



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 11:48 PM UTC

PDB ID : 8FLZ / pdb_00008flz
Title : HIV-1 gp120 complex with CJF-III-049-S
Authors : Gong, Z.; Hendrickson, W.A.
Deposited on : 2022-12-22
Resolution : 2.00 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

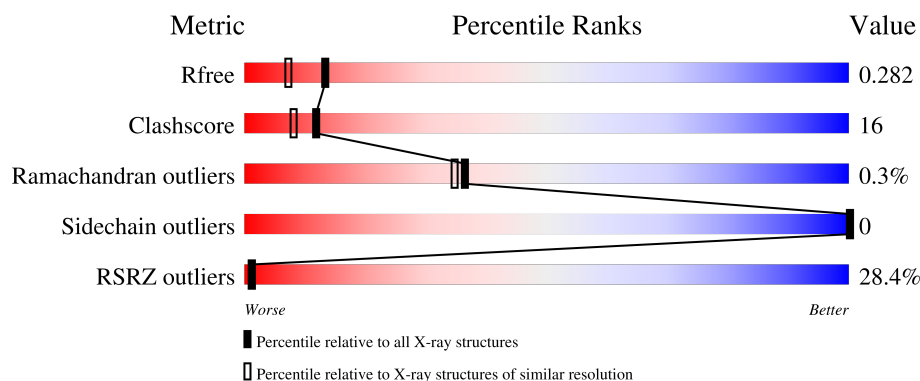
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	18% 72% 19% • 6%
1	B	358	30% 71% 20% • 6%
1	C	358	28% 72% 18% • 6%
1	D	358	30% 70% 21% • 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11219 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	A	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	B	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	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		

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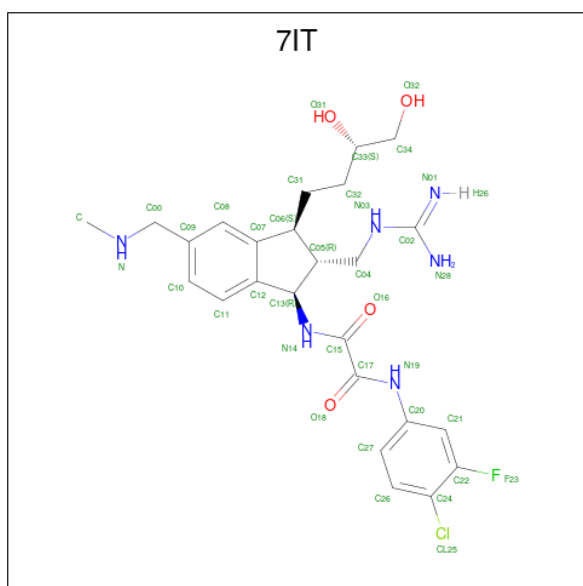
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	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	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	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	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 N 1 -{(1R,2R,3S)-2-(carbamimidamidomethyl)-3-[(3S)-3,4-dihydroxybutyl]-5-[(methylamino)methyl]-2,3-dihydro-1H-inden-1-yl}-N 2 -(4-chloro-3-fluorophenyl)ethanediamide (CCD ID: 7IT) (formula: C₂₅H₃₂ClFN₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		
3	D	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		
3	B	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		
3	C	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		

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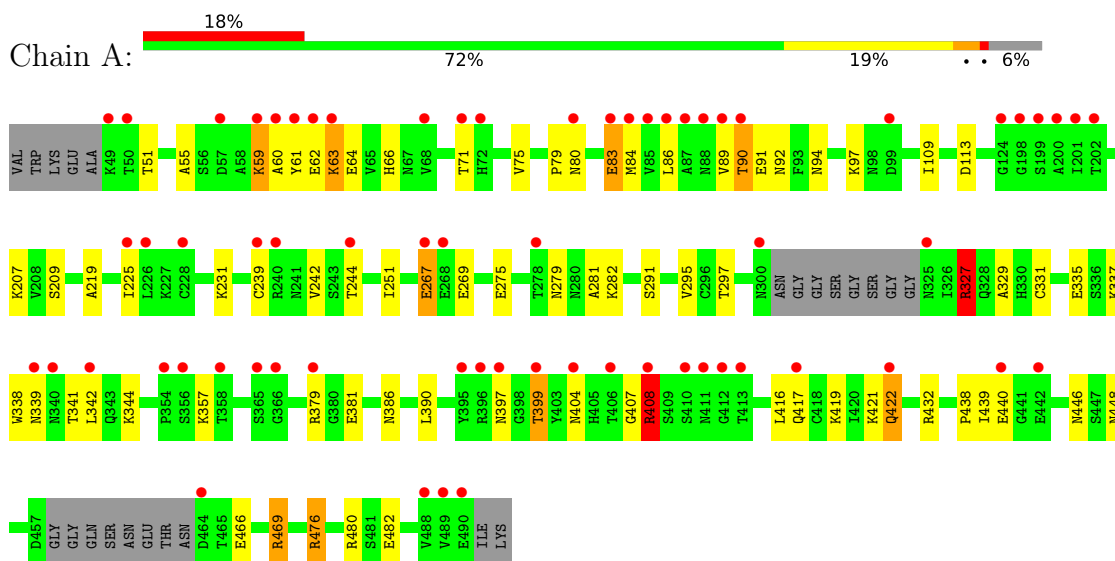
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	59	Total 59	O 59	0	0
4	B	43	Total 43	O 43	0	0
4	C	56	Total 56	O 56	0	0

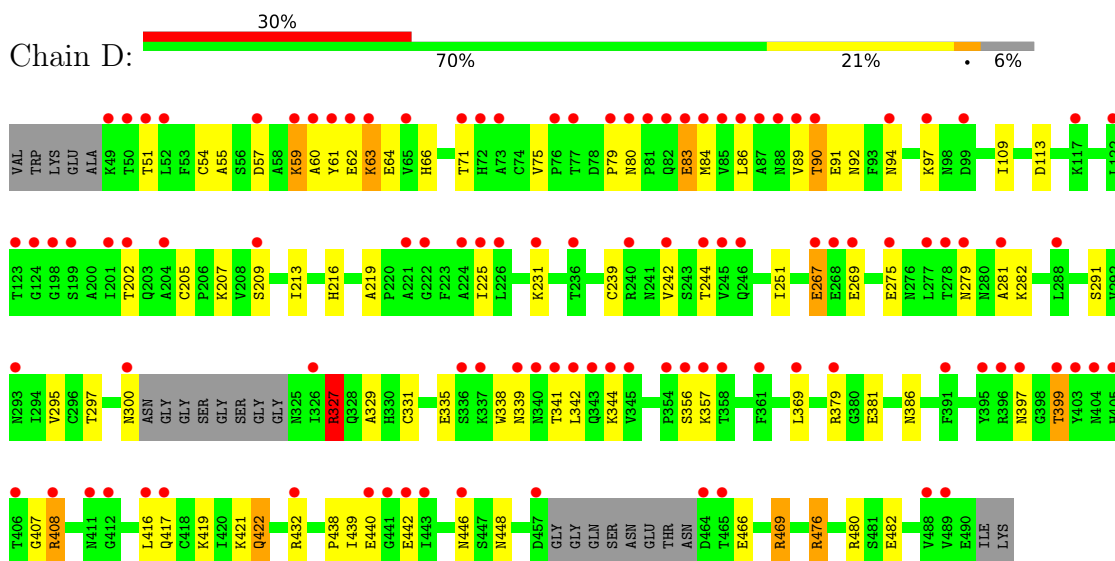
3 Residue-property plots [i](#)

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.

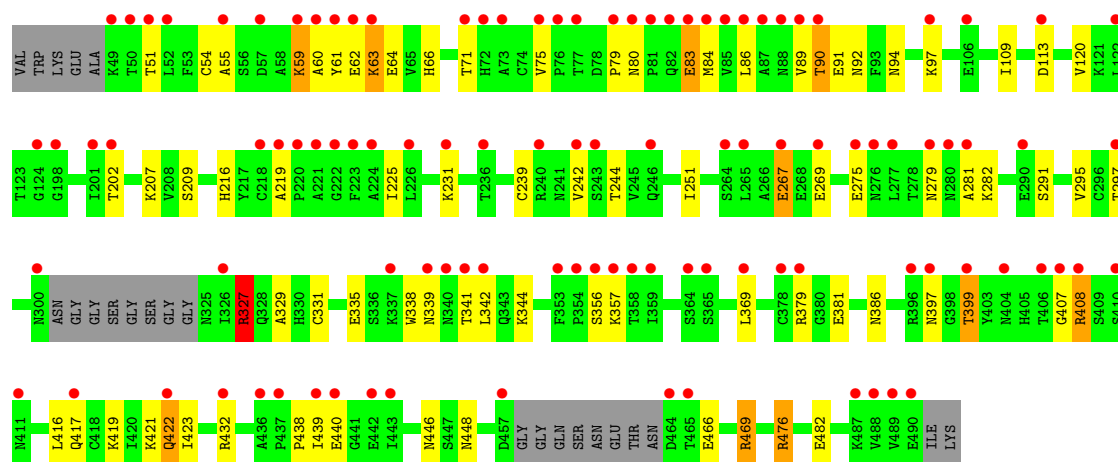
- Molecule 1: Envelope glycoprotein gp120



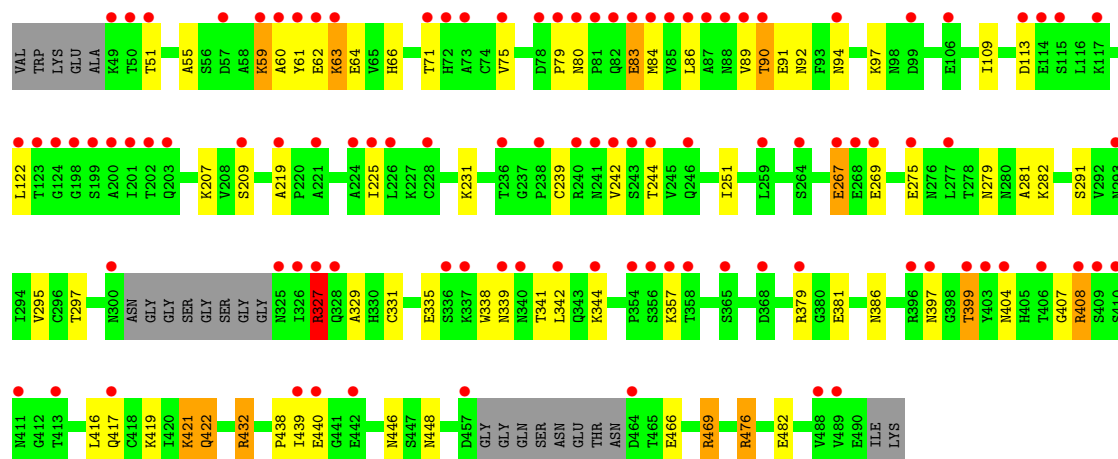
- Molecule 1: Envelope glycoprotein gp120



- Molecule 1: Envelope glycoprotein gp120



• 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	71.08Å 121.92Å 195.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.00 48.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	60.4 (48.98-2.00) 60.4 (48.98-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.263 , 0.283 0.263 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	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	11219	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 16.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7IT, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	0/2682	1.20	35/3640 (1.0%)
1	B	0.60	0/2682	1.20	35/3640 (1.0%)
1	C	0.60	0/2682	1.20	35/3640 (1.0%)
1	D	0.60	0/2682	1.20	35/3640 (1.0%)
All	All	0.60	0/10728	1.20	140/14560 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

There are no bond length outliers.

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	408	ARG	CG-CD-NE	12.06	138.54	112.00
1	A	408	ARG	CG-CD-NE	12.06	138.53	112.00
1	C	408	ARG	CG-CD-NE	12.05	138.52	112.00
1	B	408	ARG	CG-CD-NE	12.03	138.47	112.00
1	C	63	LYS	CB-CA-C	-10.67	93.08	110.79
1	A	63	LYS	CB-CA-C	-10.66	93.09	110.79
1	B	63	LYS	CB-CA-C	-10.66	93.09	110.79
1	D	63	LYS	CB-CA-C	-10.65	93.10	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	GLU	CG-CD-OE2	-8.79	98.18	118.40
1	D	83	GLU	CG-CD-OE2	-8.79	98.18	118.40
1	C	83	GLU	CG-CD-OE2	-8.78	98.20	118.40
1	A	83	GLU	CG-CD-OE2	-8.77	98.22	118.40
1	C	408	ARG	N-CA-CB	8.63	123.57	110.45
1	D	408	ARG	N-CA-CB	8.61	123.54	110.45
1	A	408	ARG	N-CA-CB	8.60	123.52	110.45
1	B	408	ARG	N-CA-CB	8.56	123.46	110.45
1	D	267	GLU	CA-CB-CG	8.46	131.02	114.10
1	A	267	GLU	CA-CB-CG	8.45	131.01	114.10
1	B	267	GLU	CA-CB-CG	8.45	131.00	114.10
1	C	267	GLU	CA-CB-CG	8.44	130.99	114.10
1	B	344	LYS	CA-CB-CG	-7.81	98.48	114.10
1	A	344	LYS	CA-CB-CG	-7.80	98.49	114.10
1	D	344	LYS	CA-CB-CG	-7.80	98.50	114.10
1	C	344	LYS	CA-CB-CG	-7.79	98.52	114.10
1	D	79	PRO	CA-C-N	-7.36	107.82	122.40
1	D	79	PRO	C-N-CA	-7.36	107.82	122.40
1	A	79	PRO	CA-C-N	-7.34	107.87	122.40
1	A	79	PRO	C-N-CA	-7.34	107.87	122.40
1	C	79	PRO	CA-C-N	-7.33	107.89	122.40
1	C	79	PRO	C-N-CA	-7.33	107.89	122.40
1	B	79	PRO	CA-C-N	-7.32	107.90	122.40
1	B	79	PRO	C-N-CA	-7.32	107.90	122.40
1	A	422	GLN	CB-CG-CD	7.24	124.90	112.60
1	D	422	GLN	CB-CG-CD	7.23	124.89	112.60
1	B	422	GLN	CB-CG-CD	7.22	124.88	112.60
1	C	422	GLN	CB-CG-CD	7.21	124.86	112.60
1	B	408	ARG	CB-CA-C	-6.93	95.96	109.76
1	A	408	ARG	CB-CA-C	-6.92	95.99	109.76
1	D	408	ARG	CB-CA-C	-6.91	96.00	109.76
1	C	408	ARG	CB-CA-C	-6.91	96.01	109.76
1	A	407	GLY	CA-C-N	-6.75	107.13	121.32
1	A	407	GLY	C-N-CA	-6.75	107.13	121.32
1	B	407	GLY	CA-C-N	-6.75	107.14	121.32
1	B	407	GLY	C-N-CA	-6.75	107.14	121.32
1	D	407	GLY	CA-C-N	-6.75	107.14	121.32
1	D	407	GLY	C-N-CA	-6.75	107.14	121.32
1	C	407	GLY	CA-C-N	-6.75	107.15	121.32
1	C	407	GLY	C-N-CA	-6.75	107.15	121.32
1	B	59	LYS	CA-C-N	-6.74	108.46	121.94
1	B	59	LYS	C-N-CA	-6.74	108.46	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	LYS	CA-C-N	-6.73	108.47	121.94
1	C	59	LYS	C-N-CA	-6.73	108.47	121.94
1	D	59	LYS	CA-C-N	-6.73	108.48	121.94
1	D	59	LYS	C-N-CA	-6.73	108.48	121.94
1	A	59	LYS	CA-C-N	-6.73	108.48	121.94
1	A	59	LYS	C-N-CA	-6.73	108.48	121.94
1	B	399	THR	OG1-CB-CG2	6.67	122.64	109.30
1	D	476	ARG	CG-CD-NE	-6.67	97.33	112.00
1	C	476	ARG	CG-CD-NE	-6.66	97.34	112.00
1	A	476	ARG	CG-CD-NE	-6.66	97.36	112.00
1	B	476	ARG	CG-CD-NE	-6.66	97.36	112.00
1	C	399	THR	OG1-CB-CG2	6.66	122.61	109.30
1	A	399	THR	OG1-CB-CG2	6.64	122.59	109.30
1	D	399	THR	OG1-CB-CG2	6.63	122.57	109.30
1	B	83	GLU	CG-CD-OE1	6.60	133.58	118.40
1	D	83	GLU	CG-CD-OE1	6.57	133.52	118.40
1	C	83	GLU	CG-CD-OE1	6.57	133.51	118.40
1	A	83	GLU	CG-CD-OE1	6.57	133.50	118.40
1	A	399	THR	CA-CB-CG2	6.55	121.64	110.50
1	D	399	THR	CA-CB-CG2	6.54	121.62	110.50
1	C	327	ARG	CG-CD-NE	-6.54	97.61	112.00
1	A	327	ARG	CG-CD-NE	-6.54	97.62	112.00
1	D	327	ARG	CG-CD-NE	-6.54	97.62	112.00
1	B	327	ARG	CG-CD-NE	-6.53	97.64	112.00
1	B	399	THR	CA-CB-CG2	6.52	121.59	110.50
1	C	399	THR	CA-CB-CG2	6.52	121.59	110.50
1	B	440	GLU	CA-CB-CG	6.46	127.02	114.10
1	C	440	GLU	CA-CB-CG	6.46	127.02	114.10
1	A	440	GLU	CA-CB-CG	6.45	127.01	114.10
1	D	440	GLU	CA-CB-CG	6.44	126.98	114.10
1	A	432	ARG	CB-CG-CD	6.37	125.96	111.30
1	B	432	ARG	CB-CG-CD	6.37	125.95	111.30
1	C	432	ARG	CB-CG-CD	6.37	125.96	111.30
1	D	432	ARG	CB-CG-CD	6.37	125.94	111.30
1	B	469	ARG	CG-CD-NE	-6.25	98.26	112.00
1	A	469	ARG	CG-CD-NE	-6.25	98.26	112.00
1	D	469	ARG	CG-CD-NE	-6.24	98.27	112.00
1	C	469	ARG	CG-CD-NE	-6.22	98.33	112.00
1	B	59	LYS	CB-CA-C	-5.81	99.95	109.53
1	A	59	LYS	CB-CA-C	-5.80	99.96	109.53
1	C	59	LYS	CB-CA-C	-5.80	99.96	109.53
1	D	59	LYS	CB-CA-C	-5.79	99.97	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ARG	CB-CG-CD	5.75	124.53	111.30
1	C	327	ARG	CB-CG-CD	5.75	124.52	111.30
1	D	327	ARG	CB-CG-CD	5.74	124.51	111.30
1	A	327	ARG	CB-CG-CD	5.74	124.50	111.30
1	D	440	GLU	N-CA-CB	5.68	118.22	110.38
1	B	440	GLU	N-CA-CB	5.66	118.20	110.38
1	A	440	GLU	N-CA-CB	5.66	118.19	110.38
1	C	440	GLU	N-CA-CB	5.65	118.17	110.38
1	B	327	ARG	CA-CB-CG	5.58	125.26	114.10
1	A	327	ARG	CA-CB-CG	5.57	125.24	114.10
1	C	327	ARG	CA-CB-CG	5.55	125.20	114.10
1	D	327	ARG	CA-CB-CG	5.54	125.18	114.10
1	D	327	ARG	CB-CA-C	-5.54	98.93	109.95
1	C	327	ARG	CB-CA-C	-5.53	98.95	109.95
1	A	327	ARG	CB-CA-C	-5.52	98.97	109.95
1	B	327	ARG	CB-CA-C	-5.50	99.01	109.95
1	D	59	LYS	CD-CE-NZ	-5.38	94.69	111.90
1	B	59	LYS	CD-CE-NZ	-5.38	94.69	111.90
1	A	59	LYS	CD-CE-NZ	-5.37	94.71	111.90
1	C	59	LYS	CD-CE-NZ	-5.37	94.72	111.90
1	C	51	THR	OG1-CB-CG2	5.33	119.96	109.30
1	B	51	THR	OG1-CB-CG2	5.32	119.93	109.30
1	A	51	THR	OG1-CB-CG2	5.30	119.90	109.30
1	D	51	THR	OG1-CB-CG2	5.28	119.86	109.30
1	A	408	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	B	408	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	D	408	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	C	408	ARG	CD-NE-CZ	-5.19	117.14	124.40
1	D	89	VAL	CA-C-O	-5.19	115.56	120.95
1	A	269	GLU	CA-CB-CG	5.18	124.46	114.10
1	C	269	GLU	CA-CB-CG	5.18	124.46	114.10
1	D	269	GLU	CA-CB-CG	5.18	124.45	114.10
1	B	269	GLU	CA-CB-CG	5.15	124.41	114.10
1	A	89	VAL	CA-C-O	-5.15	115.59	120.95
1	A	267	GLU	CB-CG-CD	5.13	121.33	112.60
1	D	267	GLU	CB-CG-CD	5.13	121.32	112.60
1	B	267	GLU	CB-CG-CD	5.13	121.32	112.60
1	C	267	GLU	CB-CG-CD	5.13	121.31	112.60
1	B	89	VAL	CA-C-O	-5.12	115.63	120.95
1	C	89	VAL	CA-C-O	-5.12	115.63	120.95
1	D	421	LYS	CA-C-N	5.07	131.82	122.79
1	D	421	LYS	C-N-CA	5.07	131.82	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	LYS	CA-C-N	5.07	131.82	122.79
1	B	421	LYS	C-N-CA	5.07	131.82	122.79
1	A	421	LYS	CA-C-N	5.05	131.78	122.79
1	A	421	LYS	C-N-CA	5.05	131.78	122.79
1	C	421	LYS	CA-C-N	5.05	131.78	122.79
1	C	421	LYS	C-N-CA	5.05	131.78	122.79

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	327	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	408	ARG	Sidechain
1	A	469	ARG	Sidechain
1	A	476	ARG	Sidechain
1	A	83	GLU	Sidechain
1	B	327	ARG	Sidechain
1	B	379	ARG	Sidechain
1	B	408	ARG	Sidechain
1	B	469	ARG	Sidechain
1	B	476	ARG	Sidechain
1	B	83	GLU	Sidechain
1	C	327	ARG	Sidechain
1	C	379	ARG	Sidechain
1	C	408	ARG	Sidechain
1	C	469	ARG	Sidechain
1	C	476	ARG	Sidechain
1	C	83	GLU	Sidechain
1	D	327	ARG	Sidechain
1	D	379	ARG	Sidechain
1	D	408	ARG	Sidechain
1	D	469	ARG	Sidechain
1	D	476	ARG	Sidechain
1	D	83	GLU	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	2539	79	1
1	B	2627	0	2542	76	1
1	C	2627	0	2539	116	0
1	D	2627	0	2542	107	1
2	A	98	0	91	4	0
2	B	84	0	78	0	0
2	C	98	0	91	3	0
2	D	84	0	78	0	1
3	A	37	0	0	0	0
3	B	37	0	0	0	0
3	C	37	0	0	0	0
3	D	37	0	0	0	0
4	A	41	0	0	4	0
4	B	43	0	0	2	0
4	C	56	0	0	1	0
4	D	59	0	0	6	0
All	All	11219	0	10500	339	2

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 16.

All (339) 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:300:ASN:HB2	1:C:80:ASN:ND2	1.41	1.34
1:D:59:LYS:NZ	1:C:60:ALA:C	2.15	1.04
1:A:408:ARG:NH2	1:C:399:THR:OG1	1.90	1.03
1:D:300:ASN:CB	1:C:80:ASN:ND2	2.23	1.01
1:D:59:LYS:HZ3	1:C:61:TYR:CA	1.74	1.00
1:D:442:GLU:HB3	1:C:80:ASN:HB3	1.45	0.98
1:D:300:ASN:CB	1:C:80:ASN:HD21	1.77	0.97
1:D:300:ASN:HB2	1:C:80:ASN:HD22	1.30	0.94
1:D:59:LYS:HZ3	1:C:61:TYR:N	1.67	0.91
1:D:300:ASN:HB2	1:C:80:ASN:HD21	1.19	0.91
1:D:59:LYS:HE3	1:C:60:ALA:HB3	1.53	0.90
1:D:59:LYS:NZ	1:C:60:ALA:O	2.05	0.88
1:B:342:LEU:HD12	1:B:342:LEU:N	1.89	0.88
1:A:342:LEU:N	1:A:342:LEU:HD12	1.89	0.87
1:C:342:LEU:N	1:C:342:LEU:HD12	1.89	0.87
2:A:505:NAG:H62	1:C:404:ASN:HD22	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:LEU:HD12	1:D:342:LEU:N	1.89	0.86
1:C:338:TRP:O	1:C:342:LEU:HD13	1.78	0.84
1:B:338:TRP:O	1:B:342:LEU:HD13	1.78	0.84
1:C:275:GLU:OE2	1:C:282:LYS:NZ	2.11	0.84
1:D:338:TRP:O	1:D:342:LEU:HD13	1.78	0.83
1:B:275:GLU:OE2	1:B:282:LYS:NZ	2.11	0.83
1:A:275:GLU:OE2	1:A:282:LYS:NZ	2.11	0.82
1:A:338:TRP:O	1:A:342:LEU:HD13	1.78	0.82
1:D:275:GLU:OE2	1:D:282:LYS:NZ	2.11	0.82
1:D:59:LYS:HZ1	1:C:60:ALA:C	1.81	0.81
1:D:442:GLU:CB	1:C:80:ASN:HB3	2.12	0.79
1:A:408:ARG:HH22	1:C:399:THR:HG1	1.25	0.79
1:C:63:LYS:HG3	1:C:209:SER:OG	1.83	0.79
1:D:63:LYS:HG3	1:D:209:SER:OG	1.83	0.79
1:D:59:LYS:CE	1:C:60:ALA:HB3	2.14	0.78
1:B:63:LYS:HG3	1:B:209:SER:OG	1.83	0.78
1:A:63:LYS:HG3	1:A:209:SER:OG	1.83	0.78
1:D:442:GLU:HB3	1:C:80:ASN:CB	2.15	0.76
1:D:59:LYS:HZ3	1:C:60:ALA:C	1.87	0.75
1:C:63:LYS:CG	1:C:209:SER:OG	2.35	0.75
1:B:63:LYS:HD2	1:B:209:SER:HB3	1.68	0.75
1:D:63:LYS:CG	1:D:209:SER:OG	2.35	0.74
1:A:63:LYS:HD2	1:A:209:SER:CB	2.18	0.74
1:D:63:LYS:HD2	1:D:209:SER:CB	2.18	0.74
1:B:63:LYS:CG	1:B:209:SER:OG	2.35	0.74
1:C:63:LYS:HD2	1:C:209:SER:CB	2.17	0.74
1:D:63:LYS:HD2	1:D:209:SER:HB3	1.68	0.74
1:B:63:LYS:HD2	1:B:209:SER:CB	2.18	0.74
1:A:63:LYS:HD2	1:A:209:SER:HB3	1.68	0.73
1:A:63:LYS:CG	1:A:209:SER:OG	2.35	0.73
1:C:63:LYS:HG3	1:C:64:GLU:N	2.04	0.72
1:C:63:LYS:HD2	1:C:209:SER:HB3	1.68	0.72
1:B:207:LYS:HD2	1:B:439:ILE:HG23	1.71	0.72
1:D:207:LYS:HD2	1:D:439:ILE:HG23	1.71	0.72
1:A:63:LYS:HG3	1:A:64:GLU:N	2.04	0.72
1:D:63:LYS:HG3	1:D:64:GLU:N	2.04	0.71
1:B:63:LYS:HG3	1:B:64:GLU:N	2.04	0.71
1:C:207:LYS:HD2	1:C:439:ILE:HG23	1.71	0.71
1:A:207:LYS:HD2	1:A:439:ILE:HG23	1.71	0.71
1:B:63:LYS:CG	1:B:64:GLU:N	2.54	0.70
1:D:63:LYS:CG	1:D:64:GLU:N	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:CG	1:C:64:GLU:HB2	2.22	0.70
1:A:63:LYS:CG	1:A:64:GLU:N	2.54	0.70
1:A:62:GLU:CG	1:A:64:GLU:HB2	2.22	0.70
1:D:59:LYS:HZ3	1:C:61:TYR:HA	1.57	0.70
1:B:62:GLU:CG	1:B:64:GLU:HB2	2.22	0.69
1:D:62:GLU:CG	1:D:64:GLU:HB2	2.22	0.69
1:A:62:GLU:HG3	1:A:64:GLU:HB2	1.76	0.68
1:D:62:GLU:HG3	1:D:64:GLU:HB2	1.75	0.68
1:B:62:GLU:HG3	1:B:64:GLU:HB2	1.75	0.68
1:B:120:VAL:HG21	1:C:122:LEU:HD11	1.77	0.67
1:C:63:LYS:CG	1:C:64:GLU:N	2.54	0.66
1:D:62:GLU:HG3	1:D:64:GLU:CB	2.26	0.66
1:B:62:GLU:HG3	1:B:64:GLU:CB	2.26	0.66
1:C:62:GLU:HG3	1:C:64:GLU:HB2	1.76	0.66
1:C:338:TRP:CZ2	1:C:342:LEU:HD21	2.30	0.66
1:A:338:TRP:CZ2	1:A:342:LEU:HD21	2.30	0.66
1:D:338:TRP:CZ2	1:D:342:LEU:HD21	2.30	0.66
1:B:202:THR:HG21	4:C:601:HOH:O	1.94	0.66
1:B:338:TRP:CZ2	1:B:342:LEU:HD21	2.30	0.66
1:C:62:GLU:HG3	1:C:64:GLU:CB	2.26	0.65
1:A:62:GLU:HG3	1:A:64:GLU:CB	2.26	0.65
1:A:480:ARG:NH1	4:A:601:HOH:O	2.10	0.65
1:D:442:GLU:CB	1:C:80:ASN:CB	2.74	0.64
1:C:59:LYS:HG3	1:C:61:TYR:CE1	2.33	0.64
1:D:59:LYS:HG3	1:D:61:TYR:CE1	2.32	0.64
1:A:59:LYS:HG3	1:A:61:TYR:CE1	2.32	0.64
1:B:342:LEU:N	1:B:342:LEU:CD1	2.61	0.64
1:D:448:ASN:ND2	4:D:601:HOH:O	1.99	0.64
1:D:342:LEU:N	1:D:342:LEU:CD1	2.61	0.63
1:B:59:LYS:HG3	1:B:61:TYR:CE1	2.33	0.63
1:A:63:LYS:HD3	4:A:618:HOH:O	1.99	0.63
1:A:342:LEU:N	1:A:342:LEU:CD1	2.61	0.63
1:C:231:LYS:HD2	1:C:267:GLU:CG	2.30	0.62
1:D:231:LYS:HD2	1:D:267:GLU:CG	2.30	0.62
1:B:84:MET:HE3	1:B:86:LEU:HD21	1.82	0.62
1:D:84:MET:HE3	1:D:86:LEU:HD21	1.82	0.62
1:A:231:LYS:HD2	1:A:267:GLU:CG	2.30	0.62
1:B:231:LYS:HD2	1:B:267:GLU:CG	2.30	0.61
1:C:84:MET:HE3	1:C:86:LEU:HD21	1.82	0.61
1:C:342:LEU:N	1:C:342:LEU:CD1	2.61	0.61
1:D:59:LYS:HE3	1:C:60:ALA:CB	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASN:ND2	1:A:281:ALA:H	1.99	0.61
1:D:279:ASN:ND2	1:D:281:ALA:H	1.99	0.61
1:D:300:ASN:CG	1:C:80:ASN:HD21	2.08	0.61
1:A:84:MET:HE3	1:A:86:LEU:HD21	1.82	0.60
1:A:62:GLU:HG3	1:A:64:GLU:H	1.67	0.60
1:D:442:GLU:OE1	1:C:80:ASN:HB2	2.01	0.60
1:C:279:ASN:ND2	1:C:281:ALA:H	1.99	0.60
1:C:62:GLU:HG3	1:C:64:GLU:H	1.67	0.60
1:D:63:LYS:HD2	1:D:209:SER:OG	2.02	0.60
1:C:357:LYS:HG3	1:C:466:GLU:HG2	1.84	0.59
1:A:63:LYS:HD2	1:A:209:SER:OG	2.02	0.59
1:B:279:ASN:ND2	1:B:281:ALA:H	1.99	0.59
1:D:357:LYS:HG3	1:D:466:GLU:HG2	1.84	0.59
1:B:63:LYS:HD2	1:B:209:SER:OG	2.02	0.59
1:B:94:ASN:OD1	1:B:97:LYS:HB2	2.03	0.59
1:A:63:LYS:HG3	1:A:209:SER:HG	1.65	0.59
1:C:63:LYS:HD2	1:C:209:SER:OG	2.02	0.59
1:B:62:GLU:HG3	1:B:64:GLU:H	1.67	0.59
1:B:357:LYS:HG3	1:B:466:GLU:HG2	1.84	0.58
1:D:62:GLU:HG3	1:D:64:GLU:H	1.67	0.58
1:A:357:LYS:HG3	1:A:466:GLU:HG2	1.84	0.58
1:A:231:LYS:HD2	1:A:267:GLU:HG2	1.86	0.58
1:D:94:ASN:OD1	1:D:97:LYS:HB2	2.03	0.58
1:C:94:ASN:OD1	1:C:97:LYS:HB2	2.03	0.58
1:D:231:LYS:HD2	1:D:267:GLU:HG2	1.86	0.58
1:A:94:ASN:OD1	1:A:97:LYS:HB2	2.03	0.57
1:B:231:LYS:HD2	1:B:267:GLU:HG2	1.86	0.57
1:C:381:GLU:OE2	1:C:438:PRO:HA	2.05	0.57
1:D:381:GLU:OE2	1:D:438:PRO:HA	2.05	0.57
1:B:381:GLU:OE2	1:B:438:PRO:HA	2.05	0.57
1:D:59:LYS:NZ	1:C:61:TYR:CA	2.59	0.57
1:A:279:ASN:HD22	1:A:281:ALA:H	1.53	0.56
1:B:97:LYS:HE3	4:B:631:HOH:O	2.04	0.56
1:C:231:LYS:HD2	1:C:267:GLU:HG2	1.86	0.56
1:C:279:ASN:HD22	1:C:281:ALA:H	1.53	0.56
1:A:64:GLU:OE2	1:A:66:HIS:HB2	2.05	0.56
1:A:381:GLU:OE2	1:A:438:PRO:HA	2.05	0.56
1:A:404:ASN:HD22	2:C:505:NAG:H62	1.70	0.56
1:B:279:ASN:HD22	1:B:281:ALA:H	1.53	0.56
1:D:279:ASN:HD22	1:D:281:ALA:H	1.53	0.56
1:D:64:GLU:OE2	1:D:66:HIS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLU:OE2	1:C:66:HIS:HB2	2.05	0.56
1:A:80:ASN:OD1	1:A:80:ASN:O	2.25	0.55
1:D:80:ASN:OD1	1:D:80:ASN:O	2.25	0.55
1:D:59:LYS:NZ	1:C:61:TYR:HA	2.20	0.55
1:B:80:ASN:OD1	1:B:80:ASN:O	2.25	0.55
1:B:64:GLU:OE2	1:B:66:HIS:HB2	2.05	0.55
1:C:339:ASN:ND2	2:C:508:NAG:H83	2.21	0.55
1:C:80:ASN:OD1	1:C:80:ASN:O	2.25	0.55
1:A:62:GLU:CG	1:A:64:GLU:CB	2.84	0.55
1:C:62:GLU:CG	1:C:64:GLU:CB	2.84	0.54
1:D:59:LYS:CE	1:C:60:ALA:CB	2.85	0.54
1:D:62:GLU:CG	1:D:64:GLU:CB	2.84	0.54
1:D:63:LYS:CD	1:D:209:SER:OG	2.56	0.54
1:B:338:TRP:CE2	1:B:342:LEU:HD21	2.43	0.54
1:A:397:ASN:O	1:A:399:THR:HG22	2.08	0.53
1:D:397:ASN:O	1:D:399:THR:HG22	2.08	0.53
1:B:62:GLU:CG	1:B:64:GLU:CB	2.84	0.53
1:B:63:LYS:CD	1:B:209:SER:OG	2.56	0.53
2:A:505:NAG:H62	1:C:404:ASN:ND2	2.16	0.53
1:B:397:ASN:O	1:B:399:THR:HG22	2.08	0.53
1:C:397:ASN:O	1:C:399:THR:HG22	2.08	0.53
1:B:120:VAL:CG2	1:C:122:LEU:HD11	2.39	0.53
1:C:63:LYS:CD	1:C:209:SER:OG	2.56	0.53
1:D:59:LYS:HZ3	1:C:61:TYR:CB	2.21	0.53
1:D:338:TRP:CE2	1:D:342:LEU:HD21	2.44	0.53
1:A:63:LYS:CD	1:A:209:SER:OG	2.56	0.53
1:A:338:TRP:CE2	1:A:342:LEU:HD21	2.43	0.53
1:D:59:LYS:CE	1:C:60:ALA:C	2.82	0.52
1:C:338:TRP:CE2	1:C:342:LEU:HD21	2.43	0.52
1:D:338:TRP:O	1:D:342:LEU:CD1	2.56	0.52
1:D:84:MET:CE	1:D:86:LEU:HD21	2.40	0.52
1:C:338:TRP:O	1:C:342:LEU:CD1	2.55	0.52
1:C:84:MET:CE	1:C:86:LEU:HD21	2.40	0.51
1:A:60:ALA:HA	1:A:71:THR:HG21	1.92	0.51
1:A:84:MET:CE	1:A:86:LEU:HD21	2.40	0.51
1:B:84:MET:CE	1:B:86:LEU:HD21	2.40	0.51
1:B:279:ASN:HD21	1:B:281:ALA:HB3	1.76	0.51
1:C:279:ASN:HD21	1:C:281:ALA:HB3	1.76	0.51
1:D:60:ALA:HA	1:D:71:THR:HG21	1.92	0.51
1:D:62:GLU:HG3	1:D:64:GLU:N	2.26	0.51
1:B:60:ALA:HA	1:B:71:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ILE:HD11	1:C:432:ARG:HD3	1.92	0.51
1:A:279:ASN:HD21	1:A:281:ALA:HB3	1.76	0.51
1:C:60:ALA:HA	1:C:71:THR:HG21	1.92	0.51
2:A:505:NAG:C6	1:C:404:ASN:HD22	2.17	0.50
1:B:62:GLU:HG3	1:B:64:GLU:N	2.26	0.50
1:C:62:GLU:HG3	1:C:64:GLU:N	2.26	0.50
1:D:207:LYS:HD2	1:D:439:ILE:CG2	2.41	0.50
1:A:338:TRP:O	1:A:342:LEU:CD1	2.55	0.50
1:A:207:LYS:HD2	1:A:439:ILE:CG2	2.41	0.50
1:D:57:ASP:O	1:C:61:TYR:HB2	2.10	0.50
1:A:331:CYS:HB2	1:A:416:LEU:HD12	1.94	0.50
1:A:62:GLU:HG3	1:A:64:GLU:N	2.26	0.50
1:A:295:VAL:HG22	1:A:446:ASN:OD1	2.12	0.50
1:D:295:VAL:HG22	1:D:446:ASN:OD1	2.12	0.49
1:D:331:CYS:HB2	1:D:416:LEU:HD12	1.94	0.49
1:C:295:VAL:HG22	1:C:446:ASN:OD1	2.12	0.49
1:D:279:ASN:HD21	1:D:281:ALA:HB3	1.76	0.49
1:C:331:CYS:HB2	1:C:416:LEU:HD12	1.94	0.49
1:A:86:LEU:HB2	1:A:242:VAL:HG23	1.95	0.49
1:B:295:VAL:HG22	1:B:446:ASN:OD1	2.12	0.49
1:D:84:MET:HB2	1:D:244:THR:CG2	2.43	0.48
1:B:341:THR:HB	1:B:342:LEU:HD12	1.95	0.48
1:B:84:MET:HB2	1:B:244:THR:CG2	2.44	0.48
1:A:422:GLN:OE1	1:A:438:PRO:HD3	2.13	0.48
1:B:338:TRP:O	1:B:342:LEU:CD1	2.55	0.48
1:C:84:MET:HB2	1:C:244:THR:CG2	2.44	0.48
1:C:422:GLN:OE1	1:C:438:PRO:HD3	2.13	0.48
1:D:86:LEU:HB2	1:D:242:VAL:HG23	1.95	0.48
1:D:341:THR:HB	1:D:342:LEU:HD12	1.95	0.48
1:B:338:TRP:NE1	1:B:342:LEU:HD22	2.29	0.48
1:C:417:GLN:OE1	1:C:417:GLN:HA	2.14	0.48
1:A:59:LYS:HB3	1:A:61:TYR:H	1.79	0.48
1:C:341:THR:HB	1:C:342:LEU:HD12	1.96	0.48
1:A:84:MET:HB2	1:A:244:THR:CG2	2.43	0.48
1:B:331:CYS:HB2	1:B:416:LEU:HD12	1.94	0.48
1:B:422:GLN:HG2	1:C:432:ARG:HH12	1.79	0.48
1:C:219:ALA:HB2	1:C:225:ILE:HG13	1.96	0.48
1:A:338:TRP:NE1	1:A:342:LEU:HD22	2.29	0.48
1:D:338:TRP:NE1	1:D:342:LEU:HD22	2.29	0.48
1:C:86:LEU:HB2	1:C:242:VAL:HG23	1.95	0.48
1:A:63:LYS:CD	4:A:618:HOH:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ALA:HB2	1:D:225:ILE:HG13	1.96	0.47
1:D:279:ASN:HD22	1:D:281:ALA:N	2.12	0.47
1:D:442:GLU:HB2	1:C:80:ASN:HD22	1.78	0.47
1:B:369:LEU:HD23	4:B:624:HOH:O	2.12	0.47
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.96	0.47
1:B:59:LYS:HB3	1:B:61:TYR:H	1.79	0.47
1:B:207:LYS:HD2	1:B:439:ILE:CG2	2.41	0.47
1:B:417:GLN:OE1	1:B:417:GLN:HA	2.14	0.47
1:D:422:GLN:OE1	1:D:438:PRO:HD3	2.14	0.47
1:B:219:ALA:HB2	1:B:225:ILE:HG13	1.96	0.47
1:B:422:GLN:OE1	1:B:438:PRO:HD3	2.13	0.47
1:D:109:ILE:O	1:D:113:ASP:HB2	2.15	0.47
1:B:279:ASN:HD22	1:B:281:ALA:N	2.12	0.47
1:A:84:MET:HB2	1:A:244:THR:HG22	1.96	0.47
1:D:291:SER:HB2	1:D:448:ASN:HB3	1.97	0.47
1:D:417:GLN:HA	1:D:417:GLN:OE1	2.14	0.47
1:C:59:LYS:HB3	1:C:61:TYR:H	1.79	0.47
1:D:202:THR:OG1	4:D:602:HOH:O	2.21	0.47
1:B:86:LEU:HB2	1:B:242:VAL:HG23	1.95	0.47
1:A:109:ILE:O	1:A:113:ASP:HB2	2.15	0.47
1:C:338:TRP:NE1	1:C:342:LEU:HD22	2.29	0.47
1:D:59:LYS:HB3	1:D:61:TYR:H	1.79	0.46
1:B:291:SER:HB2	1:B:448:ASN:HB3	1.97	0.46
1:C:109:ILE:O	1:C:113:ASP:HB2	2.15	0.46
1:B:84:MET:HB2	1:B:244:THR:HG22	1.96	0.46
1:A:291:SER:HB2	1:A:448:ASN:HB3	1.97	0.46
1:A:341:THR:HB	1:A:342:LEU:HD12	1.95	0.46
1:D:84:MET:HB2	1:D:244:THR:HG22	1.96	0.46
1:C:84:MET:HB2	1:C:244:THR:HG22	1.96	0.46
1:A:417:GLN:HA	1:A:417:GLN:OE1	2.14	0.46
1:C:279:ASN:HD22	1:C:281:ALA:N	2.12	0.46
1:C:291:SER:HB2	1:C:448:ASN:HB3	1.97	0.46
1:A:279:ASN:HD22	1:A:281:ALA:N	2.12	0.46
1:D:442:GLU:HB2	1:C:80:ASN:CB	2.46	0.46
1:B:109:ILE:O	1:B:113:ASP:HB2	2.15	0.46
1:C:207:LYS:HD2	1:C:439:ILE:CG2	2.41	0.46
1:C:91:GLU:HG3	1:C:92:ASN:H	1.81	0.45
1:C:339:ASN:ND2	2:C:508:NAG:C7	2.77	0.45
1:A:91:GLU:HG3	1:A:92:ASN:H	1.81	0.45
1:B:91:GLU:HG3	1:B:92:ASN:H	1.81	0.45
1:D:91:GLU:HG3	1:D:92:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:GLU:O	1:D:339:ASN:HB2	2.17	0.45
1:D:59:LYS:HB2	1:D:62:GLU:H	1.82	0.44
1:A:335:GLU:O	1:A:339:ASN:HB2	2.17	0.44
1:A:59:LYS:HB2	1:A:62:GLU:H	1.82	0.44
1:C:335:GLU:O	1:C:339:ASN:HB2	2.17	0.44
1:A:295:VAL:O	1:A:331:CYS:HA	2.18	0.44
1:A:337:LYS:HG2	4:A:632:HOH:O	2.16	0.44
1:A:338:TRP:CE2	1:A:342:LEU:CD2	3.01	0.44
1:A:297:THR:O	1:A:329:ALA:HB1	2.18	0.44
1:B:295:VAL:O	1:B:331:CYS:HA	2.18	0.44
1:B:335:GLU:O	1:B:339:ASN:HB2	2.17	0.44
1:D:295:VAL:O	1:D:331:CYS:HA	2.18	0.43
1:D:327:ARG:HG3	1:D:419:LYS:HE3	2.01	0.43
1:C:338:TRP:CE2	1:C:342:LEU:CD2	3.01	0.43
1:A:408:ARG:CZ	1:C:399:THR:OG1	2.63	0.43
2:A:505:NAG:C6	1:C:404:ASN:ND2	2.80	0.43
1:B:59:LYS:HB2	1:B:62:GLU:H	1.82	0.43
1:C:295:VAL:O	1:C:331:CYS:HA	2.18	0.43
1:D:338:TRP:CE2	1:D:342:LEU:CD2	3.01	0.43
1:C:91:GLU:HG3	1:C:92:ASN:N	2.34	0.43
1:B:338:TRP:CE2	1:B:342:LEU:CD2	3.01	0.43
1:C:327:ARG:HG3	1:C:419:LYS:HE3	2.01	0.43
1:D:91:GLU:HG3	1:D:92:ASN:N	2.34	0.43
1:A:91:GLU:HG3	1:A:92:ASN:N	2.34	0.43
1:D:297:THR:O	1:D:329:ALA:HB1	2.18	0.43
1:C:55:ALA:HA	1:C:75:VAL:O	2.19	0.43
1:A:90:THR:HA	1:A:239:CYS:O	2.19	0.43
1:C:59:LYS:HB2	1:C:62:GLU:H	1.83	0.43
1:B:386:ASN:O	1:B:416:LEU:HB3	2.19	0.42
1:D:251:ILE:HG12	1:D:482:GLU:HB3	2.02	0.42
1:B:55:ALA:HA	1:B:75:VAL:O	2.19	0.42
1:B:251:ILE:HG12	1:B:482:GLU:HB3	2.01	0.42
1:C:90:THR:HA	1:C:239:CYS:O	2.19	0.42
1:A:327:ARG:HG3	1:A:419:LYS:HE3	2.01	0.42
1:B:91:GLU:HG3	1:B:92:ASN:N	2.34	0.42
1:B:297:THR:O	1:B:329:ALA:HB1	2.18	0.42
1:C:297:THR:O	1:C:329:ALA:HB1	2.18	0.42
1:A:251:ILE:HG12	1:A:482:GLU:HB3	2.01	0.42
1:D:90:THR:HA	1:D:239:CYS:O	2.19	0.42
1:B:90:THR:HA	1:B:239:CYS:O	2.19	0.42
1:B:327:ARG:HG3	1:B:419:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:THR:C	1:C:342:LEU:HD12	2.45	0.42
1:A:55:ALA:HA	1:A:75:VAL:O	2.19	0.42
1:A:386:ASN:O	1:A:416:LEU:HB3	2.20	0.42
1:D:55:ALA:HA	1:D:75:VAL:O	2.19	0.42
1:B:59:LYS:N	1:B:59:LYS:CD	2.83	0.42
1:A:59:LYS:N	1:A:59:LYS:CD	2.83	0.42
1:C:59:LYS:N	1:C:59:LYS:CD	2.83	0.42
1:C:386:ASN:O	1:C:416:LEU:HB3	2.20	0.42
1:D:213:ILE:HG22	1:C:61:TYR:CZ	2.55	0.41
1:D:341:THR:C	1:D:342:LEU:HD12	2.45	0.41
1:D:386:ASN:O	1:D:416:LEU:HB3	2.20	0.41
4:D:656:HOH:O	1:C:61:TYR:HE2	2.03	0.41
1:C:421:LYS:HE3	1:C:421:LYS:HB3	1.87	0.41
1:D:480:ARG:NH1	4:D:603:HOH:O	2.22	0.41
1:C:251:ILE:HG12	1:C:482:GLU:HB3	2.01	0.41
1:C:251:ILE:HG23	1:C:482:GLU:HG3	2.03	0.41
1:D:54:CYS:HA	1:D:216:HIS:O	2.20	0.41
1:D:59:LYS:N	1:D:59:LYS:CD	2.83	0.41
1:B:341:THR:C	1:B:342:LEU:HD12	2.44	0.41
1:B:54:CYS:HA	1:B:216:HIS:O	2.21	0.41
1:D:282:LYS:HA	1:D:282:LYS:HD3	1.91	0.41
1:A:390:LEU:HD12	1:A:390:LEU:HA	1.90	0.41
1:C:279:ASN:ND2	1:C:281:ALA:HB3	2.36	0.41
1:C:381:GLU:OE1	1:C:381:GLU:HA	2.21	0.41
1:D:59:LYS:NZ	1:C:61:TYR:N	2.42	0.40
1:D:80:ASN:OD1	1:D:80:ASN:C	2.65	0.40
1:D:442:GLU:CB	1:C:80:ASN:HB2	2.51	0.40
1:A:80:ASN:OD1	1:A:80:ASN:C	2.65	0.40
1:A:381:GLU:OE1	1:A:381:GLU:HA	2.21	0.40
1:D:381:GLU:OE1	1:D:381:GLU:HA	2.21	0.40
1:D:205:CYS:HB2	4:D:624:HOH:O	2.21	0.40
1:B:381:GLU:OE1	1:B:381:GLU:HA	2.21	0.40
1:B:251:ILE:HG23	1:B:482:GLU:HG3	2.03	0.40
1:A:251:ILE:HG23	1:A:482:GLU:HG3	2.03	0.40
1:A:408:ARG:HH11	1:A:408:ARG:HD3	1.74	0.40
1:D:369:LEU:HD23	4:D:645:HOH:O	2.21	0.40

All (2) 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:A:94:ASN:ND2	2:D:506:NAG:O3[3_444]	1.64	0.56
1:D:356:SER:OG	1:B:356:SER:OG[3_454]	2.06	0.14

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/358 (92%)	312 (95%)	16 (5%)	1 (0%)	36	35
1	B	329/358 (92%)	312 (95%)	16 (5%)	1 (0%)	36	35
1	C	329/358 (92%)	312 (95%)	16 (5%)	1 (0%)	36	35
1	D	329/358 (92%)	312 (95%)	16 (5%)	1 (0%)	36	35
All	All	1316/1432 (92%)	1248 (95%)	64 (5%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/312 (95%)	297 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	297/312 (95%)	297 (100%)	0	100	100
1	C	297/312 (95%)	297 (100%)	0	100	100
1	D	297/312 (95%)	297 (100%)	0	100	100
All	All	1188/1248 (95%)	1188 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	279	ASN
1	A	404	ASN
1	A	411	ASN
1	D	72	HIS
1	D	279	ASN
1	D	339	ASN
1	D	411	ASN
1	B	72	HIS
1	B	279	ASN
1	B	280	ASN
1	B	339	ASN
1	B	411	ASN
1	C	80	ASN
1	C	279	ASN
1	C	404	ASN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	7IT	A	507	-	38,39,39	2.00	10 (26%)	43,54,54	1.56	8 (18%)
2	NAG	B	501	1	14,14,15	0.33	0	17,19,21	0.53	0
2	NAG	C	503	1	14,14,15	1.08	1 (7%)	17,19,21	0.89	0
2	NAG	A	505	1	14,14,15	0.53	0	17,19,21	0.58	0
2	NAG	B	502	1	14,14,15	0.38	0	17,19,21	0.74	1 (5%)
2	NAG	A	503	1	14,14,15	1.06	1 (7%)	17,19,21	0.89	0
2	NAG	C	504	1	14,14,15	0.68	1 (7%)	17,19,21	0.60	0
3	7IT	D	507	-	38,39,39	2.01	10 (26%)	43,54,54	1.55	9 (20%)
2	NAG	A	508	1	14,14,15	1.08	1 (7%)	17,19,21	0.83	0
2	NAG	D	505	1	14,14,15	0.52	0	17,19,21	0.58	0
2	NAG	A	502	1	14,14,15	0.37	0	17,19,21	0.73	1 (5%)
2	NAG	B	503	1	14,14,15	1.06	1 (7%)	17,19,21	0.89	0
2	NAG	A	504	1	14,14,15	0.69	1 (7%)	17,19,21	0.60	0
2	NAG	A	501	1	14,14,15	0.32	0	17,19,21	0.53	0
2	NAG	A	506	1	14,14,15	0.75	1 (7%)	17,19,21	2.00	2 (11%)
2	NAG	C	508	1	14,14,15	1.64	2 (14%)	17,19,21	0.71	0
3	7IT	C	507	-	38,39,39	2.01	10 (26%)	43,54,54	1.56	8 (18%)
2	NAG	B	504	1	14,14,15	0.69	1 (7%)	17,19,21	0.60	0
2	NAG	C	502	1	14,14,15	0.36	0	17,19,21	0.74	1 (5%)
3	7IT	B	507	-	38,39,39	2.01	10 (26%)	43,54,54	1.56	8 (18%)
2	NAG	D	502	1	14,14,15	0.37	0	17,19,21	0.73	1 (5%)
2	NAG	C	501	1	14,14,15	0.33	0	17,19,21	0.53	0
2	NAG	D	503	1	14,14,15	1.05	1 (7%)	17,19,21	0.89	0
2	NAG	B	506	1	14,14,15	0.73	0	17,19,21	2.01	2 (11%)
2	NAG	D	506	1	14,14,15	0.74	1 (7%)	17,19,21	2.00	2 (11%)
2	NAG	C	505	1	14,14,15	0.54	0	17,19,21	0.58	0
2	NAG	C	506	1	14,14,15	0.75	1 (7%)	17,19,21	2.00	2 (11%)

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	0.52	0	17,19,21	0.57	0
2	NAG	D	501	1	14,14,15	0.32	0	17,19,21	0.53	0
2	NAG	D	504	1	14,14,15	0.69	1 (7%)	17,19,21	0.60	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
3	7IT	A	507	-	-	5/27/43/43	0/3/3/3
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	503	1	-	2/6/23/26	0/1/1/1
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	503	1	-	2/6/23/26	0/1/1/1
2	NAG	C	504	1	-	2/6/23/26	0/1/1/1
3	7IT	D	507	-	-	5/27/43/43	0/3/3/3
2	NAG	A	508	1	-	2/6/23/26	0/1/1/1
2	NAG	D	505	1	-	2/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	2/6/23/26	0/1/1/1
2	NAG	A	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	506	1	-	2/6/23/26	0/1/1/1
2	NAG	C	508	1	-	2/6/23/26	0/1/1/1
3	7IT	C	507	-	-	5/27/43/43	0/3/3/3
2	NAG	B	504	1	-	2/6/23/26	0/1/1/1
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	7IT	B	507	-	-	5/27/43/43	0/3/3/3
2	NAG	D	502	1	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	503	1	-	2/6/23/26	0/1/1/1
2	NAG	B	506	1	-	2/6/23/26	0/1/1/1
2	NAG	D	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	C	506	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	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	504	1	-	2/6/23/26	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	507	7IT	C02-N03	6.29	1.45	1.33
3	B	507	7IT	C02-N03	6.28	1.45	1.33
3	A	507	7IT	C02-N03	6.26	1.45	1.33
3	D	507	7IT	C02-N03	6.26	1.45	1.33
2	C	508	NAG	O5-C1	5.58	1.53	1.43
3	D	507	7IT	C15-N14	4.54	1.43	1.34
3	B	507	7IT	C15-N14	4.53	1.43	1.34
3	A	507	7IT	C15-N14	4.50	1.43	1.34
3	C	507	7IT	C15-N14	4.49	1.43	1.34
3	D	507	7IT	C17-N19	3.93	1.43	1.35
3	C	507	7IT	C17-N19	3.92	1.43	1.35
3	B	507	7IT	C17-N19	3.92	1.43	1.35
3	A	507	7IT	C17-N19	3.92	1.43	1.35
2	A	508	NAG	C1-C2	3.68	1.57	1.52
3	D	507	7IT	C02-N01	3.47	1.44	1.32
3	A	507	7IT	C02-N01	3.47	1.44	1.32
3	B	507	7IT	C02-N01	3.46	1.44	1.32
3	C	507	7IT	C02-N01	3.45	1.44	1.32
2	C	503	NAG	C1-C2	3.36	1.56	1.52
2	B	503	NAG	C1-C2	3.32	1.56	1.52
2	A	503	NAG	C1-C2	3.30	1.56	1.52
3	B	507	7IT	C07-C06	3.29	1.56	1.51
3	D	507	7IT	C07-C06	3.29	1.56	1.51
3	A	507	7IT	C07-C06	3.28	1.55	1.51
2	D	503	NAG	C1-C2	3.27	1.56	1.52
3	C	507	7IT	C07-C06	3.26	1.55	1.51
3	B	507	7IT	O16-C15	-2.92	1.18	1.23
3	D	507	7IT	O16-C15	-2.91	1.18	1.23
3	C	507	7IT	O16-C15	-2.90	1.18	1.23
3	A	507	7IT	O16-C15	-2.90	1.18	1.23
3	C	507	7IT	C06-C05	-2.55	1.51	1.55
3	D	507	7IT	C06-C05	-2.55	1.51	1.55
3	B	507	7IT	C06-C05	-2.51	1.51	1.55
3	A	507	7IT	C06-C05	-2.50	1.51	1.55
3	C	507	7IT	C24-CL25	2.44	1.79	1.73
3	B	507	7IT	C24-CL25	2.42	1.79	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	7IT	C24-CL25	2.41	1.79	1.73
3	D	507	7IT	C24-CL25	2.40	1.79	1.73
2	D	504	NAG	O5-C1	2.28	1.47	1.43
2	A	504	NAG	O5-C1	2.27	1.47	1.43
2	B	504	NAG	O5-C1	2.27	1.47	1.43
2	C	504	NAG	O5-C1	2.23	1.47	1.43
3	B	507	7IT	O18-C17	-2.21	1.19	1.23
2	C	508	NAG	C1-C2	2.20	1.55	1.52
3	C	507	7IT	O18-C17	-2.20	1.19	1.23
3	D	507	7IT	O18-C17	-2.18	1.19	1.23
3	A	507	7IT	O18-C17	-2.18	1.19	1.23
3	B	507	7IT	C02-N28	-2.10	1.26	1.34
3	A	507	7IT	C02-N28	-2.09	1.26	1.34
3	C	507	7IT	C02-N28	-2.09	1.26	1.34
3	D	507	7IT	C02-N28	-2.08	1.26	1.34
2	C	506	NAG	O5-C1	2.07	1.47	1.43
2	A	506	NAG	O5-C1	2.07	1.47	1.43
2	D	506	NAG	O5-C1	2.03	1.47	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	506	NAG	C1-O5-C5	7.36	122.05	112.19
2	A	506	NAG	C1-O5-C5	7.34	122.02	112.19
2	D	506	NAG	C1-O5-C5	7.34	122.02	112.19
2	C	506	NAG	C1-O5-C5	7.33	122.01	112.19
3	C	507	7IT	C20-N19-C17	-3.55	121.14	127.45
3	D	507	7IT	C20-N19-C17	-3.55	121.15	127.45
3	A	507	7IT	C20-N19-C17	-3.54	121.17	127.45
3	B	507	7IT	C20-N19-C17	-3.54	121.17	127.45
3	B	507	7IT	C12-C13-N14	-3.35	104.99	114.77
3	C	507	7IT	C12-C13-N14	-3.34	104.99	114.77
3	A	507	7IT	C12-C13-N14	-3.34	105.00	114.77
3	D	507	7IT	C12-C13-N14	-3.34	105.01	114.77
3	A	507	7IT	C15-C17-N19	2.69	116.78	112.25
3	C	507	7IT	C15-C17-N19	2.67	116.76	112.25
3	B	507	7IT	C15-C17-N19	2.67	116.75	112.25
3	D	507	7IT	C15-C17-N19	2.67	116.75	112.25
3	B	507	7IT	C12-C13-C05	2.35	106.99	104.03
3	A	507	7IT	C12-C13-C05	2.34	106.98	104.03
2	C	502	NAG	C1-O5-C5	2.33	115.31	112.19
3	D	507	7IT	C12-C13-C05	2.33	106.96	104.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	507	7IT	C12-C13-C05	2.32	106.94	104.03
2	A	502	NAG	C1-O5-C5	2.32	115.29	112.19
3	C	507	7IT	C22-C24-CL25	-2.31	116.87	119.79
2	B	502	NAG	C1-O5-C5	2.31	115.28	112.19
2	D	502	NAG	C1-O5-C5	2.30	115.27	112.19
3	C	507	7IT	C08-C07-C12	-2.29	118.60	121.37
3	B	507	7IT	C22-C24-CL25	-2.28	116.91	119.79
3	A	507	7IT	C22-C24-CL25	-2.28	116.91	119.79
3	D	507	7IT	C22-C24-CL25	-2.28	116.92	119.79
3	A	507	7IT	C08-C07-C12	-2.26	118.64	121.37
3	D	507	7IT	C08-C07-C12	-2.25	118.65	121.37
3	B	507	7IT	C08-C07-C12	-2.23	118.68	121.37
2	A	506	NAG	C3-C4-C5	2.22	114.26	110.23
2	D	506	NAG	C3-C4-C5	2.21	114.25	110.23
2	B	506	NAG	C3-C4-C5	2.21	114.24	110.23
2	C	506	NAG	C3-C4-C5	2.20	114.22	110.23
3	B	507	7IT	C07-C08-C09	-2.13	119.78	122.01
3	D	507	7IT	C07-C08-C09	-2.12	119.79	122.01
3	A	507	7IT	C07-C08-C09	-2.10	119.81	122.01
3	D	507	7IT	C26-C24-CL25	2.10	122.56	118.42
3	C	507	7IT	C07-C08-C09	-2.09	119.82	122.01
3	C	507	7IT	C26-C24-CL25	2.09	122.55	118.42
3	A	507	7IT	C26-C24-CL25	2.09	122.54	118.42
3	B	507	7IT	C26-C24-CL25	2.08	122.52	118.42
3	D	507	7IT	F23-C22-C24	-2.00	116.54	118.96

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	507	7IT	C09-C00-N-C
3	A	507	7IT	C31-C32-C33-C34
3	D	507	7IT	C09-C00-N-C
3	D	507	7IT	C31-C32-C33-C34
3	B	507	7IT	C09-C00-N-C
3	B	507	7IT	C31-C32-C33-C34
3	C	507	7IT	C09-C00-N-C
3	C	507	7IT	C31-C32-C33-C34
2	A	505	NAG	O5-C5-C6-O6
2	D	505	NAG	O5-C5-C6-O6
2	B	505	NAG	O5-C5-C6-O6
2	C	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	504	NAG	O5-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	B	504	NAG	O5-C5-C6-O6
2	C	504	NAG	O5-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	B	505	NAG	C4-C5-C6-O6
2	C	505	NAG	C4-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	B	506	NAG	C4-C5-C6-O6
2	C	506	NAG	C4-C5-C6-O6
2	A	504	NAG	C4-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6
2	B	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	A	503	NAG	O5-C5-C6-O6
2	D	503	NAG	O5-C5-C6-O6
2	B	503	NAG	O5-C5-C6-O6
2	C	503	NAG	O5-C5-C6-O6
2	A	503	NAG	C4-C5-C6-O6
2	D	503	NAG	C4-C5-C6-O6
2	B	503	NAG	C4-C5-C6-O6
2	C	503	NAG	C4-C5-C6-O6
3	A	507	7IT	C32-C33-C34-O32
3	D	507	7IT	C32-C33-C34-O32
3	B	507	7IT	C32-C33-C34-O32
3	C	507	7IT	C32-C33-C34-O32
2	A	506	NAG	O5-C5-C6-O6
2	D	506	NAG	O5-C5-C6-O6
2	B	506	NAG	O5-C5-C6-O6
2	C	506	NAG	O5-C5-C6-O6
3	A	507	7IT	C31-C32-C33-O31
3	B	507	7IT	C31-C32-C33-O31
3	C	507	7IT	C31-C32-C33-O31
3	D	507	7IT	C31-C32-C33-O31
3	A	507	7IT	O31-C33-C34-O32
3	D	507	7IT	O31-C33-C34-O32

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Mol	Chain	Res	Type	Atoms
3	B	507	7IT	O31-C33-C34-O32
3	C	507	7IT	O31-C33-C34-O32

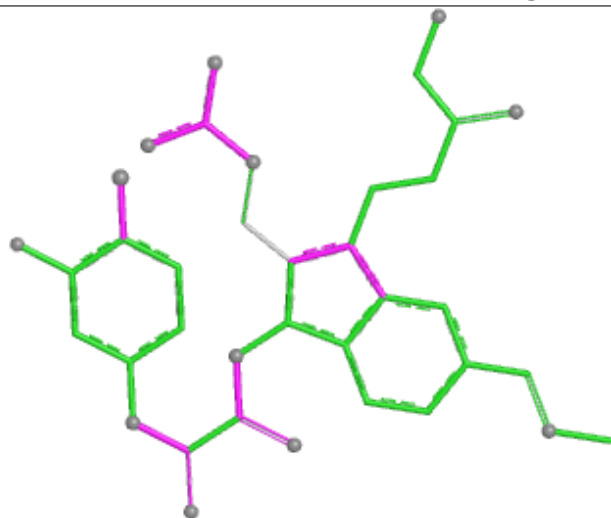
There are no ring outliers.

4 monomers are involved in 8 short contacts:

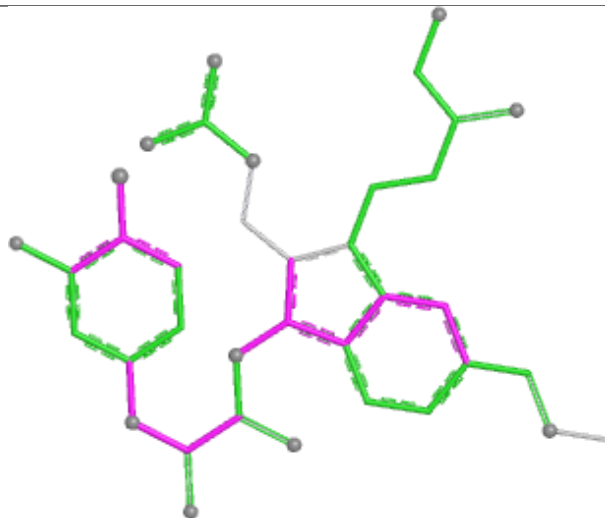
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	NAG	4	0
2	C	508	NAG	2	0
2	D	506	NAG	0	1
2	C	505	NAG	1	0

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

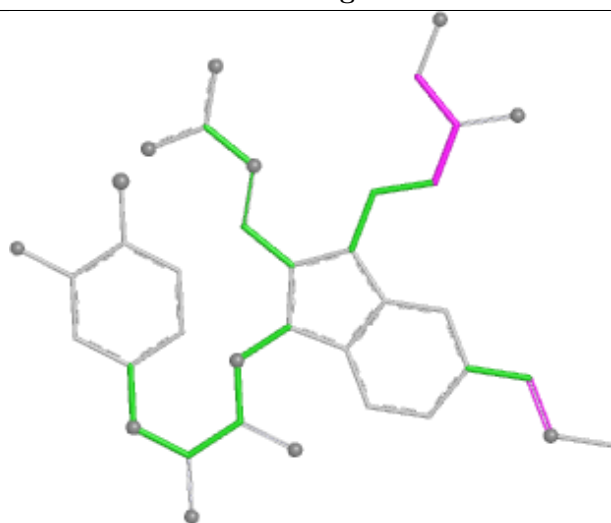
Ligand 7IT A 507



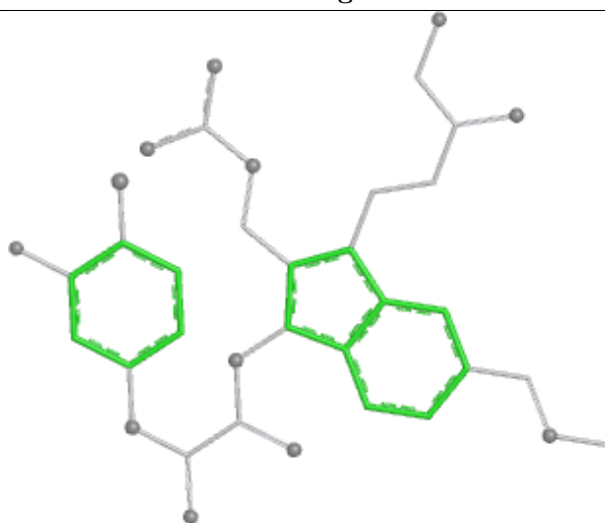
Bond lengths



Bond angles

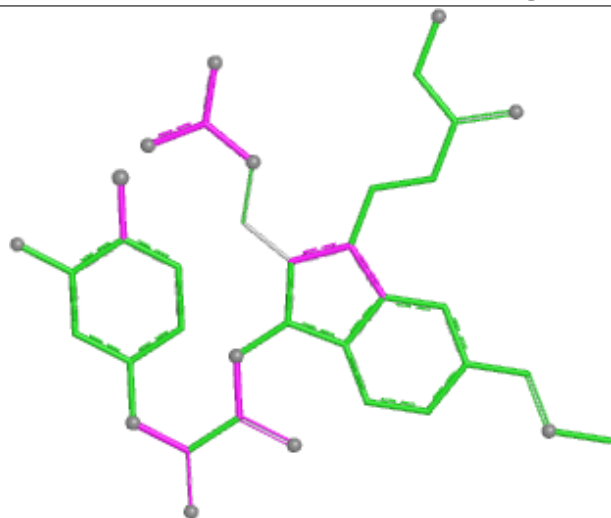


Torsions

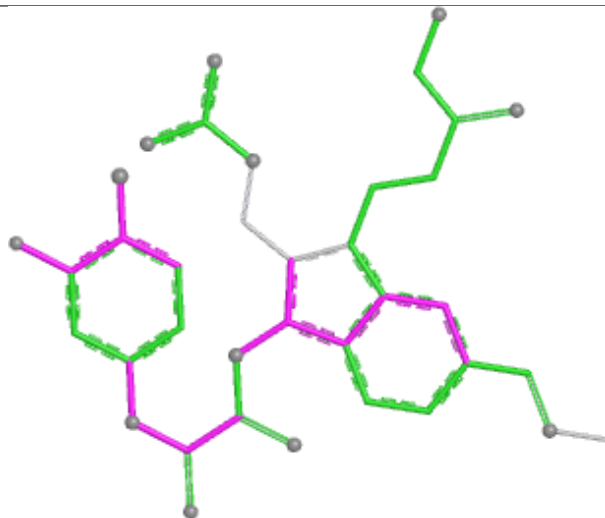


Rings

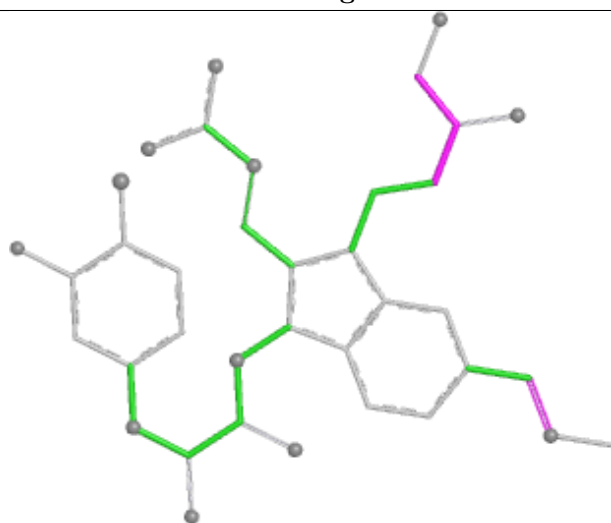
Ligand 7IT D 507



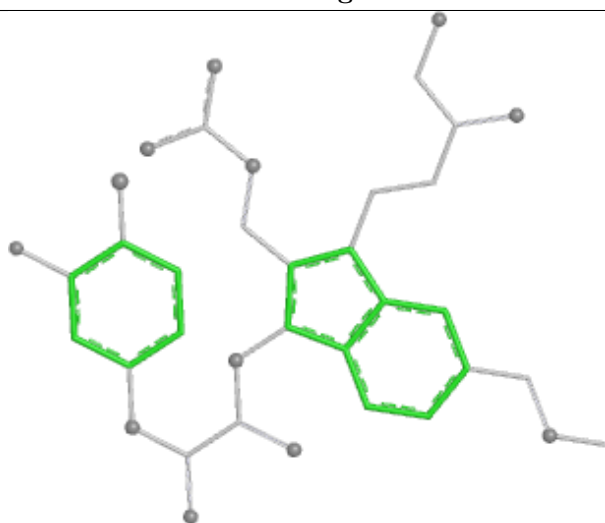
Bond lengths



Bond angles

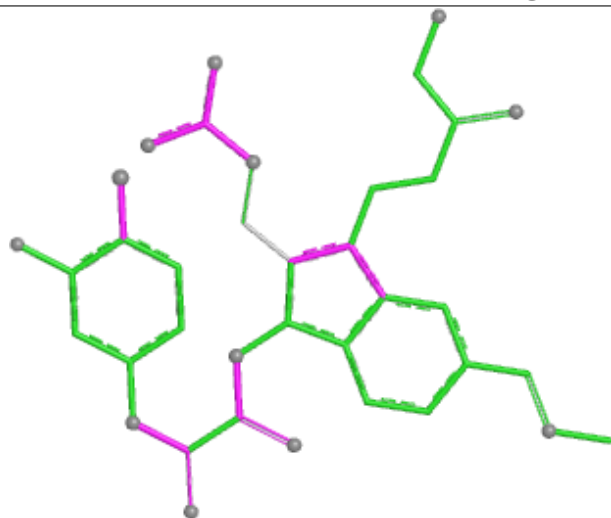


Torsions

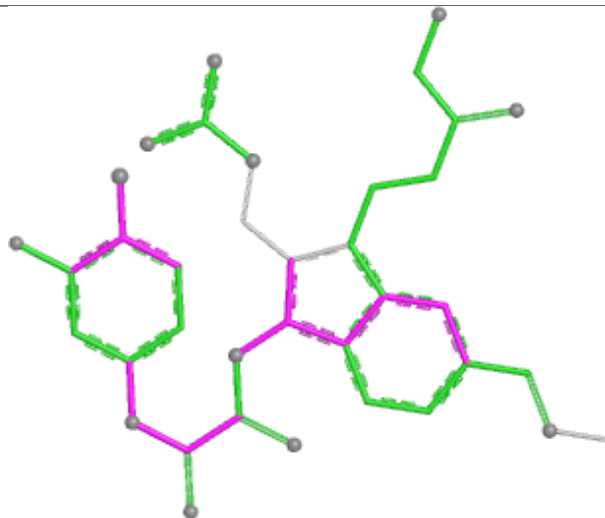


Rings

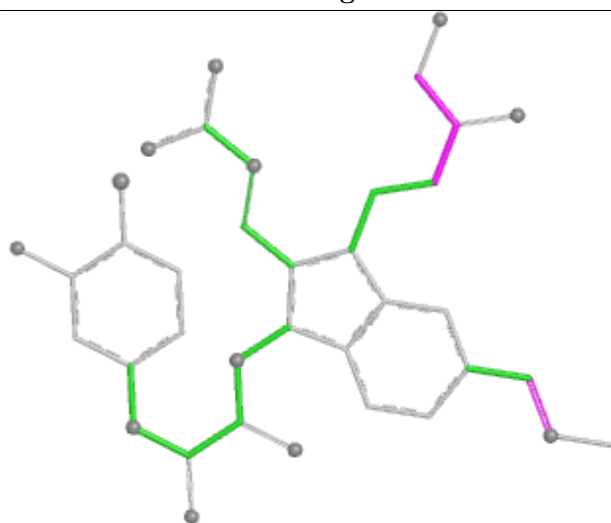
Ligand 7IT C 507



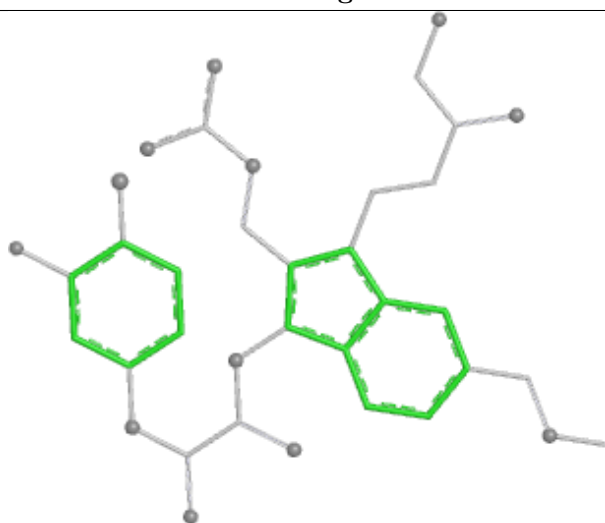
Bond lengths



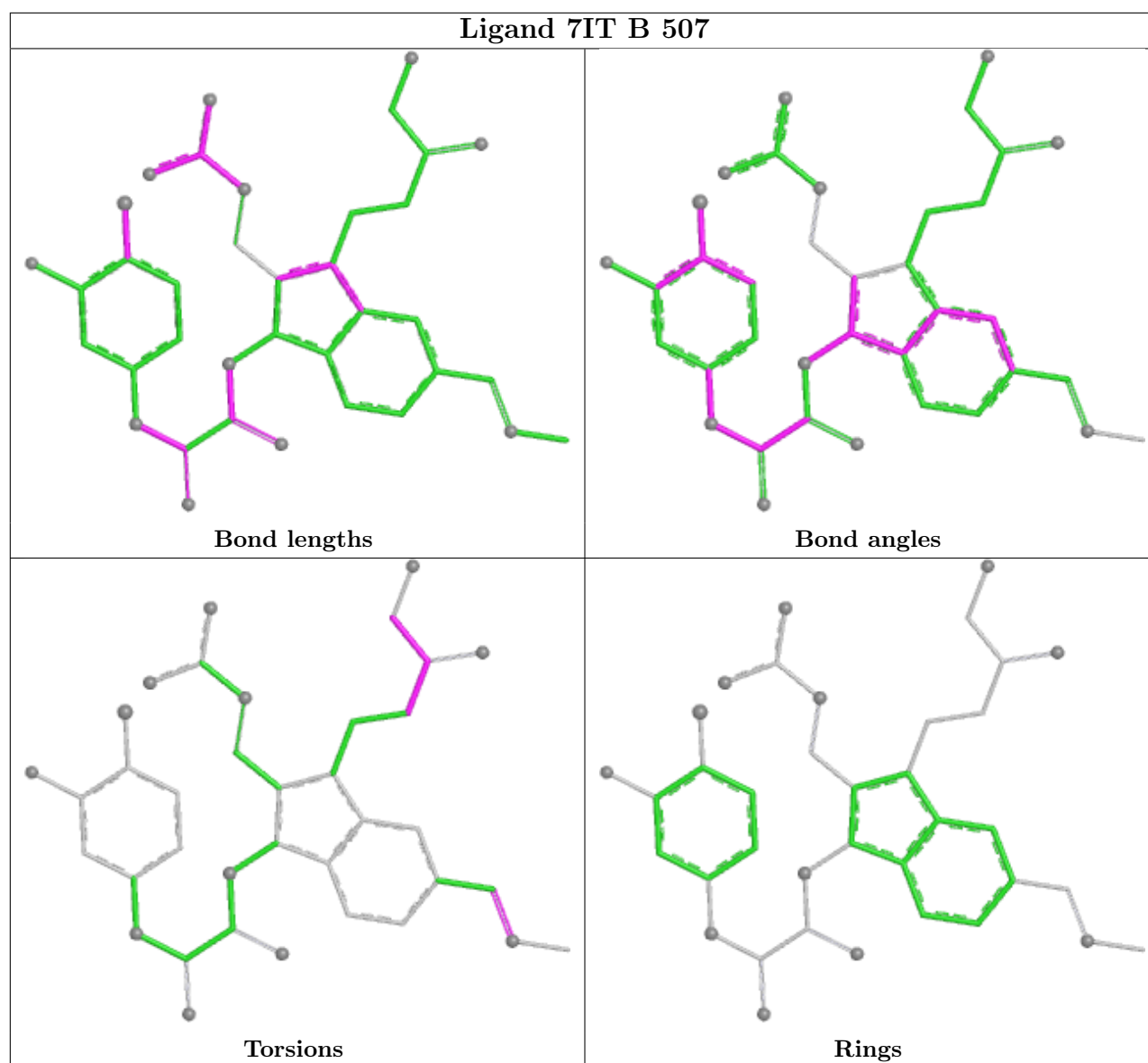
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/358 (93%)	1.17	66 (19%) 3 3	24, 41, 62, 86	0
1	B	335/358 (93%)	1.59	106 (31%) 1 1	24, 41, 62, 86	0
1	C	335/358 (93%)	1.70	102 (30%) 1 1	24, 41, 62, 86	0
1	D	335/358 (93%)	1.65	106 (31%) 1 1	24, 41, 62, 86	0
All	All	1340/1432 (93%)	1.53	380 (28%) 1 1	24, 41, 63, 86	0

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	TYR	12.8
1	C	60	ALA	12.5
1	C	198	GLY	10.5
1	C	124	GLY	8.9
1	B	89	VAL	8.2
1	C	87	ALA	7.5
1	C	122	LEU	6.9
1	A	198	GLY	6.8
1	C	80	ASN	6.7
1	D	89	VAL	6.7
1	D	124	GLY	6.5
1	C	59	LYS	6.4
1	A	87	ALA	6.3
1	A	86	LEU	6.2
1	D	59	LYS	6.2
1	C	408	ARG	6.1
1	C	89	VAL	6.0
1	D	61	TYR	5.9
1	B	87	ALA	5.9
1	A	63	LYS	5.9
1	C	63	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	356	SER	5.6
1	B	60	ALA	5.6
1	D	63	LYS	5.6
1	D	326	ILE	5.5
1	C	202	THR	5.4
1	D	87	ALA	5.4
1	D	84	MET	5.4
1	B	49	LYS	5.3
1	B	72	HIS	5.3
1	B	356	SER	5.2
1	C	85	VAL	5.1
1	C	86	LEU	5.0
1	D	60	ALA	5.0
1	B	84	MET	4.9
1	C	88	ASN	4.9
1	A	61	TYR	4.8
1	A	89	VAL	4.8
1	C	240	ARG	4.8
1	C	84	MET	4.8
1	D	88	ASN	4.7
1	C	123	THR	4.7
1	B	489	VAL	4.6
1	C	199	SER	4.6
1	B	396	ARG	4.5
1	B	342	LEU	4.5
1	A	408	ARG	4.4
1	C	356	SER	4.4
1	C	396	ARG	4.4
1	A	202	THR	4.3
1	B	63	LYS	4.3
1	B	85	VAL	4.3
1	C	49	LYS	4.3
1	A	396	ARG	4.3
1	B	88	ASN	4.3
1	D	358	THR	4.2
1	C	358	THR	4.2
1	D	342	LEU	4.2
1	A	267	GLU	4.2
1	B	358	THR	4.2
1	C	62	GLU	4.1
1	C	90	THR	4.1
1	C	200	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	124	GLY	4.1
1	B	86	LEU	4.1
1	D	267	GLU	4.1
1	B	432	ARG	4.0
1	D	300	ASN	4.0
1	B	242	VAL	4.0
1	B	240	ARG	4.0
1	A	356	SER	4.0
1	D	49	LYS	4.0
1	D	86	LEU	3.9
1	C	57	ASP	3.9
1	D	90	THR	3.9
1	B	61	TYR	3.9
1	D	396	ARG	3.9
1	C	357	LYS	3.9
1	C	244	THR	3.9
1	C	406	THR	3.8
1	C	114	GLU	3.8
1	D	202	THR	3.8
1	B	357	LYS	3.8
1	C	79	PRO	3.8
1	B	408	ARG	3.8
1	D	341	THR	3.7
1	D	404	ASN	3.7
1	C	489	VAL	3.7
1	D	72	HIS	3.7
1	D	440	GLU	3.6
1	C	82	GLN	3.6
1	C	201	ILE	3.6
1	B	81	PRO	3.6
1	D	441	GLY	3.6
1	A	379	ARG	3.6
1	D	85	VAL	3.6
1	B	220	PRO	3.6
1	A	354	PRO	3.6
1	D	369	LEU	3.6
1	C	268	GLU	3.6
1	C	440	GLU	3.5
1	B	55	ALA	3.5
1	B	422	GLN	3.5
1	A	85	VAL	3.5
1	B	97	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	201	ILE	3.5
1	D	337	LYS	3.5
1	A	300	ASN	3.5
1	D	201	ILE	3.4
1	C	81	PRO	3.4
1	C	339	ASN	3.4
1	B	57	ASP	3.4
1	B	464	ASP	3.4
1	C	113	ASP	3.4
1	C	368	ASP	3.4
1	D	242	VAL	3.4
1	D	465	THR	3.4
1	D	198	GLY	3.4
1	D	221	ALA	3.4
1	D	279	ASN	3.3
1	C	327	ARG	3.3
1	B	83	GLU	3.3
1	D	357	LYS	3.3
1	D	432	ARG	3.3
1	A	358	THR	3.3
1	A	90	THR	3.3
1	B	50	THR	3.3
1	A	88	ASN	3.3
1	C	457	ASP	3.3
1	C	336	SER	3.2
1	B	222	GLY	3.2
1	B	264	SER	3.2
1	A	488	VAL	3.2
1	B	300	ASN	3.2
1	B	246	GLN	3.2
1	D	408	ARG	3.2
1	A	489	VAL	3.2
1	D	57	ASP	3.2
1	B	399	THR	3.2
1	D	488	VAL	3.1
1	B	226	LEU	3.1
1	B	439	ILE	3.1
1	B	202	THR	3.1
1	A	397	ASN	3.1
1	D	246	GLN	3.1
1	C	342	LEU	3.1
1	D	405	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	49	LYS	3.1
1	B	417	GLN	3.1
1	A	442	GLU	3.1
1	B	442	GLU	3.1
1	C	397	ASN	3.1
1	D	97	LYS	3.0
1	B	243	SER	3.0
1	A	339	ASN	3.0
1	C	325	ASN	3.0
1	D	406	THR	3.0
1	B	354	PRO	3.0
1	B	490	GLU	3.0
1	C	379	ARG	3.0
1	A	440	GLU	3.0
1	B	465	THR	3.0
1	D	76	PRO	3.0
1	B	59	LYS	3.0
1	D	281	ALA	3.0
1	D	122	LEU	3.0
1	D	339	ASN	3.0
1	D	71	THR	3.0
1	C	51	THR	3.0
1	C	326	ILE	2.9
1	B	231	LYS	2.9
1	A	399	THR	2.9
1	D	81	PRO	2.9
1	D	354	PRO	2.9
1	C	354	PRO	2.9
1	C	106	GLU	2.9
1	A	199	SER	2.9
1	D	293	ASN	2.9
1	B	79	PRO	2.9
1	D	240	ARG	2.9
1	A	268	GLU	2.9
1	D	94	ASN	2.9
1	C	300	ASN	2.9
1	C	404	ASN	2.9
1	B	221	ALA	2.9
1	D	412	GLY	2.9
1	A	72	HIS	2.9
1	C	439	ILE	2.9
1	C	442	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	397	ASN	2.9
1	B	124	GLY	2.9
1	A	59	LYS	2.8
1	B	404	ASN	2.8
1	C	365	SER	2.8
1	A	60	ALA	2.8
1	A	406	THR	2.8
1	D	79	PRO	2.8
1	D	403	TYR	2.8
1	A	342	LEU	2.8
1	C	399	THR	2.8
1	C	242	VAL	2.8
1	C	72	HIS	2.8
1	A	226	LEU	2.8
1	D	278	THR	2.8
1	B	90	THR	2.8
1	B	337	LYS	2.8
1	C	337	LYS	2.8
1	A	228	CYS	2.8
1	B	62	GLU	2.7
1	C	488	VAL	2.7
1	B	411	ASN	2.7
1	D	82	GLN	2.7
1	B	280	ASN	2.7
1	C	411	ASN	2.7
1	A	404	ASN	2.7
1	A	490	GLU	2.7
1	C	94	ASN	2.7
1	B	457	ASP	2.7
1	B	198	GLY	2.7
1	A	417	GLN	2.6
1	D	83	GLU	2.6
1	C	413	THR	2.6
1	B	279	ASN	2.6
1	B	340	ASN	2.6
1	A	365	SER	2.6
1	C	99	ASP	2.6
1	C	464	ASP	2.6
1	C	75	VAL	2.6
1	A	240	ARG	2.6
1	C	417	GLN	2.6
1	A	50	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	244	THR	2.6
1	A	411	ASN	2.6
1	D	244	THR	2.6
1	B	406	THR	2.6
1	B	277	LEU	2.6
1	B	353	PHE	2.6
1	C	115	SER	2.6
1	B	359	ILE	2.6
1	B	488	VAL	2.6
1	C	203	GLN	2.6
1	D	442	GLU	2.6
1	B	440	GLU	2.6
1	D	397	ASN	2.6
1	B	436	ALA	2.6
1	A	84	MET	2.6
1	B	73	ALA	2.6
1	C	71	THR	2.6
1	A	99	ASP	2.6
1	C	243	SER	2.6
1	B	82	GLN	2.5
1	C	267	GLU	2.5
1	D	245	VAL	2.5
1	B	326	ILE	2.5
1	A	395	TYR	2.5
1	D	340	ASN	2.5
1	D	411	ASN	2.5
1	D	51	THR	2.5
1	A	410	SER	2.5
1	B	365	SER	2.5
1	C	328	GLN	2.5
1	A	201	ILE	2.5
1	B	443	ILE	2.5
1	A	80	ASN	2.5
1	A	57	ASP	2.5
1	D	236	THR	2.5
1	C	73	ALA	2.5
1	D	80	ASN	2.5
1	B	80	ASN	2.5
1	B	297	THR	2.5
1	D	222	GLY	2.5
1	C	275	GLU	2.4
1	D	199	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	336	SER	2.4
1	B	51	THR	2.4
1	C	410	SER	2.4
1	B	219	ALA	2.4
1	B	52	LEU	2.4
1	D	62	GLU	2.4
1	D	345	VAL	2.4
1	D	464	ASP	2.4
1	C	78	ASP	2.4
1	D	50	THR	2.4
1	B	76	PRO	2.4
1	C	221	ALA	2.4
1	D	52	LEU	2.4
1	C	340	ASN	2.4
1	A	225	ILE	2.4
1	A	239	CYS	2.4
1	B	487	LYS	2.4
1	C	259	LEU	2.4
1	D	391	PHE	2.4
1	C	264	SER	2.4
1	A	71	THR	2.4
1	D	204	ALA	2.3
1	B	224	ALA	2.3
1	B	281	ALA	2.3
1	D	416	LEU	2.3
1	B	407	GLY	2.3
1	D	225	ILE	2.3
1	B	364	SER	2.3
1	D	77	THR	2.3
1	C	293	ASN	2.3
1	A	464	ASP	2.3
1	D	269	GLU	2.3
1	B	267	GLU	2.3
1	A	278	THR	2.3
1	B	71	THR	2.3
1	A	366	GLY	2.3
1	B	379	ARG	2.3
1	D	344	LYS	2.3
1	B	290	GLU	2.3
1	D	343	GLN	2.3
1	C	225	ILE	2.3
1	D	489	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	123	THR	2.3
1	D	231	LYS	2.3
1	D	277	LEU	2.3
1	B	275	GLU	2.2
1	D	209	SER	2.2
1	D	417	GLN	2.2
1	D	443	ILE	2.2
1	C	344	LYS	2.2
1	C	224	ALA	2.2
1	B	369	LEU	2.2
1	D	275	GLU	2.2
1	C	269	GLU	2.2
1	C	246	GLN	2.2
1	A	340	ASN	2.2
1	D	224	ALA	2.2
1	B	106	GLU	2.2
1	C	219	ALA	2.2
1	D	446	ASN	2.2
1	B	339	ASN	2.2
1	D	399	THR	2.2
1	B	77	THR	2.2
1	B	236	THR	2.2
1	A	62	GLU	2.2
1	B	269	GLU	2.2
1	B	218	CYS	2.2
1	D	395	TYR	2.2
1	A	325	ASN	2.2
1	A	413	THR	2.2
1	D	457	ASP	2.2
1	B	341	THR	2.2
1	C	83	GLU	2.1
1	C	409	SER	2.1
1	D	99	ASP	2.1
1	D	268	GLU	2.1
1	B	223	PHE	2.1
1	D	73	ALA	2.1
1	D	226	LEU	2.1
1	C	277	LEU	2.1
1	B	378	CYS	2.1
1	C	236	THR	2.1
1	A	412	GLY	2.1
1	A	68	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	265	LEU	2.1
1	C	209	SER	2.1
1	B	276	ASN	2.1
1	C	241	ASN	2.1
1	A	422	GLN	2.1
1	C	50	THR	2.1
1	C	238	PRO	2.1
1	C	117	LYS	2.1
1	A	200	ALA	2.1
1	D	288	LEU	2.0
1	C	226	LEU	2.0
1	B	113	ASP	2.0
1	D	379	ARG	2.0
1	C	403	TYR	2.0
1	A	83	GLU	2.0
1	D	65	VAL	2.0
1	D	361	PHE	2.0
1	B	75	VAL	2.0
1	B	410	SER	2.0
1	B	122	LEU	2.0
1	C	228	CYS	2.0
1	D	117	LYS	2.0
1	B	437	PRO	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.

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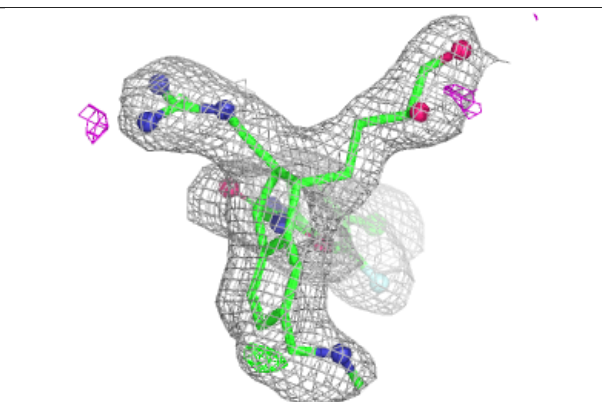
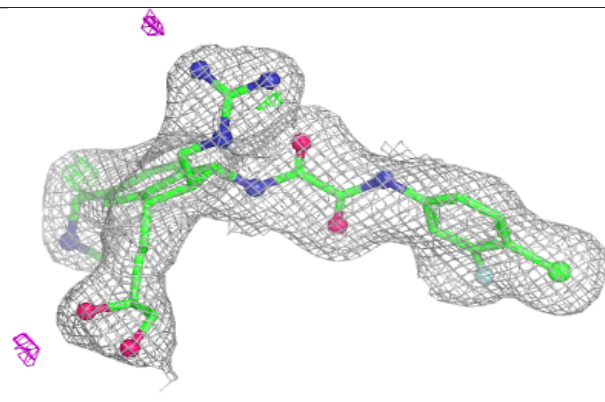
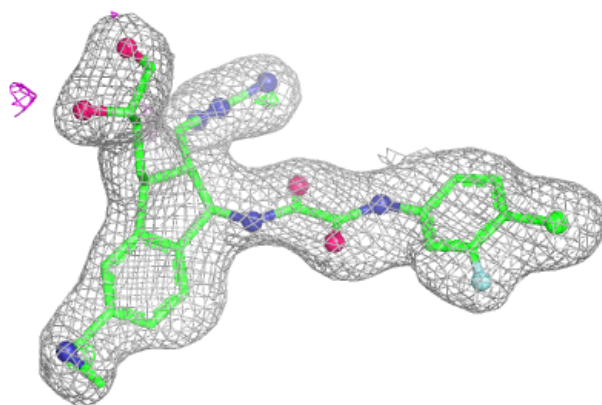
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	506	14/15	0.56	0.37	59,93,102,120	0
2	NAG	B	506	14/15	0.62	0.38	59,93,102,120	0
2	NAG	A	506	14/15	0.63	0.23	59,93,102,120	0
2	NAG	C	506	14/15	0.63	0.28	59,93,102,120	0
2	NAG	D	503	14/15	0.64	0.19	45,50,60,65	0
2	NAG	B	503	14/15	0.66	0.21	45,50,60,65	0
2	NAG	B	501	14/15	0.70	0.18	39,55,68,78	0
2	NAG	D	505	14/15	0.70	0.14	33,40,55,55	0
2	NAG	D	501	14/15	0.71	0.17	39,55,68,78	0
2	NAG	C	503	14/15	0.75	0.17	45,50,60,65	0
2	NAG	C	508	14/15	0.76	0.15	50,56,61,63	0
2	NAG	A	508	14/15	0.77	0.16	44,54,60,69	0
2	NAG	A	501	14/15	0.78	0.14	39,55,68,78	0
2	NAG	D	504	14/15	0.78	0.14	42,51,60,67	0
2	NAG	B	504	14/15	0.78	0.14	42,51,60,67	0
2	NAG	B	505	14/15	0.78	0.13	33,40,55,55	0
2	NAG	C	501	14/15	0.80	0.18	39,55,68,78	0
2	NAG	A	503	14/15	0.81	0.16	45,50,60,65	0
2	NAG	C	504	14/15	0.82	0.14	42,51,60,67	0
2	NAG	A	504	14/15	0.83	0.11	42,51,60,67	0
2	NAG	C	505	14/15	0.83	0.13	33,40,55,55	0
2	NAG	C	502	14/15	0.85	0.12	22,33,42,43	0
2	NAG	A	505	14/15	0.86	0.14	33,40,55,55	0
2	NAG	A	502	14/15	0.86	0.12	22,33,42,43	0
2	NAG	B	502	14/15	0.88	0.09	22,33,42,43	0
2	NAG	D	502	14/15	0.88	0.11	22,33,42,43	0
3	7IT	B	507	37/37	0.93	0.10	21,29,45,59	0
3	7IT	D	507	37/37	0.94	0.09	21,29,45,59	0
3	7IT	C	507	37/37	0.94	0.09	21,29,45,59	0
3	7IT	A	507	37/37	0.95	0.09	21,29,45,59	0

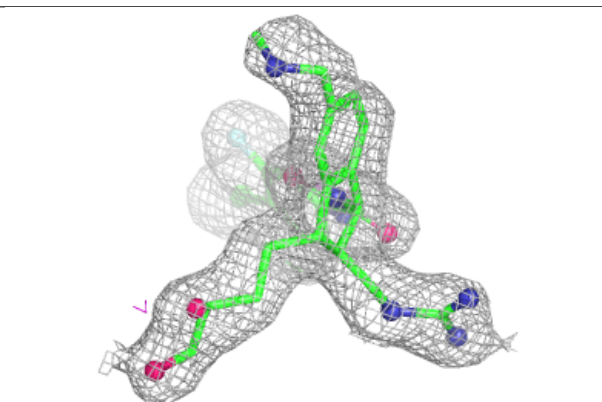
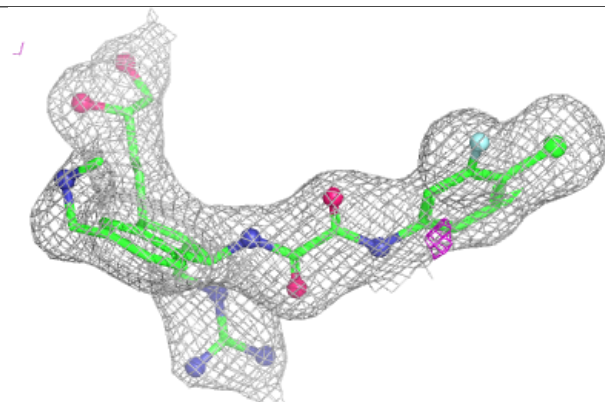
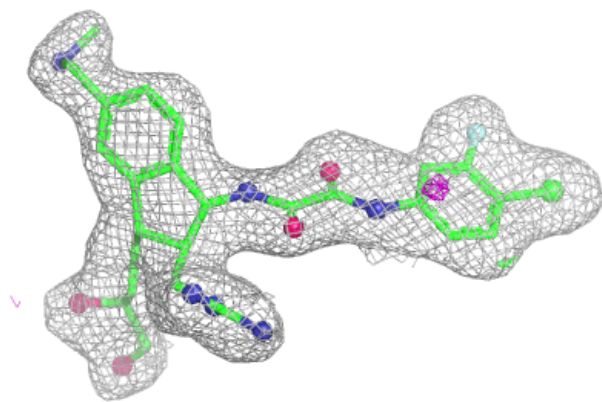
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7IT 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)

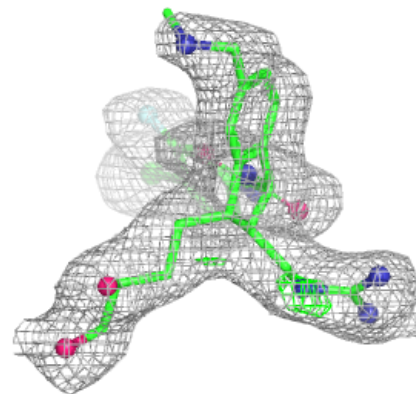
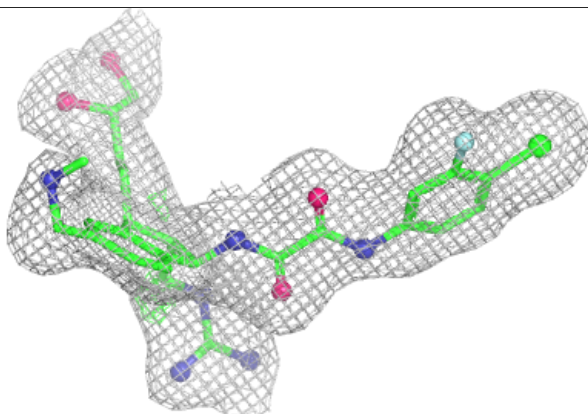
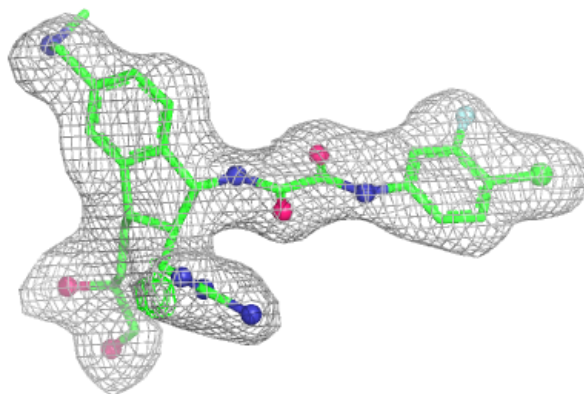
**Electron density around 7IT D 507:**

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



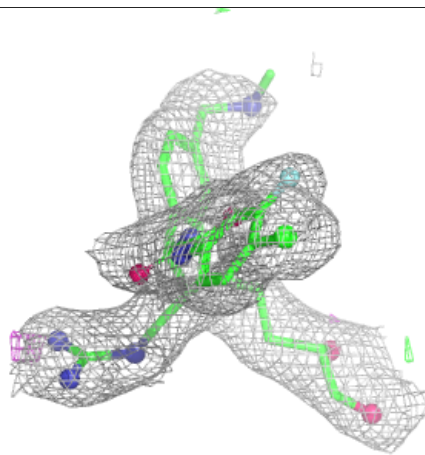
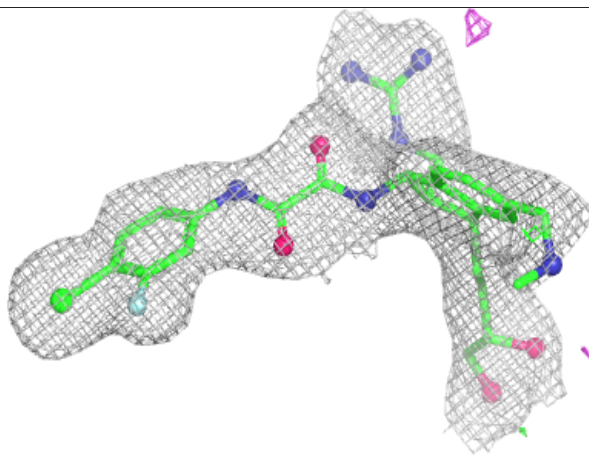
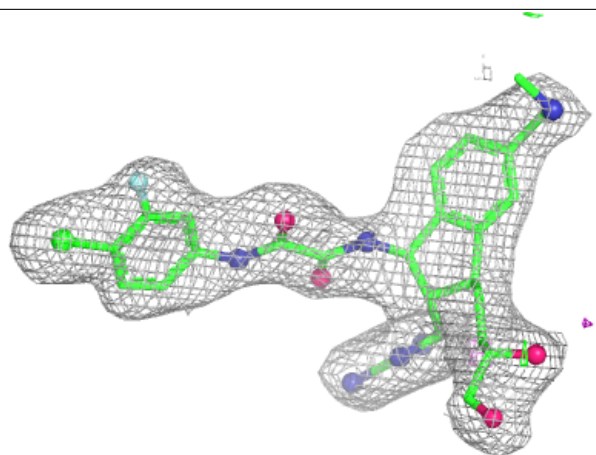
Electron density around 7IT C 507:

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



Electron density around 7IT 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.