



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:14 AM UTC

PDB ID : 5GUD / pdb_00005gud
Title : Glutamate dehydrogenase from *Corynebacterium glutamicum* (alpha-iminoglutarate/NADP+ complex)
Authors : Tomita, T.; Nishiyama, M.
Deposited on : 2016-08-28
Resolution : 1.68 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

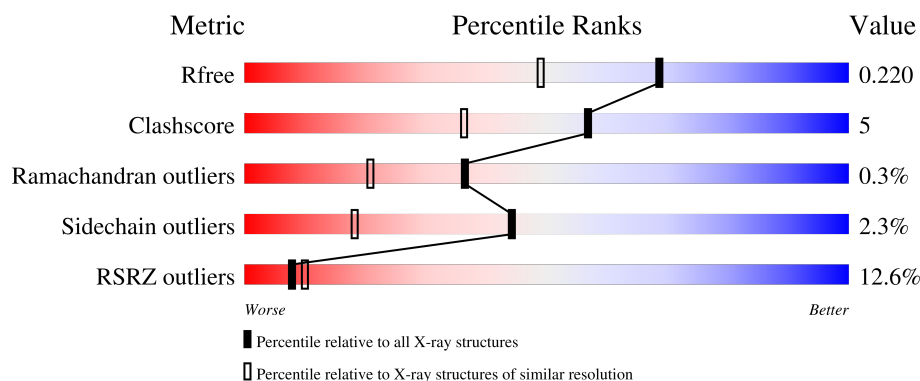
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	471	3% 86% 8% 5%
1	B	471	30% 81% 13% 5%
1	C	471	10% 85% 9% 5%
1	D	471	20% 85% 9% 5%
1	E	471	3% 90% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	471	7% 87% 7% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23954 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3449	2167	605	660	17			
1	B	446	Total	C	N	O	S	0	0	0
			3441	2162	604	659	16			
1	C	447	Total	C	N	O	S	0	1	0
			3458	2175	605	661	17			
1	D	447	Total	C	N	O	S	0	2	0
			3461	2176	607	661	17			
1	E	460	Total	C	N	O	S	0	3	0
			3559	2237	627	678	17			
1	F	447	Total	C	N	O	S	0	2	0
			3463	2177	609	660	17			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP A0A0U4QBJ6
A	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
A	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
A	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
A	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
A	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
A	-7	GLY	-	expression tag	UNP A0A0U4QBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	SER	-	expression tag	UNP A0A0U4QBJ6
A	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-2	SER	-	expression tag	UNP A0A0U4QBJ6
A	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
A	0	PHE	-	expression tag	UNP A0A0U4QBJ6
A	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
A	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
B	-23	MET	-	expression tag	UNP A0A0U4QBJ6
B	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
B	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
B	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
B	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
B	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
B	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-6	SER	-	expression tag	UNP A0A0U4QBJ6
B	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-2	SER	-	expression tag	UNP A0A0U4QBJ6
B	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
B	0	PHE	-	expression tag	UNP A0A0U4QBJ6
B	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
B	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
C	-23	MET	-	expression tag	UNP A0A0U4QBJ6
C	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
C	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-17	HIS	-	expression tag	UNP A0A0U4QBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
C	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
C	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
C	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
C	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-6	SER	-	expression tag	UNP A0A0U4QBJ6
C	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-2	SER	-	expression tag	UNP A0A0U4QBJ6
C	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
C	0	PHE	-	expression tag	UNP A0A0U4QBJ6
C	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
C	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
D	-23	MET	-	expression tag	UNP A0A0U4QBJ6
D	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
D	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
D	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
D	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
D	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
D	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-6	SER	-	expression tag	UNP A0A0U4QBJ6
D	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-2	SER	-	expression tag	UNP A0A0U4QBJ6
D	-1	GLU	-	expression tag	UNP A0A0U4QBJ6

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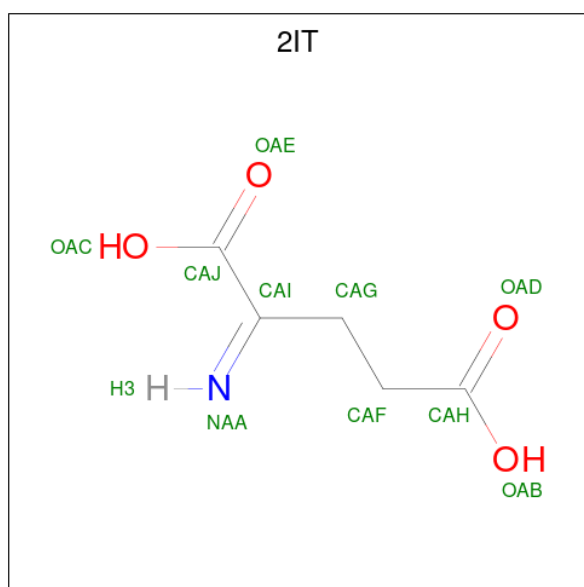
Chain	Residue	Modelled	Actual	Comment	Reference
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D	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
D	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
E	-23	MET	-	expression tag	UNP A0A0U4QBJ6
E	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
E	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
E	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
E	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
E	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
E	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-6	SER	-	expression tag	UNP A0A0U4QBJ6
E	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-2	SER	-	expression tag	UNP A0A0U4QBJ6
E	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
E	0	PHE	-	expression tag	UNP A0A0U4QBJ6
E	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
E	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
F	-23	MET	-	expression tag	UNP A0A0U4QBJ6
F	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
F	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-11	LEU	-	expression tag	UNP A0A0U4QBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
F	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
F	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
F	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-6	SER	-	expression tag	UNP A0A0U4QBJ6
F	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-2	SER	-	expression tag	UNP A0A0U4QBJ6
F	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
F	0	PHE	-	expression tag	UNP A0A0U4QBJ6
F	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
F	299	GLU	ASP	conflict	UNP A0A0U4QBJ6

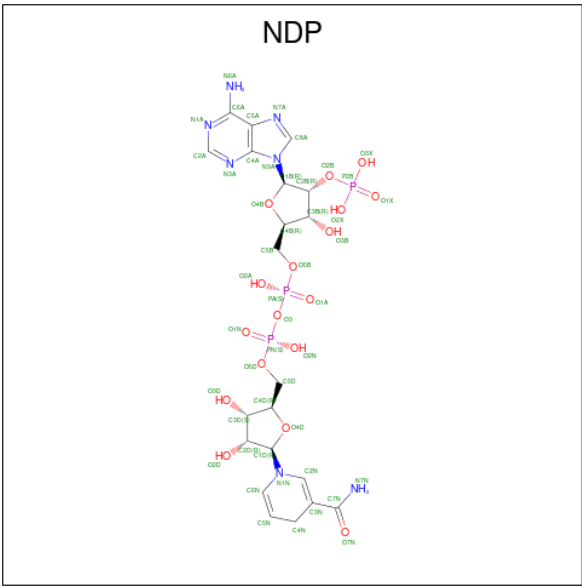
- Molecule 2 is (2Z)-2-iminopentanedioic acid (CCD ID: 2IT) (formula: C₅H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

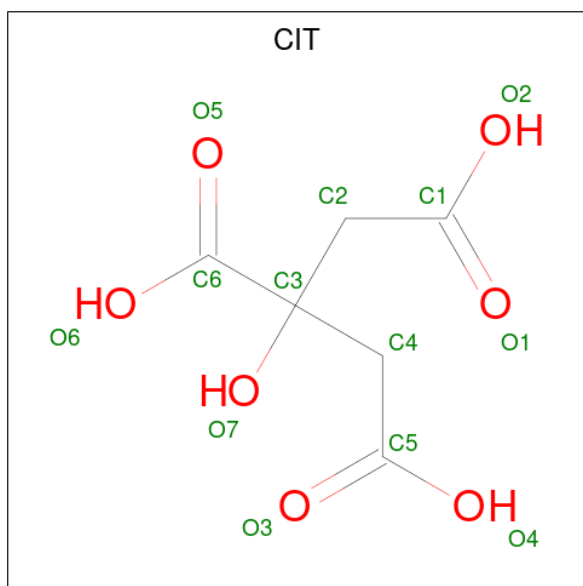
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	K	0	0
			3	3		
4	B	1	Total	K	0	0
			1	1		
4	C	2	Total	K	0	0
			2	2		
4	D	2	Total	K	0	0
			2	2		
4	E	4	Total	K	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	2	Total K 2 2	0	0

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 13 6 7	0	0

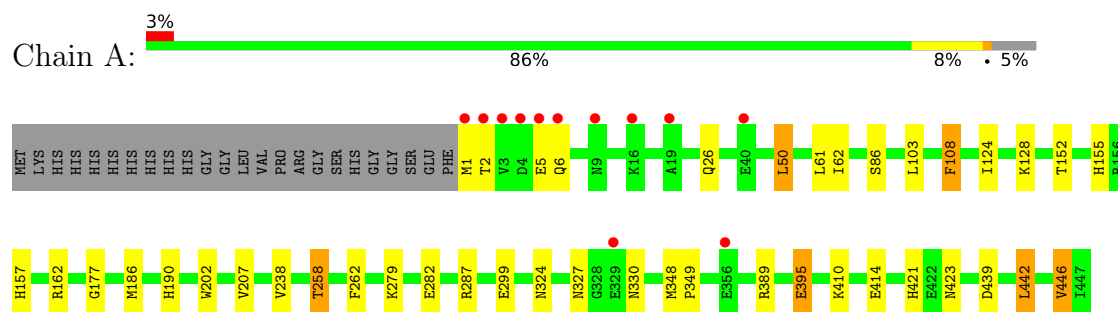
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	525	Total O 525 525	0	0
6	B	355	Total O 355 355	0	0
6	C	429	Total O 429 429	0	0
6	D	401	Total O 401 401	0	0
6	E	583	Total O 583 583	0	0
6	F	475	Total O 475 475	0	0

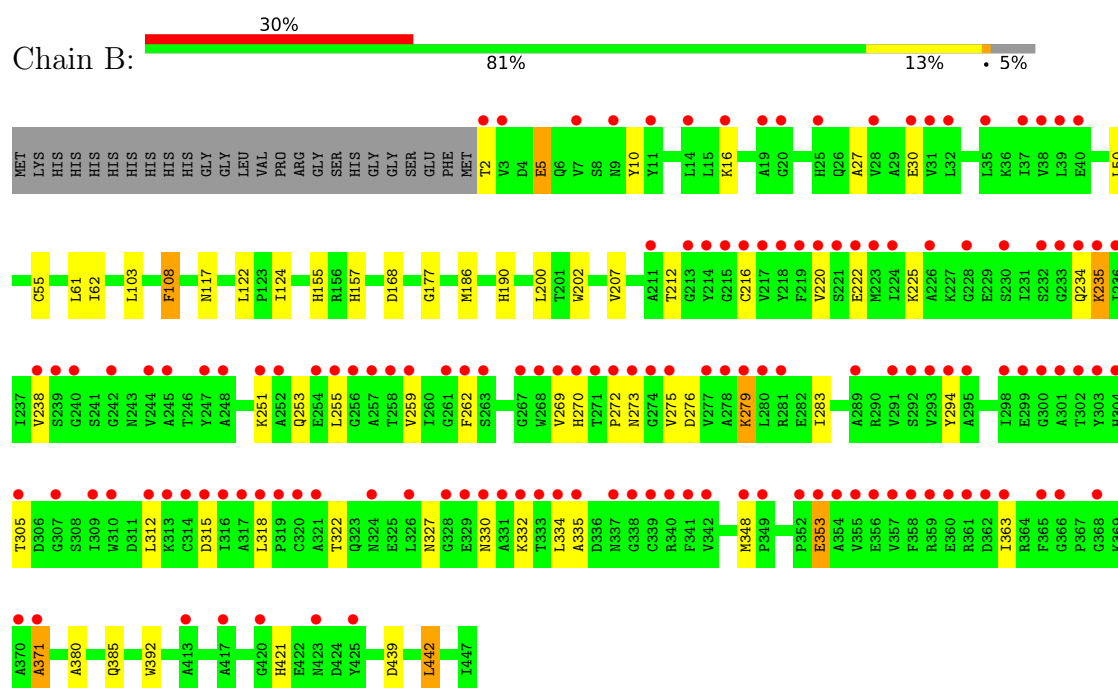
3 Residue-property plots [i](#)

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.

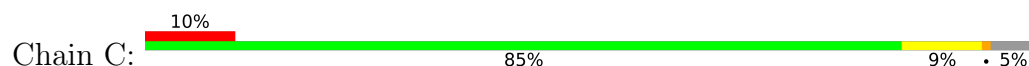
- Molecule 1: Glutamate dehydrogenase

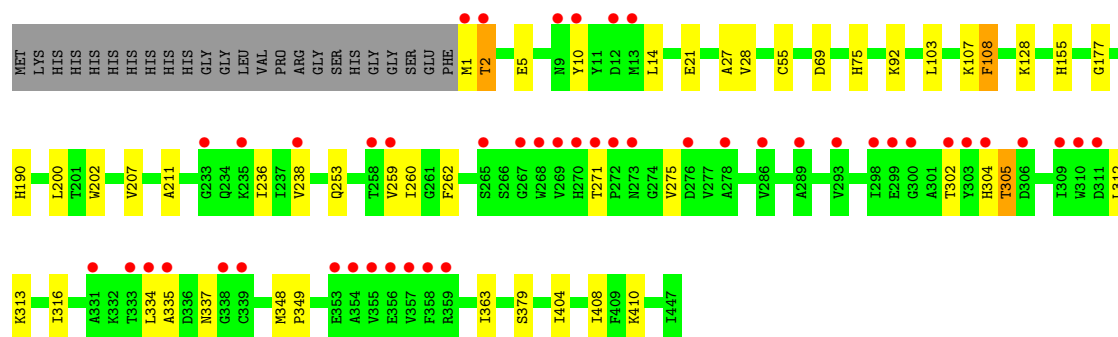


- Molecule 1: Glutamate dehydrogenase

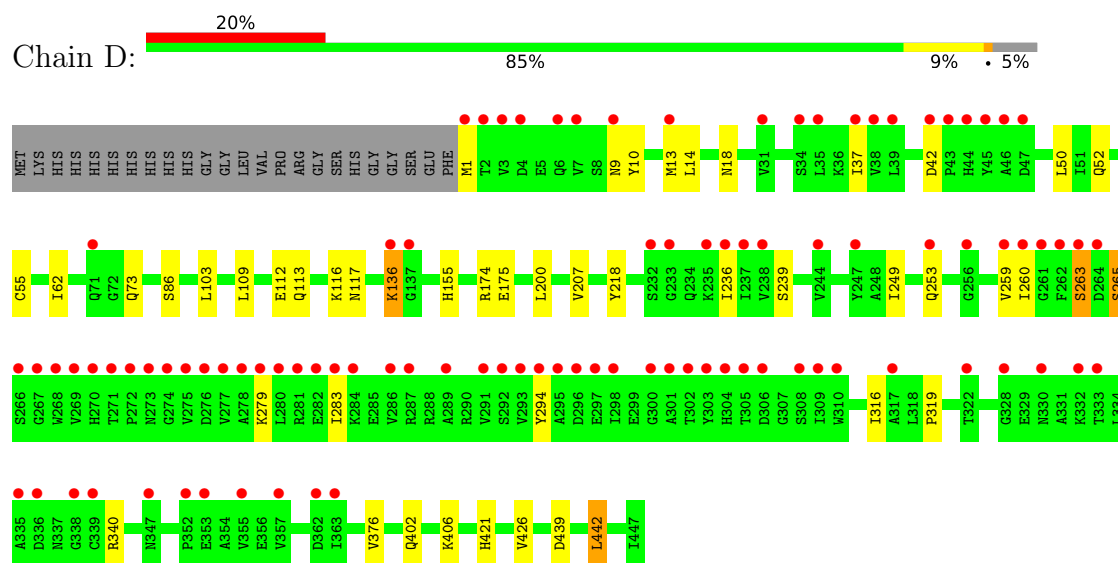


- Molecule 1: Glutamate dehydrogenase

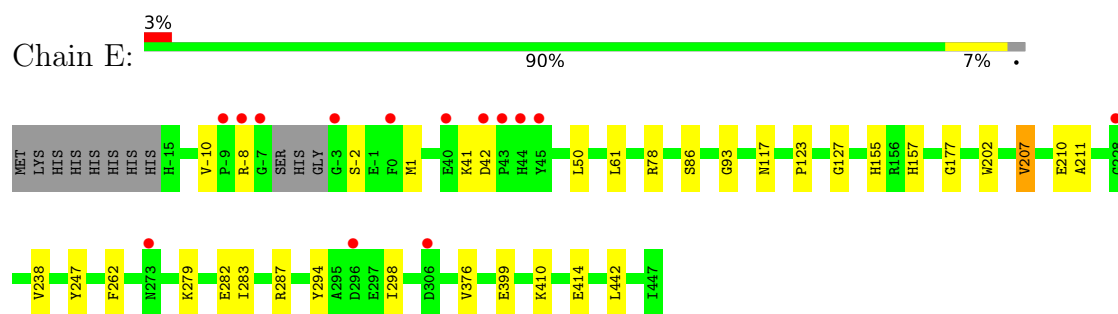




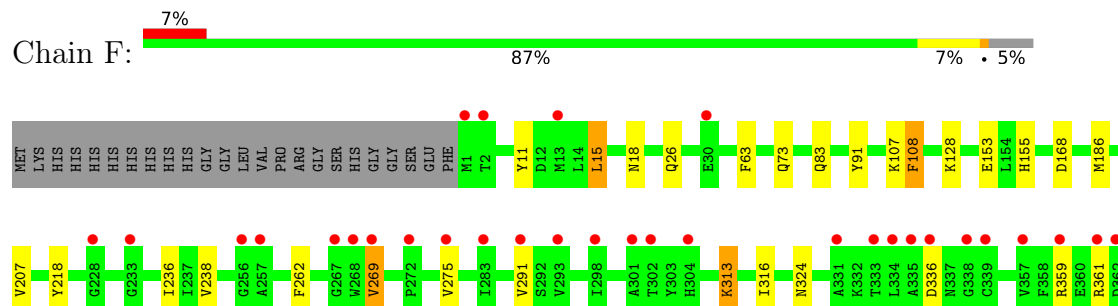
• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.59Å 127.67Å 126.63Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	30.83 – 1.68 30.83 – 1.68	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.83-1.68) 97.0 (30.83-1.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.192 , 0.226 (Not available) , 0.220	Depositor DCC
R_{free} test set	15636 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23954	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: NDP, CIT, K, 2IT

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	0.76	1/3519 (0.0%)	0.85	1/4749 (0.0%)
1	B	0.67	0/3511	0.86	1/4739 (0.0%)
1	C	0.65	0/3532	0.84	2/4767 (0.0%)
1	D	0.66	0/3537	0.86	2/4772 (0.0%)
1	E	0.72	0/3641	0.85	1/4910 (0.0%)
1	F	0.70	0/3539	0.84	0/4774
All	All	0.69	1/21279 (0.0%)	0.85	7/28711 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	VAL	CA-CB	5.54	1.60	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	VAL	CB-CA-C	6.80	118.57	111.23
1	B	371	ALA	N-CA-C	6.32	119.15	111.82
1	C	211	ALA	N-CA-C	5.99	117.80	111.28
1	E	211	ALA	N-CA-C	5.49	116.94	111.07
1	C	305	THR	N-CA-C	-5.48	107.23	114.31
1	D	263	SER	N-CA-C	5.14	116.65	108.79
1	D	260	ILE	N-CA-C	5.10	117.79	112.90

There are no chirality outliers.

There are no planarity outliers.

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	3449	0	3357	31	0
1	B	3441	0	3345	46	0
1	C	3458	0	3366	25	0
1	D	3461	0	3378	29	0
1	E	3559	0	3470	27	0
1	F	3463	0	3383	37	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	F	10	0	0	1	0
3	A	48	0	26	1	0
3	B	48	0	26	3	0
3	C	48	0	26	1	0
3	D	48	0	26	1	0
3	E	48	0	26	0	0
3	F	48	0	26	2	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	4	0	0	0	0
4	F	2	0	0	0	0
5	E	13	0	5	0	0
6	A	525	0	0	10	0
6	B	355	0	0	14	0
6	C	429	0	0	3	0
6	D	401	0	0	4	0
6	E	583	0	0	4	0
6	F	475	0	0	6	0
All	All	23954	0	20460	192	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 5.

All (192) 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)
3:F:502:NDP:H8A	6:F:950:HOH:O	1.37	1.20
1:B:225:LYS:HB2	6:B:785:HOH:O	1.54	1.05
1:C:2:THR:HG22	1:C:5:GLU:H	1.35	0.91
1:E:8:ARG:H	1:F:73:GLN:HE22	1.23	0.84
1:C:253:GLN:HE22	1:C:275:VAL:H	1.24	0.82
1:D:340:ARG:HH11	1:D:340:ARG:HG3	1.46	0.80
1:B:155:HIS:CE1	1:B:186:MET:HE2	2.17	0.79
1:A:1:MET:HE2	1:A:5:GLU:HB3	1.65	0.79
1:E:78:ARG:NH2	6:E:601:HOH:O	2.14	0.78
1:B:253:GLN:HE22	1:B:275:VAL:H	1.34	0.76
1:F:269:VAL:HG11	1:F:291:VAL:HG22	1.66	0.76
1:E:282:GLU:OE2	1:E:287:ARG:HD2	1.87	0.74
1:B:253:GLN:HE21	1:B:259:VAL:H	1.34	0.74
1:F:269:VAL:CG1	1:F:291:VAL:CG2	2.66	0.74
1:C:253:GLN:HE21	1:C:259:VAL:H	1.33	0.73
1:A:327:ASN:H	1:A:330:ASN:HD22	1.35	0.73
2:F:501:2IT:CAI	3:F:502:NDP:H41N	2.17	0.73
1:F:128:LYS:NZ	6:F:601:HOH:O	2.22	0.73
1:F:313:LYS:N	1:F:313:LYS:HD3	2.04	0.72
1:F:269:VAL:CG1	1:F:291:VAL:HG22	2.21	0.70
1:C:69:ASP:OD2	1:C:75:HIS:HE1	1.74	0.70
1:A:421:HIS:HD2	6:A:621:HOH:O	1.75	0.69
1:B:50:LEU:HD22	1:B:442:LEU:HD13	1.75	0.67
1:F:402:GLN:NE2	6:F:602:HOH:O	2.28	0.67
1:F:269:VAL:HG11	1:F:291:VAL:CG2	2.25	0.66
1:F:313:LYS:HD3	1:F:313:LYS:H	1.59	0.66
1:A:282:GLU:OE2	1:A:287:ARG:NH1	2.28	0.66
1:B:222:GLU:HA	6:B:785:HOH:O	1.95	0.65
1:B:2:THR:HG23	1:B:5:GLU:HB3	1.77	0.65
1:F:26:GLN:HE22	1:F:324:ASN:HD21	1.45	0.65
1:E:410:LYS:HE2	1:E:414:GLU:OE1	1.97	0.65
1:B:273:ASN:O	6:B:601:HOH:O	2.14	0.64
1:A:128:LYS:NZ	6:A:601:HOH:O	2.29	0.64
1:B:190:HIS:HE1	6:B:666:HOH:O	1.79	0.64
1:F:389:ARG:NH2	6:F:603:HOH:O	2.31	0.64
1:D:50:LEU:HD12	1:D:442:LEU:HD13	1.80	0.63
1:A:439:ASP:HB2	6:A:613:HOH:O	1.99	0.63
1:E:399:GLU:HG3	6:E:647:HOH:O	1.99	0.62
1:E:78:ARG:HH22	1:F:18:ASN:HD21	1.46	0.62
1:B:27:ALA:HA	1:B:348:MET:HE1	1.82	0.62
2:B:501:2IT:CAI	3:B:502:NDP:H41N	2.30	0.62
1:B:385:GLN:NE2	1:B:392:TRP:H	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLN:HE21	1:D:259:VAL:H	1.47	0.61
1:F:313:LYS:H	1:F:313:LYS:CD	2.13	0.61
1:F:269:VAL:CG1	1:F:291:VAL:HG21	2.30	0.61
1:F:381:LEU:HG	1:F:392:TRP:HZ3	1.66	0.61
1:A:190:HIS:HE1	6:A:635:HOH:O	1.83	0.61
1:B:327:ASN:H	1:B:330:ASN:HD22	1.49	0.61
1:A:50:LEU:HD23	1:A:442:LEU:HD13	1.83	0.60
1:A:258:THR:HG22	6:A:663:HOH:O	2.01	0.60
1:B:385:GLN:HE21	1:B:392:TRP:H	1.50	0.60
1:C:190:HIS:HE1	6:C:652:HOH:O	1.84	0.59
1:D:174:ARG:HD2	1:D:175:GLU:OE2	2.02	0.59
1:A:1:MET:HA	6:A:981:HOH:O	2.02	0.58
1:E:61:LEU:HD22	1:E:157:HIS:CD2	2.38	0.58
1:A:62:ILE:HD11	1:A:103:LEU:HD22	1.86	0.58
1:B:276:ASP:HB3	1:B:279:LYS:HB3	1.86	0.57
2:C:501:2IT:CAI	3:C:502:NDP:H41N	2.35	0.56
1:B:238:VAL:O	1:B:262:PHE:HA	2.05	0.56
1:D:37:ILE:H	1:D:37:ILE:HD12	1.70	0.56
1:F:218:TYR:CE2	1:F:402:GLN:HG2	2.40	0.56
1:C:27:ALA:HB2	1:C:348:MET:HE1	1.86	0.55
1:B:108:PHE:C	1:B:108:PHE:CD1	2.83	0.55
1:D:265:SER:HB2	3:D:502:NDP:O1X	2.06	0.55
1:D:340:ARG:HG3	1:D:340:ARG:NH1	2.19	0.55
1:A:26:GLN:HE22	1:A:324:ASN:HD21	1.54	0.55
1:D:62:ILE:HD11	1:D:103:LEU:HD22	1.89	0.55
1:E:-2:SER:O	1:E:1:MET:HE2	2.07	0.54
1:F:398:ASP:O	1:F:402:GLN:HG3	2.08	0.54
1:F:313:LYS:N	1:F:313:LYS:CD	2.69	0.54
2:A:501:2IT:CAI	3:A:502:NDP:H41N	2.38	0.54
1:C:108:PHE:C	1:C:108:PHE:CD1	2.86	0.54
1:E:-8:ARG:H	1:F:73:GLN:NE2	2.01	0.53
1:F:262:PHE:HE1	1:F:291:VAL:HG23	1.74	0.53
1:D:14:LEU:HG	1:D:18:ASN:HD22	1.74	0.53
1:B:234:GLN:HE21	1:B:234:GLN:HA	1.74	0.53
1:B:27:ALA:CB	1:B:348:MET:HE1	2.39	0.53
1:D:73:GLN:NE2	6:D:601:HOH:O	2.18	0.53
1:D:218:TYR:CD1	1:D:402:GLN:HG3	2.45	0.52
1:C:155:HIS:HD2	6:C:946:HOH:O	1.93	0.52
1:C:128:LYS:NZ	6:C:603:HOH:O	2.35	0.52
1:E:117:ASN:OD1	1:E:376:VAL:HG21	2.10	0.52
1:A:190:HIS:HD2	1:E:86:SER:O	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:ASP:OD1	1:F:361:ARG:NH1	2.41	0.51
1:A:238:VAL:O	1:A:262:PHE:HA	2.12	0.50
1:B:155:HIS:HD2	6:B:908:HOH:O	1.94	0.50
1:B:439:ASP:HB2	6:B:622:HOH:O	2.12	0.50
1:B:190:HIS:HD2	1:D:86:SER:O	1.95	0.50
1:B:27:ALA:CA	1:B:348:MET:HE1	2.42	0.49
1:A:61:LEU:HD22	1:A:157:HIS:CD2	2.47	0.49
1:B:220:VAL:HB	6:B:611:HOH:O	2.13	0.49
1:A:395:GLU:H	1:A:395:GLU:CD	2.19	0.49
1:F:421:HIS:HE1	6:F:975:HOH:O	1.96	0.49
1:A:108:PHE:C	1:A:108:PHE:CD1	2.90	0.49
1:A:155:HIS:HD2	6:A:1017:HOH:O	1.94	0.49
1:E:282:GLU:OE2	1:E:287:ARG:CD	2.58	0.49
1:B:50:LEU:HD22	1:B:442:LEU:CD1	2.43	0.49
1:F:108:PHE:C	1:F:108:PHE:CD1	2.90	0.49
1:F:359:ARG:NH2	1:F:424:ASP:OD2	2.31	0.49
1:F:18:ASN:HD22	1:F:107:LYS:NZ	2.11	0.48
1:B:421:HIS:HE1	6:B:894:HOH:O	1.95	0.48
1:F:155:HIS:HD2	6:F:978:HOH:O	1.95	0.48
1:A:86:SER:O	1:C:190:HIS:HD2	1.96	0.48
1:E:41:LYS:NZ	6:E:607:HOH:O	2.47	0.48
1:B:177:GLY:HA2	1:B:202:TRP:CH2	2.48	0.48
1:F:262:PHE:CE1	1:F:291:VAL:HG23	2.47	0.48
1:E:238:VAL:O	1:E:262:PHE:HA	2.14	0.48
1:F:381:LEU:HG	1:F:392:TRP:CZ3	2.49	0.48
1:A:155:HIS:CE1	1:A:186:MET:CE	2.97	0.47
1:C:27:ALA:CB	1:C:348:MET:HE1	2.43	0.47
1:D:10:TYR:OH	1:D:55:CYS:HB2	2.14	0.47
1:C:348:MET:N	1:C:349:PRO:CD	2.78	0.47
1:A:389:ARG:NH1	1:E:123:PRO:HG2	2.29	0.47
1:E:-10:VAL:CB	1:E:1:MET:HE1	2.44	0.47
1:B:30:GLU:HG3	6:B:714:HOH:O	2.14	0.47
1:B:10:TYR:OH	1:B:55:CYS:HB2	2.15	0.47
1:B:235:LYS:HD2	1:B:315:ASP:OD2	2.14	0.46
1:C:260:ILE:HA	1:C:271:THR:O	2.14	0.46
1:B:212:THR:OG1	3:B:502:NDP:H42N	2.15	0.46
1:C:14:LEU:HD13	1:C:28:VAL:HG11	1.97	0.46
1:B:27:ALA:HB2	1:B:348:MET:HE1	1.97	0.46
1:A:162:ARG:CZ	6:A:771:HOH:O	2.64	0.46
1:C:335:ALA:HB2	1:C:363:ILE:HD11	1.97	0.46
1:D:236:ILE:HG12	1:D:316:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ILE:O	1:C:408:ILE:HG13	2.16	0.46
1:F:262:PHE:CE1	1:F:291:VAL:CG2	2.99	0.45
1:A:410:LYS:HE3	1:A:414:GLU:OE2	2.16	0.45
1:E:279:LYS:HG2	1:E:298:ILE:HD11	1.98	0.45
1:F:11:TYR:CZ	1:F:15:LEU:HD21	2.50	0.45
1:C:177:GLY:HA2	1:C:202:TRP:CH2	2.51	0.45
1:C:313:LYS:HG3	1:C:337:ASN:O	2.17	0.45
1:D:117:ASN:OD1	1:D:376:VAL:HG21	2.17	0.45
1:D:283:ILE:HD13	1:D:294:TYR:HB2	1.97	0.45
1:B:270:HIS:CE1	1:B:272:PRO:HG3	2.51	0.45
1:E:50:LEU:HD12	1:E:442:LEU:HG	1.98	0.45
1:A:155:HIS:CE1	1:A:186:MET:HE3	2.51	0.45
1:B:61:LEU:HD22	1:B:157:HIS:CD2	2.51	0.44
1:B:318:LEU:HD22	6:B:611:HOH:O	2.16	0.44
1:B:332:LYS:HG2	6:B:693:HOH:O	2.16	0.44
1:A:327:ASN:H	1:A:330:ASN:ND2	2.06	0.44
1:D:340:ARG:HH11	1:D:340:ARG:CG	2.23	0.44
1:F:291:VAL:HG22	1:F:291:VAL:O	2.17	0.44
1:F:236:ILE:HG12	1:F:316:ILE:HB	2.00	0.44
1:D:73:GLN:HB3	6:D:601:HOH:O	2.18	0.44
1:D:109:LEU:O	1:D:113:GLN:HG2	2.18	0.44
1:E:1:MET:HE3	1:E:1:MET:HB2	1.80	0.44
1:B:117:ASN:HB3	1:B:124:ILE:HG13	2.00	0.44
1:B:62:ILE:HD11	1:B:103:LEU:HD22	2.00	0.44
1:B:322:THR:HG21	3:B:502:NDP:C6A	2.48	0.44
1:B:353:GLU:H	1:B:353:GLU:CD	2.25	0.44
1:E:-10:VAL:HG11	1:E:1:MET:HE1	2.01	0.43
1:A:2:THR:O	1:A:6:GLN:HG3	2.18	0.43
1:A:190:HIS:CD2	1:E:86:SER:O	2.72	0.43
1:D:10:TYR:CE1	1:D:52:GLN:HG3	2.54	0.43
1:A:177:GLY:HA2	1:A:202:TRP:CH2	2.53	0.43
1:C:10[A]:TYR:OH	1:C:55:CYS:HB2	2.19	0.43
1:D:421:HIS:HD2	6:D:709:HOH:O	2.02	0.43
1:E:93:GLY:HA3	1:E:127:GLY:O	2.18	0.43
1:C:103:LEU:HG	1:C:107:LYS:HD2	2.00	0.43
1:B:276:ASP:CG	6:B:617:HOH:O	2.62	0.43
1:B:251:LYS:O	1:B:255:LEU:HG	2.19	0.43
1:E:210:GLU:HG3	1:E:247:TYR:CD1	2.54	0.42
1:D:155:HIS:HD2	6:D:940:HOH:O	2.01	0.42
1:C:236:ILE:HG12	1:C:316:ILE:HB	2.01	0.42
1:A:152:THR:HG23	1:F:186:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LYS:HE3	6:B:785:HOH:O	2.19	0.42
1:C:238:VAL:O	1:C:262:PHE:HA	2.20	0.42
1:F:238:VAL:O	1:F:262:PHE:HA	2.20	0.42
1:F:410:LYS:HE2	1:F:414:GLU:OE1	2.19	0.42
6:B:627:HOH:O	1:D:439:ASP:HB2	2.19	0.42
1:B:216:CYS:HA	1:B:371:ALA:O	2.19	0.41
1:D:402:GLN:NE2	1:D:406:LYS:HD2	2.35	0.41
1:A:423:ASN:ND2	6:A:610:HOH:O	2.52	0.41
1:C:92:LYS:HE3	1:C:379:SER:HB3	2.03	0.41
1:A:348:MET:N	1:A:349:PRO:CD	2.84	0.41
1:B:122:LEU:HD13	1:B:380:ALA:HB3	2.01	0.41
1:C:302:THR:OG1	1:C:304:HIS:HE1	2.03	0.41
1:D:136:LYS:N	1:D:136:LYS:HE3	2.35	0.41
1:D:239:SER:OG	1:D:319:PRO:HA	2.20	0.41
1:D:249:ILE:HG12	1:D:259:VAL:HG11	2.03	0.41
1:B:335:ALA:HB2	1:B:363:ILE:HD11	2.03	0.41
1:E:207:VAL:HG12	1:E:207:VAL:O	2.19	0.41
1:C:21:GLU:CD	1:C:107:LYS:HZ3	2.29	0.41
1:D:402:GLN:HE21	1:D:406:LYS:HD2	1.85	0.41
1:E:155:HIS:HD2	6:E:1051:HOH:O	2.04	0.41
1:F:63:PHE:CG	1:F:153:GLU:HG2	2.56	0.41
1:E:177:GLY:HA2	1:E:202:TRP:CH2	2.56	0.41
1:F:83:GLN:HB3	1:F:91:TYR:CE2	2.55	0.40
1:B:279:LYS:HG2	1:B:294:TYR:CE1	2.56	0.40
1:D:112:GLU:O	1:D:116[B]:LYS:HG3	2.22	0.40
2:A:501:2IT:CAI	6:A:601:HOH:O	2.70	0.40
1:E:283:ILE:CD1	1:E:294:TYR:HA	2.51	0.40

There are no symmetry-related clashes.

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	445/471 (94%)	435 (98%)	9 (2%)	1 (0%)	43	27
1	B	444/471 (94%)	432 (97%)	10 (2%)	2 (0%)	24	8
1	C	446/471 (95%)	435 (98%)	10 (2%)	1 (0%)	43	27
1	D	447/471 (95%)	435 (97%)	11 (2%)	1 (0%)	43	27
1	E	459/471 (98%)	449 (98%)	9 (2%)	1 (0%)	43	27
1	F	447/471 (95%)	437 (98%)	8 (2%)	2 (0%)	30	13
All	All	2688/2826 (95%)	2623 (98%)	57 (2%)	8 (0%)	36	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	VAL
1	B	207	VAL
1	D	207	VAL
1	E	207	VAL
1	F	207	VAL
1	C	207	VAL
1	F	168	ASP
1	B	168	ASP

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	358/377 (95%)	349 (98%)	9 (2%)	42	16
1	B	357/377 (95%)	344 (96%)	13 (4%)	31	6
1	C	359/377 (95%)	351 (98%)	8 (2%)	45	19
1	D	360/377 (96%)	349 (97%)	11 (3%)	35	10
1	E	370/377 (98%)	369 (100%)	1 (0%)	86	81
1	F	360/377 (96%)	353 (98%)	7 (2%)	50	25
All	All	2164/2262 (96%)	2115 (98%)	49 (2%)	44	18

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	108	PHE
1	A	124	ILE
1	A	258	THR
1	A	279	LYS
1	A	299	GLU
1	A	395	GLU
1	A	442	LEU
1	A	446	VAL
1	B	5	GLU
1	B	16	LYS
1	B	108	PHE
1	B	200	LEU
1	B	235	LYS
1	B	269	VAL
1	B	279	LYS
1	B	283	ILE
1	B	305	THR
1	B	312	LEU
1	B	334	LEU
1	B	353	GLU
1	B	442	LEU
1	C	1	MET
1	C	2	THR
1	C	108	PHE
1	C	200	LEU
1	C	305	THR
1	C	312	LEU
1	C	334	LEU
1	C	410	LYS
1	D	1	MET
1	D	9	ASN
1	D	13	MET
1	D	42	ASP
1	D	136	LYS
1	D	200	LEU
1	D	263	SER
1	D	265	SER
1	D	279	LYS
1	D	426	VAL
1	D	442	LEU
1	E	42	ASP

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Mol	Chain	Res	Type
1	F	15	LEU
1	F	108	PHE
1	F	269	VAL
1	F	275	VAL
1	F	313	LYS
1	F	381	LEU
1	F	389	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	73	GLN
1	A	155	HIS
1	A	190	HIS
1	A	243	ASN
1	A	304	HIS
1	A	330	ASN
1	A	384	GLN
1	B	26	GLN
1	B	44	HIS
1	B	73	GLN
1	B	155	HIS
1	B	190	HIS
1	B	234	GLN
1	B	243	ASN
1	B	253	GLN
1	B	270	HIS
1	B	324	ASN
1	B	330	ASN
1	B	385	GLN
1	B	402	GLN
1	B	421	HIS
1	C	26	GLN
1	C	60	GLN
1	C	75	HIS
1	C	148	GLN
1	C	155	HIS
1	C	182	HIS
1	C	190	HIS
1	C	253	GLN
1	C	304	HIS

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Mol	Chain	Res	Type
1	C	324	ASN
1	D	44	HIS
1	D	60	GLN
1	D	155	HIS
1	D	182	HIS
1	D	253	GLN
1	D	304	HIS
1	D	347	ASN
1	D	384	GLN
1	D	402	GLN
1	D	421	HIS
1	E	73	GLN
1	E	155	HIS
1	E	182	HIS
1	E	304	HIS
1	E	402	GLN
1	E	421	HIS
1	F	9	ASN
1	F	18	ASN
1	F	26	GLN
1	F	60	GLN
1	F	73	GLN
1	F	155	HIS
1	F	182	HIS
1	F	243	ASN
1	F	402	GLN
1	F	421	HIS

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

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 for Mogul analysis.

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
5	CIT	E	502	-	12,12,12	0.96	0	17,17,17	1.63	4 (23%)
2	2IT	B	501	-	8,9,9	1.73	3 (37%)	6,11,11	1.42	1 (16%)
3	NDP	D	502	-	51,52,52	1.94	13 (25%)	71,80,80	1.82	15 (21%)
2	2IT	F	501	-	8,9,9	1.58	1 (12%)	6,11,11	1.43	1 (16%)
3	NDP	E	503	-	51,52,52	1.93	16 (31%)	71,80,80	1.82	12 (16%)
3	NDP	F	502	-	51,52,52	1.77	14 (27%)	71,80,80	1.77	16 (22%)
3	NDP	A	502	-	51,52,52	1.96	15 (29%)	71,80,80	1.63	10 (14%)
3	NDP	C	502	-	51,52,52	1.89	17 (33%)	71,80,80	1.74	15 (21%)
2	2IT	A	501	-	8,9,9	1.62	1 (12%)	6,11,11	1.36	0
3	NDP	B	502	-	51,52,52	1.98	16 (31%)	71,80,80	1.61	11 (15%)
2	2IT	C	501	-	8,9,9	1.72	2 (25%)	6,11,11	1.66	2 (33%)

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
5	CIT	E	502	-	-	6/16/16/16	-
2	2IT	B	501	-	-	0/6/9/9	-
3	NDP	D	502	-	-	4/34/77/77	0/5/5/5
2	2IT	F	501	-	-	1/6/9/9	-
3	NDP	E	503	-	-	5/34/77/77	0/5/5/5
3	NDP	F	502	-	-	7/34/77/77	0/5/5/5
3	NDP	A	502	-	-	2/34/77/77	0/5/5/5
3	NDP	C	502	-	-	3/34/77/77	0/5/5/5
2	2IT	A	501	-	-	3/6/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	502	-	-	4/34/77/77	0/5/5/5
2	2IT	C	501	-	-	0/6/9/9	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NDP	PN-O3	-5.58	1.53	1.59
3	D	502	NDP	C4N-C3N	-5.48	1.39	1.50
3	E	503	NDP	P2B-O2B	5.21	1.68	1.59
3	B	502	NDP	C4N-C3N	-5.12	1.40	1.50
3	C	502	NDP	C4N-C3N	-4.97	1.40	1.50
3	E	503	NDP	C4N-C3N	-4.83	1.40	1.50
3	A	502	NDP	C4N-C3N	-4.83	1.40	1.50
3	A	502	NDP	C2A-N1A	4.68	1.42	1.33
3	F	502	NDP	C2A-N3A	4.53	1.42	1.33
3	F	502	NDP	C4N-C3N	-4.46	1.41	1.50
3	B	502	NDP	P2B-O1X	4.42	1.64	1.50
3	B	502	NDP	C2A-N3A	4.12	1.41	1.33
3	D	502	NDP	C7N-C3N	-4.06	1.40	1.48
3	D	502	NDP	C2A-N1A	3.87	1.40	1.33
3	C	502	NDP	C4N-C5N	-3.82	1.39	1.49
3	B	502	NDP	C2A-N1A	3.80	1.40	1.33
3	F	502	NDP	P2B-O1X	3.78	1.62	1.50
3	E	503	NDP	C5A-C4A	-3.78	1.32	1.39
2	A	501	2IT	CAI-NAA	3.78	1.36	1.27
3	D	502	NDP	C2A-N3A	3.77	1.40	1.33
3	A	502	NDP	C2A-N3A	3.75	1.40	1.33
3	C	502	NDP	C7N-C3N	-3.69	1.40	1.48
3	C	502	NDP	C2A-N3A	3.67	1.40	1.33
3	B	502	NDP	PN-O1N	3.64	1.63	1.50
3	C	502	NDP	C2A-N1A	3.60	1.40	1.33
3	B	502	NDP	C7N-C3N	-3.60	1.41	1.48
3	D	502	NDP	C4N-C5N	-3.56	1.39	1.49
3	E	503	NDP	C2A-N3A	3.49	1.40	1.33
2	C	501	2IT	CAI-NAA	3.47	1.35	1.27
3	D	502	NDP	P2B-O1X	3.44	1.61	1.50
2	F	501	2IT	CAI-NAA	3.42	1.35	1.27
3	F	502	NDP	C7N-C3N	-3.39	1.41	1.48
3	B	502	NDP	C4N-C5N	-3.36	1.40	1.49
3	E	503	NDP	C4N-C5N	-3.36	1.40	1.49
3	E	503	NDP	C7N-C3N	-3.33	1.41	1.48
2	B	501	2IT	CAI-NAA	3.33	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	NDP	C4N-C5N	-3.30	1.40	1.49
3	D	502	NDP	PA-O1A	3.24	1.62	1.50
3	C	502	NDP	PN-O1N	3.23	1.62	1.50
3	E	503	NDP	C2A-N1A	3.22	1.39	1.33
3	D	502	NDP	C5A-N7A	-3.12	1.33	1.39
3	D	502	NDP	PA-O3	3.08	1.62	1.59
3	A	502	NDP	P2B-O1X	2.94	1.59	1.50
3	A	502	NDP	P2B-O2B	2.92	1.64	1.59
3	A	502	NDP	C7N-C3N	-2.91	1.42	1.48
3	C	502	NDP	C5A-N7A	-2.91	1.33	1.39
3	C	502	NDP	PN-O3	2.90	1.62	1.59
3	F	502	NDP	C5A-N7A	-2.83	1.33	1.39
3	D	502	NDP	C5A-C4A	-2.81	1.34	1.39
3	A	502	NDP	C4N-C5N	-2.79	1.41	1.49
3	E	503	NDP	P2B-O1X	2.79	1.59	1.50
3	F	502	NDP	C5A-C4A	-2.72	1.34	1.39
3	C	502	NDP	O3B-C3B	2.70	1.49	1.43
3	A	502	NDP	C5A-C4A	-2.66	1.34	1.39
3	E	503	NDP	PN-O3	2.64	1.62	1.59
3	D	502	NDP	C8A-N9A	-2.58	1.33	1.37
3	F	502	NDP	C2A-N1A	2.57	1.38	1.33
3	F	502	NDP	PA-O3	2.55	1.62	1.59
3	E	503	NDP	PN-O1N	2.48	1.59	1.50
3	B	502	NDP	C5A-N7A	-2.47	1.34	1.39
3	A	502	NDP	C4A-N9A	-2.46	1.32	1.37
3	E	503	NDP	C5A-N7A	-2.45	1.34	1.39
3	C	502	NDP	O4B-C1B	2.43	1.47	1.42
3	C	502	NDP	C8A-N9A	-2.40	1.33	1.37
3	E	503	NDP	C8A-N9A	-2.39	1.33	1.37
3	B	502	NDP	C5A-C4A	-2.38	1.34	1.39
3	A	502	NDP	C1B-N9A	2.36	1.52	1.46
3	B	502	NDP	C1B-N9A	2.34	1.52	1.46
3	B	502	NDP	PA-O3	2.34	1.62	1.59
3	E	503	NDP	C5A-C6A	-2.31	1.34	1.41
3	B	502	NDP	C6N-C5N	2.31	1.40	1.33
3	C	502	NDP	C5A-C4A	-2.27	1.35	1.39
3	E	503	NDP	C6N-C5N	2.26	1.40	1.33
3	A	502	NDP	C5A-C6A	-2.26	1.34	1.41
3	C	502	NDP	PA-O3	2.25	1.61	1.59
3	D	502	NDP	C5A-C6A	-2.24	1.34	1.41
3	F	502	NDP	C4A-N9A	-2.24	1.33	1.37
3	F	502	NDP	C5A-C6A	-2.23	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NDP	C6N-C5N	2.23	1.39	1.33
3	B	502	NDP	C2N-C3N	2.23	1.41	1.35
3	F	502	NDP	PA-O1A	2.22	1.58	1.50
3	C	502	NDP	P2B-O2B	2.20	1.63	1.59
3	E	503	NDP	O4B-C1B	2.17	1.47	1.42
3	B	502	NDP	PA-O1A	2.17	1.58	1.50
2	C	501	2IT	OAC-CAJ	-2.15	1.24	1.30
3	F	502	NDP	C8A-N9A	-2.13	1.33	1.37
3	C	502	NDP	C5A-C6A	-2.13	1.35	1.41
3	B	502	NDP	O3B-C3B	2.11	1.48	1.43
3	E	503	NDP	O4D-C1D	2.11	1.46	1.42
3	B	502	NDP	C5A-C6A	-2.11	1.35	1.41
3	F	502	NDP	C6N-C5N	2.11	1.39	1.33
3	A	502	NDP	PA-O3	2.06	1.61	1.59
3	C	502	NDP	P2B-O1X	2.05	1.56	1.50
2	B	501	2IT	OAC-CAJ	-2.05	1.25	1.30
3	A	502	NDP	C2N-C3N	2.04	1.40	1.35
3	C	502	NDP	C2N-C3N	2.04	1.40	1.35
2	B	501	2IT	OAB-CAH	-2.03	1.24	1.30
3	A	502	NDP	C5A-N7A	-2.01	1.35	1.39

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	NDP	N3A-C2A-N1A	-8.21	116.16	128.58
3	D	502	NDP	N3A-C2A-N1A	-7.62	117.05	128.58
3	F	502	NDP	N3A-C2A-N1A	-7.29	117.54	128.58
3	B	502	NDP	N3A-C2A-N1A	-7.18	117.72	128.58
3	A	502	NDP	N3A-C2A-N1A	-7.05	117.91	128.58
3	C	502	NDP	N3A-C2A-N1A	-6.77	118.33	128.58
3	E	503	NDP	N9A-C8A-N7A	-5.27	106.46	113.94
3	F	502	NDP	C5A-C4A-N3A	-4.67	120.29	126.72
3	E	503	NDP	C4A-N9A-C1B	-4.56	115.96	126.63
3	D	502	NDP	N9A-C8A-N7A	-4.44	107.63	113.94
3	D	502	NDP	C5A-C4A-N3A	-4.37	120.69	126.72
3	F	502	NDP	N9A-C8A-N7A	-4.31	107.82	113.94
3	C	502	NDP	N9A-C8A-N7A	-4.25	107.91	113.94
3	C	502	NDP	C5A-C4A-N3A	-4.25	120.87	126.72
3	B	502	NDP	C5A-C4A-N3A	-4.22	120.90	126.72
3	A	502	NDP	C2B-C1B-N9A	-4.13	106.95	113.75
3	B	502	NDP	N9A-C8A-N7A	-3.99	108.28	113.94
3	A	502	NDP	C3N-C2N-N1N	-3.89	117.49	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	502	CIT	O6-C6-C3	3.69	120.22	113.14
3	E	503	NDP	C2A-N3A-C4A	3.62	120.68	111.83
3	D	502	NDP	C2A-N3A-C4A	3.59	120.59	111.83
3	F	502	NDP	C2A-N3A-C4A	3.56	120.51	111.83
3	E	503	NDP	C5A-C4A-N3A	-3.51	121.89	126.72
3	E	503	NDP	C1B-N9A-C8A	3.44	134.72	127.09
2	B	501	2IT	CAF-CAG-CAI	-3.41	103.17	113.51
3	E	503	NDP	C4A-N9A-C8A	3.41	109.32	105.74
3	B	502	NDP	C2A-N3A-C4A	3.35	120.01	111.83
3	C	502	NDP	C5A-N7A-C8A	3.34	108.69	103.45
3	C	502	NDP	O4D-C1D-N1N	-3.33	101.73	108.08
3	A	502	NDP	N9A-C8A-N7A	-3.29	109.27	113.94
3	D	502	NDP	C5A-N7A-C8A	3.23	108.53	103.45
3	E	503	NDP	C5A-N7A-C8A	3.22	108.51	103.45
3	D	502	NDP	C3N-C2N-N1N	-3.22	118.48	123.20
3	D	502	NDP	O4B-C1B-C2B	-3.16	101.14	106.59
3	C	502	NDP	C2A-N3A-C4A	3.15	119.53	111.83
3	B	502	NDP	C3N-C2N-N1N	-3.01	118.79	123.20
3	F	502	NDP	C5A-N7A-C8A	2.93	108.06	103.45
3	F	502	NDP	O3X-P2B-O2B	2.93	117.25	105.85
3	F	502	NDP	N3A-C4A-N9A	2.93	132.14	127.17
3	D	502	NDP	O3X-P2B-O2B	2.92	117.23	105.85
3	B	502	NDP	C5A-N7A-C8A	2.86	107.94	103.45
3	C	502	NDP	C4A-C5A-N7A	-2.84	107.34	110.58
3	A	502	NDP	C2A-N3A-C4A	2.79	118.65	111.83
3	A	502	NDP	C5A-C4A-N3A	-2.79	122.88	126.72
3	A	502	NDP	C5A-C6A-N6A	-2.74	116.50	123.29
3	A	502	NDP	O4D-C1D-N1N	-2.71	102.92	108.08
3	D	502	NDP	C5A-C6A-N6A	-2.69	116.63	123.29
2	F	501	2IT	CAF-CAG-CAI	-2.67	105.41	113.51
3	F	502	NDP	C4A-N9A-C8A	2.67	108.54	105.74
2	C	501	2IT	CAF-CAG-CAI	-2.66	105.46	113.51
3	D	502	NDP	N3A-C4A-N9A	2.61	131.60	127.17
3	B	502	NDP	C4A-C5A-N7A	-2.58	107.63	110.58
3	E	503	NDP	C5A-C6A-N6A	-2.57	116.91	123.29
3	D	502	NDP	C4A-N9A-C8A	2.54	108.41	105.74
3	C	502	NDP	O4B-C1B-C2B	-2.53	102.22	106.59
3	C	502	NDP	C3B-C2B-C1B	-2.53	97.97	102.81
3	D	502	NDP	C4A-C5A-N7A	-2.51	107.71	110.58
3	F	502	NDP	C5A-C6A-N6A	-2.50	117.11	123.29
3	C	502	NDP	C3N-C2N-N1N	-2.45	119.60	123.20
3	B	502	NDP	C5A-C6A-N6A	-2.39	117.36	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	NDP	O4B-C1B-C2B	-2.37	102.50	106.59
3	D	502	NDP	C6A-C5A-C4A	2.37	120.41	117.18
3	C	502	NDP	N3A-C4A-N9A	2.36	131.18	127.17
3	E	503	NDP	C4A-C5A-N7A	-2.34	107.90	110.58
5	E	502	CIT	C2-C3-C6	-2.34	104.85	110.03
3	E	503	NDP	O2B-P2B-O1X	-2.34	101.00	109.33
3	F	502	NDP	C2B-C1B-N9A	-2.33	109.92	113.75
3	B	502	NDP	C5A-C4A-N9A	2.30	108.32	105.81
3	C	502	NDP	C1D-N1N-C6N	-2.29	115.93	120.77
3	C	502	NDP	C4A-N9A-C8A	2.28	108.13	105.74
3	C	502	NDP	C5A-C6A-N6A	-2.26	117.69	123.29
3	F	502	NDP	O4D-C1D-N1N	-2.24	103.81	108.08
3	F	502	NDP	C4A-C5A-N7A	-2.24	108.02	110.58
3	B	502	NDP	C6A-C5A-C4A	2.19	120.17	117.18
3	C	502	NDP	C6A-C5A-C4A	2.19	120.17	117.18
5	E	502	CIT	O2-C1-C2	2.13	121.10	114.35
3	B	502	NDP	N3A-C4A-N9A	2.12	130.77	127.17
3	D	502	NDP	C3B-C2B-C1B	-2.09	98.81	102.81
2	C	501	2IT	OAD-CAH-CAF	-2.06	116.55	123.09
5	E	502	CIT	O4-C5-C4	2.05	120.84	114.35
3	E	503	NDP	C5A-C6A-N1A	2.05	122.71	117.51
3	F	502	NDP	C6A-C5A-C4A	2.04	119.97	117.18
3	A	502	NDP	C6N-N1N-C2N	2.04	121.50	119.32
3	A	502	NDP	C1D-N1N-C6N	-2.04	116.47	120.77
3	D	502	NDP	O2A-PA-O5B	2.03	116.78	107.57
3	F	502	NDP	C5A-C6A-N1A	2.03	122.66	117.51
3	F	502	NDP	C3N-C2N-N1N	-2.01	120.26	123.20

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	NDP	C2N-C3N-C7N-N7N
3	E	503	NDP	C2N-C3N-C7N-N7N
3	F	502	NDP	C5D-O5D-PN-O1N
3	D	502	NDP	O4D-C1D-N1N-C6N
3	E	503	NDP	O4D-C1D-N1N-C6N
3	F	502	NDP	C3B-C4B-C5B-O5B
3	F	502	NDP	O4B-C4B-C5B-O5B
5	E	502	CIT	C2-C3-C6-O5
5	E	502	CIT	C2-C3-C6-O6
3	A	502	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	C	502	NDP	O4D-C1D-N1N-C6N
3	F	502	NDP	O4D-C1D-N1N-C6N
2	A	501	2IT	CAF-CAG-CAI-CAJ
2	F	501	2IT	CAF-CAG-CAI-CAJ
3	B	502	NDP	O4D-C1D-N1N-C6N
3	E	503	NDP	O4D-C4D-C5D-O5D
3	F	502	NDP	C2N-C3N-C7N-N7N
2	A	501	2IT	CAG-CAF-CAH-OAD
3	B	502	NDP	C2B-O2B-P2B-O1X
3	C	502	NDP	C2B-O2B-P2B-O1X
3	E	503	NDP	C2B-O2B-P2B-O1X
2	A	501	2IT	CAG-CAF-CAH-OAB
3	D	502	NDP	O4D-C4D-C5D-O5D
3	B	502	NDP	C2D-C1D-N1N-C6N
3	A	502	NDP	C2D-C1D-N1N-C6N
3	C	502	NDP	C2D-C1D-N1N-C6N
3	F	502	NDP	C2D-C1D-N1N-C6N
5	E	502	CIT	C4-C3-C6-O5
5	E	502	CIT	C4-C3-C6-O6
3	D	502	NDP	C2B-O2B-P2B-O1X
3	F	502	NDP	C2B-O2B-P2B-O1X
5	E	502	CIT	C3-C4-C5-O3
5	E	502	CIT	C3-C4-C5-O4
3	B	502	NDP	O4B-C4B-C5B-O5B
3	E	503	NDP	O4B-C4B-C5B-O5B

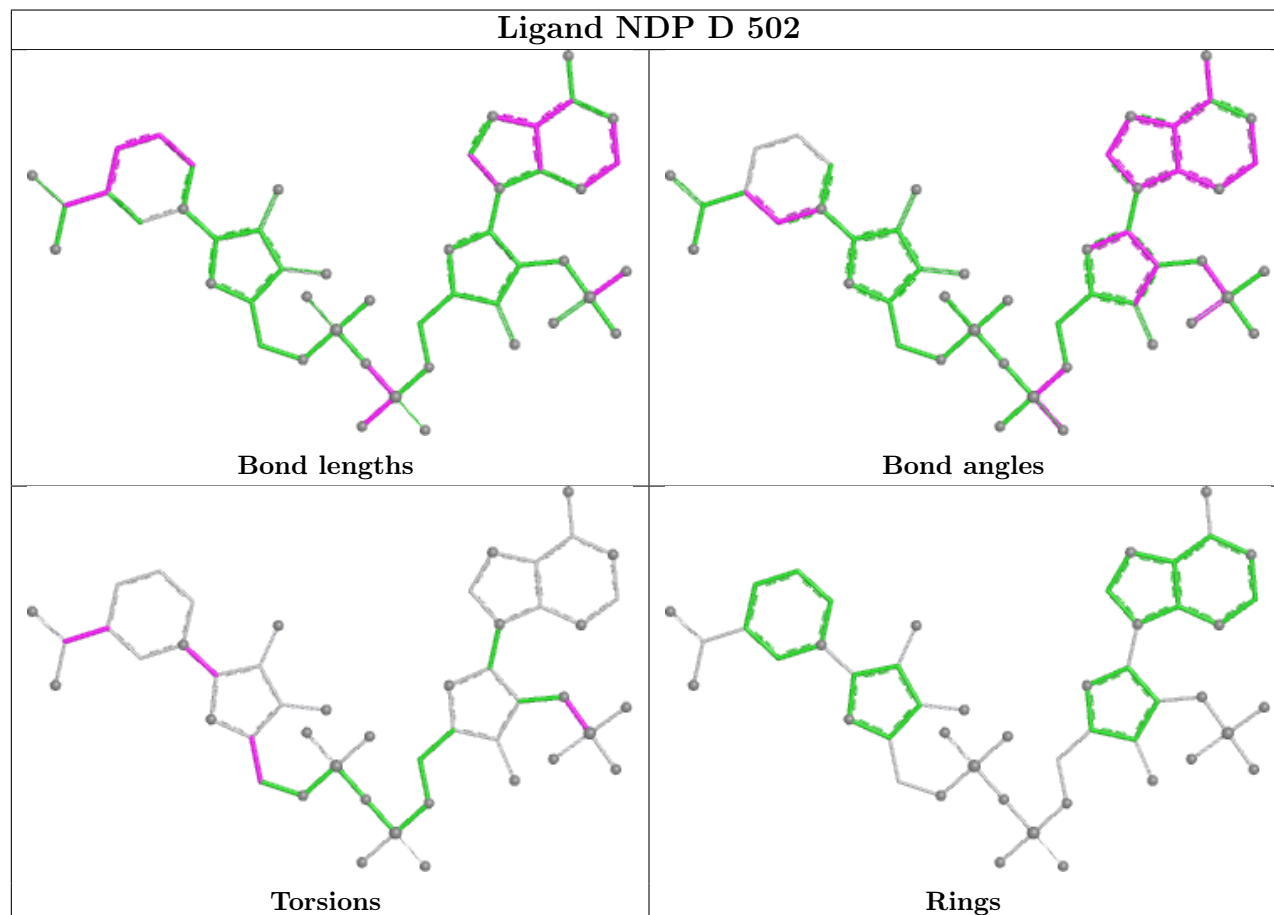
There are no ring outliers.

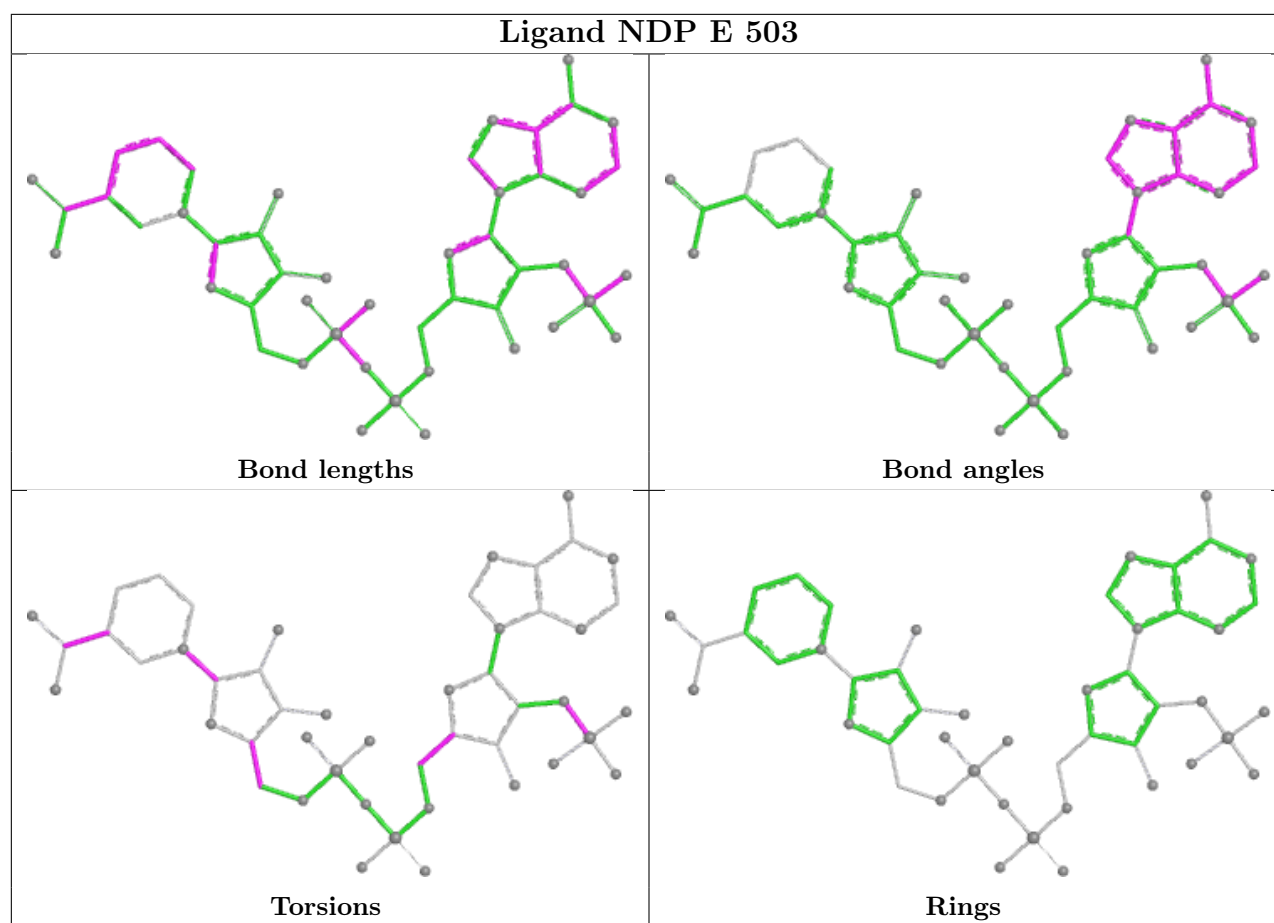
9 monomers are involved in 9 short contacts:

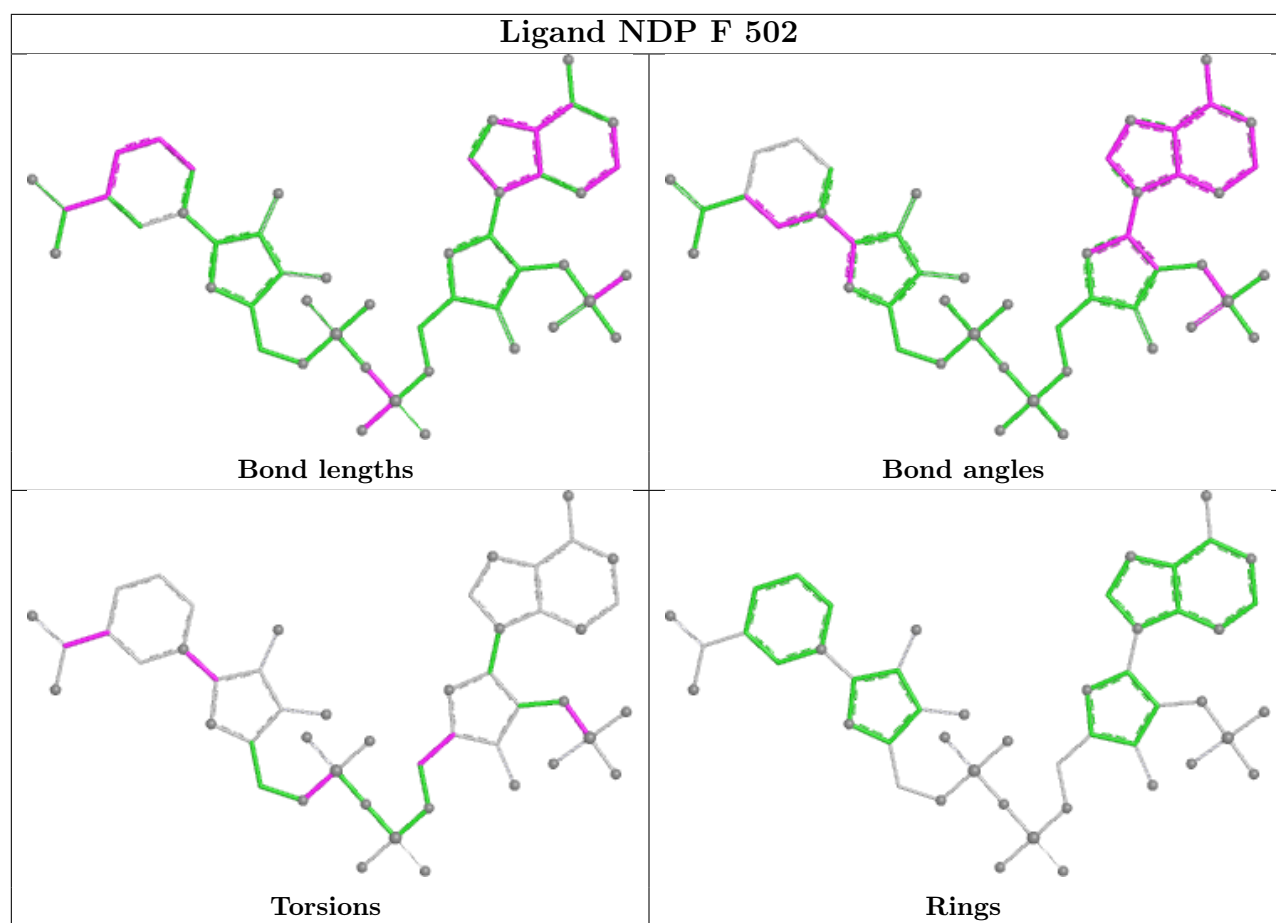
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	2IT	1	0
3	D	502	NDP	1	0
2	F	501	2IT	1	0
3	F	502	NDP	2	0
3	A	502	NDP	1	0
3	C	502	NDP	1	0
2	A	501	2IT	2	0
3	B	502	NDP	3	0
2	C	501	2IT	1	0

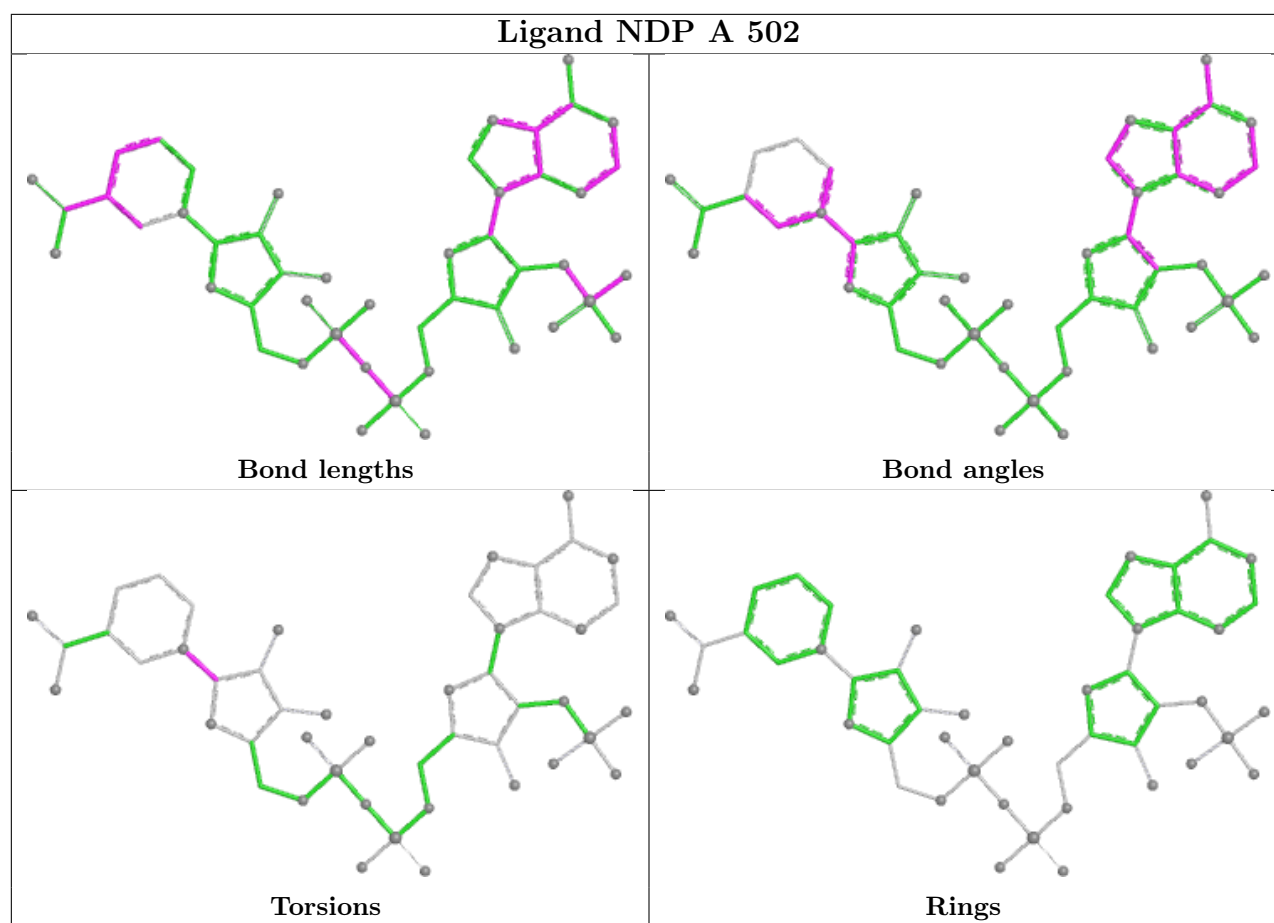
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

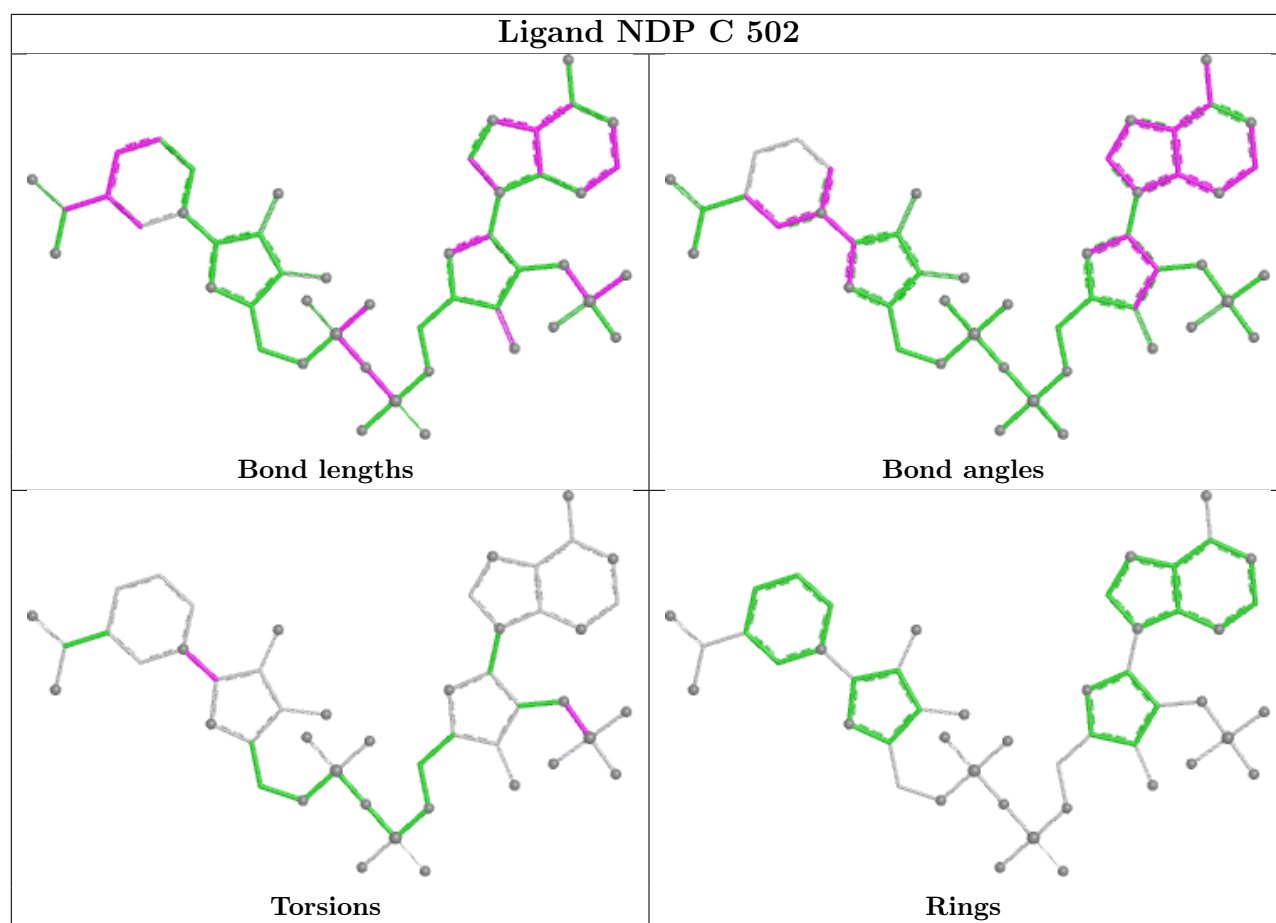
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

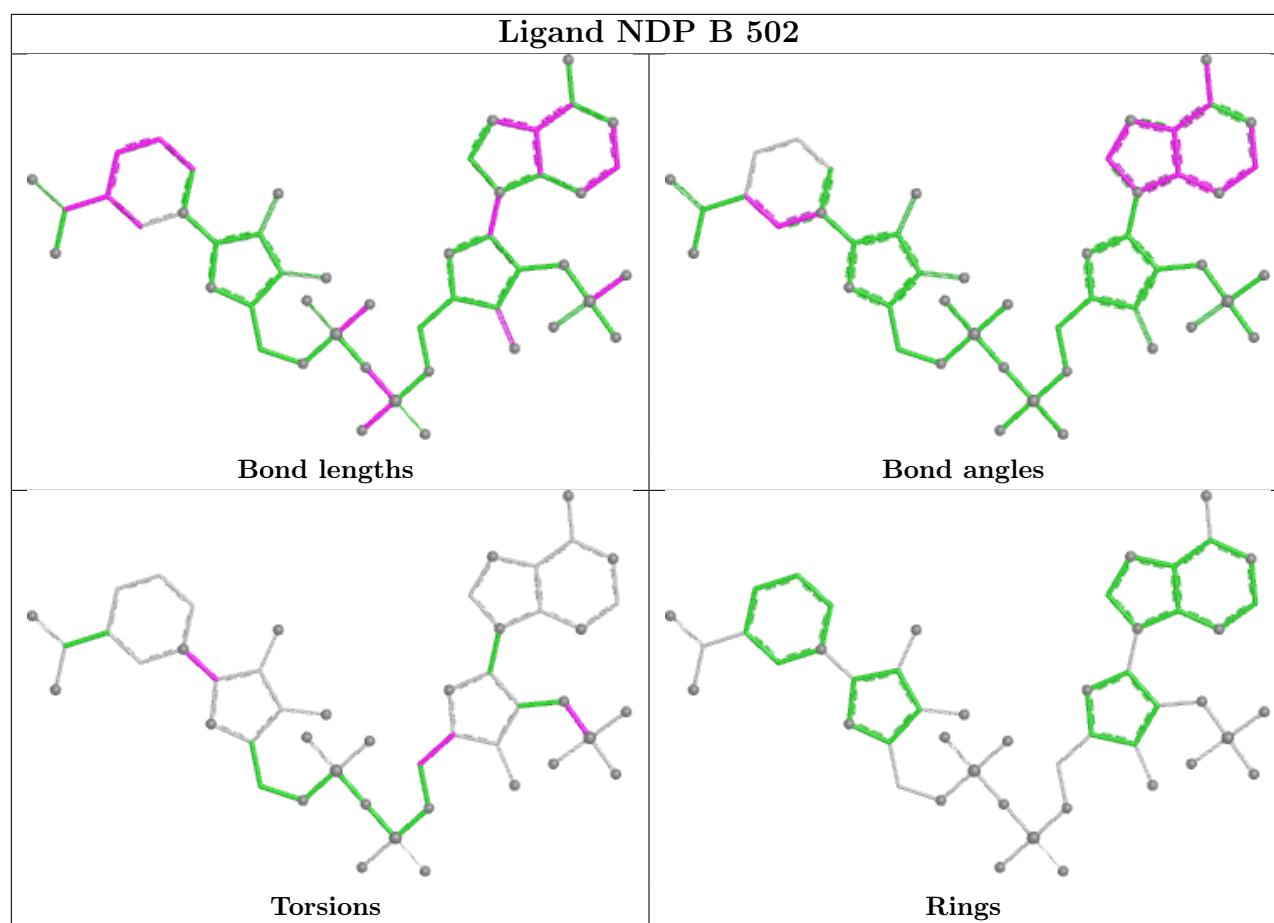












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	447/471 (94%)	0.04	12 (2%) 56 63	11, 17, 31, 50	0
1	B	446/471 (94%)	1.34	140 (31%) 1 1	14, 27, 45, 55	0
1	C	447/471 (94%)	0.58	47 (10%) 11 14	12, 22, 38, 47	1 (0%)
1	D	447/471 (94%)	0.90	96 (21%) 2 3	9, 23, 47, 64	2 (0%)
1	E	460/471 (97%)	0.05	14 (3%) 52 59	10, 17, 31, 45	3 (0%)
1	F	447/471 (94%)	0.30	31 (6%) 23 29	11, 19, 34, 44	2 (0%)
All	All	2694/2826 (95%)	0.53	340 (12%) 8 10	9, 20, 42, 64	8 (0%)

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	295	ALA	7.4
1	B	269	VAL	6.2
1	D	267	GLY	5.6
1	B	301	ALA	5.6
1	B	255	LEU	5.5
1	B	298	ILE	5.4
1	B	248	ALA	5.4
1	D	283	ILE	5.3
1	D	298	ILE	5.3
1	B	291	VAL	5.1
1	D	293	VAL	5.0
1	D	259	VAL	5.0
1	E	45	TYR	5.0
1	B	278	ALA	4.9
1	B	368	GLY	4.9
1	B	335	ALA	4.8
1	B	268	TRP	4.7
1	D	278	ALA	4.7
1	C	300	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	316	ILE	4.5
1	B	365	PHE	4.5
1	B	293	VAL	4.5
1	B	310	TRP	4.5
1	B	334	LEU	4.5
1	D	276	ASP	4.4
1	D	303	TYR	4.4
1	C	310	TRP	4.3
1	E	44	HIS	4.3
1	B	256	GLY	4.3
1	D	304	HIS	4.3
1	B	363	ILE	4.2
1	B	338	GLY	4.2
1	B	366	GLY	4.2
1	C	357	VAL	4.2
1	E	-3	GLY	4.2
1	D	2	THR	4.2
1	B	230	SER	4.1
1	B	318	LEU	4.1
1	E	43	PRO	4.1
1	D	3	VAL	4.0
1	D	292	SER	3.9
1	B	295	ALA	3.9
1	B	303	TYR	3.9
1	B	272	PRO	3.8
1	D	286	VAL	3.8
1	A	2	THR	3.8
1	B	315	ASP	3.7
1	B	340	ARG	3.7
1	E	42	ASP	3.7
1	B	357	VAL	3.6
1	B	258	THR	3.6
1	B	252	ALA	3.6
1	D	301	ALA	3.6
1	D	362	ASP	3.6
1	D	271	THR	3.6
1	F	302	THR	3.6
1	B	228	GLY	3.6
1	D	13	MET	3.6
1	D	260	ILE	3.5
1	E	0	PHE	3.5
1	D	263	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	238	VAL	3.5
1	B	300	GLY	3.5
1	D	1	MET	3.5
1	B	304	HIS	3.5
1	B	312	LEU	3.5
1	B	355	VAL	3.5
1	D	269	VAL	3.5
1	B	223	MET	3.5
1	D	280	LEU	3.4
1	B	38	VAL	3.4
1	F	228	GLY	3.4
1	C	272	PRO	3.4
1	B	257	ALA	3.3
1	B	332	LYS	3.3
1	D	44	HIS	3.3
1	B	267	GLY	3.3
1	C	334	LEU	3.3
1	D	332	LYS	3.3
1	C	278	ALA	3.3
1	D	333	THR	3.3
1	D	282	GLU	3.3
1	B	233	GLY	3.3
1	B	274	GLY	3.3
1	B	2	THR	3.3
1	D	275	VAL	3.3
1	B	302	THR	3.2
1	D	355	VAL	3.2
1	B	362	ASP	3.2
1	B	224	ILE	3.2
1	D	289	ALA	3.2
1	F	335	ALA	3.2
1	B	342	VAL	3.2
1	D	305	THR	3.2
1	B	271	THR	3.1
1	F	357	VAL	3.1
1	B	360	GLU	3.1
1	B	235	LYS	3.1
1	B	222	GLU	3.1
1	B	232	SER	3.1
1	C	10[A]	TYR	3.1
1	D	274	GLY	3.1
1	B	216	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	339	CYS	3.1
1	D	287	ARG	3.1
1	B	341	PHE	3.1
1	D	262	PHE	3.1
1	D	272	PRO	3.0
1	D	296	ASP	3.0
1	C	304	HIS	3.0
1	D	291	VAL	3.0
1	C	268	TRP	3.0
1	D	268	TRP	3.0
1	F	272	PRO	3.0
1	B	262	PHE	3.0
1	C	269	VAL	3.0
1	A	4	ASP	3.0
1	B	239	SER	3.0
1	B	245	ALA	3.0
1	B	309	ILE	3.0
1	D	236	ILE	3.0
1	D	352	PRO	3.0
1	A	3	VAL	2.9
1	B	277	VAL	2.9
1	B	359	ARG	2.9
1	D	266	SER	2.9
1	F	13	MET	2.9
1	B	7	VAL	2.9
1	B	217	VAL	2.9
1	D	38	VAL	2.9
1	B	226	ALA	2.9
1	B	321	ALA	2.9
1	C	331	ALA	2.9
1	B	9	ASN	2.9
1	D	35	LEU	2.9
1	C	338	GLY	2.9
1	C	339	CYS	2.9
1	B	356	GLU	2.9
1	B	358	PHE	2.9
1	B	3	VAL	2.9
1	C	259	VAL	2.9
1	C	335	ALA	2.9
1	D	294	TYR	2.9
1	B	213	GLY	2.9
1	B	215	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	309	ILE	2.9
1	C	271	THR	2.8
1	B	220	VAL	2.8
1	B	20	GLY	2.8
1	B	242	GLY	2.8
1	B	221	SER	2.8
1	B	330	ASN	2.8
1	D	264	ASP	2.8
1	B	370	ALA	2.8
1	D	277	VAL	2.8
1	D	37	ILE	2.8
1	D	273	ASN	2.8
1	E	-8	ARG	2.8
1	F	359	ARG	2.8
1	B	234	GLN	2.8
1	B	251	LYS	2.8
1	F	298	ILE	2.8
1	D	336	ASP	2.8
1	D	302	THR	2.8
1	F	333	THR	2.8
1	E	-7	GLY	2.8
1	B	289	ALA	2.7
1	B	218	TYR	2.7
1	B	280	LEU	2.7
1	D	47	ASP	2.7
1	C	2	THR	2.7
1	C	258	THR	2.7
1	C	270	HIS	2.7
1	D	34	SER	2.7
1	B	354	ALA	2.7
1	B	417	ALA	2.7
1	E	306	ASP	2.7
1	B	270	HIS	2.7
1	B	307	GLY	2.7
1	D	43	PRO	2.7
1	F	30	GLU	2.7
1	B	11	TYR	2.7
1	B	214	TYR	2.7
1	B	261	GLY	2.7
1	B	423	ASN	2.7
1	D	232	SER	2.6
1	C	333	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	328	GLY	2.6
1	B	39	LEU	2.6
1	B	275	VAL	2.6
1	C	355	VAL	2.6
1	F	269	VAL	2.6
1	F	275	VAL	2.6
1	D	42	ASP	2.6
1	B	371	ALA	2.6
1	B	292	SER	2.6
1	D	284	LYS	2.6
1	C	302	THR	2.6
1	B	314	CYS	2.6
1	B	263	SER	2.6
1	B	319	PRO	2.6
1	B	349	PRO	2.6
1	D	330	ASN	2.6
1	B	333	THR	2.6
1	C	309	ILE	2.6
1	B	331	ALA	2.6
1	F	233	GLY	2.5
1	C	273	ASN	2.5
1	E	273	ASN	2.5
1	B	281	ARG	2.5
1	F	291	VAL	2.5
1	C	298	ILE	2.5
1	F	283	ILE	2.5
1	D	328	GLY	2.5
1	F	267	GLY	2.5
1	B	329	GLU	2.5
1	E	40	GLU	2.5
1	C	303	TYR	2.5
1	F	301	ALA	2.5
1	B	240	GLY	2.5
1	B	279	LYS	2.5
1	B	30	GLU	2.5
1	D	297	GLU	2.5
1	B	247	TYR	2.5
1	B	294	TYR	2.5
1	D	317	ALA	2.5
1	B	420	GLY	2.5
1	C	267	GLY	2.5
1	D	233	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	338	GLY	2.5
1	D	353	GLU	2.5
1	E	296	ASP	2.4
1	B	14	LEU	2.4
1	B	352	PRO	2.4
1	B	425	TYR	2.4
1	D	237	ILE	2.4
1	D	71	GLN	2.4
1	D	235	LYS	2.4
1	B	348	MET	2.4
1	C	13	MET	2.4
1	F	1	MET	2.4
1	B	35	LEU	2.4
1	E	228	GLY	2.4
1	F	268	TRP	2.4
1	C	289	ALA	2.4
1	B	337	ASN	2.4
1	B	37	ILE	2.4
1	B	236	ILE	2.4
1	F	304	HIS	2.4
1	D	256	GLY	2.4
1	A	6	GLN	2.4
1	F	339	CYS	2.4
1	D	39	LEU	2.4
1	D	281	ARG	2.4
1	B	238	VAL	2.4
1	C	238	VAL	2.4
1	D	6	GLN	2.3
1	D	137	GLY	2.3
1	C	299	GLU	2.3
1	C	356	GLU	2.3
1	C	12	ASP	2.3
1	F	361	ARG	2.3
1	B	313	LYS	2.3
1	D	136	LYS	2.3
1	C	358	PHE	2.3
1	B	28	VAL	2.3
1	B	244	VAL	2.3
1	C	293	VAL	2.3
1	D	7	VAL	2.3
1	F	293	VAL	2.3
1	D	306	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	16	LYS	2.3
1	D	253	GLN	2.3
1	D	300	GLY	2.3
1	F	256	GLY	2.3
1	C	235	LYS	2.3
1	D	322	THR	2.3
1	B	16	LYS	2.3
1	C	311	ASP	2.3
1	A	1	MET	2.3
1	A	5	GLU	2.2
1	B	413	ALA	2.2
1	D	339	CYS	2.2
1	B	273	ASN	2.2
1	B	326	LEU	2.2
1	C	276	ASP	2.2
1	C	233	GLY	2.2
1	D	261	GLY	2.2
1	D	247	TYR	2.2
1	D	363	ILE	2.2
1	A	329	GLU	2.2
1	D	31	VAL	2.2
1	D	357	VAL	2.2
1	A	9	ASN	2.2
1	B	324	ASN	2.2
1	D	347	ASN	2.2
1	A	19	ALA	2.2
1	D	335	ALA	2.2
1	F	331	ALA	2.2
1	C	265	SER	2.2
1	D	308	SER	2.2
1	F	334	LEU	2.2
1	A	40	GLU	2.2
1	B	299	GLU	2.2
1	D	244	VAL	2.2
1	A	356	GLU	2.2
1	B	25	HIS	2.2
1	B	361	ARG	2.2
1	C	1	MET	2.1
1	D	4	ASP	2.1
1	C	286	VAL	2.1
1	B	40	GLU	2.1
1	B	254	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	2	THR	2.1
1	D	45	TYR	2.1
1	C	359	ARG	2.1
1	C	354	ALA	2.1
1	B	305	THR	2.1
1	B	219	PHE	2.1
1	B	317	ALA	2.1
1	D	279	LYS	2.1
1	D	9	ASN	2.1
1	B	353	GLU	2.1
1	C	353	GLU	2.1
1	B	32	LEU	2.1
1	D	310	TRP	2.1
1	F	338	GLY	2.0
1	B	19	ALA	2.0
1	B	211	ALA	2.0
1	C	9	ASN	2.0
1	D	46	ALA	2.0
1	F	257	ALA	2.0
1	B	31	VAL	2.0
1	F	336	ASP	2.0
1	B	320	CYS	2.0
1	E	-9	PRO	2.0
1	C	306	ASP	2.0
1	F	362	ASP	2.0
1	B	259	VAL	2.0
1	D	270	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

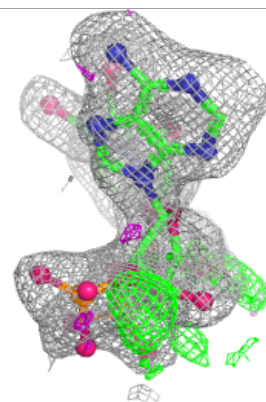
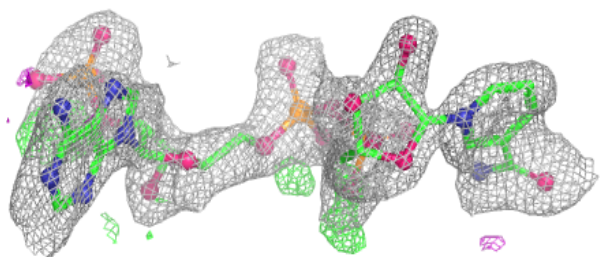
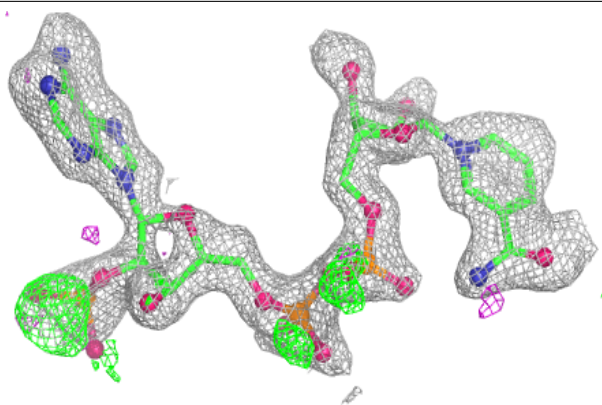
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NDP	D	502	48/48	0.89	0.12	24,35,41,43	0
4	K	C	504	1/1	0.89	0.16	43,43,43,43	0
4	K	F	504	1/1	0.90	0.15	38,38,38,38	0
5	CIT	E	502	13/13	0.90	0.09	24,26,28,28	0
2	2IT	B	501	10/10	0.92	0.09	25,28,28,28	0
3	NDP	B	502	48/48	0.92	0.10	21,27,36,38	0
2	2IT	A	501	10/10	0.93	0.10	16,19,23,24	0
3	NDP	C	502	48/48	0.94	0.09	17,21,32,34	0
4	K	E	506	1/1	0.94	0.10	31,31,31,31	0
2	2IT	F	501	10/10	0.95	0.07	17,21,24,25	0
4	K	A	505	1/1	0.95	0.08	32,32,32,32	0
3	NDP	F	502	48/48	0.96	0.08	15,19,31,34	0
2	2IT	C	501	10/10	0.96	0.07	18,22,26,27	0
3	NDP	E	503	48/48	0.97	0.06	16,22,29,32	0
3	NDP	A	502	48/48	0.97	0.07	12,15,29,31	0
4	K	E	504	1/1	0.97	0.06	28,28,28,28	0
4	K	A	503	1/1	0.98	0.05	30,30,30,30	0
4	K	D	503	1/1	0.99	0.08	22,22,22,22	0
4	K	E	501	1/1	0.99	0.02	13,13,13,13	0
4	K	B	503	1/1	0.99	0.09	25,25,25,25	0
4	K	E	505	1/1	0.99	0.07	19,19,19,19	0
4	K	C	503	1/1	0.99	0.10	23,23,23,23	0
4	K	F	503	1/1	0.99	0.05	23,23,23,23	0
4	K	A	504	1/1	0.99	0.06	21,21,21,21	0
4	K	D	501	1/1	0.99	0.03	18,18,18,18	0

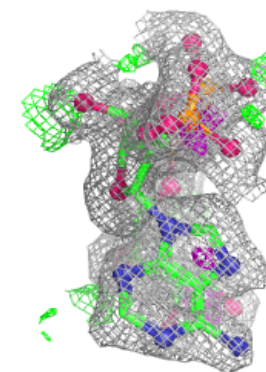
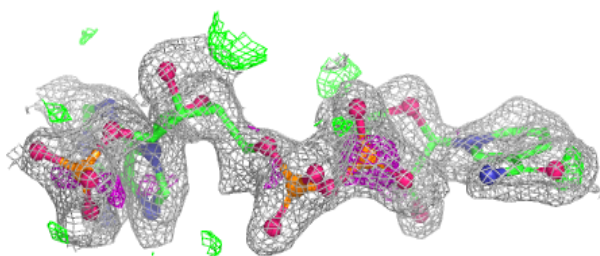
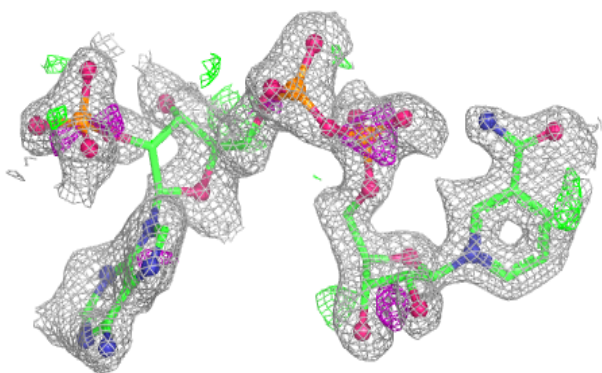
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP D 502:

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

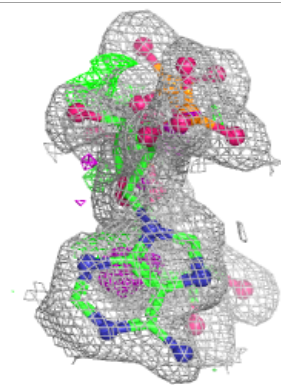
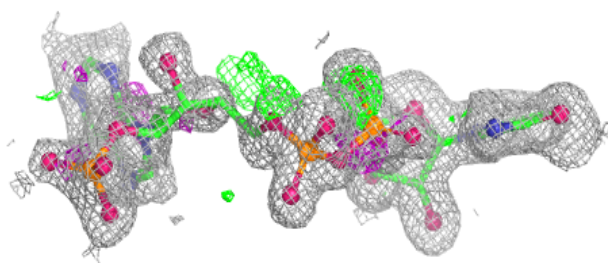
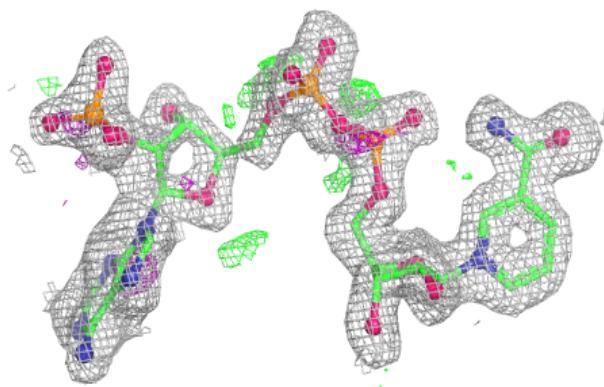
**Electron density around NDP B 502:**

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

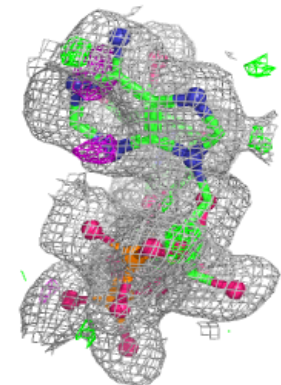
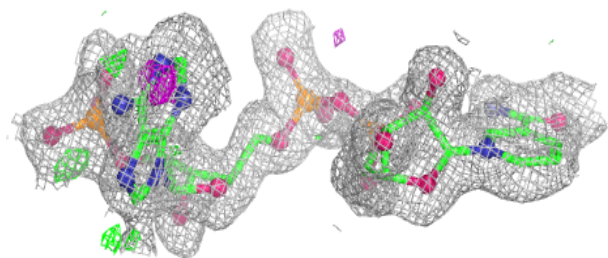
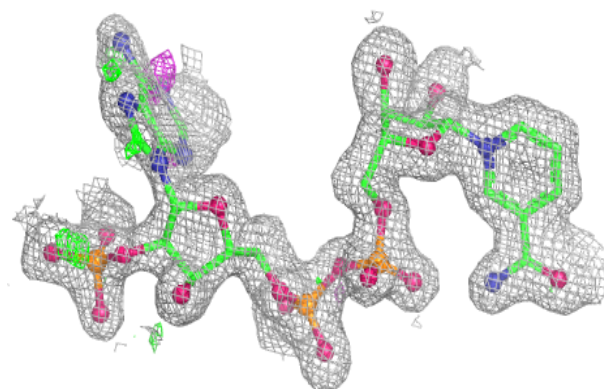


Electron density around NDP C 502:

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

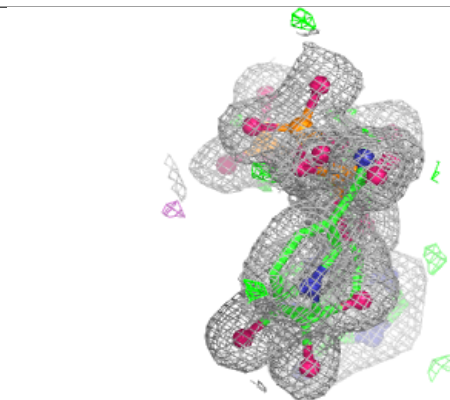
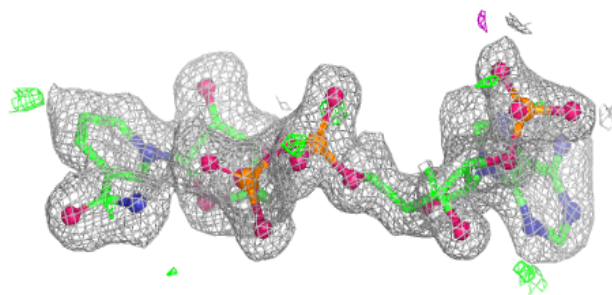
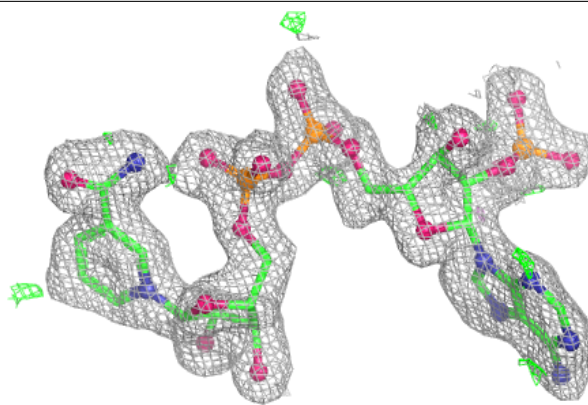
**Electron density around NDP F 502:**

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

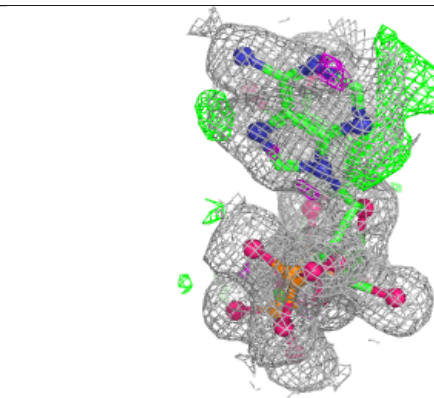
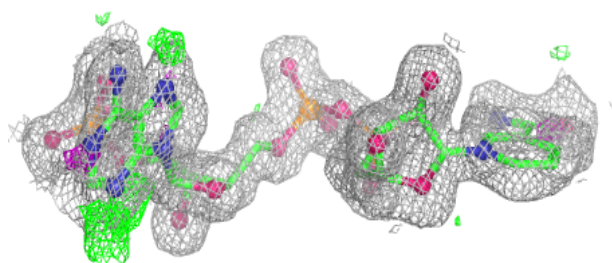
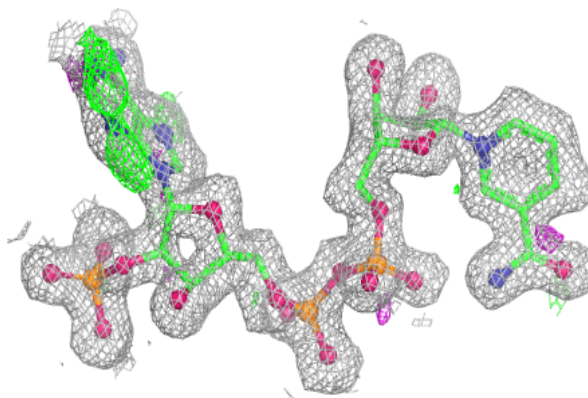


Electron density around NDP E 503:

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

**Electron density around NDP A 502:**

$2mF_o-DF_c$ (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.