



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:44 PM UTC

PDB ID : 4L04 / pdb_00004l04
Title : Crystal Structure Analysis of human IDH1 mutants in complex with NADP+ and Ca2+/alpha-Ketoglutarate
Authors : Concha, N.O.; Smallwood, A.M.
Deposited on : 2013-05-30
Resolution : 2.87 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

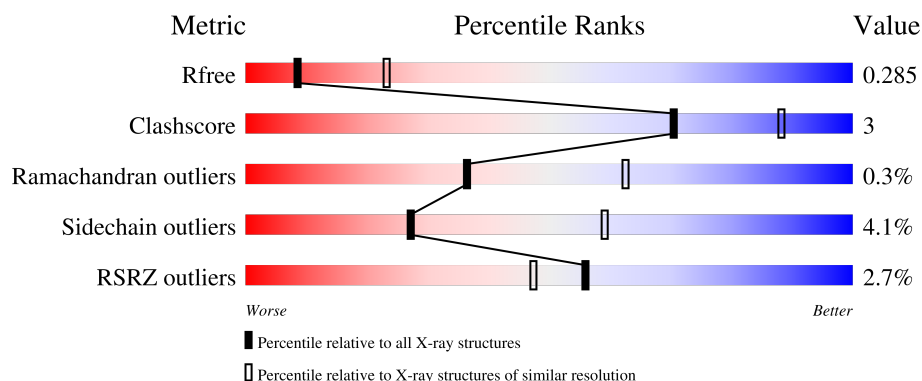
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	425	2% 83% 13% ..
1	B	425	83% 14% .
1	C	425	3% 81% 15% ..
1	D	425	4% 81% 16% .
1	E	425	3% 83% 14% .

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Mol	Chain	Length	Quality of chain
1	F	425	4% 84% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19647 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3221	2048	546	609	18			
1	B	412	Total	C	N	O	S	0	2	0
			3258	2071	553	616	18			
1	C	412	Total	C	N	O	S	0	0	0
			3206	2030	547	611	18			
1	D	412	Total	C	N	O	S	0	1	0
			3129	1982	535	596	16			
1	E	412	Total	C	N	O	S	0	1	0
			3226	2047	547	614	18			
1	F	412	Total	C	N	O	S	0	1	0
			3184	2025	543	598	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	GLY	conflict	UNP O75874
A	415	SER	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
B	97	ASN	GLY	conflict	UNP O75874
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874

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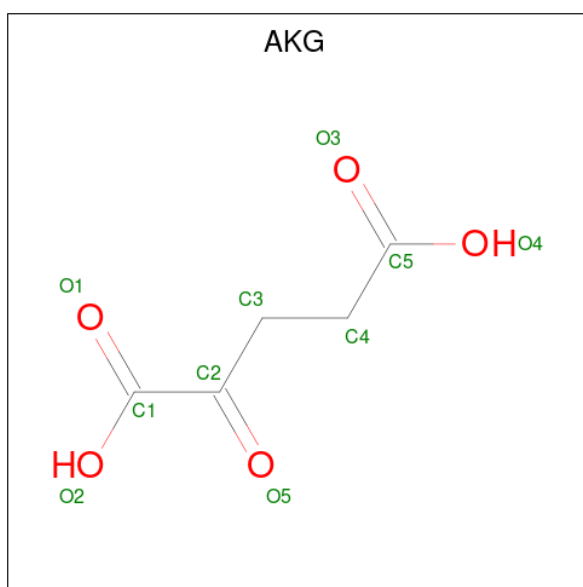
Chain	Residue	Modelled	Actual	Comment	Reference
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874
B	425	HIS	-	expression tag	UNP O75874
C	97	ASN	GLY	conflict	UNP O75874
C	415	SER	-	expression tag	UNP O75874
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874
D	97	ASN	GLY	conflict	UNP O75874
D	415	SER	-	expression tag	UNP O75874
D	416	LEU	-	expression tag	UNP O75874
D	417	GLU	-	expression tag	UNP O75874
D	418	HIS	-	expression tag	UNP O75874
D	419	HIS	-	expression tag	UNP O75874
D	420	HIS	-	expression tag	UNP O75874
D	421	HIS	-	expression tag	UNP O75874
D	422	HIS	-	expression tag	UNP O75874
D	423	HIS	-	expression tag	UNP O75874
D	424	HIS	-	expression tag	UNP O75874
D	425	HIS	-	expression tag	UNP O75874
E	97	ASN	GLY	conflict	UNP O75874
E	415	SER	-	expression tag	UNP O75874
E	416	LEU	-	expression tag	UNP O75874
E	417	GLU	-	expression tag	UNP O75874
E	418	HIS	-	expression tag	UNP O75874
E	419	HIS	-	expression tag	UNP O75874
E	420	HIS	-	expression tag	UNP O75874
E	421	HIS	-	expression tag	UNP O75874
E	422	HIS	-	expression tag	UNP O75874
E	423	HIS	-	expression tag	UNP O75874
E	424	HIS	-	expression tag	UNP O75874

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Chain	Residue	Modelled	Actual	Comment	Reference
E	425	HIS	-	expression tag	UNP O75874
F	97	ASN	GLY	conflict	UNP O75874
F	415	SER	-	expression tag	UNP O75874
F	416	LEU	-	expression tag	UNP O75874
F	417	GLU	-	expression tag	UNP O75874
F	418	HIS	-	expression tag	UNP O75874
F	419	HIS	-	expression tag	UNP O75874
F	420	HIS	-	expression tag	UNP O75874
F	421	HIS	-	expression tag	UNP O75874
F	422	HIS	-	expression tag	UNP O75874
F	423	HIS	-	expression tag	UNP O75874
F	424	HIS	-	expression tag	UNP O75874
F	425	HIS	-	expression tag	UNP O75874

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	E	1	Total	C	O	0	0
			10	5	5		

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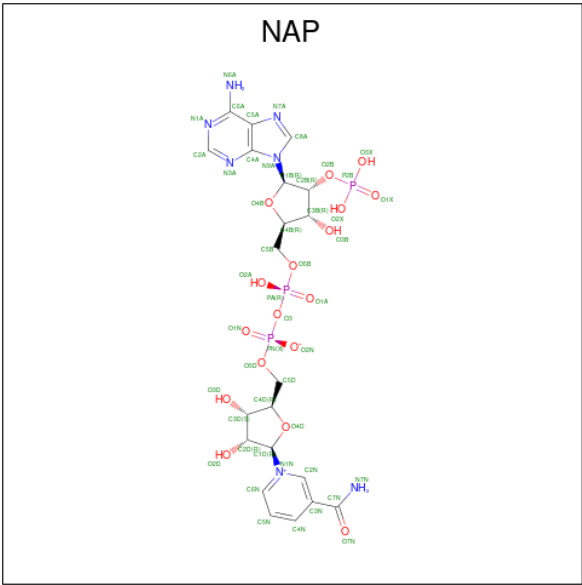
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



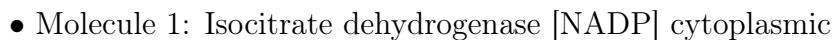
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is water.

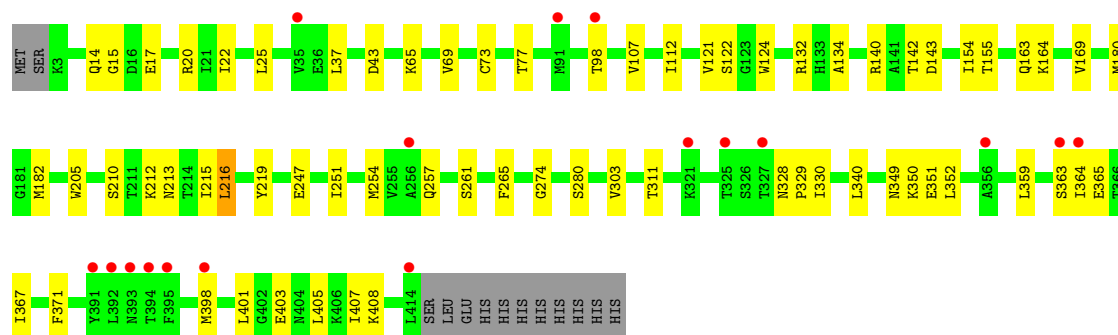
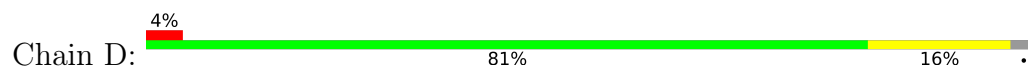
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	13	Total	O	0	0
			13	13		
5	C	16	Total	O	0	0
			16	16		
5	D	8	Total	O	0	0
			8	8		
5	E	7	Total	O	0	0
			7	7		
5	F	7	Total	O	0	0
			7	7		

- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

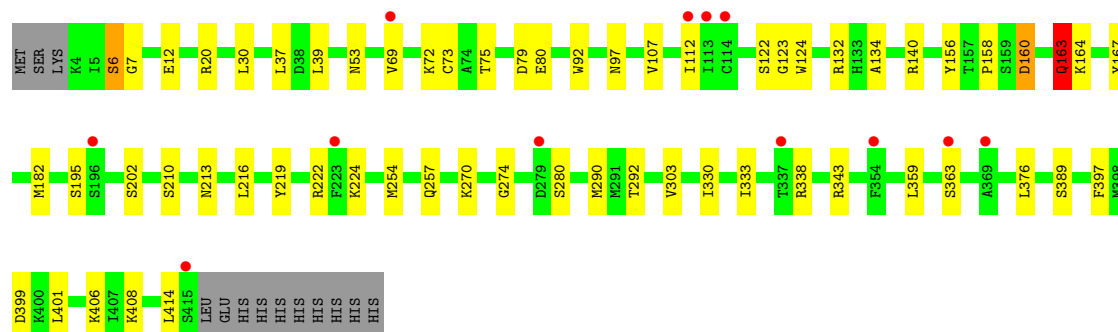
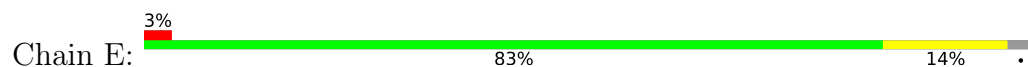




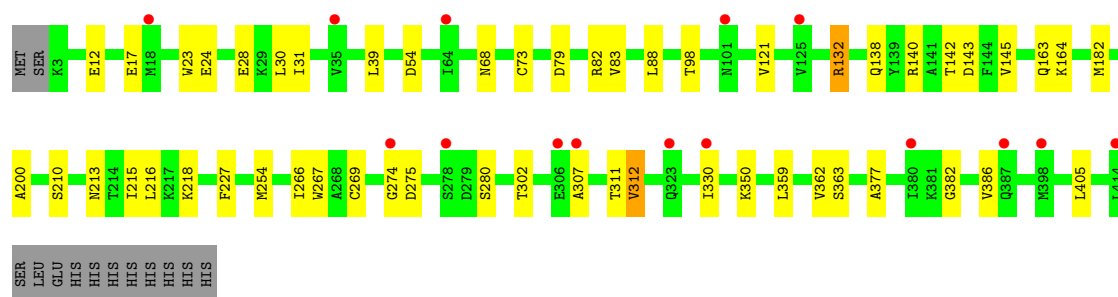
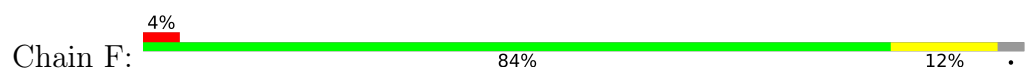
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.41Å 116.62Å 275.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 2.87 49.24 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.24-2.87) 98.2 (49.24-2.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.86Å)	Xtrriage
Refinement program	PHENIX, BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.259 (Not available) , 0.285	Depositor DCC
R_{free} test set	3578 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtrriage
Anisotropy	0.326	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19647	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.99 % 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 1.6255e-05. 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: AKG, CA, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	0/3289	1.36	11/4446 (0.2%)
1	B	0.81	0/3332	1.36	9/4499 (0.2%)
1	C	0.81	0/3272	1.37	12/4422 (0.3%)
1	D	0.81	0/3197	1.41	15/4336 (0.3%)
1	E	0.82	0/3296	1.39	11/4456 (0.2%)
1	F	0.81	0/3255	1.42	22/4406 (0.5%)
All	All	0.81	0/19641	1.39	80/26565 (0.3%)

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	163	GLN	CA-C-N	8.47	134.72	122.44
1	E	163	GLN	C-N-CA	8.47	134.72	122.44
1	E	333	ILE	N-CA-C	-7.54	103.11	110.72
1	C	77	THR	CB-CA-C	7.26	117.36	110.17
1	A	169	VAL	N-CA-C	-7.06	104.89	111.45
1	C	252	ASP	CA-CB-CG	6.87	119.47	112.60
1	B	123	GLY	N-CA-C	6.60	121.22	112.77
1	C	253	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	77	THR	CB-CA-C	6.46	117.21	109.85
1	F	163	GLN	CA-C-N	6.10	133.19	121.54
1	F	163	GLN	C-N-CA	6.10	133.19	121.54
1	C	299	ASP	CA-CB-CG	6.08	118.68	112.60
1	D	350	LYS	CA-C-N	5.93	128.14	120.44
1	D	350	LYS	C-N-CA	5.93	128.14	120.44
1	F	145	VAL	CA-C-N	5.91	126.62	122.60
1	F	145	VAL	C-N-CA	5.91	126.62	122.60
1	D	122	SER	N-CA-C	5.86	117.34	111.07
1	D	65	LYS	CA-C-N	5.82	128.00	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	LYS	C-N-CA	5.82	128.00	120.44
1	F	312	VAL	CA-C-N	5.79	128.35	120.54
1	F	312	VAL	C-N-CA	5.79	128.35	120.54
1	A	122	SER	N-CA-C	5.77	118.31	111.33
1	B	251	ILE	CA-C-N	5.76	128.79	120.79
1	B	251	ILE	C-N-CA	5.76	128.79	120.79
1	B	43	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	393	ASN	CA-CB-CG	5.69	118.29	112.60
1	F	227	PHE	CA-C-N	5.66	128.18	120.54
1	F	227	PHE	C-N-CA	5.66	128.18	120.54
1	D	121	VAL	CA-C-N	5.58	127.69	120.44
1	D	121	VAL	C-N-CA	5.58	127.69	120.44
1	F	307	ALA	CA-C-N	5.56	128.00	120.38
1	F	307	ALA	C-N-CA	5.56	128.00	120.38
1	A	146	VAL	N-CA-C	-5.55	102.06	107.55
1	F	98	THR	CA-C-N	5.53	127.73	120.60
1	F	98	THR	C-N-CA	5.53	127.73	120.60
1	A	117	ILE	N-CA-C	5.50	112.56	107.56
1	A	323	GLN	CA-C-N	5.45	128.36	120.79
1	A	323	GLN	C-N-CA	5.45	128.36	120.79
1	C	78	PRO	N-CA-C	5.42	118.98	110.80
1	E	163	GLN	N-CA-C	5.37	117.25	108.76
1	E	122	SER	N-CA-C	5.34	117.10	111.28
1	F	350	LYS	CA-C-N	5.33	127.42	120.28
1	F	350	LYS	C-N-CA	5.33	127.42	120.28
1	F	275	ASP	CA-C-N	5.31	127.36	120.56
1	F	275	ASP	C-N-CA	5.31	127.36	120.56
1	E	6	SER	CA-C-N	5.28	125.69	119.94
1	E	6	SER	C-N-CA	5.28	125.69	119.94
1	B	224	LYS	CA-C-N	5.27	127.61	120.44
1	B	224	LYS	C-N-CA	5.27	127.61	120.44
1	D	77	THR	CB-CA-C	5.26	116.00	110.17
1	C	258	ALA	CA-C-N	5.25	127.32	120.28
1	C	258	ALA	C-N-CA	5.25	127.32	120.28
1	E	123	GLY	N-CA-C	5.25	118.84	112.49
1	F	121	VAL	CA-C-N	5.24	129.06	120.63
1	F	121	VAL	C-N-CA	5.24	129.06	120.63
1	A	335	ALA	N-CA-C	-5.22	105.67	111.36
1	D	37	LEU	N-CA-C	5.22	117.74	109.50
1	D	365	GLU	CA-C-N	5.21	127.58	120.54
1	D	365	GLU	C-N-CA	5.21	127.58	120.54
1	E	79	ASP	CA-CB-CG	5.20	117.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	349	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	372	MET	N-CA-C	5.17	116.15	108.86
1	B	79	ASP	CA-CB-CG	5.16	117.75	112.60
1	A	270	LYS	N-CA-C	-5.12	103.28	110.50
1	D	169	VAL	N-CA-C	-5.11	105.44	111.00
1	E	160	ASP	CA-CB-CG	5.11	117.70	112.60
1	E	270	LYS	N-CA-C	-5.10	103.31	110.50
1	B	16	ASP	N-CA-C	5.08	117.01	109.69
1	A	393	ASN	CA-CB-CG	5.04	117.64	112.60
1	F	216	LEU	CA-C-N	5.04	127.34	120.54
1	F	216	LEU	C-N-CA	5.04	127.34	120.54
1	C	413	LYS	CA-C-N	5.03	129.51	122.36
1	C	413	LYS	C-N-CA	5.03	129.51	122.36
1	B	38	ASP	N-CA-C	-5.02	102.09	109.62
1	C	349	ASN	CA-CB-CG	5.02	117.62	112.60
1	F	377	ALA	CA-C-N	5.01	127.00	120.28
1	F	377	ALA	C-N-CA	5.01	127.00	120.28
1	C	38	ASP	N-CA-C	-5.00	99.86	108.56
1	D	216	LEU	CA-C-N	5.00	128.32	120.82
1	D	216	LEU	C-N-CA	5.00	128.32	120.82

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	3221	0	3144	24	0
1	B	3258	0	3208	24	0
1	C	3206	0	3111	27	0
1	D	3129	0	2959	25	0
1	E	3226	0	3147	27	0
1	F	3184	0	3075	21	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	48	0	25	1	0
4	B	48	0	25	0	0
4	C	48	0	25	1	0
4	D	48	0	25	0	0
4	E	48	0	25	1	0
4	F	48	0	25	0	0
5	A	18	0	0	0	0
5	B	13	0	0	0	0
5	C	16	0	0	0	0
5	D	8	0	0	0	0
5	E	7	0	0	0	0
5	F	7	0	0	0	0
All	All	19647	0	18818	132	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 3.

All (132) 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:E:163:GLN:NE2	1:E:164:LYS:H	1.59	0.99
1:C:19:THR:HG21	1:C:74:ALA:HB3	1.64	0.79
1:D:205:TRP:HB3	1:D:265:PHE:HA	1.75	0.68
1:E:163:GLN:HA	1:E:163:GLN:OE1	1.90	0.64
1:A:142:THR:HG21	1:B:167:TYR:HB3	1.80	0.64
1:F:132:ARG:HB2	1:F:274:GLY:HA3	1.80	0.62
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.82	0.62
1:E:69:VAL:HG11	1:E:343:ARG:HD2	1.82	0.62
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.82	0.61
1:E:112:ILE:HD13	1:E:330:ILE:HG22	1.83	0.61
1:D:17:GLU:HB2	1:D:311:THR:HB	1.82	0.61
1:E:158:PRO:HD2	1:E:163:GLN:O	2.00	0.61
1:A:155:THR:HB	1:A:166:THR:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASN:HA	1:B:302:THR:HG23	1.83	0.60
1:B:180:MET:HE2	1:B:182:MET:HE2	1.84	0.60
1:E:163:GLN:CD	1:E:164:LYS:H	2.09	0.58
1:E:182:MET:HE3	1:F:182:MET:HE3	1.85	0.58
1:E:107:VAL:HG23	1:E:134:ALA:HB2	1.85	0.58
1:A:219:TYR:HB2	1:B:143:ASP:HB2	1.85	0.57
1:D:155[A]:THR:HG21	1:D:164:LYS:HE3	1.86	0.56
1:D:107:VAL:HG23	1:D:134:ALA:HB2	1.87	0.56
1:D:398:MET:HA	1:D:401:LEU:HD12	1.87	0.56
1:C:16:ASP:O	1:C:19:THR:HG22	2.06	0.56
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.87	0.56
1:A:340:LEU:HD22	1:A:352:LEU:HD11	1.88	0.55
1:C:22:ILE:HD11	1:C:327:THR:HB	1.88	0.55
1:C:158:PRO:HG2	1:C:163:GLN:HB2	1.88	0.54
1:D:14:GLN:HB2	1:D:43:ASP:HA	1.89	0.54
1:D:340:LEU:HD22	1:D:352:LEU:HD11	1.90	0.53
1:E:216:LEU:HD21	1:F:138:GLN:HB3	1.90	0.53
1:C:19:THR:HG23	1:C:73:CYS:SG	2.48	0.53
1:E:132:ARG:HG3	1:E:274:GLY:HA3	1.91	0.53
1:C:333:ILE:O	1:C:337:THR:HG23	2.08	0.53
1:A:215:ILE:HG23	1:B:97:ASN:HD21	1.75	0.52
1:B:158:PRO:HD2	1:B:163:GLN:O	2.11	0.51
1:E:97:ASN:HD21	1:F:215:ILE:HD12	1.75	0.51
1:A:256:ALA:O	1:B:283:GLN:HG2	2.11	0.51
1:D:257:GLN:O	1:D:261:SER:HB3	2.11	0.51
1:E:290:MET:HG3	1:E:376:LEU:HD21	1.93	0.51
1:F:17:GLU:HB2	1:F:311:THR:HB	1.93	0.51
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.93	0.50
1:C:412:ALA:C	1:C:414:LEU:H	2.18	0.50
1:F:24:GLU:O	1:F:28:GLU:HG2	2.12	0.50
1:A:14:GLN:HB2	1:A:43:ASP:HA	1.93	0.50
2:A:501:AKG:H42	4:A:504:NAP:C4N	2.41	0.50
1:D:112:ILE:HD13	1:D:330:ILE:HG22	1.93	0.50
1:D:22:ILE:HG21	1:D:329:PRO:HB3	1.93	0.49
1:B:209:LEU:HD23	1:B:248:HIS:HD2	1.77	0.49
1:D:403:GLU:O	1:D:407:ILE:HG12	2.12	0.49
1:C:112:ILE:HD13	1:C:330:ILE:HG22	1.94	0.49
1:E:7:GLY:HA3	1:E:37:LEU:HD23	1.94	0.49
1:B:141:ALA:HB1	1:B:180:MET:CE	2.43	0.48
1:A:7:GLY:HA3	1:A:37:LEU:HD23	1.95	0.48
1:E:210:SER:HB3	1:E:254:MET:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:MET:HE1	1:D:216:LEU:HD22	1.96	0.48
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.94	0.47
1:C:138:GLN:HG3	1:C:182:MET:HE1	1.96	0.47
1:E:53:ASN:HA	1:E:92:TRP:CH2	2.50	0.47
1:A:68:ASN:HA	1:A:302:THR:HG23	1.97	0.47
1:B:24:GLU:O	1:B:28:GLU:HG2	2.15	0.47
1:F:132:ARG:CB	1:F:274:GLY:HA3	2.45	0.47
1:C:219:TYR:HB2	1:D:143:ASP:HB2	1.97	0.47
1:A:403:GLU:O	1:A:407:ILE:HG12	2.15	0.47
1:F:68:ASN:O	1:F:302:THR:HA	2.15	0.47
1:A:359:LEU:HD13	1:A:405:LEU:HD22	1.97	0.46
1:B:47:GLU:H	1:B:47:GLU:CD	2.22	0.46
1:F:210:SER:HB3	1:F:254:MET:HG2	1.96	0.46
1:D:210:SER:HB3	1:D:254:MET:HG2	1.97	0.46
1:F:83:VAL:HA	1:F:88:LEU:HD12	1.98	0.46
1:C:317:ARG:HH11	1:C:320:GLN:HE22	1.63	0.46
1:A:25:LEU:HB3	1:A:398:MET:HE2	1.96	0.46
1:A:154:ILE:HG23	1:A:167:TYR:HB2	1.98	0.46
1:A:24:GLU:O	1:A:28:GLU:HB2	2.16	0.45
1:B:210:SER:HA	1:B:249:ARG:O	2.17	0.45
1:F:330:ILE:HD12	1:F:363:SER:HB3	1.97	0.45
1:A:315:HIS:HA	1:A:318:MET:HE3	1.98	0.45
1:E:330:ILE:HD12	1:E:363:SER:HB3	1.99	0.45
1:A:143:ASP:HB2	1:B:219:TYR:HB2	1.98	0.45
1:D:132:ARG:HG3	1:D:274:GLY:HA3	2.00	0.44
1:E:80:GLU:H	1:E:80:GLU:CD	2.26	0.44
1:F:267:TRP:CD1	1:F:269:CYS:HG	2.35	0.44
1:F:200:ALA:HA	1:F:266:ILE:HG13	1.99	0.44
1:C:11:VAL:HG12	1:C:13:MET:HE2	1.98	0.44
1:E:338:ARG:HA	1:E:338:ARG:HD3	1.80	0.44
1:F:23:TRP:CE3	1:F:73:CYS:HB2	2.53	0.44
1:A:412:ALA:C	1:A:414:LEU:H	2.26	0.43
1:C:7:GLY:HA3	1:C:37:LEU:HD23	2.00	0.43
1:D:180:MET:HE2	1:D:182:MET:HE2	2.00	0.43
1:F:30:LEU:HD13	1:F:359:LEU:HD11	2.01	0.43
1:E:12:GLU:HB2	1:E:39:LEU:HD11	2.00	0.43
1:A:124:TRP:HB3	1:A:285:TYR:CE1	2.54	0.43
1:A:182:MET:HE3	1:B:182:MET:HE3	2.01	0.43
1:A:210:SER:HA	1:A:249:ARG:O	2.19	0.43
1:C:312:VAL:HG13	4:C:503:NAP:H3B	2.01	0.43
1:B:213:ASN:O	1:B:217:LYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LYS:HG2	1:D:251:ILE:HG22	2.01	0.43
1:D:22:ILE:HA	1:D:25:LEU:HD12	2.00	0.42
1:B:201:LEU:HD23	1:B:244:ILE:HD11	2.00	0.42
1:C:143:ASP:HB2	1:D:219:TYR:HB2	2.01	0.42
1:E:156:TYR:CE2	1:E:158:PRO:HD3	2.53	0.42
1:E:397:PHE:CE2	1:E:401:LEU:HD11	2.54	0.42
1:D:367:ILE:HA	1:D:371:PHE:O	2.20	0.42
1:F:362:VAL:HG21	1:F:405:LEU:HA	2.01	0.42
1:F:359:LEU:HD13	1:F:405:LEU:HD13	2.00	0.42
1:A:283:GLN:HG2	1:B:256:ALA:O	2.19	0.42
1:E:167:TYR:HB3	1:F:142:THR:HG21	2.02	0.42
1:C:123:GLY:O	1:C:262:GLU:HA	2.20	0.41
1:B:57:THR:HG21	1:B:95:PRO:HA	2.02	0.41
1:C:97:ASN:HD21	1:D:215:ILE:HD12	1.85	0.41
1:C:120:LEU:HD12	1:C:283:GLN:O	2.20	0.41
1:D:330:ILE:HD12	1:D:363:SER:HB3	2.01	0.41
1:C:71:VAL:HG11	1:C:336:TRP:HA	2.03	0.41
1:E:72:LYS:HG2	1:E:73:CYS:O	2.20	0.41
1:C:121:VAL:HG11	1:C:124:TRP:CE2	2.56	0.41
1:B:23:TRP:CD1	1:B:27:LYS:HE2	2.55	0.41
1:C:200:ALA:HA	1:C:266:ILE:HG13	2.03	0.41
1:C:30:LEU:O	1:C:355:PHE:HZ	2.03	0.41
1:E:75:THR:O	4:E:503:NAP:H2N	2.21	0.41
1:E:30:LEU:HD22	1:E:359:LEU:HD11	2.03	0.41
1:F:382:GLY:O	1:F:386:VAL:HG23	2.21	0.41
1:C:201:LEU:HD23	1:C:244:ILE:HD11	2.02	0.41
1:C:210:SER:HB3	1:C:254:MET:HG2	2.01	0.41
1:B:126:LYS:O	1:B:263:GLY:HA3	2.21	0.40
1:D:328:ASN:OD1	1:D:330:ILE:HG12	2.21	0.40
1:E:219:TYR:HB2	1:F:143:ASP:HB2	2.02	0.40
1:A:156:TYR:CE1	1:B:146:VAL:HG13	2.56	0.40
1:B:125:VAL:HG22	1:B:262:GLU:HB2	2.03	0.40
1:D:15:GLY:HA3	1:D:73:CYS:SG	2.60	0.40
1:F:79:ASP:H	1:F:82:ARG:HB2	1.87	0.40
1:C:282:ALA:HB2	1:C:291:MET:SD	2.61	0.40
1:D:359:LEU:HD13	1:D:405:LEU:HD22	2.02	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	409/425 (96%)	389 (95%)	19 (5%)	1 (0%)	43	70
1	B	412/425 (97%)	391 (95%)	19 (5%)	2 (0%)	24	51
1	C	410/425 (96%)	384 (94%)	26 (6%)	0	100	100
1	D	411/425 (97%)	386 (94%)	23 (6%)	2 (0%)	24	51
1	E	411/425 (97%)	389 (95%)	21 (5%)	1 (0%)	43	70
1	F	411/425 (97%)	387 (94%)	22 (5%)	2 (0%)	24	51
All	All	2464/2550 (97%)	2326 (94%)	130 (5%)	8 (0%)	36	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	TRP
1	D	163	GLN
1	E	124	TRP
1	F	164	LYS
1	A	124	TRP
1	B	271	ASN
1	D	124	TRP
1	F	31	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/362 (93%)	326 (97%)	11 (3%)	33	65
1	B	345/362 (95%)	328 (95%)	17 (5%)	22	51
1	C	333/362 (92%)	319 (96%)	14 (4%)	26	58
1	D	312/362 (86%)	299 (96%)	13 (4%)	26	58
1	E	339/362 (94%)	321 (95%)	18 (5%)	20	49
1	F	326/362 (90%)	317 (97%)	9 (3%)	38	70
All	All	1992/2172 (92%)	1910 (96%)	82 (4%)	27	59

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	69	VAL
1	A	90	GLN
1	A	94	SER
1	A	140	ARG
1	A	155	THR
1	A	173	GLU
1	A	303	VAL
1	A	312	VAL
1	A	332	SER
1	A	394	THR
1	B	47	GLU
1	B	107	VAL
1	B	151	LYS
1	B	164	LYS
1	B	165	VAL
1	B	212	LYS
1	B	252	ASP
1	B	303	VAL
1	B	304	GLU
1	B	312	VAL
1	B	314[A]	ARG
1	B	314[B]	ARG
1	B	325	THR
1	B	333	ILE
1	B	348	ASN
1	B	388	ARG

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Mol	Chain	Res	Type
1	B	414	LEU
1	C	19	THR
1	C	20	ARG
1	C	30	LEU
1	C	47	GLU
1	C	140	ARG
1	C	155	THR
1	C	157	THR
1	C	252	ASP
1	C	280	SER
1	C	303	VAL
1	C	312	VAL
1	C	326	SER
1	C	332	SER
1	C	399	ASP
1	D	20	ARG
1	D	69	VAL
1	D	98	THR
1	D	140	ARG
1	D	142	THR
1	D	154	ILE
1	D	213	ASN
1	D	247	GLU
1	D	280	SER
1	D	303	VAL
1	D	351	GLU
1	D	364	ILE
1	D	408	LYS
1	E	6	SER
1	E	20	ARG
1	E	140	ARG
1	E	160	ASP
1	E	163	GLN
1	E	195	SER
1	E	202	SER
1	E	213	ASN
1	E	222	ARG
1	E	224	LYS
1	E	280	SER
1	E	292	THR
1	E	303	VAL
1	E	389	SER

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Mol	Chain	Res	Type
1	E	399	ASP
1	E	406	LYS
1	E	408	LYS
1	E	414	LEU
1	F	12	GLU
1	F	39	LEU
1	F	54	ASP
1	F	132	ARG
1	F	140	ARG
1	F	213	ASN
1	F	218	LYS
1	F	280	SER
1	F	312	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	101	ASN
1	A	315	HIS
1	B	53	ASN
1	B	67	HIS
1	B	68	ASN
1	B	97	ASN
1	B	101	ASN
1	B	213	ASN
1	B	228	GLN
1	B	357	ASN
1	C	101	ASN
1	C	198	GLN
1	C	234	GLN
1	C	242	GLN
1	C	320	GLN
1	C	357	ASN
1	C	404	ASN
1	D	101	ASN
1	D	242	GLN
1	D	283	GLN
1	D	357	ASN
1	D	404	ASN
1	E	68	ASN
1	E	96	ASN

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Mol	Chain	Res	Type
1	E	97	ASN
1	E	163	GLN
1	E	194	HIS
1	E	198	GLN
1	E	234	GLN
1	E	257	GLN
1	E	309	HIS
1	E	323	GLN
1	E	348	ASN
1	E	404	ASN
1	F	53	ASN
1	F	55	GLN
1	F	90	GLN
1	F	96	ASN
1	F	242	GLN
1	F	404	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](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
2	AKG	D	501	3	9,9,9	1.90	1 (11%)	11,11,11	1.25	1 (9%)
4	NAP	E	503	-	50,52,52	1.70	4 (8%)	71,80,80	1.52	10 (14%)
2	AKG	B	501	3	9,9,9	1.87	1 (11%)	11,11,11	1.62	2 (18%)
4	NAP	D	503	-	50,52,52	1.79	7 (14%)	71,80,80	1.49	8 (11%)
4	NAP	F	503	-	50,52,52	1.74	4 (8%)	71,80,80	1.53	10 (14%)
4	NAP	A	504	-	50,52,52	1.78	6 (12%)	71,80,80	1.35	8 (11%)
2	AKG	E	501	3	9,9,9	2.05	1 (11%)	11,11,11	1.49	1 (9%)
4	NAP	B	502	-	50,52,52	1.67	5 (10%)	71,80,80	1.52	9 (12%)
4	NAP	C	503	-	50,52,52	1.77	3 (6%)	71,80,80	1.51	7 (9%)
2	AKG	A	501	3	9,9,9	1.98	1 (11%)	11,11,11	1.63	2 (18%)
2	AKG	F	501	3	9,9,9	1.79	1 (11%)	11,11,11	1.68	2 (18%)
2	AKG	C	501	3	9,9,9	1.82	1 (11%)	11,11,11	1.39	1 (9%)

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	AKG	D	501	3	-	5/9/9/9	-
4	NAP	E	503	-	-	11/35/67/67	0/5/5/5
2	AKG	B	501	3	-	1/9/9/9	-
4	NAP	D	503	-	-	5/35/67/67	0/5/5/5
4	NAP	F	503	-	-	11/35/67/67	0/5/5/5
4	NAP	A	504	-	-	11/35/67/67	0/5/5/5
2	AKG	E	501	3	-	6/9/9/9	-
4	NAP	B	502	-	-	9/35/67/67	0/5/5/5
4	NAP	C	503	-	-	10/35/67/67	0/5/5/5
2	AKG	A	501	3	-	6/9/9/9	-
2	AKG	F	501	3	-	6/9/9/9	-
2	AKG	C	501	3	-	5/9/9/9	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NAP	O7N-C7N	9.69	1.42	1.24
4	D	503	NAP	O7N-C7N	9.42	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	503	NAP	O7N-C7N	9.25	1.41	1.24
4	E	503	NAP	O7N-C7N	9.19	1.41	1.24
4	A	504	NAP	O7N-C7N	9.09	1.41	1.24
4	B	502	NAP	O7N-C7N	8.49	1.39	1.24
2	E	501	AKG	C2-C1	-5.32	1.45	1.53
2	A	501	AKG	C2-C1	-5.06	1.45	1.53
2	B	501	AKG	C2-C1	-4.80	1.46	1.53
2	D	501	AKG	C2-C1	-4.70	1.46	1.53
2	C	501	AKG	C2-C1	-4.52	1.46	1.53
2	F	501	AKG	C2-C1	-4.44	1.46	1.53
4	C	503	NAP	C2A-N3A	3.45	1.40	1.33
4	A	504	NAP	C2A-N1A	3.26	1.39	1.33
4	A	504	NAP	C2A-N3A	3.14	1.39	1.33
4	C	503	NAP	C2A-N1A	3.01	1.39	1.33
4	D	503	NAP	C2A-N3A	2.96	1.39	1.33
4	E	503	NAP	C2A-N1A	2.92	1.39	1.33
4	B	502	NAP	C2A-N1A	2.90	1.39	1.33
4	E	503	NAP	C2A-N3A	2.84	1.39	1.33
4	A	504	NAP	PA-O3	2.83	1.62	1.59
4	D	503	NAP	C2A-N1A	2.82	1.38	1.33
4	F	503	NAP	C2A-N1A	2.81	1.38	1.33
4	F	503	NAP	C2A-N3A	2.80	1.38	1.33
4	D	503	NAP	C2N-N1N	2.77	1.38	1.35
4	B	502	NAP	C2A-N3A	2.74	1.38	1.33
4	F	503	NAP	C2N-N1N	2.67	1.37	1.35
4	D	503	NAP	PN-O3	2.51	1.62	1.59
4	B	502	NAP	PA-O3	2.50	1.62	1.59
4	D	503	NAP	PA-O3	2.48	1.62	1.59
4	A	504	NAP	C2N-N1N	2.35	1.37	1.35
4	B	502	NAP	C2N-N1N	2.34	1.37	1.35
4	A	504	NAP	PN-O3	2.33	1.62	1.59
4	E	503	NAP	C8A-N7A	2.29	1.36	1.31
4	D	503	NAP	C8A-N7A	2.03	1.35	1.31

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	NAP	N3A-C2A-N1A	-6.63	118.55	128.58
4	E	503	NAP	N3A-C2A-N1A	-5.97	119.54	128.58
4	F	503	NAP	N3A-C2A-N1A	-5.96	119.57	128.58
4	D	503	NAP	N3A-C2A-N1A	-5.79	119.82	128.58
4	C	503	NAP	C5A-C4A-N3A	-5.34	119.37	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	NAP	N3A-C2A-N1A	-5.27	120.60	128.58
4	D	503	NAP	C5A-C4A-N3A	-5.21	119.55	126.72
4	F	503	NAP	C5A-C4A-N3A	-5.04	119.77	126.72
4	C	503	NAP	N3A-C2A-N1A	-4.90	121.17	128.58
4	E	503	NAP	C5A-C4A-N3A	-4.67	120.29	126.72
4	B	502	NAP	C5A-C4A-N3A	-4.12	121.05	126.72
4	A	504	NAP	C5A-C4A-N3A	-4.11	121.06	126.72
2	B	501	AKG	O1-C1-C2	-3.96	116.89	121.81
4	F	503	NAP	C2A-N3A-C4A	3.91	121.38	111.83
4	D	503	NAP	C2A-N3A-C4A	3.80	121.11	111.83
4	C	503	NAP	C2A-N3A-C4A	3.72	120.91	111.83
2	A	501	AKG	C3-C2-C1	3.71	122.15	115.86
4	E	503	NAP	C2A-N3A-C4A	3.67	120.80	111.83
4	B	502	NAP	C2A-N3A-C4A	3.66	120.76	111.83
4	C	503	NAP	N3A-C4A-N9A	3.59	133.28	127.17
4	E	503	NAP	C5A-N7A-C8A	3.56	109.05	103.45
4	B	502	NAP	C5A-N7A-C8A	3.52	108.98	103.45
2	F	501	AKG	C3-C2-C1	3.49	121.78	115.86
4	D	503	NAP	N3A-C4A-N9A	3.41	132.96	127.17
4	F	503	NAP	C5A-N7A-C8A	3.38	108.77	103.45
4	B	502	NAP	N9A-C8A-N7A	-3.32	109.22	113.94
4	B	502	NAP	C3N-C7N-N7N	3.31	121.82	117.74
2	E	501	AKG	O1-C1-C2	-3.29	117.72	121.81
4	E	503	NAP	N9A-C8A-N7A	-3.24	109.34	113.94
4	D	503	NAP	C5A-N7A-C8A	3.18	108.45	103.45
4	A	504	NAP	C2A-N3A-C4A	3.14	119.51	111.83
4	F	503	NAP	N3A-C4A-N9A	3.12	132.47	127.17
4	C	503	NAP	C5A-N7A-C8A	3.07	108.27	103.45
4	F	503	NAP	N9A-C8A-N7A	-2.98	109.71	113.94
4	D	503	NAP	N9A-C8A-N7A	-2.95	109.75	113.94
4	E	503	NAP	C4A-C5A-N7A	-2.85	107.32	110.58
4	A	504	NAP	N3A-C4A-N9A	2.85	132.02	127.17
4	C	503	NAP	N9A-C8A-N7A	-2.84	109.90	113.94
4	E	503	NAP	N3A-C4A-N9A	2.82	131.96	127.17
2	D	501	AKG	C3-C2-C1	2.79	120.60	115.86
4	A	504	NAP	C5A-N7A-C8A	2.76	107.78	103.45
4	B	502	NAP	C4A-C5A-N7A	-2.72	107.47	110.58
4	E	503	NAP	C3N-C7N-N7N	2.72	121.09	117.74
4	A	504	NAP	N9A-C8A-N7A	-2.70	110.10	113.94
4	F	503	NAP	C4A-C5A-N7A	-2.67	107.53	110.58
4	B	502	NAP	N3A-C4A-N9A	2.57	131.53	127.17
4	F	503	NAP	C6N-N1N-C2N	-2.55	119.71	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AKG	O2-C1-C2	2.35	120.10	113.59
4	D	503	NAP	C4A-C5A-N7A	-2.31	107.94	110.58
4	D	503	NAP	C3N-C7N-N7N	2.24	120.50	117.74
2	F	501	AKG	C4-C3-C2	-2.24	108.72	112.91
4	C	503	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
4	A	504	NAP	C4A-C5A-N7A	-2.19	108.08	110.58
4	E	503	NAP	O4B-C4B-C5B	2.19	116.34	109.33
4	F	503	NAP	C3N-C7N-N7N	2.19	120.43	117.74
4	F	503	NAP	O4B-C1B-N9A	2.17	112.26	108.09
4	A	504	NAP	C3N-C7N-N7N	2.17	120.41	117.74
2	C	501	AKG	C3-C2-C1	2.15	119.51	115.86
4	B	502	NAP	C2A-N1A-C6A	2.05	122.09	118.73
4	E	503	NAP	O7N-C7N-N7N	-2.02	119.69	122.62
2	A	501	AKG	O3-C5-C4	-2.01	116.72	123.09

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AKG	O1-C1-C2-O5
2	A	501	AKG	O1-C1-C2-C3
2	A	501	AKG	O2-C1-C2-C3
2	C	501	AKG	C2-C3-C4-C5
2	D	501	AKG	O2-C1-C2-C3
2	E	501	AKG	O1-C1-C2-C3
2	E	501	AKG	O2-C1-C2-C3
2	F	501	AKG	O2-C1-C2-C3
2	F	501	AKG	C1-C2-C3-C4
4	A	504	NAP	C5B-O5B-PA-O1A
4	A	504	NAP	C5B-O5B-PA-O3
4	A	504	NAP	C5D-O5D-PN-O3
4	A	504	NAP	C5D-O5D-PN-O1N
4	A	504	NAP	C5D-O5D-PN-O2N
4	A	504	NAP	O4D-C1D-N1N-C2N
4	A	504	NAP	O4D-C1D-N1N-C6N
4	A	504	NAP	C2D-C1D-N1N-C2N
4	B	502	NAP	C5B-O5B-PA-O1A
4	B	502	NAP	C5D-O5D-PN-O3
4	B	502	NAP	C5D-O5D-PN-O1N
4	B	502	NAP	C5D-O5D-PN-O2N
4	B	502	NAP	O4D-C1D-N1N-C2N
4	B	502	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
4	C	503	NAP	C5D-O5D-PN-O3
4	C	503	NAP	C5D-O5D-PN-O2N
4	C	503	NAP	O4D-C1D-N1N-C2N
4	C	503	NAP	O4D-C1D-N1N-C6N
4	E	503	NAP	C5D-O5D-PN-O3
4	E	503	NAP	C5D-O5D-PN-O1N
4	E	503	NAP	O4D-C1D-N1N-C2N
4	E	503	NAP	O4D-C1D-N1N-C6N
4	F	503	NAP	C5B-O5B-PA-O1A
4	F	503	NAP	C5B-O5B-PA-O2A
4	F	503	NAP	C5B-O5B-PA-O3
4	F	503	NAP	C5D-O5D-PN-O3
4	F	503	NAP	C5D-O5D-PN-O1N
4	F	503	NAP	C5D-O5D-PN-O2N
4	C	503	NAP	O4B-C4B-C5B-O5B
4	E	503	NAP	O4B-C4B-C5B-O5B
4	F	503	NAP	O4D-C4D-C5D-O5D
4	E	503	NAP	C3B-C4B-C5B-O5B
2	B	501	AKG	C2-C3-C4-C5
2	D	501	AKG	C2-C3-C4-C5
2	F	501	AKG	C2-C3-C4-C5
4	F	503	NAP	C3D-C4D-C5D-O5D
4	C	503	NAP	C3B-C4B-C5B-O5B
2	E	501	AKG	O1-C1-C2-O5
2	D	501	AKG	O1-C1-C2-C3
2	A	501	AKG	C1-C2-C3-C4
4	A	504	NAP	C1B-C2B-O2B-P2B
4	E	503	NAP	PN-O3-PA-O2A
4	B	502	NAP	C5B-O5B-PA-O2A
4	B	502	NAP	C5B-O5B-PA-O3
4	C	503	NAP	C5D-O5D-PN-O1N
4	E	503	NAP	C5D-O5D-PN-O2N
4	C	503	NAP	C1B-C2B-O2B-P2B
2	F	501	AKG	O5-C2-C3-C4
4	C	503	NAP	PN-O3-PA-O2A
4	F	503	NAP	PN-O3-PA-O2A
2	E	501	AKG	C2-C3-C4-C5
2	F	501	AKG	C3-C4-C5-O4
4	A	504	NAP	C2D-C1D-N1N-C6N
4	B	502	NAP	C2D-C1D-N1N-C2N
4	E	503	NAP	C2D-C1D-N1N-C2N
2	F	501	AKG	C3-C4-C5-O3

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Mol	Chain	Res	Type	Atoms
4	F	503	NAP	C1B-C2B-O2B-P2B
4	D	503	NAP	O4D-C1D-N1N-C2N
2	C	501	AKG	C3-C4-C5-O4
2	D	501	AKG	C3-C4-C5-O4
2	D	501	AKG	C3-C4-C5-O3
4	F	503	NAP	PN-O3-PA-O1A
2	E	501	AKG	C3-C4-C5-O4
2	C	501	AKG	C3-C4-C5-O3
2	A	501	AKG	C3-C4-C5-O4
2	A	501	AKG	C3-C4-C5-O3
2	C	501	AKG	C1-C2-C3-C4
2	E	501	AKG	C3-C4-C5-O3
4	C	503	NAP	PN-O3-PA-O1A
4	D	503	NAP	PN-O3-PA-O1A
4	D	503	NAP	PN-O3-PA-O2A
4	E	503	NAP	PN-O3-PA-O1A
4	D	503	NAP	C2B-O2B-P2B-O2X
4	E	503	NAP	O4D-C4D-C5D-O5D
4	D	503	NAP	C2B-O2B-P2B-O1X
4	A	504	NAP	C3B-C2B-O2B-P2B
2	C	501	AKG	O5-C2-C3-C4

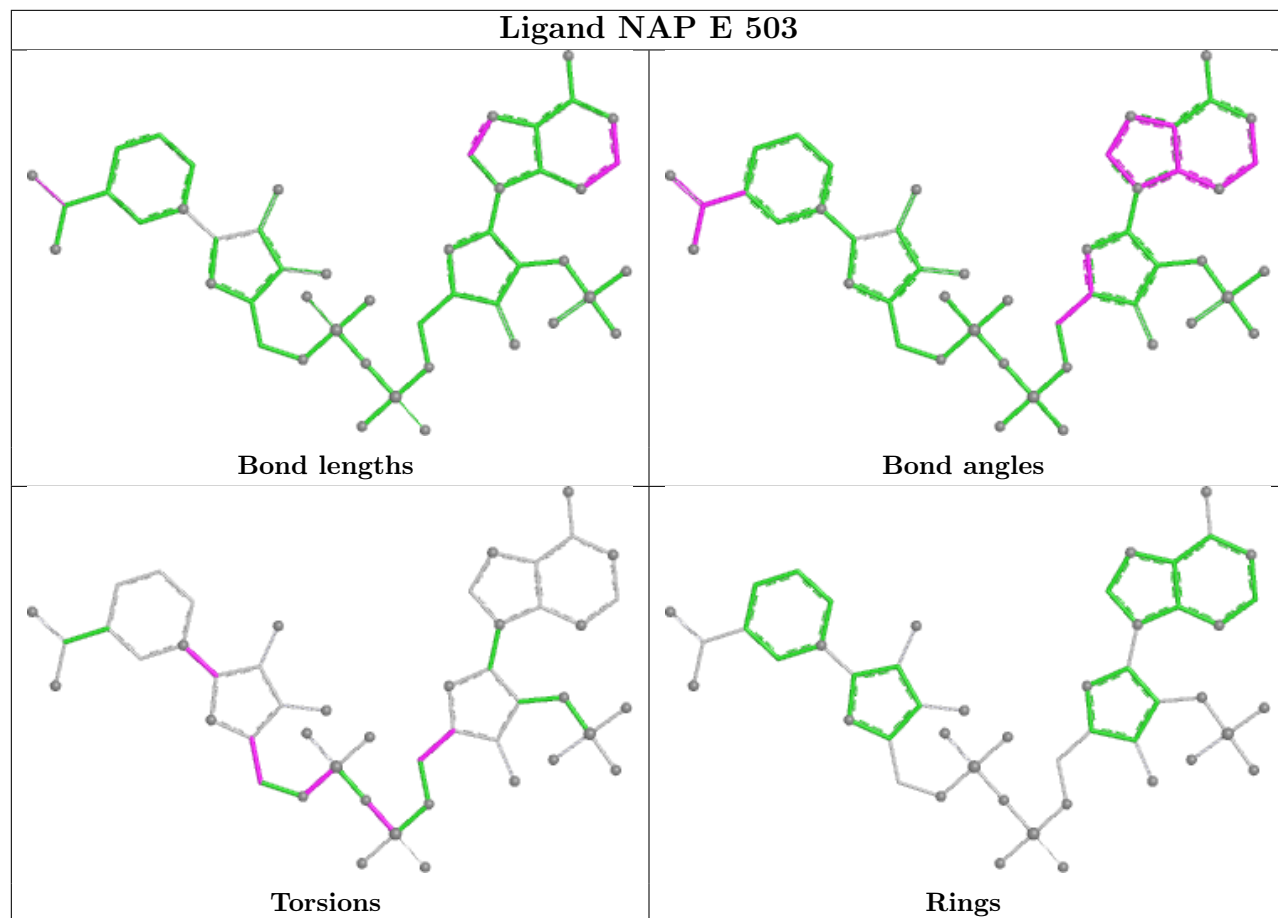
There are no ring outliers.

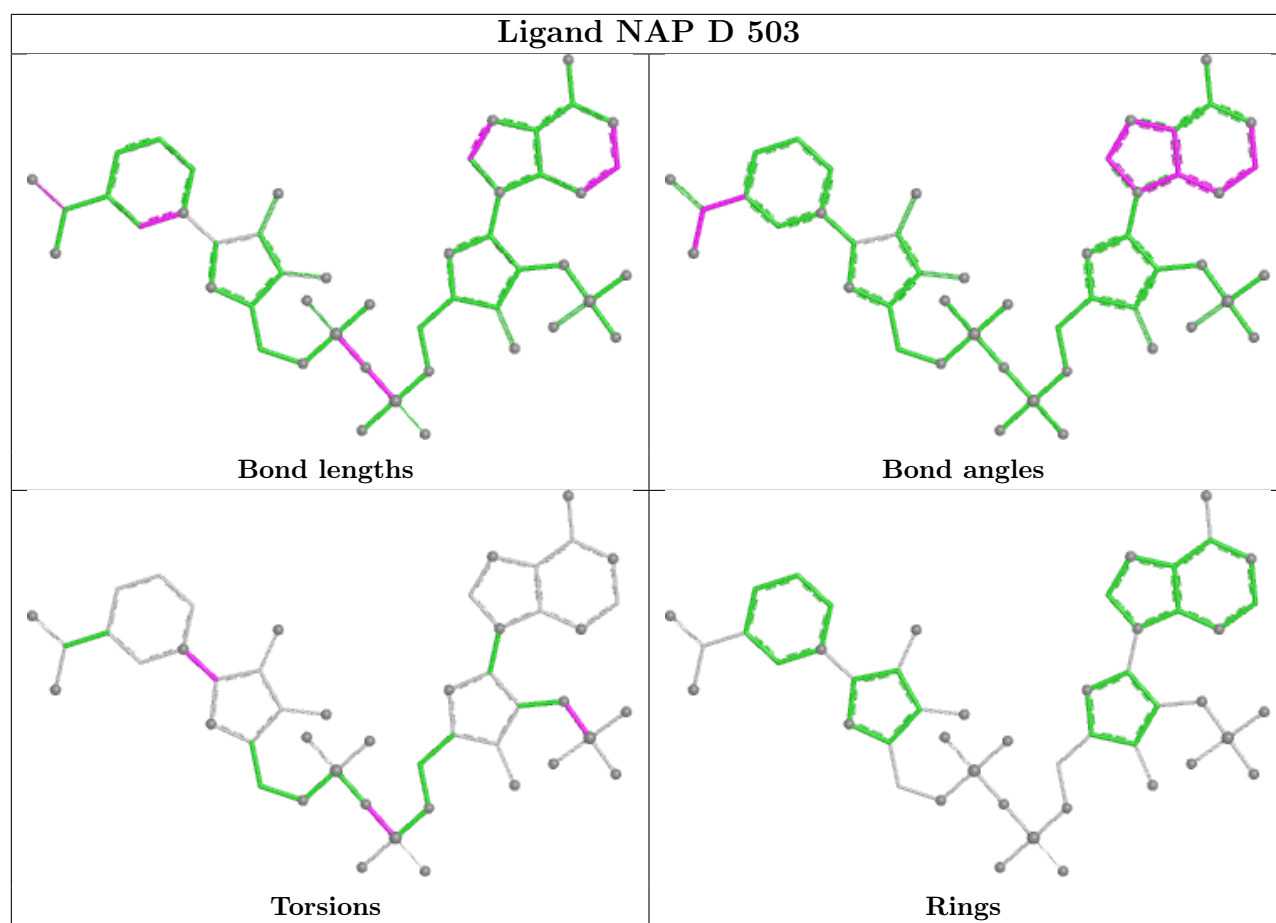
4 monomers are involved in 3 short contacts:

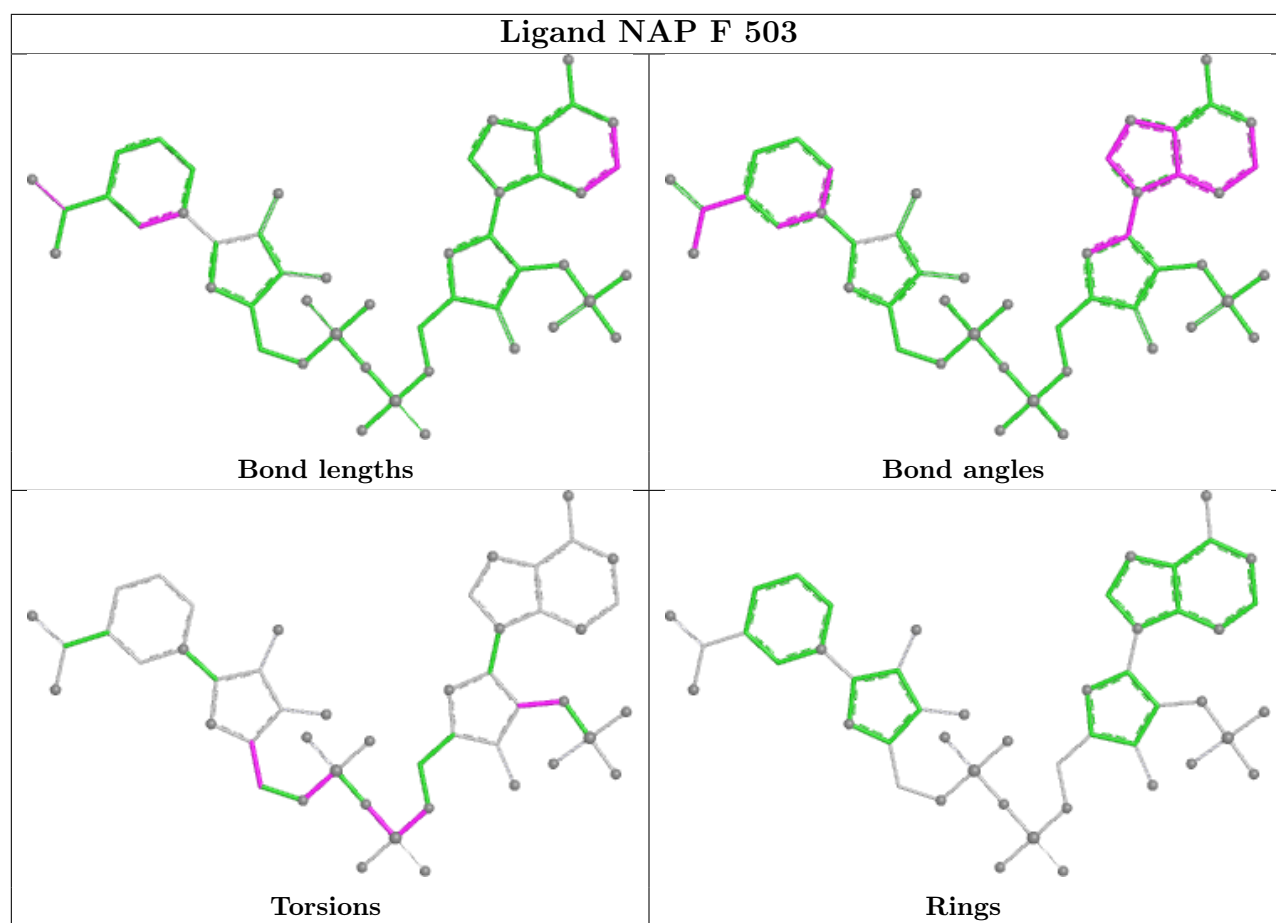
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	503	NAP	1	0
4	A	504	NAP	1	0
4	C	503	NAP	1	0
2	A	501	AKG	1	0

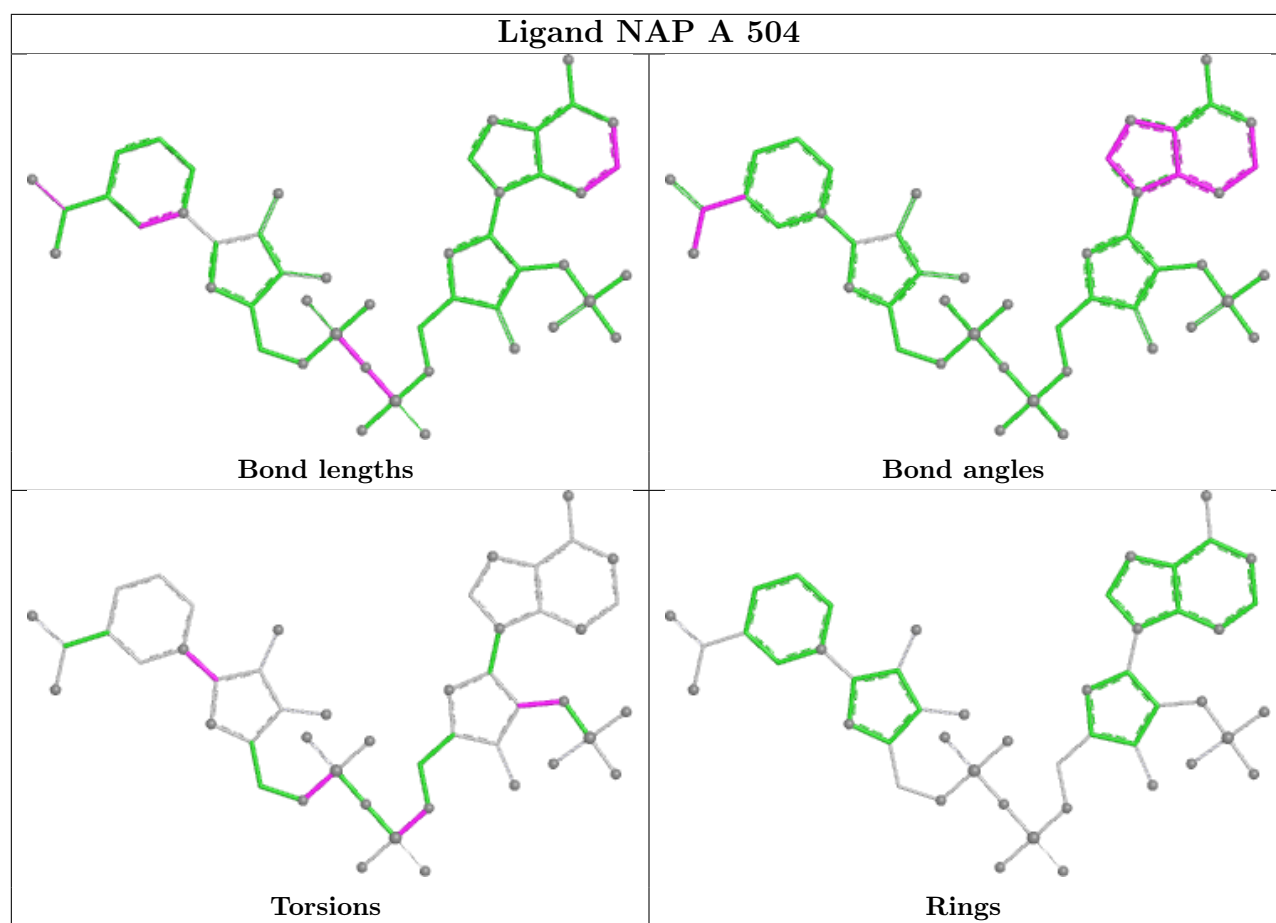
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

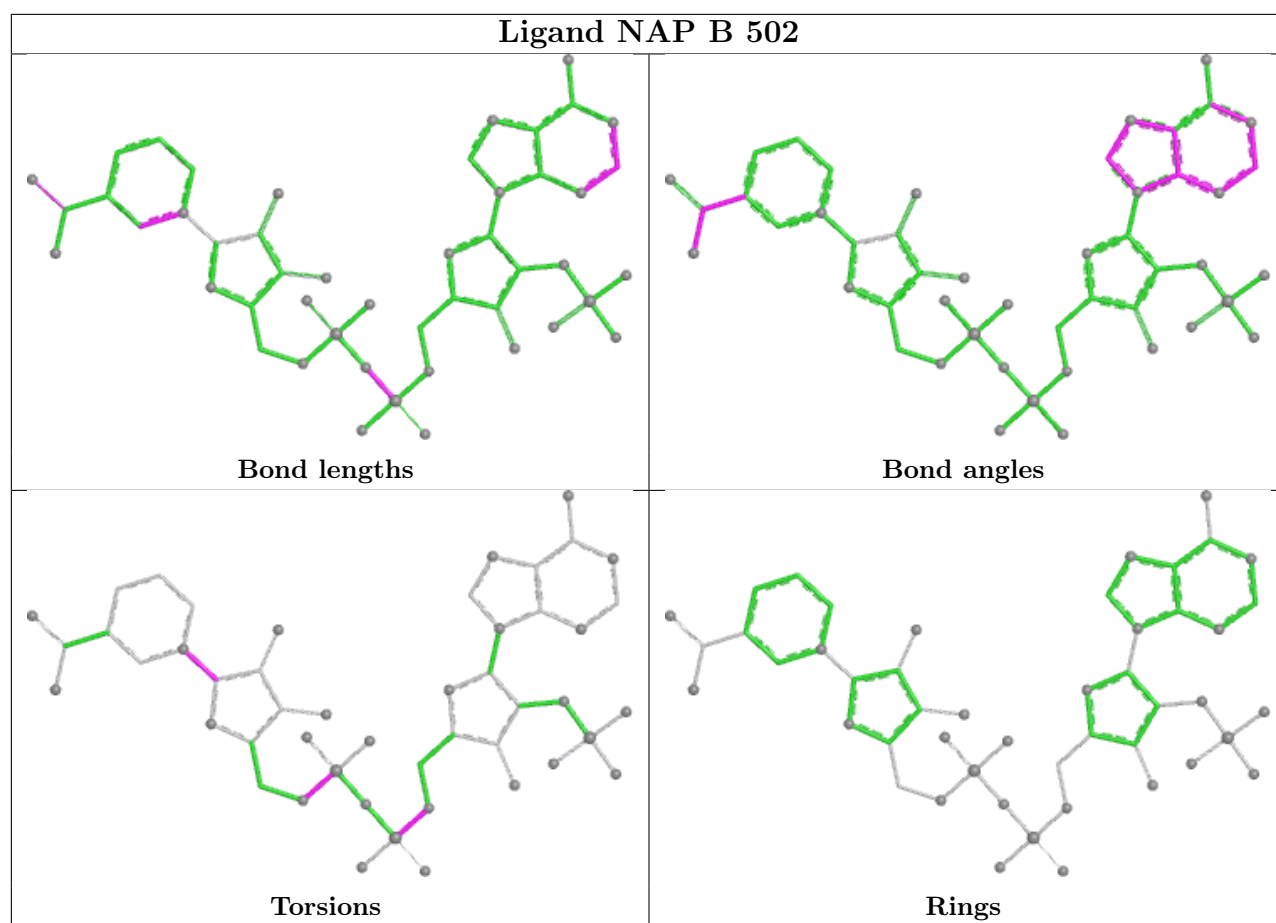
equivalents in the CSD to analyse the geometry.

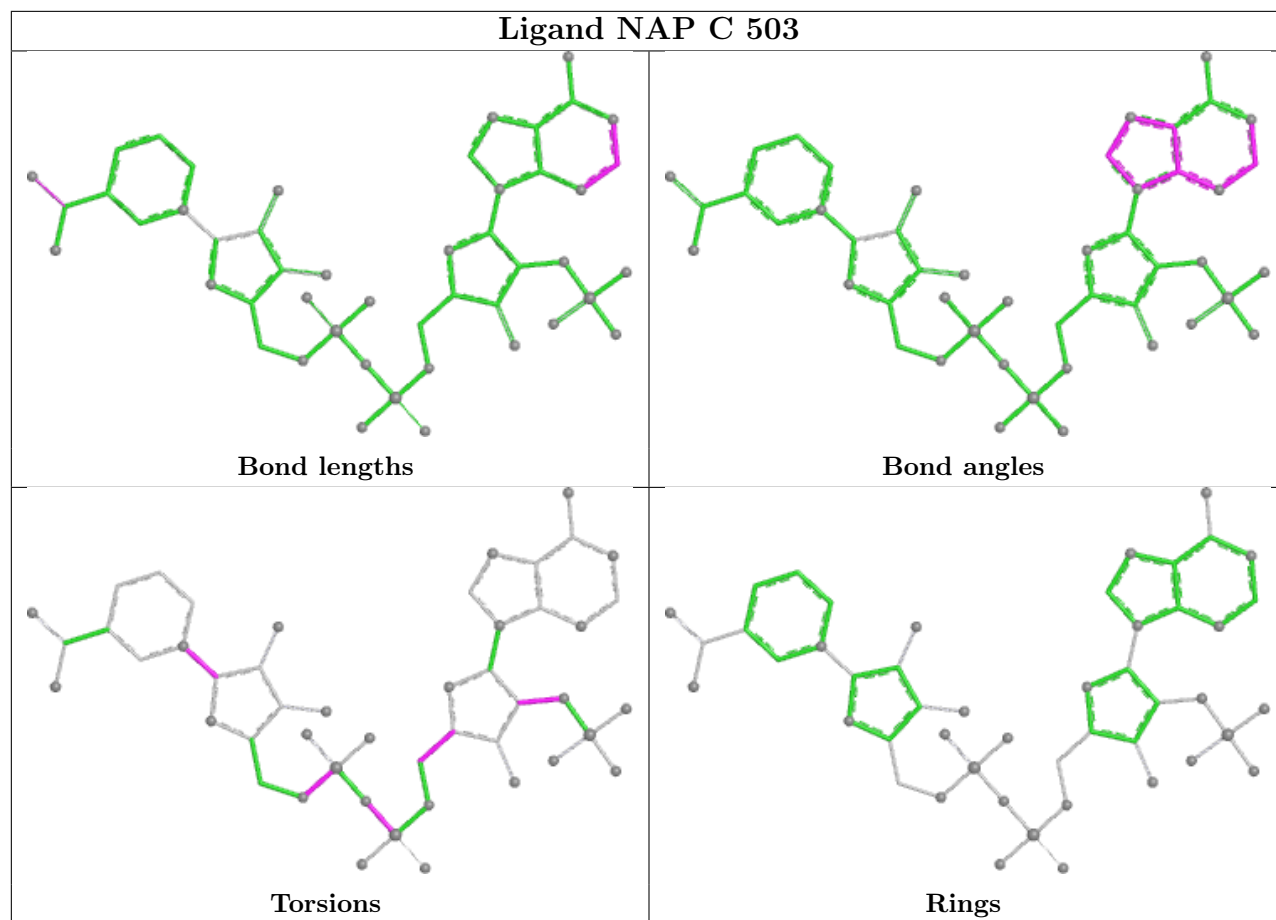












5.7 Other polymers [i](#)

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	411/425 (96%)	0.13	9 (2%)	62 53	39, 69, 98, 124	0
1	B	412/425 (96%)	-0.26	1 (0%)	91 89	30, 55, 79, 94	2 (0%)
1	C	412/425 (96%)	0.21	13 (3%)	50 41	40, 69, 96, 130	0
1	D	412/425 (96%)	0.30	17 (4%)	41 33	33, 83, 116, 147	1 (0%)
1	E	412/425 (96%)	0.23	12 (2%)	53 45	40, 71, 101, 121	1 (0%)
1	F	412/425 (96%)	0.33	15 (3%)	46 38	33, 81, 112, 151	1 (0%)
All	All	2471/2550 (96%)	0.16	67 (2%)	56 47	30, 70, 105, 151	5 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	SER	5.7
1	F	18	MET	5.3
1	F	380	ILE	5.1
1	D	394	THR	5.0
1	A	415	SER	4.7
1	C	409	LEU	4.3
1	C	414	LEU	3.8
1	E	196	SER	3.8
1	E	337	THR	3.5
1	E	114	CYS	3.4
1	D	414	LEU	3.3
1	E	363	SER	3.3
1	D	393	ASN	3.2
1	F	64	ILE	3.2
1	E	279	ASP	3.1
1	D	98	THR	3.1
1	F	35	VAL	3.0
1	C	131	GLY	3.0
1	E	369	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	414	LEU	3.0
1	D	35	VAL	2.9
1	F	414	LEU	2.9
1	A	319	TYR	2.8
1	F	330	ILE	2.8
1	C	398	MET	2.7
1	A	90	GLN	2.7
1	E	69	VAL	2.6
1	E	113	ILE	2.6
1	A	31	ILE	2.6
1	D	256	ALA	2.6
1	D	321	LYS	2.5
1	C	372	MET	2.5
1	A	44	LEU	2.5
1	D	356	ALA	2.5
1	D	364	ILE	2.4
1	D	392	LEU	2.4
1	C	390	ASP	2.4
1	F	398	MET	2.4
1	D	391	TYR	2.4
1	D	395	PHE	2.4
1	C	190	GLU	2.4
1	E	112	ILE	2.3
1	C	281	VAL	2.3
1	C	124	TRP	2.3
1	D	327	THR	2.3
1	D	91	MET	2.3
1	F	101	ASN	2.2
1	F	323	GLN	2.2
1	F	306	GLU	2.2
1	F	125	VAL	2.2
1	C	278	SER	2.2
1	C	356	ALA	2.2
1	C	226	ILE	2.2
1	B	414	LEU	2.2
1	F	387	GLN	2.1
1	F	307	ALA	2.1
1	A	327	THR	2.1
1	C	387	GLN	2.1
1	F	274	GLY	2.1
1	D	325	THR	2.1
1	E	354	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	415	SER	2.1
1	F	278	SER	2.1
1	A	190	GLU	2.1
1	D	398	MET	2.0
1	A	336	TRP	2.0
1	E	223	PHE	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.

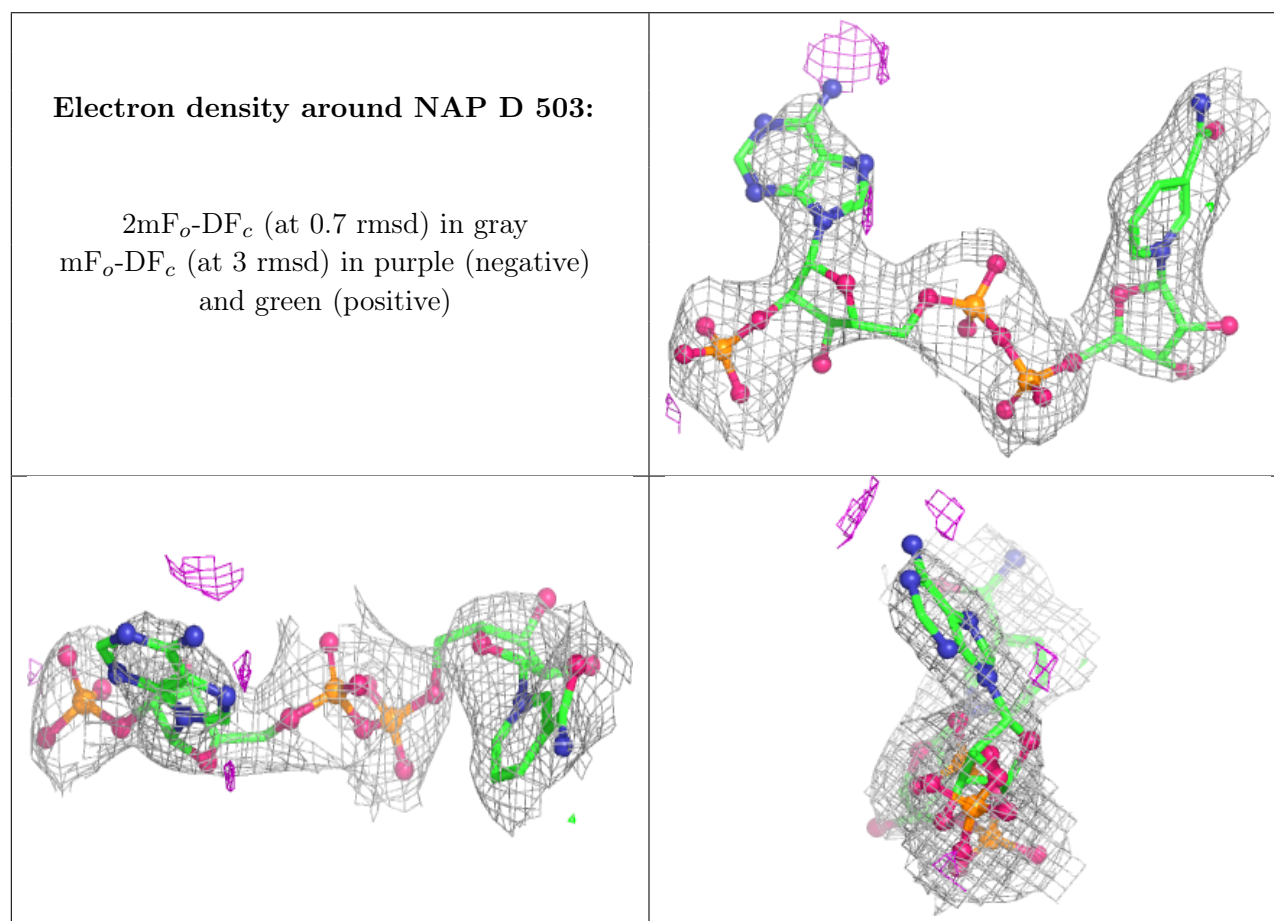
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAP	D	503	48/48	0.84	0.12	98,109,113,114	0
2	AKG	F	501	10/10	0.85	0.16	86,90,99,99	0
4	NAP	F	503	48/48	0.86	0.12	84,99,103,105	0
2	AKG	D	501	10/10	0.88	0.14	100,101,102,102	0
2	AKG	C	501	10/10	0.88	0.18	79,85,88,88	0
2	AKG	E	501	10/10	0.89	0.18	91,96,98,98	0
2	AKG	A	501	10/10	0.91	0.12	74,77,79,79	0
2	AKG	B	501	10/10	0.91	0.11	41,55,58,58	0
4	NAP	E	503	48/48	0.92	0.10	54,68,77,79	0
3	CA	A	502	1/1	0.93	0.12	70,70,70,70	0
4	NAP	C	503	48/48	0.94	0.09	50,61,74,75	0
3	CA	D	502	1/1	0.95	0.08	70,70,70,70	0
3	CA	E	502	1/1	0.95	0.10	72,72,72,72	0
3	CA	F	502	1/1	0.95	0.07	74,74,74,74	0
4	NAP	A	504	48/48	0.95	0.09	43,59,68,71	0
4	NAP	B	502	48/48	0.96	0.08	44,51,59,62	0
3	CA	C	502	1/1	0.97	0.08	62,62,62,62	0

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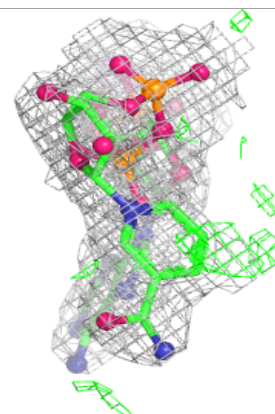
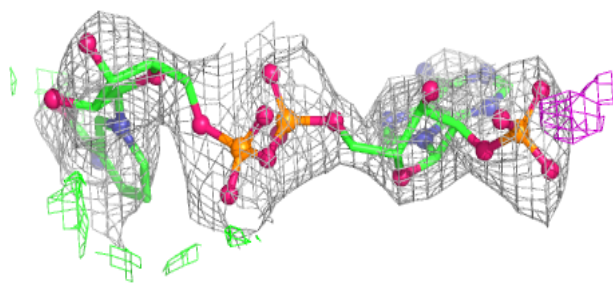
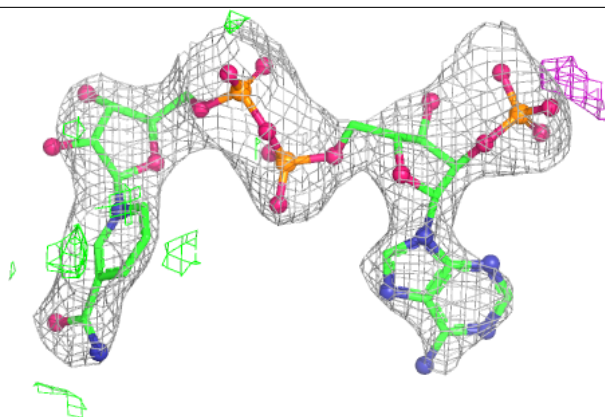
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	503	1/1	0.99	0.04	53,53,53,53	0

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.

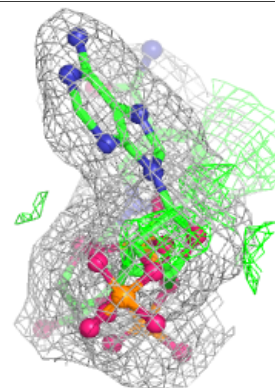
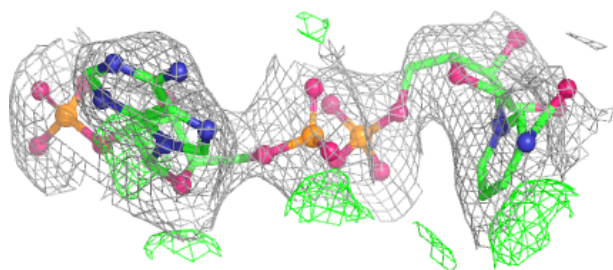
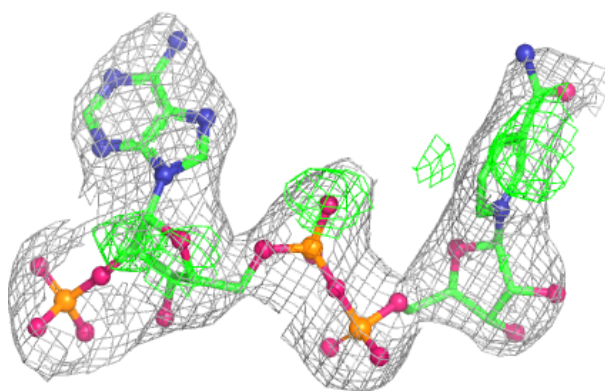


Electron density around NAP F 503:

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

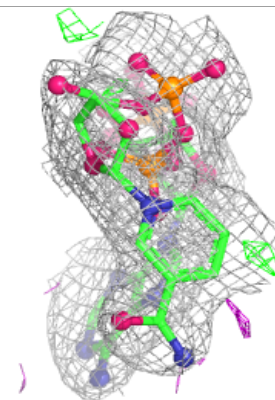
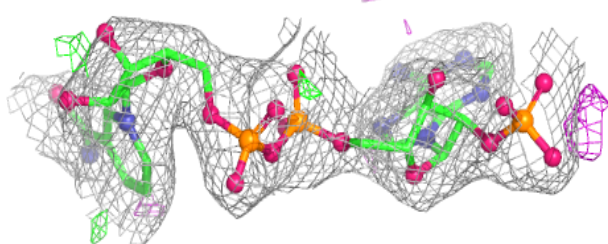
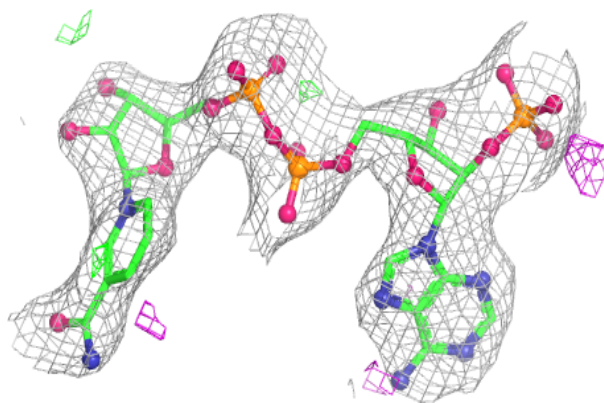
**Electron density around NAP E 503:**

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

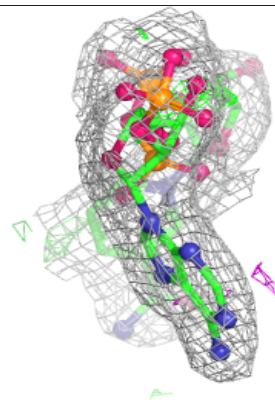
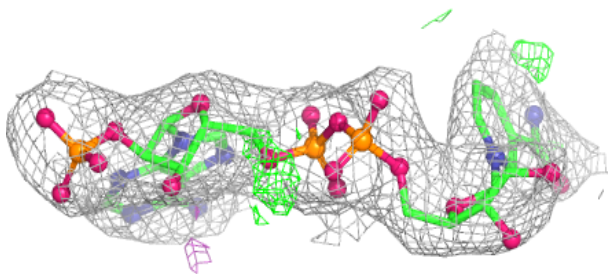
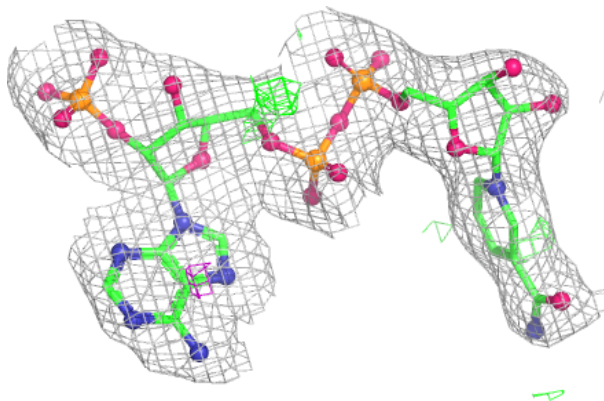


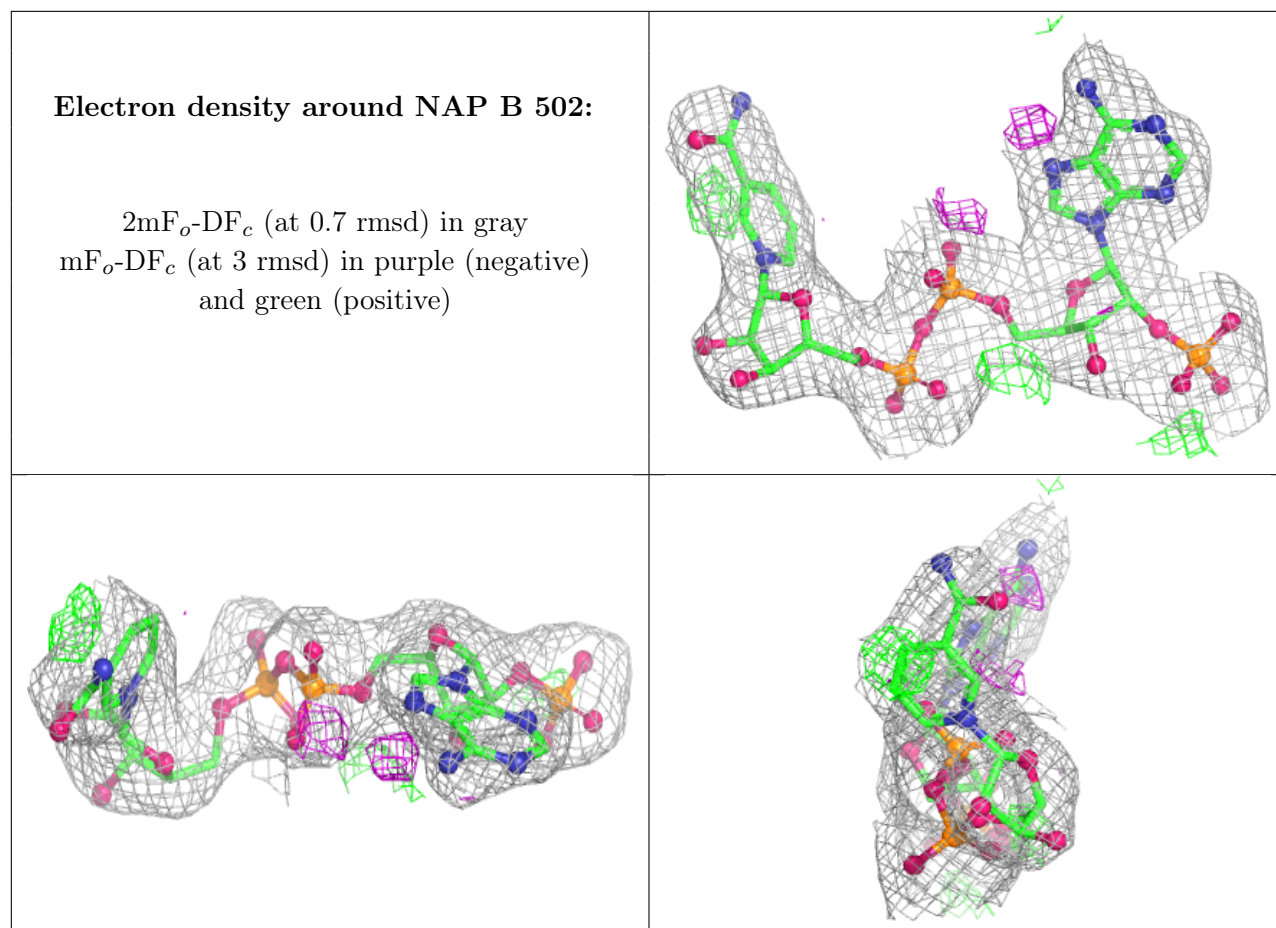
Electron density around NAP C 503:

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

**Electron density around NAP A 504:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.