



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:34 PM UTC

PDB ID : 3GR6 / pdb_00003gr6
Title : Crystal structure of the staphylococcus aureus enoyl-acyl carrier protein reductase (fabI) in complex with NADP and triclosan
Authors : Priyadarshi, A.; Hwang, K.Y.
Deposited on : 2009-03-25
Resolution : 2.28 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

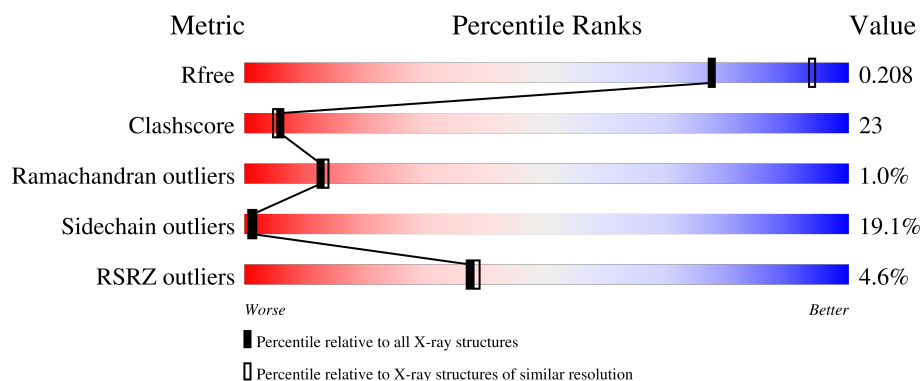
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	260	
1	D	260	
1	G	260	
1	J	260	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TCL	A	371	-	-	X	-
3	TCL	D	258	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8334 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.

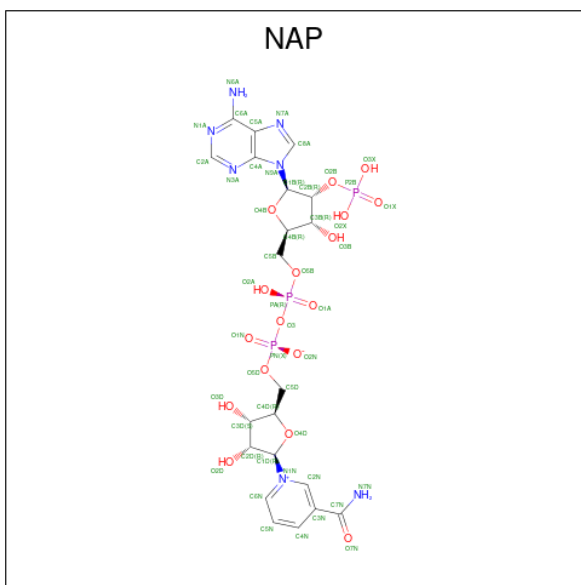
- Molecule 1 is a protein called Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1963	1238	339	382	4			
1	D	260	Total	C	N	O	S	0	0	0
			1994	1258	344	387	5			
1	G	254	Total	C	N	O	S	0	0	0
			1955	1232	338	381	4			
1	J	260	Total	C	N	O	S	0	0	0
			1994	1258	344	387	5			

There are 16 discrepancies between the modelled and reference sequences:

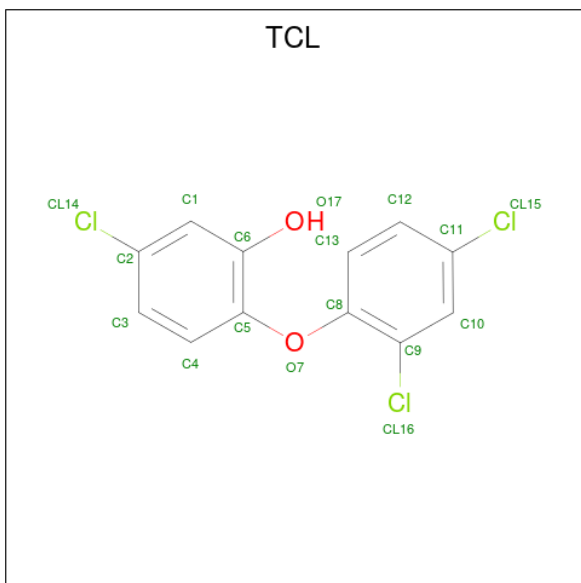
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	LEU	-	expression tag	UNP Q6GI75
A	-2	ALA	-	expression tag	UNP Q6GI75
A	-1	ALA	-	expression tag	UNP Q6GI75
A	0	ALA	-	expression tag	UNP Q6GI75
D	-3	LEU	-	expression tag	UNP Q6GI75
D	-2	ALA	-	expression tag	UNP Q6GI75
D	-1	ALA	-	expression tag	UNP Q6GI75
D	0	ALA	-	expression tag	UNP Q6GI75
G	-3	LEU	-	expression tag	UNP Q6GI75
G	-2	ALA	-	expression tag	UNP Q6GI75
G	-1	ALA	-	expression tag	UNP Q6GI75
G	0	ALA	-	expression tag	UNP Q6GI75
J	-3	LEU	-	expression tag	UNP Q6GI75
J	-2	ALA	-	expression tag	UNP Q6GI75
J	-1	ALA	-	expression tag	UNP Q6GI75
J	0	ALA	-	expression tag	UNP Q6GI75

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	J	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is TRICLOSAN (CCD ID: TCL) (formula: $C_{12}H_7Cl_3O_2$).



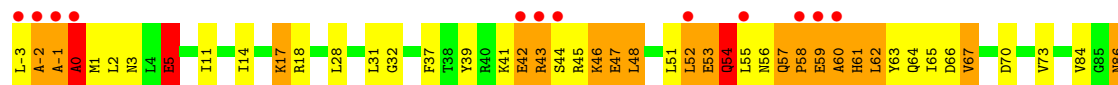
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	D	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	G	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	J	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	D	49	Total	O	0	0
			49	49		
4	G	42	Total	O	0	0
			42	42		
4	J	36	Total	O	0	0
			36	36		



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.56Å 118.44Å 149.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.28 47.09 – 2.28	Depositor EDS
% Data completeness (in resolution range)	90.9 (47.09-2.28) 90.9 (47.09-2.28)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.264 0.209 , 0.208	Depositor DCC
R_{free} test set	2895 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8334	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: TCL, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.52	10/1990 (0.5%)	1.55	32/2682 (1.2%)
1	D	1.55	10/2021 (0.5%)	1.57	32/2724 (1.2%)
1	G	1.49	8/1982 (0.4%)	1.60	38/2671 (1.4%)
1	J	1.45	11/2021 (0.5%)	1.55	30/2724 (1.1%)
All	All	1.50	39/8014 (0.5%)	1.57	132/10801 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	1	4
1	G	0	3
1	J	0	6
All	All	1	16

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	-1	ALA	C-N	14.93	1.53	1.33
1	D	210	GLU	CD-OE1	-12.74	1.01	1.25
1	J	47	GLU	C-N	11.96	1.50	1.33
1	D	47	GLU	C-N	10.29	1.46	1.33
1	D	209	LYS	C-N	8.53	1.45	1.34
1	G	155	GLN	C-O	8.53	1.33	1.24
1	J	3	ASN	C-N	8.48	1.46	1.33
1	J	162	VAL	CA-CB	7.89	1.65	1.54
1	A	84	VAL	N-CA	7.35	1.52	1.46
1	J	28	LEU	C-N	7.08	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	14	ILE	CA-CB	7.02	1.62	1.54
1	D	94	ILE	N-CA	-6.72	1.37	1.46
1	G	73	VAL	CA-CB	6.33	1.61	1.54
1	A	73	VAL	CA-CB	6.28	1.62	1.54
1	A	53	GLU	CA-C	6.26	1.60	1.52
1	A	224	VAL	CA-CB	6.24	1.63	1.54
1	G	20	ILE	CA-CB	6.20	1.62	1.54
1	G	103	ARG	CA-C	6.15	1.58	1.53
1	D	185	VAL	CA-CB	6.13	1.62	1.54
1	D	169	ALA	CA-CB	-5.70	1.44	1.53
1	J	248	VAL	CA-C	5.53	1.57	1.52
1	J	183	ILE	CA-CB	5.48	1.60	1.54
1	J	127	ILE	CA-CB	5.43	1.61	1.54
1	A	157	TYR	C-O	-5.42	1.17	1.24
1	G	158	ASN	C-O	-5.41	1.19	1.24
1	A	4	LEU	CA-C	5.41	1.59	1.53
1	J	156	ASN	N-CA	5.38	1.52	1.46
1	G	84	VAL	CA-CB	5.37	1.61	1.54
1	G	144	ALA	CA-CB	-5.33	1.45	1.53
1	J	106	PHE	C-O	-5.32	1.17	1.24
1	A	192	PRO	CA-C	5.29	1.59	1.52
1	A	61	HIS	C-O	-5.29	1.17	1.24
1	D	57	GLN	CA-C	5.26	1.59	1.52
1	A	56	ASN	CA-C	5.25	1.59	1.52
1	D	208	LEU	C-N	-5.12	1.26	1.34
1	J	67	VAL	CA-C	5.12	1.59	1.52
1	A	15	ALA	CA-CB	5.11	1.61	1.53
1	G	53	GLU	CA-C	5.05	1.59	1.52
1	D	114	PHE	C-O	-5.03	1.18	1.24

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	N-CA-C	15.36	128.52	108.24
1	G	4	LEU	N-CA-C	11.02	125.47	107.73
1	J	0	ALA	N-CA-C	10.89	134.01	110.80
1	G	155	GLN	N-CA-C	10.23	123.39	111.11
1	J	0	ALA	CA-C-N	9.98	137.65	120.58
1	J	0	ALA	C-N-CA	9.98	137.65	120.58
1	G	47	GLU	O-C-N	9.67	132.37	122.12
1	D	155	GLN	CA-C-N	-9.51	107.55	122.67
1	D	155	GLN	C-N-CA	-9.51	107.55	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	158	ASN	CB-CA-C	-9.10	104.85	117.23
1	D	127	ILE	CB-CA-C	-8.97	99.84	112.22
1	D	86	ASN	N-CA-C	8.76	122.38	110.55
1	A	53	GLU	CA-C-N	8.70	137.35	121.70
1	A	53	GLU	C-N-CA	8.70	137.35	121.70
1	A	165	ALA	N-CA-C	-8.59	102.00	111.36
1	D	54	GLN	N-CA-C	8.41	134.56	111.00
1	J	127	ILE	CB-CA-C	-8.37	101.03	112.24
1	J	0	ALA	CB-CA-C	-8.36	93.78	110.42
1	J	61	HIS	N-CA-C	8.25	128.37	110.80
1	J	54	GLN	N-CA-C	8.19	133.94	111.00
1	G	127	ILE	CB-CA-C	-8.03	101.30	112.14
1	A	54	GLN	N-CA-C	7.88	133.05	111.00
1	D	155	GLN	N-CA-C	7.85	120.60	111.02
1	G	185	VAL	CB-CA-C	7.63	120.49	110.12
1	D	-1	ALA	N-CA-C	-7.48	102.08	112.25
1	J	5	GLU	CA-C-N	-7.47	107.26	121.54
1	J	5	GLU	C-N-CA	-7.47	107.26	121.54
1	G	43	ARG	N-CA-C	7.47	121.30	112.93
1	D	210	GLU	CG-CD-OE1	-7.46	101.23	118.40
1	A	83	ASP	N-CA-C	7.38	120.77	111.69
1	J	86	ASN	N-CA-C	7.23	119.86	110.53
1	J	155	GLN	CA-C-N	-7.20	111.00	122.95
1	J	155	GLN	C-N-CA	-7.20	111.00	122.95
1	A	84	VAL	CB-CA-C	-7.17	103.60	110.70
1	D	-1	ALA	CA-C-N	-7.09	111.44	122.08
1	D	-1	ALA	C-N-CA	-7.09	111.44	122.08
1	D	53	GLU	CA-C-N	7.07	134.42	121.70
1	D	53	GLU	C-N-CA	7.07	134.42	121.70
1	A	56	ASN	CB-CA-C	6.92	118.31	109.80
1	A	42	GLU	CA-C-N	6.87	129.81	120.54
1	A	42	GLU	C-N-CA	6.87	129.81	120.54
1	G	55	LEU	N-CA-CB	6.84	120.99	110.80
1	A	57	GLN	N-CA-C	6.83	124.91	109.81
1	G	18	ARG	CB-CA-C	6.82	121.48	110.09
1	D	131	GLU	N-CA-C	6.82	118.71	111.28
1	G	54	GLN	N-CA-CB	-6.82	98.92	110.50
1	G	54	GLN	CB-CA-C	6.76	122.95	110.10
1	D	185	VAL	N-CA-C	6.73	117.72	107.77
1	J	42	GLU	N-CA-C	6.72	125.12	110.80
1	G	53	GLU	O-C-N	-6.71	115.07	123.05
1	D	1	MET	N-CA-C	6.67	121.16	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	220	ASN	N-CA-C	6.65	120.21	110.17
1	J	130	HIS	N-CA-C	6.61	119.32	111.33
1	D	157	TYR	CB-CA-C	6.58	122.54	110.11
1	A	86	ASN	CB-CA-C	6.51	126.11	111.78
1	D	185	VAL	CB-CA-C	6.49	119.18	110.42
1	A	104	GLY	N-CA-C	-6.45	94.61	113.30
1	J	18	ARG	CB-CA-C	6.42	120.81	110.09
1	D	208	LEU	O-C-N	6.38	128.73	122.09
1	G	194	ARG	CG-CD-NE	-6.33	98.07	112.00
1	G	6	ASN	N-CA-CB	-6.19	107.11	114.17
1	A	4	LEU	CA-C-N	6.15	132.01	121.86
1	A	4	LEU	C-N-CA	6.15	132.01	121.86
1	A	155	GLN	N-CA-C	6.12	118.48	111.02
1	J	229	THR	N-CA-C	-6.10	104.55	112.23
1	J	155	GLN	N-CA-C	6.02	118.36	111.02
1	J	101	ASP	N-CA-C	6.01	117.52	110.97
1	A	127	ILE	CB-CA-C	-5.97	103.98	112.22
1	G	25	ALA	CA-C-N	5.93	128.54	120.54
1	G	25	ALA	C-N-CA	5.93	128.54	120.54
1	A	53	GLU	CA-C-O	-5.89	114.79	120.92
1	A	5	GLU	CA-C-N	-5.84	114.74	125.02
1	A	5	GLU	C-N-CA	-5.84	114.74	125.02
1	D	51	LEU	N-CA-C	5.79	118.37	111.71
1	A	155	GLN	CA-C-N	-5.76	113.51	122.67
1	A	155	GLN	C-N-CA	-5.76	113.51	122.67
1	A	255	ILE	CA-C-N	5.71	131.98	121.70
1	A	255	ILE	C-N-CA	5.71	131.98	121.70
1	J	197	SER	N-CA-C	5.68	118.25	111.71
1	A	53	GLU	O-C-N	-5.68	115.47	122.68
1	G	222	ASP	N-CA-C	5.67	118.48	109.81
1	J	59	GLU	N-CA-C	-5.66	104.51	111.75
1	G	57	GLN	N-CA-C	5.64	122.28	109.81
1	G	53	GLU	CA-C-N	5.62	131.82	121.70
1	G	53	GLU	C-N-CA	5.62	131.82	121.70
1	G	42	GLU	N-CA-C	5.61	122.74	110.80
1	J	177	ASP	N-CA-C	5.60	117.38	111.28
1	A	58	PRO	N-CA-C	-5.59	100.96	112.47
1	D	57	GLN	N-CA-C	5.55	122.08	109.81
1	G	54	GLN	N-CA-C	5.55	126.55	111.00
1	A	43	ARG	CA-CB-CG	5.50	125.10	114.10
1	D	230	ALA	CA-C-N	5.49	127.95	120.54
1	D	230	ALA	C-N-CA	5.49	127.95	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	86	ASN	CB-CA-C	5.43	120.03	110.36
1	J	239	SER	N-CA-CB	-5.42	100.95	109.78
1	G	256	LYS	N-CA-C	5.39	126.10	111.00
1	D	36	VAL	N-CA-C	-5.36	100.47	108.46
1	D	86	ASN	CB-CA-C	5.33	120.36	109.76
1	G	246	ILE	N-CA-CB	5.32	117.07	111.00
1	J	53	GLU	CA-C-N	5.27	131.19	121.70
1	J	53	GLU	C-N-CA	5.27	131.19	121.70
1	A	185	VAL	CB-CA-C	5.25	118.57	110.28
1	D	105	ARG	CB-CG-CD	-5.25	99.23	111.30
1	G	217	LEU	N-CA-C	5.24	118.77	112.38
1	J	5	GLU	N-CA-C	5.22	116.78	111.14
1	D	4	LEU	CA-CB-CG	5.22	134.56	116.30
1	G	207	ILE	CA-C-N	5.22	127.27	120.28
1	G	207	ILE	C-N-CA	5.22	127.27	120.28
1	D	3	ASN	CA-C-N	-5.21	114.06	122.24
1	D	3	ASN	C-N-CA	-5.21	114.06	122.24
1	G	47	GLU	CA-C-N	-5.20	113.55	120.63
1	G	47	GLU	C-N-CA	-5.20	113.55	120.63
1	G	234	LEU	N-CA-C	5.19	118.39	111.75
1	G	214	ARG	N-CA-C	5.18	119.96	113.43
1	D	237	LEU	CA-CB-CG	5.18	134.43	116.30
1	A	73	VAL	N-CA-CB	5.18	118.35	110.58
1	J	70	ASP	CA-C-N	5.14	127.13	120.44
1	J	70	ASP	C-N-CA	5.14	127.13	120.44
1	G	171	VAL	N-CA-C	5.14	115.36	110.42
1	J	158	ASN	N-CA-C	5.13	117.24	108.67
1	D	157	TYR	N-CA-C	-5.13	105.32	112.45
1	G	85	GLY	CA-C-N	-5.11	113.90	123.05
1	G	85	GLY	C-N-CA	-5.11	113.90	123.05
1	A	165	ALA	CA-C-N	5.07	127.07	120.28
1	A	165	ALA	C-N-CA	5.07	127.07	120.28
1	G	239	SER	N-CA-C	5.07	121.60	110.80
1	A	80	ILE	N-CA-C	-5.06	105.46	110.62
1	G	116	LEU	N-CA-C	5.04	116.47	111.07
1	G	4	LEU	CA-C-N	5.03	131.15	121.54
1	G	4	LEU	C-N-CA	5.03	131.15	121.54
1	J	87	ILE	N-CA-CB	-5.02	105.50	112.52
1	D	185	VAL	N-CA-CB	5.01	118.64	111.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	86	ASN	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Peptide
1	A	2	LEU	Peptide
1	A	58	PRO	Peptide
1	D	-2	ALA	Peptide
1	D	0	ALA	Peptide
1	D	57	GLN	Peptide
1	D	58	PRO	Peptide
1	G	103	ARG	Peptide
1	G	57	GLN	Peptide
1	G	58	PRO	Peptide
1	J	-1	ALA	Peptide
1	J	-2	ALA	Peptide
1	J	-3	LEU	Peptide
1	J	0	ALA	Peptide
1	J	41	LYS	Peptide
1	J	58	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	1979	107	0
1	D	1994	0	2017	92	0
1	G	1955	0	1968	86	0
1	J	1994	0	2017	105	0
2	A	48	0	23	7	0
2	D	48	0	23	10	0
2	G	48	0	23	3	0
2	J	48	0	23	7	0
3	A	17	0	6	6	0
3	D	17	0	6	6	0
3	G	17	0	6	3	0
3	J	17	0	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	41	0	0	0	0
4	D	49	0	0	1	0
4	G	42	0	0	0	0
4	J	36	0	0	1	0
All	All	8334	0	8097	373	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLU:HB3	1:D:61:HIS:N	1.48	1.27
1:G:59:GLU:N	1:G:60:ALA:HA	1.45	1.24
1:G:59:GLU:CB	1:G:61:HIS:H	1.53	1.21
1:A:59:GLU:CB	1:A:61:HIS:H	1.52	1.20
1:D:59:GLU:CB	1:D:61:HIS:H	1.53	1.19
1:A:57:GLN:H	1:A:57:GLN:NE2	1.41	1.19
1:G:59:GLU:HB3	1:G:61:HIS:N	1.61	1.16
1:A:59:GLU:N	1:A:60:ALA:HA	1.61	1.16
1:D:136:MET:HE2	1:D:140:GLY:HA3	1.24	1.13
1:D:59:GLU:N	1:D:60:ALA:HA	1.61	1.11
1:A:59:GLU:HB3	1:A:61:HIS:N	1.67	1.10
1:A:256:LYS:HG3	1:A:256:LYS:OXT	1.52	1.09
1:D:59:GLU:HB3	1:D:61:HIS:H	0.97	1.06
1:G:59:GLU:N	1:G:60:ALA:CA	2.19	1.06
1:J:59:GLU:N	1:J:60:ALA:HA	1.69	1.06
1:J:58:PRO:C	1:J:60:ALA:HA	1.81	1.05
1:J:59:GLU:HB3	1:J:61:HIS:N	1.72	1.05
1:D:41:LYS:HD2	1:D:43:ARG:HD2	1.38	1.04
1:A:59:GLU:HB3	1:A:61:HIS:H	1.21	1.03
1:A:57:GLN:H	1:A:57:GLN:CD	1.67	1.02
1:A:136:MET:HE2	1:A:140:GLY:HA3	1.40	0.99
1:D:1:MET:HE1	1:G:31:LEU:CD1	1.93	0.98
1:J:59:GLU:CB	1:J:61:HIS:H	1.77	0.97
1:A:57:GLN:NE2	1:A:57:GLN:N	2.13	0.95
1:D:1:MET:HE1	1:G:31:LEU:HD13	1.49	0.94
1:D:59:GLU:N	1:D:60:ALA:CA	2.31	0.94
1:G:59:GLU:CB	1:G:61:HIS:N	2.26	0.94
1:J:59:GLU:N	1:J:60:ALA:CA	2.31	0.94
1:J:59:GLU:CB	1:J:61:HIS:N	2.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:GLU:O	1:G:6:ASN:HB2	1.65	0.93
1:J:-1:ALA:HA	1:J:1:MET:H	1.31	0.93
1:A:59:GLU:N	1:A:60:ALA:CA	2.30	0.93
1:G:124:SER:HA	1:G:127:ILE:HD11	1.49	0.93
1:D:1:MET:CE	1:G:31:LEU:HD11	2.00	0.91
1:D:-3:LEU:H3	1:D:-1:ALA:H	1.18	0.91
1:G:157:TYR:OH	3:G:258:TCL:CL16	2.24	0.90
1:J:58:PRO:O	1:J:60:ALA:HA	1.70	0.90
1:A:59:GLU:CB	1:A:61:HIS:N	2.28	0.89
1:G:59:GLU:H	1:G:60:ALA:CA	1.79	0.89
1:G:59:GLU:HB3	1:G:61:HIS:H	1.21	0.88
1:A:5:GLU:O	1:A:6:ASN:HB2	1.71	0.88
1:G:59:GLU:H	1:G:60:ALA:HA	1.06	0.86
1:A:99:MET:HE2	1:A:103:ARG:HG3	1.56	0.85
1:D:59:GLU:H	1:D:60:ALA:HA	1.39	0.85
1:J:57:GLN:HB2	1:J:58:PRO:CD	2.07	0.84
1:J:57:GLN:HB2	1:J:58:PRO:HD3	1.57	0.84
1:A:52:LEU:CD2	1:A:60:ALA:H	1.90	0.84
1:A:59:GLU:HB2	1:A:61:HIS:H	1.41	0.83
1:J:86:ASN:HB2	1:J:135:LEU:O	1.78	0.83
1:A:204:PHE:HA	1:A:207:ILE:HG12	1.61	0.83
1:G:59:GLU:HB2	1:G:61:HIS:H	1.43	0.83
1:G:136:MET:HE2	1:G:140:GLY:HA3	1.61	0.82
1:D:59:GLU:HB3	1:D:61:HIS:CA	2.09	0.82
1:G:57:GLN:H	1:G:57:GLN:NE2	1.78	0.82
1:G:58:PRO:C	1:G:60:ALA:HA	2.04	0.82
1:A:52:LEU:HD22	1:A:60:ALA:H	1.45	0.82
1:D:1:MET:HE3	1:G:31:LEU:HD11	1.62	0.81
1:J:58:PRO:O	1:J:60:ALA:CA	2.29	0.81
1:D:147:TYR:CD1	2:D:257:NAP:H5N	2.16	0.80
1:A:147:TYR:CD1	2:A:361:NAP:H5N	2.16	0.80
1:D:124:SER:HA	1:D:127:ILE:HD11	1.63	0.80
1:A:58:PRO:C	1:A:60:ALA:HA	2.06	0.79
1:D:58:PRO:C	1:D:60:ALA:HA	2.07	0.79
1:G:86:ASN:HB2	1:G:135:LEU:O	1.83	0.79
1:J:157:TYR:OH	3:J:258:TCL:CL16	2.38	0.78
1:D:246:ILE:HD12	1:G:246:ILE:HD12	1.66	0.78
1:D:157:TYR:OH	3:D:258:TCL:CL16	2.38	0.78
1:A:209:LYS:O	1:A:213:GLU:HG3	1.85	0.77
1:D:86:ASN:HB2	1:D:135:LEU:O	1.84	0.77
1:D:256:LYS:NZ	1:J:207:ILE:HG22	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:GLN:CD	1:J:155:GLN:H	1.92	0.77
1:A:60:ALA:O	1:A:61:HIS:C	2.27	0.76
1:D:136:MET:CE	1:D:140:GLY:HA3	2.12	0.76
1:J:57:GLN:CD	1:J:57:GLN:H	1.94	0.75
1:D:192:PRO:HA	2:D:257:NAP:O7N	1.86	0.75
1:G:146:THR:O	2:G:257:NAP:H6N	1.88	0.74
1:J:58:PRO:C	1:J:60:ALA:CA	2.59	0.74
1:D:59:GLU:CA	1:D:61:HIS:H	1.99	0.74
1:D:1:MET:CE	1:G:31:LEU:CD1	2.60	0.72
1:A:46:LYS:HE3	1:A:49:GLU:OE1	1.89	0.72
1:A:204:PHE:HA	1:A:207:ILE:CD1	2.19	0.72
1:G:57:GLN:H	1:G:57:GLN:CD	1.97	0.72
1:A:59:GLU:H	1:A:60:ALA:HA	1.49	0.72
1:G:5:GLU:O	1:G:6:ASN:CB	2.36	0.72
1:J:45:ARG:NH2	1:J:59:GLU:OE1	2.23	0.71
1:A:204:PHE:CD1	1:A:207:ILE:HD11	2.26	0.71
1:D:209:LYS:O	1:D:213:GLU:HG2	1.91	0.70
1:G:35:LEU:H	1:G:56:ASN:HD21	1.37	0.70
1:A:155:GLN:CD	1:A:155:GLN:H	1.98	0.70
1:G:136:MET:CE	1:G:140:GLY:HA3	2.21	0.70
1:D:59:GLU:H	1:D:60:ALA:CA	2.00	0.69
1:A:204:PHE:HA	1:A:207:ILE:CG1	2.22	0.69
1:D:124:SER:HA	1:D:127:ILE:CD1	2.23	0.69
1:D:39:TYR:CE1	1:D:64:GLN:HG3	2.28	0.69
1:J:219:ARG:HD3	4:J:266:HOH:O	1.91	0.69
1:A:204:PHE:O	1:A:207:ILE:HG12	1.93	0.68
1:G:57:GLN:NE2	1:G:57:GLN:N	2.39	0.68
1:J:112:GLU:H	1:J:112:GLU:CD	2.00	0.68
1:J:209:LYS:O	1:J:213:GLU:HG3	1.93	0.68
1:A:210:GLU:OE2	1:G:256:LYS:HE3	1.93	0.68
1:A:146:THR:O	2:A:361:NAP:H6N	1.94	0.68
1:A:2:LEU:C	1:A:2:LEU:HD23	2.19	0.67
1:A:2:LEU:HA	1:A:3:ASN:HB2	1.75	0.67
1:A:4:LEU:HG	1:A:5:GLU:HG3	1.76	0.67
1:G:124:SER:HA	1:G:127:ILE:CD1	2.24	0.67
1:A:201:VAL:CG2	3:A:371:TCL:O17	2.43	0.66
1:J:146:THR:O	2:J:257:NAP:H6N	1.95	0.66
1:G:57:GLN:CD	1:G:57:GLN:N	2.52	0.66
1:A:204:PHE:C	1:A:207:ILE:HG12	2.21	0.66
1:J:204:PHE:O	1:J:207:ILE:HG12	1.96	0.66
1:J:59:GLU:HB2	1:J:61:HIS:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:MET:HE2	1:D:140:GLY:CA	2.15	0.66
1:A:204:PHE:CA	1:A:207:ILE:HG12	2.25	0.65
1:J:57:GLN:H	1:J:57:GLN:NE2	1.93	0.65
1:J:-2:ALA:HA	1:J:-1:ALA:O	1.96	0.65
1:D:147:TYR:HD1	2:D:257:NAP:H5N	1.61	0.65
1:G:256:LYS:OXT	1:G:256:LYS:HG3	1.94	0.65
1:D:59:GLU:H	1:D:61:HIS:N	1.94	0.65
1:D:256:LYS:OXT	1:D:256:LYS:HG3	1.97	0.65
1:A:124:SER:HA	1:A:127:ILE:HD11	1.79	0.64
1:D:146:THR:O	2:D:257:NAP:H6N	1.97	0.64
1:A:35:LEU:H	1:A:56:ASN:HD21	1.45	0.64
1:A:143:VAL:HG23	1:A:234:LEU:HD13	1.79	0.64
1:A:204:PHE:CE2	1:A:208:LEU:HD22	2.33	0.64
1:J:210:GLU:OE2	1:J:214:ARG:NH1	2.30	0.64
1:A:35:LEU:H	1:A:56:ASN:ND2	1.96	0.63
1:D:-3:LEU:H3	1:D:-1:ALA:N	1.94	0.63
1:D:-2:ALA:HB1	1:D:0:ALA:H	1.62	0.63
2:D:257:NAP:C4N	3:D:258:TCL:C11	2.76	0.63
1:J:89:GLY:HA2	1:J:136:MET:HE1	1.81	0.63
1:A:99:MET:CE	1:A:103:ARG:HG3	2.29	0.63
1:A:54:GLN:HG3	1:A:55:LEU:H	1.62	0.63
1:J:217:LEU:O	1:J:219:ARG:HG2	1.99	0.62
1:D:256:LYS:HE2	1:J:155:GLN:OE1	1.99	0.62
1:J:204:PHE:CE2	1:J:208:LEU:HD22	2.34	0.62
1:J:57:GLN:OE1	1:J:58:PRO:HD2	1.99	0.62
1:J:-1:ALA:HA	1:J:1:MET:N	2.10	0.62
1:J:-1:ALA:HB1	1:J:2:LEU:H	1.65	0.62
1:A:4:LEU:HG	1:A:5:GLU:H	1.64	0.62
1:J:52:LEU:HD21	1:J:60:ALA:HB3	1.81	0.62
1:J:42:GLU:OE1	1:J:42:GLU:HA	2.00	0.61
1:J:44:SER:O	1:J:48:LEU:HB2	2.01	0.61
1:D:188:ILE:HG23	1:D:248:VAL:HG23	1.83	0.61
1:A:155:GLN:CD	1:A:155:GLN:N	2.60	0.60
1:G:194:ARG:NH2	1:G:205:ASN:OD1	2.30	0.60
1:A:214:ARG:HH22	1:A:256:LYS:HB3	1.67	0.60
1:D:256:LYS:HZ1	1:J:207:ILE:HG22	1.67	0.60
1:J:59:GLU:H	1:J:61:HIS:H	1.50	0.60
1:A:41:LYS:HE2	2:A:361:NAP:O3X	2.02	0.59
3:G:258:TCL:C8	3:G:258:TCL:O17	2.50	0.59
3:J:258:TCL:C8	3:J:258:TCL:O17	2.51	0.59
1:D:57:GLN:H	1:D:57:GLN:CD	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLU:HB3	1:D:61:HIS:HA	1.85	0.59
3:D:258:TCL:C8	3:D:258:TCL:O17	2.50	0.58
1:J:57:GLN:CD	1:J:57:GLN:N	2.60	0.58
1:A:60:ALA:O	1:A:61:HIS:O	2.21	0.58
1:D:2:LEU:HD13	1:D:237:LEU:HD22	1.84	0.57
2:A:361:NAP:C3N	3:A:371:TCL:C13	2.82	0.57
1:A:157:TYR:OH	3:A:371:TCL:CL16	2.51	0.57
3:A:371:TCL:O17	3:A:371:TCL:C8	2.52	0.57
1:D:210:GLU:OE1	1:J:256:LYS:NZ	2.36	0.57
1:J:130:HIS:HD2	1:J:131:GLU:OE1	1.87	0.57
1:A:124:SER:HA	1:A:127:ILE:CD1	2.34	0.57
1:A:58:PRO:O	1:A:60:ALA:HA	2.05	0.57
1:D:99:MET:HE2	1:D:100:GLU:HA	1.87	0.56
1:A:123:TYR:CE2	1:A:127:ILE:HG12	2.40	0.56
1:A:193:ILE:N	2:A:361:NAP:O7N	2.32	0.56
1:A:210:GLU:OE2	1:G:256:LYS:CE	2.53	0.56
1:J:59:GLU:N	1:J:61:HIS:H	2.02	0.56
1:D:210:GLU:CD	1:J:256:LYS:NZ	2.64	0.56
1:J:209:LYS:O	1:J:213:GLU:CG	2.54	0.56
1:J:59:GLU:CA	1:J:61:HIS:H	2.19	0.56
1:D:22:PHE:CZ	1:D:51:LEU:HD22	2.41	0.56
1:J:143:VAL:HG23	1:J:234:LEU:HD13	1.87	0.55
1:G:197:SER:HB3	3:G:258:TCL:C4	2.36	0.55
2:D:257:NAP:O2D	3:D:258:TCL:CL16	2.54	0.55
1:J:155:GLN:CD	1:J:155:GLN:N	2.64	0.55
1:J:57:GLN:CB	1:J:58:PRO:CD	2.83	0.54
1:J:194:ARG:HH11	1:J:194:ARG:HG2	1.72	0.54
1:D:59:GLU:CB	1:D:61:HIS:N	2.29	0.54
1:D:256:LYS:HZ3	1:J:207:ILE:HG22	1.72	0.54
1:A:106:PHE:HE1	1:D:170:ASN:ND2	2.06	0.54
1:A:201:VAL:HG23	3:A:371:TCL:O17	2.07	0.54
1:J:5:GLU:O	1:J:32:GLY:O	2.26	0.54
1:G:35:LEU:H	1:G:56:ASN:ND2	2.06	0.53
1:A:57:GLN:CD	1:A:57:GLN:N	2.37	0.53
1:A:89:GLY:HA2	1:A:136:MET:HE3	1.91	0.53
1:J:205:ASN:O	1:J:209:LYS:CD	2.57	0.53
1:A:2:LEU:CA	1:A:3:ASN:HB2	2.39	0.53
1:J:136:MET:HE2	1:J:140:GLY:HA3	1.89	0.53
1:D:3:ASN:O	1:D:7:LYS:CD	2.57	0.53
1:D:219:ARG:NH2	1:D:225:GLU:OE1	2.42	0.53
1:D:59:GLU:N	1:D:61:HIS:H	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HD12	1:J:246:ILE:HD12	1.92	0.52
1:G:132:ALA:O	1:G:136:MET:HG3	2.09	0.52
1:J:37:PHE:HB2	1:J:62:LEU:HD12	1.92	0.52
1:G:116:LEU:HD11	1:G:120:ILE:HD11	1.92	0.52
1:D:58:PRO:O	1:D:60:ALA:HA	2.09	0.52
1:G:4:LEU:HG	1:G:5:GLU:H	1.74	0.52
1:G:58:PRO:O	1:G:60:ALA:HA	2.09	0.52
1:D:210:GLU:O	1:D:214:ARG:HB2	2.09	0.52
1:D:102:LEU:HD23	1:D:157:TYR:O	2.10	0.52
1:J:37:PHE:CE2	1:J:52:LEU:HD11	2.45	0.52
1:G:40:ARG:HD3	2:G:257:NAP:C5A	2.40	0.52
1:A:89:GLY:HA2	1:A:136:MET:CE	2.40	0.51
1:G:89:GLY:HA2	1:G:141:SER:O	2.09	0.51
1:D:59:GLU:H	1:D:61:HIS:H	1.57	0.51
1:D:219:ARG:HH22	1:D:225:GLU:CD	2.18	0.51
1:D:124:SER:O	1:D:127:ILE:HD12	2.11	0.51
1:A:88:ASP:C	1:A:136:MET:HE3	2.36	0.51
1:G:24:VAL:HG22	1:G:227:GLY:HA2	1.93	0.51
1:J:67:VAL:HG22	2:J:257:NAP:N1A	2.26	0.51
1:D:57:GLN:CD	1:D:57:GLN:N	2.69	0.51
2:D:257:NAP:C4N	3:D:258:TCL:C10	2.88	0.51
1:J:17:LYS:HB3	1:J:51:LEU:HD21	1.93	0.51
1:A:228:LYS:HZ2	1:J:239:SER:HB2	1.74	0.51
1:D:71:GLU:HG3	1:D:75:ASN:ND2	2.26	0.51
1:D:88:ASP:C	1:D:136:MET:HE3	2.36	0.50
1:G:42:GLU:O	1:G:42:GLU:HG3	2.11	0.50
1:J:59:GLU:CA	1:J:61:HIS:N	2.75	0.50
1:G:194:ARG:NH1	1:G:208:LEU:CD1	2.75	0.50
1:J:52:LEU:HD23	1:J:60:ALA:H	1.77	0.50
1:J:205:ASN:O	1:J:209:LYS:HD3	2.11	0.50
1:A:56:ASN:HA	1:A:57:GLN:NE2	2.26	0.50
1:J:44:SER:HA	1:J:47:GLU:HB2	1.93	0.50
1:G:4:LEU:HG	1:G:5:GLU:HG3	1.94	0.50
1:A:35:LEU:O	1:A:60:ALA:HB1	2.12	0.49
1:D:114:PHE:HA	1:D:159:VAL:HG21	1.94	0.49
1:J:59:GLU:N	1:J:61:HIS:N	2.60	0.49
1:A:5:GLU:O	1:A:6:ASN:CB	2.43	0.49
1:D:-3:LEU:N	1:D:-2:ALA:HA	2.27	0.49
1:D:41:LYS:CD	1:D:43:ARG:HD2	2.26	0.49
1:G:59:GLU:CA	1:G:61:HIS:H	2.22	0.49
1:A:54:GLN:HG3	1:A:55:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:ASN:O	1:G:4:LEU:HB2	2.13	0.49
1:J:59:GLU:HB3	1:J:61:HIS:CA	2.41	0.49
1:D:103:ARG:NH2	4:D:409:HOH:O	2.46	0.49
1:A:123:TYR:CE2	1:A:127:ILE:CG1	2.96	0.49
1:A:87:ILE:HG22	1:A:136:MET:HG3	1.95	0.48
2:A:361:NAP:C3N	3:A:371:TCL:C12	2.90	0.48
1:G:49:GLU:HG2	1:G:62:LEU:HD21	1.94	0.48
1:J:-2:ALA:HA	1:J:-1:ALA:C	2.37	0.48
1:A:18:ARG:HG3	1:A:195:THR:HA	1.96	0.48
1:A:204:PHE:HA	1:A:207:ILE:HD11	1.96	0.48
1:D:217:LEU:O	1:D:219:ARG:HG2	2.13	0.48
1:J:54:GLN:HE21	1:J:54:GLN:HB3	1.42	0.48
1:A:199:LYS:NZ	1:A:199:LYS:CB	2.76	0.48
1:A:217:LEU:HD13	1:J:242:THR:HG21	1.94	0.48
1:G:209:LYS:O	1:G:213:GLU:HG3	2.13	0.48
1:G:48:LEU:O	1:G:52:LEU:HG	2.12	0.48
1:G:155:GLN:CD	1:G:155:GLN:H	2.21	0.48
1:G:71:GLU:HG3	1:G:75:ASN:ND2	2.28	0.48
1:D:59:GLU:H	1:D:60:ALA:C	2.22	0.48
1:G:59:GLU:H	1:G:61:HIS:N	2.12	0.48
1:A:214:ARG:NH2	1:A:256:LYS:HB3	2.28	0.48
1:D:256:LYS:OXT	1:D:256:LYS:CG	2.60	0.48
1:G:177:ASP:OD1	1:J:105:ARG:NH1	2.46	0.48
1:A:107:SER:O	1:D:130:HIS:HB2	2.14	0.48
1:D:54:GLN:HG3	1:D:55:LEU:H	1.79	0.48
1:D:59:GLU:N	1:D:61:HIS:N	2.62	0.48
1:A:59:GLU:CA	1:A:61:HIS:H	2.20	0.47
1:D:197:SER:HB3	3:D:258:TCL:C4	2.44	0.47
1:A:86:ASN:HB2	1:A:135:LEU:O	2.14	0.47
1:A:136:MET:HE2	1:A:140:GLY:CA	2.28	0.47
1:G:39:TYR:CE1	1:G:64:GLN:HG3	2.50	0.47
1:J:59:GLU:H	1:J:61:HIS:N	2.12	0.47
1:J:249:ASP:O	1:J:250:SER:HB2	2.14	0.47
1:J:42:GLU:OE1	1:J:42:GLU:CA	2.62	0.47
1:J:201:VAL:CG2	3:J:258:TCL:O17	2.62	0.47
1:A:256:LYS:HB2	1:G:154:VAL:HG22	1.96	0.47
1:G:184:ARG:HD2	1:G:241:VAL:O	2.14	0.47
1:J:39:TYR:CE1	1:J:64:GLN:HG3	2.49	0.47
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.78	0.47
1:A:37:PHE:CE2	1:A:60:ALA:HB3	2.50	0.47
1:A:204:PHE:O	1:A:207:ILE:CG1	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:GLU:CD	1:G:112:GLU:H	2.23	0.47
1:J:58:PRO:O	1:J:60:ALA:N	2.48	0.46
1:D:217:LEU:HB2	1:D:250:SER:HB3	1.96	0.46
1:G:81:GLY:HA2	1:G:85:GLY:O	2.15	0.46
1:J:52:LEU:CD2	1:J:60:ALA:H	2.27	0.46
1:J:63:TYR:N	1:J:63:TYR:CD2	2.83	0.46
1:A:37:PHE:HE2	1:A:60:ALA:HB3	1.80	0.46
1:A:4:LEU:CG	1:A:5:GLU:H	2.26	0.46
1:J:-2:ALA:HB1	1:J:0:ALA:HB3	1.97	0.46
1:G:8:THR:HA	1:G:34:LYS:O	2.16	0.46
1:J:67:VAL:HG22	2:J:257:NAP:C6A	2.46	0.46
1:D:-3:LEU:HD23	1:D:-1:ALA:HB2	1.98	0.46
1:G:179:GLY:N	1:G:180:PRO:CD	2.79	0.46
1:A:52:LEU:HD21	1:A:60:ALA:H	1.77	0.46
1:D:5:GLU:CD	1:D:5:GLU:H	2.21	0.46
1:G:123:TYR:CE2	1:J:111:ARG:HB2	2.51	0.46
1:G:124:SER:O	1:G:127:ILE:HD12	2.16	0.46
1:J:46:LYS:HA	1:J:46:LYS:HD3	1.70	0.46
1:D:99:MET:HE2	1:D:100:GLU:CA	2.46	0.45
1:J:178:LEU:O	1:J:181:ASP:HB2	2.16	0.45
1:J:236:ASP:O	1:J:239:SER:HB2	2.16	0.45
1:A:52:LEU:HD22	1:A:60:ALA:N	2.23	0.45
1:J:58:PRO:C	1:J:60:ALA:N	2.71	0.45
1:J:213:GLU:O	1:J:218:LYS:HE3	2.16	0.45
1:A:112:GLU:CD	1:A:112:GLU:H	2.23	0.45
1:D:193:ILE:H	2:D:257:NAP:C7N	2.28	0.45
1:G:217:LEU:HB2	1:G:250:SER:HB3	1.98	0.45
1:D:143:VAL:CG2	1:D:234:LEU:HD13	2.47	0.45
1:G:12:MET:HB3	1:G:94:ILE:HD11	1.97	0.45
1:G:81:GLY:HA3	1:G:135:LEU:HD21	1.97	0.45
1:A:125:LEU:HD13	1:A:144:ALA:HB2	1.99	0.45
1:J:57:GLN:NE2	1:J:57:GLN:N	2.62	0.45
1:D:53:GLU:H	1:D:53:GLU:HG3	1.61	0.44
1:D:59:GLU:CA	1:D:61:HIS:N	2.74	0.44
1:D:178:LEU:HB3	1:D:183:ILE:HB	1.99	0.44
1:J:205:ASN:O	1:J:209:LYS:HD2	2.16	0.44
1:G:40:ARG:HD3	2:G:257:NAP:C6A	2.48	0.44
1:G:217:LEU:HD22	1:G:250:SER:HA	1.98	0.44
1:D:67:VAL:HG22	2:D:257:NAP:N1A	2.32	0.44
1:D:38:THR:HA	1:D:63:TYR:O	2.18	0.44
1:J:127:ILE:H	1:J:127:ILE:HG13	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:HB2	2:A:361:NAP:C6N	2.48	0.44
1:G:143:VAL:HG23	1:G:234:LEU:HD13	1.99	0.44
1:G:59:GLU:HB3	1:G:61:HIS:CA	2.43	0.44
1:A:58:PRO:C	1:A:60:ALA:CA	2.83	0.43
1:A:228:LYS:NZ	1:J:239:SER:CB	2.81	0.43
1:A:5:GLU:C	1:A:7:LYS:H	2.26	0.43
1:A:246:ILE:HD12	1:J:246:ILE:CD1	2.48	0.43
1:G:53:GLU:H	1:G:53:GLU:HG3	1.62	0.43
1:J:219:ARG:HH22	1:J:225:GLU:CD	2.26	0.43
1:G:38:THR:HG21	1:G:65:ILE:HD12	2.00	0.43
1:G:105:ARG:HD3	1:J:177:ASP:OD1	2.18	0.43
1:A:34:LYS:HA	1:A:56:ASN:HD21	1.84	0.43
1:D:184:ARG:HG2	1:D:242:THR:HB	2.01	0.43
1:J:204:PHE:HA	1:J:207:ILE:CD1	2.49	0.43
1:J:216:PRO:HD2	1:J:251:GLY:C	2.44	0.42
1:J:192:PRO:C	1:J:193:ILE:HG13	2.44	0.42
1:J:214:ARG:NH2	1:J:256:LYS:HB3	2.35	0.42
1:G:5:GLU:H	1:G:5:GLU:HG3	1.57	0.42
1:G:38:THR:HA	1:G:63:TYR:O	2.20	0.42
1:G:54:GLN:HG3	1:G:55:LEU:H	1.84	0.42
1:A:17:LYS:HE3	1:A:18:ARG:NH1	2.35	0.42
1:A:28:LEU:HD11	1:A:234:LEU:HD23	2.01	0.42
1:G:153:ALA:HA	1:J:173:TYR:CZ	2.55	0.42
1:A:3:ASN:O	1:A:4:LEU:HB2	2.19	0.42
1:A:209:LYS:O	1:A:213:GLU:CG	2.64	0.42
1:G:105:ARG:HB2	1:G:108:GLU:OE1	2.20	0.42
1:G:216:PRO:HD2	1:G:251:GLY:C	2.44	0.42
1:A:105:ARG:O	1:A:106:PHE:C	2.63	0.41
1:A:196:LEU:O	1:A:199:LYS:HG2	2.20	0.41
1:D:216:PRO:HD2	1:D:251:GLY:C	2.45	0.41
1:A:45:ARG:NE	1:A:49:GLU:OE2	2.53	0.41
1:A:204:PHE:HD1	1:A:207:ILE:HD11	1.80	0.41
1:D:18:ARG:O	1:D:195:THR:HG22	2.20	0.41
1:D:193:ILE:N	2:D:257:NAP:O7N	2.50	0.41
1:G:42:GLU:O	1:G:42:GLU:CG	2.69	0.41
1:J:214:ARG:HH21	1:J:256:LYS:HB3	1.86	0.41
1:D:-2:ALA:C	1:D:0:ALA:H	2.29	0.41
1:D:4:LEU:HB2	1:D:9:TYR:OH	2.21	0.41
1:J:147:TYR:HB2	2:J:257:NAP:C6N	2.51	0.41
1:D:130:HIS:HD2	1:D:131:GLU:OE1	2.03	0.41
1:D:231:ALA:O	1:D:235:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:LEU:O	1:G:199:LYS:HG2	2.21	0.41
1:J:65:ILE:O	2:J:257:NAP:H2A	2.21	0.41
1:G:31:LEU:HD12	1:G:31:LEU:HA	1.93	0.41
1:G:141:SER:HB3	1:G:234:LEU:HD12	2.03	0.41
1:A:18:ARG:O	1:A:195:THR:HG22	2.21	0.41
1:A:106:PHE:CE1	1:D:170:ASN:ND2	2.88	0.41
1:A:256:LYS:OXT	1:A:256:LYS:CG	2.34	0.41
1:G:207:ILE:HD12	1:G:207:ILE:HG21	1.74	0.41
1:J:158:ASN:HB3	1:J:159:VAL:H	1.20	0.41
1:J:66:ASP:HA	2:J:257:NAP:N1A	2.36	0.40
1:J:204:PHE:HA	1:J:207:ILE:HD11	2.03	0.40
1:A:3:ASN:HD22	1:A:3:ASN:HA	1.70	0.40
1:G:40:ARG:HE	1:G:40:ARG:HB3	1.55	0.40
2:J:257:NAP:H2D	2:J:257:NAP:H2N	1.64	0.40
1:A:117:ALA:O	1:A:121:SER:HB2	2.21	0.40
1:J:189:SER:HB2	1:J:245:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

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	253/260 (97%)	230 (91%)	20 (8%)	3 (1%)	10	10
1	D	258/260 (99%)	236 (92%)	21 (8%)	1 (0%)	30	36
1	G	252/260 (97%)	229 (91%)	20 (8%)	3 (1%)	10	10
1	J	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	10	10
All	All	1021/1040 (98%)	932 (91%)	79 (8%)	10 (1%)	12	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	58	PRO
1	J	54	GLN
1	A	52	LEU
1	G	58	PRO
1	D	54	GLN
1	G	42	GLU
1	J	43	ARG
1	J	60	ALA
1	G	149	GLY

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	209/211 (99%)	173 (83%)	36 (17%)	2	1
1	D	211/211 (100%)	162 (77%)	49 (23%)	1	0
1	G	208/211 (99%)	170 (82%)	38 (18%)	2	1
1	J	211/211 (100%)	174 (82%)	37 (18%)	2	1
All	All	839/844 (99%)	679 (81%)	160 (19%)	1	1

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	ASN
1	A	4	LEU
1	A	17	LYS
1	A	26	LYS
1	A	31	LEU
1	A	43	ARG
1	A	46	LYS
1	A	48	LEU
1	A	52	LEU
1	A	57	GLN
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	73	VAL
1	A	87	ILE
1	A	99	MET
1	A	100	GLU
1	A	103	ARG
1	A	112	GLU
1	A	115	LEU
1	A	127	ILE
1	A	138	GLU
1	A	154	VAL
1	A	155	GLN
1	A	178	LEU
1	A	185	VAL
1	A	196	LEU
1	A	199	LYS
1	A	208	LEU
1	A	209	LYS
1	A	213	GLU
1	A	217	LEU
1	A	220	ASN
1	A	224	VAL
1	A	234	LEU
1	A	236	ASP
1	A	255	ILE
1	D	-3	LEU
1	D	1	MET
1	D	2	LEU
1	D	4	LEU
1	D	5	GLU
1	D	17	LYS
1	D	18	ARG
1	D	26	LYS
1	D	31	LEU
1	D	34	LYS
1	D	43	ARG
1	D	48	LEU
1	D	50	LYS
1	D	52	LEU
1	D	53	GLU
1	D	54	GLN
1	D	55	LEU
1	D	56	ASN

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Mol	Chain	Res	Type
1	D	57	GLN
1	D	62	LEU
1	D	73	VAL
1	D	78	GLU
1	D	84	VAL
1	D	87	ILE
1	D	93	SER
1	D	99	MET
1	D	103	ARG
1	D	112	GLU
1	D	115	LEU
1	D	127	ILE
1	D	128	VAL
1	D	138	GLU
1	D	154	VAL
1	D	178	LEU
1	D	183	ILE
1	D	185	VAL
1	D	196	LEU
1	D	207	ILE
1	D	209	LYS
1	D	213	GLU
1	D	214	ARG
1	D	217	LEU
1	D	220	ASN
1	D	224	VAL
1	D	234	LEU
1	D	236	ASP
1	D	237	LEU
1	D	239	SER
1	D	256	LYS
1	G	5	GLU
1	G	6	ASN
1	G	17	LYS
1	G	18	ARG
1	G	26	LYS
1	G	31	LEU
1	G	34	LYS
1	G	47	GLU
1	G	53	GLU
1	G	55	LEU
1	G	57	GLN

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Mol	Chain	Res	Type
1	G	62	LEU
1	G	64	GLN
1	G	73	VAL
1	G	82	LYS
1	G	84	VAL
1	G	87	ILE
1	G	93	SER
1	G	99	MET
1	G	102	LEU
1	G	103	ARG
1	G	105	ARG
1	G	112	GLU
1	G	115	LEU
1	G	126	THR
1	G	127	ILE
1	G	178	LEU
1	G	185	VAL
1	G	194	ARG
1	G	196	LEU
1	G	199	LYS
1	G	207	ILE
1	G	217	LEU
1	G	219	ARG
1	G	224	VAL
1	G	234	LEU
1	G	239	SER
1	G	256	LYS
1	J	5	GLU
1	J	11	ILE
1	J	17	LYS
1	J	31	LEU
1	J	43	ARG
1	J	46	LYS
1	J	48	LEU
1	J	52	LEU
1	J	53	GLU
1	J	54	GLN
1	J	55	LEU
1	J	56	ASN
1	J	57	GLN
1	J	62	LEU
1	J	73	VAL

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Mol	Chain	Res	Type
1	J	84	VAL
1	J	87	ILE
1	J	103	ARG
1	J	112	GLU
1	J	115	LEU
1	J	127	ILE
1	J	154	VAL
1	J	155	GLN
1	J	158	ASN
1	J	178	LEU
1	J	185	VAL
1	J	194	ARG
1	J	196	LEU
1	J	208	LEU
1	J	209	LYS
1	J	213	GLU
1	J	216	PRO
1	J	217	LEU
1	J	224	VAL
1	J	234	LEU
1	J	246	ILE
1	J	255	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	6	ASN
1	A	56	ASN
1	A	57	GLN
1	A	130	HIS
1	A	170	ASN
1	A	220	ASN
1	D	3	ASN
1	D	54	GLN
1	D	56	ASN
1	D	75	ASN
1	D	130	HIS
1	D	170	ASN
1	D	220	ASN
1	G	6	ASN
1	G	54	GLN

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Mol	Chain	Res	Type
1	G	56	ASN
1	G	57	GLN
1	G	68	GLN
1	G	170	ASN
1	J	3	ASN
1	J	54	GLN
1	J	56	ASN
1	J	57	GLN
1	J	64	GLN
1	J	130	HIS
1	J	170	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	NAP	G	257	-	50,52,52	5.29	9 (18%)	71,80,80	3.45	29 (40%)
2	NAP	J	257	-	50,52,52	4.45	12 (24%)	71,80,80	4.13	33 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	D	257	-	50,52,52	5.65	10 (20%)	71,80,80	4.41	24 (33%)
2	NAP	A	361	-	50,52,52	4.96	13 (26%)	71,80,80	3.20	28 (39%)
3	TCL	A	371	-	18,18,18	2.05	5 (27%)	25,25,25	0.97	2 (8%)
3	TCL	J	258	-	18,18,18	2.05	5 (27%)	25,25,25	0.97	2 (8%)
3	TCL	D	258	-	18,18,18	2.05	5 (27%)	25,25,25	0.96	2 (8%)
3	TCL	G	258	-	18,18,18	2.04	5 (27%)	25,25,25	0.97	2 (8%)

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	NAP	G	257	-	-	6/35/67/67	0/5/5/5
2	NAP	J	257	-	-	5/35/67/67	0/5/5/5
2	NAP	D	257	-	-	6/35/67/67	0/5/5/5
2	NAP	A	361	-	-	5/35/67/67	0/5/5/5
3	TCL	A	371	-	-	2/4/4/4	0/2/2/2
3	TCL	J	258	-	-	2/4/4/4	0/2/2/2
3	TCL	D	258	-	-	2/4/4/4	0/2/2/2
3	TCL	G	258	-	-	2/4/4/4	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	257	NAP	C2N-N1N	26.13	1.63	1.35
2	D	257	NAP	C2N-N1N	25.35	1.62	1.35
2	A	361	NAP	C2N-N1N	23.21	1.60	1.35
2	D	257	NAP	C7N-N7N	-17.78	1.00	1.33
2	J	257	NAP	C4N-C3N	15.54	1.63	1.39
2	G	257	NAP	C2N-C3N	14.73	1.62	1.39
2	G	257	NAP	C3N-C7N	-13.76	1.30	1.50
2	A	361	NAP	C2N-C3N	13.75	1.60	1.39
2	D	257	NAP	C4N-C3N	13.29	1.59	1.39
2	J	257	NAP	C2N-C3N	13.15	1.59	1.39
2	D	257	NAP	C2N-C3N	12.39	1.58	1.39
2	J	257	NAP	C6N-C5N	12.07	1.63	1.38
2	J	257	NAP	C7N-N7N	-11.87	1.11	1.33
2	J	257	NAP	O7N-C7N	10.86	1.44	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	NAP	C5N-C4N	10.85	1.57	1.38
2	A	361	NAP	C6N-N1N	10.69	1.59	1.35
2	A	361	NAP	C7N-N7N	-10.21	1.14	1.33
2	G	257	NAP	C6N-C5N	10.11	1.59	1.38
2	D	257	NAP	C5N-C4N	9.10	1.54	1.38
2	J	257	NAP	C2N-N1N	9.02	1.44	1.35
2	A	361	NAP	C6N-C5N	8.58	1.56	1.38
2	D	257	NAP	C6N-C5N	8.56	1.56	1.38
2	D	257	NAP	C6N-N1N	8.41	1.54	1.35
2	G	257	NAP	C6N-N1N	6.76	1.50	1.35
2	G	257	NAP	O4D-C1D	6.70	1.49	1.40
2	G	257	NAP	C7N-N7N	-6.50	1.21	1.33
3	A	371	TCL	C8-C9	5.31	1.48	1.39
3	J	258	TCL	C8-C9	5.30	1.48	1.39
3	G	258	TCL	C8-C9	5.28	1.48	1.39
3	D	258	TCL	C8-C9	5.25	1.48	1.39
3	D	258	TCL	C6-C5	4.89	1.48	1.40
3	J	258	TCL	C6-C5	4.86	1.48	1.40
3	A	371	TCL	C6-C5	4.84	1.48	1.40
3	G	258	TCL	C6-C5	4.82	1.48	1.40
2	D	257	NAP	O4D-C1D	4.73	1.47	1.40
2	G	257	NAP	O7N-C7N	4.19	1.31	1.24
2	A	361	NAP	O4D-C1D	3.83	1.45	1.40
2	D	257	NAP	C2A-N1A	3.67	1.40	1.33
2	J	257	NAP	O4D-C1D	3.50	1.45	1.40
2	J	257	NAP	C8A-N7A	3.47	1.38	1.31
2	A	361	NAP	O7N-C7N	-3.17	1.18	1.24
2	A	361	NAP	C2A-N1A	3.16	1.39	1.33
2	J	257	NAP	P2B-O2B	2.82	1.64	1.59
3	D	258	TCL	C9-CL16	2.71	1.80	1.73
2	J	257	NAP	C5N-C4N	-2.71	1.34	1.38
3	A	371	TCL	C9-CL16	2.70	1.80	1.73
3	J	258	TCL	C9-CL16	2.69	1.80	1.73
3	G	258	TCL	C9-CL16	2.69	1.80	1.73
2	G	257	NAP	PA-O3	2.58	1.62	1.59
2	A	361	NAP	O4B-C4B	-2.55	1.39	1.45
2	A	361	NAP	P2B-O2B	2.53	1.64	1.59
2	A	361	NAP	C5A-N7A	-2.49	1.34	1.39
2	A	361	NAP	C2A-N3A	2.46	1.38	1.33
3	D	258	TCL	C11-CL15	2.40	1.80	1.74
2	J	257	NAP	C2A-N3A	2.40	1.38	1.33
3	J	258	TCL	C11-CL15	2.39	1.80	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	371	TCL	C2-CL14	2.39	1.80	1.74
3	J	258	TCL	C2-CL14	2.38	1.80	1.74
3	D	258	TCL	C2-CL14	2.37	1.80	1.74
3	A	371	TCL	C11-CL15	2.36	1.79	1.74
3	G	258	TCL	C2-CL14	2.35	1.79	1.74
3	G	258	TCL	C11-CL15	2.35	1.79	1.74
2	D	257	NAP	PN-O3	-2.10	1.57	1.59
2	J	257	NAP	C3D-C4D	-2.07	1.47	1.53

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	257	NAP	O7N-C7N-N7N	22.11	154.56	122.62
2	D	257	NAP	O7N-C7N-C3N	-18.36	97.14	119.60
2	A	361	NAP	C2N-C3N-C4N	-14.78	101.07	118.26
2	J	257	NAP	C2N-N1N-C1D	-12.61	91.29	119.13
2	J	257	NAP	O7N-C7N-C3N	-12.27	104.59	119.60
2	G	257	NAP	C6N-N1N-C1D	11.55	142.40	119.73
2	J	257	NAP	C6N-N1N-C1D	11.38	142.06	119.73
2	G	257	NAP	C2N-N1N-C1D	-10.81	95.27	119.13
2	J	257	NAP	C2N-C3N-C7N	10.64	150.18	119.46
2	J	257	NAP	O7N-C7N-N7N	10.39	137.63	122.62
2	D	257	NAP	C6N-C5N-C4N	9.55	133.21	119.45
2	G	257	NAP	C5N-C4N-C3N	9.13	129.34	120.36
2	D	257	NAP	C5N-C6N-N1N	-8.80	108.38	120.38
2	A	361	NAP	C4N-C3N-C7N	-8.48	97.96	121.06
2	J	257	NAP	C4N-C3N-C7N	-8.46	98.01	121.06
2	G	257	NAP	C2N-C3N-C7N	8.15	142.99	119.46
2	A	361	NAP	C4D-O4D-C1D	8.02	117.27	109.92
2	G	257	NAP	C4N-C3N-C7N	-7.83	99.75	121.06
2	G	257	NAP	N3A-C2A-N1A	-7.71	116.91	128.58
2	D	257	NAP	C3N-C7N-N7N	-7.67	108.29	117.74
2	J	257	NAP	C4D-O4D-C1D	7.53	116.82	109.92
2	A	361	NAP	C5N-C6N-N1N	-7.00	110.83	120.38
2	J	257	NAP	N9A-C8A-N7A	-6.82	104.26	113.94
2	G	257	NAP	C4D-O4D-C1D	6.48	115.86	109.92
2	D	257	NAP	C4N-C3N-C7N	-6.33	103.83	121.06
2	J	257	NAP	N3A-C2A-N1A	-5.85	119.72	128.58
2	D	257	NAP	C2N-C3N-C4N	-5.78	111.54	118.26
2	A	361	NAP	N3A-C2A-N1A	-5.75	119.88	128.58
2	J	257	NAP	C2N-C3N-C4N	-5.61	111.73	118.26
2	A	361	NAP	N9A-C8A-N7A	-5.44	106.22	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	257	NAP	N9A-C8A-N7A	-5.36	106.33	113.94
2	J	257	NAP	C5A-C4A-N3A	-5.31	119.40	126.72
2	J	257	NAP	C5A-N7A-C8A	5.29	111.77	103.45
2	A	361	NAP	C6N-N1N-C1D	5.11	129.75	119.73
2	D	257	NAP	C2N-C3N-C7N	5.05	134.03	119.46
2	D	257	NAP	C4D-O4D-C1D	4.96	114.46	109.92
2	A	361	NAP	C5A-N7A-C8A	4.94	111.21	103.45
2	J	257	NAP	C6N-N1N-C2N	4.59	125.78	121.88
2	D	257	NAP	N3A-C2A-N1A	-4.56	121.68	128.58
2	D	257	NAP	C6N-N1N-C1D	4.48	128.53	119.73
2	J	257	NAP	C2A-N3A-C4A	4.46	122.73	111.83
2	J	257	NAP	O3-PA-O1A	-4.41	97.45	110.70
2	J	257	NAP	C4A-N9A-C8A	4.33	110.28	105.74
2	D	257	NAP	O4B-C1B-C2B	-4.30	99.18	106.59
2	D	257	NAP	C2N-N1N-C1D	-4.28	109.69	119.13
2	G	257	NAP	C3N-C7N-N7N	4.12	122.82	117.74
2	G	257	NAP	C5A-N7A-C8A	4.07	109.85	103.45
2	A	361	NAP	C2N-N1N-C1D	-3.95	110.42	119.13
2	D	257	NAP	O2D-C2D-C3D	-3.93	99.22	111.82
2	A	361	NAP	C4A-C5A-N7A	-3.92	106.09	110.58
2	G	257	NAP	C6N-N1N-C2N	-3.85	118.60	121.88
2	G	257	NAP	C2A-N1A-C6A	3.74	124.88	118.73
2	G	257	NAP	C4A-N9A-C8A	3.72	109.65	105.74
2	J	257	NAP	N3A-C4A-N9A	3.68	133.43	127.17
2	G	257	NAP	C5A-C4A-N3A	-3.68	121.65	126.72
2	A	361	NAP	O4B-C1B-N9A	3.68	115.15	108.09
2	J	257	NAP	C4A-C5A-N7A	-3.52	106.56	110.58
2	G	257	NAP	C2A-N3A-C4A	3.49	120.37	111.83
2	G	257	NAP	C5N-C6N-N1N	-3.40	115.75	120.38
2	J	257	NAP	O4B-C1B-C2B	-3.39	100.74	106.59
2	A	361	NAP	O2A-PA-O3	3.38	116.41	107.27
2	A	361	NAP	C2B-C1B-N9A	-3.27	108.37	113.75
2	J	257	NAP	O5D-C5D-C4D	3.21	119.91	108.99
2	G	257	NAP	O4D-C4D-C5D	3.20	119.59	109.33
2	A	361	NAP	C6N-C5N-C4N	-3.19	114.85	119.45
2	J	257	NAP	O4D-C4D-C5D	3.17	119.50	109.33
2	J	257	NAP	O2D-C2D-C3D	-3.17	101.66	111.82
2	G	257	NAP	O3D-C3D-C4D	-3.15	102.03	111.08
2	J	257	NAP	O3D-C3D-C4D	-3.08	102.24	111.08
2	G	257	NAP	O4B-C1B-N9A	3.02	113.90	108.09
2	A	361	NAP	C6N-N1N-C2N	-2.90	119.41	121.88
2	G	257	NAP	C2N-C3N-C4N	-2.90	114.89	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	NAP	C5N-C4N-C3N	2.87	123.19	120.36
2	G	257	NAP	N3A-C4A-N9A	2.85	132.01	127.17
2	A	361	NAP	C4A-N9A-C8A	2.79	108.67	105.74
2	J	257	NAP	C3B-C2B-C1B	-2.77	97.50	102.81
2	A	361	NAP	O4B-C1B-C2B	-2.75	101.85	106.59
2	A	361	NAP	O2N-PN-O1N	2.70	125.00	112.44
2	D	257	NAP	O3D-C3D-C4D	-2.69	103.36	111.08
2	A	361	NAP	C5A-C4A-N3A	-2.66	123.05	126.72
2	D	257	NAP	O4D-C4D-C5D	2.59	117.63	109.33
2	D	257	NAP	O2A-PA-O3	2.58	114.25	107.27
2	J	257	NAP	O4B-C1B-N9A	2.58	113.05	108.09
2	G	257	NAP	O4B-C1B-C2B	-2.58	102.15	106.59
2	G	257	NAP	O2N-PN-O3	2.57	114.23	107.27
2	J	257	NAP	O5B-C5B-C4B	-2.49	100.51	108.99
2	A	361	NAP	O3-PN-O1N	-2.48	103.24	110.70
2	G	257	NAP	O3-PN-O1N	-2.48	103.25	110.70
2	A	361	NAP	O4D-C4D-C3D	-2.48	100.23	105.15
2	J	257	NAP	C5N-C6N-N1N	-2.47	117.01	120.38
2	G	257	NAP	C5B-C4B-C3B	-2.46	106.34	115.21
2	G	257	NAP	C4A-C5A-N7A	-2.44	107.79	110.58
2	A	361	NAP	C2N-C3N-C7N	2.41	126.43	119.46
2	D	257	NAP	C5A-C4A-N3A	-2.40	123.41	126.72
2	A	361	NAP	C4A-N9A-C1B	-2.39	121.04	126.63
2	D	257	NAP	C5N-C4N-C3N	-2.37	118.04	120.36
3	A	371	TCL	O7-C5-C6	2.35	120.56	116.59
3	J	258	TCL	O7-C5-C6	2.34	120.54	116.59
2	J	257	NAP	C3N-C7N-N7N	-2.34	114.86	117.74
3	G	258	TCL	O7-C5-C6	2.33	120.53	116.59
3	D	258	TCL	O7-C5-C6	2.32	120.52	116.59
2	D	257	NAP	O2B-P2B-O1X	-2.31	101.11	109.33
2	D	257	NAP	C5D-C4D-C3D	-2.30	106.94	115.21
2	D	257	NAP	O2N-PN-O1N	2.29	123.10	112.44
2	A	361	NAP	C2A-N3A-C4A	2.27	117.37	111.83
2	J	257	NAP	O3D-C3D-C2D	-2.26	104.58	111.82
2	G	257	NAP	O2N-PN-O1N	2.22	122.77	112.44
2	J	257	NAP	O3-PN-O1N	-2.21	104.05	110.70
2	A	361	NAP	C2A-N1A-C6A	2.18	122.31	118.73
2	A	361	NAP	O2D-C2D-C3D	-2.15	104.91	111.82
2	G	257	NAP	O7N-C7N-N7N	-2.15	119.51	122.62
2	J	257	NAP	O2X-P2B-O2B	2.12	114.10	105.85
2	G	257	NAP	C4B-O4B-C1B	-2.10	104.82	109.47
2	D	257	NAP	O4B-C1B-N9A	2.09	112.11	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	NAP	O5B-C5B-C4B	-2.09	101.87	108.99
2	J	257	NAP	C4B-O4B-C1B	-2.07	104.90	109.47
2	D	257	NAP	C2A-N3A-C4A	2.06	116.86	111.83
3	D	258	TCL	C4-C3-C2	2.05	121.30	119.24
3	J	258	TCL	C4-C3-C2	2.04	121.29	119.24
3	G	258	TCL	C13-C12-C11	2.04	121.29	119.24
3	A	371	TCL	C13-C12-C11	2.04	121.29	119.24
2	J	257	NAP	O3B-C3B-C2B	-2.01	105.56	111.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	361	NAP	C5D-O5D-PN-O3
2	A	361	NAP	C5D-O5D-PN-O1N
2	D	257	NAP	C5D-O5D-PN-O3
2	D	257	NAP	C5D-O5D-PN-O1N
2	D	257	NAP	C5D-O5D-PN-O2N
2	G	257	NAP	C5D-O5D-PN-O3
2	G	257	NAP	C5D-O5D-PN-O1N
2	G	257	NAP	C5D-O5D-PN-O2N
2	G	257	NAP	O4D-C1D-N1N-C6N
2	G	257	NAP	C2D-C1D-N1N-C6N
2	J	257	NAP	C5D-O5D-PN-O3
3	A	371	TCL	C6-C5-O7-C8
3	D	258	TCL	C6-C5-O7-C8
3	D	258	TCL	C4-C5-O7-C8
3	G	258	TCL	C6-C5-O7-C8
3	G	258	TCL	C4-C5-O7-C8
3	J	258	TCL	C6-C5-O7-C8
3	A	371	TCL	C4-C5-O7-C8
3	J	258	TCL	C4-C5-O7-C8
2	A	361	NAP	C2N-C3N-C7N-O7N
2	A	361	NAP	PA-O3-PN-O2N
2	D	257	NAP	C5B-O5B-PA-O1A
2	J	257	NAP	C5D-O5D-PN-O1N
2	J	257	NAP	C2B-O2B-P2B-O3X
2	J	257	NAP	C2D-C1D-N1N-C6N
2	J	257	NAP	O4D-C1D-N1N-C6N
2	A	361	NAP	PA-O3-PN-O1N
2	D	257	NAP	O4B-C4B-C5B-O5B
2	D	257	NAP	PA-O3-PN-O2N

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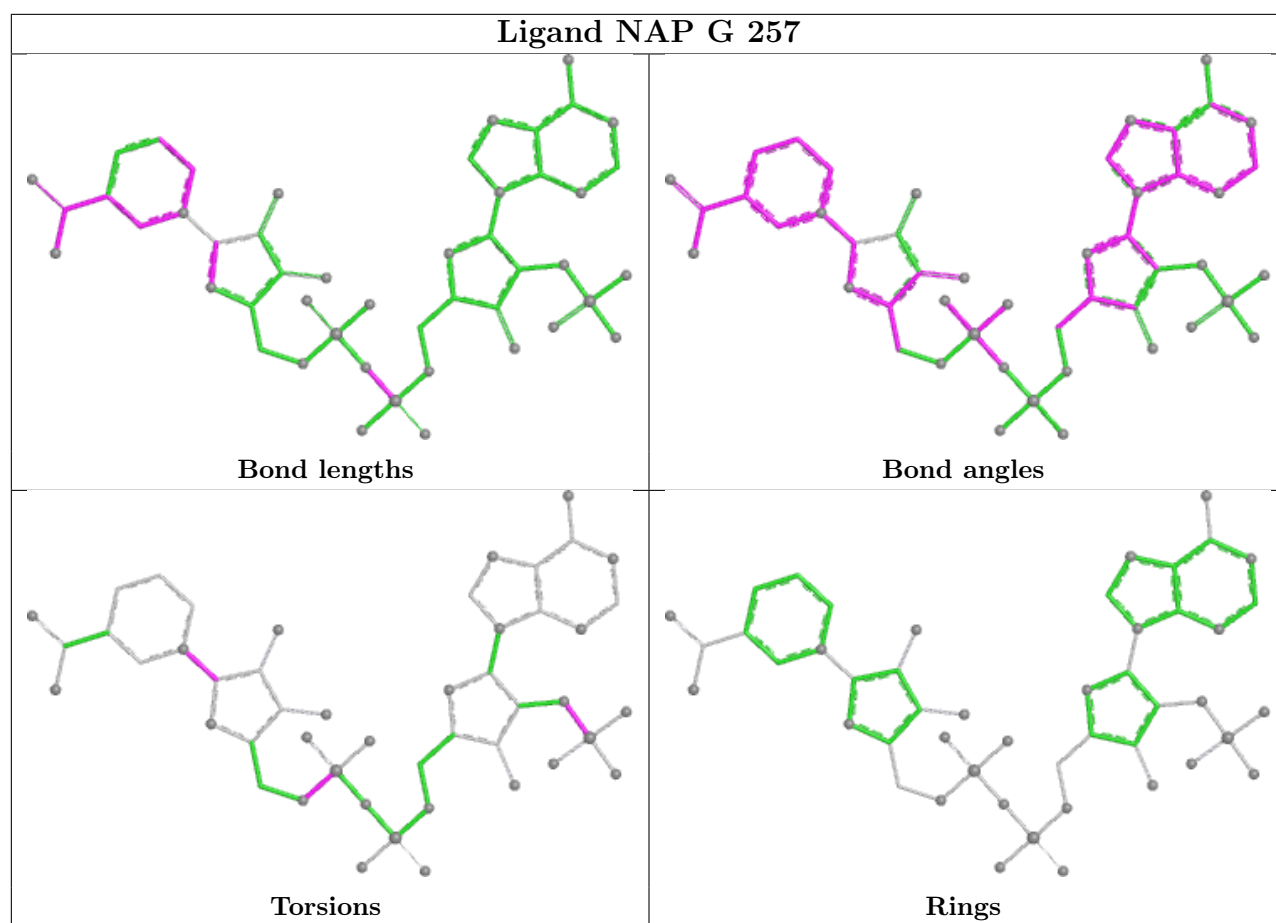
Mol	Chain	Res	Type	Atoms
2	G	257	NAP	C2B-O2B-P2B-O1X

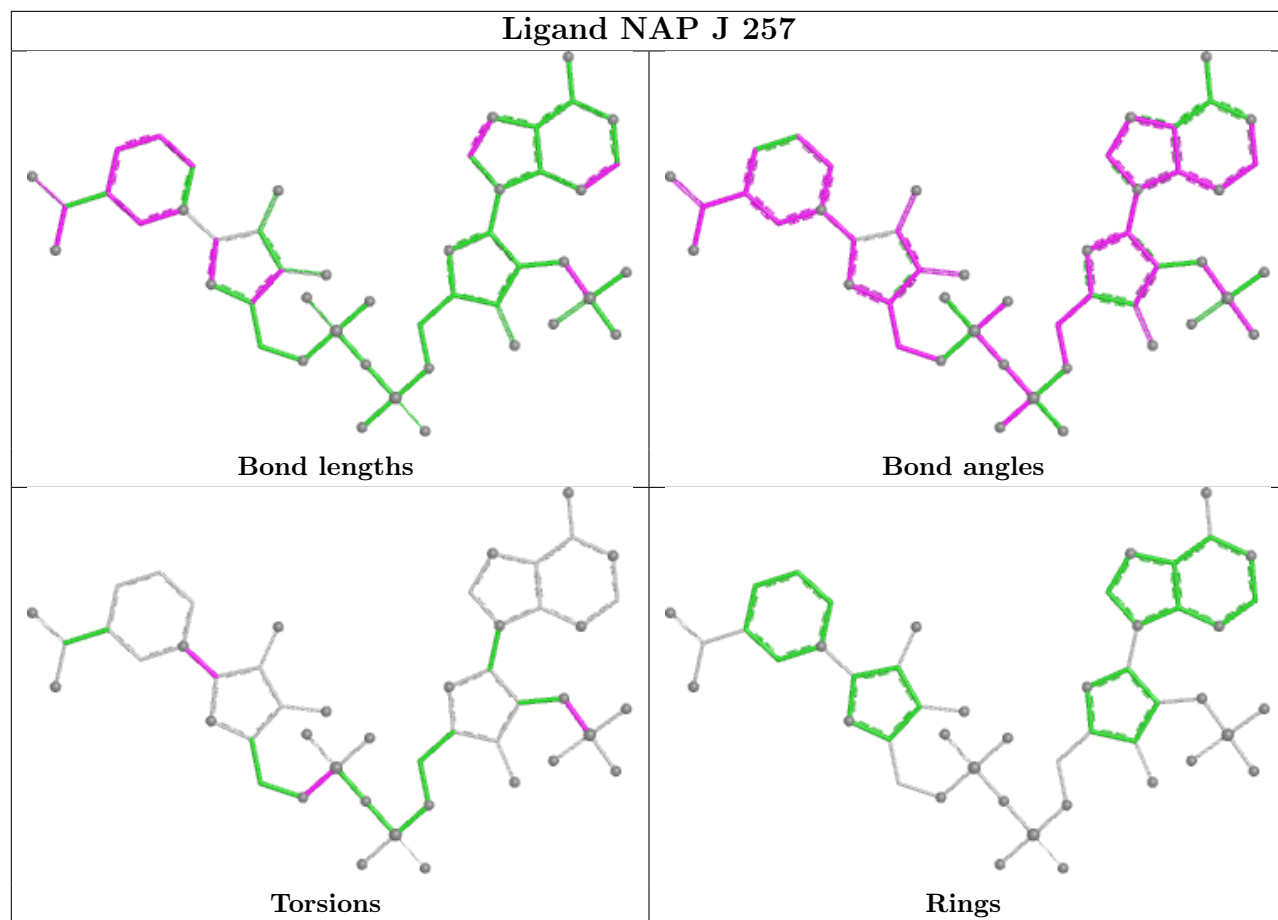
There are no ring outliers.

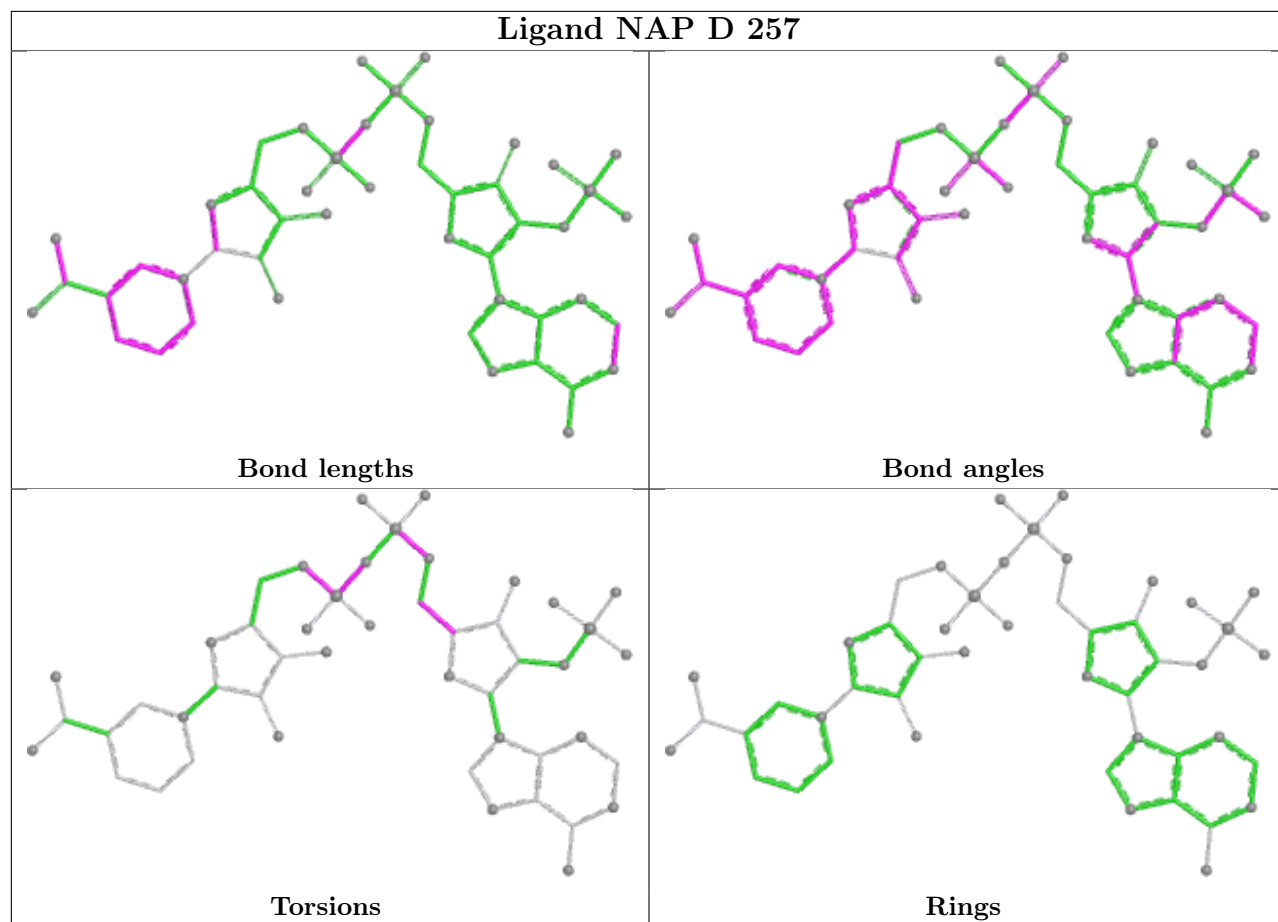
8 monomers are involved in 40 short contacts:

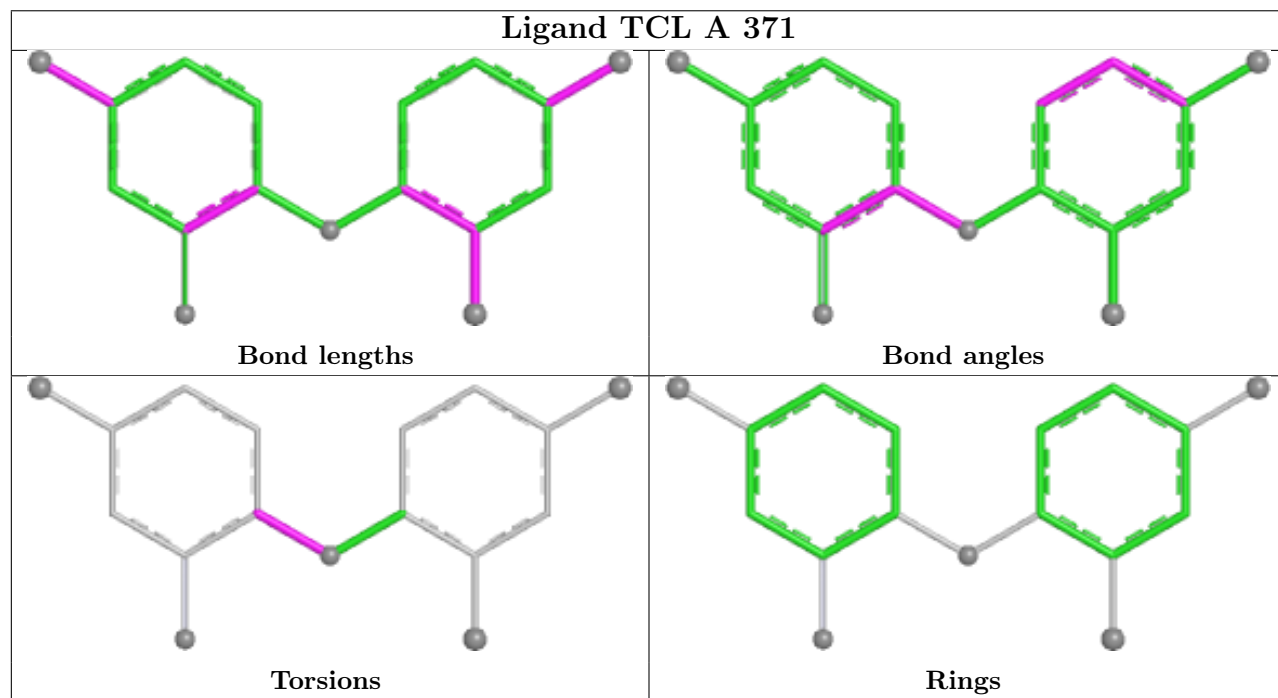
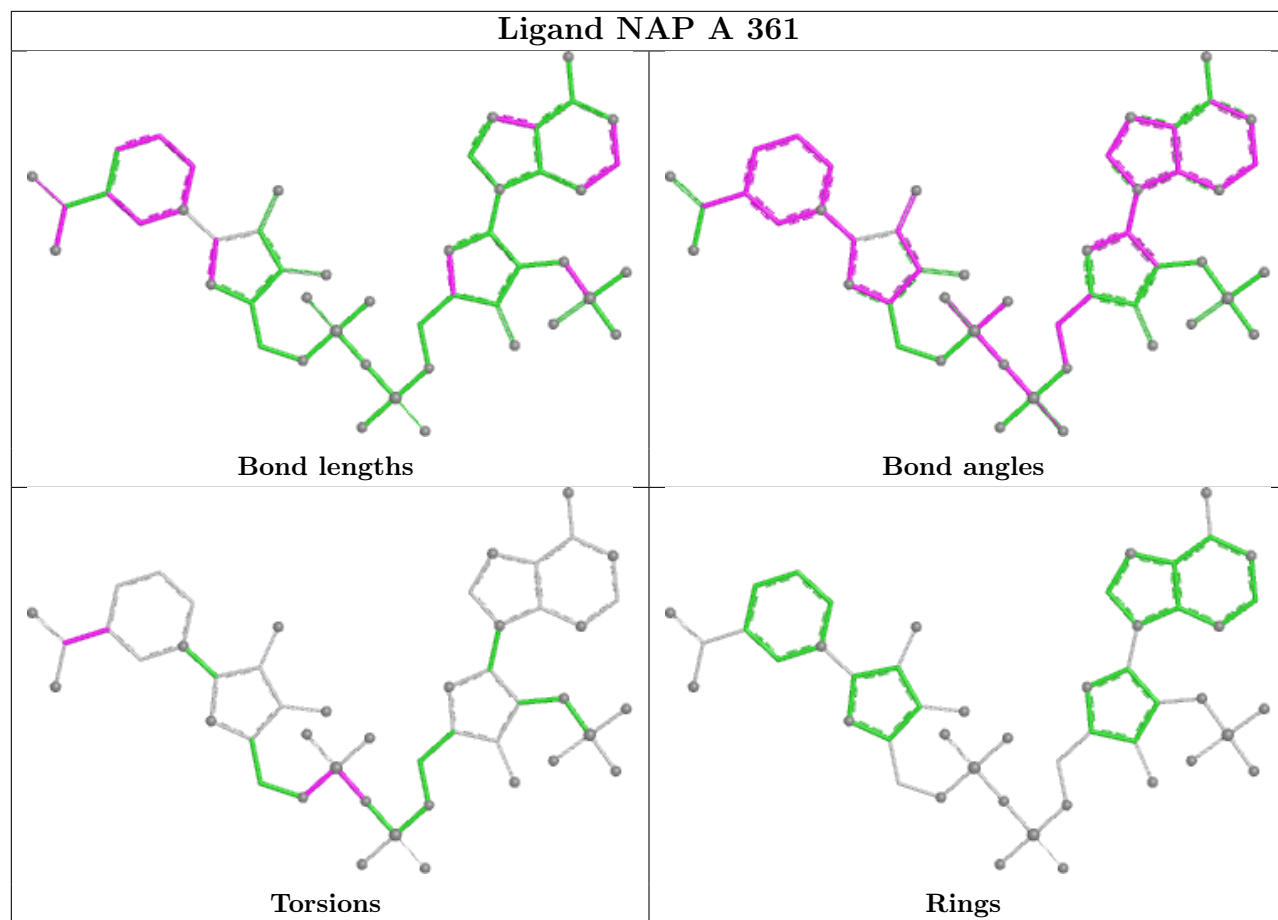
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	257	NAP	3	0
2	J	257	NAP	7	0
2	D	257	NAP	10	0
2	A	361	NAP	7	0
3	A	371	TCL	6	0
3	J	258	TCL	3	0
3	D	258	TCL	6	0
3	G	258	TCL	3	0

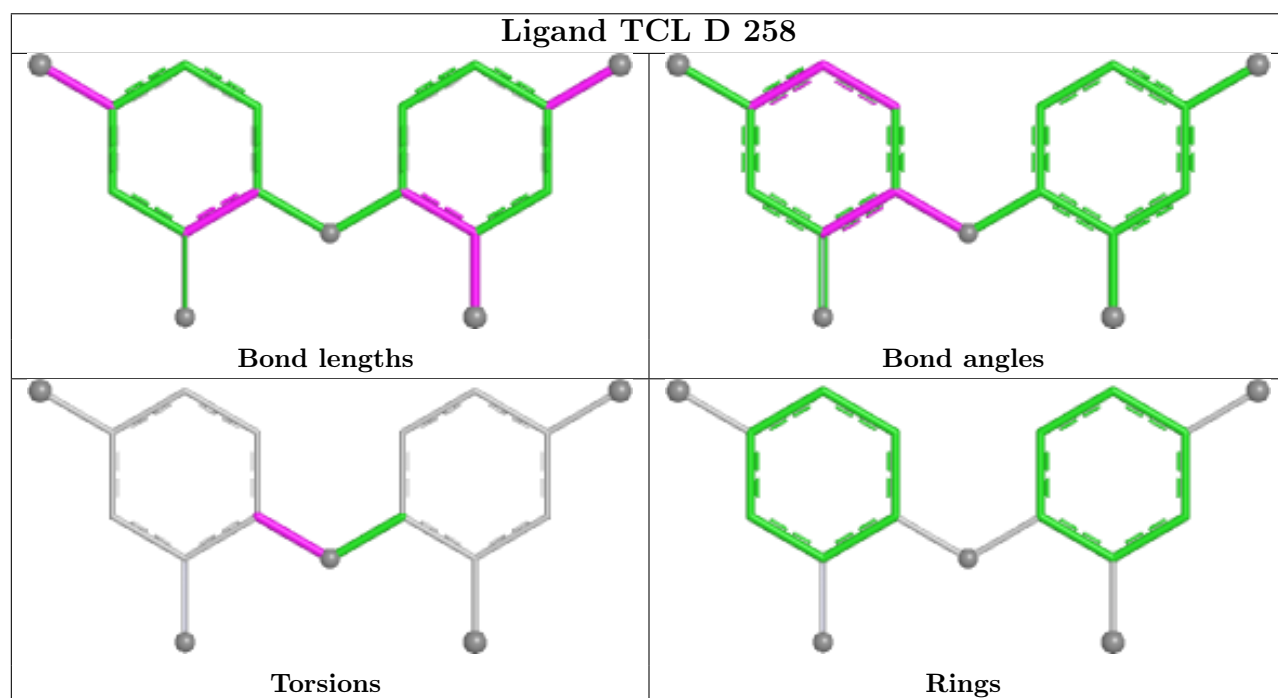
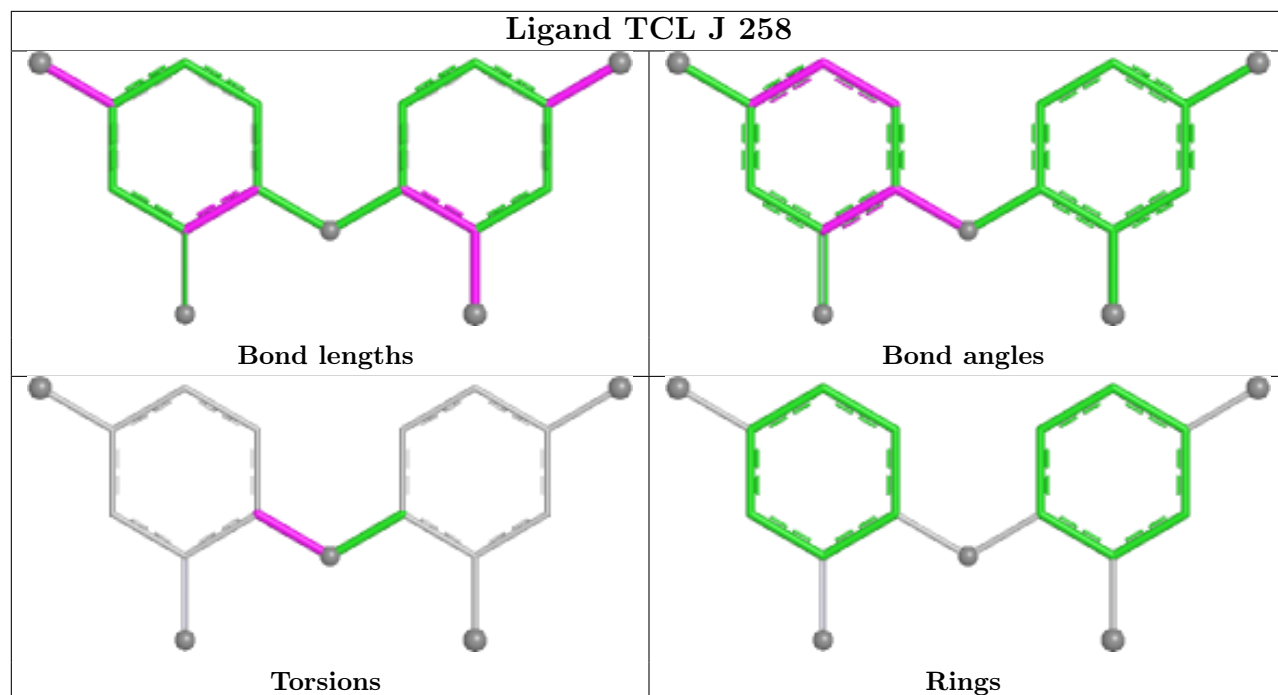
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

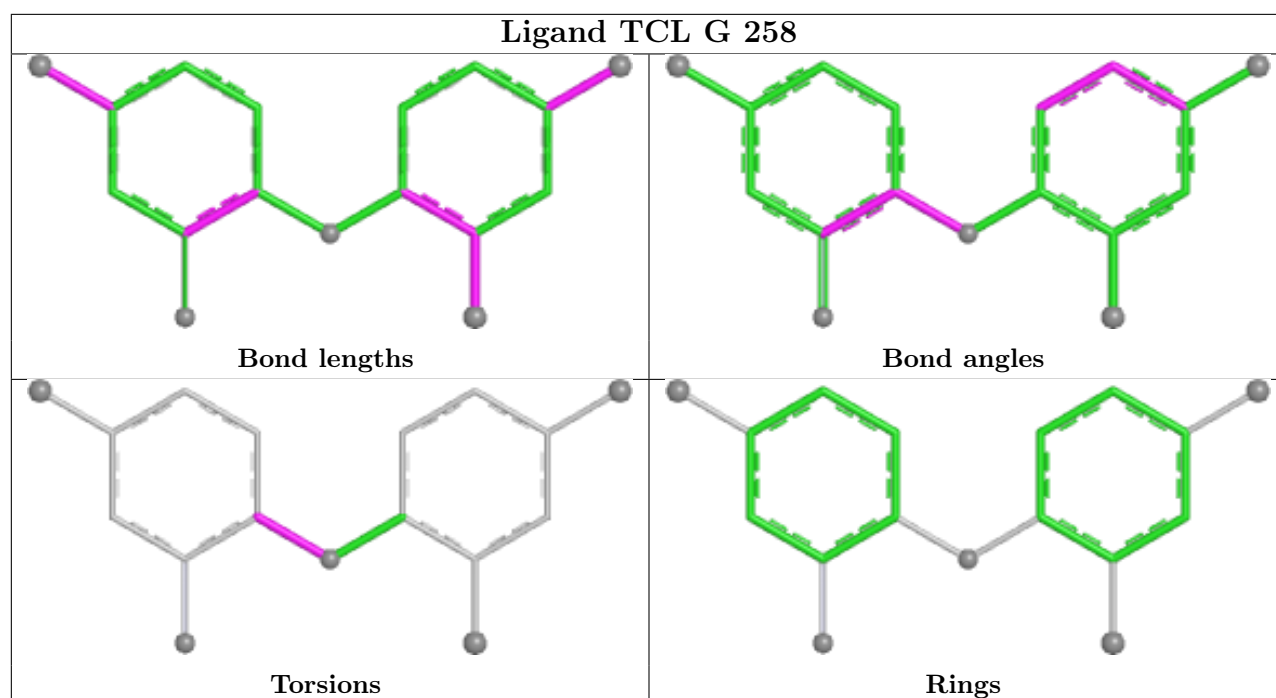












5.7 Other polymers [i](#)

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	255/260 (98%)	-0.39	7 (2%) 56 58	6, 16, 31, 50	0
1	D	260/260 (100%)	-0.19	10 (3%) 44 46	8, 19, 40, 52	0
1	G	254/260 (97%)	-0.23	15 (5%) 28 29	8, 18, 40, 60	0
1	J	260/260 (100%)	-0.12	15 (5%) 29 30	7, 19, 48, 60	0
All	All	1029/1040 (98%)	-0.23	47 (4%) 37 38	6, 18, 41, 60	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	60	ALA	8.7
1	J	60	ALA	7.5
1	A	60	ALA	7.4
1	G	60	ALA	5.3
1	A	2	LEU	5.3
1	J	-2	ALA	5.1
1	G	4	LEU	4.8
1	D	-3	LEU	4.7
1	J	55	LEU	4.3
1	J	103	ARG	4.0
1	D	-1	ALA	3.9
1	J	0	ALA	3.7
1	G	3	ASN	3.7
1	G	43	ARG	3.5
1	J	43	ARG	3.5
1	D	59	GLU	3.4
1	A	207	ILE	3.3
1	J	59	GLU	3.2
1	G	53	GLU	3.1
1	J	-1	ALA	3.1
1	J	44	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	-3	LEU	2.9
1	D	99	MET	2.9
1	D	0	ALA	2.8
1	G	47	GLU	2.7
1	D	52	LEU	2.7
1	A	4	LEU	2.7
1	G	155	GLN	2.7
1	G	99	MET	2.6
1	G	55	LEU	2.5
1	A	59	GLU	2.5
1	A	155	GLN	2.5
1	G	59	GLU	2.4
1	J	207	ILE	2.3
1	A	3	ASN	2.3
1	G	6	ASN	2.3
1	D	103	ARG	2.3
1	G	42	GLU	2.3
1	J	52	LEU	2.2
1	G	44	SER	2.2
1	J	155	GLN	2.2
1	G	58	PRO	2.2
1	G	46	LYS	2.2
1	D	55	LEU	2.1
1	D	104	GLY	2.1
1	J	58	PRO	2.0
1	J	42	GLU	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](#)

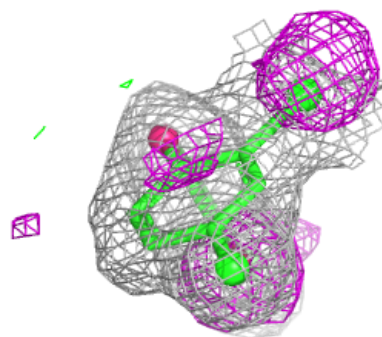
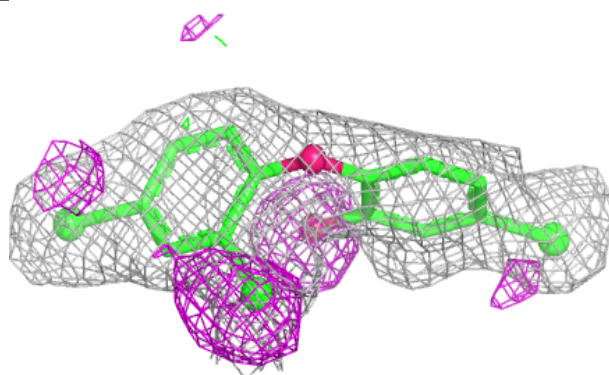
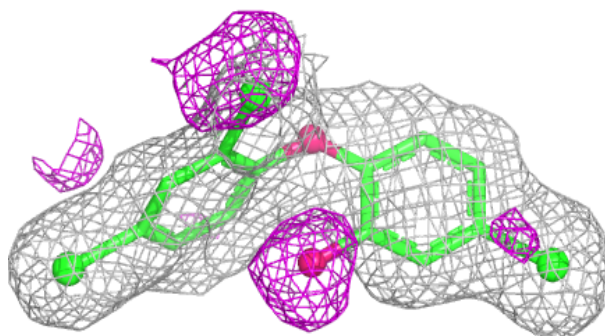
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	TCL	D	258	17/17	0.85	0.14	25,29,35,42	0
3	TCL	J	258	17/17	0.87	0.13	19,25,34,39	0
3	TCL	A	371	17/17	0.90	0.12	16,21,28,32	0
3	TCL	G	258	17/17	0.92	0.10	18,20,26,32	0
2	NAP	J	257	48/48	0.93	0.09	14,20,32,33	0
2	NAP	G	257	48/48	0.94	0.09	9,16,33,41	0
2	NAP	D	257	48/48	0.94	0.09	5,16,24,30	0
2	NAP	A	361	48/48	0.97	0.06	6,14,24,27	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.

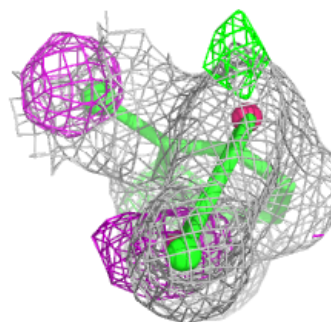
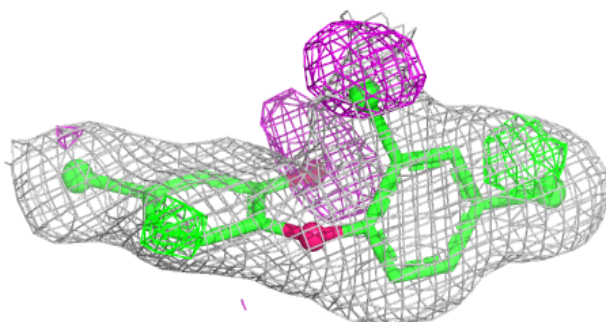
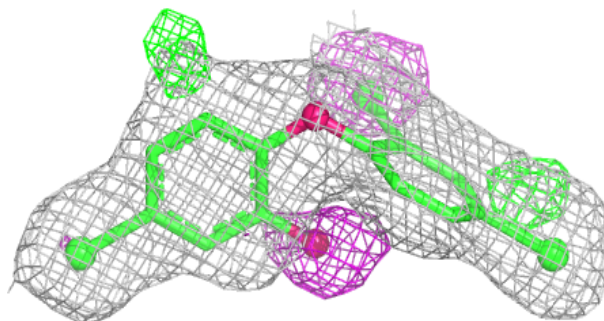
Electron density around TCL D 258:

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

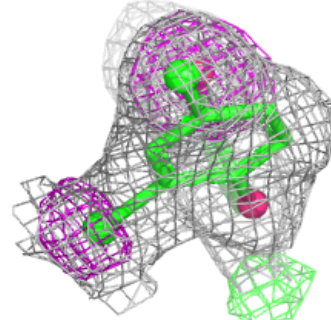
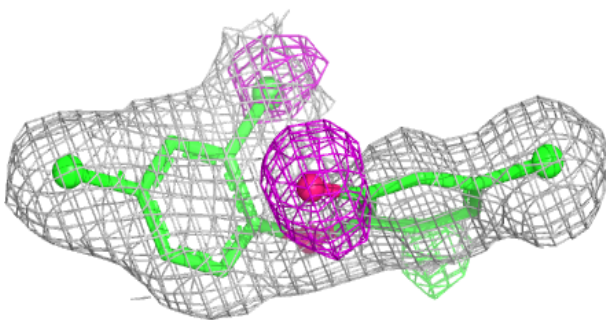
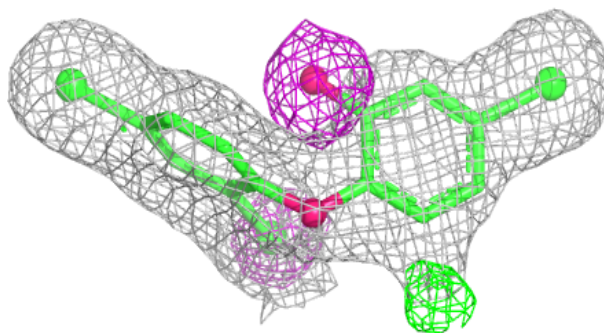


Electron density around TCL J 258:

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

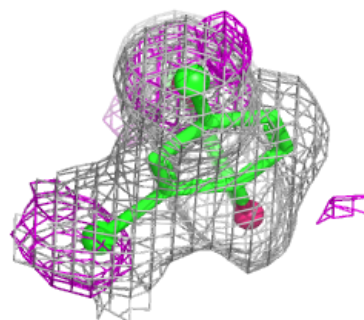
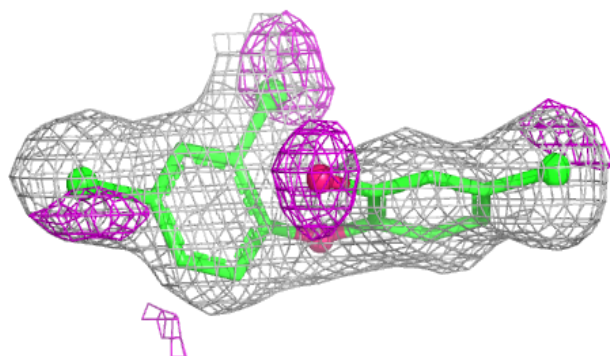
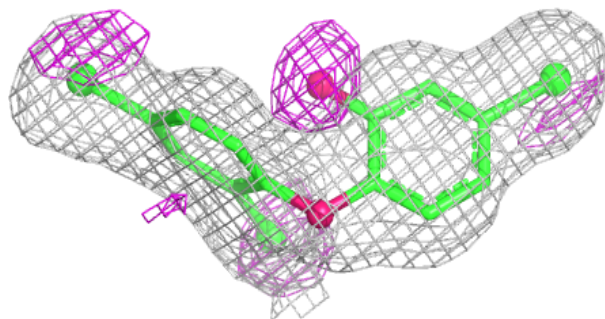
**Electron density around TCL A 371:**

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

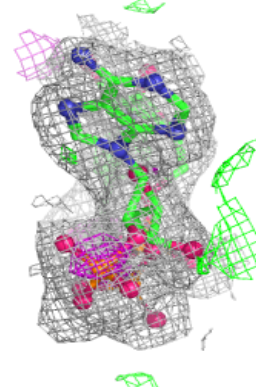
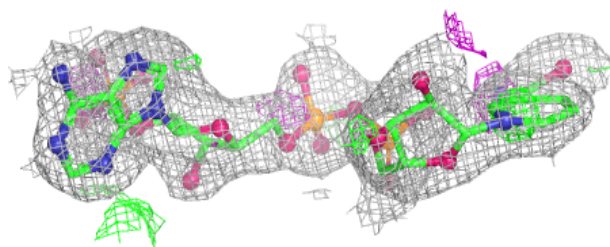
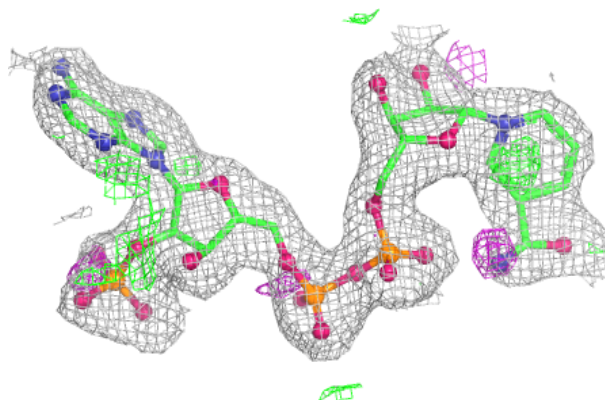


Electron density around TCL G 258:

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

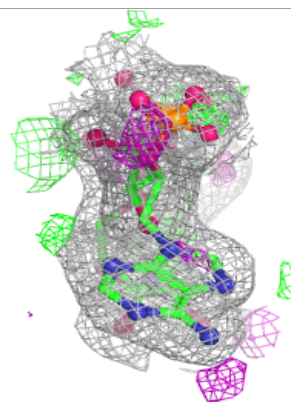
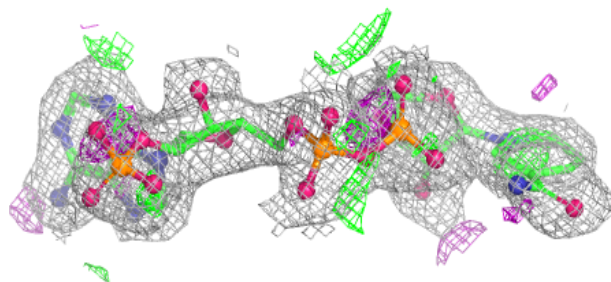
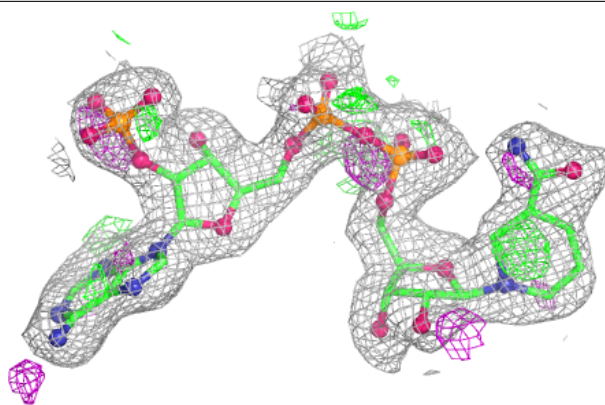
**Electron density around NAP J 257:**

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

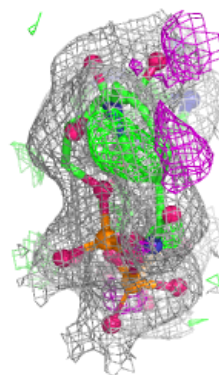
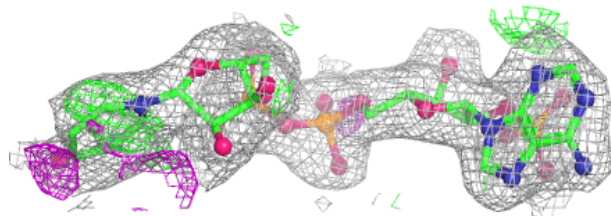
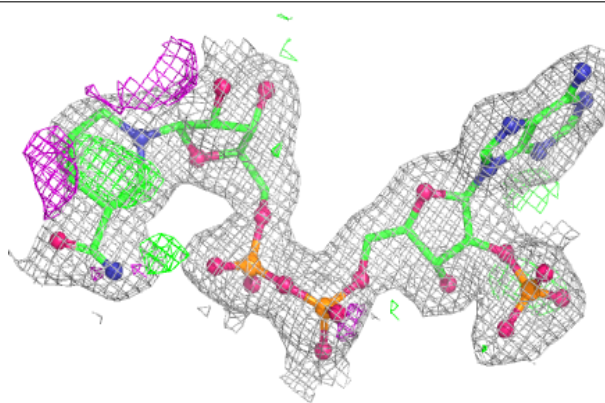


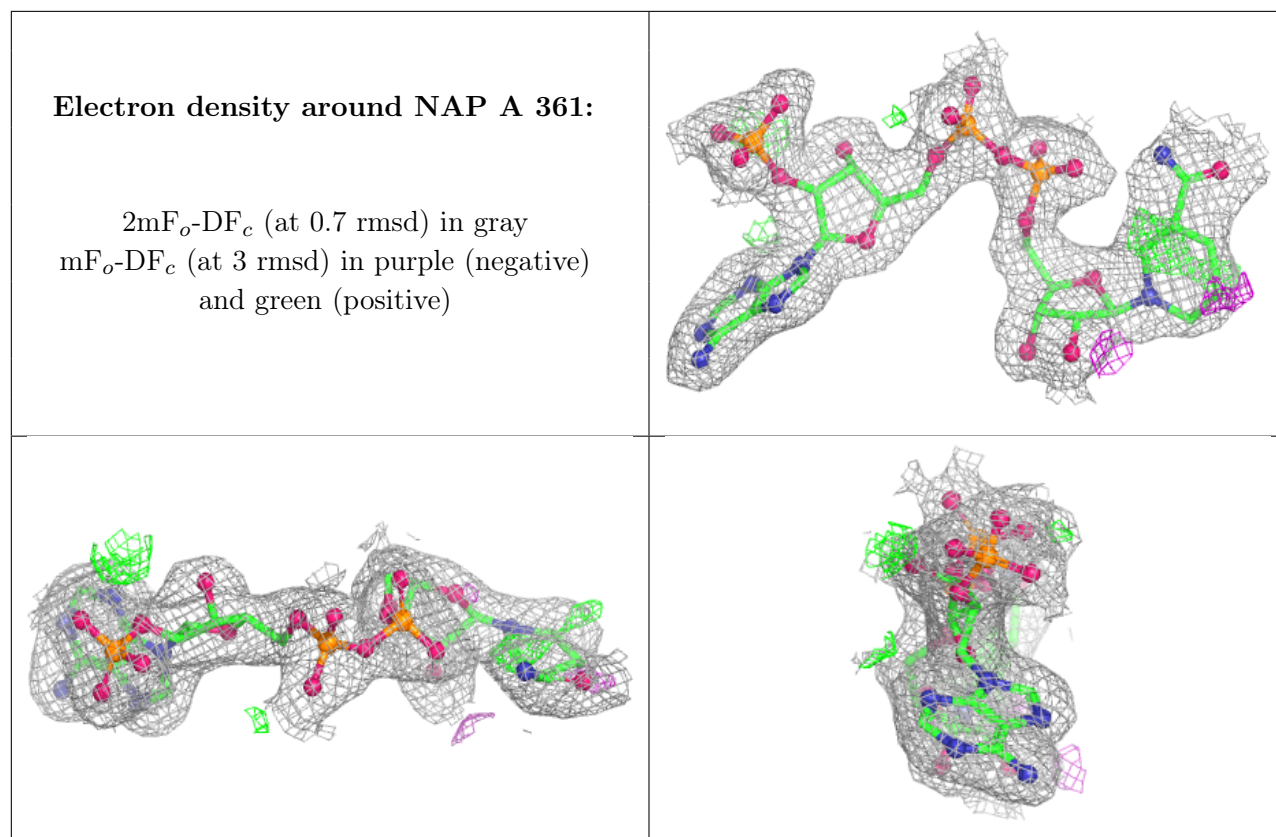
Electron density around NAP G 257:

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

**Electron density around NAP D 257:**

$2mF_o-DF_c$ (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.