



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 01:45 PM EDT

PDB ID : 8FM4 / pdb_00008fm4
Title : HIV-1 gp120 complex with CJF-IV-047
Authors : Gong, Z.; Hendrickson, W.A.
Deposited on : 2022-12-22
Resolution : 2.18 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

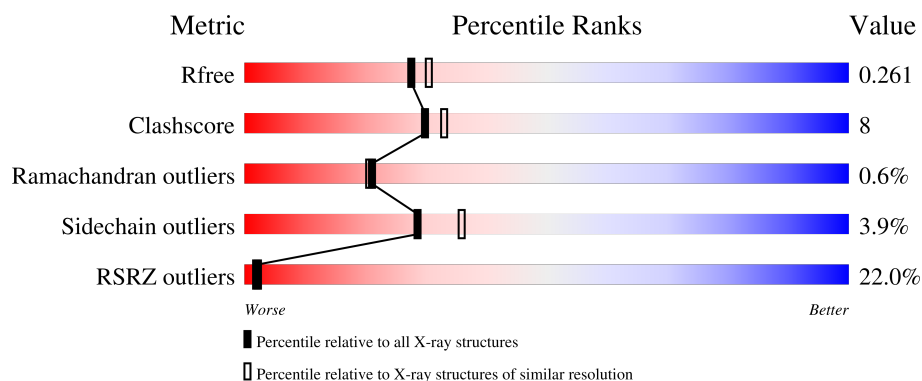
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 11224 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	D	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			

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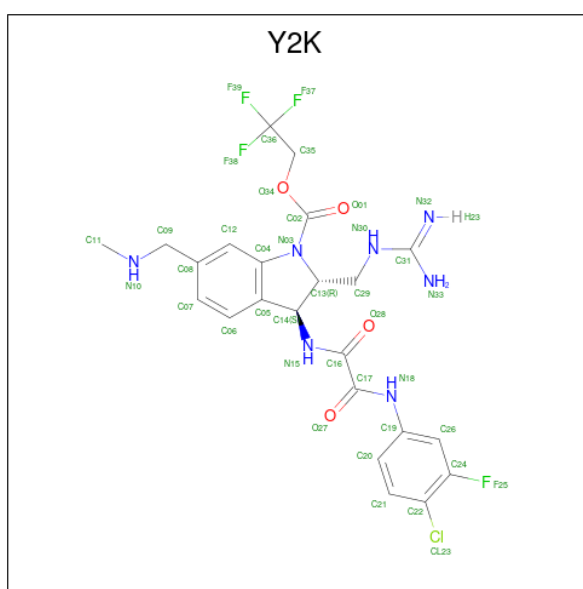
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 3 is 2,2,2-trifluoroethyl (2R,3S)-2-(carbamimidamidomethyl)-3-[2-(4-chloro-3-fluoranylino)(oxo)acetamido]-6-[(methylamino)methyl]-2,3-dihydro-1H-indole-1-carboxylate (CCD ID: Y2K) (formula: C₂₃H₂₄ClF₄N₇O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	F	N	O	0	0
			39	23	1	4	7	4		
3	D	1	Total	C	Cl	F	N	O	0	0
			39	23	1	4	7	4		
3	A	1	Total	C	Cl	F	N	O	0	0
			39	23	1	4	7	4		
3	C	1	Total	C	Cl	F	N	O	0	0
			39	23	1	4	7	4		

- Molecule 4 is water.

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

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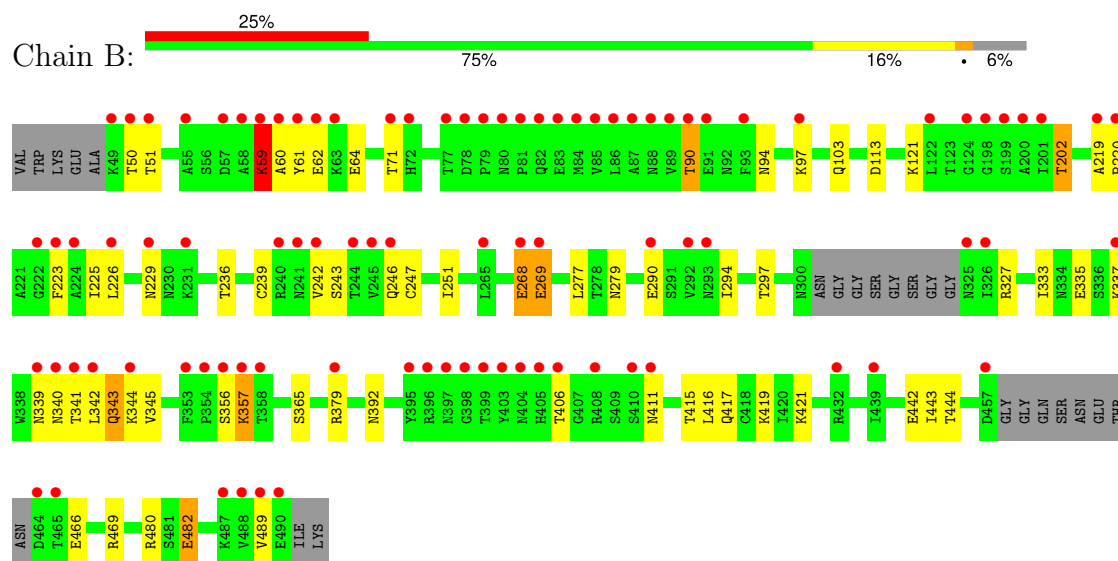
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	58	Total 58	O 58	0	0
4	A	41	Total 41	O 41	0	0
4	C	54	Total 54	O 54	0	0

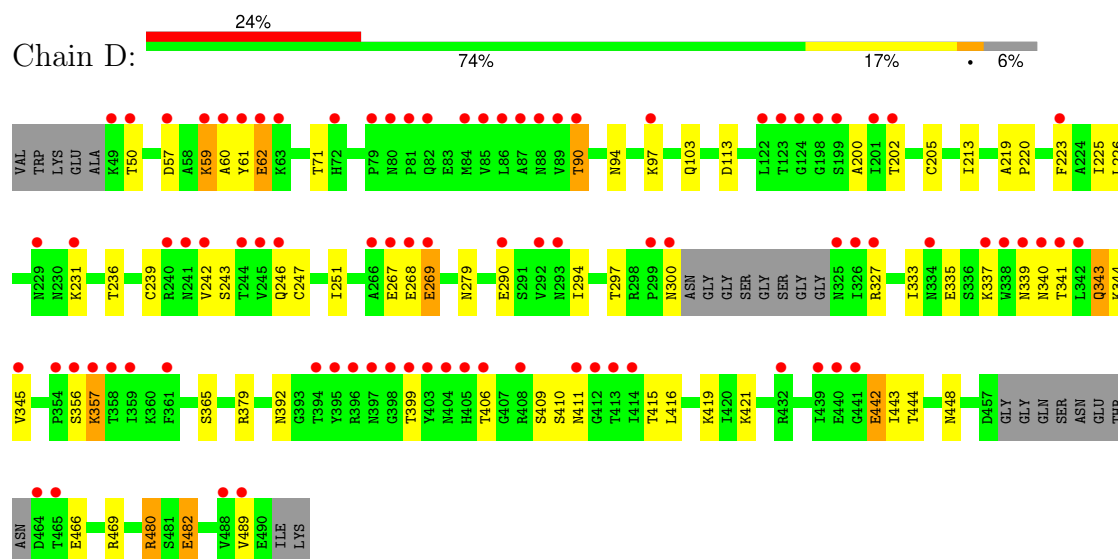
3 Residue-property plots [i](#)

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: Envelope glycoprotein gp120

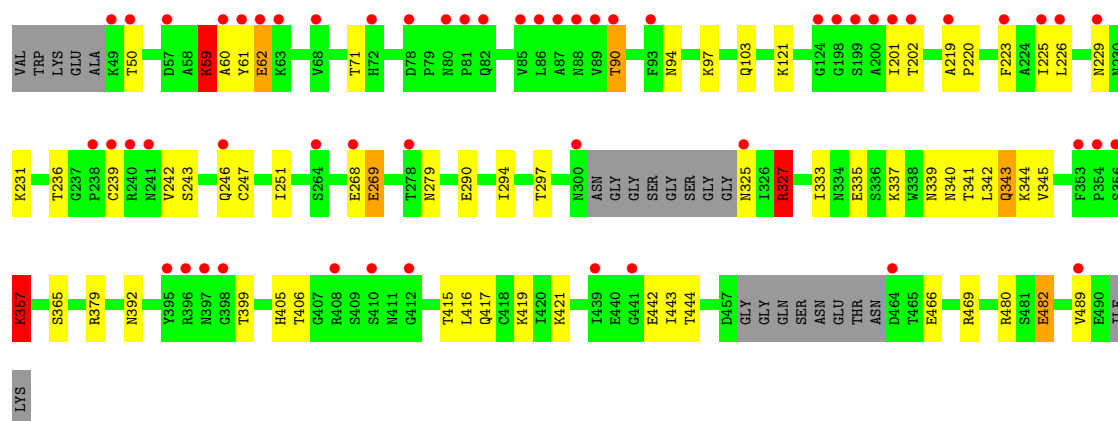


• Molecule 1: Envelope glycoprotein gp120



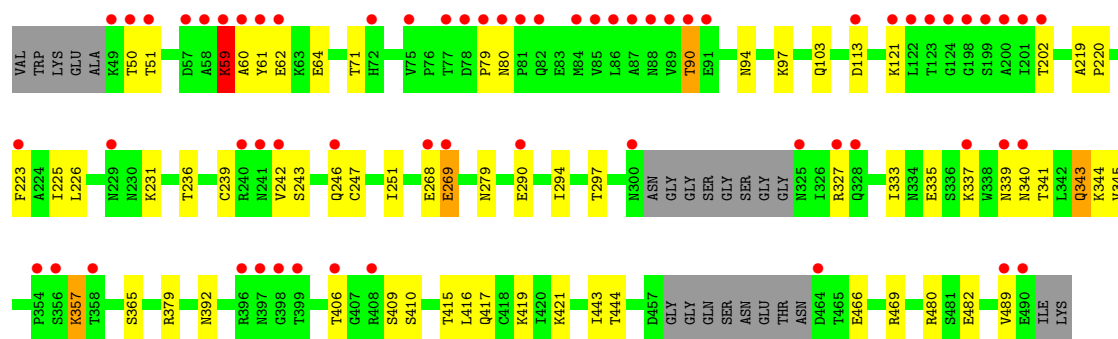
• Molecule 1: Envelope glycoprotein gp120

Chain A: 



• Molecule 1: Envelope glycoprotein gp120

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.91Å 121.26Å 194.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.18 48.65 – 2.18	Depositor EDS
% Data completeness (in resolution range)	73.4 (48.65-2.18) 73.4 (48.65-2.18)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.237 , 0.261 0.237 , 0.261	Depositor DCC
R_{free} test set	2000 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11224	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.23% 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: NAG, Y2K

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	0.57	1/2682 (0.0%)	0.97	13/3640 (0.4%)
1	B	0.57	1/2682 (0.0%)	0.96	13/3640 (0.4%)
1	C	0.57	1/2682 (0.0%)	0.96	13/3640 (0.4%)
1	D	0.57	1/2682 (0.0%)	0.97	13/3640 (0.4%)
All	All	0.57	4/10728 (0.0%)	0.96	52/14560 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	LYS	CB-CG	-5.15	1.37	1.52
1	A	59	LYS	CB-CG	-5.14	1.37	1.52
1	B	59	LYS	CB-CG	-5.13	1.37	1.52
1	C	59	LYS	CB-CG	-5.13	1.37	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	LYS	CG-CD-CE	-14.18	78.68	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	LYS	CG-CD-CE	-14.18	78.69	111.30
1	B	59	LYS	CG-CD-CE	-14.18	78.69	111.30
1	A	59	LYS	CG-CD-CE	-14.18	78.70	111.30
1	B	344	LYS	CA-CB-CG	-7.19	99.71	114.10
1	D	344	LYS	CA-CB-CG	-7.19	99.72	114.10
1	C	344	LYS	CA-CB-CG	-7.18	99.74	114.10
1	A	344	LYS	CA-CB-CG	-7.18	99.75	114.10
1	C	327	ARG	CG-CD-NE	-7.13	96.32	112.00
1	A	327	ARG	CG-CD-NE	-7.12	96.34	112.00
1	D	327	ARG	CG-CD-NE	-7.12	96.34	112.00
1	B	327	ARG	CG-CD-NE	-7.11	96.36	112.00
1	D	327	ARG	CA-CB-CG	6.89	127.89	114.10
1	C	327	ARG	CA-CB-CG	6.89	127.88	114.10
1	B	327	ARG	CA-CB-CG	6.89	127.88	114.10
1	A	327	ARG	CA-CB-CG	6.88	127.87	114.10
1	A	59	LYS	CB-CG-CD	6.63	126.55	111.30
1	B	59	LYS	CB-CG-CD	6.63	126.54	111.30
1	D	59	LYS	CB-CG-CD	6.62	126.53	111.30
1	C	59	LYS	CB-CG-CD	6.61	126.50	111.30
1	A	327	ARG	CA-C-N	-5.92	113.83	122.65
1	A	327	ARG	C-N-CA	-5.92	113.83	122.65
1	D	327	ARG	CA-C-N	-5.88	113.89	122.65
1	D	327	ARG	C-N-CA	-5.88	113.89	122.65
1	B	327	ARG	CA-C-N	-5.87	113.90	122.65
1	B	327	ARG	C-N-CA	-5.87	113.90	122.65
1	C	327	ARG	CA-C-N	-5.86	113.91	122.65
1	C	327	ARG	C-N-CA	-5.86	113.91	122.65
1	B	327	ARG	CB-CG-CD	5.55	124.06	111.30
1	D	327	ARG	CB-CG-CD	5.55	124.06	111.30
1	C	327	ARG	CB-CG-CD	5.54	124.04	111.30
1	A	327	ARG	CB-CG-CD	5.54	124.03	111.30
1	D	357	LYS	N-CA-CB	-5.54	101.39	110.52
1	C	357	LYS	N-CA-CB	-5.53	101.40	110.52
1	A	357	LYS	N-CA-CB	-5.52	101.41	110.52
1	B	357	LYS	N-CA-CB	-5.51	101.43	110.52
1	A	327	ARG	CB-CA-C	-5.42	99.81	110.11
1	B	327	ARG	CB-CA-C	-5.40	99.84	110.11
1	C	327	ARG	CB-CA-C	-5.40	99.86	110.11
1	D	327	ARG	CB-CA-C	-5.39	99.86	110.11
1	B	480	ARG	CG-CD-NE	-5.27	100.41	112.00
1	A	480	ARG	CG-CD-NE	-5.27	100.41	112.00
1	A	269	GLU	N-CA-C	5.25	118.21	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	480	ARG	CG-CD-NE	-5.25	100.44	112.00
1	C	480	ARG	CG-CD-NE	-5.25	100.46	112.00
1	B	269	GLU	N-CA-C	5.24	118.19	110.59
1	C	269	GLU	N-CA-C	5.23	118.17	110.59
1	D	269	GLU	N-CA-C	5.20	118.12	110.59
1	A	343	GLN	CA-CB-CG	5.19	124.48	114.10
1	D	343	GLN	CA-CB-CG	5.18	124.45	114.10
1	B	343	GLN	CA-CB-CG	5.17	124.45	114.10
1	C	343	GLN	CA-CB-CG	5.17	124.44	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	379	ARG	Sidechain
1	A	469	ARG	Sidechain
1	B	379	ARG	Sidechain
1	B	469	ARG	Sidechain
1	C	379	ARG	Sidechain
1	C	469	ARG	Sidechain
1	D	379	ARG	Sidechain
1	D	469	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	37	1
1	B	2627	0	2542	35	2
1	C	2627	0	2540	73	0
1	D	2627	0	2542	71	2
2	A	98	0	91	4	0
2	B	84	0	78	2	0
2	C	98	0	91	4	0
2	D	84	0	78	2	1
3	A	39	0	0	0	0
3	B	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	39	0	0	0	0
3	D	39	0	0	0	0
4	A	41	0	0	1	0
4	B	43	0	0	3	0
4	C	54	0	0	1	0
4	D	58	0	0	7	0
All	All	11224	0	10502	183	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 8.

All (183) 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:D:59:LYS:HZ2	1:C:61:TYR:N	1.17	1.36
1:D:300:ASN:HB2	1:C:80:ASN:ND2	1.61	1.17
1:D:59:LYS:NZ	1:C:61:TYR:N	2.04	1.06
1:D:59:LYS:HZ2	1:C:60:ALA:C	1.65	1.03
1:D:442:GLU:HB3	1:C:80:ASN:HB2	1.42	1.02
1:D:300:ASN:HB2	1:C:80:ASN:HD21	1.12	0.98
1:D:59:LYS:HE3	1:C:60:ALA:HB3	1.53	0.88
1:D:59:LYS:HZ3	1:C:61:TYR:HD2	1.23	0.83
1:D:59:LYS:HE3	1:C:60:ALA:CB	2.09	0.81
1:D:59:LYS:NZ	1:C:61:TYR:CD2	2.50	0.80
1:D:300:ASN:CB	1:C:80:ASN:ND2	2.44	0.79
1:D:59:LYS:CE	1:C:60:ALA:HB3	2.14	0.78
1:D:59:LYS:NZ	1:C:61:TYR:HD2	1.84	0.75
1:D:246:GLN:HG3	1:D:247:CYS:SG	2.30	0.71
1:B:246:GLN:HG3	1:B:247:CYS:SG	2.30	0.71
1:D:59:LYS:HZ2	1:C:61:TYR:H	1.33	0.71
1:A:246:GLN:HG3	1:A:247:CYS:SG	2.30	0.71
1:C:246:GLN:HG3	1:C:247:CYS:SG	2.30	0.71
1:D:59:LYS:NZ	1:C:60:ALA:C	2.41	0.70
1:C:113:ASP:OD1	4:C:601:HOH:O	2.09	0.70
1:D:113:ASP:OD1	4:D:603:HOH:O	2.11	0.69
1:C:335:GLU:O	1:C:339:ASN:HB2	1.93	0.69
1:A:335:GLU:O	1:A:339:ASN:HB2	1.93	0.68
1:B:335:GLU:O	1:B:339:ASN:HB2	1.93	0.68
1:D:335:GLU:O	1:D:339:ASN:HB2	1.93	0.68
1:D:300:ASN:CB	1:C:80:ASN:HD21	2.01	0.66
1:D:290:GLU:OE2	1:D:337:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:GLU:OE2	1:C:337:LYS:NZ	2.30	0.64
1:A:290:GLU:OE2	1:A:337:LYS:NZ	2.30	0.63
1:B:290:GLU:OE2	1:B:337:LYS:NZ	2.30	0.63
1:D:57:ASP:O	1:C:61:TYR:HB2	2.00	0.61
1:D:267:GLU:O	4:D:604:HOH:O	2.16	0.61
1:C:251:ILE:HG23	1:C:482:GLU:HG3	1.84	0.60
1:D:59:LYS:HZ3	1:C:61:TYR:CB	2.15	0.59
1:D:335:GLU:OE1	1:D:409:SER:OG	2.17	0.59
1:C:226:LEU:HD12	1:C:489:VAL:HG11	1.84	0.59
1:D:226:LEU:HD12	1:D:489:VAL:HG11	1.84	0.59
1:D:251:ILE:HG23	1:D:482:GLU:HG3	1.84	0.59
1:C:339:ASN:ND2	2:C:508:NAG:H83	2.18	0.58
1:B:268:GLU:OE2	1:B:268:GLU:HA	2.03	0.58
1:A:226:LEU:HD12	1:A:489:VAL:HG11	1.84	0.58
1:B:251:ILE:HG23	1:B:482:GLU:HG3	1.84	0.58
1:B:226:LEU:HD12	1:B:489:VAL:HG11	1.84	0.58
1:D:297:THR:HG22	1:D:444:THR:HG23	1.86	0.58
1:A:251:ILE:HG23	1:A:482:GLU:HG3	1.84	0.57
1:D:300:ASN:ND2	1:C:80:ASN:ND2	2.51	0.57
1:B:297:THR:HG22	1:B:444:THR:HG23	1.86	0.57
1:D:300:ASN:HD22	1:C:80:ASN:ND2	2.02	0.57
1:C:59:LYS:HG3	1:C:61:TYR:CZ	2.39	0.57
1:C:297:THR:HG22	1:C:444:THR:HG23	1.86	0.57
1:A:59:LYS:HG3	1:A:61:TYR:CE1	2.40	0.57
1:B:59:LYS:HG3	1:B:61:TYR:CE1	2.40	0.57
1:A:297:THR:HG22	1:A:444:THR:HG23	1.86	0.56
1:B:59:LYS:HG3	1:B:61:TYR:CZ	2.39	0.56
1:A:419:LYS:HD3	1:A:421:LYS:HG2	1.88	0.56
1:A:59:LYS:HG3	1:A:61:TYR:CZ	2.39	0.56
1:C:59:LYS:HG3	1:C:61:TYR:CE1	2.40	0.56
1:D:213:ILE:HG22	1:C:61:TYR:CZ	2.41	0.56
1:D:419:LYS:HD3	1:D:421:LYS:HG2	1.88	0.55
1:D:59:LYS:HZ3	1:C:61:TYR:HB3	1.71	0.55
1:C:335:GLU:HB3	2:C:508:NAG:H62	1.89	0.55
1:B:419:LYS:HD3	1:B:421:LYS:HG2	1.88	0.55
1:B:294:ILE:HD12	1:B:333:ILE:HD11	1.89	0.54
1:A:340:ASN:O	1:A:343:GLN:HB3	2.07	0.54
1:C:340:ASN:O	1:C:343:GLN:HB3	2.07	0.54
1:C:419:LYS:HD3	1:C:421:LYS:HG2	1.88	0.54
1:D:294:ILE:HD12	1:D:333:ILE:HD11	1.89	0.54
1:C:294:ILE:HD12	1:C:333:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:GLU:OE1	1:C:409:SER:OG	2.17	0.53
1:C:357:LYS:HG3	1:C:466:GLU:HG2	1.89	0.53
1:D:357:LYS:HG3	1:D:466:GLU:HG2	1.89	0.53
1:D:442:GLU:HB3	1:C:80:ASN:CB	2.26	0.53
1:A:357:LYS:HG3	1:A:466:GLU:HG2	1.90	0.53
1:B:340:ASN:O	1:B:343:GLN:HB3	2.07	0.53
1:D:340:ASN:O	1:D:343:GLN:HB3	2.07	0.53
1:B:357:LYS:HG3	1:B:466:GLU:HG2	1.89	0.53
1:D:59:LYS:HG3	1:D:61:TYR:CE1	2.43	0.53
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.89	0.53
1:A:333:ILE:HD12	1:A:416:LEU:HD11	1.91	0.53
1:D:59:LYS:NZ	1:C:61:TYR:CB	2.72	0.52
1:C:333:ILE:HD12	1:C:416:LEU:HD11	1.91	0.52
1:D:59:LYS:CE	1:C:60:ALA:C	2.83	0.52
1:C:50:THR:O	1:C:103:GLN:NE2	2.42	0.52
1:B:333:ILE:HD12	1:B:416:LEU:HD11	1.91	0.52
1:D:333:ILE:HD12	1:D:416:LEU:HD11	1.91	0.51
1:A:50:THR:O	1:A:103:GLN:NE2	2.42	0.51
1:B:50:THR:O	1:B:103:GLN:NE2	2.42	0.51
1:D:448:ASN:ND2	4:D:602:HOH:O	2.08	0.51
1:A:90:THR:HA	1:A:239:CYS:O	2.12	0.50
1:D:90:THR:HA	1:D:239:CYS:O	2.12	0.50
1:D:50:THR:O	1:D:103:GLN:NE2	2.42	0.50
1:C:90:THR:HA	1:C:239:CYS:O	2.12	0.50
1:D:59:LYS:HZ2	1:C:61:TYR:CA	2.15	0.49
1:B:90:THR:HA	1:B:239:CYS:O	2.12	0.49
1:D:297:THR:HA	1:D:443:ILE:O	2.13	0.49
1:B:297:THR:HA	1:B:443:ILE:O	2.13	0.49
1:D:57:ASP:O	1:C:61:TYR:CB	2.61	0.49
1:A:297:THR:HA	1:A:443:ILE:O	2.13	0.49
1:C:297:THR:HA	1:C:443:ILE:O	2.13	0.48
1:A:405:HIS:H	2:A:508:NAG:H81	1.79	0.48
1:D:200:ALA:O	4:D:605:HOH:O	2.20	0.47
1:C:226:LEU:HD23	1:C:243:SER:O	2.15	0.47
1:D:59:LYS:HE3	1:C:60:ALA:C	2.39	0.47
1:B:226:LEU:HD23	1:B:243:SER:O	2.15	0.47
1:D:480:ARG:NH1	4:D:601:HOH:O	2.04	0.46
1:D:226:LEU:HD23	1:D:243:SER:O	2.15	0.46
1:A:226:LEU:HD23	1:A:243:SER:O	2.15	0.46
1:B:392:ASN:OD1	1:B:406:THR:HB	2.16	0.46
1:C:392:ASN:OD1	1:C:406:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASN:OD1	1:D:406:THR:HB	2.16	0.45
1:B:94:ASN:ND2	1:B:97:LYS:HD2	2.31	0.45
1:D:205:CYS:HB2	4:D:619:HOH:O	2.15	0.45
1:A:392:ASN:OD1	1:A:406:THR:HB	2.16	0.45
1:B:219:ALA:HB2	1:B:225:ILE:HG13	1.99	0.45
1:D:269:GLU:HB3	2:D:503:NAG:O6	2.17	0.45
1:A:94:ASN:ND2	1:A:97:LYS:HD2	2.31	0.45
1:C:220:PRO:O	1:C:223:PHE:HB2	2.17	0.45
1:B:269:GLU:HB3	2:B:503:NAG:O6	2.17	0.45
1:B:279:ASN:HB2	2:B:506:NAG:H61	1.99	0.45
1:C:94:ASN:ND2	1:C:97:LYS:HD2	2.31	0.45
1:C:279:ASN:HB2	2:C:506:NAG:H61	1.99	0.45
1:D:220:PRO:O	1:D:223:PHE:HB2	2.17	0.45
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.98	0.45
1:A:269:GLU:HB3	2:A:503:NAG:O6	2.17	0.45
4:B:633:HOH:O	1:C:202:THR:HG23	2.15	0.44
1:D:94:ASN:ND2	1:D:97:LYS:HD2	2.32	0.44
1:A:220:PRO:O	1:A:223:PHE:HB2	2.17	0.44
1:A:339:ASN:ND2	2:A:508:NAG:H83	2.33	0.44
1:C:60:ALA:HB2	1:C:71:THR:HG21	2.00	0.44
1:C:269:GLU:HB3	2:C:503:NAG:O6	2.17	0.44
1:D:60:ALA:HB2	1:D:71:THR:HG21	2.00	0.44
1:C:219:ALA:HB2	1:C:225:ILE:HG13	1.98	0.44
1:D:219:ALA:HB2	1:D:225:ILE:HG13	1.98	0.44
4:D:649:HOH:O	1:C:61:TYR:HE2	1.99	0.44
1:A:279:ASN:HB2	2:A:506:NAG:H61	1.99	0.44
1:D:279:ASN:HB2	2:D:506:NAG:H61	1.99	0.44
1:C:62:GLU:HG3	1:C:64:GLU:HB3	2.00	0.44
1:D:300:ASN:CB	1:C:80:ASN:HD22	2.29	0.44
1:B:60:ALA:HB2	1:B:71:THR:HG21	2.00	0.44
1:C:297:THR:HG22	1:C:444:THR:OG1	2.18	0.43
1:D:59:LYS:HB3	1:D:61:TYR:CE2	2.53	0.43
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.83	0.43
1:B:220:PRO:O	1:B:223:PHE:HB2	2.17	0.43
1:B:226:LEU:CD1	1:B:489:VAL:HG11	2.48	0.43
1:D:297:THR:HG22	1:D:444:THR:OG1	2.18	0.43
1:B:62:GLU:HG3	1:B:64:GLU:HB3	2.00	0.43
1:C:226:LEU:CD1	1:C:489:VAL:HG11	2.48	0.43
1:A:60:ALA:HB2	1:A:71:THR:HG21	2.00	0.43
1:D:300:ASN:CG	1:C:80:ASN:ND2	2.77	0.43
1:D:226:LEU:CD1	1:D:489:VAL:HG11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:THR:HG22	1:B:444:THR:OG1	2.18	0.43
1:A:226:LEU:CD1	1:A:489:VAL:HG11	2.48	0.43
1:A:325:ASN:OD1	1:A:327:ARG:HB2	2.18	0.43
1:A:50:THR:HB	1:A:223:PHE:CE1	2.54	0.42
1:B:50:THR:HB	1:B:223:PHE:CE1	2.54	0.42
1:D:442:GLU:HG2	1:C:79:PRO:O	2.19	0.42
1:A:297:THR:HG22	1:A:444:THR:OG1	2.18	0.42
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.83	0.42
1:A:226:LEU:HD12	1:A:489:VAL:CG1	2.49	0.42
1:C:50:THR:HB	1:C:223:PHE:CE1	2.54	0.42
1:B:59:LYS:HB2	1:B:62:GLU:H	1.85	0.41
1:B:59:LYS:HB3	1:B:61:TYR:CE2	2.55	0.41
1:D:231:LYS:CB	1:D:268:GLU:HG2	2.51	0.41
1:A:59:LYS:HB2	1:A:62:GLU:H	1.85	0.41
1:A:406:THR:HG22	4:A:639:HOH:O	2.19	0.41
1:C:59:LYS:HB2	1:C:62:GLU:H	1.85	0.41
1:C:231:LYS:CB	1:C:268:GLU:HG2	2.51	0.41
1:D:50:THR:HB	1:D:223:PHE:CE1	2.55	0.41
1:C:59:LYS:HB3	1:C:61:TYR:CE2	2.55	0.41
1:C:297:THR:HG22	1:C:444:THR:CG2	2.51	0.41
1:D:59:LYS:HB2	1:D:62:GLU:H	1.84	0.41
1:B:341:THR:O	1:B:345:VAL:HG23	2.21	0.41
1:B:97:LYS:HE3	4:B:623:HOH:O	2.20	0.41
1:B:277:LEU:HA	4:B:608:HOH:O	2.21	0.41
1:D:59:LYS:NZ	1:C:61:TYR:HB3	2.35	0.41
1:A:231:LYS:CB	1:A:268:GLU:HG2	2.51	0.41
1:A:341:THR:O	1:A:345:VAL:HG23	2.21	0.41
1:A:59:LYS:HB3	1:A:61:TYR:CE2	2.55	0.41
1:C:226:LEU:HD12	1:C:489:VAL:CG1	2.49	0.40
1:D:59:LYS:HG3	1:D:61:TYR:CZ	2.56	0.40
1:D:59:LYS:NZ	1:C:61:TYR:H	2.02	0.40
1:D:341:THR:O	1:D:345:VAL:HG23	2.21	0.40
1:C:341:THR:O	1:C:345:VAL:HG23	2.21	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:356:SER:OG	1:D:356:SER:OG[3_444]	1.91	0.29
1:A:94:ASN:ND2	2:D:506:NAG:O3[3_444]	2.11	0.09
1:B:202:THR:O	1:D:202:THR:OG1[4_455]	2.19	0.01

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	329/358 (92%)	313 (95%)	14 (4%)	2 (1%)	21	20
1	B	329/358 (92%)	313 (95%)	14 (4%)	2 (1%)	21	20
1	C	329/358 (92%)	313 (95%)	14 (4%)	2 (1%)	21	20
1	D	329/358 (92%)	313 (95%)	14 (4%)	2 (1%)	21	20
All	All	1316/1432 (92%)	1252 (95%)	56 (4%)	8 (1%)	21	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	365	SER
1	D	365	SER
1	A	365	SER
1	C	365	SER
1	B	90	THR
1	D	90	THR
1	A	90	THR
1	C	90	THR

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	297/312 (95%)	282 (95%)	15 (5%)	21	24
1	B	297/312 (95%)	283 (95%)	14 (5%)	23	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	297/312 (95%)	289 (97%)	8 (3%)	39	50
1	D	297/312 (95%)	288 (97%)	9 (3%)	36	46
All	All	1188/1248 (95%)	1142 (96%)	46 (4%)	28	36

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	THR
1	B	59	LYS
1	B	113	ASP
1	B	121	LYS
1	B	202	THR
1	B	229	ASN
1	B	236	THR
1	B	242	VAL
1	B	268	GLU
1	B	411	ASN
1	B	415	THR
1	B	417	GLN
1	B	442	GLU
1	B	482	GLU
1	D	62	GLU
1	D	236	THR
1	D	242	VAL
1	D	399	THR
1	D	410	SER
1	D	411	ASN
1	D	415	THR
1	D	442	GLU
1	D	482	GLU
1	A	59	LYS
1	A	62	GLU
1	A	121	LYS
1	A	201	ILE
1	A	202	THR
1	A	229	ASN
1	A	236	THR
1	A	242	VAL
1	A	327	ARG
1	A	357	LYS
1	A	399	THR

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Mol	Chain	Res	Type
1	A	415	THR
1	A	417	GLN
1	A	442	GLU
1	A	482	GLU
1	C	51	THR
1	C	59	LYS
1	C	121	LYS
1	C	236	THR
1	C	242	VAL
1	C	410	SER
1	C	415	THR
1	C	417	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	B	246	GLN
1	B	343	GLN
1	D	229	ASN
1	D	246	GLN
1	D	300	ASN
1	D	343	GLN
1	D	404	ASN
1	A	241	ASN
1	A	246	GLN
1	A	411	ASN
1	C	80	ASN
1	C	229	ASN
1	C	246	GLN
1	C	343	GLN
1	C	411	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	C	504	1	14,14,15	0.72	1 (7%)	17,19,21	0.46	0
2	NAG	D	506	1	14,14,15	0.67	1 (7%)	17,19,21	2.30	2 (11%)
2	NAG	C	505	1	14,14,15	0.59	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	C	503	1	14,14,15	1.31	2 (14%)	17,19,21	0.83	0
2	NAG	C	508	1	14,14,15	1.21	1 (7%)	17,19,21	0.94	1 (5%)
3	Y2K	D	507	-	40,41,41	2.78	16 (40%)	53,59,59	2.49	20 (37%)
2	NAG	A	508	1	14,14,15	0.64	1 (7%)	17,19,21	0.94	2 (11%)
3	Y2K	A	507	-	40,41,41	2.78	16 (40%)	53,59,59	2.49	20 (37%)
2	NAG	D	505	1	14,14,15	0.59	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	B	506	1	14,14,15	0.67	1 (7%)	17,19,21	2.30	2 (11%)
2	NAG	A	504	1	14,14,15	0.72	1 (7%)	17,19,21	0.46	0
2	NAG	D	503	1	14,14,15	1.31	2 (14%)	17,19,21	0.83	0
2	NAG	A	505	1	14,14,15	0.59	1 (7%)	17,19,21	0.78	1 (5%)
3	Y2K	B	507	-	40,41,41	2.78	16 (40%)	53,59,59	2.49	20 (37%)
2	NAG	A	502	1	14,14,15	0.78	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	B	504	1	14,14,15	0.72	1 (7%)	17,19,21	0.46	0
2	NAG	A	503	1	14,14,15	1.31	2 (14%)	17,19,21	0.83	0
2	NAG	D	501	1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	D	502	1	14,14,15	0.79	1 (7%)	17,19,21	0.83	1 (5%)
3	Y2K	C	507	-	40,41,41	2.78	16 (40%)	53,59,59	2.49	20 (37%)
2	NAG	C	501	1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	D	504	1	14,14,15	0.72	1 (7%)	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	505	1	14,14,15	0.59	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	B	501	1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	B	503	1	14,14,15	1.31	2 (14%)	17,19,21	0.83	0
2	NAG	B	502	1	14,14,15	0.78	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	C	506	1	14,14,15	0.67	1 (7%)	17,19,21	2.30	2 (11%)
2	NAG	C	502	1	14,14,15	0.78	1 (7%)	17,19,21	0.84	1 (5%)
2	NAG	A	506	1	14,14,15	0.67	1 (7%)	17,19,21	2.30	2 (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
2	NAG	C	504	1	-	2/6/23/26	0/1/1/1
2	NAG	D	506	1	-	3/6/23/26	0/1/1/1
2	NAG	C	505	1	-	2/6/23/26	0/1/1/1
2	NAG	C	503	1	-	2/6/23/26	0/1/1/1
2	NAG	C	508	1	-	4/6/23/26	0/1/1/1
3	Y2K	D	507	-	-	1/30/46/46	0/3/3/3
2	NAG	A	508	1	-	4/6/23/26	0/1/1/1
3	Y2K	A	507	-	-	1/30/46/46	0/3/3/3
2	NAG	D	505	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	504	1	-	2/6/23/26	0/1/1/1
2	NAG	D	503	1	-	2/6/23/26	0/1/1/1
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
3	Y2K	B	507	-	-	1/30/46/46	0/3/3/3
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	503	1	-	2/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	502	1	-	0/6/23/26	0/1/1/1
3	Y2K	C	507	-	-	1/30/46/46	0/3/3/3
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	504	1	-	2/6/23/26	0/1/1/1
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	2/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	C	506	1	-	3/6/23/26	0/1/1/1
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	506	1	-	3/6/23/26	0/1/1/1

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	507	Y2K	C31-N30	7.74	1.48	1.33
3	A	507	Y2K	C31-N30	7.74	1.48	1.33
3	D	507	Y2K	C31-N30	7.74	1.48	1.33
3	B	507	Y2K	C31-N30	7.74	1.48	1.33
3	B	507	Y2K	C02-N03	6.49	1.46	1.37
3	C	507	Y2K	C02-N03	6.48	1.46	1.37
3	A	507	Y2K	C02-N03	6.48	1.46	1.37
3	D	507	Y2K	C02-N03	6.48	1.46	1.37
3	C	507	Y2K	C17-N18	6.02	1.48	1.35
3	A	507	Y2K	C17-N18	6.02	1.48	1.35
3	D	507	Y2K	C17-N18	6.02	1.48	1.35
3	B	507	Y2K	C17-N18	6.02	1.48	1.35
3	C	507	Y2K	C13-N03	-5.98	1.40	1.47
3	B	507	Y2K	C13-N03	-5.98	1.40	1.47
3	A	507	Y2K	C13-N03	-5.97	1.40	1.47
3	D	507	Y2K	C13-N03	-5.97	1.40	1.47
3	B	507	Y2K	C16-N15	4.67	1.43	1.34
3	A	507	Y2K	C16-N15	4.67	1.43	1.34
3	C	507	Y2K	C16-N15	4.67	1.43	1.34
3	D	507	Y2K	C16-N15	4.67	1.43	1.34
2	C	508	NAG	O5-C1	4.34	1.51	1.43
3	D	507	Y2K	C31-N32	4.16	1.47	1.32
3	A	507	Y2K	C31-N32	4.16	1.47	1.32
3	B	507	Y2K	C31-N32	4.16	1.47	1.32
3	C	507	Y2K	C31-N32	4.16	1.47	1.32
3	A	507	Y2K	O28-C16	-4.03	1.15	1.23
3	D	507	Y2K	O28-C16	-4.03	1.15	1.23
3	B	507	Y2K	O28-C16	-4.03	1.15	1.23
3	C	507	Y2K	O28-C16	-4.03	1.15	1.23
2	A	503	NAG	O5-C1	3.83	1.50	1.43
2	D	503	NAG	O5-C1	3.83	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	NAG	O5-C1	3.83	1.50	1.43
2	C	503	NAG	O5-C1	3.82	1.50	1.43
2	C	503	NAG	C1-C2	2.91	1.56	1.52
2	B	503	NAG	C1-C2	2.91	1.56	1.52
2	A	503	NAG	C1-C2	2.90	1.56	1.52
2	D	503	NAG	C1-C2	2.90	1.56	1.52
3	A	507	Y2K	C14-N15	-2.90	1.40	1.46
3	D	507	Y2K	C14-N15	-2.89	1.40	1.46
3	B	507	Y2K	C14-N15	-2.89	1.40	1.46
3	C	507	Y2K	C14-N15	-2.89	1.40	1.46
2	D	502	NAG	O5-C1	2.77	1.48	1.43
2	B	502	NAG	O5-C1	2.77	1.48	1.43
2	C	502	NAG	O5-C1	2.77	1.48	1.43
2	A	502	NAG	O5-C1	2.77	1.48	1.43
3	C	507	Y2K	C22-CL23	2.63	1.79	1.73
3	A	507	Y2K	C22-CL23	2.63	1.79	1.73
3	D	507	Y2K	C22-CL23	2.63	1.79	1.73
3	B	507	Y2K	C22-CL23	2.63	1.79	1.73
3	B	507	Y2K	C14-C13	-2.61	1.52	1.55
3	C	507	Y2K	C14-C13	-2.60	1.52	1.55
3	D	507	Y2K	C14-C13	-2.60	1.52	1.55
3	A	507	Y2K	C14-C13	-2.60	1.52	1.55
3	B	507	Y2K	C16-C17	-2.42	1.48	1.53
3	C	507	Y2K	C16-C17	-2.42	1.48	1.53
3	D	507	Y2K	C16-C17	-2.42	1.48	1.53
3	A	507	Y2K	C16-C17	-2.42	1.48	1.53
2	A	504	NAG	O5-C1	2.35	1.47	1.43
2	C	504	NAG	O5-C1	2.35	1.47	1.43
2	D	504	NAG	O5-C1	2.35	1.47	1.43
2	B	504	NAG	O5-C1	2.35	1.47	1.43
3	D	507	Y2K	O27-C17	-2.33	1.19	1.23
3	C	507	Y2K	O27-C17	-2.33	1.19	1.23
3	A	507	Y2K	O27-C17	-2.33	1.19	1.23
3	B	507	Y2K	O27-C17	-2.33	1.19	1.23
3	B	507	Y2K	C19-N18	2.18	1.46	1.41
3	D	507	Y2K	C19-N18	2.18	1.46	1.41
3	C	507	Y2K	C19-N18	2.18	1.46	1.41
3	A	507	Y2K	C19-N18	2.17	1.46	1.41
3	B	507	Y2K	C05-C14	2.14	1.56	1.50
3	C	507	Y2K	C05-C14	2.14	1.56	1.50
3	D	507	Y2K	C05-C14	2.14	1.56	1.50
3	A	507	Y2K	C05-C14	2.14	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	506	NAG	O5-C1	2.12	1.47	1.43
2	C	506	NAG	O5-C1	2.12	1.47	1.43
2	B	506	NAG	O5-C1	2.12	1.47	1.43
3	B	507	Y2K	C35-C36	2.12	1.57	1.48
3	A	507	Y2K	C35-C36	2.12	1.57	1.48
2	A	506	NAG	O5-C1	2.12	1.47	1.43
3	D	507	Y2K	C35-C36	2.12	1.57	1.48
3	C	507	Y2K	C35-C36	2.12	1.57	1.48
3	D	507	Y2K	C09-C08	2.11	1.56	1.51
3	A	507	Y2K	C09-C08	2.11	1.56	1.51
3	B	507	Y2K	C09-C08	2.11	1.56	1.51
3	C	507	Y2K	C09-C08	2.11	1.56	1.51
2	A	505	NAG	O5-C1	2.05	1.47	1.43
2	B	505	NAG	O5-C1	2.05	1.47	1.43
2	C	505	NAG	O5-C1	2.05	1.47	1.43
2	D	505	NAG	O5-C1	2.05	1.47	1.43
2	A	508	NAG	O5-C1	2.05	1.47	1.43

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	507	Y2K	C13-C14-N15	-9.85	104.25	115.01
3	C	507	Y2K	C13-C14-N15	-9.85	104.25	115.01
3	A	507	Y2K	C13-C14-N15	-9.84	104.25	115.01
3	B	507	Y2K	C13-C14-N15	-9.84	104.26	115.01
2	D	506	NAG	C1-O5-C5	8.61	123.73	112.19
2	B	506	NAG	C1-O5-C5	8.61	123.73	112.19
2	A	506	NAG	C1-O5-C5	8.61	123.72	112.19
2	C	506	NAG	C1-O5-C5	8.61	123.72	112.19
3	B	507	Y2K	C04-N03-C13	5.92	116.25	109.75
3	A	507	Y2K	C04-N03-C13	5.92	116.25	109.75
3	C	507	Y2K	C04-N03-C13	5.92	116.25	109.75
3	D	507	Y2K	C04-N03-C13	5.92	116.25	109.75
3	C	507	Y2K	C05-C04-N03	-4.47	105.87	109.42
3	A	507	Y2K	C05-C04-N03	-4.47	105.87	109.42
3	B	507	Y2K	C05-C04-N03	-4.46	105.87	109.42
3	D	507	Y2K	C05-C04-N03	-4.46	105.87	109.42
3	A	507	Y2K	C35-O34-C02	-4.32	109.72	115.94
3	C	507	Y2K	C35-O34-C02	-4.32	109.72	115.94
3	B	507	Y2K	C35-O34-C02	-4.31	109.72	115.94
3	D	507	Y2K	C35-O34-C02	-4.31	109.73	115.94
3	B	507	Y2K	C05-C14-N15	-3.91	103.34	114.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	507	Y2K	C05-C14-N15	-3.91	103.34	114.77
3	A	507	Y2K	C05-C14-N15	-3.91	103.34	114.77
3	D	507	Y2K	C05-C14-N15	-3.91	103.35	114.77
3	A	507	Y2K	C19-C26-C24	-3.84	115.61	118.82
3	C	507	Y2K	C19-C26-C24	-3.83	115.61	118.82
3	B	507	Y2K	C19-C26-C24	-3.83	115.61	118.82
3	D	507	Y2K	C19-C26-C24	-3.83	115.61	118.82
3	C	507	Y2K	C24-C22-CL23	-3.60	115.25	119.79
3	D	507	Y2K	C24-C22-CL23	-3.59	115.25	119.79
3	B	507	Y2K	C24-C22-CL23	-3.59	115.26	119.79
3	A	507	Y2K	C24-C22-CL23	-3.59	115.26	119.79
3	C	507	Y2K	C19-N18-C17	-3.37	121.46	127.45
3	D	507	Y2K	C19-N18-C17	-3.37	121.47	127.45
3	A	507	Y2K	C19-N18-C17	-3.37	121.47	127.45
3	B	507	Y2K	C19-N18-C17	-3.37	121.47	127.45
3	D	507	Y2K	O34-C02-O01	-3.09	119.39	124.76
3	B	507	Y2K	O34-C02-O01	-3.09	119.39	124.76
3	C	507	Y2K	O34-C02-O01	-3.09	119.39	124.76
3	A	507	Y2K	O34-C02-O01	-3.08	119.39	124.76
3	C	507	Y2K	C21-C22-C24	2.96	121.58	119.04
3	B	507	Y2K	C21-C22-C24	2.96	121.58	119.04
3	D	507	Y2K	C21-C22-C24	2.96	121.58	119.04
3	A	507	Y2K	C21-C22-C24	2.96	121.58	119.04
2	C	506	NAG	C3-C4-C5	2.91	115.51	110.23
2	D	506	NAG	C3-C4-C5	2.91	115.51	110.23
2	A	506	NAG	C3-C4-C5	2.91	115.51	110.23
2	B	506	NAG	C3-C4-C5	2.91	115.50	110.23
2	C	508	NAG	C1-O5-C5	2.91	116.08	112.19
3	D	507	Y2K	O34-C02-N03	2.81	115.04	111.04
3	B	507	Y2K	O34-C02-N03	2.81	115.03	111.04
3	A	507	Y2K	O34-C02-N03	2.80	115.03	111.04
3	C	507	Y2K	O34-C02-N03	2.80	115.03	111.04
2	A	508	NAG	C4-C3-C2	-2.52	107.32	111.02
3	C	507	Y2K	C21-C22-CL23	2.39	123.13	118.42
3	D	507	Y2K	C21-C22-CL23	2.39	123.13	118.42
3	A	507	Y2K	C21-C22-CL23	2.39	123.13	118.42
3	B	507	Y2K	C21-C22-CL23	2.39	123.13	118.42
3	B	507	Y2K	C12-C04-N03	2.34	132.70	128.59
3	C	507	Y2K	C12-C04-N03	2.34	132.70	128.59
3	D	507	Y2K	C12-C04-N03	2.34	132.69	128.59
3	A	507	Y2K	C12-C04-N03	2.34	132.69	128.59
2	C	502	NAG	C1-O5-C5	2.33	115.31	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	NAG	C1-O5-C5	2.33	115.30	112.19
2	D	502	NAG	C1-O5-C5	2.33	115.30	112.19
2	A	502	NAG	C1-O5-C5	2.32	115.30	112.19
2	C	505	NAG	C1-O5-C5	2.18	115.11	112.19
3	B	507	Y2K	C07-C06-C05	-2.18	117.51	121.12
3	D	507	Y2K	C07-C06-C05	-2.18	117.51	121.12
3	A	507	Y2K	C07-C06-C05	-2.18	117.51	121.12
3	C	507	Y2K	C07-C06-C05	-2.18	117.51	121.12
2	D	505	NAG	C1-O5-C5	2.18	115.11	112.19
2	A	505	NAG	C1-O5-C5	2.18	115.10	112.19
3	B	507	Y2K	C20-C19-C26	2.18	122.29	119.66
3	A	507	Y2K	C20-C19-C26	2.18	122.29	119.66
2	B	505	NAG	C1-O5-C5	2.18	115.10	112.19
3	D	507	Y2K	C20-C19-C26	2.17	122.28	119.66
3	C	507	Y2K	C20-C19-C26	2.17	122.28	119.66
3	B	507	Y2K	C06-C05-C04	2.14	122.13	120.03
3	D	507	Y2K	C06-C05-C04	2.14	122.12	120.03
3	C	507	Y2K	C06-C05-C04	2.14	122.12	120.03
3	A	507	Y2K	C06-C05-C04	2.13	122.12	120.03
3	B	507	Y2K	C17-C16-N15	2.11	118.79	113.73
3	D	507	Y2K	C17-C16-N15	2.11	118.79	113.73
3	C	507	Y2K	C17-C16-N15	2.11	118.79	113.73
3	A	507	Y2K	C17-C16-N15	2.11	118.79	113.73
3	D	507	Y2K	C20-C21-C22	-2.07	117.12	119.98
3	C	507	Y2K	C20-C21-C22	-2.07	117.12	119.98
3	B	507	Y2K	C20-C21-C22	-2.07	117.13	119.98
3	A	507	Y2K	C20-C21-C22	-2.06	117.13	119.98
3	D	507	Y2K	C09-C08-C07	-2.06	116.73	120.94
3	C	507	Y2K	C09-C08-C07	-2.06	116.73	120.94
3	B	507	Y2K	C09-C08-C07	-2.06	116.73	120.94
3	A	507	Y2K	C09-C08-C07	-2.06	116.73	120.94
2	A	508	NAG	C1-O5-C5	2.05	114.94	112.19
3	C	507	Y2K	C04-C12-C08	-2.05	117.09	120.28
3	A	507	Y2K	C04-C12-C08	-2.05	117.09	120.28
3	D	507	Y2K	C04-C12-C08	-2.05	117.09	120.28
3	B	507	Y2K	C04-C12-C08	-2.05	117.09	120.28

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	505	NAG	O5-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
2	C	505	NAG	O5-C5-C6-O6
2	B	506	NAG	C4-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	C	506	NAG	C4-C5-C6-O6
2	B	503	NAG	O5-C5-C6-O6
2	D	503	NAG	O5-C5-C6-O6
2	A	503	NAG	O5-C5-C6-O6
2	C	503	NAG	O5-C5-C6-O6
2	B	506	NAG	O5-C5-C6-O6
2	D	506	NAG	O5-C5-C6-O6
2	A	506	NAG	O5-C5-C6-O6
2	C	506	NAG	O5-C5-C6-O6
2	B	504	NAG	O5-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	A	504	NAG	O5-C5-C6-O6
2	C	504	NAG	O5-C5-C6-O6
2	B	505	NAG	C4-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	C	505	NAG	C4-C5-C6-O6
2	B	503	NAG	C4-C5-C6-O6
2	D	503	NAG	C4-C5-C6-O6
2	A	503	NAG	C4-C5-C6-O6
2	C	503	NAG	C4-C5-C6-O6
2	B	504	NAG	C4-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6
2	A	504	NAG	C4-C5-C6-O6
2	C	504	NAG	C4-C5-C6-O6
2	A	508	NAG	C8-C7-N2-C2
2	A	508	NAG	O7-C7-N2-C2
2	C	508	NAG	C8-C7-N2-C2
2	C	508	NAG	O7-C7-N2-C2
2	C	508	NAG	C4-C5-C6-O6
2	C	508	NAG	O5-C5-C6-O6
2	A	508	NAG	C4-C5-C6-O6
2	B	506	NAG	C1-C2-N2-C7
2	D	506	NAG	C1-C2-N2-C7
2	A	506	NAG	C1-C2-N2-C7
2	C	506	NAG	C1-C2-N2-C7

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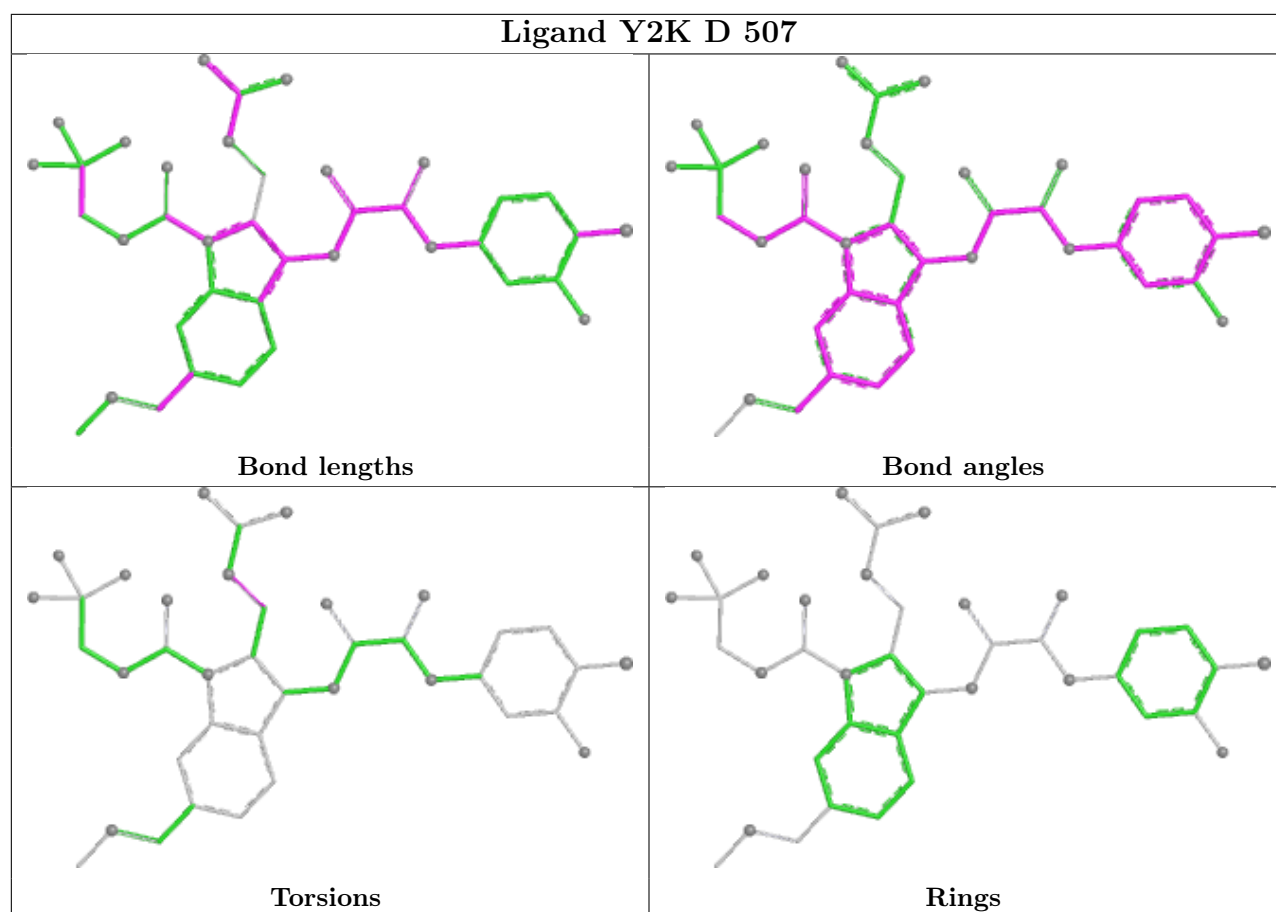
Mol	Chain	Res	Type	Atoms
3	B	507	Y2K	C13-C29-N30-C31
3	D	507	Y2K	C13-C29-N30-C31
3	A	507	Y2K	C13-C29-N30-C31
3	C	507	Y2K	C13-C29-N30-C31
2	A	508	NAG	O5-C5-C6-O6

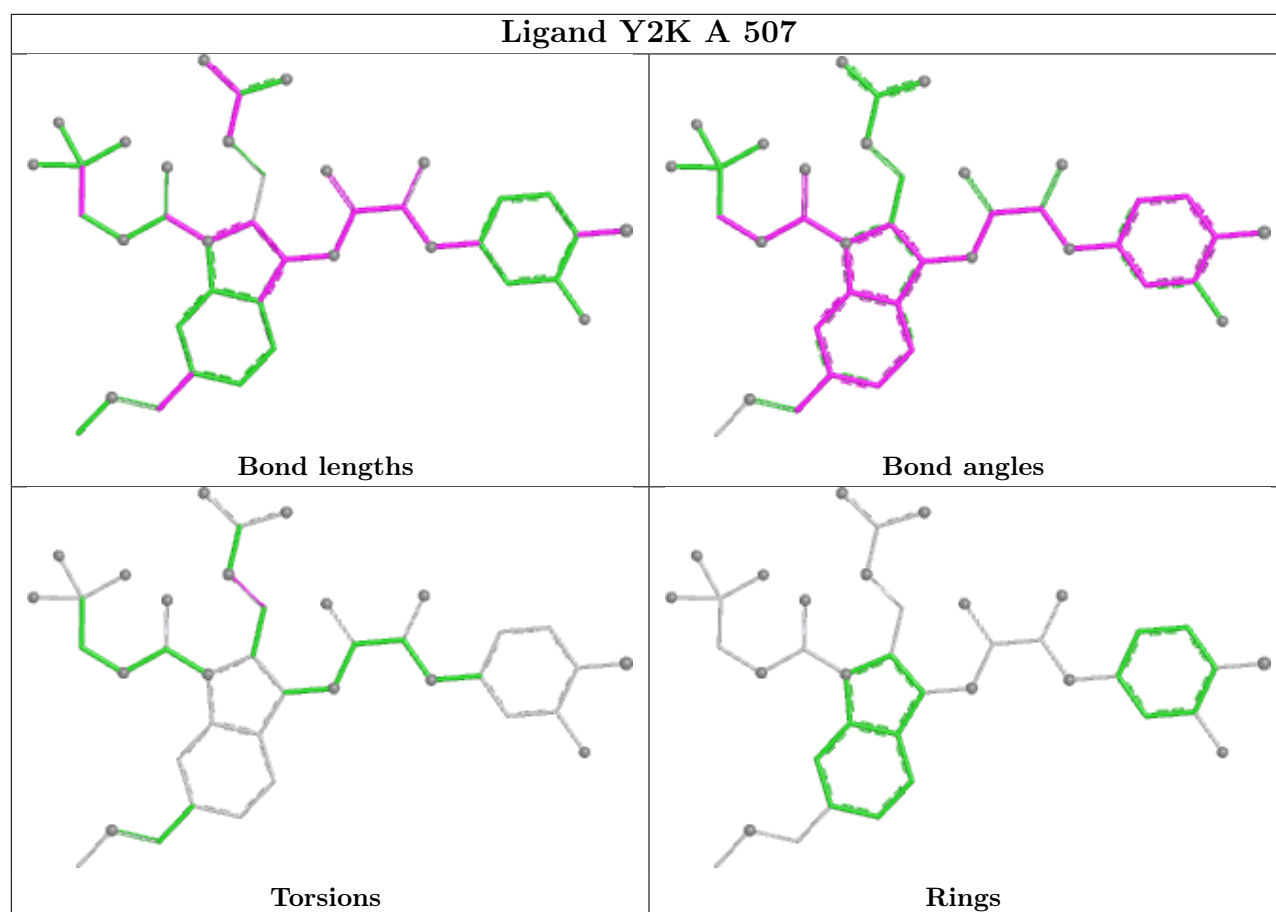
There are no ring outliers.

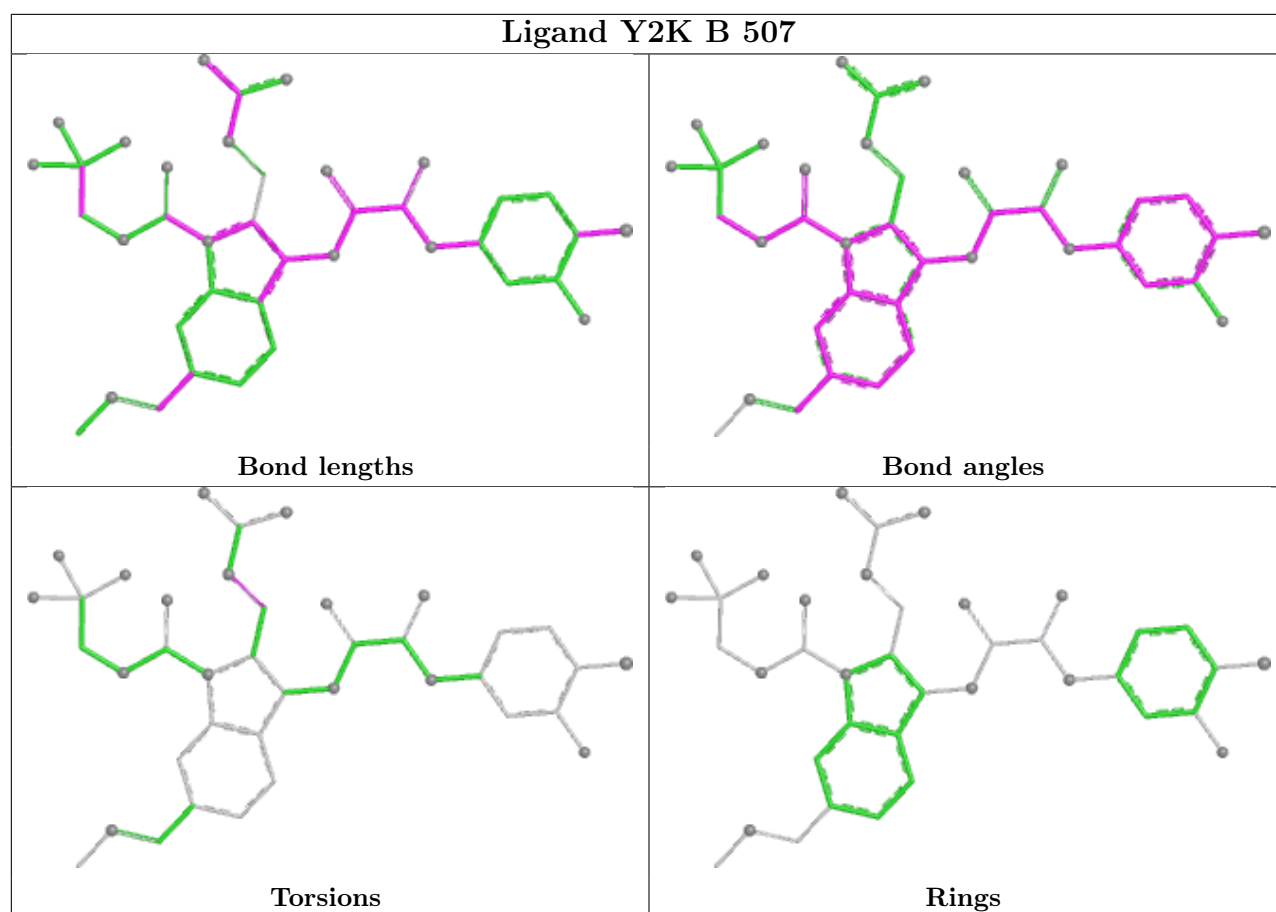
10 monomers are involved in 13 short contacts:

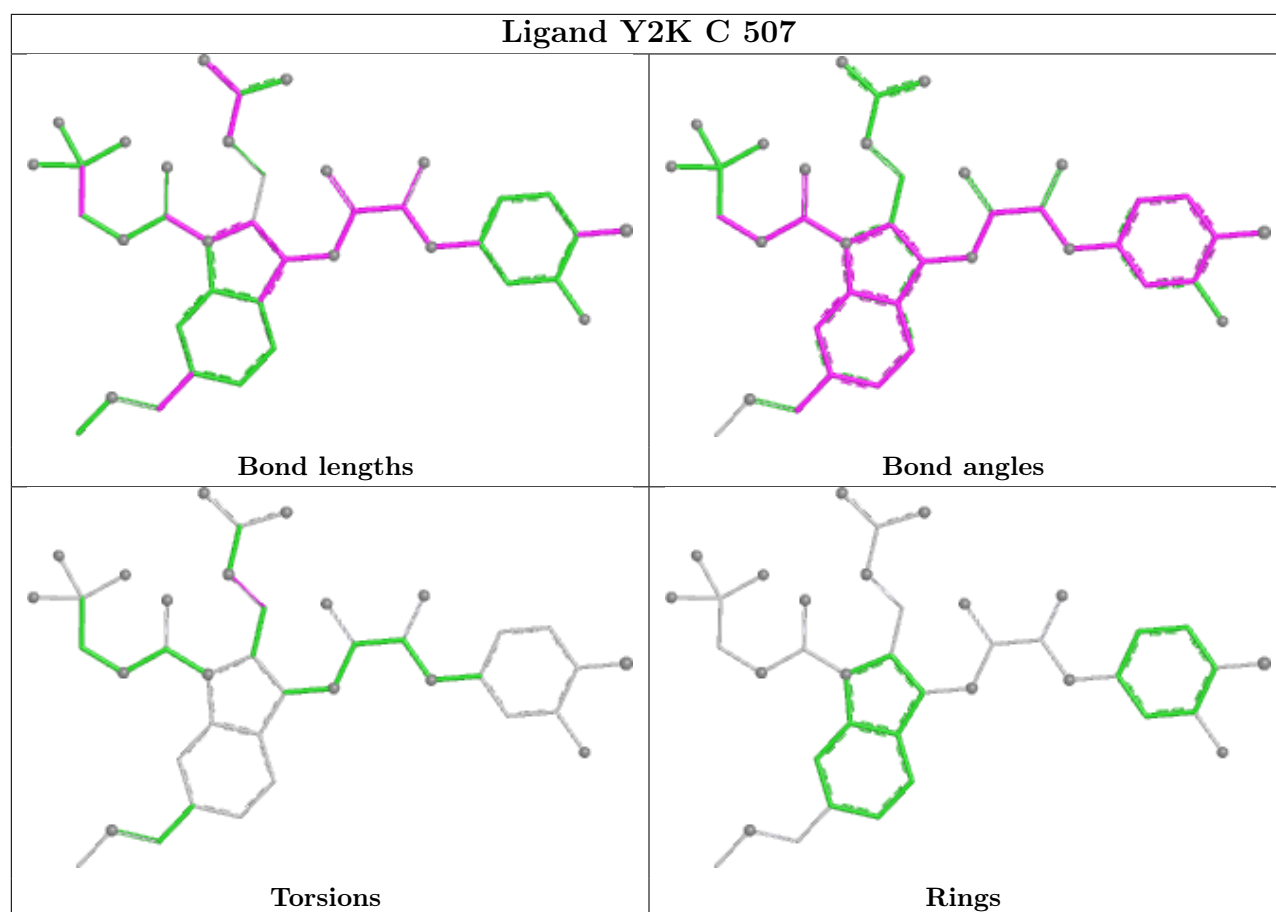
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	506	NAG	1	1
2	C	503	NAG	1	0
2	C	508	NAG	2	0
2	A	508	NAG	2	0
2	B	506	NAG	1	0
2	D	503	NAG	1	0
2	A	503	NAG	1	0
2	B	503	NAG	1	0
2	C	506	NAG	1	0
2	A	506	NAG	1	0

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.









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%)	0.93	55 (16%) 4 4	25, 42, 67, 89	0
1	B	335/358 (93%)	1.21	91 (27%) 1 1	26, 46, 79, 106	0
1	C	335/358 (93%)	1.14	63 (18%) 3 3	24, 40, 71, 122	0
1	D	335/358 (93%)	1.32	86 (25%) 1 1	27, 46, 76, 100	0
All	All	1340/1432 (93%)	1.15	295 (22%) 2 2	24, 44, 74, 122	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	TYR	11.3
1	C	60	ALA	11.1
1	C	198	GLY	9.1
1	C	124	GLY	7.2
1	C	199	SER	6.8
1	A	198	GLY	6.6
1	C	59	LYS	6.5
1	C	122	LEU	6.1
1	B	60	ALA	5.8
1	D	59	LYS	5.8
1	D	61	TYR	5.6
1	B	72	HIS	5.4
1	B	61	TYR	5.4
1	D	60	ALA	5.2
1	A	124	GLY	5.1
1	A	89	VAL	4.9
1	C	123	THR	4.9
1	D	439	ILE	4.8
1	C	81	PRO	4.8
1	A	87	ALA	4.8
1	C	87	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	85	VAL	4.7
1	A	86	LEU	4.7
1	D	397	ASN	4.6
1	D	81	PRO	4.6
1	D	72	HIS	4.6
1	C	202	THR	4.6
1	D	124	GLY	4.5
1	D	89	VAL	4.5
1	C	80	ASN	4.5
1	B	57	ASP	4.4
1	C	88	ASN	4.4
1	B	490	GLU	4.4
1	A	356	SER	4.3
1	B	50	THR	4.2
1	C	49	LYS	4.2
1	A	90	THR	4.1
1	C	57	ASP	4.1
1	D	341	THR	4.1
1	C	200	ALA	4.1
1	D	408	ARG	4.0
1	D	246	GLN	4.0
1	D	356	SER	4.0
1	B	356	SER	4.0
1	B	87	ALA	3.9
1	B	49	LYS	3.9
1	C	89	VAL	3.9
1	C	84	MET	3.9
1	B	269	GLU	3.8
1	A	354	PRO	3.8
1	B	89	VAL	3.8
1	C	356	SER	3.7
1	C	72	HIS	3.7
1	D	84	MET	3.7
1	D	88	ASN	3.7
1	C	240	ARG	3.7
1	D	240	ARG	3.7
1	B	81	PRO	3.6
1	B	226	LEU	3.6
1	D	293	ASN	3.6
1	B	231	LYS	3.6
1	C	246	GLN	3.6
1	A	200	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	79	PRO	3.6
1	B	59	LYS	3.5
1	D	300	ASN	3.5
1	A	412	GLY	3.5
1	D	85	VAL	3.5
1	D	406	THR	3.5
1	B	340	ASN	3.5
1	A	61	TYR	3.5
1	D	465	THR	3.5
1	B	396	ARG	3.5
1	C	91	GLU	3.5
1	B	397	ASN	3.5
1	D	326	ILE	3.4
1	B	84	MET	3.4
1	D	87	ALA	3.4
1	D	396	ARG	3.4
1	C	86	LEU	3.4
1	A	88	ASN	3.4
1	A	489	VAL	3.4
1	A	300	ASN	3.4
1	B	439	ILE	3.4
1	D	82	GLN	3.4
1	A	50	THR	3.3
1	B	85	VAL	3.3
1	C	79	PRO	3.3
1	B	223	PHE	3.3
1	D	441	GLY	3.3
1	A	223	PHE	3.3
1	C	396	ARG	3.2
1	B	224	ALA	3.2
1	B	88	ASN	3.2
1	D	86	LEU	3.2
1	C	489	VAL	3.2
1	D	339	ASN	3.2
1	D	345	VAL	3.1
1	D	268	GLU	3.1
1	C	398	GLY	3.1
1	C	78	ASP	3.1
1	D	198	GLY	3.1
1	B	86	LEU	3.1
1	D	90	THR	3.1
1	B	242	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	82	GLN	3.1
1	A	60	ALA	3.0
1	C	408	ARG	3.0
1	D	299	PRO	3.0
1	D	404	ASN	3.0
1	D	399	THR	3.0
1	B	122	LEU	3.0
1	B	339	ASN	3.0
1	D	201	ILE	3.0
1	D	49	LYS	3.0
1	D	223	PHE	3.0
1	B	265	LEU	2.9
1	A	241	ASN	2.9
1	B	201	ILE	2.9
1	D	358	THR	2.9
1	A	278	THR	2.9
1	B	246	GLN	2.9
1	A	396	ARG	2.9
1	B	198	GLY	2.9
1	B	357	LYS	2.9
1	B	489	VAL	2.9
1	B	399	THR	2.9
1	C	82	GLN	2.9
1	D	267	GLU	2.9
1	D	361	PHE	2.9
1	D	403	TYR	2.9
1	A	199	SER	2.9
1	D	398	GLY	2.9
1	B	488	VAL	2.9
1	A	202	THR	2.9
1	B	63	LYS	2.9
1	C	241	ASN	2.9
1	D	464	ASP	2.8
1	A	410	SER	2.8
1	B	240	ARG	2.8
1	D	269	GLU	2.8
1	B	229	ASN	2.8
1	B	464	ASP	2.8
1	C	300	ASN	2.8
1	D	202	THR	2.8
1	A	49	LYS	2.8
1	C	406	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	489	VAL	2.8
1	A	85	VAL	2.8
1	B	432	ARG	2.7
1	A	72	HIS	2.7
1	B	55	ALA	2.7
1	B	354	PRO	2.7
1	C	328	GLN	2.7
1	B	241	ASN	2.7
1	D	241	ASN	2.7
1	A	229	ASN	2.7
1	D	432	ARG	2.7
1	D	50	THR	2.7
1	C	51	THR	2.7
1	B	79	PRO	2.7
1	C	340	ASN	2.7
1	C	242	VAL	2.7
1	D	337	LYS	2.7
1	B	51	THR	2.7
1	A	464	ASP	2.7
1	C	113	ASP	2.7
1	B	268	GLU	2.6
1	D	440	GLU	2.6
1	B	465	THR	2.6
1	C	325	ASN	2.6
1	B	97	LYS	2.6
1	D	199	SER	2.6
1	C	337	LYS	2.6
1	A	239	CYS	2.6
1	B	406	THR	2.6
1	D	354	PRO	2.6
1	A	226	LEU	2.6
1	B	93	PHE	2.6
1	C	339	ASN	2.6
1	C	77	THR	2.6
1	C	464	ASP	2.6
1	C	223	PHE	2.5
1	C	268	GLU	2.5
1	B	326	ILE	2.5
1	A	68	VAL	2.5
1	B	408	ARG	2.5
1	A	408	ARG	2.5
1	B	244	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	395	TYR	2.5
1	A	78	ASP	2.5
1	A	264	SER	2.5
1	C	327	ARG	2.5
1	B	78	ASP	2.5
1	B	342	LEU	2.5
1	B	325	ASN	2.5
1	A	62	GLU	2.4
1	A	268	GLU	2.4
1	C	90	THR	2.4
1	B	219	ALA	2.4
1	D	357	LYS	2.4
1	B	124	GLY	2.4
1	D	229	ASN	2.4
1	B	82	GLN	2.4
1	B	457	ASP	2.4
1	D	414	ILE	2.4
1	A	439	ILE	2.4
1	B	395	TYR	2.4
1	B	341	THR	2.4
1	B	200	ALA	2.4
1	B	80	ASN	2.4
1	C	229	ASN	2.4
1	B	353	PHE	2.4
1	A	57	ASP	2.4
1	B	410	SER	2.4
1	A	63	LYS	2.4
1	C	358	THR	2.4
1	C	58	ALA	2.4
1	D	80	ASN	2.4
1	D	245	VAL	2.4
1	B	358	THR	2.4
1	C	269	GLU	2.3
1	B	293	ASN	2.3
1	B	404	ASN	2.3
1	D	122	LEU	2.3
1	A	246	GLN	2.3
1	C	397	ASN	2.3
1	D	231	LYS	2.3
1	D	405	HIS	2.3
1	B	83	GLU	2.3
1	D	338	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	412	GLY	2.3
1	A	93	PHE	2.3
1	B	245	VAL	2.3
1	B	90	THR	2.3
1	B	220	PRO	2.3
1	A	240	ARG	2.3
1	B	62	GLU	2.3
1	C	62	GLU	2.3
1	C	290	GLU	2.3
1	B	71	THR	2.3
1	D	394	THR	2.3
1	D	325	ASN	2.3
1	B	58	ALA	2.3
1	B	344	LYS	2.3
1	D	62	GLU	2.2
1	D	342	LEU	2.2
1	B	91	GLU	2.2
1	B	379	ARG	2.2
1	D	123	THR	2.2
1	A	201	ILE	2.2
1	C	50	THR	2.2
1	D	242	VAL	2.2
1	D	488	VAL	2.2
1	C	121	LYS	2.2
1	D	359	ILE	2.2
1	D	413	THR	2.2
1	A	225	ILE	2.2
1	B	337	LYS	2.2
1	D	340	ASN	2.2
1	B	290	GLU	2.1
1	D	290	GLU	2.1
1	C	75	VAL	2.1
1	A	80	ASN	2.1
1	D	57	ASP	2.1
1	D	244	THR	2.1
1	C	399	THR	2.1
1	C	201	ILE	2.1
1	A	398	GLY	2.1
1	A	219	ALA	2.1
1	C	490	GLU	2.1
1	B	77	THR	2.1
1	C	354	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	292	VAL	2.1
1	D	63	LYS	2.1
1	B	411	ASN	2.1
1	D	334	ASN	2.1
1	D	411	ASN	2.1
1	A	81	PRO	2.1
1	B	398	GLY	2.1
1	D	97	LYS	2.1
1	B	199	SER	2.1
1	D	266	ALA	2.1
1	A	397	ASN	2.0
1	D	327	ARG	2.0
1	B	405	HIS	2.0
1	A	238	PRO	2.0
1	B	222	GLY	2.0
1	B	403	TYR	2.0
1	A	395	TYR	2.0
1	B	292	VAL	2.0
1	A	353	PHE	2.0
1	A	325	ASN	2.0
1	B	487	LYS	2.0
1	A	441	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(Å ²)	Q<0.9
2	NAG	A	506	14/15	0.55	0.26	81,95,106,112	0

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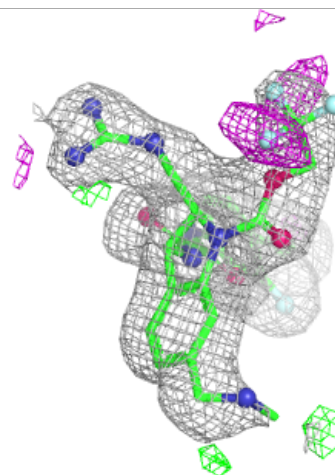
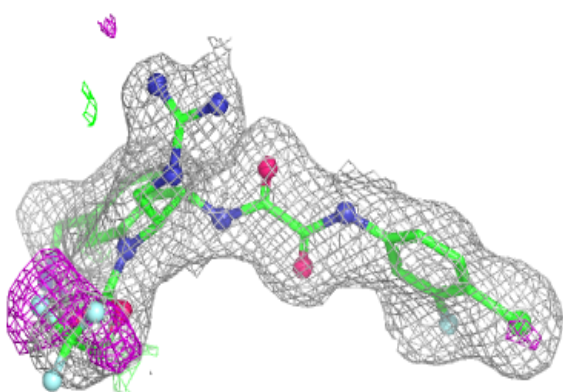
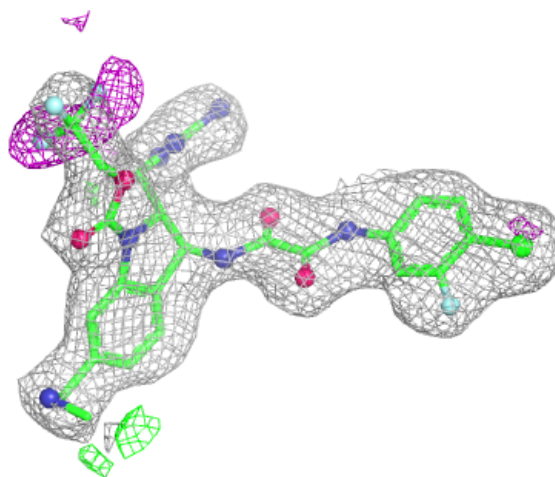
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	506	14/15	0.57	0.28	59,65,73,78	0
2	NAG	B	506	14/15	0.64	0.24	47,59,66,68	0
2	NAG	C	506	14/15	0.64	0.22	57,67,75,82	0
2	NAG	D	503	14/15	0.72	0.19	58,65,71,79	0
2	NAG	B	501	14/15	0.76	0.15	43,54,60,61	0
2	NAG	D	501	14/15	0.77	0.15	40,52,61,66	0
2	NAG	B	503	14/15	0.79	0.18	62,63,71,74	0
2	NAG	B	504	14/15	0.79	0.14	45,54,60,60	0
2	NAG	D	505	14/15	0.80	0.16	60,63,68,69	0
2	NAG	C	508	14/15	0.80	0.14	50,58,59,62	0
2	NAG	C	503	14/15	0.82	0.15	53,57,60,66	0
2	NAG	A	504	14/15	0.83	0.13	44,51,60,67	0
2	NAG	C	504	14/15	0.84	0.13	30,42,51,52	0
2	NAG	A	501	14/15	0.84	0.13	43,54,60,69	0
2	NAG	D	504	14/15	0.84	0.14	51,56,60,62	0
2	NAG	A	508	14/15	0.85	0.12	49,54,58,62	0
2	NAG	C	505	14/15	0.85	0.14	35,42,46,49	0
2	NAG	C	501	14/15	0.87	0.11	34,45,49,60	0
2	NAG	A	503	14/15	0.87	0.12	48,52,55,57	0
2	NAG	B	505	14/15	0.87	0.12	53,57,60,64	0
2	NAG	A	505	14/15	0.88	0.13	34,40,46,52	0
2	NAG	D	502	14/15	0.89	0.11	34,41,45,50	0
2	NAG	B	502	14/15	0.91	0.10	31,42,45,47	0
3	Y2K	B	507	39/39	0.91	0.11	25,33,53,66	0
2	NAG	C	502	14/15	0.92	0.09	26,36,39,44	0
2	NAG	A	502	14/15	0.93	0.08	28,37,46,46	0
3	Y2K	D	507	39/39	0.93	0.11	25,35,58,75	0
3	Y2K	A	507	39/39	0.93	0.10	25,31,55,76	0
3	Y2K	C	507	39/39	0.93	0.11	23,30,58,76	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.

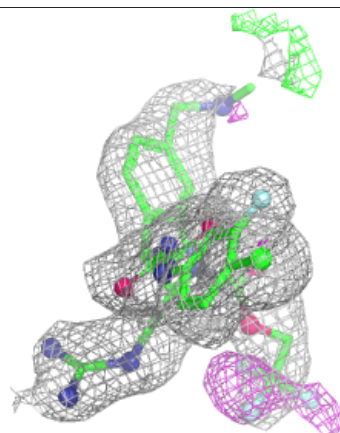
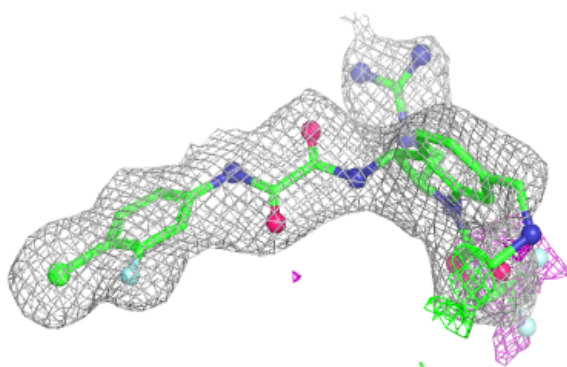
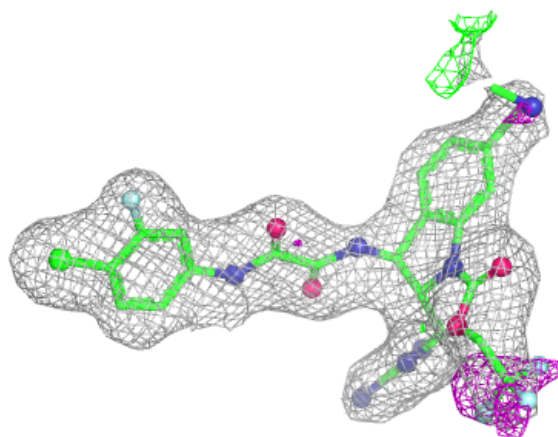
Electron density around Y2K B 507:

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



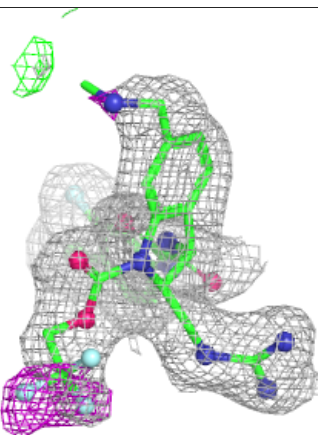
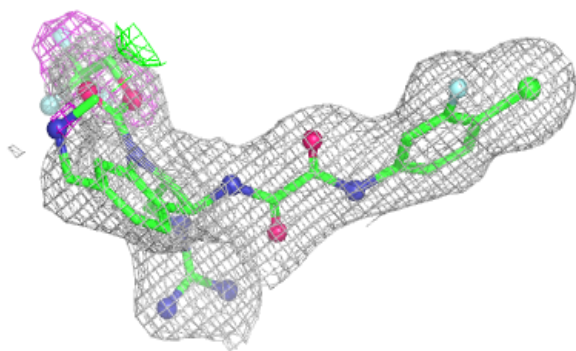
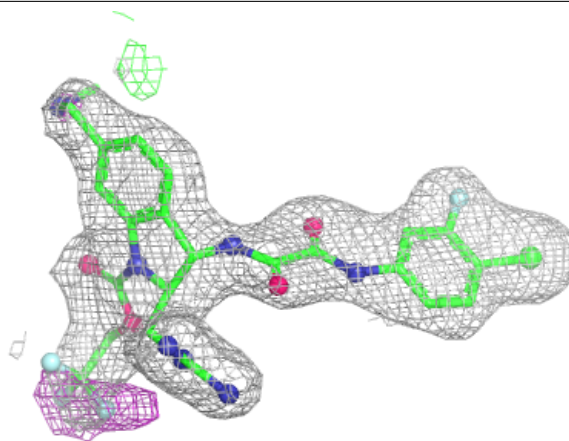
Electron density around Y2K D 507:

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



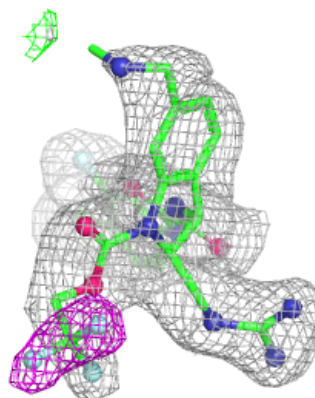
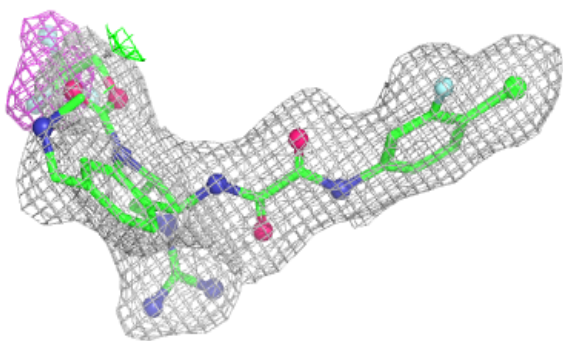
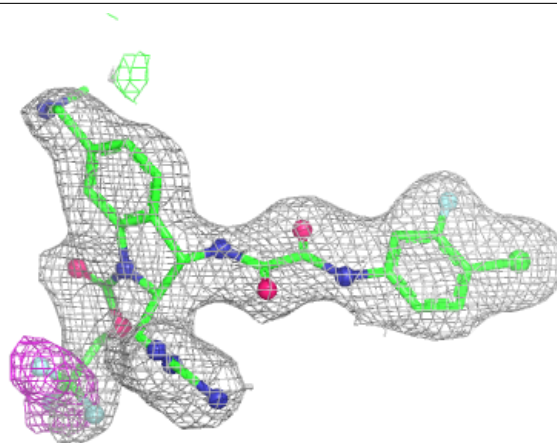
Electron density around Y2K A 507:

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



Electron density around Y2K 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.