



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:15 AM UTC

PDB ID : 1OFG / pdb_00001ofg
Title : GLUCOSE-FRUCTOSE OXIDOREDUCTASE
Authors : Kingston, R.L.; Scopes, R.K.; Baker, E.N.
Deposited on : 1996-10-17
Resolution : 2.70 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

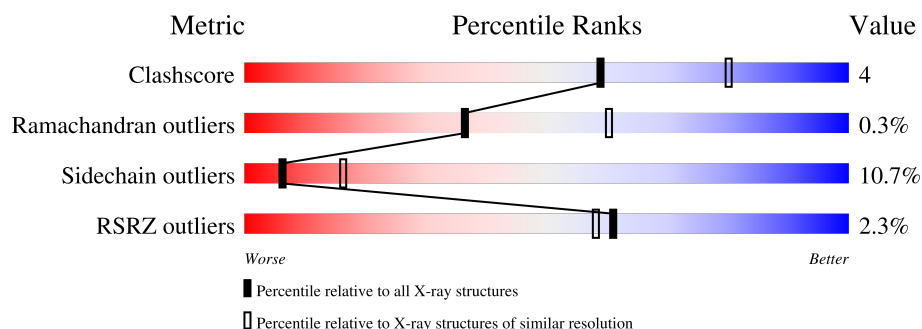
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	381	2% 76% 20% ..
1	B	381	2% 76% 20% ..
1	C	381	4% 76% 20% .
1	D	381	2% 77% 19% .
1	E	381	4% 77% 19% .
1	F	381	% 76% 20% ..

2 Entry composition ⓘ

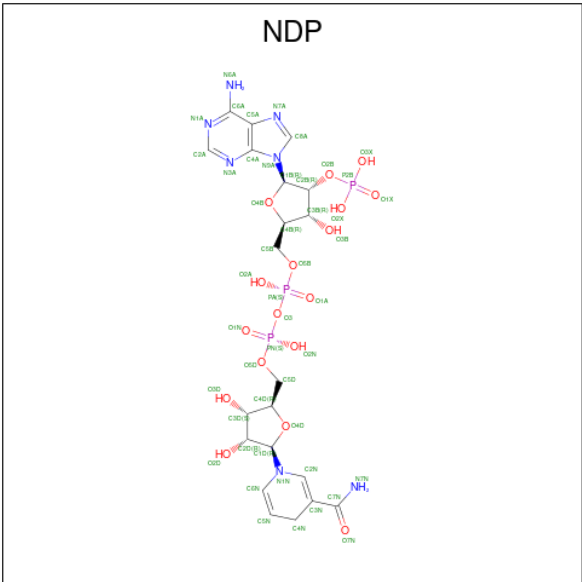
There are 3 unique types of molecules in this entry. The entry contains 18498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-FRUCTOSE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	B	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	C	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	D	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	E	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	F	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

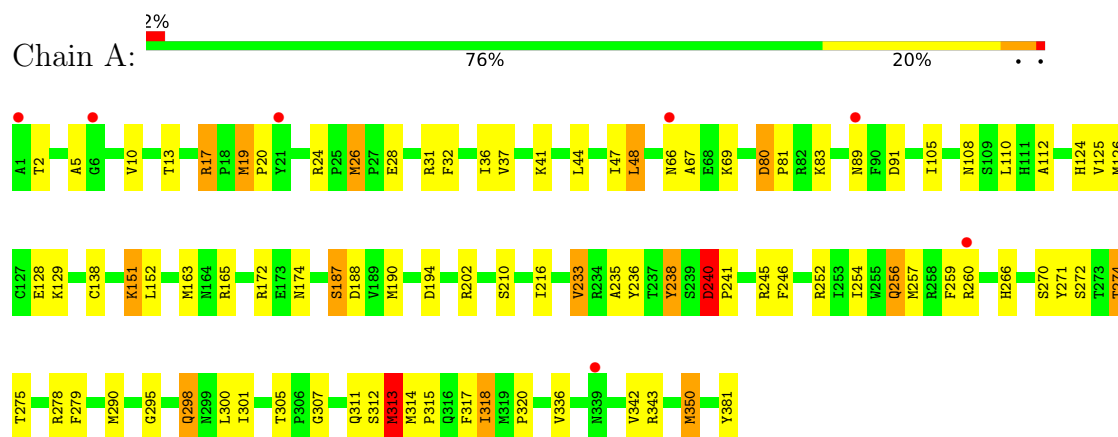
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	140	Total	O	0	0
			140	140		
3	C	139	Total	O	0	0
			139	139		
3	D	139	Total	O	0	0
			139	139		
3	E	139	Total	O	0	0
			139	139		
3	F	141	Total	O	0	0
			141	141		

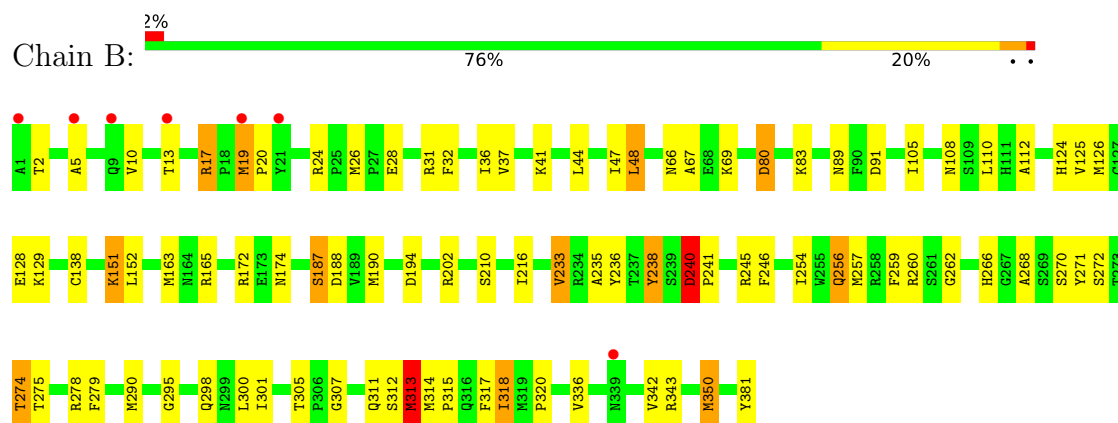
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

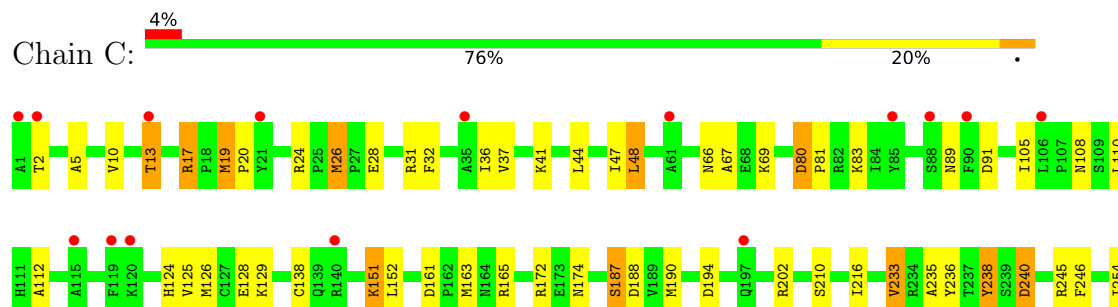
• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

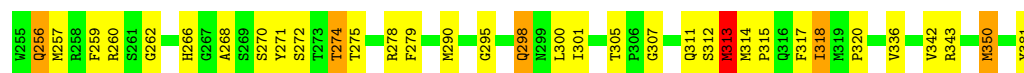


• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

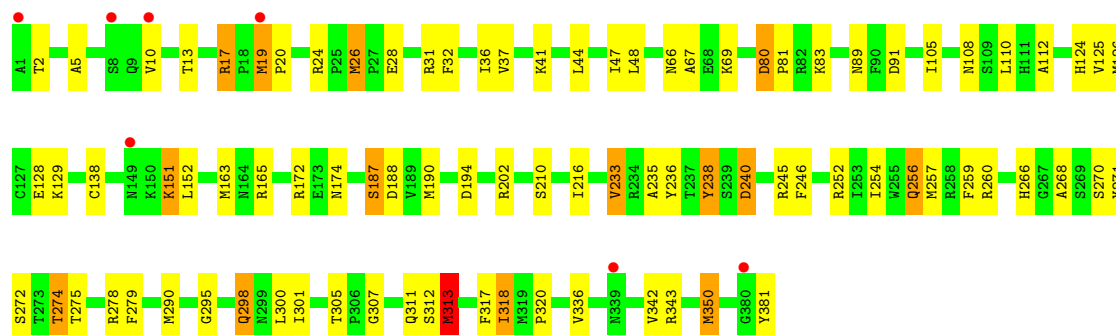
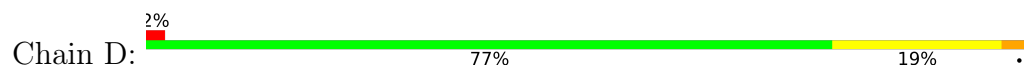


• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

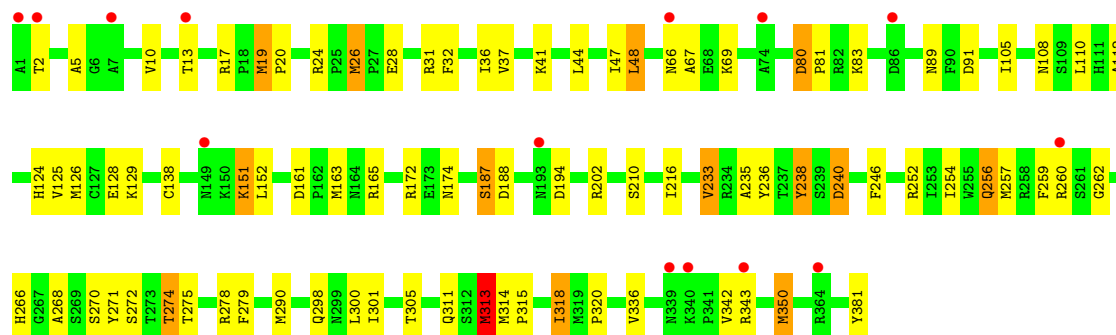
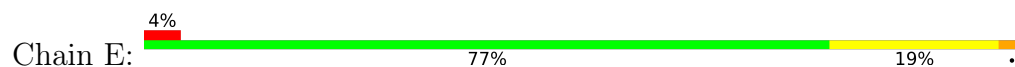




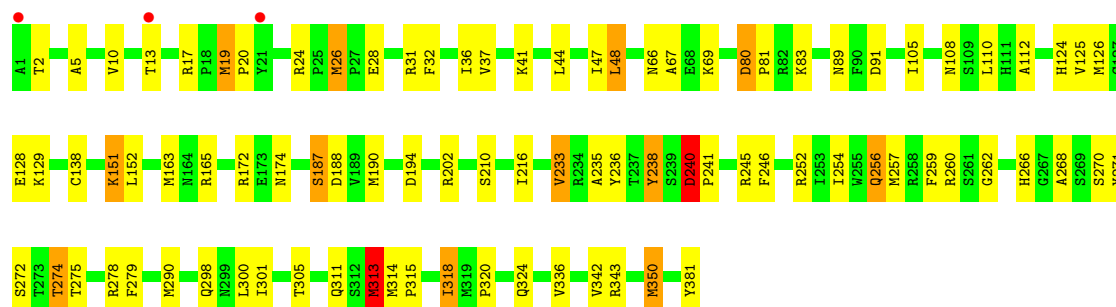
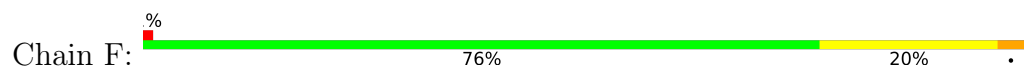
• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE



• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE



• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.49Å 283.69Å 116.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.70) 91.4 (50.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.69Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.203 , (Not available) 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18498	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8857e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.92	6/2959 (0.2%)	1.49	35/4019 (0.9%)
1	B	0.92	6/2959 (0.2%)	1.49	35/4019 (0.9%)
1	C	0.92	6/2959 (0.2%)	1.49	37/4019 (0.9%)
1	D	0.92	6/2959 (0.2%)	1.49	35/4019 (0.9%)
1	E	0.92	6/2959 (0.2%)	1.49	37/4019 (0.9%)
1	F	0.92	6/2959 (0.2%)	1.49	36/4019 (0.9%)
All	All	0.92	36/17754 (0.2%)	1.49	215/24114 (0.9%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	381	TYR	C-O	7.17	1.37	1.23
1	E	381	TYR	C-O	7.15	1.37	1.23
1	D	381	TYR	C-O	7.15	1.37	1.23
1	A	381	TYR	C-O	7.13	1.37	1.23
1	B	381	TYR	C-O	7.11	1.37	1.23
1	C	381	TYR	C-O	7.08	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	350	MET	SD-CE	-5.54	1.65	1.79
1	A	350	MET	SD-CE	-5.53	1.65	1.79
1	D	350	MET	SD-CE	-5.52	1.65	1.79
1	E	350	MET	SD-CE	-5.51	1.65	1.79
1	F	350	MET	SD-CE	-5.50	1.65	1.79
1	C	350	MET	SD-CE	-5.50	1.65	1.79
1	B	238	TYR	CA-CB	5.42	1.63	1.53
1	A	238	TYR	CA-CB	5.42	1.63	1.53
1	E	238	TYR	CA-CB	5.38	1.63	1.53
1	D	238	TYR	CA-CB	5.37	1.63	1.53
1	C	238	TYR	CA-CB	5.36	1.63	1.53
1	F	238	TYR	CA-CB	5.35	1.62	1.53
1	B	10	VAL	CA-C	-5.33	1.48	1.53
1	A	10	VAL	CA-C	-5.31	1.48	1.53
1	F	10	VAL	CA-C	-5.30	1.48	1.53
1	B	381	TYR	C-OXT	-5.28	1.12	1.23
1	A	381	TYR	C-OXT	-5.28	1.12	1.23
1	C	381	TYR	C-OXT	-5.28	1.12	1.23
1	E	381	TYR	C-OXT	-5.26	1.13	1.23
1	D	381	TYR	C-OXT	-5.26	1.13	1.23
1	F	381	TYR	C-OXT	-5.24	1.13	1.23
1	D	10	VAL	CA-C	-5.22	1.49	1.53
1	C	10	VAL	CA-C	-5.22	1.49	1.53
1	E	10	VAL	CA-C	-5.21	1.49	1.53
1	F	163	MET	SD-CE	-5.12	1.66	1.79
1	A	163	MET	SD-CE	-5.12	1.66	1.79
1	E	163	MET	SD-CE	-5.11	1.66	1.79
1	B	163	MET	SD-CE	-5.11	1.66	1.79
1	C	163	MET	SD-CE	-5.10	1.66	1.79
1	D	163	MET	SD-CE	-5.10	1.66	1.79

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	N-CA-CB	-9.19	101.45	111.10
1	D	24	ARG	N-CA-CB	-9.18	101.46	111.10
1	A	47	ILE	N-CA-C	9.17	119.19	110.30
1	C	24	ARG	N-CA-CB	-9.17	101.47	111.10
1	D	47	ILE	N-CA-C	9.16	119.18	110.30
1	F	47	ILE	N-CA-C	9.15	119.18	110.30
1	B	47	ILE	N-CA-C	9.14	119.17	110.30
1	B	24	ARG	N-CA-CB	-9.12	101.52	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	24	ARG	N-CA-CB	-9.12	101.52	111.10
1	C	47	ILE	N-CA-C	9.11	119.14	110.30
1	E	24	ARG	N-CA-CB	-9.09	101.55	111.10
1	E	47	ILE	N-CA-C	9.09	119.12	110.30
1	D	305	THR	N-CA-C	-8.75	98.08	108.14
1	E	305	THR	N-CA-C	-8.75	98.08	108.14
1	F	305	THR	N-CA-C	-8.74	98.08	108.14
1	A	305	THR	N-CA-C	-8.74	98.09	108.14
1	B	305	THR	N-CA-C	-8.74	98.09	108.14
1	C	305	THR	N-CA-C	-8.71	98.12	108.14
1	D	298	GLN	N-CA-C	8.65	123.30	111.54
1	F	298	GLN	N-CA-C	8.60	123.23	111.54
1	B	298	GLN	N-CA-C	8.60	123.23	111.54
1	C	298	GLN	N-CA-C	8.59	123.22	111.54
1	E	298	GLN	N-CA-C	8.59	123.22	111.54
1	A	298	GLN	N-CA-C	8.59	123.22	111.54
1	C	210	SER	N-CA-C	8.54	121.53	111.71
1	D	210	SER	N-CA-C	8.53	121.52	111.71
1	B	210	SER	N-CA-C	8.52	121.50	111.71
1	A	210	SER	N-CA-C	8.48	121.47	111.71
1	F	210	SER	N-CA-C	8.48	121.47	111.71
1	E	210	SER	N-CA-C	8.46	121.44	111.71
1	C	246	PHE	N-CA-C	7.28	120.80	112.57
1	B	246	PHE	N-CA-C	7.28	120.80	112.57
1	F	246	PHE	N-CA-C	7.28	120.79	112.57
1	D	246	PHE	N-CA-C	7.27	120.79	112.57
1	A	246	PHE	N-CA-C	7.27	120.78	112.57
1	E	246	PHE	N-CA-C	7.23	120.75	112.57
1	F	313	MET	N-CA-C	-7.10	97.87	107.88
1	E	313	MET	N-CA-C	-7.10	97.87	107.88
1	B	313	MET	N-CA-C	-7.08	97.89	107.88
1	A	313	MET	N-CA-C	-7.08	97.90	107.88
1	D	313	MET	N-CA-C	-7.07	97.92	107.88
1	C	313	MET	N-CA-C	-7.06	97.93	107.88
1	A	240	ASP	CA-C-N	7.01	126.71	119.56
1	A	240	ASP	C-N-CA	7.01	126.71	119.56
1	E	240	ASP	CA-C-N	7.01	126.71	119.56
1	E	240	ASP	C-N-CA	7.01	126.71	119.56
1	D	67	ALA	N-CA-C	6.99	118.98	111.36
1	A	67	ALA	N-CA-C	6.99	118.98	111.36
1	F	240	ASP	CA-C-N	6.99	126.69	119.56
1	F	240	ASP	C-N-CA	6.99	126.69	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	ASP	CA-C-N	6.97	126.67	119.56
1	C	240	ASP	C-N-CA	6.97	126.67	119.56
1	B	240	ASP	CA-C-N	6.96	126.66	119.56
1	B	240	ASP	C-N-CA	6.96	126.66	119.56
1	D	240	ASP	CA-C-N	6.96	126.66	119.56
1	D	240	ASP	C-N-CA	6.96	126.66	119.56
1	E	67	ALA	N-CA-C	6.95	118.94	111.36
1	F	67	ALA	N-CA-C	6.94	118.93	111.36
1	B	67	ALA	N-CA-C	6.94	118.92	111.36
1	C	67	ALA	N-CA-C	6.93	118.92	111.36
1	A	19	MET	N-CA-C	-6.66	101.26	109.65
1	B	31	ARG	N-CA-C	6.66	120.66	112.54
1	B	19	MET	N-CA-C	-6.65	101.27	109.65
1	E	274	THR	N-CA-C	6.65	118.91	110.33
1	C	19	MET	N-CA-C	-6.65	101.27	109.65
1	D	31	ARG	N-CA-C	6.64	120.64	112.54
1	D	19	MET	N-CA-C	-6.63	101.29	109.65
1	E	19	MET	N-CA-C	-6.63	101.30	109.65
1	C	274	THR	N-CA-C	6.63	118.88	110.33
1	A	31	ARG	N-CA-C	6.62	120.62	112.54
1	C	31	ARG	N-CA-C	6.62	120.62	112.54
1	B	274	THR	N-CA-C	6.62	118.87	110.33
1	E	31	ARG	N-CA-C	6.62	120.61	112.54
1	F	19	MET	N-CA-C	-6.62	101.31	109.65
1	F	274	THR	N-CA-C	6.61	118.86	110.33
1	D	274	THR	N-CA-C	6.61	118.85	110.33
1	A	274	THR	N-CA-C	6.60	118.85	110.33
1	D	80	ASP	CA-C-N	6.57	126.20	119.56
1	D	80	ASP	C-N-CA	6.57	126.20	119.56
1	F	31	ARG	N-CA-C	6.57	120.56	112.54
1	B	80	ASP	CA-C-N	6.57	126.19	119.56
1	B	80	ASP	C-N-CA	6.57	126.19	119.56
1	F	80	ASP	CA-C-N	6.56	126.19	119.56
1	F	80	ASP	C-N-CA	6.56	126.19	119.56
1	C	80	ASP	CA-C-N	6.55	126.17	119.56
1	C	80	ASP	C-N-CA	6.55	126.17	119.56
1	E	80	ASP	CA-C-N	6.53	126.16	119.56
1	E	80	ASP	C-N-CA	6.53	126.16	119.56
1	A	80	ASP	CA-C-N	6.53	126.15	119.56
1	A	80	ASP	C-N-CA	6.53	126.15	119.56
1	A	41	LYS	N-CA-C	6.50	118.02	111.07
1	F	41	LYS	N-CA-C	6.49	118.01	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	LYS	N-CA-C	6.49	118.01	111.07
1	B	41	LYS	N-CA-C	6.48	118.00	111.07
1	C	41	LYS	N-CA-C	6.48	118.00	111.07
1	E	41	LYS	N-CA-C	6.45	117.97	111.07
1	A	108	ASN	N-CA-C	6.20	124.00	110.80
1	E	108	ASN	N-CA-C	6.19	123.99	110.80
1	B	108	ASN	N-CA-C	6.18	123.97	110.80
1	F	108	ASN	N-CA-C	6.17	123.95	110.80
1	C	108	ASN	N-CA-C	6.16	123.93	110.80
1	D	108	ASN	N-CA-C	6.16	123.93	110.80
1	E	10	VAL	CB-CA-C	-6.08	105.28	110.94
1	A	10	VAL	CB-CA-C	-6.03	105.33	110.94
1	F	10	VAL	CB-CA-C	-6.02	105.34	110.94
1	C	10	VAL	CB-CA-C	-6.01	105.35	110.94
1	D	10	VAL	CB-CA-C	-5.99	105.37	110.94
1	B	10	VAL	CB-CA-C	-5.99	105.37	110.94
1	C	235	ALA	N-CA-C	5.82	117.70	108.79
1	D	126	MET	N-CA-C	-5.82	99.03	108.52
1	C	126	MET	N-CA-C	-5.80	99.06	108.52
1	B	126	MET	N-CA-C	-5.80	99.06	108.52
1	E	235	ALA	N-CA-C	5.80	117.67	108.79
1	A	235	ALA	N-CA-C	5.79	117.66	108.79
1	F	126	MET	N-CA-C	-5.79	99.08	108.52
1	E	126	MET	N-CA-C	-5.78	99.09	108.52
1	A	126	MET	N-CA-C	-5.78	99.10	108.52
1	F	235	ALA	N-CA-C	5.78	117.63	108.79
1	B	235	ALA	N-CA-C	5.77	117.62	108.79
1	D	235	ALA	N-CA-C	5.75	117.59	108.79
1	C	194	ASP	CA-C-N	5.61	125.13	119.19
1	C	194	ASP	C-N-CA	5.61	125.13	119.19
1	F	194	ASP	CA-C-N	5.60	125.12	119.19
1	F	194	ASP	C-N-CA	5.60	125.12	119.19
1	B	194	ASP	CA-C-N	5.58	125.11	119.19
1	B	194	ASP	C-N-CA	5.58	125.11	119.19
1	A	194	ASP	CA-C-N	5.58	125.10	119.19
1	A	194	ASP	C-N-CA	5.58	125.10	119.19
1	E	194	ASP	CA-C-N	5.57	125.09	119.19
1	E	194	ASP	C-N-CA	5.57	125.09	119.19
1	D	194	ASP	CA-C-N	5.57	125.09	119.19
1	D	194	ASP	C-N-CA	5.57	125.09	119.19
1	B	125	VAL	N-CA-C	5.51	115.82	108.11
1	A	37	VAL	N-CA-C	5.50	115.51	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	125	VAL	N-CA-C	5.50	115.80	108.11
1	D	37	VAL	N-CA-C	5.49	115.49	107.37
1	C	125	VAL	N-CA-C	5.48	115.79	108.11
1	E	37	VAL	N-CA-C	5.48	115.48	107.37
1	D	125	VAL	N-CA-C	5.48	115.78	108.11
1	E	125	VAL	N-CA-C	5.48	115.78	108.11
1	C	37	VAL	N-CA-C	5.47	115.46	107.37
1	A	125	VAL	N-CA-C	5.45	115.75	108.11
1	F	37	VAL	N-CA-C	5.45	115.44	107.37
1	B	37	VAL	N-CA-C	5.44	115.42	107.37
1	C	202	ARG	CA-C-N	5.41	127.53	120.28
1	C	202	ARG	C-N-CA	5.41	127.53	120.28
1	A	202	ARG	CA-C-N	5.40	127.52	120.28
1	A	202	ARG	C-N-CA	5.40	127.52	120.28
1	D	202	ARG	CA-C-N	5.40	127.51	120.28
1	D	202	ARG	C-N-CA	5.40	127.51	120.28
1	E	202	ARG	CA-C-N	5.37	127.48	120.28
1	E	202	ARG	C-N-CA	5.37	127.48	120.28
1	F	202	ARG	CA-C-N	5.37	127.48	120.28
1	F	202	ARG	C-N-CA	5.37	127.48	120.28
1	B	202	ARG	CA-C-N	5.36	127.46	120.28
1	B	202	ARG	C-N-CA	5.36	127.46	120.28
1	D	272	SER	N-CA-C	5.34	119.77	112.88
1	E	272	SER	N-CA-C	5.34	119.77	112.88
1	B	89	ASN	CA-C-N	5.33	127.68	120.38
1	B	89	ASN	C-N-CA	5.33	127.68	120.38
1	B	194	ASP	N-CA-C	-5.32	102.94	109.65
1	A	89	ASN	CA-C-N	5.31	127.66	120.38
1	A	89	ASN	C-N-CA	5.31	127.66	120.38
1	A	194	ASP	N-CA-C	-5.31	102.96	109.65
1	D	194	ASP	N-CA-C	-5.31	102.96	109.65
1	A	272	SER	N-CA-C	5.31	119.73	112.88
1	C	194	ASP	N-CA-C	-5.31	102.96	109.65
1	C	259	PHE	CA-C-N	5.30	127.91	120.28
1	C	259	PHE	C-N-CA	5.30	127.91	120.28
1	F	194	ASP	N-CA-C	-5.30	102.97	109.65
1	E	194	ASP	N-CA-C	-5.30	102.97	109.65
1	C	272	SER	N-CA-C	5.29	119.71	112.88
1	F	272	SER	N-CA-C	5.29	119.71	112.88
1	B	259	PHE	CA-C-N	5.29	127.90	120.28
1	B	259	PHE	C-N-CA	5.29	127.90	120.28
1	D	259	PHE	CA-C-N	5.29	127.90	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	PHE	C-N-CA	5.29	127.90	120.28
1	E	89	ASN	CA-C-N	5.29	127.63	120.38
1	E	89	ASN	C-N-CA	5.29	127.63	120.38
1	F	89	ASN	CA-C-N	5.29	127.63	120.38
1	F	89	ASN	C-N-CA	5.29	127.63	120.38
1	C	89	ASN	CA-C-N	5.29	127.62	120.38
1	C	89	ASN	C-N-CA	5.29	127.62	120.38
1	B	272	SER	N-CA-C	5.28	119.69	112.88
1	F	112	ALA	N-CA-C	5.28	117.04	111.28
1	D	174	ASN	N-CA-C	5.28	118.99	112.24
1	E	259	PHE	CA-C-N	5.28	127.88	120.28
1	E	259	PHE	C-N-CA	5.28	127.88	120.28
1	F	259	PHE	CA-C-N	5.28	127.88	120.28
1	F	259	PHE	C-N-CA	5.28	127.88	120.28
1	E	174	ASN	N-CA-C	5.27	118.99	112.24
1	A	112	ALA	N-CA-C	5.27	117.02	111.28
1	F	174	ASN	N-CA-C	5.27	118.98	112.24
1	D	112	ALA	N-CA-C	5.27	117.02	111.28
1	C	112	ALA	N-CA-C	5.26	117.02	111.28
1	D	89	ASN	CA-C-N	5.26	127.58	120.38
1	D	89	ASN	C-N-CA	5.26	127.58	120.38
1	A	259	PHE	CA-C-N	5.25	127.84	120.28
1	A	259	PHE	C-N-CA	5.25	127.84	120.28
1	C	174	ASN	N-CA-C	5.25	118.96	112.24
1	A	174	ASN	N-CA-C	5.25	118.96	112.24
1	B	112	ALA	N-CA-C	5.23	116.98	111.28
1	B	174	ASN	N-CA-C	5.22	118.92	112.24
1	E	112	ALA	N-CA-C	5.19	116.94	111.28
1	F	5	ALA	N-CA-C	5.12	117.53	111.33
1	E	5	ALA	N-CA-C	5.11	117.52	111.33
1	A	5	ALA	N-CA-C	5.11	117.51	111.33
1	C	5	ALA	N-CA-C	5.11	117.51	111.33
1	B	5	ALA	N-CA-C	5.09	117.50	111.33
1	D	5	ALA	N-CA-C	5.07	117.47	111.33
1	E	161	ASP	CA-C-N	5.02	124.62	119.05
1	E	161	ASP	C-N-CA	5.02	124.62	119.05
1	F	324	GLN	N-CA-C	5.01	117.47	111.71
1	C	161	ASP	CA-C-N	5.00	124.60	119.05
1	C	161	ASP	C-N-CA	5.00	124.60	119.05

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	TYR	Sidechain
1	B	238	TYR	Sidechain
1	C	238	TYR	Sidechain
1	D	238	TYR	Sidechain
1	E	238	TYR	Sidechain
1	F	238	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2895	0	2783	32	0
1	B	2895	0	2783	31	0
1	C	2895	0	2783	35	0
1	D	2895	0	2783	31	0
1	E	2895	0	2783	25	0
1	F	2895	0	2783	27	0
2	A	48	0	26	2	0
2	B	48	0	26	2	0
2	C	48	0	26	1	0
2	D	48	0	26	2	0
2	E	48	0	26	0	0
2	F	48	0	26	0	0
3	A	142	0	0	3	0
3	B	140	0	0	2	0
3	C	139	0	0	3	0
3	D	139	0	0	3	0
3	E	139	0	0	1	0
3	F	141	0	0	1	0
All	All	18498	0	16854	153	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 4.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:MET:HE3	1:C:20:PRO:HD2	1.69	0.74
1:A:19:MET:HE3	1:A:20:PRO:HD2	1.69	0.73
1:B:19:MET:HE3	1:B:20:PRO:HD2	1.69	0.73
1:D:19:MET:HE3	1:D:20:PRO:HD2	1.69	0.73
1:E:19:MET:HE3	1:E:20:PRO:HD2	1.69	0.73
1:F:19:MET:HE3	1:F:20:PRO:HD2	1.69	0.73
1:F:187:SER:HB3	1:F:270:SER:HB3	1.75	0.69
1:A:187:SER:HB3	1:A:270:SER:HB3	1.75	0.69
1:B:187:SER:HB3	1:B:270:SER:HB3	1.75	0.69
1:C:187:SER:HB3	1:C:270:SER:HB3	1.75	0.69
1:D:187:SER:HB3	1:D:270:SER:HB3	1.75	0.69
1:E:187:SER:HB3	1:E:270:SER:HB3	1.75	0.68
1:A:124:HIS:HD2	1:A:151:LYS:H	1.43	0.67
1:E:124:HIS:HD2	1:E:151:LYS:H	1.43	0.67
1:D:124:HIS:HD2	1:D:151:LYS:H	1.43	0.67
1:C:124:HIS:HD2	1:C:151:LYS:H	1.43	0.67
1:B:124:HIS:HD2	1:B:151:LYS:H	1.43	0.67
1:F:124:HIS:HD2	1:F:151:LYS:H	1.43	0.66
1:A:256:GLN:HE22	1:B:236:TYR:HB3	1.61	0.65
1:A:236:TYR:HB3	1:B:256:GLN:HE22	1.63	0.64
1:E:236:TYR:HB3	1:F:256:GLN:HE22	1.65	0.62
1:E:256:GLN:HE22	1:F:236:TYR:HB3	1.65	0.61
3:B:554:HOH:O	1:C:17:ARG:HD3	2.01	0.60
1:B:307:GLY:O	1:D:312:SER:HA	2.02	0.59
1:C:256:GLN:HE22	1:D:236:TYR:HB3	1.68	0.59
1:A:254:ILE:HD13	1:B:266:HIS:HB3	1.85	0.59
1:A:266:HIS:HB3	1:B:254:ILE:HD13	1.84	0.59
1:E:254:ILE:HD13	1:F:266:HIS:HB3	1.87	0.57
1:C:236:TYR:HB3	1:D:256:GLN:HE22	1.70	0.57
1:E:266:HIS:HB3	1:F:254:ILE:HD13	1.87	0.56
1:A:17:ARG:HD2	2:D:500:NDP:C2A	2.36	0.55
3:A:546:HOH:O	1:D:17:ARG:HD3	2.06	0.55
1:C:266:HIS:HB3	1:D:254:ILE:HD13	1.89	0.54
1:B:17:ARG:HD3	3:C:564:HOH:O	2.08	0.53
1:A:312:SER:HA	1:C:307:GLY:O	2.08	0.53
2:A:500:NDP:C2A	1:D:17:ARG:HD2	2.39	0.53
1:D:66:ASN:HB3	1:D:69:LYS:HE2	1.91	0.53
1:F:66:ASN:HB3	1:F:69:LYS:HE2	1.91	0.53
1:A:66:ASN:HB3	1:A:69:LYS:HE2	1.91	0.52
1:B:66:ASN:HB3	1:B:69:LYS:HE2	1.91	0.52
1:B:312:SER:HA	1:D:307:GLY:O	2.09	0.52
1:C:254:ILE:HD13	1:D:266:HIS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASN:HB3	1:C:69:LYS:HE2	1.91	0.52
1:E:66:ASN:HB3	1:E:69:LYS:HE2	1.91	0.52
1:A:17:ARG:HD3	3:D:571:HOH:O	2.08	0.52
1:A:307:GLY:O	1:C:312:SER:HA	2.10	0.52
1:C:298:GLN:HB3	3:C:509:HOH:O	2.12	0.49
1:B:295:GLY:HA2	1:C:317:PHE:CE1	2.47	0.48
1:E:80:ASP:HA	1:E:81:PRO:HD2	1.63	0.48
1:E:300:LEU:HD12	1:E:313:MET:HB3	1.96	0.47
1:A:80:ASP:HA	1:A:81:PRO:HD2	1.63	0.47
1:C:278:ARG:HD2	3:C:636:HOH:O	2.14	0.47
1:B:17:ARG:HD2	2:C:500:NDP:C2A	2.44	0.47
1:A:252:ARG:NH2	1:B:262:GLY:O	2.40	0.47
1:A:300:LEU:HD12	1:A:313:MET:HB3	1.96	0.47
1:C:300:LEU:HD12	1:C:313:MET:HB3	1.97	0.46
1:F:300:LEU:HD12	1:F:313:MET:HB3	1.96	0.46
2:B:500:NDP:C2A	1:C:17:ARG:HD2	2.46	0.46
1:C:80:ASP:HA	1:C:81:PRO:HD2	1.63	0.46
1:E:278:ARG:HD2	3:E:782:HOH:O	2.15	0.46
1:A:278:ARG:HD2	3:A:618:HOH:O	2.14	0.46
1:C:314:MET:HA	1:C:315:PRO:HD3	1.75	0.46
1:B:300:LEU:HD12	1:B:313:MET:HB3	1.97	0.46
1:B:317:PHE:CE1	1:C:295:GLY:HA2	2.51	0.46
1:D:300:LEU:HD12	1:D:313:MET:HB3	1.96	0.46
1:D:298:GLN:HB3	3:D:508:HOH:O	2.15	0.46
1:C:266:HIS:ND1	1:D:266:HIS:ND1	2.58	0.45
1:E:48:LEU:HD12	1:E:48:LEU:HA	1.81	0.45
1:E:233:VAL:HG22	1:E:257:MET:HG2	1.99	0.45
1:C:26:MET:HE3	1:C:26:MET:HB3	1.73	0.45
1:D:26:MET:HE3	1:D:26:MET:HB3	1.73	0.45
1:D:80:ASP:HA	1:D:81:PRO:HD2	1.63	0.45
1:C:233:VAL:HG22	1:C:257:MET:HG2	1.98	0.45
1:A:233:VAL:HG22	1:A:257:MET:HG2	1.99	0.44
1:A:32:PHE:HE1	1:A:336:VAL:HG11	1.83	0.44
1:B:240:ASP:HA	1:B:241:PRO:HD2	1.73	0.44
1:C:32:PHE:HE1	1:C:336:VAL:HG11	1.83	0.44
1:F:240:ASP:HA	1:F:241:PRO:HD2	1.73	0.44
1:B:233:VAL:HG22	1:B:257:MET:HG2	1.98	0.44
1:E:32:PHE:HE1	1:E:336:VAL:HG11	1.83	0.44
1:F:233:VAL:HG22	1:F:257:MET:HG2	1.98	0.44
1:D:32:PHE:HE1	1:D:336:VAL:HG11	1.83	0.44
1:D:233:VAL:HG22	1:D:257:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLY:HA2	1:D:317:PHE:CE1	2.53	0.44
1:E:279:PHE:HB2	1:E:290:MET:HB2	2.00	0.44
1:C:138:CYS:HB3	1:C:350:MET:HG3	2.00	0.43
1:F:290:MET:HG2	1:F:301:ILE:HG22	2.00	0.43
1:B:290:MET:HG2	1:B:301:ILE:HG22	2.00	0.43
1:F:278:ARG:HD2	3:F:642:HOH:O	2.16	0.43
1:E:252:ARG:NH2	1:F:262:GLY:O	2.44	0.43
1:A:138:CYS:HB3	1:A:350:MET:HG3	2.00	0.43
1:C:279:PHE:HB2	1:C:290:MET:HB2	2.00	0.43
1:A:279:PHE:HB2	1:A:290:MET:HB2	2.00	0.43
1:E:138:CYS:HB3	1:E:350:MET:HG3	2.00	0.43
1:C:290:MET:HG2	1:C:301:ILE:HG22	2.00	0.43
1:D:278:ARG:HD2	3:D:522:HOH:O	2.18	0.43
1:E:26:MET:HB3	1:E:26:MET:HE3	1.73	0.43
1:D:138:CYS:HB3	1:D:350:MET:HG3	2.00	0.43
1:B:32:PHE:HE1	1:B:336:VAL:HG11	1.83	0.43
1:B:138:CYS:HB3	1:B:350:MET:HG3	2.00	0.43
1:F:318:ILE:HG13	1:F:320:PRO:HG3	2.01	0.43
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.81	0.43
1:A:317:PHE:CE1	1:D:295:GLY:HA2	2.54	0.43
1:B:279:PHE:HB2	1:B:290:MET:HB2	2.00	0.43
1:B:318:ILE:HG13	1:B:320:PRO:HG3	2.01	0.43
1:C:318:ILE:HG13	1:C:320:PRO:HG3	2.01	0.43
1:D:318:ILE:HG13	1:D:320:PRO:HG3	2.01	0.43
1:A:314:MET:HA	1:A:315:PRO:HD3	1.75	0.43
1:A:318:ILE:HG13	1:A:320:PRO:HG3	2.01	0.43
1:D:279:PHE:HB2	1:D:290:MET:HB2	2.00	0.42
1:F:26:MET:HB3	1:F:26:MET:HE3	1.73	0.42
1:F:32:PHE:HE1	1:F:336:VAL:HG11	1.83	0.42
1:F:279:PHE:HB2	1:F:290:MET:HB2	2.00	0.42
1:E:318:ILE:HG13	1:E:320:PRO:HG3	2.01	0.42
1:F:138:CYS:HB3	1:F:350:MET:HG3	2.00	0.42
1:B:317:PHE:CZ	1:C:295:GLY:HA2	2.54	0.42
1:D:290:MET:HG2	1:D:301:ILE:HG22	2.00	0.42
1:E:290:MET:HG2	1:E:301:ILE:HG22	2.00	0.42
1:E:314:MET:HA	1:E:315:PRO:HD3	1.75	0.42
1:A:290:MET:HG2	1:A:301:ILE:HG22	2.00	0.42
1:B:295:GLY:HA2	1:C:317:PHE:CZ	2.55	0.42
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.81	0.41
1:F:48:LEU:HD12	1:F:48:LEU:HA	1.81	0.41
1:F:314:MET:HA	1:F:315:PRO:HD3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:HA	1:A:241:PRO:HD2	1.73	0.41
1:C:48:LEU:HD12	1:C:48:LEU:HA	1.81	0.41
1:A:298:GLN:HB3	3:A:633:HOH:O	2.19	0.41
1:F:80:ASP:HA	1:F:81:PRO:HD2	1.63	0.41
1:A:17:ARG:HD2	2:D:500:NDP:H2A	2.02	0.41
1:A:26:MET:HB3	1:A:26:MET:HE3	1.73	0.41
1:C:262:GLY:O	1:D:252:ARG:NH2	2.49	0.41
2:A:500:NDP:H2A	1:D:17:ARG:HD2	2.03	0.41
1:C:80:ASP:HB3	1:C:83:LYS:HG3	2.03	0.41
1:C:190:MET:HB3	1:C:245:ARG:HH21	1.86	0.40
1:D:190:MET:HB3	1:D:245:ARG:HH21	1.86	0.40
1:E:262:GLY:O	1:F:252:ARG:NH2	2.49	0.40
1:B:80:ASP:HB3	1:B:83:LYS:HG3	2.03	0.40
1:B:190:MET:HB3	1:B:245:ARG:HH21	1.86	0.40
1:B:254:ILE:HG12	1:B:268:ALA:HB2	2.02	0.40
1:B:278:ARG:HD2	3:B:504:HOH:O	2.19	0.40
1:B:314:MET:HA	1:B:315:PRO:HD3	1.75	0.40
1:D:80:ASP:HB3	1:D:83:LYS:HG3	2.03	0.40
1:D:254:ILE:HG12	1:D:268:ALA:HB2	2.03	0.40
1:E:254:ILE:HG12	1:E:268:ALA:HB2	2.02	0.40
1:E:266:HIS:ND1	1:F:266:HIS:ND1	2.61	0.40
1:F:190:MET:HB3	1:F:245:ARG:HH21	1.86	0.40
1:F:254:ILE:HG12	1:F:268:ALA:HB2	2.03	0.40
1:F:80:ASP:HB3	1:F:83:LYS:HG3	2.03	0.40
1:A:80:ASP:HB3	1:A:83:LYS:HG3	2.03	0.40
1:A:190:MET:HB3	1:A:245:ARG:HH21	1.86	0.40
2:B:500:NDP:N6A	1:C:13:THR:O	2.51	0.40
1:C:254:ILE:HG12	1:C:268:ALA:HB2	2.03	0.40
1:E:80:ASP:HB3	1:E:83:LYS:HG3	2.03	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	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	36	60
1	B	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	36	60
1	C	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	36	60
1	D	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	36	60
1	E	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	36	60
1	F	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	36	60
All	All	2274/2286 (100%)	2190 (96%)	78 (3%)	6 (0%)	36	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	THR
1	B	275	THR
1	C	275	THR
1	D	275	THR
1	E	275	THR
1	F	275	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/308 (94%)	259 (89%)	31 (11%)	6	16
1	B	290/308 (94%)	259 (89%)	31 (11%)	6	16
1	C	290/308 (94%)	259 (89%)	31 (11%)	6	16
1	D	290/308 (94%)	259 (89%)	31 (11%)	6	16
1	E	290/308 (94%)	259 (89%)	31 (11%)	6	16
1	F	290/308 (94%)	259 (89%)	31 (11%)	6	16
All	All	1740/1848 (94%)	1554 (89%)	186 (11%)	6	16

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	13	THR
1	A	17	ARG
1	A	26	MET
1	A	28	GLU
1	A	36	ILE
1	A	44	LEU
1	A	48	LEU
1	A	91	ASP
1	A	105	ILE
1	A	110	LEU
1	A	128	GLU
1	A	129	LYS
1	A	151	LYS
1	A	152	LEU
1	A	165	ARG
1	A	172	ARG
1	A	187	SER
1	A	188	ASP
1	A	216	ILE
1	A	233	VAL
1	A	240	ASP
1	A	256	GLN
1	A	260	ARG
1	A	271	TYR
1	A	274	THR
1	A	311	GLN
1	A	313	MET
1	A	318	ILE
1	A	342	VAL
1	A	343	ARG
1	B	2	THR
1	B	13	THR
1	B	17	ARG
1	B	26	MET
1	B	28	GLU
1	B	36	ILE
1	B	44	LEU
1	B	48	LEU
1	B	91	ASP
1	B	105	ILE
1	B	110	LEU
1	B	128	GLU

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Mol	Chain	Res	Type
1	B	129	LYS
1	B	151	LYS
1	B	152	LEU
1	B	165	ARG
1	B	172	ARG
1	B	187	SER
1	B	188	ASP
1	B	216	ILE
1	B	233	VAL
1	B	240	ASP
1	B	256	GLN
1	B	260	ARG
1	B	271	TYR
1	B	274	THR
1	B	311	GLN
1	B	313	MET
1	B	318	ILE
1	B	342	VAL
1	B	343	ARG
1	C	2	THR
1	C	13	THR
1	C	17	ARG
1	C	26	MET
1	C	28	GLU
1	C	36	ILE
1	C	44	LEU
1	C	48	LEU
1	C	91	ASP
1	C	105	ILE
1	C	110	LEU
1	C	128	GLU
1	C	129	LYS
1	C	151	LYS
1	C	152	LEU
1	C	165	ARG
1	C	172	ARG
1	C	187	SER
1	C	188	ASP
1	C	216	ILE
1	C	233	VAL
1	C	240	ASP
1	C	256	GLN

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Mol	Chain	Res	Type
1	C	260	ARG
1	C	271	TYR
1	C	274	THR
1	C	311	GLN
1	C	313	MET
1	C	318	ILE
1	C	342	VAL
1	C	343	ARG
1	D	2	THR
1	D	13	THR
1	D	17	ARG
1	D	26	MET
1	D	28	GLU
1	D	36	ILE
1	D	44	LEU
1	D	48	LEU
1	D	91	ASP
1	D	105	ILE
1	D	110	LEU
1	D	128	GLU
1	D	129	LYS
1	D	151	LYS
1	D	152	LEU
1	D	165	ARG
1	D	172	ARG
1	D	187	SER
1	D	188	ASP
1	D	216	ILE
1	D	233	VAL
1	D	240	ASP
1	D	256	GLN
1	D	260	ARG
1	D	271	TYR
1	D	274	THR
1	D	311	GLN
1	D	313	MET
1	D	318	ILE
1	D	342	VAL
1	D	343	ARG
1	E	2	THR
1	E	13	THR
1	E	17	ARG

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Mol	Chain	Res	Type
1	E	26	MET
1	E	28	GLU
1	E	36	ILE
1	E	44	LEU
1	E	48	LEU
1	E	91	ASP
1	E	105	ILE
1	E	110	LEU
1	E	128	GLU
1	E	129	LYS
1	E	151	LYS
1	E	152	LEU
1	E	165	ARG
1	E	172	ARG
1	E	187	SER
1	E	188	ASP
1	E	216	ILE
1	E	233	VAL
1	E	240	ASP
1	E	256	GLN
1	E	260	ARG
1	E	271	TYR
1	E	274	THR
1	E	311	GLN
1	E	313	MET
1	E	318	ILE
1	E	342	VAL
1	E	343	ARG
1	F	2	THR
1	F	13	THR
1	F	17	ARG
1	F	26	MET
1	F	28	GLU
1	F	36	ILE
1	F	44	LEU
1	F	48	LEU
1	F	91	ASP
1	F	105	ILE
1	F	110	LEU
1	F	128	GLU
1	F	129	LYS
1	F	151	LYS

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Mol	Chain	Res	Type
1	F	152	LEU
1	F	165	ARG
1	F	172	ARG
1	F	187	SER
1	F	188	ASP
1	F	216	ILE
1	F	233	VAL
1	F	240	ASP
1	F	256	GLN
1	F	260	ARG
1	F	271	TYR
1	F	274	THR
1	F	311	GLN
1	F	313	MET
1	F	318	ILE
1	F	342	VAL
1	F	343	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	124	HIS
1	A	149	ASN
1	A	186	ASN
1	A	256	GLN
1	A	328	GLN
1	A	338	ASN
1	B	46	GLN
1	B	124	HIS
1	B	149	ASN
1	B	186	ASN
1	B	328	GLN
1	B	338	ASN
1	C	46	GLN
1	C	124	HIS
1	C	149	ASN
1	C	186	ASN
1	C	256	GLN
1	C	328	GLN
1	C	338	ASN
1	D	46	GLN

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Mol	Chain	Res	Type
1	D	124	HIS
1	D	186	ASN
1	D	328	GLN
1	D	338	ASN
1	E	46	GLN
1	E	124	HIS
1	E	149	ASN
1	E	186	ASN
1	E	328	GLN
1	E	338	ASN
1	F	46	GLN
1	F	124	HIS
1	F	149	ASN
1	F	186	ASN
1	F	256	GLN
1	F	328	GLN
1	F	338	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](#)

6 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	NDP	E	500	-	51,52,52	1.87	8 (15%)	71,80,80	1.57	10 (14%)
2	NDP	B	500	-	51,52,52	1.87	8 (15%)	71,80,80	1.57	10 (14%)
2	NDP	A	500	-	51,52,52	1.87	8 (15%)	71,80,80	1.57	10 (14%)
2	NDP	F	500	-	51,52,52	1.87	8 (15%)	71,80,80	1.57	10 (14%)
2	NDP	D	500	-	51,52,52	1.88	8 (15%)	71,80,80	1.57	10 (14%)
2	NDP	C	500	-	51,52,52	1.88	8 (15%)	71,80,80	1.57	10 (14%)

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	NDP	E	500	-	-	2/34/77/77	0/5/5/5
2	NDP	B	500	-	-	2/34/77/77	0/5/5/5
2	NDP	A	500	-	-	2/34/77/77	0/5/5/5
2	NDP	F	500	-	-	2/34/77/77	0/5/5/5
2	NDP	D	500	-	-	2/34/77/77	0/5/5/5
2	NDP	C	500	-	-	2/34/77/77	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	NDP	PA-O3	-7.14	1.51	1.59
2	B	500	NDP	PA-O3	-7.11	1.51	1.59
2	D	500	NDP	PA-O3	-7.10	1.51	1.59
2	C	500	NDP	PA-O3	-7.08	1.51	1.59
2	E	500	NDP	PA-O3	-7.07	1.51	1.59
2	A	500	NDP	PA-O3	-7.05	1.51	1.59
2	A	500	NDP	C4N-C3N	-5.56	1.39	1.50
2	D	500	NDP	C4N-C3N	-5.51	1.39	1.50
2	E	500	NDP	C4N-C3N	-5.50	1.39	1.50
2	F	500	NDP	C4N-C3N	-5.49	1.39	1.50
2	C	500	NDP	C4N-C3N	-5.48	1.39	1.50
2	B	500	NDP	C4N-C3N	-5.47	1.39	1.50
2	D	500	NDP	PN-O3	5.30	1.65	1.59
2	E	500	NDP	PN-O3	5.30	1.65	1.59
2	C	500	NDP	PN-O3	5.29	1.65	1.59
2	B	500	NDP	PN-O3	5.23	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NDP	PN-O3	5.21	1.65	1.59
2	F	500	NDP	PN-O3	5.19	1.65	1.59
2	C	500	NDP	P2B-O2B	-4.87	1.51	1.59
2	B	500	NDP	P2B-O2B	-4.85	1.51	1.59
2	E	500	NDP	P2B-O2B	-4.85	1.51	1.59
2	D	500	NDP	P2B-O2B	-4.83	1.51	1.59
2	F	500	NDP	P2B-O2B	-4.82	1.51	1.59
2	A	500	NDP	P2B-O2B	-4.81	1.51	1.59
2	B	500	NDP	C4N-C5N	-3.04	1.41	1.49
2	F	500	NDP	C4N-C5N	-3.03	1.41	1.49
2	E	500	NDP	C4N-C5N	-3.03	1.41	1.49
2	A	500	NDP	C4N-C5N	-3.02	1.41	1.49
2	C	500	NDP	C4N-C5N	-3.02	1.41	1.49
2	D	500	NDP	C4N-C5N	-3.01	1.41	1.49
2	C	500	NDP	PN-O5D	-2.80	1.48	1.59
2	D	500	NDP	PN-O5D	-2.80	1.48	1.59
2	F	500	NDP	PN-O5D	-2.79	1.48	1.59
2	B	500	NDP	PN-O5D	-2.78	1.48	1.59
2	A	500	NDP	PN-O5D	-2.78	1.48	1.59
2	E	500	NDP	PN-O5D	-2.77	1.48	1.59
2	A	500	NDP	PA-O5B	-2.42	1.49	1.59
2	C	500	NDP	PA-O5B	-2.41	1.50	1.59
2	E	500	NDP	PA-O5B	-2.40	1.50	1.59
2	F	500	NDP	PA-O5B	-2.40	1.50	1.59
2	D	500	NDP	PA-O5B	-2.40	1.50	1.59
2	B	500	NDP	PA-O5B	-2.39	1.50	1.59
2	F	500	NDP	C6N-C5N	2.10	1.39	1.33
2	D	500	NDP	C6N-C5N	2.08	1.39	1.33
2	B	500	NDP	C6N-C5N	2.07	1.39	1.33
2	A	500	NDP	C6N-C5N	2.07	1.39	1.33
2	E	500	NDP	C6N-C5N	2.06	1.39	1.33
2	C	500	NDP	C6N-C5N	2.06	1.39	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NDP	C1D-N1N-C2N	-6.50	110.44	121.14
2	E	500	NDP	C1D-N1N-C2N	-6.49	110.44	121.14
2	C	500	NDP	C1D-N1N-C2N	-6.47	110.47	121.14
2	F	500	NDP	C1D-N1N-C2N	-6.46	110.49	121.14
2	D	500	NDP	C1D-N1N-C2N	-6.46	110.50	121.14
2	A	500	NDP	C1D-N1N-C2N	-6.45	110.51	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	NDP	C4A-N9A-C1B	4.53	137.22	126.63
2	E	500	NDP	C4A-N9A-C1B	4.52	137.21	126.63
2	A	500	NDP	C4A-N9A-C1B	4.52	137.20	126.63
2	B	500	NDP	C4A-N9A-C1B	4.51	137.18	126.63
2	F	500	NDP	C4A-N9A-C1B	4.51	137.17	126.63
2	D	500	NDP	C4A-N9A-C1B	4.50	137.15	126.63
2	E	500	NDP	O2A-PA-O3	-4.27	95.72	107.27
2	A	500	NDP	O2A-PA-O3	-4.27	95.73	107.27
2	D	500	NDP	O2A-PA-O3	-4.26	95.76	107.27
2	B	500	NDP	O2A-PA-O3	-4.26	95.76	107.27
2	C	500	NDP	O2A-PA-O3	-4.26	95.77	107.27
2	F	500	NDP	O2A-PA-O3	-4.25	95.80	107.27
2	A	500	NDP	C1B-N9A-C8A	-4.08	118.03	127.09
2	C	500	NDP	C1B-N9A-C8A	-4.07	118.05	127.09
2	E	500	NDP	C1B-N9A-C8A	-4.07	118.05	127.09
2	B	500	NDP	C1B-N9A-C8A	-4.07	118.06	127.09
2	F	500	NDP	C1B-N9A-C8A	-4.06	118.08	127.09
2	D	500	NDP	C1B-N9A-C8A	-4.05	118.10	127.09
2	B	500	NDP	C1D-N1N-C6N	4.03	129.30	120.77
2	D	500	NDP	C1D-N1N-C6N	4.01	129.25	120.77
2	F	500	NDP	C1D-N1N-C6N	4.01	129.25	120.77
2	C	500	NDP	C1D-N1N-C6N	4.01	129.25	120.77
2	E	500	NDP	C1D-N1N-C6N	4.01	129.25	120.77
2	A	500	NDP	C1D-N1N-C6N	4.00	129.23	120.77
2	D	500	NDP	O3-PA-O1A	2.99	119.71	110.70
2	F	500	NDP	O3-PA-O1A	2.99	119.70	110.70
2	A	500	NDP	O3-PA-O1A	2.99	119.70	110.70
2	B	500	NDP	O3-PA-O1A	2.99	119.70	110.70
2	E	500	NDP	O3-PA-O1A	2.99	119.69	110.70
2	C	500	NDP	O3-PA-O1A	2.98	119.68	110.70
2	D	500	NDP	O4D-C1D-N1N	-2.89	102.58	108.08
2	E	500	NDP	O4D-C1D-N1N	-2.89	102.58	108.08
2	F	500	NDP	O4D-C1D-N1N	-2.89	102.58	108.08
2	A	500	NDP	O4D-C1D-N1N	-2.87	102.61	108.08
2	B	500	NDP	O4D-C1D-N1N	-2.87	102.61	108.08
2	C	500	NDP	O4D-C1D-N1N	-2.86	102.63	108.08
2	B	500	NDP	O2N-PN-O3	2.30	113.49	107.27
2	A	500	NDP	O2N-PN-O3	2.30	113.48	107.27
2	F	500	NDP	O2N-PN-O3	2.29	113.47	107.27
2	C	500	NDP	O2N-PN-O3	2.28	113.45	107.27
2	E	500	NDP	O2N-PN-O3	2.28	113.43	107.27
2	D	500	NDP	O2N-PN-O3	2.27	113.41	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NDP	C2D-C1D-N1N	-2.08	108.19	113.31
2	C	500	NDP	C2D-C1D-N1N	-2.08	108.19	113.31
2	E	500	NDP	C2D-C1D-N1N	-2.07	108.21	113.31
2	D	500	NDP	C2D-C1D-N1N	-2.07	108.22	113.31
2	F	500	NDP	C2D-C1D-N1N	-2.07	108.22	113.31
2	C	500	NDP	O3-PN-O1N	-2.06	104.50	110.70
2	B	500	NDP	O3-PN-O1N	-2.06	104.51	110.70
2	A	500	NDP	C2D-C1D-N1N	-2.06	108.25	113.31
2	D	500	NDP	O3-PN-O1N	-2.05	104.53	110.70
2	A	500	NDP	O3-PN-O1N	-2.05	104.53	110.70
2	E	500	NDP	O3-PN-O1N	-2.05	104.55	110.70
2	F	500	NDP	O3-PN-O1N	-2.05	104.55	110.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NDP	O4D-C1D-N1N-C2N
2	B	500	NDP	O4D-C1D-N1N-C2N
2	C	500	NDP	O4D-C1D-N1N-C2N
2	D	500	NDP	O4D-C1D-N1N-C2N
2	E	500	NDP	O4D-C1D-N1N-C2N
2	F	500	NDP	O4D-C1D-N1N-C2N
2	A	500	NDP	C2D-C1D-N1N-C2N
2	B	500	NDP	C2D-C1D-N1N-C2N
2	C	500	NDP	C2D-C1D-N1N-C2N
2	D	500	NDP	C2D-C1D-N1N-C2N
2	E	500	NDP	C2D-C1D-N1N-C2N
2	F	500	NDP	C2D-C1D-N1N-C2N

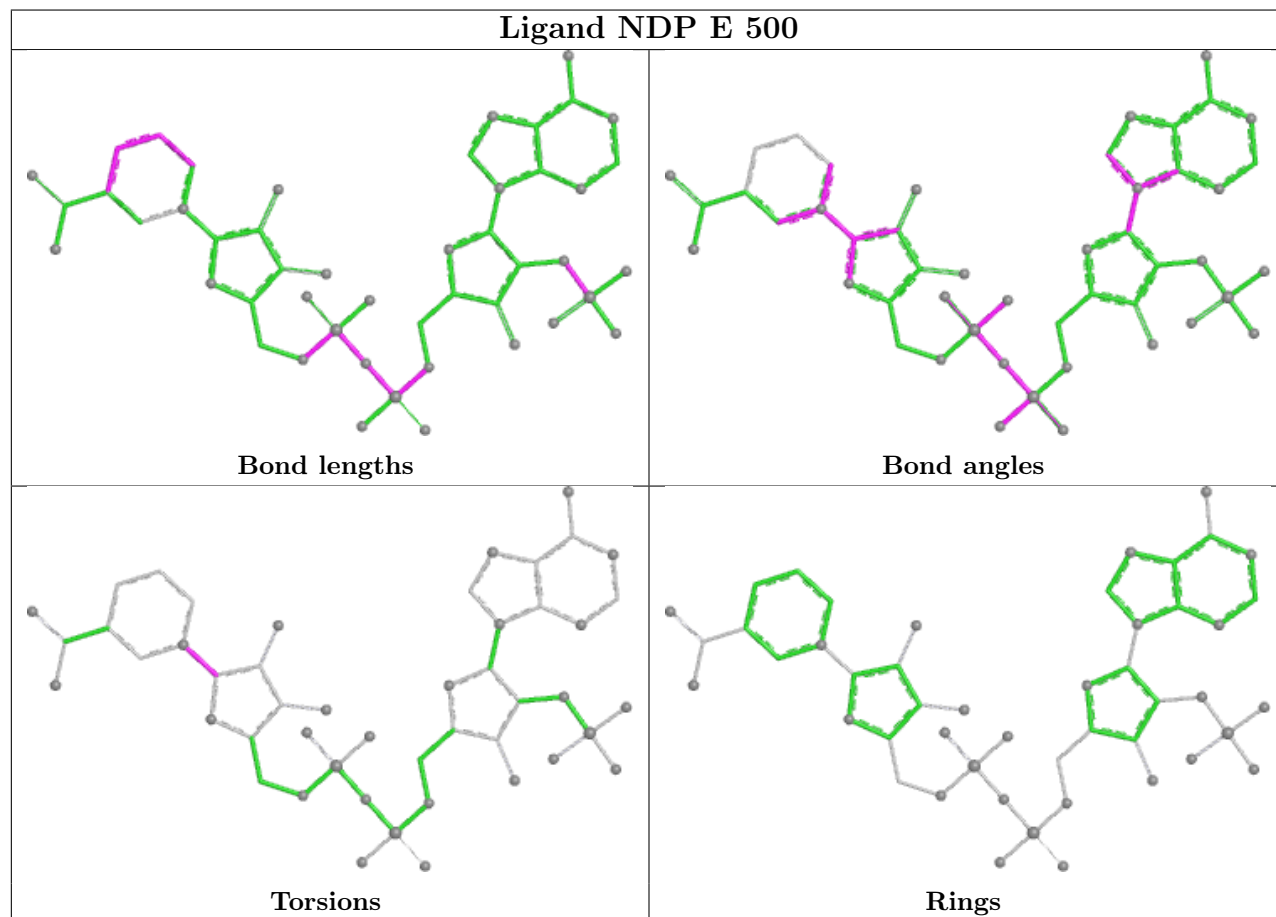
There are no ring outliers.

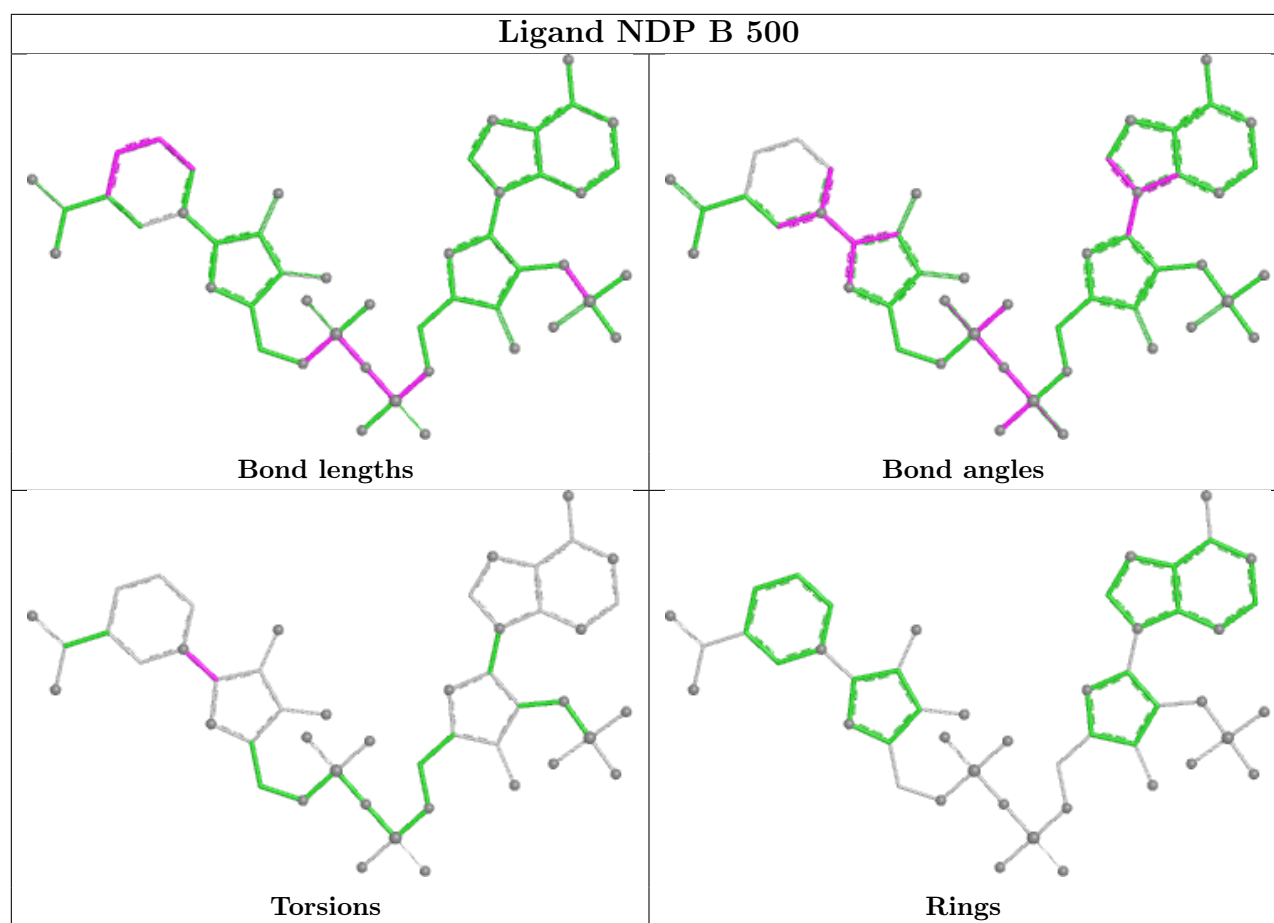
4 monomers are involved in 7 short contacts:

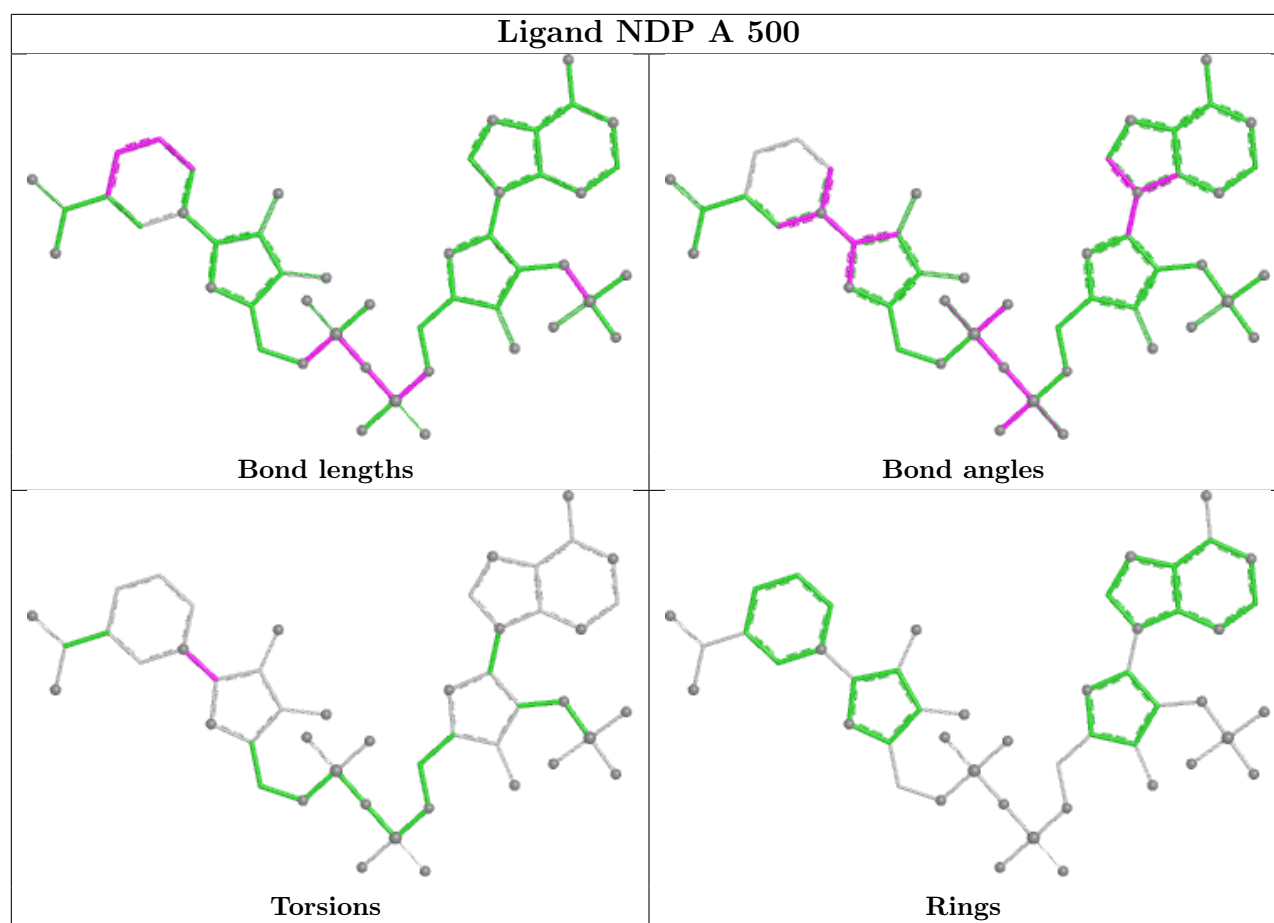
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	NDP	2	0
2	A	500	NDP	2	0
2	D	500	NDP	2	0
2	C	500	NDP	1	0

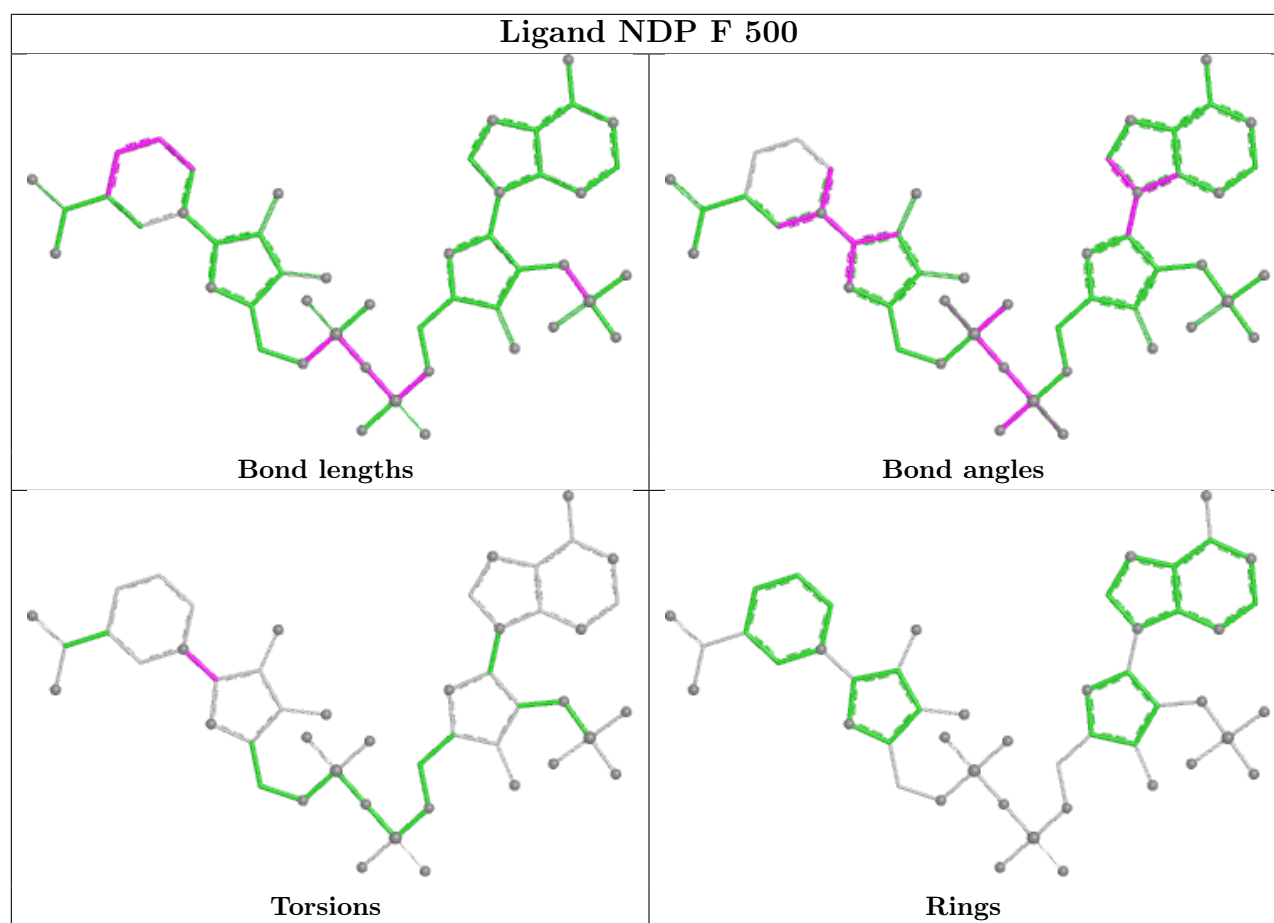
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

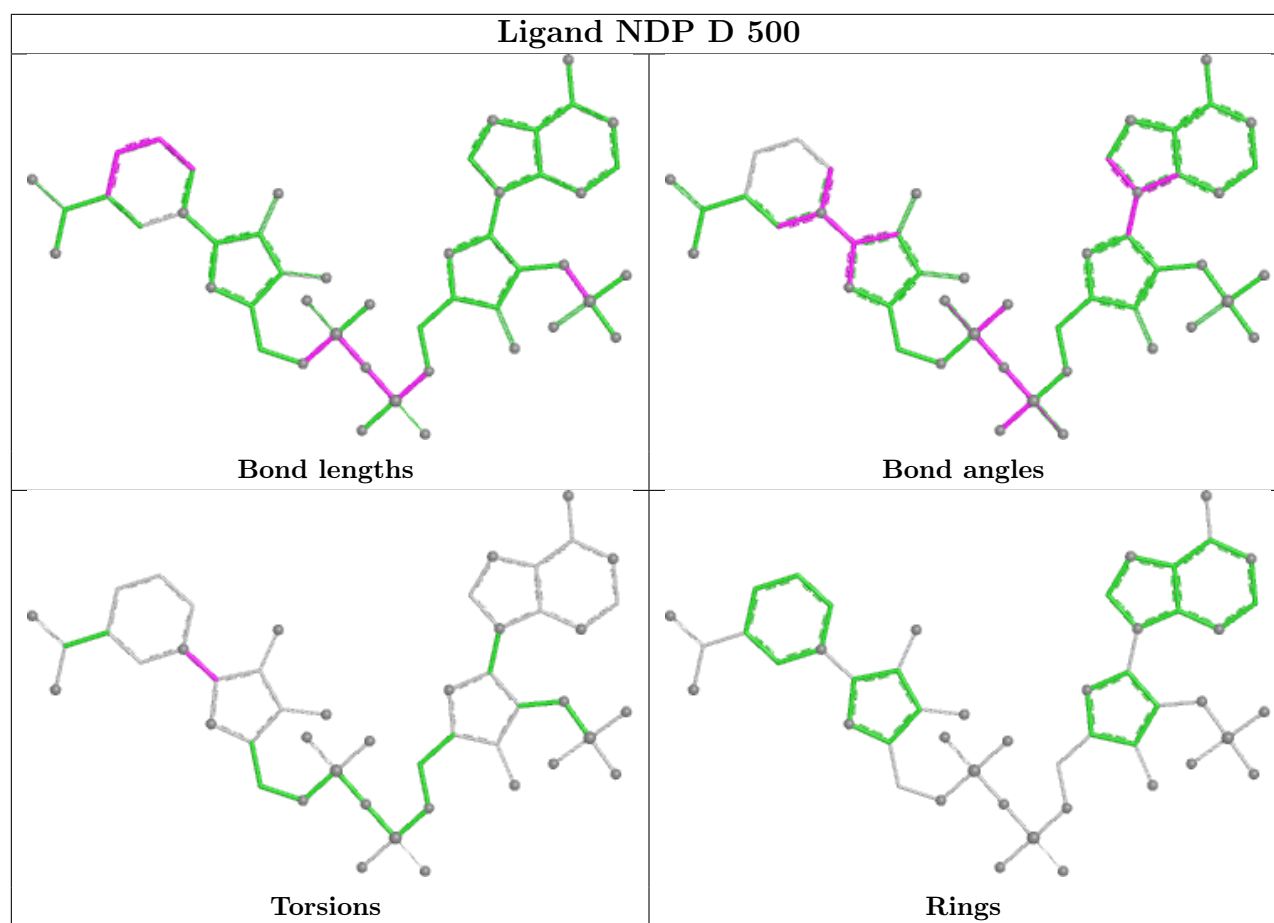
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

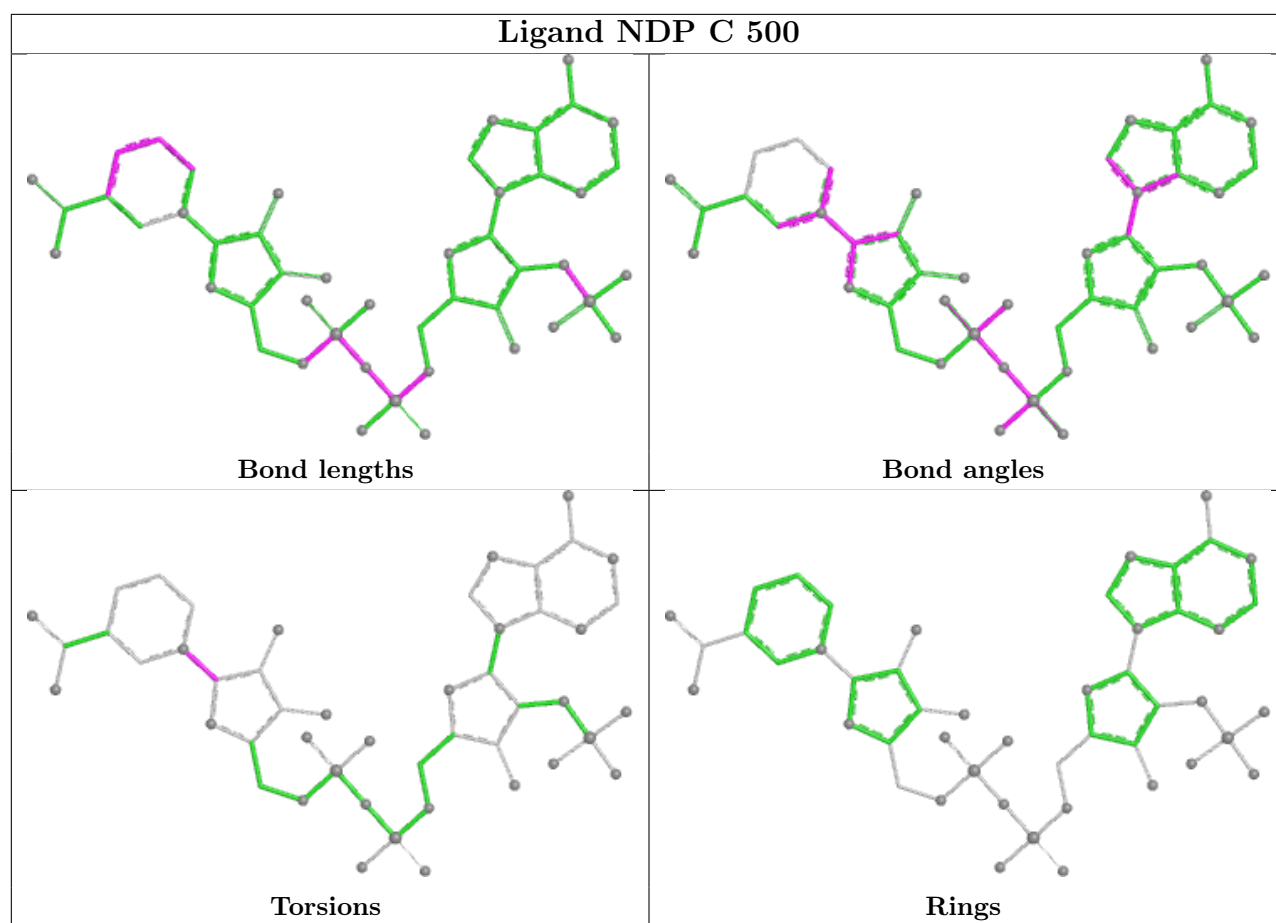












5.7 Other polymers [i](#)

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	381/381 (100%)	0.42	7 (1%) 67 65	29, 40, 62, 72	0
1	B	381/381 (100%)	0.41	7 (1%) 67 65	29, 40, 62, 72	0
1	C	381/381 (100%)	0.62	15 (3%) 43 39	29, 40, 62, 72	0
1	D	381/381 (100%)	0.39	7 (1%) 67 65	29, 40, 62, 72	0
1	E	381/381 (100%)	0.50	14 (3%) 45 41	29, 40, 62, 72	0
1	F	381/381 (100%)	0.33	3 (0%) 82 81	29, 40, 62, 72	0
All	All	2286/2286 (100%)	0.44	53 (2%) 61 58	29, 40, 62, 72	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	4.6
1	E	1	ALA	3.9
1	F	13	THR	3.3
1	C	115	ALA	3.2
1	D	1	ALA	3.2
1	E	149	ASN	3.0
1	F	1	ALA	3.0
1	A	6	GLY	2.9
1	E	340	LYS	2.9
1	A	1	ALA	2.8
1	C	13	THR	2.8
1	C	1	ALA	2.7
1	C	90	PHE	2.7
1	D	339	ASN	2.7
1	E	193	ASN	2.7
1	B	21	TYR	2.7
1	E	339	ASN	2.6
1	A	66	ASN	2.6
1	B	13	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	119	PHE	2.5
1	E	74	ALA	2.5
1	E	343	ARG	2.5
1	E	66	ASN	2.5
1	C	120	LYS	2.4
1	B	9	GLN	2.4
1	C	85	TYR	2.4
1	B	19	MET	2.4
1	E	86	ASP	2.3
1	C	35	ALA	2.3
1	D	10	VAL	2.3
1	F	21	TYR	2.3
1	A	339	ASN	2.3
1	C	197	GLN	2.3
1	E	7	ALA	2.3
1	C	88	SER	2.3
1	E	364	ARG	2.2
1	A	89	ASN	2.2
1	D	8	SER	2.2
1	D	149	ASN	2.2
1	E	13	THR	2.2
1	C	140	ARG	2.2
1	C	106	LEU	2.2
1	D	380	GLY	2.2
1	A	21	TYR	2.1
1	B	5	ALA	2.1
1	C	2	THR	2.1
1	B	339	ASN	2.1
1	D	19	MET	2.1
1	C	21	TYR	2.1
1	A	260	ARG	2.1
1	C	61	ALA	2.0
1	E	260	ARG	2.0
1	E	2	THR	2.0

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

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

6.3 Carbohydrates [i](#)

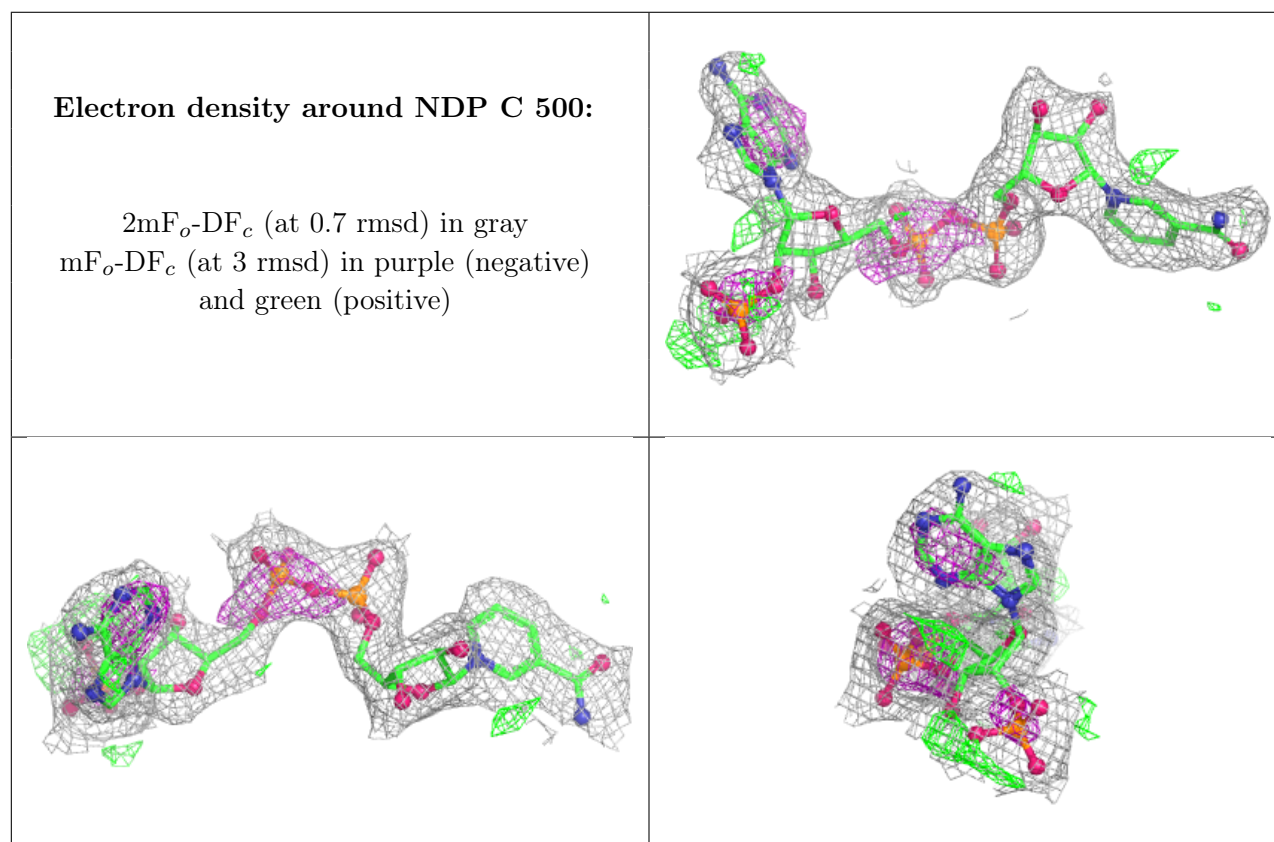
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

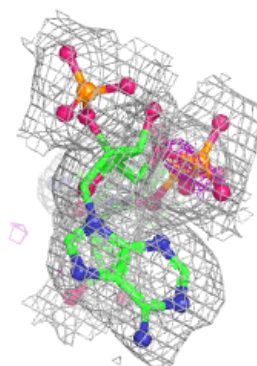
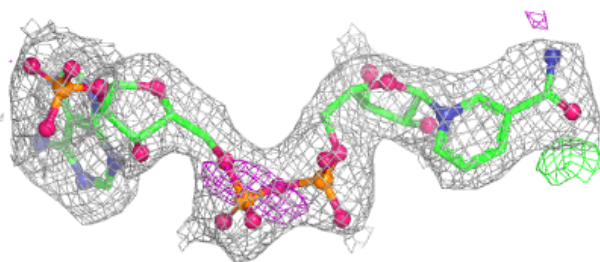
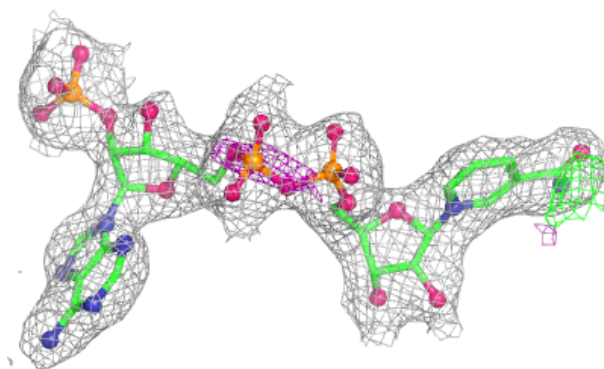
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	C	500	48/48	0.90	0.13	38,40,41,41	0
2	NDP	B	500	48/48	0.94	0.10	38,40,41,41	0
2	NDP	F	500	48/48	0.95	0.09	38,40,41,41	0
2	NDP	D	500	48/48	0.96	0.09	38,40,41,41	0
2	NDP	E	500	48/48	0.97	0.09	38,40,41,41	0
2	NDP	A	500	48/48	0.97	0.09	38,40,41,41	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.

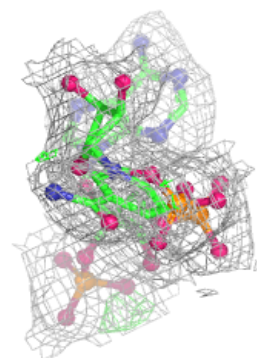
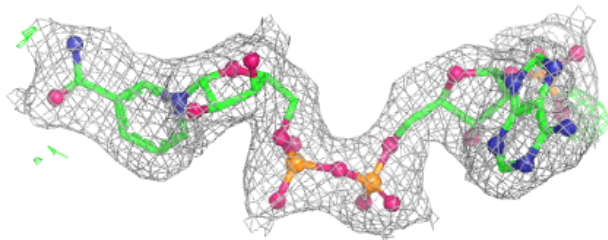
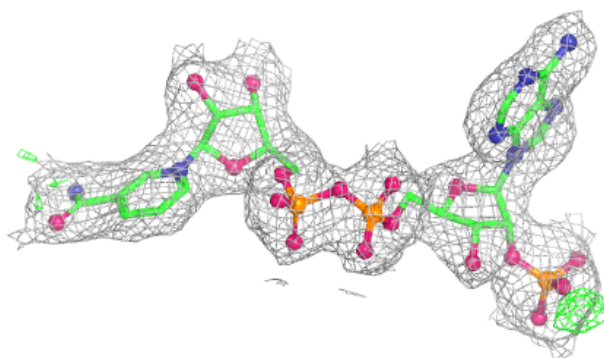


Electron density around NDP B 500:

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

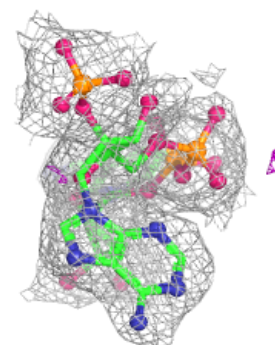
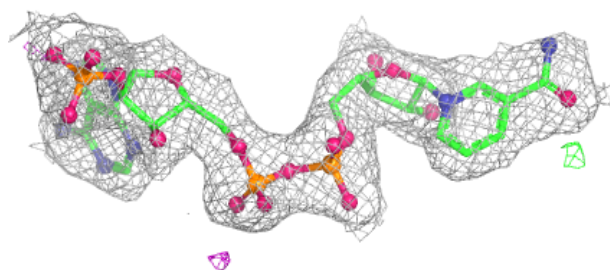
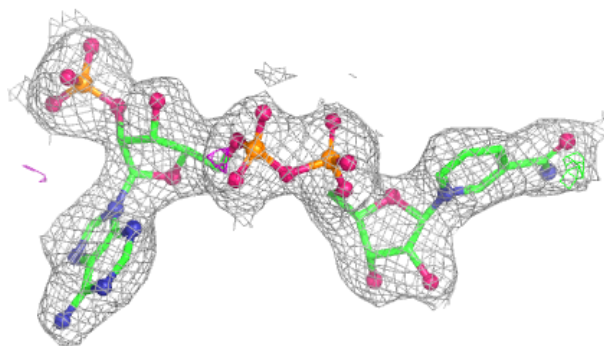
**Electron density around NDP F 500:**

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

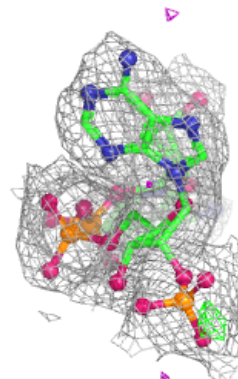
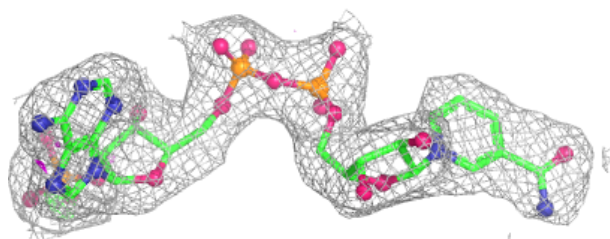
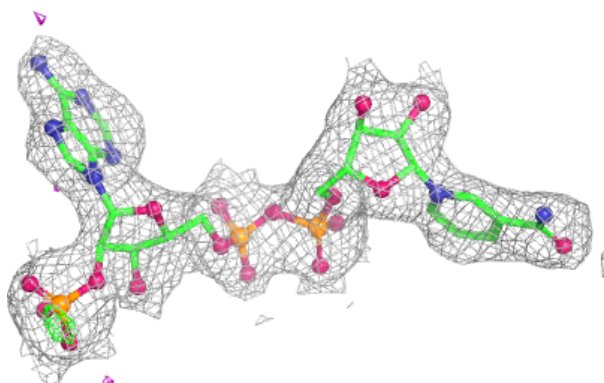


Electron density around NDP D 500:

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

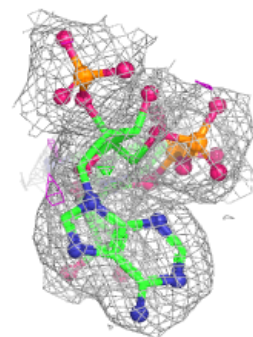
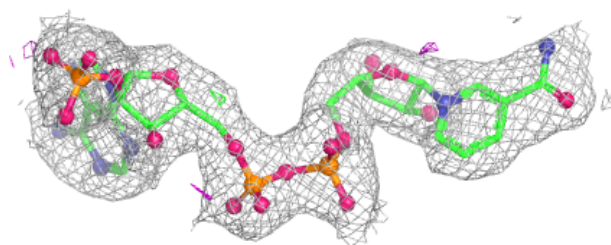
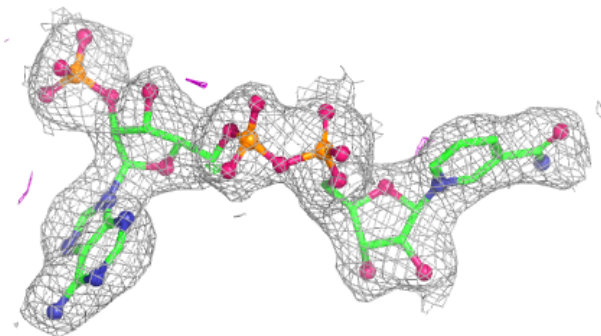
**Electron density around NDP E 500:**

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



Electron density around NDP A 500:

$2mF_o-DF_c$ (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.