



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:54 AM UTC

PDB ID : 8FM8 / pdb_00008fm8
Title : HIV-1 gp120 complex with CJC-IV-046
Authors : Gong, Z.; Hendrickson, W.A.
Deposited on : 2022-12-22
Resolution : 2.47 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

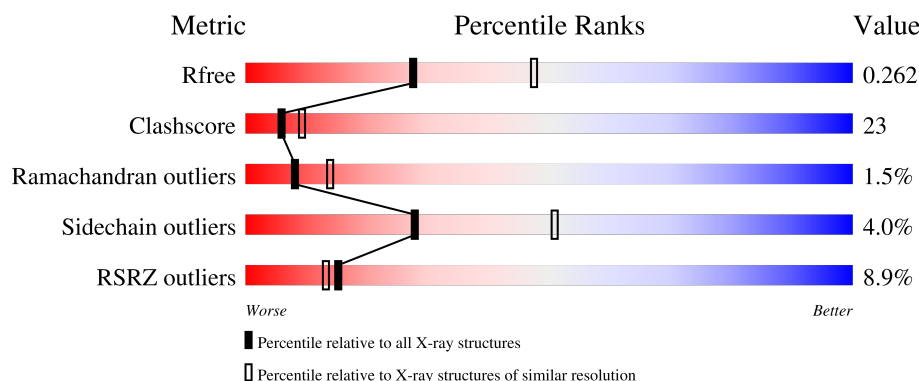
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	5% 59% 29% 5% 6%
1	B	358	12% 59% 29% 5% 6%
1	C	358	9% 59% 30% • 6%
1	D	358	8% 61% 28% • 6%

2 Entry composition [i](#)

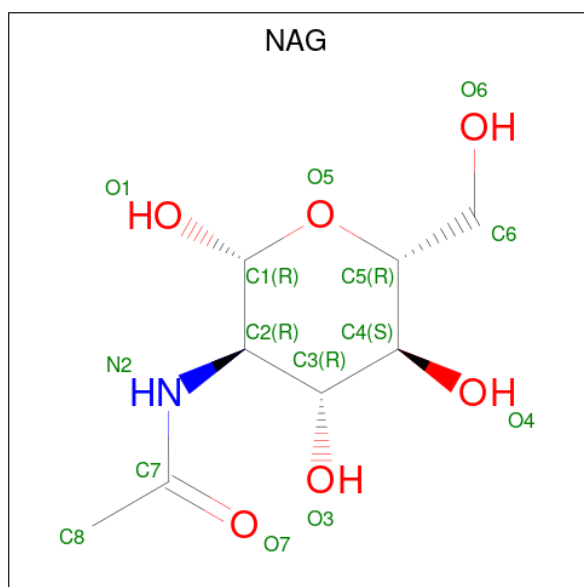
There are 5 unique types of molecules in this entry. The entry contains 11282 atoms, of which 5 are hydrogens and 0 are deuteriums.

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	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			
1	A	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	B	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	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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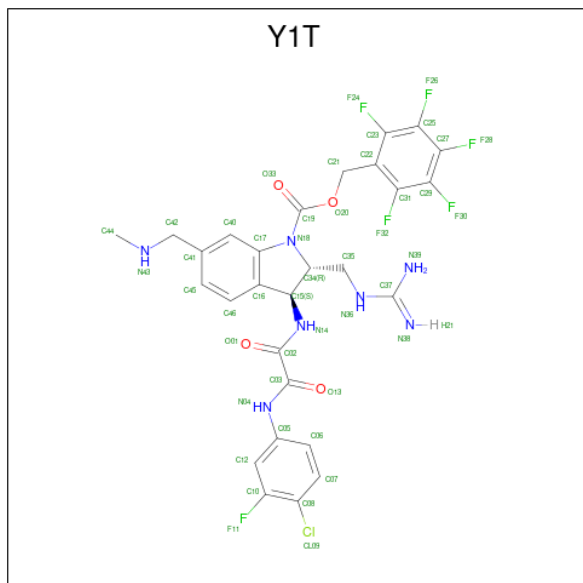
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	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	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		

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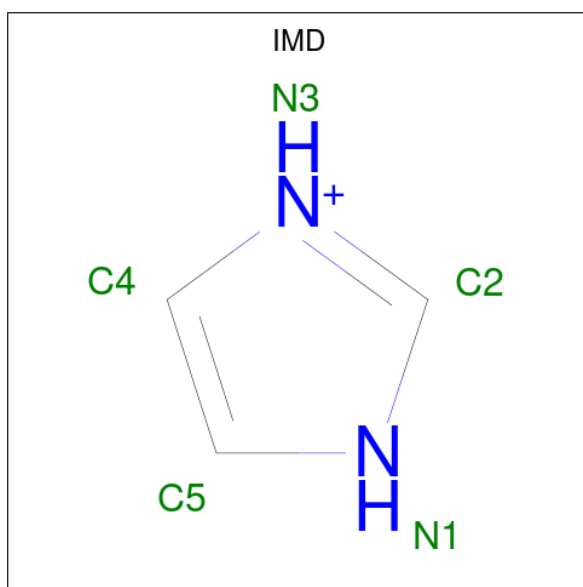
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (pentafluorophenyl)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: Y1T) (formula: $C_{28}H_{24}ClF_6N_7O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	Cl	F	N	O	0	0
			46	28	1	6	7	4		
3	D	1	Total	C	Cl	F	N	O	0	0
			46	28	1	6	7	4		
3	A	1	Total	C	Cl	F	N	O	0	0
			46	28	1	6	7	4		
3	B	1	Total	C	Cl	F	N	O	0	0
			46	28	1	6	7	4		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	N	0	0
			10	3	5	2		

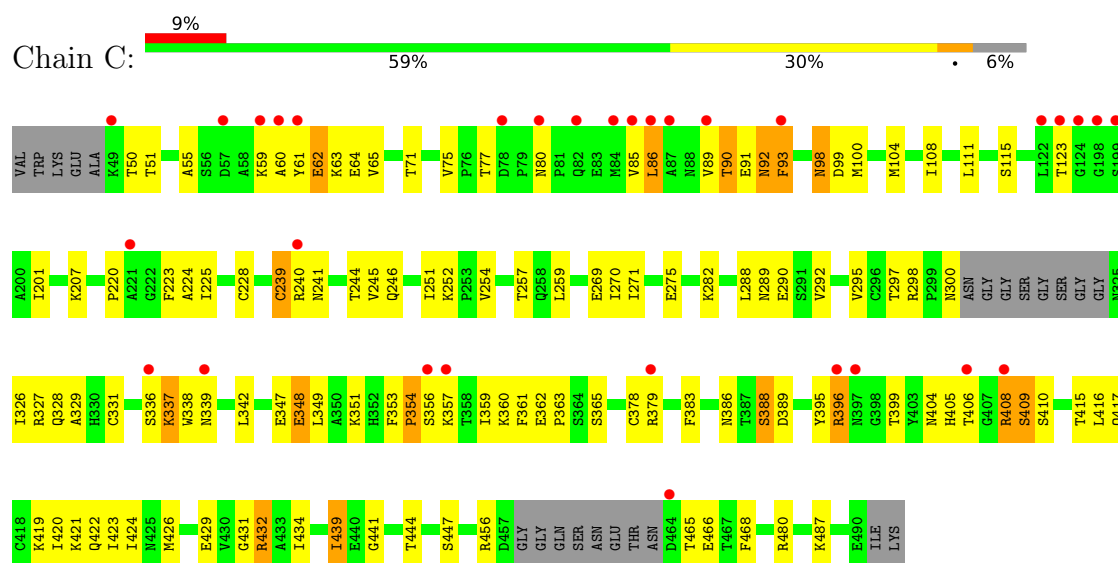
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	70	Total	O	0	0
			70	70		
5	D	53	Total	O	0	0
			53	53		
5	A	68	Total	O	0	0
			68	68		
5	B	53	Total	O	0	0
			53	53		

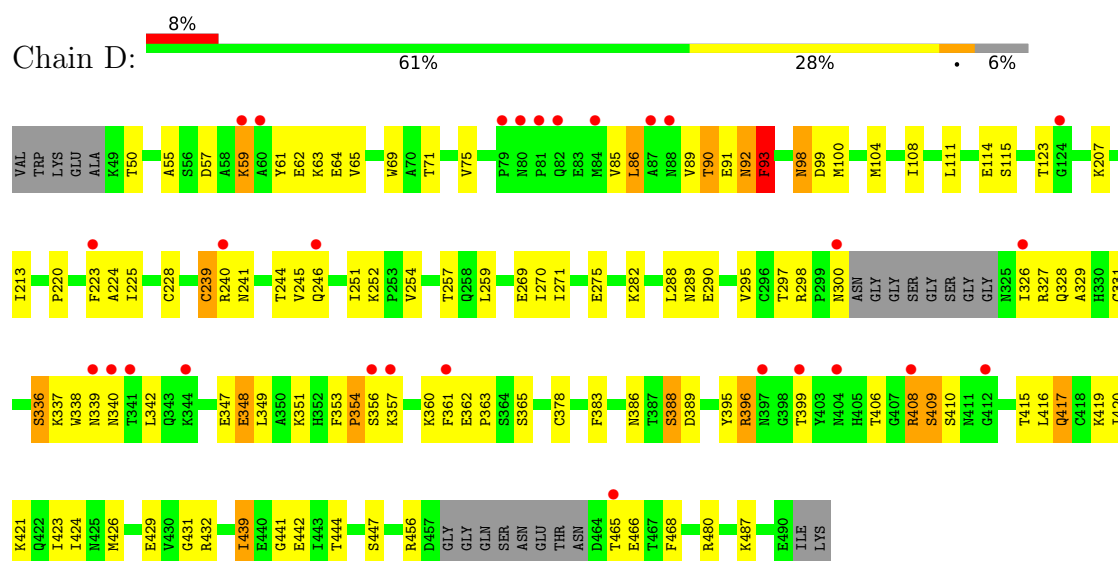
3 Residue-property plots

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.53Å 121.79Å 194.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.47 48.65 – 2.47	Depositor EDS
% Data completeness (in resolution range)	69.5 (48.65-2.47) 69.4 (48.65-2.47)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.217 , 0.263 0.220 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.6	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	0.91	EDS
Total number of atoms	11282	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.60% 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: Y1T, NAG, IMD

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	0.60	0/2682	0.97	16/3640 (0.4%)
1	B	0.60	0/2682	0.97	16/3640 (0.4%)
1	C	0.60	0/2682	0.97	16/3640 (0.4%)
1	D	0.60	0/2682	0.97	16/3640 (0.4%)
All	All	0.60	0/10728	0.97	64/14560 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	ARG	CB-CG-CD	7.70	129.00	111.30
1	D	408	ARG	CB-CG-CD	7.68	128.97	111.30
1	C	408	ARG	CB-CG-CD	7.68	128.96	111.30
1	A	408	ARG	CB-CG-CD	7.67	128.94	111.30
1	C	408	ARG	CA-CB-CG	-7.61	98.87	114.10
1	A	408	ARG	CA-CB-CG	-7.61	98.89	114.10
1	D	408	ARG	CA-CB-CG	-7.60	98.90	114.10
1	B	408	ARG	CA-CB-CG	-7.58	98.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	388	SER	CA-C-N	-6.85	110.78	122.56
1	D	388	SER	C-N-CA	-6.85	110.78	122.56
1	C	388	SER	CA-C-N	-6.83	110.81	122.56
1	C	388	SER	C-N-CA	-6.83	110.81	122.56
1	A	388	SER	CA-C-N	-6.82	110.83	122.56
1	A	388	SER	C-N-CA	-6.82	110.83	122.56
1	B	388	SER	CA-C-N	-6.81	110.84	122.56
1	B	388	SER	C-N-CA	-6.81	110.84	122.56
1	C	396	ARG	CA-C-N	-6.56	114.00	122.79
1	C	396	ARG	C-N-CA	-6.56	114.00	122.79
1	B	396	ARG	CA-C-N	-6.56	114.00	122.79
1	B	396	ARG	C-N-CA	-6.56	114.00	122.79
1	D	396	ARG	CA-C-N	-6.55	114.01	122.79
1	D	396	ARG	C-N-CA	-6.55	114.01	122.79
1	A	396	ARG	CA-C-N	-6.54	114.02	122.79
1	A	396	ARG	C-N-CA	-6.54	114.02	122.79
1	C	432	ARG	CB-CG-CD	6.44	126.12	111.30
1	A	432	ARG	CB-CG-CD	6.42	126.06	111.30
1	D	432	ARG	CB-CG-CD	6.41	126.05	111.30
1	B	432	ARG	CB-CG-CD	6.41	126.05	111.30
1	D	337	LYS	CA-CB-CG	-6.39	101.33	114.10
1	B	337	LYS	CA-CB-CG	-6.38	101.35	114.10
1	A	337	LYS	CA-CB-CG	-6.37	101.36	114.10
1	C	337	LYS	CA-CB-CG	-6.36	101.38	114.10
1	C	71	THR	CA-C-N	-6.03	111.82	122.26
1	C	71	THR	C-N-CA	-6.03	111.82	122.26
1	D	71	THR	CA-C-N	-6.02	111.84	122.26
1	D	71	THR	C-N-CA	-6.02	111.84	122.26
1	A	71	THR	CA-C-N	-6.01	111.86	122.26
1	A	71	THR	C-N-CA	-6.01	111.86	122.26
1	B	71	THR	CA-C-N	-5.99	111.89	122.26
1	B	71	THR	C-N-CA	-5.99	111.89	122.26
1	A	337	LYS	CB-CG-CD	5.72	124.47	111.30
1	C	337	LYS	CB-CG-CD	5.71	124.44	111.30
1	D	337	LYS	CB-CG-CD	5.70	124.41	111.30
1	B	337	LYS	CB-CG-CD	5.70	124.40	111.30
1	B	432	ARG	CA-CB-CG	-5.30	103.50	114.10
1	D	432	ARG	CA-CB-CG	-5.29	103.52	114.10
1	A	432	ARG	CA-CB-CG	-5.28	103.54	114.10
1	C	432	ARG	CA-CB-CG	-5.27	103.56	114.10
1	D	239	CYS	CA-C-N	5.24	127.76	120.63
1	D	239	CYS	C-N-CA	5.24	127.76	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	CYS	CA-C-N	5.21	127.72	120.63
1	B	239	CYS	C-N-CA	5.21	127.72	120.63
1	C	239	CYS	CA-C-N	5.21	127.71	120.63
1	C	239	CYS	C-N-CA	5.21	127.71	120.63
1	A	239	CYS	CA-C-N	5.18	127.67	120.63
1	A	239	CYS	C-N-CA	5.18	127.67	120.63
1	D	92	ASN	CA-C-N	-5.15	114.17	122.82
1	D	92	ASN	C-N-CA	-5.15	114.17	122.82
1	A	92	ASN	CA-C-N	-5.15	114.17	122.82
1	A	92	ASN	C-N-CA	-5.15	114.17	122.82
1	B	92	ASN	CA-C-N	-5.13	114.19	122.82
1	B	92	ASN	C-N-CA	-5.13	114.19	122.82
1	C	92	ASN	CA-C-N	-5.11	114.24	122.82
1	C	92	ASN	C-N-CA	-5.11	114.24	122.82

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	GLU	Sidechain
1	A	396	ARG	Sidechain
1	A	93	PHE	Sidechain
1	B	348	GLU	Sidechain
1	B	396	ARG	Sidechain
1	B	93	PHE	Sidechain
1	C	348	GLU	Sidechain
1	C	396	ARG	Sidechain
1	C	93	PHE	Sidechain
1	D	348	GLU	Sidechain
1	D	396	ARG	Sidechain
1	D	93	PHE	Sidechain

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	2542	121	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2627	0	2542	117	0
1	C	2627	0	2542	148	1
1	D	2627	0	2542	128	0
2	A	84	0	78	11	0
2	B	84	0	78	6	0
2	C	84	0	78	8	0
2	D	84	0	78	6	0
3	A	46	0	0	0	0
3	B	46	0	0	0	0
3	C	46	0	0	0	0
3	D	46	0	0	1	0
4	A	5	5	5	2	0
5	A	68	0	0	4	0
5	B	53	0	0	10	0
5	C	70	0	0	5	0
5	D	53	0	0	1	0
All	All	11277	5	10485	492	1

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 23.

All (492) 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:61:TYR:HD2	1:D:59:LYS:NZ	1.27	1.27
1:C:61:TYR:CD2	1:D:59:LYS:NZ	2.11	1.17
1:B:432:ARG:NH2	5:B:601:HOH:O	1.77	1.16
1:C:60:ALA:HB3	1:D:59:LYS:HE2	1.35	1.05
2:C:503:NAG:H83	2:C:503:NAG:H3	1.40	1.01
2:A:503:NAG:H3	2:A:503:NAG:H83	1.40	1.00
2:D:503:NAG:H3	2:D:503:NAG:H83	1.40	0.99
2:B:503:NAG:H3	2:B:503:NAG:H83	1.40	0.99
1:C:60:ALA:C	1:D:59:LYS:HE3	1.88	0.97
1:C:80:ASN:HB2	1:D:442:GLU:HB3	1.49	0.93
1:C:61:TYR:HD2	1:D:59:LYS:HZ2	0.93	0.92
1:C:61:TYR:H	1:D:59:LYS:HZ1	1.14	0.91
1:C:61:TYR:N	1:D:59:LYS:HZ1	1.70	0.89
1:C:61:TYR:N	1:D:59:LYS:HE3	1.86	0.89
2:D:503:NAG:H3	2:D:503:NAG:C8	2.08	0.84
2:B:503:NAG:H3	2:B:503:NAG:C8	2.08	0.84
2:C:503:NAG:H3	2:C:503:NAG:C8	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:LYS:HG2	1:D:61:TYR:CZ	2.14	0.83
2:A:503:NAG:H3	2:A:503:NAG:C8	2.08	0.83
1:B:464:ASP:OD1	5:B:602:HOH:O	1.97	0.82
1:C:408:ARG:NH1	1:A:399:THR:HB	1.93	0.82
1:B:59:LYS:HG2	1:B:61:TYR:CZ	2.14	0.82
1:C:60:ALA:C	1:D:59:LYS:CE	2.53	0.81
1:C:404:ASN:HD22	2:A:505:NAG:H62	1.45	0.81
1:A:59:LYS:HG2	1:A:61:TYR:CZ	2.14	0.81
1:A:98:ASN:C	1:A:98:ASN:HD22	1.89	0.81
1:D:98:ASN:C	1:D:98:ASN:HD22	1.89	0.80
1:C:98:ASN:C	1:C:98:ASN:HD22	1.89	0.80
1:B:98:ASN:C	1:B:98:ASN:HD22	1.89	0.80
1:C:85:VAL:O	1:C:86:LEU:HG	1.82	0.80
1:A:59:LYS:H	1:A:59:LYS:HD2	1.48	0.79
1:A:85:VAL:O	1:A:86:LEU:HG	1.82	0.79
1:D:59:LYS:H	1:D:59:LYS:HD2	1.48	0.79
1:C:61:TYR:N	1:D:59:LYS:CE	2.45	0.79
1:D:85:VAL:O	1:D:86:LEU:HG	1.82	0.78
1:B:59:LYS:H	1:B:59:LYS:HD2	1.48	0.78
1:C:60:ALA:CB	1:D:59:LYS:HE2	2.11	0.78
1:B:85:VAL:O	1:B:86:LEU:HG	1.81	0.78
1:B:59:LYS:HD2	1:B:59:LYS:N	1.99	0.77
1:D:59:LYS:HD2	1:D:59:LYS:N	1.99	0.77
1:A:59:LYS:HD2	1:A:59:LYS:N	1.99	0.77
1:B:379:ARG:NH1	5:B:604:HOH:O	2.17	0.76
2:C:503:NAG:H83	2:C:503:NAG:C3	2.16	0.75
2:D:503:NAG:H83	2:D:503:NAG:C3	2.16	0.74
1:C:61:TYR:N	1:D:59:LYS:NZ	2.36	0.73
2:B:503:NAG:H83	2:B:503:NAG:C3	2.16	0.73
1:C:80:ASN:HB2	1:D:442:GLU:CB	2.18	0.72
1:C:422:GLN:HG3	5:C:635:HOH:O	1.89	0.72
1:D:86:LEU:HB3	1:D:89:VAL:CG2	2.20	0.71
1:C:86:LEU:HB3	1:C:89:VAL:CG2	2.20	0.71
1:A:86:LEU:HB3	1:A:89:VAL:CG2	2.20	0.71
1:B:86:LEU:HB3	1:B:89:VAL:CG2	2.20	0.71
1:A:90:THR:HA	1:A:239:CYS:O	1.91	0.70
2:A:503:NAG:H83	2:A:503:NAG:C3	2.16	0.70
1:D:90:THR:HA	1:D:239:CYS:O	1.91	0.70
1:C:90:THR:HA	1:C:239:CYS:O	1.91	0.70
1:C:408:ARG:HH12	1:A:399:THR:CG2	2.05	0.70
2:C:505:NAG:H62	1:A:404:ASN:HD22	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:PHE:HB3	1:D:357:LYS:HE2	1.75	0.69
1:C:419:LYS:HD3	1:C:421:LYS:HG2	1.75	0.69
1:B:90:THR:HA	1:B:239:CYS:O	1.91	0.69
1:D:419:LYS:HD3	1:D:421:LYS:HG2	1.75	0.69
1:A:419:LYS:HD3	1:A:421:LYS:HG2	1.75	0.69
1:B:353:PHE:HB3	1:B:357:LYS:HE2	1.75	0.68
1:A:93:PHE:CD1	1:A:487:LYS:HD3	2.29	0.68
1:A:49:LYS:HE2	5:A:617:HOH:O	1.94	0.68
1:C:80:ASN:CB	1:D:442:GLU:HB3	2.21	0.68
1:B:419:LYS:HD3	1:B:421:LYS:HG2	1.76	0.68
1:C:93:PHE:CD1	1:C:487:LYS:HD3	2.29	0.68
1:C:80:ASN:HB2	1:D:442:GLU:H	1.59	0.67
1:C:98:ASN:HD21	1:C:100:MET:HG3	1.59	0.67
1:C:353:PHE:HB3	1:C:357:LYS:HE2	1.75	0.67
1:D:98:ASN:HD21	1:D:100:MET:HG3	1.59	0.67
1:A:98:ASN:HD21	1:A:100:MET:HG3	1.59	0.67
1:A:353:PHE:HB3	1:A:357:LYS:HE2	1.75	0.67
1:C:408:ARG:HH12	1:A:399:THR:HG22	1.60	0.67
1:B:98:ASN:HD21	1:B:100:MET:HG3	1.59	0.66
1:A:207:LYS:HD2	1:A:439:ILE:HG23	1.79	0.65
1:A:405:HIS:O	4:A:508:IMD:C2	2.45	0.65
1:C:207:LYS:HD2	1:C:439:ILE:HG23	1.79	0.65
1:B:419:LYS:NZ	5:B:603:HOH:O	2.12	0.64
1:D:207:LYS:HD2	1:D:439:ILE:HG23	1.79	0.64
1:D:298:ARG:HG2	1:D:328:GLN:O	1.98	0.64
1:B:298:ARG:HG2	1:B:328:GLN:O	1.98	0.64
1:B:207:LYS:HD2	1:B:439:ILE:HG23	1.79	0.64
1:A:298:ARG:HG2	1:A:328:GLN:O	1.98	0.63
1:C:275:GLU:OE2	1:C:282:LYS:HE3	1.99	0.63
1:C:298:ARG:HG2	1:C:328:GLN:O	1.98	0.63
1:B:275:GLU:OE2	1:B:282:LYS:HE3	1.99	0.63
1:D:62:GLU:OE2	1:D:64:GLU:HB2	1.99	0.63
1:A:275:GLU:OE2	1:A:282:LYS:HE3	1.99	0.63
1:C:61:TYR:CB	1:D:57:ASP:O	2.46	0.63
1:D:275:GLU:OE2	1:D:282:LYS:HE3	1.99	0.63
1:D:92:ASN:C	1:D:93:PHE:HD1	2.07	0.63
1:B:62:GLU:OE2	1:B:64:GLU:HB2	1.99	0.62
1:B:92:ASN:C	1:B:93:PHE:HD1	2.07	0.62
1:D:86:LEU:HB3	1:D:89:VAL:HG21	1.81	0.62
1:A:86:LEU:HB3	1:A:89:VAL:HG21	1.81	0.62
1:A:241:ASN:ND2	5:A:601:HOH:O	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:TYR:HB2	1:D:57:ASP:O	2.00	0.62
1:C:98:ASN:ND2	1:C:100:MET:H	1.98	0.62
1:D:98:ASN:ND2	1:D:100:MET:H	1.98	0.62
1:B:79:PRO:HA	5:B:613:HOH:O	2.00	0.62
1:C:290:GLU:OE2	1:C:337:LYS:NZ	2.23	0.61
1:A:98:ASN:ND2	1:A:100:MET:H	1.98	0.61
1:B:98:ASN:ND2	1:B:100:MET:H	1.98	0.61
1:B:362:GLU:HG2	2:B:505:NAG:H82	1.82	0.61
1:C:86:LEU:HB3	1:C:89:VAL:HG21	1.81	0.61
1:D:123:THR:HG21	1:D:429:GLU:OE1	2.01	0.61
1:D:417:GLN:HA	1:D:417:GLN:OE1	2.01	0.61
1:B:86:LEU:HB3	1:B:89:VAL:HG21	1.81	0.61
1:C:123:THR:HG21	1:C:429:GLU:OE1	2.01	0.60
1:C:362:GLU:HG2	2:C:505:NAG:H82	1.82	0.60
1:B:417:GLN:OE1	1:B:417:GLN:HA	2.01	0.60
1:B:123:THR:HG21	1:B:429:GLU:OE1	2.01	0.60
1:C:432:ARG:HH22	1:B:422:GLN:HG2	1.65	0.60
1:D:362:GLU:HG2	2:D:505:NAG:H82	1.82	0.60
1:D:297:THR:OG1	1:D:444:THR:OG1	2.20	0.60
1:A:297:THR:OG1	1:A:444:THR:OG1	2.20	0.60
1:A:123:THR:HG21	1:A:429:GLU:OE1	2.01	0.60
1:D:240:ARG:HD2	1:D:241:ASN:CB	2.32	0.60
1:A:362:GLU:HG2	2:A:505:NAG:H82	1.83	0.60
1:C:417:GLN:OE1	1:C:417:GLN:HA	2.02	0.60
1:C:408:ARG:NH1	1:A:399:THR:CG2	2.65	0.59
1:D:290:GLU:OE1	2:D:503:NAG:H81	2.02	0.59
1:D:297:THR:O	1:D:329:ALA:HB1	2.02	0.59
1:A:297:THR:O	1:A:329:ALA:HB1	2.02	0.59
1:A:86:LEU:HB3	1:A:89:VAL:HG23	1.85	0.59
1:A:240:ARG:HD2	1:A:241:ASN:CB	2.32	0.59
1:B:240:ARG:HD2	1:B:241:ASN:CB	2.32	0.59
1:C:80:ASN:OD1	1:D:300:ASN:CB	2.51	0.59
1:C:240:ARG:HD2	1:C:241:ASN:CB	2.32	0.59
1:C:297:THR:O	1:C:329:ALA:HB1	2.02	0.59
1:B:226:LEU:HG	1:B:489:VAL:HG11	1.83	0.59
1:B:297:THR:O	1:B:329:ALA:HB1	2.02	0.59
1:C:297:THR:OG1	1:C:444:THR:OG1	2.20	0.59
1:A:55:ALA:HA	1:A:75:VAL:O	2.03	0.59
1:B:290:GLU:OE1	2:B:503:NAG:H81	2.02	0.59
1:D:55:ALA:HA	1:D:75:VAL:O	2.03	0.59
1:C:59:LYS:HG2	1:C:61:TYR:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ASN:ND2	2:A:505:NAG:H62	2.14	0.58
1:A:417:GLN:HA	1:A:417:GLN:OE1	2.02	0.58
1:A:290:GLU:OE1	2:A:503:NAG:H81	2.02	0.58
1:C:290:GLU:OE1	2:C:503:NAG:H81	2.02	0.58
1:C:408:ARG:NH1	1:A:399:THR:CB	2.65	0.58
1:B:55:ALA:HA	1:B:75:VAL:O	2.03	0.58
1:B:297:THR:HG1	1:B:444:THR:HG1	1.50	0.58
1:C:86:LEU:HB3	1:C:89:VAL:HG23	1.85	0.58
1:B:297:THR:OG1	1:B:444:THR:OG1	2.20	0.58
1:B:266:ALA:HB1	5:B:631:HOH:O	2.03	0.58
1:C:55:ALA:HA	1:C:75:VAL:O	2.03	0.58
1:C:406:THR:HG21	5:C:652:HOH:O	2.02	0.58
1:A:338:TRP:NE1	1:A:342:LEU:HD12	2.20	0.57
1:D:98:ASN:HD21	1:D:100:MET:CG	2.18	0.57
1:D:338:TRP:NE1	1:D:342:LEU:HD12	2.20	0.57
1:C:61:TYR:H	1:D:59:LYS:NZ	1.94	0.57
3:D:507:Y1T:C44	5:D:631:HOH:O	2.51	0.57
1:A:98:ASN:HD21	1:A:100:MET:CG	2.18	0.57
1:B:86:LEU:HB3	1:B:89:VAL:HG23	1.85	0.57
1:B:98:ASN:HD21	1:B:100:MET:CG	2.18	0.57
1:B:338:TRP:NE1	1:B:342:LEU:HD12	2.20	0.57
1:C:59:LYS:HG2	1:C:61:TYR:OH	2.06	0.56
1:C:98:ASN:HD21	1:C:100:MET:CG	2.18	0.56
1:C:338:TRP:NE1	1:C:342:LEU:HD12	2.20	0.56
1:D:86:LEU:HB3	1:D:89:VAL:HG23	1.85	0.56
1:D:85:VAL:O	1:D:86:LEU:CG	2.53	0.56
1:A:68:VAL:CG1	1:A:72:HIS:HE1	2.19	0.56
1:C:357:LYS:HD2	1:C:466:GLU:HG2	1.88	0.55
1:B:363:PRO:HB3	1:B:388:SER:HA	1.89	0.55
1:B:421:LYS:NZ	5:B:603:HOH:O	2.39	0.55
1:C:65:VAL:HG21	1:C:115:SER:HB3	1.89	0.55
1:A:65:VAL:HG21	1:A:115:SER:HB3	1.89	0.55
1:D:65:VAL:HG21	1:D:115:SER:HB3	1.88	0.55
1:D:363:PRO:HB3	1:D:388:SER:HA	1.89	0.55
1:A:300:ASN:OD1	1:A:441:GLY:HA2	2.06	0.55
1:A:357:LYS:HD2	1:A:466:GLU:HG2	1.88	0.55
1:B:65:VAL:HG21	1:B:115:SER:HB3	1.89	0.55
1:B:300:ASN:OD1	1:B:441:GLY:HA2	2.07	0.55
1:D:357:LYS:HD2	1:D:466:GLU:HG2	1.88	0.55
1:D:297:THR:HG1	1:D:444:THR:HG1	1.54	0.55
1:B:104:MET:HE1	1:B:251:ILE:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:PRO:HB3	1:C:388:SER:HA	1.89	0.55
1:C:85:VAL:O	1:C:86:LEU:CG	2.53	0.55
1:C:300:ASN:OD1	1:C:441:GLY:HA2	2.07	0.55
1:A:363:PRO:HB3	1:A:388:SER:HA	1.88	0.54
1:B:357:LYS:HD2	1:B:466:GLU:HG2	1.88	0.54
1:D:342:LEU:HD22	1:D:361:PHE:CE2	2.42	0.54
1:A:104:MET:HE1	1:A:251:ILE:CG2	2.37	0.54
1:C:61:TYR:CZ	1:D:213:ILE:HG22	2.42	0.54
1:D:300:ASN:OD1	1:D:441:GLY:HA2	2.07	0.54
1:A:349:LEU:HD13	1:A:468:PHE:CE2	2.43	0.54
1:B:342:LEU:HD22	1:B:361:PHE:CE2	2.42	0.54
1:C:349:LEU:HD13	1:C:468:PHE:CE2	2.43	0.54
1:D:327:ARG:HG2	1:D:420:ILE:O	2.08	0.54
1:C:104:MET:HE1	1:C:251:ILE:CG2	2.37	0.54
1:C:327:ARG:HG2	1:C:420:ILE:O	2.08	0.54
1:B:408:ARG:HG2	1:B:409:SER:N	2.22	0.54
1:D:104:MET:HE1	1:D:251:ILE:CG2	2.37	0.54
1:D:349:LEU:HD13	1:D:468:PHE:CE2	2.43	0.54
1:A:342:LEU:HD22	1:A:361:PHE:CE2	2.42	0.54
1:A:298:ARG:NH1	1:A:326:ILE:O	2.38	0.54
1:A:85:VAL:O	1:A:86:LEU:CG	2.53	0.54
1:A:408:ARG:HG2	1:A:409:SER:N	2.22	0.54
1:A:327:ARG:HG2	1:A:420:ILE:O	2.08	0.53
1:B:327:ARG:HG2	1:B:420:ILE:O	2.08	0.53
1:C:342:LEU:HD22	1:C:361:PHE:CE2	2.42	0.53
1:C:65:VAL:CG2	1:C:115:SER:HB3	2.38	0.53
1:D:207:LYS:HD2	1:D:439:ILE:CG2	2.39	0.53
1:A:65:VAL:CG2	1:A:115:SER:HB3	2.38	0.53
1:B:65:VAL:CG2	1:B:115:SER:HB3	2.38	0.53
1:C:90:THR:O	1:C:90:THR:HG22	2.08	0.53
1:C:240:ARG:HD2	1:C:241:ASN:N	2.24	0.53
1:D:408:ARG:HG2	1:D:409:SER:N	2.22	0.53
1:D:65:VAL:CG2	1:D:115:SER:HB3	2.38	0.53
1:C:406:THR:CG2	5:C:652:HOH:O	2.56	0.53
1:A:90:THR:HG22	1:A:90:THR:O	2.08	0.53
1:A:362:GLU:HG2	2:A:505:NAG:C8	2.39	0.53
1:B:298:ARG:NH1	1:B:326:ILE:O	2.38	0.53
1:C:207:LYS:HD2	1:C:439:ILE:CG2	2.39	0.53
1:C:224:ALA:HB1	1:C:244:THR:CG2	2.39	0.53
1:C:240:ARG:HD2	1:C:241:ASN:H	1.74	0.53
1:A:456:ARG:HD2	1:A:466:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HD13	1:B:468:PHE:CE2	2.43	0.53
1:D:362:GLU:HG2	2:D:505:NAG:C8	2.39	0.53
1:B:456:ARG:HD2	1:B:466:GLU:OE2	2.09	0.53
1:C:456:ARG:HD2	1:C:466:GLU:OE2	2.09	0.53
1:A:62:GLU:OE2	1:A:64:GLU:HB2	2.09	0.53
1:A:240:ARG:HD2	1:A:241:ASN:N	2.24	0.53
1:B:207:LYS:HD2	1:B:439:ILE:CG2	2.39	0.53
1:B:240:ARG:HD2	1:B:241:ASN:H	1.74	0.53
1:B:246:GLN:OE1	1:B:246:GLN:HA	2.09	0.53
1:A:246:GLN:OE1	1:A:246:GLN:HA	2.08	0.52
1:C:408:ARG:HG2	1:C:409:SER:N	2.22	0.52
1:A:240:ARG:HD2	1:A:241:ASN:H	1.74	0.52
1:B:90:THR:O	1:B:90:THR:HG22	2.08	0.52
1:D:298:ARG:NH1	1:D:326:ILE:O	2.38	0.52
1:D:456:ARG:HD2	1:D:466:GLU:OE2	2.09	0.52
1:A:68:VAL:HG13	1:A:72:HIS:HE1	1.75	0.52
1:A:207:LYS:HD2	1:A:439:ILE:CG2	2.39	0.52
1:C:62:GLU:OE2	1:C:64:GLU:HB2	2.09	0.52
1:D:90:THR:O	1:D:90:THR:HG22	2.08	0.52
1:D:246:GLN:OE1	1:D:246:GLN:HA	2.08	0.52
1:B:224:ALA:HB1	1:B:244:THR:CG2	2.39	0.52
1:B:240:ARG:HD2	1:B:241:ASN:N	2.24	0.52
1:C:362:GLU:HG2	2:C:505:NAG:C8	2.39	0.52
1:B:85:VAL:O	1:B:86:LEU:CG	2.53	0.52
1:B:362:GLU:HG2	2:B:505:NAG:C8	2.39	0.52
1:D:269:GLU:O	1:D:271:ILE:HG12	2.10	0.52
1:A:224:ALA:HB1	1:A:244:THR:CG2	2.40	0.52
1:C:246:GLN:HA	1:C:246:GLN:OE1	2.08	0.52
1:A:232:THR:HA	1:A:271:ILE:HD11	1.91	0.52
1:B:93:PHE:CE2	1:B:228:CYS:HB2	2.45	0.52
1:B:98:ASN:C	1:B:98:ASN:ND2	2.61	0.52
1:D:240:ARG:HD2	1:D:241:ASN:N	2.24	0.51
1:B:232:THR:HA	1:B:271:ILE:HD11	1.92	0.51
1:C:269:GLU:O	1:C:271:ILE:HG12	2.10	0.51
1:D:111:LEU:C	1:D:111:LEU:HD23	2.36	0.51
1:D:240:ARG:HD2	1:D:241:ASN:HB3	1.93	0.51
1:D:240:ARG:HD2	1:D:241:ASN:H	1.74	0.51
1:D:224:ALA:HB1	1:D:244:THR:CG2	2.39	0.51
1:D:386:ASN:O	1:D:416:LEU:HD22	2.11	0.51
1:A:386:ASN:O	1:A:416:LEU:HD22	2.11	0.51
1:C:386:ASN:O	1:C:416:LEU:HD22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASN:O	1:B:416:LEU:HD22	2.11	0.51
1:D:93:PHE:CE2	1:D:228:CYS:HB2	2.46	0.51
1:D:348:GLU:HA	1:D:351:LYS:HD2	1.92	0.51
1:A:348:GLU:HA	1:A:351:LYS:HD2	1.92	0.51
1:B:111:LEU:C	1:B:111:LEU:HD23	2.36	0.51
1:A:111:LEU:HD23	1:A:111:LEU:C	2.36	0.50
1:C:225:ILE:HB	1:C:245:VAL:HG23	1.93	0.50
1:C:379:ARG:NH1	5:C:603:HOH:O	2.44	0.50
1:B:240:ARG:HD2	1:B:241:ASN:HB3	1.93	0.50
1:C:111:LEU:HD23	1:C:111:LEU:C	2.36	0.50
1:B:464:ASP:HA	5:B:602:HOH:O	2.12	0.50
1:C:405:HIS:O	4:A:508:IMD:N3	2.44	0.50
1:B:98:ASN:ND2	1:B:100:MET:N	2.59	0.50
1:D:225:ILE:HB	1:D:245:VAL:HG23	1.93	0.50
1:B:225:ILE:HB	1:B:245:VAL:HG23	1.94	0.50
1:D:98:ASN:ND2	1:D:100:MET:N	2.59	0.50
1:C:348:GLU:HA	1:C:351:LYS:HD2	1.92	0.50
1:C:62:GLU:OE1	1:C:62:GLU:HA	2.12	0.50
1:B:348:GLU:HA	1:B:351:LYS:HD2	1.92	0.50
1:C:98:ASN:ND2	1:C:100:MET:N	2.59	0.49
1:C:240:ARG:HD2	1:C:241:ASN:HB3	1.93	0.49
1:C:432:ARG:NH2	1:B:422:GLN:CG	2.75	0.49
1:A:240:ARG:HD2	1:A:241:ASN:HB3	1.93	0.49
1:A:62:GLU:OE1	1:A:62:GLU:HA	2.12	0.49
1:B:277:LEU:HA	5:B:608:HOH:O	2.11	0.49
1:C:432:ARG:NH2	1:B:422:GLN:HG2	2.28	0.49
1:A:98:ASN:ND2	1:A:100:MET:N	2.59	0.49
1:B:85:VAL:C	1:B:86:LEU:HG	2.37	0.49
1:A:85:VAL:C	1:A:86:LEU:HG	2.37	0.48
1:B:240:ARG:HG2	5:B:640:HOH:O	2.13	0.48
1:A:93:PHE:CE2	1:A:228:CYS:HB2	2.48	0.48
1:C:85:VAL:C	1:C:86:LEU:HG	2.37	0.48
1:A:225:ILE:HB	1:A:245:VAL:HG23	1.94	0.48
1:A:92:ASN:O	1:A:93:PHE:HD1	1.96	0.48
1:C:298:ARG:NH1	1:C:326:ILE:O	2.38	0.48
1:B:395:TYR:HA	1:B:399:THR:O	2.14	0.48
1:C:93:PHE:CE2	1:C:228:CYS:HB2	2.48	0.48
1:A:395:TYR:HA	1:A:399:THR:O	2.14	0.48
1:A:406:THR:HG21	5:A:648:HOH:O	2.14	0.48
1:C:92:ASN:O	1:C:93:PHE:HD1	1.96	0.48
1:D:92:ASN:C	1:D:93:PHE:CD1	2.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ILE:HD11	1:B:434:ILE:HD12	1.96	0.47
1:B:93:PHE:CD1	1:B:93:PHE:N	2.82	0.47
1:A:331:CYS:O	1:A:415:THR:HA	2.15	0.47
1:D:59:LYS:CB	1:D:61:TYR:CE2	2.98	0.47
1:D:85:VAL:C	1:D:86:LEU:HG	2.37	0.47
1:B:59:LYS:CB	1:B:61:TYR:CE2	2.98	0.47
1:C:59:LYS:CB	1:C:61:TYR:CE2	2.98	0.47
1:C:423:ILE:C	1:C:424:ILE:HD13	2.40	0.47
1:D:269:GLU:HA	1:D:289:ASN:ND2	2.29	0.47
1:A:91:GLU:HG2	1:A:487:LYS:NZ	2.30	0.47
1:A:269:GLU:HA	1:A:289:ASN:ND2	2.29	0.47
1:B:423:ILE:C	1:B:424:ILE:HD13	2.40	0.47
1:C:269:GLU:HA	1:C:289:ASN:HD22	1.79	0.47
1:C:331:CYS:O	1:C:415:THR:HA	2.15	0.47
1:C:389:ASP:OD1	1:C:408:ARG:N	2.48	0.47
1:D:92:ASN:O	1:D:93:PHE:HD1	1.97	0.47
1:D:295:VAL:O	1:D:331:CYS:HA	2.15	0.47
1:D:389:ASP:OD1	1:D:408:ARG:N	2.48	0.47
1:A:295:VAL:O	1:A:331:CYS:HA	2.15	0.47
1:B:295:VAL:O	1:B:331:CYS:HA	2.15	0.47
1:D:91:GLU:HG2	1:D:487:LYS:NZ	2.30	0.47
1:D:269:GLU:HA	1:D:289:ASN:HD22	1.79	0.47
1:D:395:TYR:HA	1:D:399:THR:O	2.14	0.47
1:A:63:LYS:HA	1:A:63:LYS:HD3	1.80	0.47
1:B:92:ASN:C	1:B:93:PHE:CD1	2.90	0.47
1:B:269:GLU:HA	1:B:289:ASN:HD22	1.79	0.47
1:B:389:ASP:OD1	1:B:408:ARG:N	2.48	0.47
1:B:409:SER:OG	1:B:410:SER:N	2.48	0.47
1:A:59:LYS:CB	1:A:61:TYR:CE2	2.98	0.47
1:A:389:ASP:OD1	1:A:408:ARG:N	2.48	0.47
1:C:269:GLU:HA	1:C:289:ASN:ND2	2.29	0.47
1:C:395:TYR:HA	1:C:399:THR:O	2.14	0.47
1:A:98:ASN:HD22	1:A:100:MET:N	2.13	0.47
1:B:92:ASN:O	1:B:93:PHE:HD1	1.97	0.47
1:C:91:GLU:HG2	1:C:487:LYS:NZ	2.30	0.46
1:C:98:ASN:HD22	1:C:100:MET:H	1.63	0.46
1:C:342:LEU:HD22	1:C:361:PHE:CD2	2.51	0.46
1:D:93:PHE:CD1	1:D:93:PHE:N	2.82	0.46
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.79	0.46
1:B:269:GLU:HA	1:B:289:ASN:ND2	2.29	0.46
1:B:98:ASN:HD22	1:B:100:MET:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:CYS:O	1:B:415:THR:HA	2.15	0.46
1:B:342:LEU:HD22	1:B:361:PHE:CD2	2.50	0.46
1:D:98:ASN:HD22	1:D:100:MET:H	1.63	0.46
1:B:268:GLU:HB3	1:B:269:GLU:HG2	1.97	0.46
1:C:220:PRO:HG2	1:C:223:PHE:HD2	1.81	0.46
1:C:409:SER:OG	1:C:410:SER:N	2.48	0.46
1:D:423:ILE:C	1:D:424:ILE:HD13	2.40	0.46
1:B:63:LYS:HA	1:B:63:LYS:HD3	1.80	0.46
1:C:98:ASN:HD22	1:C:100:MET:N	2.13	0.46
1:D:104:MET:HE1	1:D:251:ILE:HG22	1.98	0.46
1:A:220:PRO:HG2	1:A:223:PHE:HD2	1.81	0.46
1:A:409:SER:OG	1:A:410:SER:N	2.48	0.46
1:B:50:THR:HG21	1:B:223:PHE:CD2	2.51	0.46
1:C:59:LYS:HB3	1:C:61:TYR:CE2	2.51	0.46
1:D:240:ARG:HH11	1:D:241:ASN:CB	2.29	0.46
1:D:331:CYS:O	1:D:415:THR:HA	2.15	0.46
1:A:68:VAL:O	1:A:72:HIS:ND1	2.48	0.46
1:A:98:ASN:HD22	1:A:100:MET:H	1.63	0.46
1:B:252:LYS:O	1:B:254:VAL:HG23	2.16	0.46
1:A:423:ILE:C	1:A:424:ILE:HD13	2.40	0.46
1:B:91:GLU:HG2	1:B:487:LYS:NZ	2.30	0.46
1:C:295:VAL:O	1:C:331:CYS:HA	2.15	0.46
1:D:220:PRO:HG2	1:D:223:PHE:HD2	1.81	0.46
1:D:409:SER:OG	1:D:410:SER:N	2.48	0.46
1:A:49:LYS:CE	5:A:617:HOH:O	2.60	0.46
1:A:342:LEU:HD22	1:A:361:PHE:CD2	2.51	0.46
1:B:98:ASN:HD22	1:B:100:MET:N	2.13	0.46
1:B:104:MET:HE1	1:B:251:ILE:HG22	1.98	0.46
1:D:98:ASN:HD22	1:D:100:MET:N	2.13	0.46
2:C:505:NAG:C6	1:A:404:ASN:HD22	2.27	0.45
1:D:50:THR:HG21	1:D:223:PHE:CD2	2.51	0.45
1:A:104:MET:HE1	1:A:251:ILE:HG22	1.98	0.45
1:A:240:ARG:HH11	1:A:241:ASN:CB	2.29	0.45
1:B:220:PRO:HG2	1:B:223:PHE:HD2	1.81	0.45
1:D:336:SER:O	1:D:339:ASN:HB2	2.16	0.45
1:A:50:THR:HG21	1:A:223:PHE:CD2	2.51	0.45
1:A:290:GLU:OE2	1:A:337:LYS:NZ	2.23	0.45
1:B:98:ASN:HD22	1:B:99:ASP:N	2.14	0.45
1:D:252:LYS:O	1:D:254:VAL:HG23	2.16	0.45
1:A:336:SER:O	1:A:339:ASN:HB2	2.17	0.45
1:D:342:LEU:HD22	1:D:361:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASN:HD22	1:C:99:ASP:N	2.14	0.45
1:C:98:ASN:HD21	1:C:100:MET:CB	2.30	0.45
1:A:252:LYS:O	1:A:254:VAL:HG23	2.16	0.45
1:C:240:ARG:HH11	1:C:241:ASN:CB	2.29	0.45
1:C:336:SER:O	1:C:339:ASN:HB2	2.16	0.45
1:C:50:THR:HG21	1:C:223:PHE:CD2	2.51	0.45
1:B:336:SER:O	1:B:339:ASN:HB2	2.16	0.45
1:C:98:ASN:C	1:C:98:ASN:ND2	2.61	0.45
1:B:240:ARG:HH11	1:B:241:ASN:CB	2.29	0.45
1:C:104:MET:HE1	1:C:251:ILE:HG22	1.98	0.45
1:B:59:LYS:HG2	1:B:61:TYR:OH	2.17	0.45
1:C:252:LYS:O	1:C:254:VAL:HG23	2.16	0.45
1:C:80:ASN:ND2	1:D:442:GLU:HB2	2.31	0.44
1:A:59:LYS:HG2	1:A:61:TYR:OH	2.17	0.44
1:A:91:GLU:HG2	1:A:487:LYS:HZ3	1.82	0.44
1:C:257:THR:O	1:C:259:LEU:N	2.50	0.44
1:C:360:LYS:HD3	1:C:465:THR:HG21	2.00	0.44
1:B:98:ASN:HD21	1:B:100:MET:CB	2.30	0.44
1:D:426:MET:CE	1:D:431:GLY:HA3	2.48	0.44
1:A:98:ASN:HD21	1:A:100:MET:CB	2.30	0.44
1:C:80:ASN:OD1	1:D:300:ASN:HB3	2.17	0.44
1:C:378:CYS:HB3	1:C:383:PHE:CE1	2.53	0.44
1:A:426:MET:HE2	1:A:431:GLY:C	2.43	0.44
1:B:426:MET:HE2	1:B:431:GLY:C	2.43	0.44
1:B:426:MET:CE	1:B:431:GLY:HA3	2.48	0.44
1:C:426:MET:HE2	1:C:431:GLY:C	2.43	0.44
1:D:59:LYS:HG2	1:D:61:TYR:OH	2.17	0.44
1:A:353:PHE:HA	1:A:354:PRO:HD3	1.79	0.44
1:C:60:ALA:CA	1:D:59:LYS:HE2	2.48	0.43
1:D:98:ASN:HD22	1:D:99:ASP:N	2.14	0.43
1:D:338:TRP:NE1	1:D:342:LEU:CD1	2.81	0.43
1:C:241:ASN:ND2	5:C:602:HOH:O	2.42	0.43
1:C:426:MET:CE	1:C:431:GLY:HA3	2.48	0.43
1:D:98:ASN:HD21	1:D:100:MET:CB	2.30	0.43
1:D:426:MET:HE2	1:D:431:GLY:C	2.43	0.43
1:B:338:TRP:NE1	1:B:342:LEU:CD1	2.81	0.43
1:D:419:LYS:HD3	1:D:421:LYS:CG	2.47	0.43
1:A:98:ASN:HD22	1:A:99:ASP:N	2.14	0.43
1:A:360:LYS:HD3	1:A:465:THR:HG21	2.00	0.43
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.53	0.43
1:C:80:ASN:HB2	1:D:442:GLU:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:THR:OG1	1:C:240:ARG:HA	2.19	0.43
1:C:91:GLU:HG2	1:C:487:LYS:HZ3	1.83	0.43
1:B:90:THR:OG1	1:B:240:ARG:HA	2.19	0.43
1:B:257:THR:O	1:B:259:LEU:N	2.50	0.43
1:B:360:LYS:HD3	1:B:465:THR:HG21	2.00	0.43
1:C:123:THR:HG22	1:C:431:GLY:HA3	2.01	0.43
1:D:123:THR:HG22	1:D:431:GLY:HA3	2.01	0.43
1:A:275:GLU:OE2	1:A:282:LYS:CE	2.67	0.43
1:C:275:GLU:OE2	1:C:282:LYS:CE	2.67	0.43
1:C:338:TRP:NE1	1:C:342:LEU:CD1	2.81	0.43
1:D:360:LYS:HD3	1:D:465:THR:HG21	2.00	0.43
1:D:378:CYS:HB3	1:D:383:PHE:CE1	2.53	0.43
1:A:419:LYS:HD3	1:A:421:LYS:CG	2.47	0.43
1:A:257:THR:O	1:A:259:LEU:N	2.51	0.43
1:A:426:MET:CE	1:A:431:GLY:HA3	2.48	0.42
1:B:123:THR:HG22	1:B:431:GLY:HA3	2.01	0.42
1:A:90:THR:OG1	1:A:240:ARG:HA	2.19	0.42
1:D:257:THR:O	1:D:259:LEU:N	2.50	0.42
1:A:65:VAL:HB	1:A:115:SER:HB3	2.01	0.42
1:A:224:ALA:HB1	1:A:244:THR:HG22	2.01	0.42
1:B:378:CYS:HB3	1:B:383:PHE:CE1	2.53	0.42
1:A:338:TRP:NE1	1:A:342:LEU:CD1	2.81	0.42
1:C:404:ASN:HD22	2:A:505:NAG:C6	2.24	0.42
1:C:419:LYS:HD3	1:C:421:LYS:CG	2.47	0.42
1:D:63:LYS:HA	1:D:63:LYS:HD3	1.80	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.79	0.42
1:D:270:ILE:HG12	1:D:288:LEU:HA	2.02	0.42
1:B:270:ILE:HG12	1:B:288:LEU:HA	2.02	0.42
1:D:90:THR:OG1	1:D:240:ARG:HA	2.19	0.42
1:A:104:MET:O	1:A:108:ILE:HG12	2.20	0.42
1:D:104:MET:O	1:D:108:ILE:HG12	2.20	0.42
1:B:104:MET:O	1:B:108:ILE:HG12	2.20	0.42
1:B:275:GLU:OE2	1:B:282:LYS:CE	2.67	0.42
1:D:353:PHE:HA	1:D:354:PRO:HD3	1.79	0.42
1:A:123:THR:HG22	1:A:431:GLY:HA3	2.01	0.42
1:D:269:GLU:H	1:D:269:GLU:HG2	1.52	0.41
1:B:65:VAL:HB	1:B:115:SER:HB3	2.01	0.41
1:C:59:LYS:HG2	1:C:61:TYR:CE2	2.56	0.41
1:C:65:VAL:HB	1:C:115:SER:HB3	2.01	0.41
1:C:353:PHE:HA	1:C:354:PRO:HD3	1.79	0.41
1:D:65:VAL:HB	1:D:115:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HG12	1:A:288:LEU:HA	2.02	0.41
1:C:63:LYS:HA	1:C:63:LYS:HD3	1.80	0.41
1:C:104:MET:O	1:C:108:ILE:HG12	2.20	0.41
1:C:292:VAL:HG22	1:C:337:LYS:HG2	2.03	0.41
1:B:226:LEU:HG	1:B:489:VAL:CG1	2.48	0.41
1:C:61:TYR:CA	1:D:59:LYS:HE3	2.49	0.41
1:D:69:TRP:CD1	1:D:114:GLU:OE1	2.74	0.41
1:A:69:TRP:CD1	1:A:114:GLU:OE1	2.74	0.41
1:C:270:ILE:HG12	1:C:288:LEU:HA	2.02	0.41
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.87	0.41
1:B:226:LEU:HD23	1:B:226:LEU:HA	1.87	0.41
1:C:85:VAL:HG12	1:C:86:LEU:H	1.86	0.41
1:D:406:THR:O	1:D:406:THR:HG22	2.21	0.41
1:C:269:GLU:O	1:C:270:ILE:C	2.64	0.40
1:D:85:VAL:HG12	1:D:86:LEU:H	1.86	0.40
1:B:69:TRP:CD1	1:B:114:GLU:OE1	2.74	0.40
1:C:404:ASN:ND2	2:A:505:NAG:C6	2.82	0.40
1:A:269:GLU:O	1:A:270:ILE:C	2.64	0.40
1:A:406:THR:O	1:A:406:THR:HG22	2.21	0.40
1:D:269:GLU:O	1:D:270:ILE:C	2.64	0.40
1:A:344:LYS:HZ3	2:A:503:NAG:C8	2.35	0.40
1:C:224:ALA:HB1	1:C:244:THR:HG22	2.04	0.40
1:A:349:LEU:HD13	1:A:468:PHE:CZ	2.57	0.40
1:B:255:VAL:HG13	1:B:475:MET:SD	2.62	0.40

All (1) 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:C:201:ILE:CD1	1:A:201:ILE:CD1[2_455]	2.16	0.04

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%)	306 (93%)	18 (6%)	5 (2%)	8	14
1	B	329/358 (92%)	306 (93%)	18 (6%)	5 (2%)	8	14
1	C	329/358 (92%)	306 (93%)	18 (6%)	5 (2%)	8	14
1	D	329/358 (92%)	306 (93%)	18 (6%)	5 (2%)	8	14
All	All	1316/1432 (92%)	1224 (93%)	72 (6%)	20 (2%)	8	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	439	ILE
1	D	439	ILE
1	A	439	ILE
1	B	439	ILE
1	C	86	LEU
1	C	90	THR
1	C	365	SER
1	D	86	LEU
1	D	90	THR
1	D	365	SER
1	A	86	LEU
1	A	90	THR
1	A	365	SER
1	B	86	LEU
1	B	90	THR
1	B	365	SER
1	C	354	PRO
1	D	354	PRO
1	A	354	PRO
1	B	354	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/312 (95%)	285 (96%)	12 (4%)	28	51
1	B	297/312 (95%)	283 (95%)	14 (5%)	23	44
1	C	297/312 (95%)	287 (97%)	10 (3%)	32	57
1	D	297/312 (95%)	286 (96%)	11 (4%)	30	54
All	All	1188/1248 (95%)	1141 (96%)	47 (4%)	28	51

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	51	THR
1	C	62	GLU
1	C	77	THR
1	C	98	ASN
1	C	347	GLU
1	C	356	SER
1	C	359	ILE
1	C	409	SER
1	C	447	SER
1	C	480	ARG
1	D	59	LYS
1	D	93	PHE
1	D	98	ASN
1	D	336	SER
1	D	340	ASN
1	D	347	GLU
1	D	356	SER
1	D	409	SER
1	D	417	GLN
1	D	447	SER
1	D	480	ARG
1	A	59	LYS
1	A	62	GLU
1	A	72	HIS
1	A	77	THR
1	A	98	ASN
1	A	244	THR
1	A	271	ILE
1	A	347	GLU
1	A	356	SER
1	A	409	SER
1	A	447	SER
1	A	480	ARG

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Mol	Chain	Res	Type
1	B	59	LYS
1	B	93	PHE
1	B	97	LYS
1	B	98	ASN
1	B	269	GLU
1	B	271	ILE
1	B	336	SER
1	B	347	GLU
1	B	356	SER
1	B	409	SER
1	B	417	GLN
1	B	419	LYS
1	B	447	SER
1	B	489	VAL

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

Mol	Chain	Res	Type
1	C	98	ASN
1	C	229	ASN
1	C	241	ASN
1	C	404	ASN
1	C	422	GLN
1	D	98	ASN
1	D	229	ASN
1	D	241	ASN
1	D	422	GLN
1	A	98	ASN
1	A	229	ASN
1	A	241	ASN
1	A	422	GLN
1	B	98	ASN
1	B	229	ASN
1	B	241	ASN

5.3.3 RNA ⓘ

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](#)

29 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	B	506	1	14,14,15	1.11	2 (14%)	17,19,21	1.18	2 (11%)
2	NAG	C	505	1	14,14,15	0.74	0	17,19,21	0.50	0
2	NAG	B	504	1	14,14,15	0.89	1 (7%)	17,19,21	0.59	0
2	NAG	D	501	1	14,14,15	0.46	0	17,19,21	0.51	0
2	NAG	B	503	1	14,14,15	0.85	1 (7%)	17,19,21	0.67	0
2	NAG	A	503	1	14,14,15	0.85	1 (7%)	17,19,21	0.68	0
2	NAG	A	501	1	14,14,15	0.46	0	17,19,21	0.51	0
2	NAG	D	502	1	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
2	NAG	A	505	1	14,14,15	0.75	0	17,19,21	0.50	0
2	NAG	C	502	1	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
3	Y1T	C	507	-	48,49,49	2.26	13 (27%)	65,71,71	2.25	20 (30%)
2	NAG	B	502	1	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
4	IMD	A	508	-	5,5,5	0.76	0	5,5,5	0.45	0
2	NAG	D	503	1	14,14,15	0.85	1 (7%)	17,19,21	0.67	0
2	NAG	D	504	1	14,14,15	0.89	1 (7%)	17,19,21	0.59	0
2	NAG	C	506	1	14,14,15	1.11	2 (14%)	17,19,21	1.18	2 (11%)
2	NAG	A	504	1	14,14,15	0.89	1 (7%)	17,19,21	0.59	0
2	NAG	D	505	1	14,14,15	0.74	0	17,19,21	0.50	0
2	NAG	B	501	1	14,14,15	0.46	0	17,19,21	0.50	0

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	1.11	2 (14%)	17,19,21	1.18	2 (11%)
2	NAG	A	502	1	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
2	NAG	B	505	1	14,14,15	0.74	0	17,19,21	0.50	0
3	Y1T	A	507	-	48,49,49	2.26	13 (27%)	65,71,71	2.25	20 (30%)
3	Y1T	D	507	-	48,49,49	2.26	14 (29%)	65,71,71	2.25	20 (30%)
2	NAG	C	504	1	14,14,15	0.89	1 (7%)	17,19,21	0.59	0
2	NAG	C	501	1	14,14,15	0.46	0	17,19,21	0.51	0
2	NAG	A	506	1	14,14,15	1.11	2 (14%)	17,19,21	1.18	2 (11%)
3	Y1T	B	507	-	48,49,49	2.26	13 (27%)	65,71,71	2.25	20 (30%)
2	NAG	C	503	1	14,14,15	0.85	1 (7%)	17,19,21	0.67	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	B	506	1	-	2/6/23/26	0/1/1/1
2	NAG	C	505	1	-	2/6/23/26	0/1/1/1
2	NAG	B	504	1	-	0/6/23/26	0/1/1/1
2	NAG	D	501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	503	1	-	5/6/23/26	0/1/1/1
2	NAG	A	503	1	-	5/6/23/26	0/1/1/1
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	D	502	1	-	2/6/23/26	0/1/1/1
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
2	NAG	C	502	1	-	2/6/23/26	0/1/1/1
3	Y1T	C	507	-	-	3/29/45/45	0/4/4/4
2	NAG	B	502	1	-	2/6/23/26	0/1/1/1
4	IMD	A	508	-	-	-	0/1/1/1
2	NAG	D	503	1	-	5/6/23/26	0/1/1/1
2	NAG	D	504	1	-	0/6/23/26	0/1/1/1
2	NAG	C	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	D	505	1	-	2/6/23/26	0/1/1/1
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
2	NAG	D	506	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	502	1	-	2/6/23/26	0/1/1/1
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1
3	Y1T	A	507	-	-	3/29/45/45	0/4/4/4
3	Y1T	D	507	-	-	3/29/45/45	0/4/4/4
2	NAG	C	504	1	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1	-	2/6/23/26	0/1/1/1
2	NAG	A	506	1	-	2/6/23/26	0/1/1/1
3	Y1T	B	507	-	-	3/29/45/45	0/4/4/4
2	NAG	C	503	1	-	5/6/23/26	0/1/1/1

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	507	Y1T	C37-N36	6.69	1.46	1.33
3	A	507	Y1T	C37-N36	6.69	1.46	1.33
3	D	507	Y1T	C37-N36	6.69	1.46	1.33
3	B	507	Y1T	C37-N36	6.69	1.46	1.33
3	B	507	Y1T	C19-N18	5.46	1.45	1.37
3	C	507	Y1T	C19-N18	5.46	1.45	1.37
3	A	507	Y1T	C19-N18	5.46	1.45	1.37
3	D	507	Y1T	C19-N18	5.46	1.45	1.37
3	C	507	Y1T	C15-C34	-5.16	1.49	1.55
3	D	507	Y1T	C15-C34	-5.16	1.49	1.55
3	B	507	Y1T	C15-C34	-5.16	1.49	1.55
3	A	507	Y1T	C15-C34	-5.15	1.49	1.55
3	A	507	Y1T	C03-N04	4.78	1.45	1.35
3	C	507	Y1T	C03-N04	4.77	1.45	1.35
3	D	507	Y1T	C03-N04	4.77	1.45	1.35
3	B	507	Y1T	C03-N04	4.77	1.45	1.35
3	D	507	Y1T	C17-N18	4.60	1.49	1.40
3	A	507	Y1T	C17-N18	4.60	1.49	1.40
3	B	507	Y1T	C17-N18	4.60	1.49	1.40
3	C	507	Y1T	C17-N18	4.59	1.49	1.40
3	D	507	Y1T	C02-N14	4.58	1.43	1.34
3	C	507	Y1T	C02-N14	4.58	1.43	1.34
3	B	507	Y1T	C02-N14	4.58	1.43	1.34
3	A	507	Y1T	C02-N14	4.58	1.43	1.34
3	A	507	Y1T	C37-N38	3.75	1.45	1.32
3	B	507	Y1T	C37-N38	3.75	1.45	1.32
3	C	507	Y1T	C37-N38	3.75	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	Y1T	C37-N38	3.75	1.45	1.32
2	B	506	NAG	O5-C1	-3.08	1.38	1.43
2	A	506	NAG	O5-C1	-3.08	1.38	1.43
2	C	506	NAG	O5-C1	-3.08	1.38	1.43
2	D	506	NAG	O5-C1	-3.08	1.38	1.43
2	B	504	NAG	O5-C1	2.97	1.48	1.43
2	A	504	NAG	O5-C1	2.97	1.48	1.43
2	D	504	NAG	O5-C1	2.97	1.48	1.43
2	C	504	NAG	O5-C1	2.97	1.48	1.43
3	D	507	Y1T	O20-C19	2.91	1.40	1.34
3	B	507	Y1T	O20-C19	2.90	1.40	1.34
3	C	507	Y1T	O20-C19	2.90	1.40	1.34
3	A	507	Y1T	O20-C19	2.90	1.40	1.34
3	B	507	Y1T	F32-C31	2.44	1.38	1.34
3	C	507	Y1T	F32-C31	2.44	1.38	1.34
3	A	507	Y1T	F32-C31	2.44	1.38	1.34
3	D	507	Y1T	F32-C31	2.44	1.38	1.34
3	D	507	Y1T	O01-C02	-2.41	1.19	1.23
3	C	507	Y1T	O01-C02	-2.41	1.19	1.23
3	B	507	Y1T	O01-C02	-2.41	1.19	1.23
3	A	507	Y1T	O01-C02	-2.41	1.19	1.23
2	A	506	NAG	C1-C2	2.30	1.55	1.52
2	D	506	NAG	C1-C2	2.30	1.55	1.52
2	B	506	NAG	C1-C2	2.30	1.55	1.52
2	C	506	NAG	C1-C2	2.29	1.55	1.52
2	D	503	NAG	C2-N2	-2.27	1.42	1.46
2	A	503	NAG	C2-N2	-2.27	1.42	1.46
2	C	503	NAG	C2-N2	-2.26	1.42	1.46
2	B	503	NAG	C2-N2	-2.26	1.42	1.46
3	A	507	Y1T	F24-C23	2.22	1.38	1.34
3	B	507	Y1T	F24-C23	2.21	1.38	1.34
3	C	507	Y1T	F24-C23	2.21	1.38	1.34
3	D	507	Y1T	F24-C23	2.21	1.38	1.34
3	B	507	Y1T	C37-N39	-2.13	1.26	1.34
3	C	507	Y1T	C37-N39	-2.13	1.26	1.34
3	D	507	Y1T	C37-N39	-2.13	1.26	1.34
3	A	507	Y1T	C37-N39	-2.13	1.26	1.34
3	C	507	Y1T	C08-CL09	2.01	1.78	1.73
3	B	507	Y1T	C08-CL09	2.01	1.78	1.73
3	D	507	Y1T	C08-CL09	2.01	1.78	1.73
3	A	507	Y1T	C08-CL09	2.01	1.78	1.73
3	D	507	Y1T	O13-C03	-2.00	1.19	1.23

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	507	Y1T	C34-C15-N14	-11.25	102.72	115.01
3	C	507	Y1T	C34-C15-N14	-11.25	102.72	115.01
3	A	507	Y1T	C34-C15-N14	-11.25	102.72	115.01
3	D	507	Y1T	C34-C15-N14	-11.24	102.73	115.01
3	D	507	Y1T	O20-C19-N18	4.00	116.73	111.04
3	A	507	Y1T	O20-C19-N18	3.99	116.72	111.04
3	C	507	Y1T	O20-C19-N18	3.99	116.72	111.04
3	B	507	Y1T	O20-C19-N18	3.99	116.72	111.04
3	C	507	Y1T	C16-C15-N14	-3.92	103.31	114.77
3	D	507	Y1T	C16-C15-N14	-3.92	103.31	114.77
3	A	507	Y1T	C16-C15-N14	-3.92	103.31	114.77
3	B	507	Y1T	C16-C15-N14	-3.92	103.32	114.77
3	D	507	Y1T	C05-N04-C03	-3.80	120.70	127.45
3	A	507	Y1T	C05-N04-C03	-3.80	120.70	127.45
3	C	507	Y1T	C05-N04-C03	-3.80	120.70	127.45
3	B	507	Y1T	C05-N04-C03	-3.80	120.71	127.45
3	D	507	Y1T	C31-C22-C23	3.48	120.00	115.91
3	A	507	Y1T	C31-C22-C23	3.48	120.00	115.91
3	B	507	Y1T	C31-C22-C23	3.48	120.00	115.91
3	C	507	Y1T	C31-C22-C23	3.48	120.00	115.91
2	A	502	NAG	C1-O5-C5	3.40	116.75	112.19
2	D	502	NAG	C1-O5-C5	3.40	116.74	112.19
2	A	506	NAG	C4-C3-C2	3.40	116.00	111.02
2	B	506	NAG	C4-C3-C2	3.40	116.00	111.02
2	C	502	NAG	C1-O5-C5	3.40	116.74	112.19
2	B	502	NAG	C1-O5-C5	3.40	116.74	112.19
2	D	506	NAG	C4-C3-C2	3.40	116.00	111.02
2	C	506	NAG	C4-C3-C2	3.39	115.99	111.02
3	D	507	Y1T	C16-C17-N18	-3.09	106.97	109.42
3	A	507	Y1T	C16-C17-N18	-3.09	106.97	109.42
3	B	507	Y1T	C16-C17-N18	-3.09	106.97	109.42
3	C	507	Y1T	C16-C17-N18	-3.08	106.97	109.42
3	C	507	Y1T	O20-C21-C22	-2.96	102.88	107.62
3	A	507	Y1T	O20-C21-C22	-2.96	102.88	107.62
3	B	507	Y1T	O20-C21-C22	-2.96	102.88	107.62
3	D	507	Y1T	O20-C21-C22	-2.96	102.88	107.62
3	C	507	Y1T	C05-C12-C10	-2.89	116.40	118.82
3	A	507	Y1T	C05-C12-C10	-2.89	116.40	118.82
3	D	507	Y1T	C05-C12-C10	-2.89	116.40	118.82
3	B	507	Y1T	C05-C12-C10	-2.88	116.40	118.82
3	A	507	Y1T	C40-C17-N18	2.84	133.57	128.59
3	B	507	Y1T	C40-C17-N18	2.84	133.57	128.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	507	Y1T	C40-C17-N18	2.84	133.57	128.59
3	D	507	Y1T	C40-C17-N18	2.84	133.56	128.59
2	C	506	NAG	C3-C4-C5	2.79	115.29	110.23
2	D	506	NAG	C3-C4-C5	2.79	115.28	110.23
2	A	506	NAG	C3-C4-C5	2.78	115.28	110.23
2	B	506	NAG	C3-C4-C5	2.78	115.28	110.23
3	D	507	Y1T	C06-C07-C08	-2.77	116.16	119.98
3	A	507	Y1T	C06-C07-C08	-2.77	116.16	119.98
3	C	507	Y1T	C06-C07-C08	-2.76	116.16	119.98
3	B	507	Y1T	C06-C07-C08	-2.76	116.17	119.98
3	D	507	Y1T	C22-C23-C25	-2.66	119.31	122.36
3	B	507	Y1T	C22-C23-C25	-2.66	119.32	122.36
3	C	507	Y1T	C22-C23-C25	-2.66	119.32	122.36
3	A	507	Y1T	C22-C23-C25	-2.66	119.32	122.36
3	C	507	Y1T	C02-C03-N04	2.47	116.42	112.25
3	A	507	Y1T	C02-C03-N04	2.47	116.42	112.25
3	B	507	Y1T	C02-C03-N04	2.47	116.42	112.25
3	D	507	Y1T	C02-C03-N04	2.47	116.41	112.25
3	C	507	Y1T	C42-C41-C45	-2.34	116.17	120.94
3	A	507	Y1T	C42-C41-C45	-2.34	116.17	120.94
3	B	507	Y1T	C42-C41-C45	-2.34	116.17	120.94
3	D	507	Y1T	C42-C41-C45	-2.34	116.17	120.94
3	D	507	Y1T	C22-C31-C29	-2.32	119.70	122.36
3	A	507	Y1T	C22-C31-C29	-2.32	119.70	122.36
3	C	507	Y1T	C22-C31-C29	-2.32	119.71	122.36
3	B	507	Y1T	C22-C31-C29	-2.32	119.71	122.36
3	A	507	Y1T	C07-C06-C05	2.30	122.95	120.30
3	D	507	Y1T	C07-C06-C05	2.30	122.95	120.30
3	C	507	Y1T	C07-C06-C05	2.30	122.94	120.30
3	B	507	Y1T	C07-C06-C05	2.30	122.94	120.30
3	D	507	Y1T	C10-C08-CL09	-2.28	116.91	119.79
3	A	507	Y1T	C10-C08-CL09	-2.28	116.91	119.79
3	B	507	Y1T	C10-C08-CL09	-2.28	116.91	119.79
3	C	507	Y1T	C10-C08-CL09	-2.28	116.92	119.79
3	C	507	Y1T	C46-C16-C17	2.24	122.22	120.03
3	B	507	Y1T	C46-C16-C17	2.24	122.22	120.03
3	A	507	Y1T	C46-C16-C17	2.23	122.22	120.03
3	D	507	Y1T	C46-C16-C17	2.23	122.22	120.03
3	B	507	Y1T	C07-C08-CL09	2.20	122.77	118.42
3	A	507	Y1T	C07-C08-CL09	2.20	122.77	118.42
3	D	507	Y1T	C07-C08-CL09	2.20	122.76	118.42
3	C	507	Y1T	C07-C08-CL09	2.20	122.76	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	507	Y1T	O20-C19-O33	-2.06	121.17	124.76
3	A	507	Y1T	O20-C19-O33	-2.06	121.18	124.76
3	B	507	Y1T	O20-C19-O33	-2.06	121.18	124.76
3	C	507	Y1T	O20-C19-O33	-2.06	121.18	124.76
3	A	507	Y1T	C03-C02-N14	2.04	118.62	113.73
3	B	507	Y1T	C03-C02-N14	2.04	118.62	113.73
3	C	507	Y1T	C03-C02-N14	2.04	118.62	113.73
3	D	507	Y1T	C03-C02-N14	2.04	118.62	113.73

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	507	Y1T	C41-C42-N43-C44
3	D	507	Y1T	C41-C42-N43-C44
3	A	507	Y1T	C41-C42-N43-C44
3	B	507	Y1T	C41-C42-N43-C44
2	C	505	NAG	O5-C5-C6-O6
2	D	505	NAG	O5-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
2	B	505	NAG	O5-C5-C6-O6
2	C	501	NAG	O5-C5-C6-O6
2	D	501	NAG	O5-C5-C6-O6
2	A	501	NAG	O5-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
2	C	503	NAG	O5-C5-C6-O6
2	D	503	NAG	O5-C5-C6-O6
2	A	503	NAG	O5-C5-C6-O6
2	B	503	NAG	O5-C5-C6-O6
2	C	501	NAG	C4-C5-C6-O6
2	D	501	NAG	C4-C5-C6-O6
2	A	501	NAG	C4-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6
2	C	505	NAG	C4-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	B	505	NAG	C4-C5-C6-O6
2	C	503	NAG	C4-C5-C6-O6
2	D	503	NAG	C4-C5-C6-O6
2	A	503	NAG	C4-C5-C6-O6
2	B	503	NAG	C4-C5-C6-O6
2	C	503	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	503	NAG	O7-C7-N2-C2
2	D	503	NAG	C8-C7-N2-C2
2	D	503	NAG	O7-C7-N2-C2
2	A	503	NAG	C8-C7-N2-C2
2	A	503	NAG	O7-C7-N2-C2
2	B	503	NAG	C8-C7-N2-C2
2	B	503	NAG	O7-C7-N2-C2
2	C	503	NAG	C3-C2-N2-C7
2	D	503	NAG	C3-C2-N2-C7
2	A	503	NAG	C3-C2-N2-C7
2	B	503	NAG	C3-C2-N2-C7
2	C	502	NAG	O5-C5-C6-O6
2	D	502	NAG	O5-C5-C6-O6
2	A	502	NAG	O5-C5-C6-O6
2	B	502	NAG	O5-C5-C6-O6
2	C	502	NAG	C4-C5-C6-O6
2	D	502	NAG	C4-C5-C6-O6
2	A	502	NAG	C4-C5-C6-O6
2	B	502	NAG	C4-C5-C6-O6
2	C	506	NAG	C4-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	B	506	NAG	C4-C5-C6-O6
3	C	507	Y1T	C34-C35-N36-C37
3	D	507	Y1T	C34-C35-N36-C37
3	A	507	Y1T	C34-C35-N36-C37
3	B	507	Y1T	C34-C35-N36-C37
3	C	507	Y1T	C15-C34-C35-N36
3	D	507	Y1T	C15-C34-C35-N36
3	A	507	Y1T	C15-C34-C35-N36
3	B	507	Y1T	C15-C34-C35-N36
2	C	506	NAG	O5-C5-C6-O6
2	D	506	NAG	O5-C5-C6-O6
2	A	506	NAG	O5-C5-C6-O6
2	B	506	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 34 short contacts:

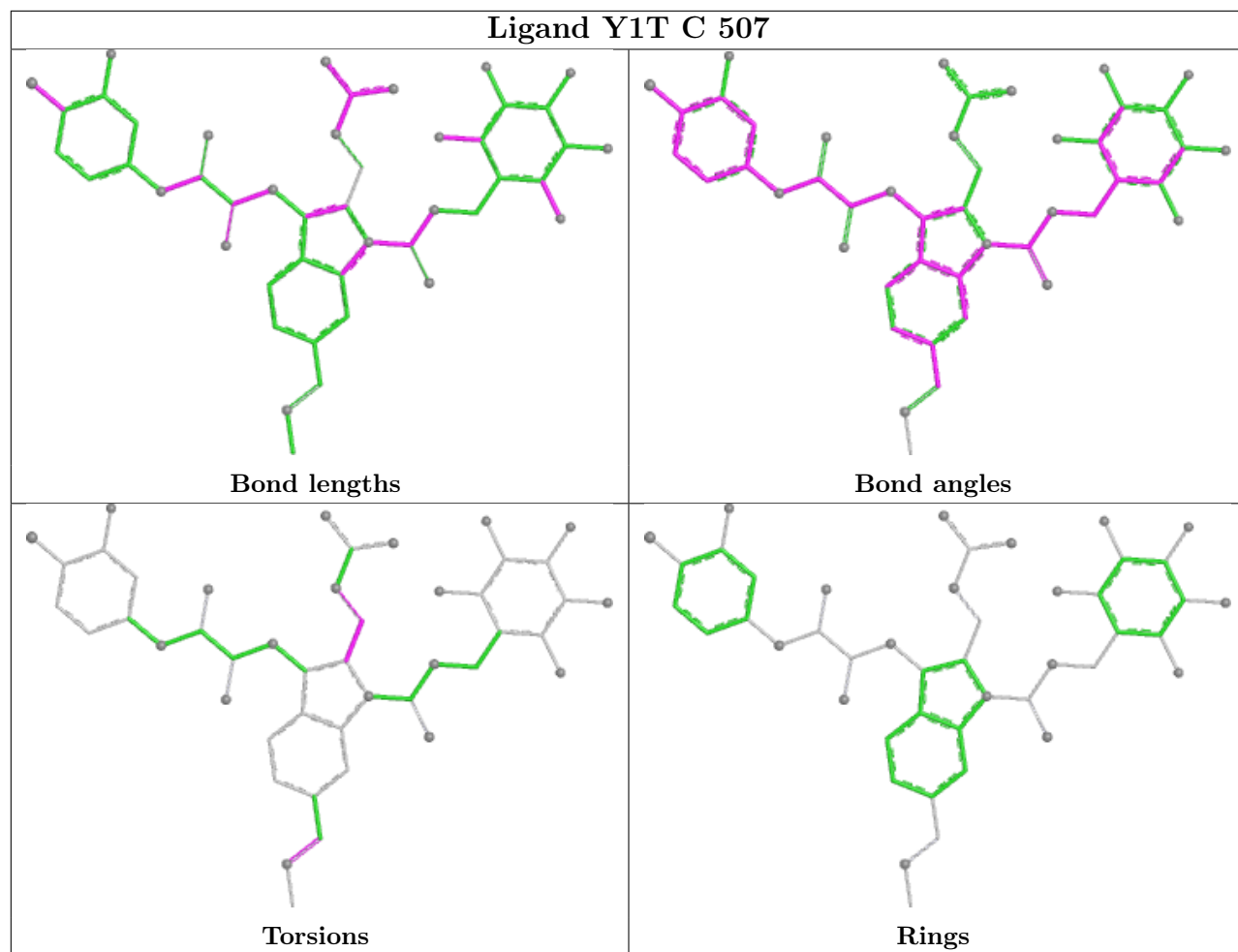
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	505	NAG	4	0
2	B	503	NAG	4	0

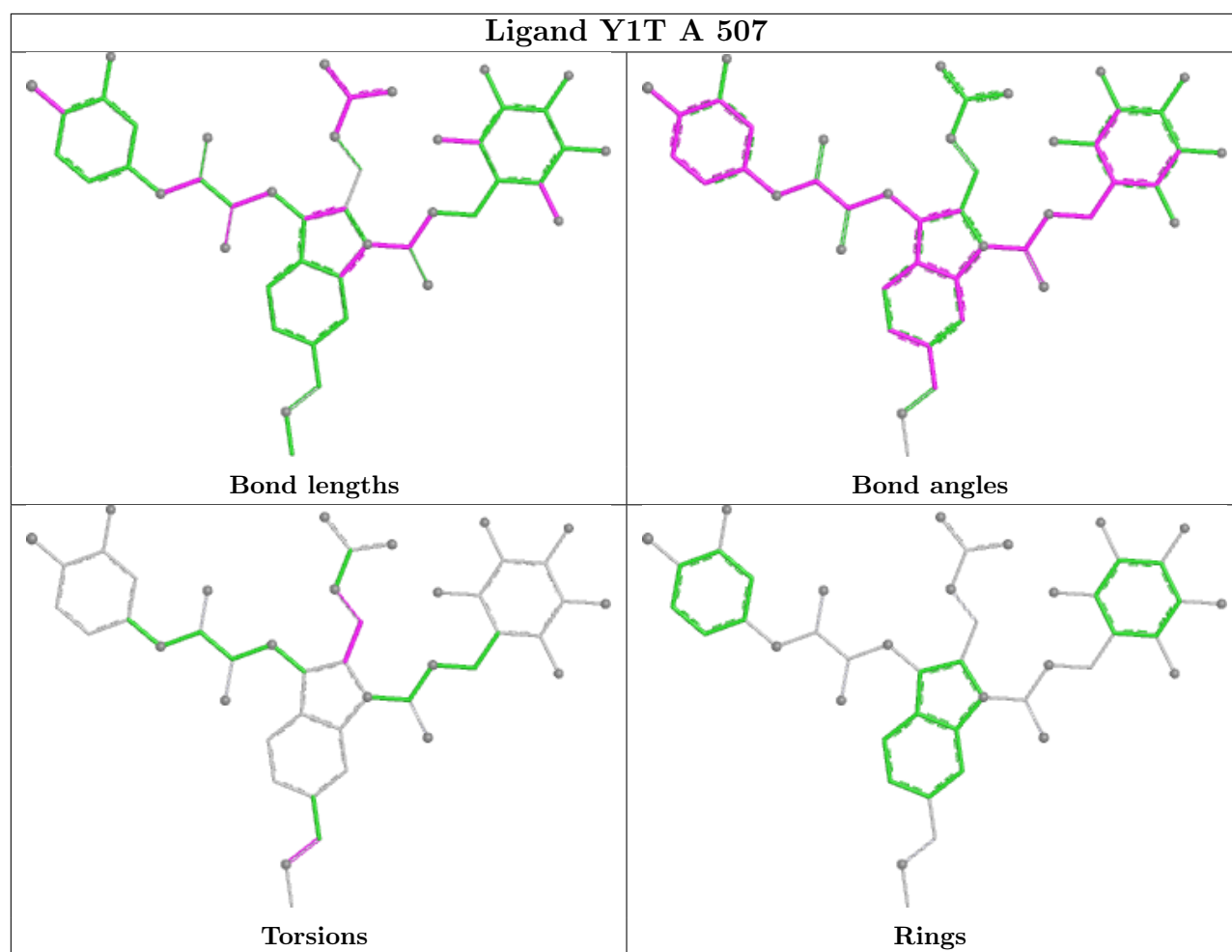
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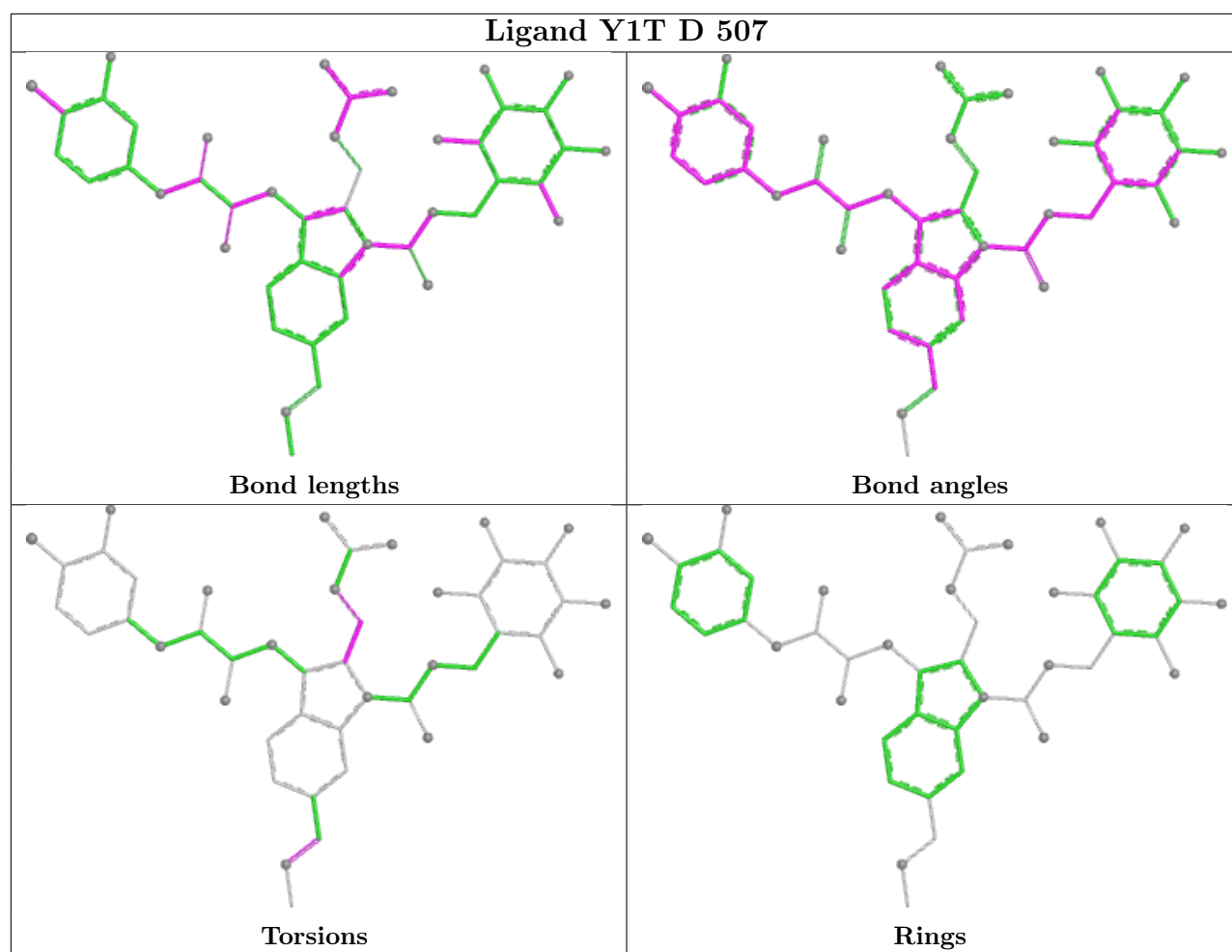
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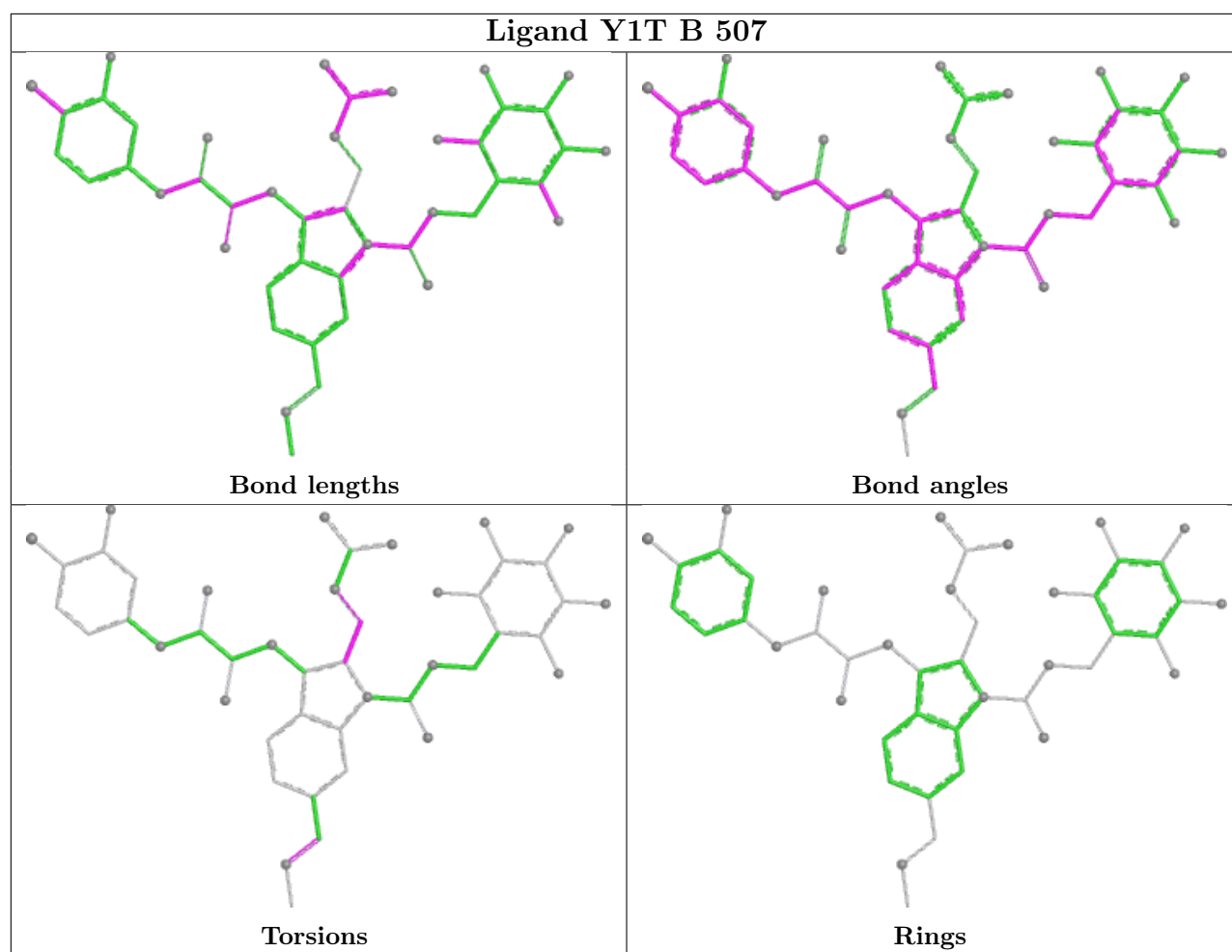
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	NAG	5	0
2	A	505	NAG	6	0
4	A	508	IMD	2	0
2	D	503	NAG	4	0
2	D	505	NAG	2	0
2	B	505	NAG	2	0
3	D	507	Y1T	1	0
2	C	503	NAG	4	0

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%)	0.36	18 (5%) 31 28	18, 38, 63, 76	0
1	B	335/358 (93%)	0.65	42 (12%) 8 6	20, 45, 74, 92	0
1	C	335/358 (93%)	0.45	31 (9%) 14 12	16, 35, 67, 88	0
1	D	335/358 (93%)	0.63	28 (8%) 17 14	22, 43, 72, 89	0
All	All	1340/1432 (93%)	0.52	119 (8%) 15 13	16, 40, 70, 92	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	60	ALA	8.2
1	C	61	TYR	7.7
1	C	124	GLY	5.5
1	C	59	LYS	4.8
1	C	198	GLY	4.5
1	C	123	THR	4.0
1	C	80	ASN	3.9
1	B	201	ILE	3.8
1	D	84	MET	3.8
1	A	93	PHE	3.7
1	C	82	GLN	3.6
1	A	202	THR	3.6
1	B	91	GLU	3.5
1	D	399	THR	3.5
1	D	397	ASN	3.4
1	B	61	TYR	3.4
1	C	122	LEU	3.3
1	B	240	ARG	3.3
1	C	199	SER	3.3
1	D	412	GLY	3.3
1	A	198	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	59	LYS	3.3
1	D	300	ASN	3.2
1	D	88	ASN	3.2
1	D	341	THR	3.2
1	A	300	ASN	3.2
1	B	349	LEU	3.2
1	D	240	ARG	3.1
1	C	49	LYS	3.0
1	B	358	THR	3.0
1	C	87	ALA	3.0
1	D	344	LYS	3.0
1	A	61	TYR	3.0
1	D	339	ASN	3.0
1	B	60	ALA	2.9
1	C	84	MET	2.9
1	B	88	ASN	2.8
1	B	345	VAL	2.8
1	B	489	VAL	2.7
1	D	465	THR	2.7
1	B	464	ASP	2.7
1	C	93	PHE	2.7
1	D	408	ARG	2.7
1	A	396	ARG	2.7
1	D	60	ALA	2.6
1	C	464	ASP	2.6
1	C	57	ASP	2.6
1	D	81	PRO	2.6
1	A	464	ASP	2.6
1	A	86	LEU	2.6
1	D	79	PRO	2.5
1	D	326	ILE	2.5
1	B	93	PHE	2.5
1	C	339	ASN	2.5
1	A	62	GLU	2.5
1	A	82	GLN	2.5
1	C	89	VAL	2.5
1	C	356	SER	2.5
1	B	399	THR	2.5
1	B	86	LEU	2.5
1	D	340	ASN	2.5
1	D	356	SER	2.5
1	B	49	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	72	HIS	2.4
1	C	379	ARG	2.4
1	C	408	ARG	2.4
1	B	408	ARG	2.4
1	B	397	ASN	2.4
1	A	397	ASN	2.4
1	B	59	LYS	2.4
1	B	340	ASN	2.4
1	B	357	LYS	2.3
1	D	404	ASN	2.3
1	B	339	ASN	2.3
1	A	87	ALA	2.3
1	B	222	GLY	2.3
1	B	343	GLN	2.3
1	B	224	ALA	2.3
1	C	396	ARG	2.3
1	B	356	SER	2.3
1	B	226	LEU	2.3
1	B	300	ASN	2.3
1	B	50	THR	2.3
1	D	82	GLN	2.3
1	C	221	ALA	2.2
1	C	336	SER	2.2
1	C	357	LYS	2.2
1	D	80	ASN	2.2
1	D	87	ALA	2.2
1	D	124	GLY	2.2
1	A	113	ASP	2.2
1	B	84	MET	2.2
1	A	124	GLY	2.1
1	C	78	ASP	2.1
1	B	97	LYS	2.1
1	B	231	LYS	2.1
1	D	223	PHE	2.1
1	C	85	VAL	2.1
1	A	90	THR	2.1
1	C	240	ARG	2.1
1	D	361	PHE	2.1
1	B	246	GLN	2.1
1	A	200	ALA	2.1
1	C	397	ASN	2.1
1	B	90	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	398	GLY	2.1
1	B	83	GLU	2.1
1	C	86	LEU	2.1
1	C	406	THR	2.1
1	B	365	SER	2.1
1	D	246	GLN	2.0
1	B	85	VAL	2.0
1	B	488	VAL	2.0
1	B	346	GLY	2.0
1	D	357	LYS	2.0
1	A	59	LYS	2.0
1	B	58	ALA	2.0
1	B	202	THR	2.0
1	B	72	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	506	14/15	0.74	0.18	60,68,87,89	0
2	NAG	D	503	14/15	0.75	0.15	55,63,68,76	0
2	NAG	B	501	14/15	0.75	0.15	44,64,73,84	0
2	NAG	D	506	14/15	0.77	0.24	48,56,78,101	0
2	NAG	B	503	14/15	0.80	0.18	43,62,79,85	0
2	NAG	C	506	14/15	0.81	0.14	37,55,68,79	0
2	NAG	D	505	14/15	0.81	0.13	50,56,62,64	0
2	NAG	D	501	14/15	0.83	0.14	39,47,65,67	0
4	IMD	A	508	5/5	0.83	0.17	39,50,64,76	0

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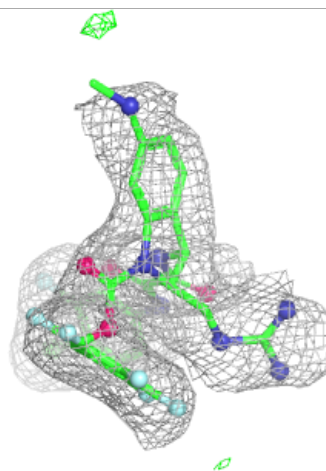
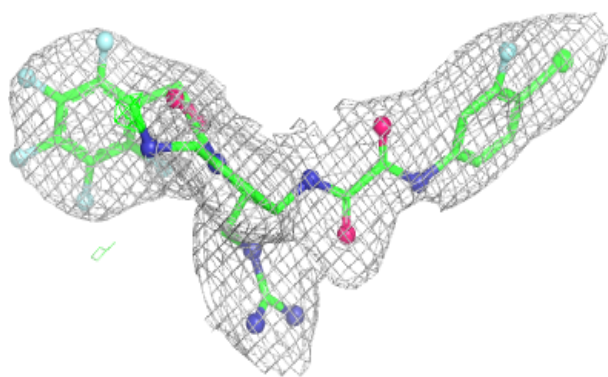
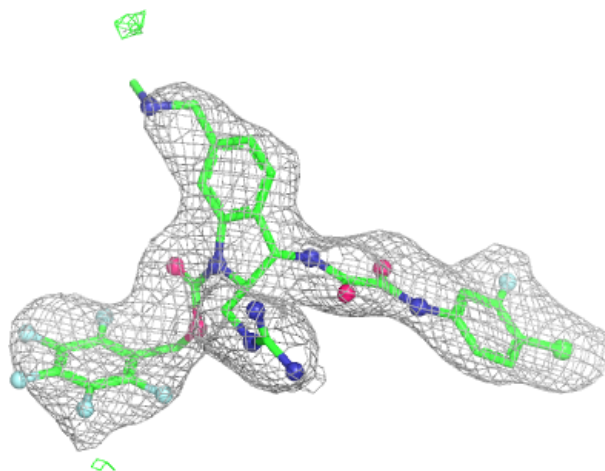
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	506	14/15	0.84	0.19	31,44,66,71	0
2	NAG	B	504	14/15	0.84	0.12	38,51,58,60	0
2	NAG	A	503	14/15	0.86	0.13	42,51,67,70	0
2	NAG	B	505	14/15	0.86	0.11	44,49,59,63	0
2	NAG	A	501	14/15	0.87	0.10	36,52,65,68	0
2	NAG	C	503	14/15	0.87	0.10	42,48,58,64	0
2	NAG	D	504	14/15	0.87	0.13	39,53,61,64	0
2	NAG	C	505	14/15	0.89	0.11	22,34,43,53	0
2	NAG	C	501	14/15	0.90	0.10	26,38,53,67	0
2	NAG	A	504	14/15	0.90	0.09	36,42,57,65	0
2	NAG	C	504	14/15	0.90	0.10	22,35,50,63	0
2	NAG	B	502	14/15	0.91	0.11	35,43,47,49	0
2	NAG	D	502	14/15	0.91	0.10	22,35,45,46	0
2	NAG	A	505	14/15	0.91	0.12	22,30,60,63	0
2	NAG	A	502	14/15	0.92	0.09	21,28,36,41	0
3	Y1T	C	507	46/46	0.94	0.09	16,26,55,70	0
3	Y1T	B	507	46/46	0.94	0.10	17,31,73,91	0
2	NAG	C	502	14/15	0.94	0.09	24,33,39,40	0
3	Y1T	D	507	46/46	0.95	0.09	20,33,59,74	0
3	Y1T	A	507	46/46	0.95	0.09	18,28,62,76	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.

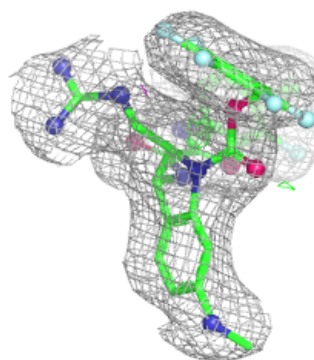
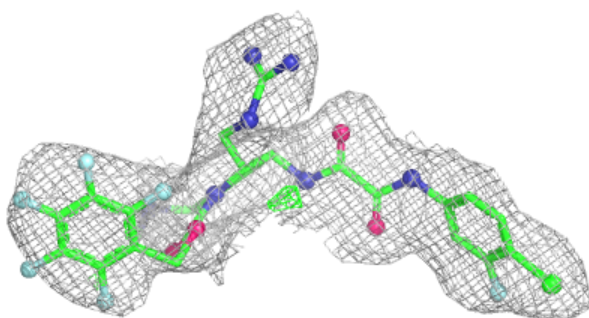
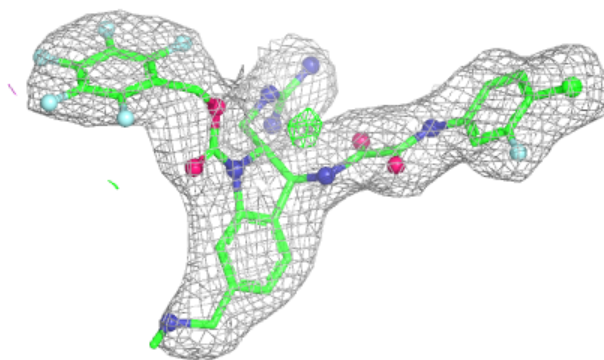
Electron density around Y1T C 507:

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

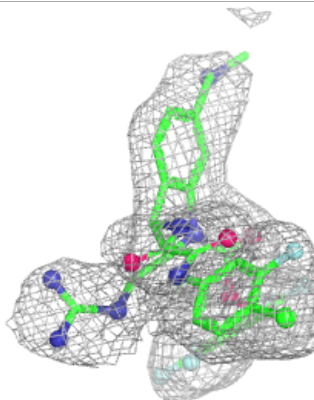
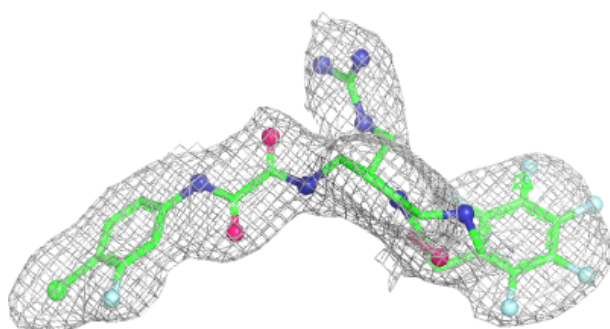
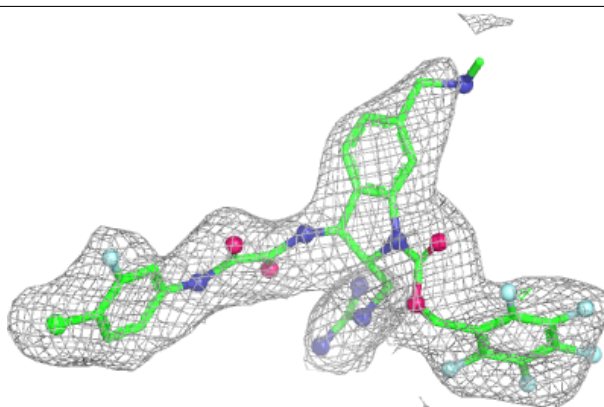


Electron density around Y1T B 507:

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

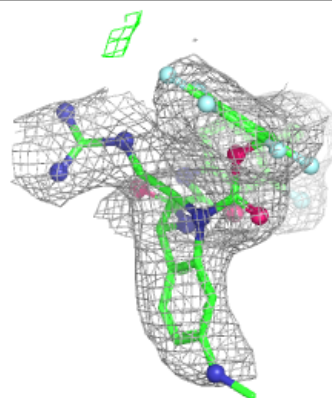
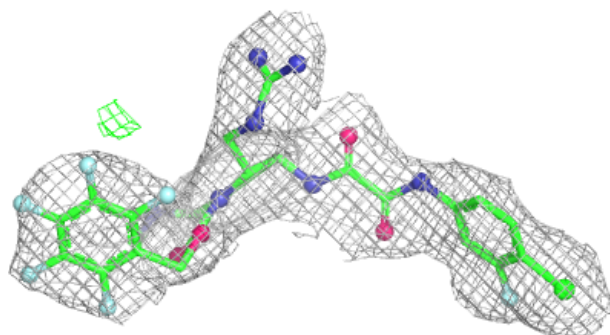
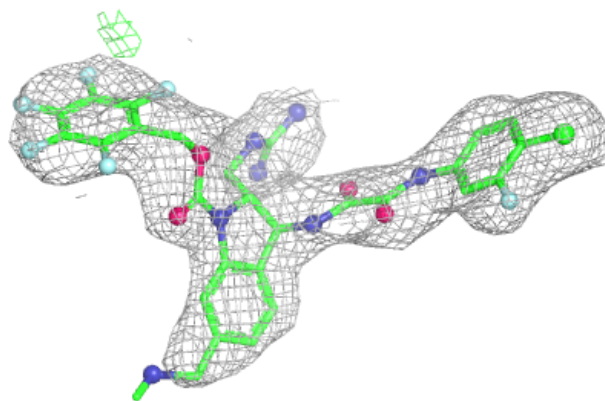
**Electron density around Y1T D 507:**

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



Electron density around Y1T 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.