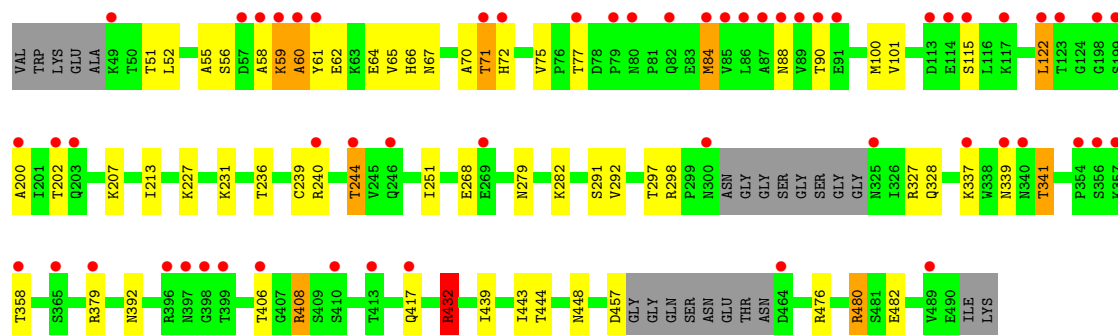
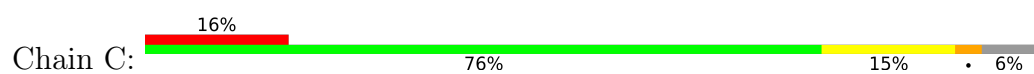
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	43	Total 43 O 43	0	0

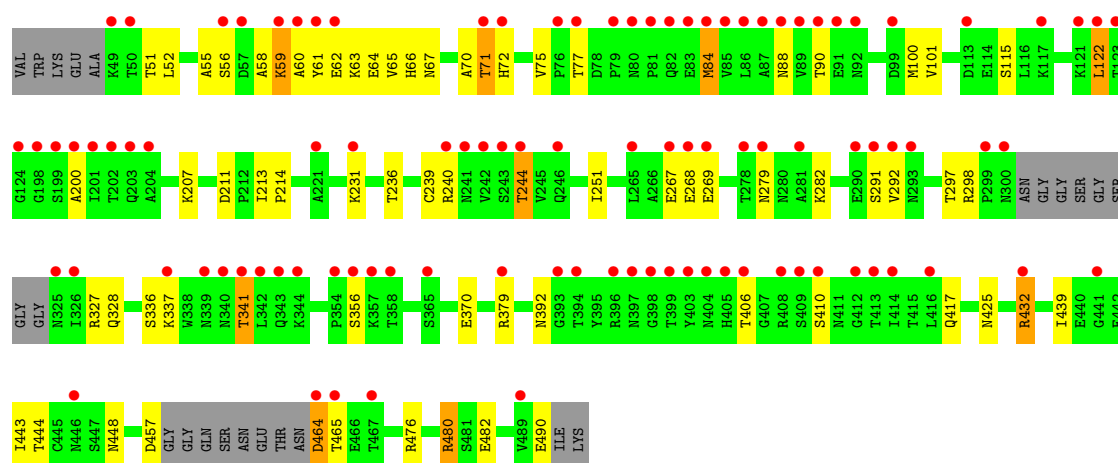
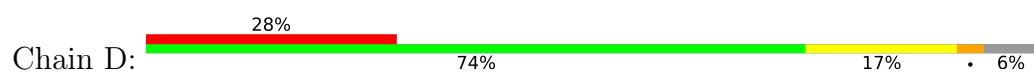
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total 40	O 40	0	0
4	C	55	Total 55	O 55	0	0
4	D	58	Total 58	O 58	0	0



• Molecule 1: Envelope glycoprotein gp120



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.80Å 120.89Å 195.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 2.08 48.79 – 2.08	Depositor EDS
% Data completeness (in resolution range)	70.8 (48.79-2.08) 70.8 (48.79-2.08)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.253 , 0.273 0.253 , 0.273	Depositor DCC
R_{free} test set	2000 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11208	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 16.49% 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: Y1O, NAG

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	0.45	1/2682 (0.0%)	0.84	8/3640 (0.2%)
1	B	0.45	1/2682 (0.0%)	0.84	8/3640 (0.2%)
1	C	0.45	1/2682 (0.0%)	0.84	8/3640 (0.2%)
1	D	0.45	1/2682 (0.0%)	0.84	7/3640 (0.2%)
All	All	0.45	4/10728 (0.0%)	0.84	31/14560 (0.2%)

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	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	THR	CB-CG2	-6.47	1.31	1.52
1	A	244	THR	CB-CG2	-6.46	1.31	1.52
1	D	244	THR	CB-CG2	-6.44	1.31	1.52
1	B	244	THR	CB-CG2	-6.42	1.31	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	MET	CB-CG-SD	-8.50	87.21	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	MET	CB-CG-SD	-8.49	87.23	112.70
1	B	84	MET	CB-CG-SD	-8.48	87.27	112.70
1	C	84	MET	CB-CG-SD	-8.47	87.28	112.70
1	B	122	LEU	CB-CG-CD2	-7.21	89.06	110.70
1	D	122	LEU	CB-CG-CD2	-7.21	89.07	110.70
1	C	122	LEU	CB-CG-CD2	-7.21	89.08	110.70
1	A	122	LEU	CB-CG-CD2	-7.20	89.09	110.70
1	B	71	THR	CA-C-N	-5.46	113.94	122.73
1	B	71	THR	C-N-CA	-5.46	113.94	122.73
1	C	71	THR	CA-C-N	-5.44	113.97	122.73
1	C	71	THR	C-N-CA	-5.44	113.97	122.73
1	A	71	THR	CA-C-N	-5.42	114.01	122.73
1	A	71	THR	C-N-CA	-5.42	114.01	122.73
1	D	71	THR	CA-C-N	-5.41	114.02	122.73
1	D	71	THR	C-N-CA	-5.41	114.02	122.73
1	B	59	LYS	CA-CB-CG	-5.35	103.40	114.10
1	A	59	LYS	CA-CB-CG	-5.35	103.41	114.10
1	D	59	LYS	CA-CB-CG	-5.34	103.41	114.10
1	C	59	LYS	CA-CB-CG	-5.34	103.43	114.10
1	D	432	ARG	CB-CG-CD	5.17	123.19	111.30
1	C	432	ARG	CB-CG-CD	5.17	123.19	111.30
1	B	432	ARG	CB-CG-CD	5.16	123.17	111.30
1	D	122	LEU	CB-CG-CD1	5.15	126.16	110.70
1	A	432	ARG	CB-CG-CD	5.15	123.15	111.30
1	C	122	LEU	CB-CG-CD1	5.15	126.15	110.70
1	A	122	LEU	CB-CG-CD1	5.15	126.14	110.70
1	B	122	LEU	CB-CG-CD1	5.14	126.12	110.70
1	B	408	ARG	CB-CG-CD	-5.01	99.77	111.30
1	A	408	ARG	CB-CG-CD	-5.01	99.77	111.30
1	C	408	ARG	CB-CG-CD	-5.01	99.79	111.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	327	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	432	ARG	Sidechain
1	A	480	ARG	Sidechain
1	A	88	ASN	Peptide
1	B	327	ARG	Sidechain
1	B	379	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	432	ARG	Sidechain
1	B	480	ARG	Sidechain
1	B	88	ASN	Peptide
1	C	327	ARG	Sidechain
1	C	379	ARG	Sidechain
1	C	432	ARG	Sidechain
1	C	480	ARG	Sidechain
1	C	88	ASN	Peptide
1	D	327	ARG	Sidechain
1	D	379	ARG	Sidechain
1	D	432	ARG	Sidechain
1	D	480	ARG	Sidechain
1	D	88	ASN	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	2627	0	2540	35	2
1	B	2627	0	2542	34	2
1	C	2627	0	2540	45	0
1	D	2627	0	2542	45	1
2	A	98	0	91	3	0
2	B	84	0	78	2	0
2	C	98	0	91	5	0
2	D	84	0	78	3	1
3	A	35	0	0	0	0
3	B	35	0	0	0	0
3	C	35	0	0	0	0
3	D	35	0	0	0	0
4	A	40	0	0	3	0
4	B	43	0	0	1	0
4	C	55	0	0	1	0
4	D	58	0	0	3	0
All	All	11208	0	10502	156	3

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 7.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ALA:O	1:D:59:LYS:HE3	1.60	1.02
1:C:60:ALA:C	1:D:59:LYS:HE3	1.90	0.94
1:C:59:LYS:NZ	1:D:211:ASP:OD2	2.03	0.92
1:A:124:GLY:O	4:A:601:HOH:O	1.88	0.90
1:D:267:GLU:O	4:D:601:HOH:O	1.89	0.89
1:D:448:ASN:ND2	4:D:602:HOH:O	1.97	0.86
1:A:422:GLN:NE2	4:A:602:HOH:O	2.08	0.85
1:A:404:ASN:ND2	1:C:408:ARG:HA	1.93	0.83
1:B:489:VAL:HG22	1:B:490:GLU:HB2	1.67	0.74
1:D:84:MET:SD	1:D:244:THR:CG2	2.78	0.72
1:A:84:MET:SD	1:A:244:THR:CG2	2.78	0.72
1:C:84:MET:SD	1:C:244:THR:CG2	2.78	0.72
1:B:84:MET:SD	1:B:244:THR:CG2	2.78	0.71
1:C:60:ALA:HB2	1:D:61:TYR:CZ	2.26	0.71
1:C:60:ALA:HB2	1:D:61:TYR:OH	1.91	0.69
1:C:337:LYS:O	1:C:341:THR:HG23	1.96	0.66
1:A:337:LYS:O	1:A:341:THR:HG23	1.96	0.65
1:D:337:LYS:O	1:D:341:THR:HG23	1.96	0.65
1:B:337:LYS:O	1:B:341:THR:HG23	1.96	0.65
1:A:231:LYS:HG3	1:A:268:GLU:OE2	1.97	0.65
2:C:503:NAG:H3	2:C:503:NAG:H83	1.79	0.65
1:B:231:LYS:HG3	1:B:268:GLU:OE2	1.97	0.64
2:D:503:NAG:H83	2:D:503:NAG:H3	1.79	0.64
1:D:231:LYS:HG3	1:D:268:GLU:OE2	1.97	0.64
1:D:67:ASN:O	1:D:71:THR:OG1	2.16	0.63
2:A:503:NAG:H83	2:A:503:NAG:H3	1.79	0.63
1:C:67:ASN:O	1:C:71:THR:OG1	2.16	0.63
2:B:503:NAG:H83	2:B:503:NAG:H3	1.79	0.63
1:C:231:LYS:HG3	1:C:268:GLU:OE2	1.97	0.63
1:A:67:ASN:O	1:A:71:THR:OG1	2.16	0.62
1:B:67:ASN:O	1:B:71:THR:OG1	2.16	0.61
1:C:339:ASN:ND2	2:C:508:NAG:H83	2.16	0.61
1:A:251:ILE:HG23	1:A:482:GLU:HG3	1.88	0.56
1:B:251:ILE:HG23	1:B:482:GLU:HG3	1.88	0.56
1:D:490:GLU:O	4:D:603:HOH:O	2.18	0.56
1:D:251:ILE:HG23	1:D:482:GLU:HG3	1.88	0.55
1:A:480:ARG:NH1	4:A:605:HOH:O	2.39	0.55
1:C:251:ILE:HG23	1:C:482:GLU:HG3	1.88	0.54
1:B:90:THR:HA	1:B:239:CYS:O	2.07	0.54
1:D:90:THR:HA	1:D:239:CYS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASN:OD1	1:D:406:THR:HB	2.08	0.54
1:A:84:MET:SD	1:A:244:THR:HG22	2.48	0.54
1:A:90:THR:HA	1:A:239:CYS:O	2.07	0.54
1:A:404:ASN:HD22	1:C:408:ARG:HA	1.73	0.54
1:B:84:MET:SD	1:B:244:THR:HG22	2.48	0.54
1:A:392:ASN:OD1	1:A:406:THR:HB	2.08	0.54
1:C:84:MET:SD	1:C:244:THR:HG22	2.48	0.53
1:C:90:THR:HA	1:C:239:CYS:O	2.07	0.53
1:B:392:ASN:OD1	1:B:406:THR:HB	2.08	0.53
2:B:503:NAG:H3	2:B:503:NAG:C8	2.39	0.53
1:C:417:GLN:HA	1:C:417:GLN:OE1	2.09	0.53
2:C:503:NAG:H3	2:C:503:NAG:C8	2.39	0.53
1:D:84:MET:SD	1:D:244:THR:HG22	2.48	0.53
1:B:417:GLN:HA	1:B:417:GLN:OE1	2.09	0.53
1:B:422:GLN:HG2	1:C:432:ARG:NH2	2.24	0.53
1:C:392:ASN:OD1	1:C:406:THR:HB	2.08	0.53
1:D:417:GLN:HA	1:D:417:GLN:OE1	2.09	0.53
1:B:476:ARG:O	1:B:480:ARG:HG3	2.09	0.52
1:C:476:ARG:O	1:C:480:ARG:HG3	2.09	0.52
1:D:84:MET:SD	1:D:244:THR:HG21	2.49	0.52
1:D:476:ARG:O	1:D:480:ARG:HG3	2.09	0.52
2:D:503:NAG:H3	2:D:503:NAG:C8	2.39	0.52
2:A:503:NAG:H3	2:A:503:NAG:C8	2.39	0.52
1:A:476:ARG:O	1:A:480:ARG:HG3	2.09	0.52
1:B:84:MET:SD	1:B:244:THR:HG21	2.49	0.52
1:A:84:MET:SD	1:A:244:THR:HG21	2.49	0.52
1:B:101:VAL:HG12	1:B:476:ARG:HG2	1.93	0.51
1:A:101:VAL:HG12	1:A:476:ARG:HG2	1.92	0.51
1:C:60:ALA:CB	1:D:61:TYR:OH	2.58	0.51
1:C:84:MET:SD	1:C:244:THR:HG21	2.49	0.51
1:A:417:GLN:HA	1:A:417:GLN:OE1	2.09	0.51
1:C:101:VAL:HG12	1:C:476:ARG:HG2	1.92	0.51
1:A:292:VAL:CG2	1:A:341:THR:HG21	2.41	0.50
1:D:101:VAL:HG12	1:D:476:ARG:HG2	1.92	0.50
1:D:292:VAL:CG2	1:D:341:THR:HG21	2.42	0.50
1:B:122:LEU:HD12	1:B:200:ALA:HB2	1.93	0.50
1:C:292:VAL:CG2	1:C:341:THR:HG21	2.41	0.50
1:D:122:LEU:HD12	1:D:200:ALA:HB2	1.93	0.50
1:C:122:LEU:HD12	1:C:200:ALA:HB2	1.94	0.50
1:A:122:LEU:HD12	1:A:200:ALA:HB2	1.93	0.50
1:A:56:SER:C	1:A:77:THR:HG23	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:SER:C	1:C:77:THR:HG23	2.37	0.50
1:B:56:SER:C	1:B:77:THR:HG23	2.37	0.49
1:B:298:ARG:HG2	1:B:328:GLN:O	2.13	0.49
1:B:292:VAL:CG2	1:B:341:THR:HG21	2.41	0.49
1:D:207:LYS:HD2	1:D:439:ILE:HG23	1.94	0.49
1:D:298:ARG:HG2	1:D:328:GLN:O	2.13	0.49
1:B:207:LYS:HD2	1:B:439:ILE:HG23	1.94	0.49
1:A:207:LYS:HD2	1:A:439:ILE:HG23	1.94	0.49
1:A:298:ARG:HG2	1:A:328:GLN:O	2.13	0.49
1:D:56:SER:C	1:D:77:THR:HG23	2.37	0.48
1:B:422:GLN:HG2	1:C:432:ARG:HH22	1.78	0.48
1:C:298:ARG:HG2	1:C:328:GLN:O	2.13	0.48
1:C:207:LYS:HD2	1:C:439:ILE:HG23	1.94	0.48
1:B:279:ASN:OD1	1:B:282:LYS:HG2	2.14	0.47
1:C:227:LYS:HE2	4:C:649:HOH:O	2.14	0.47
1:B:58:ALA:HB2	1:B:70:ALA:HB3	1.97	0.47
1:A:279:ASN:OD1	1:A:282:LYS:HG2	2.15	0.47
1:C:297:THR:OG1	1:C:444:THR:OG1	2.32	0.47
1:D:279:ASN:OD1	1:D:282:LYS:HG2	2.14	0.47
1:D:58:ALA:HB2	1:D:70:ALA:HB3	1.97	0.47
1:C:60:ALA:CA	1:D:61:TYR:OH	2.63	0.47
1:C:279:ASN:OD1	1:C:282:LYS:HG2	2.14	0.46
1:B:291:SER:HB2	1:B:448:ASN:HB3	1.98	0.46
1:D:291:SER:HB2	1:D:448:ASN:HB3	1.98	0.46
1:A:55:ALA:HA	1:A:75:VAL:O	2.16	0.46
1:C:60:ALA:O	1:D:59:LYS:CE	2.49	0.46
1:C:291:SER:HB2	1:C:448:ASN:HB3	1.97	0.46
1:D:55:ALA:HA	1:D:75:VAL:O	2.16	0.46
1:A:58:ALA:HB2	1:A:70:ALA:HB3	1.97	0.45
1:C:58:ALA:HB2	1:C:70:ALA:HB3	1.97	0.45
1:B:55:ALA:HA	1:B:75:VAL:O	2.16	0.45
1:B:297:THR:OG1	1:B:444:THR:OG1	2.32	0.45
1:A:52:LEU:HD11	1:A:100:MET:HG2	1.99	0.45
1:A:291:SER:HB2	1:A:448:ASN:HB3	1.98	0.45
1:D:292:VAL:HG21	1:D:341:THR:HG21	1.99	0.45
1:C:292:VAL:HG21	1:C:341:THR:HG21	1.99	0.45
1:C:52:LEU:HD11	1:C:100:MET:HG2	1.99	0.45
1:B:292:VAL:HG21	1:B:341:THR:HG21	1.99	0.44
1:D:297:THR:HG1	1:D:444:THR:HG1	1.62	0.44
1:C:55:ALA:HA	1:C:75:VAL:O	2.16	0.44
1:A:297:THR:HG1	1:A:444:THR:HG1	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LEU:HD11	1:D:100:MET:HG2	1.99	0.44
1:A:292:VAL:HG21	1:A:341:THR:HG21	1.99	0.43
1:D:62:GLU:OE2	1:D:64:GLU:HB2	2.18	0.43
1:A:90:THR:HA	1:A:240:ARG:HA	2.01	0.43
1:D:90:THR:HA	1:D:240:ARG:HA	2.01	0.43
1:B:52:LEU:HD11	1:B:100:MET:HG2	1.99	0.43
1:C:62:GLU:OE2	1:C:64:GLU:HB2	2.18	0.43
2:D:503:NAG:H83	2:D:503:NAG:C3	2.48	0.43
1:C:60:ALA:CB	1:D:61:TYR:CZ	2.98	0.42
1:D:269:GLU:H	1:D:269:GLU:HG2	1.52	0.42
1:C:90:THR:HA	1:C:240:ARG:HA	2.01	0.42
1:B:90:THR:HA	1:B:240:ARG:HA	2.01	0.42
1:B:65:VAL:HB	1:B:115:SER:HB3	2.02	0.42
1:D:464:ASP:HB3	1:D:465:THR:H	1.26	0.42
1:A:405:HIS:H	2:A:508:NAG:H81	1.84	0.42
1:C:297:THR:HA	1:C:443:ILE:O	2.20	0.42
1:C:65:VAL:HB	1:C:115:SER:HB3	2.02	0.41
1:D:297:THR:HA	1:D:443:ILE:O	2.20	0.41
1:A:65:VAL:HB	1:A:115:SER:HB3	2.02	0.41
1:A:297:THR:HA	1:A:443:ILE:O	2.20	0.41
1:B:464:ASP:HB3	1:B:465:THR:H	1.26	0.41
2:C:503:NAG:H83	2:C:503:NAG:C3	2.48	0.41
1:B:379:ARG:NH2	4:B:603:HOH:O	2.53	0.41
1:A:66:HIS:HB3	1:A:213:ILE:HG12	2.03	0.41
1:D:65:VAL:HB	1:D:115:SER:HB3	2.02	0.41
1:C:61:TYR:CE2	1:D:214:PRO:CD	3.04	0.41
1:C:66:HIS:HB3	1:C:213:ILE:HG12	2.03	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.78	0.41
2:C:503:NAG:C8	2:C:503:NAG:C3	2.99	0.41
1:B:297:THR:HA	1:B:443:ILE:O	2.20	0.40
1:D:66:HIS:HB3	1:D:213:ILE:HG12	2.03	0.40
1:B:66:HIS:HB3	1:B:213:ILE:HG12	2.02	0.40
1:B:295:VAL:O	1:B:331:CYS:HA	2.22	0.40
1:D:370:GLU:CD	1:D:425:ASN:HB2	2.47	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:GLU:OE1	1:A:80:ASN:ND2[3_444]	1.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:ND2	2:D:506:NAG:O3[3_444]	2.10	0.10
1:B:356:SER:OG	1:D:356:SER:OG[3_444]	2.13	0.07

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	329/358 (92%)	308 (94%)	19 (6%)	2 (1%)	21	17
1	B	329/358 (92%)	308 (94%)	20 (6%)	1 (0%)	36	36
1	C	329/358 (92%)	308 (94%)	20 (6%)	1 (0%)	36	36
1	D	329/358 (92%)	308 (94%)	20 (6%)	1 (0%)	36	36
All	All	1316/1432 (92%)	1232 (94%)	79 (6%)	5 (0%)	30	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	60	ALA
1	A	60	ALA
1	C	60	ALA
1	D	60	ALA
1	A	392	ASN

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	297/312 (95%)	289 (97%)	8 (3%)	39	43
1	B	297/312 (95%)	287 (97%)	10 (3%)	32	34
1	C	297/312 (95%)	290 (98%)	7 (2%)	43	47
1	D	297/312 (95%)	288 (97%)	9 (3%)	36	39
All	All	1188/1248 (95%)	1154 (97%)	34 (3%)	37	40

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	THR
1	B	62	GLU
1	B	72	HIS
1	B	113	ASP
1	B	236	THR
1	B	336	SER
1	B	341	THR
1	B	399	THR
1	B	464	ASP
1	B	489	VAL
1	A	51	THR
1	A	62	GLU
1	A	72	HIS
1	A	113	ASP
1	A	236	THR
1	A	341	THR
1	A	399	THR
1	A	464	ASP
1	C	51	THR
1	C	72	HIS
1	C	202	THR
1	C	236	THR
1	C	341	THR
1	C	358	THR
1	C	457	ASP
1	D	51	THR
1	D	63	LYS
1	D	72	HIS
1	D	236	THR
1	D	336	SER
1	D	341	THR
1	D	410	SER
1	D	457	ASP

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Mol	Chain	Res	Type
1	D	464	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	293	ASN
1	A	293	ASN
1	A	404	ASN
1	C	293	ASN
1	C	404	ASN
1	D	246	GLN
1	D	293	ASN

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](#)

30 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	$\# Z > 2$
2	NAG	D	506	1	14,14,15	0.63	0	17,19,21	1.82	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	503	1	14,14,15	0.47	0	17,19,21	1.40	1 (5%)
3	Y1O	C	507	-	36,37,37	2.50	12 (33%)	46,52,52	2.20	14 (30%)
2	NAG	A	504	1	14,14,15	0.53	0	17,19,21	0.44	0
2	NAG	A	508	1	14,14,15	0.38	0	17,19,21	0.89	1 (5%)
2	NAG	C	503	1	14,14,15	0.47	0	17,19,21	1.40	1 (5%)
2	NAG	B	501	1	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	D	502	1	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
2	NAG	D	505	1	14,14,15	0.30	0	17,19,21	0.49	0
3	Y1O	A	507	-	36,37,37	2.50	12 (33%)	46,52,52	2.20	14 (30%)
2	NAG	D	503	1	14,14,15	0.47	0	17,19,21	1.40	1 (5%)
2	NAG	A	505	1	14,14,15	0.30	0	17,19,21	0.49	0
2	NAG	C	504	1	14,14,15	0.53	0	17,19,21	0.44	0
2	NAG	B	506	1	14,14,15	0.63	0	17,19,21	1.82	2 (11%)
2	NAG	A	503	1	14,14,15	0.47	0	17,19,21	1.40	1 (5%)
2	NAG	B	502	1	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
2	NAG	C	508	1	14,14,15	0.92	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	D	504	1	14,14,15	0.53	0	17,19,21	0.44	0
2	NAG	A	506	1	14,14,15	0.63	0	17,19,21	1.82	2 (11%)
3	Y1O	D	507	-	36,37,37	2.50	12 (33%)	46,52,52	2.20	14 (30%)
2	NAG	C	505	1	14,14,15	0.30	0	17,19,21	0.49	0
2	NAG	C	501	1	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	C	506	1	14,14,15	0.63	0	17,19,21	1.82	2 (11%)
2	NAG	D	501	1	14,14,15	0.29	0	17,19,21	0.44	0
3	Y1O	B	507	-	36,37,37	2.50	12 (33%)	46,52,52	2.20	14 (30%)
2	NAG	C	502	1	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
2	NAG	B	505	1	14,14,15	0.30	0	17,19,21	0.49	0
2	NAG	A	502	1	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
2	NAG	B	504	1	14,14,15	0.53	0	17,19,21	0.44	0
2	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	506	1	-	3/6/23/26	0/1/1/1
2	NAG	B	503	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y1O	C	507	-	-	1/26/42/42	0/3/3/3
2	NAG	A	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	508	1	-	2/6/23/26	0/1/1/1
2	NAG	C	503	1	-	5/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	502	1	-	0/6/23/26	0/1/1/1
2	NAG	D	505	1	-	0/6/23/26	0/1/1/1
3	Y1O	A	507	-	-	1/26/42/42	0/3/3/3
2	NAG	D	503	1	-	5/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	C	504	1	-	2/6/23/26	0/1/1/1
2	NAG	B	506	1	-	3/6/23/26	0/1/1/1
2	NAG	A	503	1	-	5/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	C	508	1	-	4/6/23/26	0/1/1/1
2	NAG	D	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	506	1	-	3/6/23/26	0/1/1/1
3	Y1O	D	507	-	-	1/26/42/42	0/3/3/3
2	NAG	C	505	1	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	506	1	-	3/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
3	Y1O	B	507	-	-	1/26/42/42	0/3/3/3
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	507	Y1O	C09-N08	6.26	1.45	1.33
3	B	507	Y1O	C09-N08	6.26	1.45	1.33
3	A	507	Y1O	C09-N08	6.26	1.45	1.33
3	D	507	Y1O	C09-N08	6.26	1.45	1.33
3	D	507	Y1O	C02-N05	5.61	1.45	1.37
3	B	507	Y1O	C02-N05	5.61	1.45	1.37
3	A	507	Y1O	C02-N05	5.60	1.45	1.37
3	C	507	Y1O	C02-N05	5.60	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	Y1O	C14-N13	4.76	1.44	1.34
3	B	507	Y1O	C14-N13	4.76	1.44	1.34
3	C	507	Y1O	C14-N13	4.76	1.44	1.34
3	A	507	Y1O	C14-N13	4.75	1.44	1.34
3	A	507	Y1O	C06-N05	-4.63	1.42	1.47
3	D	507	Y1O	C06-N05	-4.63	1.42	1.47
3	C	507	Y1O	C06-N05	-4.63	1.42	1.47
3	B	507	Y1O	C06-N05	-4.62	1.42	1.47
3	A	507	Y1O	C15-N16	4.51	1.45	1.35
3	C	507	Y1O	C15-N16	4.51	1.45	1.35
3	D	507	Y1O	C15-N16	4.51	1.45	1.35
3	B	507	Y1O	C15-N16	4.51	1.45	1.35
3	C	507	Y1O	C12-N13	-3.89	1.38	1.46
3	A	507	Y1O	C12-N13	-3.89	1.38	1.46
3	D	507	Y1O	C12-N13	-3.89	1.38	1.46
3	B	507	Y1O	C12-N13	-3.89	1.38	1.46
3	B	507	Y1O	C12-C06	-3.62	1.51	1.55
3	C	507	Y1O	C12-C06	-3.61	1.51	1.55
3	A	507	Y1O	C12-C06	-3.61	1.51	1.55
3	D	507	Y1O	C12-C06	-3.60	1.51	1.55
2	C	508	NAG	O5-C1	2.95	1.48	1.43
3	A	507	Y1O	C28-C12	2.95	1.59	1.50
3	C	507	Y1O	C28-C12	2.95	1.59	1.50
3	B	507	Y1O	C28-C12	2.95	1.59	1.50
3	D	507	Y1O	C28-C12	2.94	1.59	1.50
3	A	507	Y1O	O03-C02	2.80	1.38	1.34
3	D	507	Y1O	O03-C02	2.80	1.38	1.34
3	C	507	Y1O	O03-C02	2.80	1.38	1.34
3	B	507	Y1O	O03-C02	2.80	1.38	1.34
3	A	507	Y1O	C09-N10	2.75	1.44	1.34
3	D	507	Y1O	C09-N10	2.75	1.44	1.34
3	B	507	Y1O	C09-N10	2.75	1.44	1.34
3	C	507	Y1O	C09-N10	2.75	1.44	1.34
3	A	507	Y1O	O26-C14	-2.71	1.18	1.23
3	D	507	Y1O	O26-C14	-2.71	1.18	1.23
3	B	507	Y1O	O26-C14	-2.71	1.18	1.23
3	C	507	Y1O	O26-C14	-2.70	1.18	1.23
3	A	507	Y1O	O25-C15	-2.44	1.18	1.23
3	D	507	Y1O	O25-C15	-2.43	1.19	1.23
3	B	507	Y1O	O25-C15	-2.43	1.19	1.23
3	C	507	Y1O	O25-C15	-2.43	1.19	1.23

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	507	Y1O	C06-C12-N13	-7.69	106.61	115.01
3	B	507	Y1O	C06-C12-N13	-7.69	106.61	115.01
3	A	507	Y1O	C06-C12-N13	-7.69	106.61	115.01
3	C	507	Y1O	C06-C12-N13	-7.68	106.61	115.01
2	A	506	NAG	C1-O5-C5	6.80	121.30	112.19
2	C	506	NAG	C1-O5-C5	6.80	121.29	112.19
2	D	506	NAG	C1-O5-C5	6.80	121.29	112.19
2	B	506	NAG	C1-O5-C5	6.80	121.29	112.19
3	A	507	Y1O	O03-C02-N05	5.70	119.26	111.06
3	C	507	Y1O	O03-C02-N05	5.70	119.26	111.06
3	B	507	Y1O	O03-C02-N05	5.70	119.26	111.06
3	D	507	Y1O	O03-C02-N05	5.70	119.26	111.06
2	B	503	NAG	C2-N2-C7	4.78	129.31	122.90
2	A	503	NAG	C2-N2-C7	4.78	129.31	122.90
2	C	503	NAG	C2-N2-C7	4.78	129.31	122.90
2	D	503	NAG	C2-N2-C7	4.78	129.30	122.90
3	A	507	Y1O	C27-N05-C06	4.05	114.20	109.75
3	D	507	Y1O	C27-N05-C06	4.05	114.20	109.75
3	B	507	Y1O	C27-N05-C06	4.05	114.20	109.75
3	C	507	Y1O	C27-N05-C06	4.05	114.20	109.75
3	A	507	Y1O	O03-C02-O01	-3.75	117.79	124.60
3	D	507	Y1O	O03-C02-O01	-3.75	117.80	124.60
3	C	507	Y1O	O03-C02-O01	-3.75	117.80	124.60
3	B	507	Y1O	O03-C02-O01	-3.75	117.80	124.60
3	C	507	Y1O	C14-C15-N16	3.44	118.07	112.25
3	B	507	Y1O	C14-C15-N16	3.44	118.06	112.25
3	D	507	Y1O	C14-C15-N16	3.44	118.06	112.25
3	A	507	Y1O	C14-C15-N16	3.44	118.06	112.25
3	B	507	Y1O	C04-O03-C02	-3.43	111.44	115.29
3	C	507	Y1O	C04-O03-C02	-3.43	111.44	115.29
3	D	507	Y1O	C04-O03-C02	-3.43	111.44	115.29
3	A	507	Y1O	C04-O03-C02	-3.43	111.44	115.29
3	A	507	Y1O	C17-N16-C15	-2.98	122.16	127.45
3	B	507	Y1O	C17-N16-C15	-2.98	122.17	127.45
3	C	507	Y1O	C17-N16-C15	-2.98	122.17	127.45
3	D	507	Y1O	C17-N16-C15	-2.98	122.17	127.45
2	A	508	NAG	C1-O5-C5	2.79	115.93	112.19
2	C	502	NAG	C1-O5-C5	2.73	115.84	112.19
2	D	502	NAG	C1-O5-C5	2.73	115.84	112.19
2	A	502	NAG	C1-O5-C5	2.73	115.84	112.19
2	B	502	NAG	C1-O5-C5	2.73	115.84	112.19
3	B	507	Y1O	C28-C12-N13	-2.41	107.73	114.77
3	C	507	Y1O	C28-C12-N13	-2.41	107.73	114.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	507	Y1O	C28-C12-N13	-2.41	107.74	114.77
3	A	507	Y1O	C28-C12-N13	-2.40	107.74	114.77
3	B	507	Y1O	C28-C27-N05	-2.36	107.55	109.42
3	A	507	Y1O	C28-C27-N05	-2.36	107.55	109.42
3	D	507	Y1O	C28-C27-N05	-2.36	107.55	109.42
3	C	507	Y1O	C28-C27-N05	-2.36	107.55	109.42
3	D	507	Y1O	C19-C21-CL22	-2.35	116.83	119.79
3	A	507	Y1O	C19-C21-CL22	-2.34	116.83	119.79
3	B	507	Y1O	C19-C21-CL22	-2.34	116.83	119.79
3	C	507	Y1O	C19-C21-CL22	-2.34	116.83	119.79
2	C	506	NAG	C3-C4-C5	2.29	114.39	110.23
2	D	506	NAG	C3-C4-C5	2.29	114.38	110.23
2	B	506	NAG	C3-C4-C5	2.29	114.38	110.23
2	A	506	NAG	C3-C4-C5	2.29	114.38	110.23
2	C	508	NAG	C1-O5-C5	2.26	115.22	112.19
3	C	507	Y1O	C31-C32-N33	-2.19	107.41	112.67
3	D	507	Y1O	C31-C32-N33	-2.19	107.41	112.67
3	B	507	Y1O	C31-C32-N33	-2.19	107.41	112.67
3	A	507	Y1O	C31-C32-N33	-2.19	107.41	112.67
3	A	507	Y1O	C23-C21-C19	2.15	120.88	119.04
3	D	507	Y1O	C23-C21-C19	2.15	120.88	119.04
3	B	507	Y1O	C23-C21-C19	2.14	120.88	119.04
3	C	507	Y1O	C23-C21-C19	2.14	120.87	119.04
3	C	507	Y1O	C15-C14-N13	2.07	118.69	113.73
3	D	507	Y1O	C15-C14-N13	2.07	118.69	113.73
3	B	507	Y1O	C15-C14-N13	2.07	118.69	113.73
3	A	507	Y1O	C15-C14-N13	2.07	118.69	113.73
3	A	507	Y1O	C35-C27-N05	2.06	132.20	128.59
3	B	507	Y1O	C35-C27-N05	2.05	132.19	128.59
3	D	507	Y1O	C35-C27-N05	2.05	132.19	128.59
3	C	507	Y1O	C35-C27-N05	2.05	132.19	128.59

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	503	NAG	O5-C5-C6-O6
2	A	503	NAG	O5-C5-C6-O6
2	C	503	NAG	O5-C5-C6-O6
2	D	503	NAG	O5-C5-C6-O6
2	B	503	NAG	C4-C5-C6-O6
2	A	503	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	503	NAG	C4-C5-C6-O6
2	D	503	NAG	C4-C5-C6-O6
2	B	504	NAG	O5-C5-C6-O6
2	A	504	NAG	O5-C5-C6-O6
2	C	504	NAG	O5-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	B	504	NAG	C4-C5-C6-O6
2	A	504	NAG	C4-C5-C6-O6
2	C	504	NAG	C4-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6
2	B	503	NAG	C8-C7-N2-C2
2	B	503	NAG	O7-C7-N2-C2
2	A	503	NAG	C8-C7-N2-C2
2	A	503	NAG	O7-C7-N2-C2
2	A	508	NAG	C8-C7-N2-C2
2	A	508	NAG	O7-C7-N2-C2
2	C	503	NAG	C8-C7-N2-C2
2	C	503	NAG	O7-C7-N2-C2
2	C	508	NAG	C8-C7-N2-C2
2	C	508	NAG	O7-C7-N2-C2
2	D	503	NAG	C8-C7-N2-C2
2	D	503	NAG	O7-C7-N2-C2
2	B	506	NAG	C4-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	C	506	NAG	C4-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	B	503	NAG	C3-C2-N2-C7
2	A	503	NAG	C3-C2-N2-C7
2	C	503	NAG	C3-C2-N2-C7
2	D	503	NAG	C3-C2-N2-C7
2	C	508	NAG	C4-C5-C6-O6
2	B	506	NAG	O5-C5-C6-O6
2	A	506	NAG	O5-C5-C6-O6
2	C	506	NAG	O5-C5-C6-O6
2	C	508	NAG	O5-C5-C6-O6
2	D	506	NAG	O5-C5-C6-O6
3	B	507	Y1O	C06-C07-N08-C09
3	A	507	Y1O	C06-C07-N08-C09
3	C	507	Y1O	C06-C07-N08-C09
3	D	507	Y1O	C06-C07-N08-C09
2	B	506	NAG	C1-C2-N2-C7
2	A	506	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	C	506	NAG	C1-C2-N2-C7
2	D	506	NAG	C1-C2-N2-C7

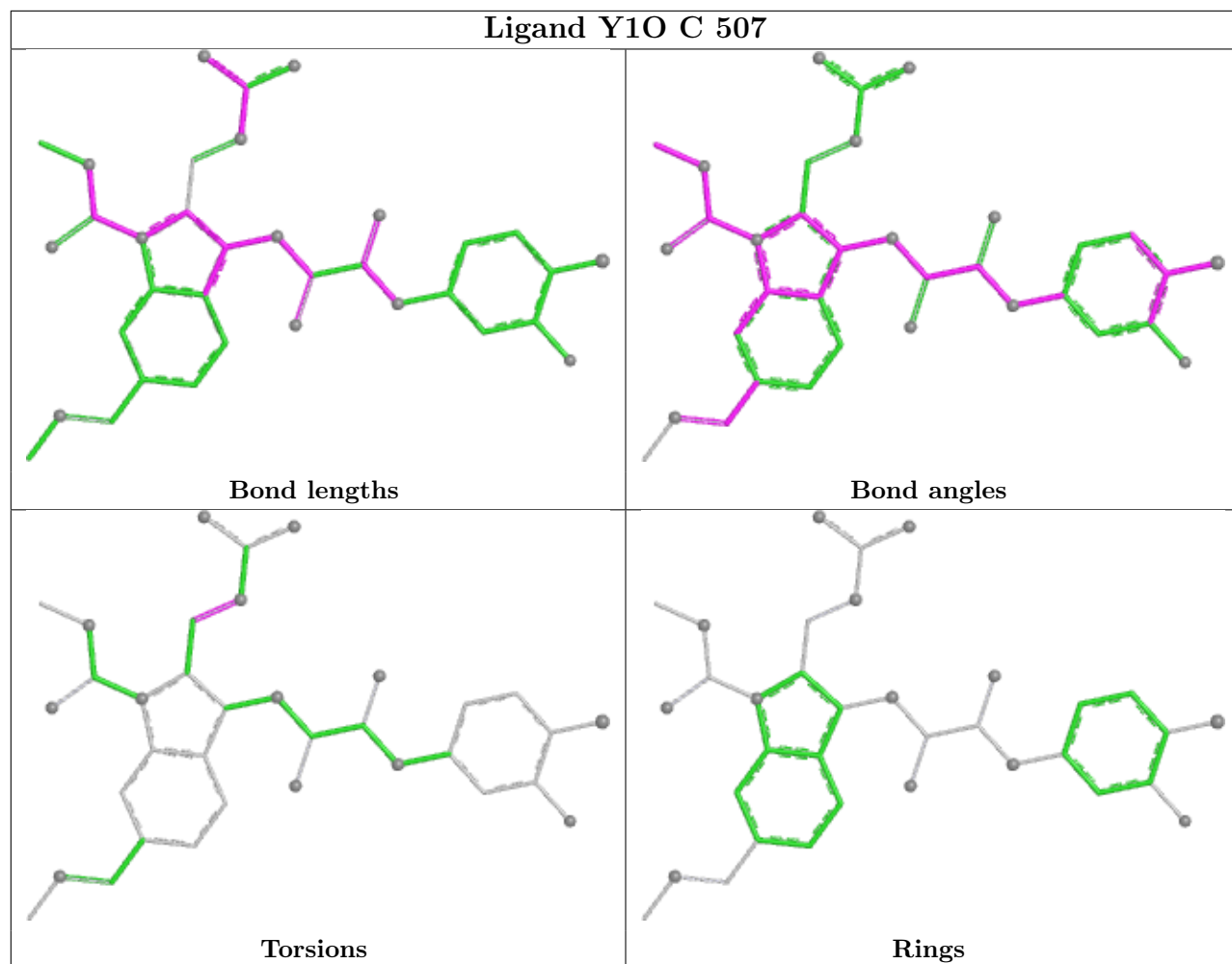
There are no ring outliers.

7 monomers are involved in 14 short contacts:

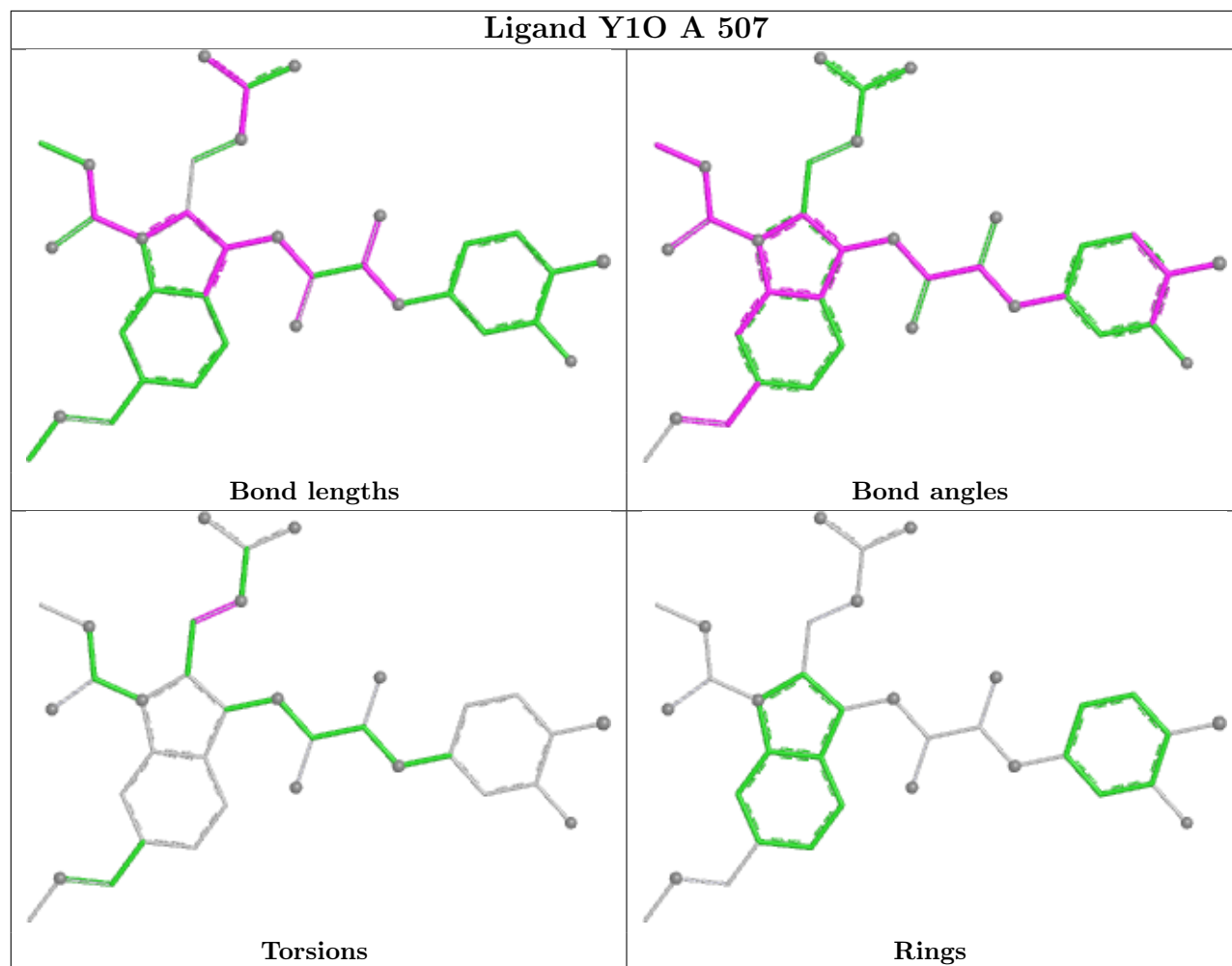
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	506	NAG	0	1
2	B	503	NAG	2	0
2	A	508	NAG	1	0
2	C	503	NAG	4	0
2	D	503	NAG	3	0
2	A	503	NAG	2	0
2	C	508	NAG	1	0

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

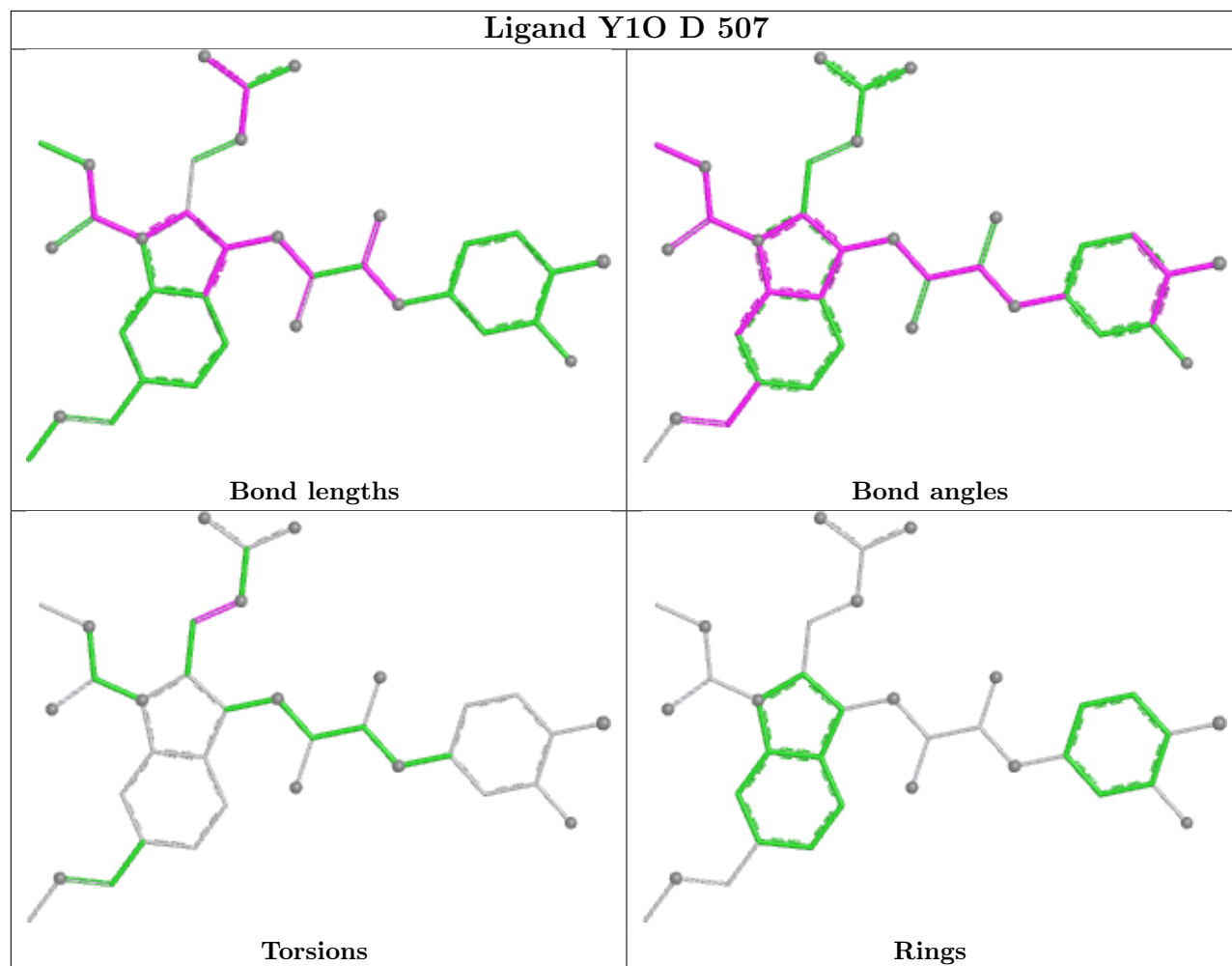
Ligand Y1O C 507

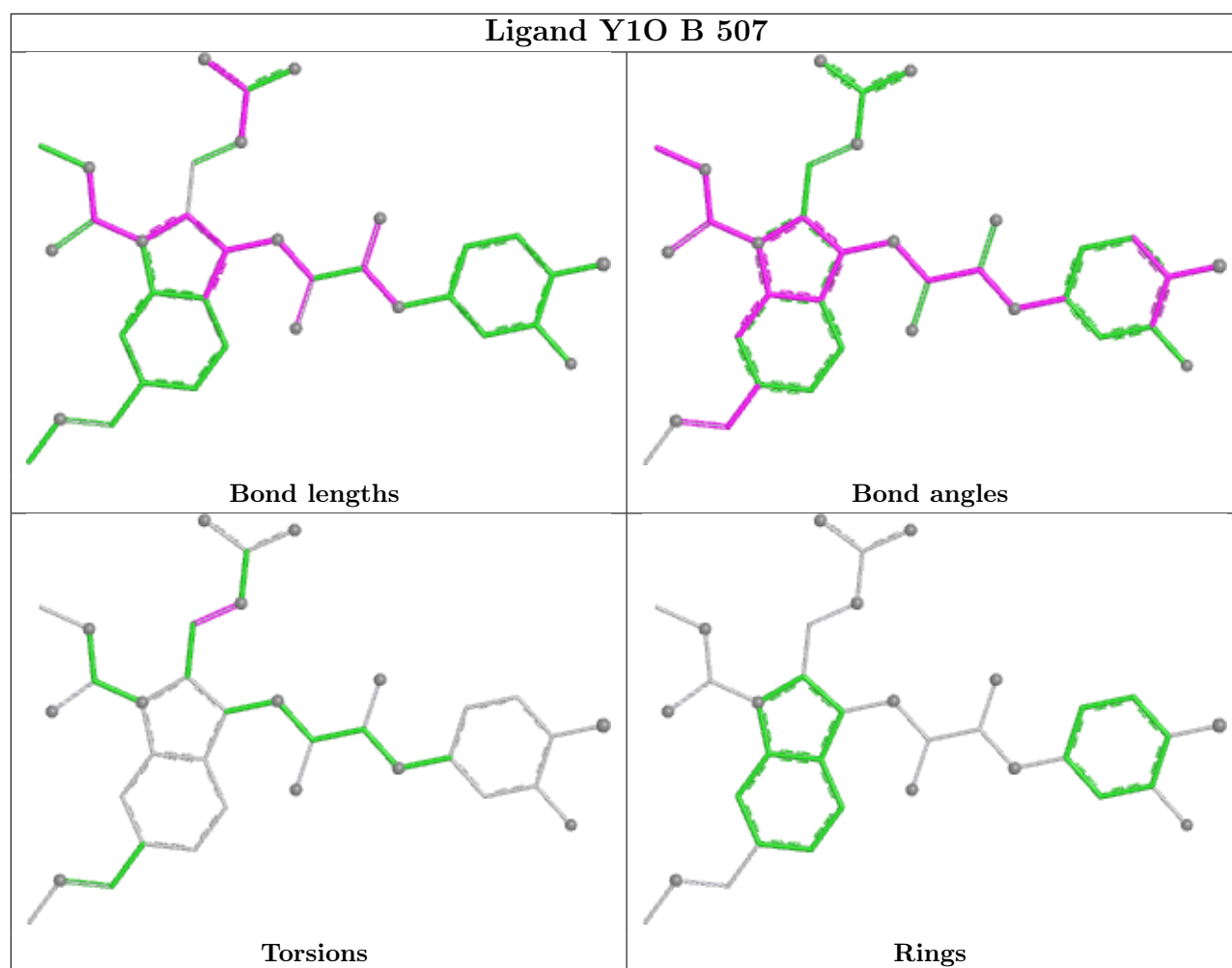


Ligand Y1O A 507



Ligand Y1O D 507





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	335/358 (93%)	1.31	75 (22%) 2 2	26, 41, 68, 129	0
1	B	335/358 (93%)	1.43	102 (30%) 1 1	25, 43, 78, 113	0
1	C	335/358 (93%)	0.99	56 (16%) 4 4	24, 39, 65, 90	0
1	D	335/358 (93%)	1.55	100 (29%) 1 1	27, 44, 76, 132	0
All	All	1340/1432 (93%)	1.32	333 (24%) 2 2	24, 41, 73, 132	0

All (333) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TYR	12.7
1	D	61	TYR	11.3
1	A	60	ALA	9.7
1	D	57	ASP	9.7
1	A	198	GLY	9.4
1	D	124	GLY	9.0
1	D	60	ALA	8.0
1	A	199	SER	7.9
1	D	84	MET	7.5
1	A	80	ASN	7.5
1	B	61	TYR	7.4
1	B	60	ALA	7.4
1	D	198	GLY	7.3
1	A	89	VAL	7.2
1	B	57	ASP	7.1
1	A	124	GLY	7.0
1	C	84	MET	6.9
1	B	122	LEU	6.8
1	A	86	LEU	6.6
1	C	60	ALA	6.4
1	B	198	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	87	ALA	6.0
1	B	124	GLY	5.9
1	D	85	VAL	5.8
1	A	85	VAL	5.7
1	C	85	VAL	5.7
1	A	202	THR	5.6
1	C	89	VAL	5.6
1	D	122	LEU	5.5
1	B	84	MET	5.5
1	A	72	HIS	5.4
1	D	72	HIS	5.3
1	A	81	PRO	5.2
1	D	123	THR	5.2
1	A	57	ASP	5.1
1	B	72	HIS	5.0
1	B	87	ALA	4.8
1	A	122	LEU	4.8
1	C	80	ASN	4.8
1	C	87	ALA	4.8
1	A	412	GLY	4.8
1	A	123	THR	4.8
1	D	86	LEU	4.7
1	B	199	SER	4.6
1	B	85	VAL	4.5
1	B	489	VAL	4.5
1	B	86	LEU	4.5
1	C	86	LEU	4.5
1	A	397	ASN	4.5
1	D	80	ASN	4.5
1	D	89	VAL	4.5
1	A	90	THR	4.4
1	D	341	THR	4.4
1	D	356	SER	4.4
1	A	200	ALA	4.4
1	A	464	ASP	4.4
1	D	340	ASN	4.3
1	D	408	ARG	4.3
1	D	79	PRO	4.3
1	D	326	ILE	4.2
1	B	89	VAL	4.1
1	B	231	LYS	4.1
1	D	87	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	49	LYS	4.1
1	A	62	GLU	4.1
1	C	240	ARG	4.0
1	B	325	ASN	4.0
1	D	339	ASN	4.0
1	A	50	THR	4.0
1	B	356	SER	4.0
1	D	199	SER	4.0
1	A	356	SER	4.0
1	A	84	MET	3.9
1	C	199	SER	3.9
1	B	242	VAL	3.9
1	A	79	PRO	3.9
1	A	59	LYS	3.8
1	B	339	ASN	3.8
1	D	77	THR	3.8
1	B	81	PRO	3.8
1	C	325	ASN	3.7
1	D	403	TYR	3.7
1	B	269	GLU	3.7
1	D	201	ILE	3.7
1	B	226	LEU	3.7
1	D	396	ARG	3.6
1	D	90	THR	3.6
1	B	432	ARG	3.6
1	D	50	THR	3.6
1	D	406	THR	3.6
1	B	224	ALA	3.6
1	C	88	ASN	3.6
1	C	72	HIS	3.6
1	C	356	SER	3.6
1	A	278	THR	3.6
1	B	358	THR	3.5
1	D	240	ARG	3.5
1	B	49	LYS	3.5
1	D	397	ASN	3.5
1	A	354	PRO	3.5
1	B	365	SER	3.5
1	C	61	TYR	3.5
1	A	396	ARG	3.5
1	D	204	ALA	3.5
1	B	59	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	71	THR	3.5
1	D	88	ASN	3.4
1	A	63	LYS	3.4
1	B	123	THR	3.4
1	A	88	ASN	3.4
1	C	406	THR	3.4
1	B	243	SER	3.3
1	B	340	ASN	3.3
1	C	397	ASN	3.3
1	B	79	PRO	3.3
1	B	221	ALA	3.3
1	A	328	GLN	3.3
1	D	81	PRO	3.3
1	B	408	ARG	3.3
1	D	300	ASN	3.3
1	D	49	LYS	3.3
1	B	464	ASP	3.3
1	D	464	ASP	3.3
1	D	291	SER	3.2
1	C	198	GLY	3.2
1	A	82	GLN	3.2
1	A	240	ARG	3.2
1	B	398	GLY	3.2
1	D	268	GLU	3.2
1	B	240	ARG	3.2
1	B	90	THR	3.2
1	A	407	GLY	3.2
1	C	202	THR	3.2
1	D	299	PRO	3.2
1	C	59	LYS	3.2
1	C	489	VAL	3.1
1	D	489	VAL	3.1
1	B	465	THR	3.1
1	D	465	THR	3.1
1	D	82	GLN	3.1
1	A	113	ASP	3.1
1	D	71	THR	3.1
1	B	88	ASN	3.1
1	B	203	GLN	3.1
1	B	397	ASN	3.1
1	B	201	ILE	3.1
1	B	50	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	71	THR	3.1
1	C	340	ASN	3.1
1	C	354	PRO	3.1
1	D	293	ASN	3.1
1	B	490	GLU	3.1
1	D	404	ASN	3.0
1	B	62	GLU	3.0
1	D	99	ASP	3.0
1	A	489	VAL	3.0
1	A	411	ASN	3.0
1	B	55	ALA	3.0
1	D	242	VAL	3.0
1	C	113	ASP	3.0
1	B	223	PHE	3.0
1	C	82	GLN	3.0
1	A	49	LYS	3.0
1	A	78	ASP	3.0
1	D	76	PRO	3.0
1	C	357	LYS	2.9
1	B	422	GLN	2.9
1	D	290	GLU	2.9
1	B	58	ALA	2.9
1	B	394	THR	2.9
1	D	358	THR	2.9
1	B	379	ARG	2.9
1	C	90	THR	2.9
1	D	269	GLU	2.9
1	A	68	VAL	2.8
1	A	244	THR	2.8
1	D	62	GLU	2.8
1	B	396	ARG	2.8
1	D	203	GLN	2.8
1	C	58	ALA	2.8
1	D	413	THR	2.8
1	A	325	ASN	2.8
1	A	395	TYR	2.8
1	B	200	ALA	2.8
1	D	342	LEU	2.8
1	B	51	THR	2.8
1	D	432	ARG	2.8
1	B	82	GLN	2.8
1	B	236	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	396	ARG	2.7
1	B	411	ASN	2.7
1	C	200	ALA	2.7
1	D	221	ALA	2.7
1	B	202	THR	2.7
1	D	343	GLN	2.7
1	A	340	ASN	2.7
1	B	344	LYS	2.7
1	D	246	GLN	2.7
1	C	71	THR	2.7
1	A	99	ASP	2.7
1	B	80	ASN	2.6
1	D	279	ASN	2.6
1	D	325	ASN	2.6
1	D	231	LYS	2.6
1	D	337	LYS	2.6
1	B	399	THR	2.6
1	B	353	PHE	2.6
1	A	410	SER	2.6
1	D	405	HIS	2.6
1	A	279	ASN	2.6
1	C	339	ASN	2.6
1	B	77	THR	2.6
1	B	244	THR	2.6
1	A	406	THR	2.6
1	D	200	ALA	2.6
1	C	410	SER	2.6
1	D	365	SER	2.6
1	D	83	GLU	2.5
1	B	245	VAL	2.5
1	A	300	ASN	2.5
1	C	123	THR	2.5
1	D	56	SER	2.5
1	B	357	LYS	2.5
1	B	457	ASP	2.5
1	B	406	THR	2.5
1	A	327	ARG	2.5
1	D	379	ARG	2.5
1	A	269	GLU	2.5
1	B	354	PRO	2.5
1	A	238	PRO	2.5
1	D	441	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	78	ASP	2.4
1	A	268	GLU	2.4
1	C	115	SER	2.4
1	C	399	THR	2.4
1	B	233	PHE	2.4
1	B	91	GLU	2.4
1	B	290	GLU	2.4
1	B	65	VAL	2.4
1	B	359	ILE	2.4
1	A	246	GLN	2.4
1	A	339	ASN	2.4
1	C	57	ASP	2.4
1	C	464	ASP	2.4
1	D	414	ILE	2.4
1	A	226	LEU	2.4
1	B	246	GLN	2.4
1	C	246	GLN	2.4
1	B	327	ARG	2.4
1	A	413	THR	2.4
1	C	77	THR	2.4
1	C	358	THR	2.4
1	D	202	THR	2.4
1	A	276	ASN	2.3
1	D	412	GLY	2.3
1	B	326	ILE	2.3
1	A	336	SER	2.3
1	A	239	CYS	2.3
1	A	267	GLU	2.3
1	C	417	GLN	2.3
1	B	436	ALA	2.3
1	B	280	ASN	2.3
1	B	93	PHE	2.3
1	B	488	VAL	2.3
1	D	267	GLU	2.3
1	D	244	THR	2.3
1	B	92	ASN	2.3
1	D	92	ASN	2.3
1	D	446	ASN	2.3
1	B	393	GLY	2.3
1	C	398	GLY	2.3
1	D	121	LYS	2.3
1	D	409	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	328	GLN	2.3
1	D	354	PRO	2.3
1	B	404	ASN	2.3
1	B	113	ASP	2.3
1	A	222	GLY	2.3
1	A	408	ARG	2.2
1	C	300	ASN	2.2
1	C	122	LEU	2.2
1	C	379	ARG	2.2
1	A	201	ILE	2.2
1	C	244	THR	2.2
1	D	59	LYS	2.2
1	B	395	TYR	2.2
1	B	336	SER	2.2
1	C	79	PRO	2.2
1	D	278	THR	2.2
1	B	99	ASP	2.2
1	D	113	ASP	2.2
1	D	292	VAL	2.2
1	C	91	GLU	2.2
1	C	365	SER	2.2
1	B	229	ASN	2.2
1	A	241	ASN	2.2
1	B	76	PRO	2.1
1	B	267	GLU	2.1
1	D	91	GLU	2.1
1	D	393	GLY	2.1
1	B	265	LEU	2.1
1	D	416	LEU	2.1
1	A	337	LYS	2.1
1	D	344	LYS	2.1
1	D	357	LYS	2.1
1	B	279	ASN	2.1
1	B	300	ASN	2.1
1	A	91	GLU	2.1
1	B	220	PRO	2.1
1	B	232	THR	2.1
1	C	413	THR	2.1
1	D	398	GLY	2.1
1	D	281	ALA	2.1
1	C	117	LYS	2.1
1	D	243	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	410	SER	2.1
1	D	241	ASN	2.1
1	A	358	THR	2.1
1	A	432	ARG	2.1
1	D	117	LYS	2.1
1	A	221	ALA	2.1
1	C	114	GLU	2.1
1	C	203	GLN	2.1
1	D	394	THR	2.1
1	A	326	ILE	2.1
1	C	337	LYS	2.1
1	B	68	VAL	2.1
1	B	73	ALA	2.1
1	A	114	GLU	2.0
1	C	269	GLU	2.0
1	D	265	LEU	2.0
1	D	399	THR	2.0
1	D	467	THR	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(Å ²)	Q<0.9
2	NAG	D	506	14/15	0.57	0.31	64,66,75,81	0
2	NAG	A	506	14/15	0.58	0.24	72,87,96,106	0
2	NAG	C	506	14/15	0.62	0.19	50,61,67,72	0
2	NAG	D	503	14/15	0.63	0.22	56,66,73,76	0
2	NAG	B	506	14/15	0.65	0.24	46,52,60,63	0

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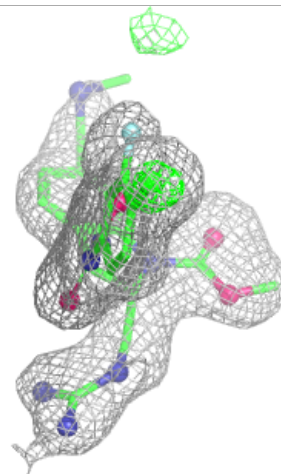
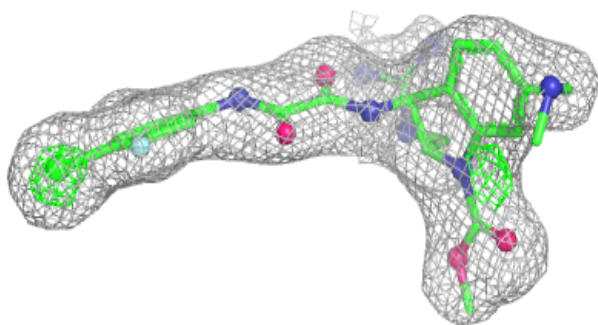
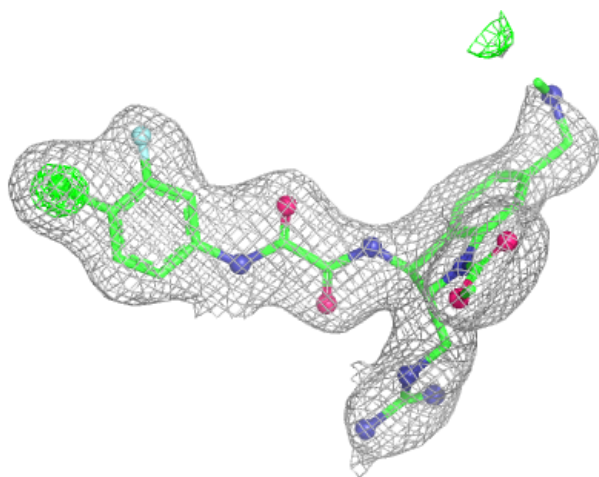
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	505	14/15	0.72	0.17	54,56,60,61	0
2	NAG	B	501	14/15	0.74	0.15	41,53,58,60	0
2	NAG	B	503	14/15	0.74	0.20	57,61,71,74	0
2	NAG	B	504	14/15	0.75	0.15	43,50,55,57	0
2	NAG	D	501	14/15	0.77	0.15	39,52,60,61	0
2	NAG	A	503	14/15	0.78	0.16	47,52,56,57	0
2	NAG	C	508	14/15	0.78	0.14	49,54,57,58	0
2	NAG	D	504	14/15	0.79	0.14	48,50,55,56	0
2	NAG	C	503	14/15	0.79	0.15	49,53,55,57	0
2	NAG	C	504	14/15	0.79	0.13	28,43,50,50	0
2	NAG	A	508	14/15	0.80	0.14	50,55,57,59	0
2	NAG	B	505	14/15	0.80	0.15	50,53,55,61	0
2	NAG	A	504	14/15	0.82	0.12	42,47,53,58	0
2	NAG	A	501	14/15	0.83	0.13	43,52,57,66	0
2	NAG	C	505	14/15	0.84	0.14	35,42,45,49	0
2	NAG	A	505	14/15	0.87	0.14	37,42,47,48	0
2	NAG	C	501	14/15	0.87	0.10	37,43,49,54	0
2	NAG	B	502	14/15	0.89	0.10	30,40,43,45	0
2	NAG	D	502	14/15	0.89	0.11	32,39,45,46	0
2	NAG	A	502	14/15	0.90	0.10	26,37,42,44	0
2	NAG	C	502	14/15	0.91	0.10	28,33,36,40	0
3	Y1O	D	507	35/35	0.93	0.10	25,33,48,48	0
3	Y1O	A	507	35/35	0.94	0.09	27,31,39,51	0
3	Y1O	C	507	35/35	0.94	0.10	23,29,39,49	0
3	Y1O	B	507	35/35	0.94	0.09	25,32,37,43	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.

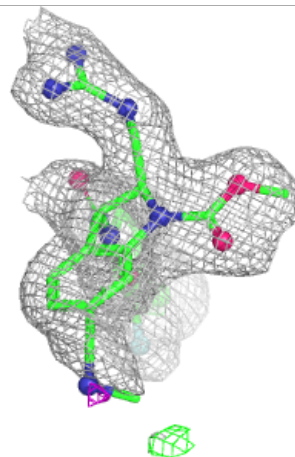
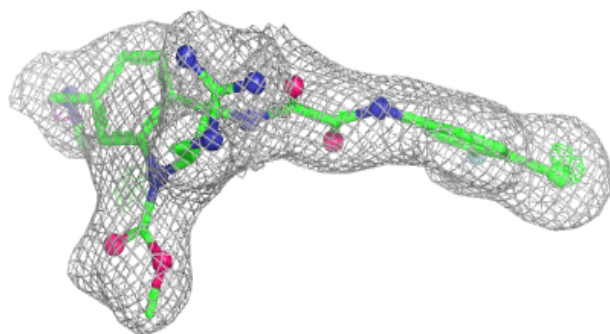
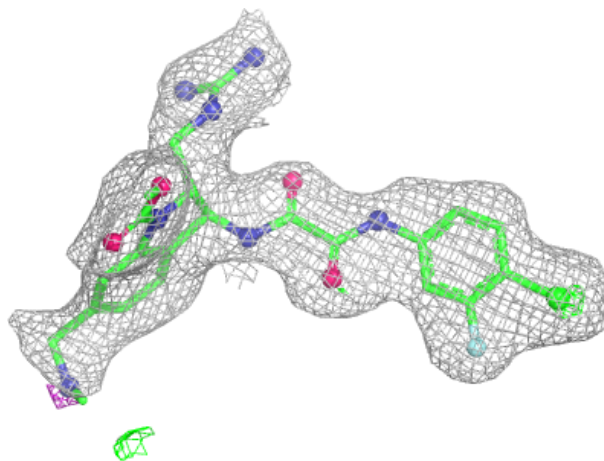
Electron density around Y1O D 507:

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



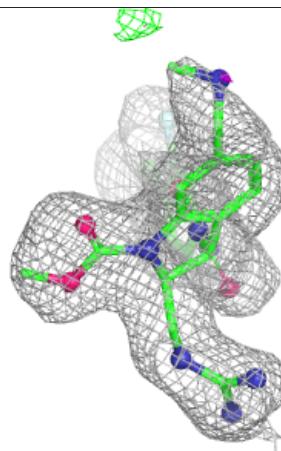
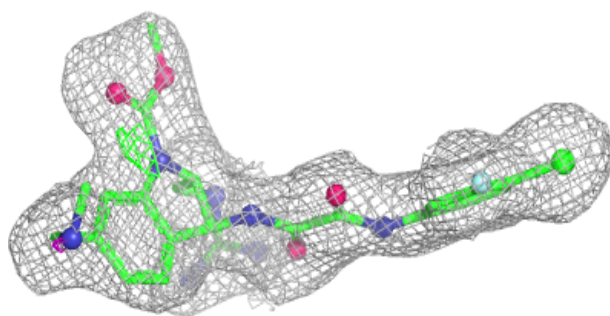
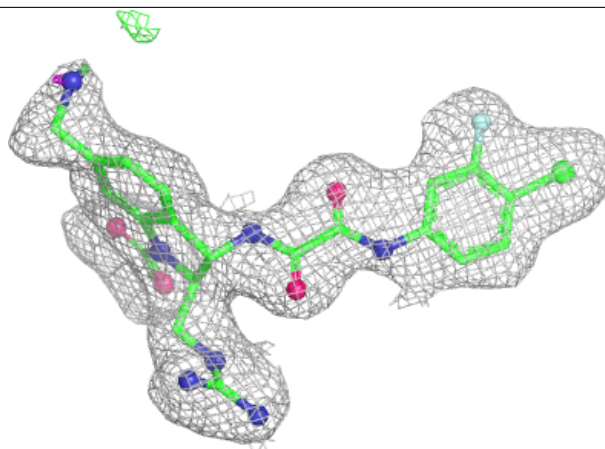
Electron density around Y1O A 507:

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



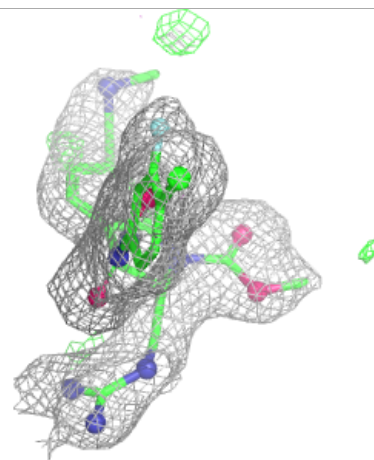
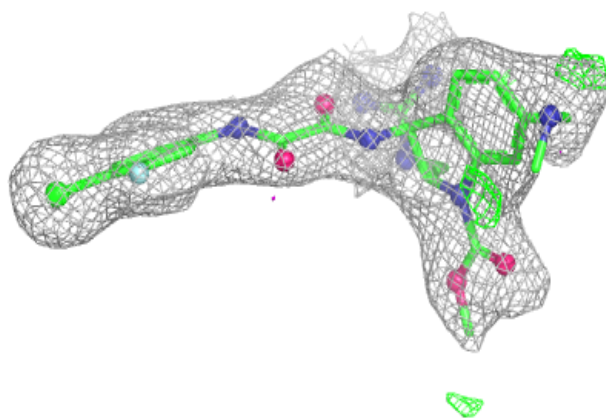
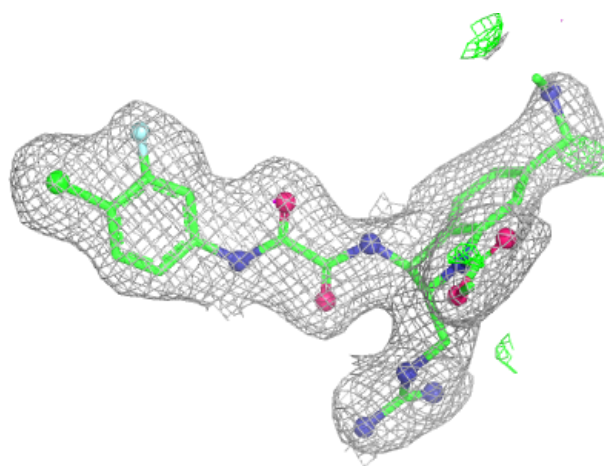
Electron density around Y1O C 507:

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



Electron density around Y1O B 507:

$2mF_o-DF_c$ (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.