



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:00 PM UTC

PDB ID : 4L06 / pdb_00004l06
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 : 2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

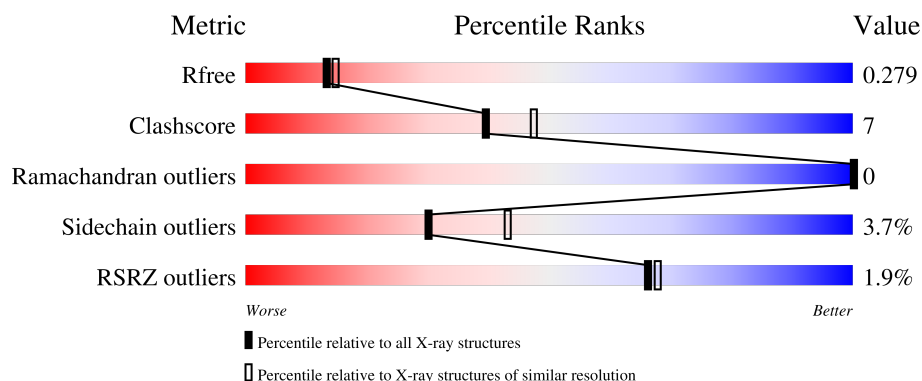
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	425	
1	B	425	
1	C	425	
1	D	425	
1	E	425	

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Mol	Chain	Length	Quality of chain
1	F	425	% 82% 14% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19823 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	413	Total	C	N	O	S	0	1	0
			3231	2050	548	615	18			
1	B	412	Total	C	N	O	S	0	2	0
			3220	2046	545	611	18			
1	C	411	Total	C	N	O	S	0	0	0
			3234	2052	549	615	18			
1	D	411	Total	C	N	O	S	0	1	0
			3168	2006	541	603	18			
1	E	413	Total	C	N	O	S	0	1	0
			3232	2051	547	616	18			
1	F	412	Total	C	N	O	S	0	1	0
			3255	2068	552	617	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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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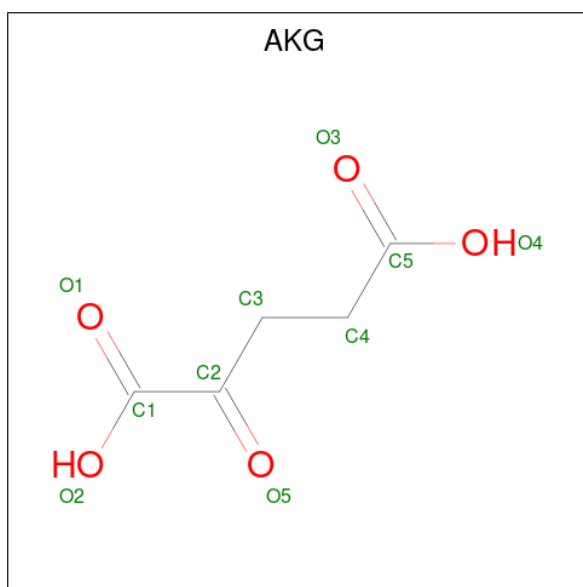
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Chain	Residue	Modelled	Actual	Comment	Reference
E	425	HIS	-	expression tag	UNP O75874
F	139	ASP	TYR	engineered mutation	UNP O75874
F	415	SER	-	expression tag	UNP O75874
F	416	LEU	-	expression tag	UNP O75874
F	417	GLU	-	expression tag	UNP O75874
F	418	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 CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

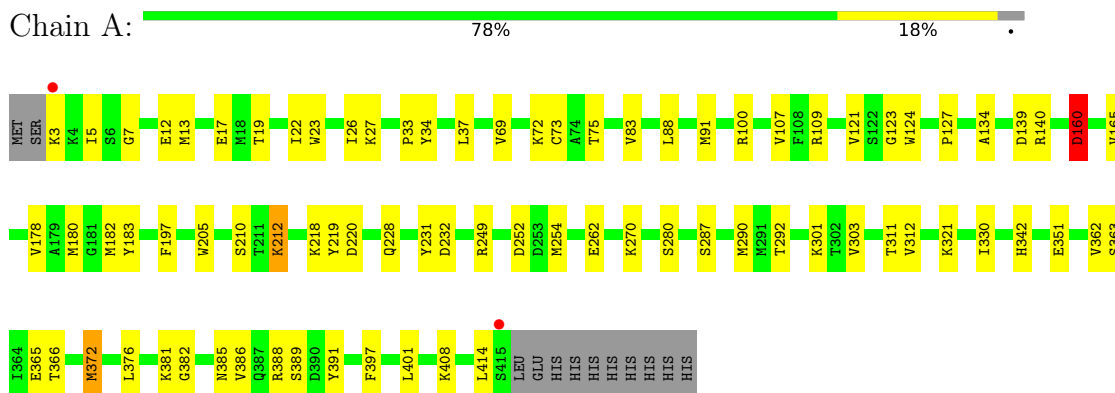
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	14	Total	O	0	0
			14	14		
5	C	16	Total	O	0	0
			16	16		
5	D	6	Total	O	0	0
			6	6		
5	E	25	Total	O	0	0
			25	25		
5	F	21	Total	O	0	0
			21	21		

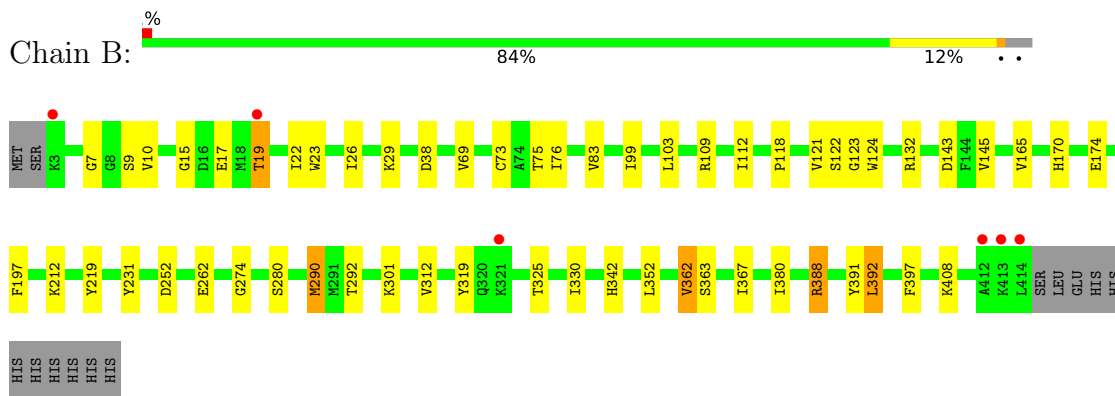
3 Residue-property plots [i](#)

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

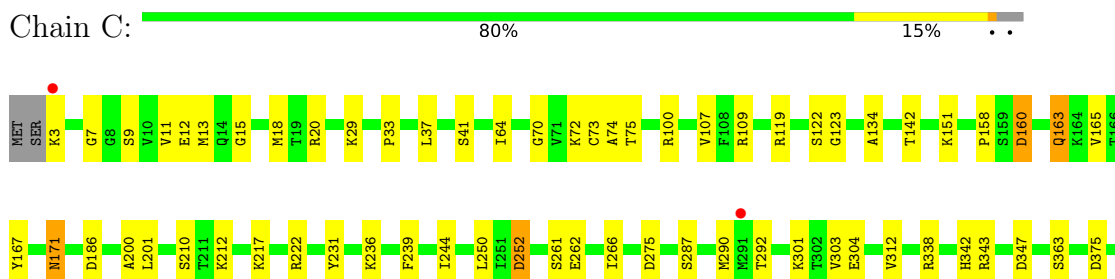
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

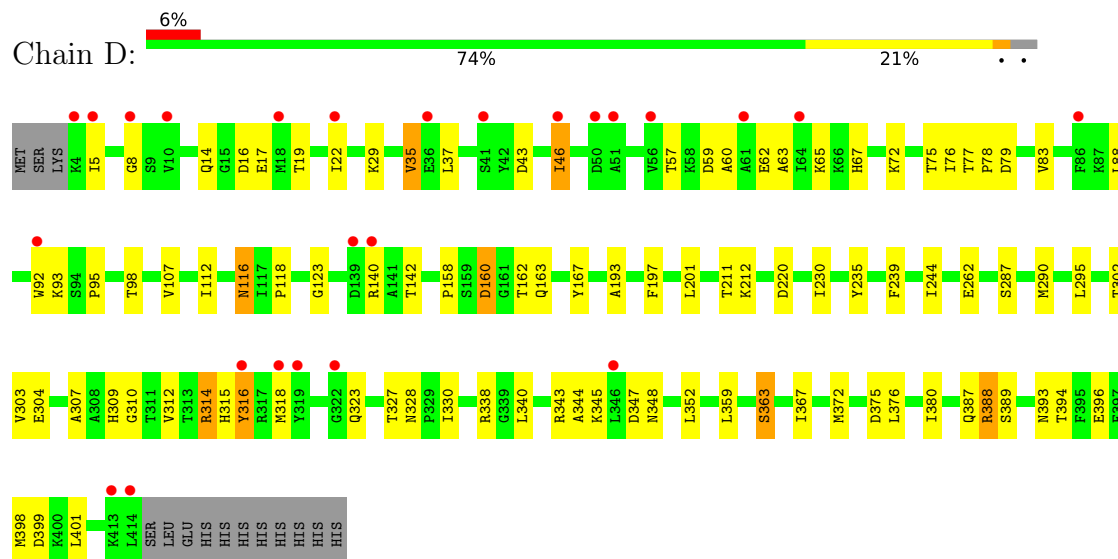


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

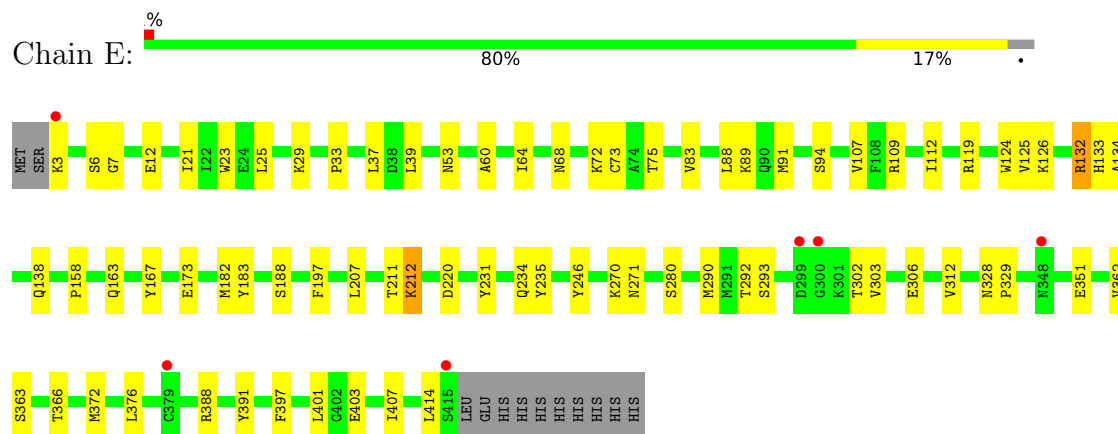




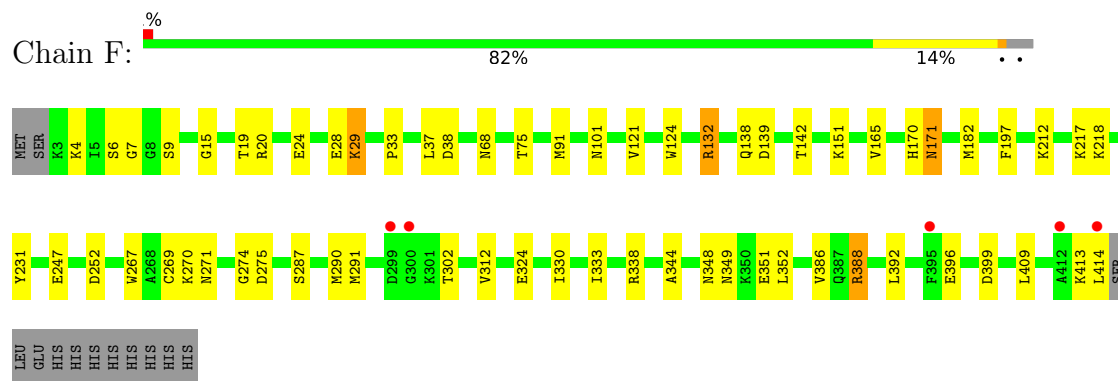
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



• 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	96.22Å 116.55Å 275.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.17 – 2.28 72.17 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.17-2.28) 99.8 (72.17-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.224 , 0.270 (Not available) , 0.279	Depositor DCC
R_{free} test set	7083 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19823	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 67.21 % 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 5.3413e-06. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, AKG, 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	0.28	0/3301	0.51	0/4462
1	B	0.25	0/3293	0.47	0/4451
1	C	0.27	0/3301	0.49	0/4456
1	D	0.25	0/3237	0.50	0/4383
1	E	0.28	0/3302	0.51	0/4463
1	F	0.27	0/3325	0.48	0/4486
All	All	0.27	0/19759	0.49	0/26701

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ASP	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3231	0	3149	49	0
1	B	3220	0	3139	32	0
1	C	3234	0	3175	39	0
1	D	3168	0	3043	66	0
1	E	3232	0	3149	44	0
1	F	3255	0	3217	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	48	0	25	2	0
3	B	48	0	25	3	0
3	C	48	0	25	2	0
3	D	48	0	25	6	0
3	E	48	0	25	0	0
3	F	48	0	25	1	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
4	C	10	0	4	1	0
4	D	10	0	4	0	0
4	E	10	0	4	0	0
4	F	10	0	4	0	0
5	A	47	0	0	3	0
5	B	14	0	0	0	0
5	C	16	0	0	0	0
5	D	6	0	0	0	0
5	E	25	0	0	0	0
5	F	21	0	0	1	0
All	All	19823	0	19046	259	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 7.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LYS:NZ	1:D:399:ASP:OD1	2.04	0.90
1:C:3:LYS:N	1:C:33:PRO:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:GLU:OE1	1:F:388:ARG:NH1	2.13	0.81
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.65	0.77
1:D:340:LEU:HD22	1:D:352:LEU:HD11	1.66	0.76
1:D:98:THR:HA	1:D:140:ARG:HH22	1.53	0.74
1:C:217:LYS:NZ	1:D:78:PRO:O	2.23	0.70
1:A:127:PRO:HG2	1:A:205:TRP:HH2	1.58	0.69
1:D:83:VAL:HG13	1:D:88:LEU:HB2	1.74	0.69
1:F:151:LYS:NZ	1:F:171:ASN:OD1	2.23	0.68
1:F:132:ARG:NH1	1:F:271:ASN:OD1	2.25	0.68
1:C:29:LYS:NZ	1:C:399:ASP:OD1	2.26	0.68
1:A:139:ASP:OD2	5:A:611:HOH:O	2.10	0.67
1:C:151:LYS:NZ	1:C:171:ASN:OD1	2.25	0.67
1:F:132:ARG:HB2	1:F:274:GLY:HA3	1.78	0.65
1:D:344:ALA:HB2	1:D:352:LEU:HB3	1.79	0.65
1:F:388:ARG:NE	1:F:388:ARG:O	2.32	0.62
1:C:167:TYR:HB3	1:D:142:THR:HG21	1.82	0.62
1:B:212:LYS:NZ	1:B:252:ASP:OD2	2.32	0.62
1:D:314:ARG:HH21	1:D:315:HIS:CD2	2.17	0.62
1:F:392:LEU:HD23	1:F:396:GLU:HB3	1.81	0.62
1:E:220:ASP:OD1	1:E:270:LYS:NZ	2.31	0.61
1:F:29:LYS:NZ	1:F:399:ASP:OD1	2.31	0.61
1:C:119:ARG:NH2	1:C:122:SER:O	2.30	0.60
1:E:125:VAL:HG23	1:E:126:LYS:HG3	1.84	0.60
1:D:22:ILE:HD11	1:D:327:THR:HB	1.83	0.59
1:A:365:GLU:OE2	1:A:408:LYS:NZ	2.34	0.59
1:F:287:SER:HB3	1:F:290:MET:HG2	1.84	0.59
1:D:359:LEU:O	1:D:363:SER:OG	2.22	0.58
1:E:351:GLU:OE1	1:E:351:GLU:N	2.37	0.58
1:D:310:GLY:HA3	3:D:502:NAP:H52N	1.85	0.58
1:B:388:ARG:NH2	1:B:391:TYR:O	2.37	0.57
1:C:212:LYS:NZ	1:C:252:ASP:OD1	2.37	0.57
1:D:309:HIS:CE1	3:D:502:NAP:H61A	2.23	0.57
1:E:91:MET:HE3	1:F:217:LYS:HD3	1.85	0.57
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.39	0.57
1:A:301:LYS:O	1:A:342:HIS:NE2	2.32	0.57
1:D:62:GLU:HA	1:D:65:LYS:HB2	1.87	0.57
1:E:133:HIS:NE2	1:E:188:SER:OG	2.30	0.56
1:D:116:ASN:ND2	1:D:367:ILE:O	2.35	0.56
1:D:363:SER:HA	1:D:401:LEU:HD21	1.86	0.56
1:D:17:GLU:HA	1:D:316:TYR:CZ	2.41	0.56
1:D:78:PRO:HG2	1:D:92:TRP:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:HB3	1:A:254:MET:HG2	1.87	0.56
1:C:301:LYS:O	1:C:342:HIS:NE2	2.38	0.56
1:D:160:ASP:OD2	1:D:162:THR:OG1	2.19	0.55
1:F:212:LYS:NZ	1:F:252:ASP:OD2	2.36	0.55
1:D:67:HIS:O	1:D:343:ARG:NH1	2.40	0.55
1:E:109:ARG:HA	1:E:292:THR:O	2.06	0.55
1:B:112:ILE:HB	1:B:290:MET:HB3	1.88	0.55
1:D:72:LYS:HZ3	1:D:75:THR:HG23	1.72	0.55
1:F:7:GLY:HA3	1:F:37:LEU:HD23	1.88	0.55
1:C:201:LEU:HD23	1:C:244:ILE:HD11	1.88	0.54
1:D:22:ILE:HG12	1:D:394:THR:HG21	1.89	0.54
1:A:381:LYS:O	1:A:385:ASN:ND2	2.29	0.54
1:C:403:GLU:O	1:C:407:ILE:HG12	2.08	0.54
1:E:403:GLU:O	1:E:407:ILE:HG12	2.08	0.54
1:D:344:ALA:O	1:D:348:ASN:N	2.40	0.54
1:E:197:PHE:CZ	1:E:231:TYR:HB2	2.42	0.54
1:A:3:LYS:N	1:A:33:PRO:O	2.41	0.54
1:A:7:GLY:HA3	1:A:37:LEU:HD23	1.90	0.54
1:E:119:ARG:NH1	1:E:124:TRP:O	2.41	0.53
1:A:180:MET:HE2	1:A:182:MET:HE2	1.91	0.53
1:A:12:GLU:OE2	1:A:27:LYS:NZ	2.29	0.52
1:A:127:PRO:HG2	1:A:205:TRP:CH2	2.42	0.52
1:D:211:THR:HB	1:D:220:ASP:HB3	1.91	0.52
1:B:392:LEU:HD12	1:B:397:PHE:HA	1.91	0.52
1:D:112:ILE:N	1:D:290:MET:O	2.38	0.52
1:E:138[B]:GLN:HG2	1:E:182:MET:HE1	1.92	0.52
1:B:75:THR:O	3:B:502:NAP:H2N	2.10	0.52
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.92	0.52
1:E:68:ASN:HA	1:E:302:THR:HG23	1.92	0.52
1:E:91:MET:HE1	1:F:217:LYS:HB3	1.92	0.52
1:B:10:VAL:HG13	1:B:69:VAL:HG12	1.92	0.52
3:B:502:NAP:O1X	3:B:502:NAP:O3B	2.22	0.52
1:D:201:LEU:HD23	1:D:244:ILE:HD11	1.92	0.52
1:E:132:ARG:NH1	1:E:271:ASN:OD1	2.43	0.52
1:A:83:VAL:HG21	1:A:91:MET:HG2	1.92	0.51
1:E:107:VAL:HG23	1:E:134:ALA:HB2	1.91	0.51
1:E:3:LYS:HA	1:E:33:PRO:O	2.11	0.51
1:D:314:ARG:HH21	1:D:315:HIS:HD2	1.59	0.51
1:C:142:THR:HG21	1:D:167:TYR:HB3	1.93	0.51
1:C:107:VAL:HG23	1:C:134:ALA:HB2	1.92	0.51
1:C:287:SER:HB3	1:C:290:MET:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:GLN:HB2	1:E:235:TYR:CD1	2.46	0.51
1:A:100:ARG:HD2	5:A:611:HOH:O	2.10	0.51
1:E:53:ASN:OD1	1:E:89:LYS:NZ	2.44	0.50
1:C:7:GLY:HA3	1:C:37:LEU:HD23	1.94	0.50
1:D:388:ARG:NH2	1:D:396:GLU:OE1	2.45	0.50
1:A:321:LYS:NZ	5:A:634:HOH:O	2.38	0.50
1:A:160:ASP:OD2	1:A:160:ASP:N	2.31	0.50
1:C:239:PHE:CD2	1:C:244:ILE:HG13	2.47	0.50
1:E:211:THR:HB	1:E:220:ASP:HB3	1.93	0.50
1:F:9:SER:OG	1:F:38:ASP:OD2	2.30	0.50
1:D:14:GLN:HB2	1:D:43:ASP:HA	1.95	0.49
1:E:397:PHE:CE2	1:E:401:LEU:HD11	2.46	0.49
1:D:328:ASN:ND2	1:D:375:ASP:OD2	2.33	0.49
1:F:267:TRP:CD1	1:F:269:CYS:HG	2.30	0.49
1:C:9:SER:O	1:C:343:ARG:NH1	2.38	0.49
1:A:287:SER:HB3	1:A:290:MET:HG2	1.94	0.49
1:D:307:ALA:HB1	1:D:309:HIS:CD2	2.48	0.49
3:D:502:NAP:O1X	3:D:502:NAP:O3B	2.29	0.49
1:F:197:PHE:CZ	1:F:231:TYR:HB2	2.48	0.48
1:A:107:VAL:HG23	1:A:134:ALA:HB2	1.95	0.48
1:B:109:ARG:HA	1:B:292:THR:O	2.13	0.48
1:F:75:THR:O	3:F:502:NAP:H2N	2.13	0.48
1:A:123:GLY:O	1:A:262:GLU:HA	2.13	0.48
1:D:343:ARG:O	1:D:347:ASP:N	2.41	0.48
1:F:101:ASN:HD21	1:F:139:ASP:HB3	1.78	0.48
1:A:228:GLN:NE2	1:A:232:ASP:OD1	2.44	0.48
1:A:351:GLU:OE1	1:A:351:GLU:N	2.31	0.48
1:E:362:VAL:O	1:E:366:THR:OG1	2.28	0.48
1:A:17:GLU:HB2	1:A:311:THR:HB	1.96	0.48
1:C:160:ASP:OD1	1:C:160:ASP:N	2.35	0.48
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.95	0.47
1:C:290:MET:HE3	1:C:290:MET:HB3	1.82	0.47
1:A:75:THR:O	3:A:502:NAP:H2N	2.14	0.47
1:D:107:VAL:HG22	1:D:295:LEU:HD13	1.95	0.47
1:D:77:THR:HG23	1:D:93:LYS:O	2.14	0.47
3:A:502:NAP:O1X	3:A:502:NAP:O3B	2.28	0.47
1:C:13:MET:HE1	1:C:64:ILE:HD11	1.96	0.47
1:D:193:ALA:HB3	1:D:230:ILE:HD12	1.97	0.47
1:A:5:ILE:HG12	1:A:34:TYR:O	2.14	0.47
1:E:372:MET:HB2	1:E:376:LEU:HB2	1.96	0.47
1:C:12:GLU:OE1	1:C:41:SER:OG	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:THR:O	3:D:502:NAP:H1D	2.14	0.47
1:B:99:ILE:O	1:B:103:LEU:HG	2.14	0.47
1:D:367:ILE:HG23	1:D:372:MET:HG2	1.97	0.47
1:F:413:LYS:HD3	1:F:413:LYS:HA	1.67	0.47
1:B:301:LYS:O	1:B:342:HIS:NE2	2.44	0.46
1:C:72:LYS:HG2	1:C:73:CYS:O	2.15	0.46
1:D:5:ILE:O	1:D:35:VAL:HA	2.15	0.46
1:B:123:GLY:O	1:B:262:GLU:HA	2.15	0.46
1:E:29:LYS:HB3	1:E:29:LYS:HE2	1.70	0.46
1:E:366:THR:HG21	1:E:401:LEU:HD23	1.97	0.46
1:C:375:ASP:OD1	1:C:375:ASP:N	2.47	0.46
1:F:270:LYS:NZ	5:F:613:HOH:O	2.48	0.46
1:A:372:MET:HE2	1:A:376:LEU:HB3	1.98	0.46
1:D:375:ASP:OD1	1:D:375:ASP:N	2.44	0.46
1:A:22:ILE:O	1:A:26:ILE:HG13	2.16	0.46
1:A:83:VAL:HA	1:A:88:LEU:HD12	1.98	0.46
1:A:180:MET:CE	1:A:182:MET:HE2	2.46	0.46
1:A:362:VAL:O	1:A:366:THR:OG1	2.26	0.46
1:B:132:ARG:HG3	1:B:274:GLY:HA3	1.97	0.46
1:C:18:MET:HE3	1:C:18:MET:HA	1.97	0.46
1:F:91:MET:HE3	1:F:91:MET:HB2	1.81	0.46
1:F:121:VAL:HG11	1:F:124:TRP:CE2	2.51	0.46
1:B:69:VAL:HG22	1:B:342:HIS:HD2	1.81	0.45
1:E:83:VAL:HA	1:E:88:LEU:HD12	1.98	0.45
1:A:397:PHE:CE2	1:A:401:LEU:HD11	2.51	0.45
3:C:502:NAP:H51N	3:C:502:NAP:O2A	2.16	0.45
1:E:12:GLU:HB2	1:E:39:LEU:HD11	1.98	0.45
1:A:121:VAL:HG11	1:A:124:TRP:CE2	2.51	0.45
1:A:183:TYR:CD1	1:B:170:HIS:HB2	2.51	0.45
1:C:261:SER:OG	1:C:262:GLU:N	2.50	0.45
1:D:328:ASN:OD1	1:D:330:ILE:HG12	2.17	0.45
1:D:338:ARG:HA	1:D:338:ARG:HD3	1.77	0.45
1:B:9:SER:HA	1:B:38:ASP:O	2.15	0.45
1:B:29:LYS:HE2	1:B:29:LYS:HB3	1.77	0.45
1:E:158:PRO:HD2	1:E:163:GLN:O	2.17	0.45
1:B:388:ARG:O	1:B:388:ARG:NE	2.29	0.45
1:D:46:ILE:HD12	1:D:46:ILE:HA	1.82	0.45
1:D:309:HIS:CD2	1:D:309:HIS:H	2.35	0.45
1:D:393:ASN:ND2	1:D:396:GLU:OE1	2.50	0.45
1:E:7:GLY:HA3	1:E:37:LEU:HD23	1.98	0.45
1:C:15:GLY:O	1:C:20:ARG:NH1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:GLY:HA2	1:F:352:LEU:HD22	1.99	0.44
1:A:382:GLY:O	1:A:386:VAL:HG23	2.18	0.44
1:D:363:SER:O	1:D:367:ILE:HG13	2.18	0.44
1:E:397:PHE:CZ	1:E:401:LEU:HD21	2.52	0.44
1:F:15:GLY:O	1:F:20:ARG:NH1	2.48	0.44
1:B:17:GLU:CD	1:B:76:ILE:HD11	2.43	0.44
1:C:275:ASP:OD2	1:D:212:LYS:NZ	2.51	0.44
1:E:112:ILE:HB	1:E:290:MET:HB3	2.00	0.44
1:E:397:PHE:O	1:E:401:LEU:HG	2.18	0.44
1:A:210:SER:HA	1:A:249:ARG:O	2.17	0.44
1:A:72:LYS:HG2	1:A:73:CYS:O	2.17	0.43
1:A:165:VAL:HG22	1:C:165:VAL:HG13	2.00	0.43
1:A:220:ASP:OD1	1:A:270:LYS:NZ	2.40	0.43
1:A:178:VAL:HG11	1:B:219:TYR:HA	2.01	0.43
1:E:167:TYR:HB3	1:F:142:THR:HG21	1.98	0.43
1:B:118:PRO:HD3	1:B:380:ILE:HG12	2.00	0.43
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.53	0.43
1:F:330:ILE:HD13	1:F:333:ILE:HD12	2.00	0.43
1:A:351:GLU:H	1:A:351:GLU:CD	2.24	0.43
1:E:212:LYS:NZ	1:F:275:ASP:OD2	2.46	0.43
1:C:11:VAL:O	1:C:70:GLY:HA2	2.18	0.43
1:D:17:GLU:HA	1:D:316:TYR:CE2	2.53	0.43
1:E:60:ALA:O	1:E:64:ILE:HG13	2.18	0.43
1:F:138:GLN:HG3	1:F:182:MET:HE1	2.01	0.43
1:D:318:MET:O	1:D:323:GLN:HB2	2.19	0.43
1:F:4:LYS:HG2	1:F:33:PRO:O	2.19	0.43
1:C:186:ASP:OD2	1:C:222:ARG:NH2	2.51	0.43
3:D:502:NAP:HO3A	3:D:502:NAP:P2B	2.41	0.43
1:E:183:TYR:CD1	1:F:170:HIS:HB2	2.53	0.43
1:B:23:TRP:CD2	1:B:73:CYS:HB2	2.54	0.43
1:D:372:MET:HB3	1:D:376:LEU:HB2	2.01	0.42
1:D:59:ASP:O	1:D:63:ALA:N	2.50	0.42
1:B:15:GLY:N	1:B:73:CYS:HB3	2.34	0.42
1:F:338:ARG:HD3	1:F:338:ARG:HA	1.75	0.42
1:D:8:GLY:N	1:D:37:LEU:HD23	2.35	0.42
1:F:218:LYS:HA	1:F:218:LYS:HD3	1.74	0.42
1:A:388:ARG:NH1	1:A:391:TYR:O	2.53	0.42
1:B:22:ILE:O	1:B:26:ILE:HG13	2.19	0.42
3:B:502:NAP:HO3A	3:B:502:NAP:P2B	2.41	0.42
1:F:344:ALA:HB2	1:F:352:LEU:HB3	2.00	0.42
1:D:78:PRO:CG	1:D:92:TRP:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:THR:HB	1:B:73:CYS:SG	2.60	0.42
1:B:319:TYR:HB2	1:B:325:THR:HG21	2.01	0.42
1:C:231:TYR:O	1:C:236:LYS:HB2	2.20	0.42
1:F:68:ASN:HA	1:F:302:THR:HG23	2.02	0.42
1:A:212:LYS:NZ	1:A:252:ASP:OD1	2.44	0.42
1:D:16:ASP:HB2	1:D:76:ILE:HG13	2.02	0.42
1:F:24:GLU:O	1:F:28:GLU:HG3	2.20	0.42
1:D:140:ARG:HD3	1:D:140:ARG:HA	1.71	0.42
1:D:75:THR:O	3:D:502:NAP:H2N	2.20	0.41
1:D:118:PRO:HD3	1:D:380:ILE:HG12	2.01	0.41
1:E:293:SER:HB3	1:E:306:GLU:HG3	2.02	0.41
1:C:338:ARG:HD3	1:C:338:ARG:HA	1.85	0.41
1:D:158:PRO:HD2	1:D:163:GLN:O	2.19	0.41
1:C:100:ARG:NH2	4:C:503:AKG:O1	2.47	0.41
1:A:372:MET:HE3	1:A:372:MET:HB3	1.86	0.41
1:C:75:THR:O	3:C:502:NAP:H2N	2.21	0.41
1:A:109:ARG:HA	1:A:292:THR:O	2.20	0.41
1:C:109:ARG:HA	1:C:292:THR:O	2.21	0.41
1:C:158:PRO:HD2	1:C:163:GLN:O	2.20	0.41
1:F:132:ARG:O	1:F:132:ARG:HG3	2.20	0.41
1:D:239:PHE:CD2	1:D:244:ILE:HG13	2.56	0.41
1:A:219:TYR:HB2	1:B:143:ASP:HB2	2.03	0.41
1:B:121:VAL:HG11	1:B:124:TRP:CE2	2.56	0.41
1:E:207:LEU:O	1:E:246:TYR:HA	2.21	0.41
1:E:328:ASN:HA	1:E:329:PRO:HD3	1.93	0.41
1:A:13:MET:HE3	1:A:72:LYS:HB2	2.02	0.41
1:C:15:GLY:HA3	1:C:74:ALA:O	2.21	0.41
1:D:57:THR:HG21	1:D:95:PRO:HA	2.03	0.41
1:D:197:PHE:HB3	1:D:235:TYR:CD2	2.56	0.41
1:E:21:ILE:H	1:E:21:ILE:HG12	1.67	0.41
1:B:7:GLY:HA2	1:B:352:LEU:HD22	2.02	0.41
1:D:19:THR:HA	1:D:22:ILE:HB	2.02	0.41
1:E:72:LYS:HG2	1:E:73:CYS:O	2.20	0.41
1:F:6:SER:O	1:F:349:ASN:ND2	2.53	0.41
1:F:132:ARG:NH1	1:F:275:ASP:HB2	2.36	0.41
1:A:218:LYS:HB3	1:B:145:VAL:HG23	2.03	0.40
1:B:9:SER:OG	1:B:38:ASP:OD2	2.32	0.40
1:D:79:ASP:O	1:D:83:VAL:HG23	2.21	0.40
1:D:123:GLY:O	1:D:262:GLU:HA	2.21	0.40
1:E:72:LYS:HZ3	1:E:75:THR:HG23	1.85	0.40
1:E:83:VAL:HG21	1:E:91:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TRP:CD2	1:A:73:CYS:HB2	2.56	0.40
1:C:200:ALA:HA	1:C:266:ILE:HG13	2.03	0.40
1:D:372:MET:HB2	1:D:372:MET:HE3	1.79	0.40
1:A:165:VAL:HG13	1:C:165:VAL:HG22	2.03	0.40
1:C:123:GLY:O	1:C:262:GLU:HA	2.21	0.40
1:E:25:LEU:HD23	1:E:25:LEU:HA	1.94	0.40
1:E:388:ARG:NH1	1:E:391:TYR:O	2.54	0.40
1:D:60:ALA:HA	1:D:63:ALA:HB3	2.02	0.40
1:D:394:THR:O	1:D:398:MET:HG2	2.22	0.40
1:E:23:TRP:CD2	1:E:73:CYS:HB2	2.57	0.40
1:F:409:LEU:HD23	1:F:409:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/425 (97%)	404 (98%)	8 (2%)	0	100	100
1	B	412/425 (97%)	398 (97%)	14 (3%)	0	100	100
1	C	409/425 (96%)	401 (98%)	8 (2%)	0	100	100
1	D	410/425 (96%)	397 (97%)	13 (3%)	0	100	100
1	E	412/425 (97%)	397 (96%)	15 (4%)	0	100	100
1	F	411/425 (97%)	399 (97%)	12 (3%)	0	100	100
All	All	2466/2550 (97%)	2396 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	339/361 (94%)	328 (97%)	11 (3%)	34	49
1	B	336/361 (93%)	324 (96%)	12 (4%)	31	44
1	C	342/361 (95%)	329 (96%)	13 (4%)	29	42
1	D	325/361 (90%)	309 (95%)	16 (5%)	22	31
1	E	339/361 (94%)	329 (97%)	10 (3%)	37	52
1	F	346/361 (96%)	333 (96%)	13 (4%)	29	42
All	All	2027/2166 (94%)	1952 (96%)	75 (4%)	30	43

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	69	VAL
1	A	140	ARG
1	A	160	ASP
1	A	212	LYS
1	A	280	SER
1	A	303	VAL
1	A	312	VAL
1	A	372	MET
1	A	389	SER
1	A	414	LEU
1	B	19	THR
1	B	83	VAL
1	B	122	SER
1	B	165	VAL
1	B	174	GLU
1	B	280	SER
1	B	290	MET
1	B	312	VAL
1	B	362	VAL
1	B	367	ILE
1	B	388	ARG

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Mol	Chain	Res	Type
1	B	392	LEU
1	C	160	ASP
1	C	163	GLN
1	C	171	ASN
1	C	210	SER
1	C	250	LEU
1	C	252	ASP
1	C	303	VAL
1	C	304	GLU
1	C	312	VAL
1	C	347	ASP
1	C	363	SER
1	C	381	LYS
1	C	389	SER
1	D	35	VAL
1	D	46	ILE
1	D	116	ASN
1	D	160	ASP
1	D	287	SER
1	D	302	THR
1	D	303	VAL
1	D	304	GLU
1	D	312	VAL
1	D	314	ARG
1	D	316	TYR
1	D	345	LYS
1	D	363	SER
1	D	387	GLN
1	D	388	ARG
1	D	389	SER
1	E	6	SER
1	E	94	SER
1	E	132	ARG
1	E	173	GLU
1	E	212	LYS
1	E	280	SER
1	E	303	VAL
1	E	312	VAL
1	E	363	SER
1	E	414	LEU
1	F	19	THR
1	F	29	LYS

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Mol	Chain	Res	Type
1	F	132	ARG
1	F	165	VAL
1	F	171	ASN
1	F	247	GLU
1	F	291	MET
1	F	312	VAL
1	F	348	ASN
1	F	351	GLU
1	F	386	VAL
1	F	388	ARG
1	F	414	LEU

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	171	ASN
1	A	213	ASN
1	A	357	ASN
1	B	67	HIS
1	B	68	ASN
1	B	213	ASN
1	B	238	GLN
1	C	48	ASN
1	C	67	HIS
1	C	68	ASN
1	C	228	GLN
1	C	238	GLN
1	C	320	GLN
1	D	14	GLN
1	D	68	ASN
1	D	96	ASN
1	D	277	GLN
1	E	14	GLN
1	E	67	HIS
1	E	385	ASN
1	F	101	ASN
1	F	198	GLN
1	F	238	GLN
1	F	277	GLN
1	F	320	GLN
1	F	357	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
3	NAP	A	502	-	50,52,52	1.66	4 (8%)	71,80,80	1.49	9 (12%)
3	NAP	B	502	-	50,52,52	1.71	7 (14%)	71,80,80	1.50	10 (14%)
4	AKG	E	503	2	9,9,9	1.81	1 (11%)	11,11,11	1.82	2 (18%)
3	NAP	E	502	-	50,52,52	1.68	4 (8%)	71,80,80	1.59	9 (12%)
4	AKG	D	503	2	9,9,9	1.81	1 (11%)	11,11,11	1.84	4 (36%)
3	NAP	D	502	-	50,52,52	1.69	7 (14%)	71,80,80	1.57	14 (19%)
3	NAP	F	502	-	50,52,52	1.74	6 (12%)	71,80,80	1.47	9 (12%)
4	AKG	F	503	2	9,9,9	1.82	1 (11%)	11,11,11	1.83	3 (27%)
3	NAP	C	502	-	50,52,52	1.63	4 (8%)	71,80,80	1.61	16 (22%)
4	AKG	C	503	2	9,9,9	1.75	1 (11%)	11,11,11	1.84	4 (36%)
4	AKG	B	503	2	9,9,9	1.83	1 (11%)	11,11,11	1.73	2 (18%)
4	AKG	A	503	2	9,9,9	1.73	1 (11%)	11,11,11	1.71	4 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	502	-	-	12/35/67/67	0/5/5/5
3	NAP	B	502	-	-	16/35/67/67	0/5/5/5
4	AKG	E	503	2	-	0/9/9/9	-
3	NAP	E	502	-	-	10/35/67/67	0/5/5/5
4	AKG	D	503	2	-	1/9/9/9	-
3	NAP	D	502	-	-	14/35/67/67	0/5/5/5
3	NAP	F	502	-	-	11/35/67/67	0/5/5/5
4	AKG	F	503	2	-	0/9/9/9	-
3	NAP	C	502	-	-	9/35/67/67	0/5/5/5
4	AKG	C	503	2	-	0/9/9/9	-
4	AKG	B	503	2	-	0/9/9/9	-
4	AKG	A	503	2	-	0/9/9/9	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	NAP	O7N-C7N	9.55	1.41	1.24
3	A	502	NAP	O7N-C7N	9.27	1.41	1.24
3	B	502	NAP	O7N-C7N	9.15	1.41	1.24
3	D	502	NAP	O7N-C7N	9.15	1.41	1.24
3	F	502	NAP	O7N-C7N	9.09	1.41	1.24
3	C	502	NAP	O7N-C7N	8.98	1.40	1.24
4	B	503	AKG	C2-C1	-4.64	1.46	1.53
4	D	503	AKG	C2-C1	-4.61	1.46	1.53
4	F	503	AKG	C2-C1	-4.61	1.46	1.53
4	E	503	AKG	C2-C1	-4.49	1.46	1.53
4	C	503	AKG	C2-C1	-4.39	1.46	1.53
4	A	503	AKG	C2-C1	-4.23	1.47	1.53
3	F	502	NAP	PA-O3	3.34	1.63	1.59
3	F	502	NAP	PN-O3	3.21	1.63	1.59
3	D	502	NAP	C8A-N7A	2.84	1.37	1.31
3	A	502	NAP	C2A-N3A	2.80	1.38	1.33
3	C	502	NAP	C8A-N7A	2.65	1.36	1.31
3	B	502	NAP	PA-O3	2.65	1.62	1.59
3	E	502	NAP	C2A-N3A	2.62	1.38	1.33
3	D	502	NAP	C2A-N3A	2.61	1.38	1.33
3	B	502	NAP	C2A-N3A	2.60	1.38	1.33
3	C	502	NAP	C2A-N3A	2.53	1.38	1.33
3	E	502	NAP	C8A-N7A	2.48	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAP	C2A-N1A	2.48	1.38	1.33
3	E	502	NAP	C2A-N1A	2.47	1.38	1.33
3	F	502	NAP	C2A-N3A	2.46	1.38	1.33
3	A	502	NAP	C2A-N1A	2.45	1.38	1.33
3	A	502	NAP	C8A-N7A	2.45	1.36	1.31
3	C	502	NAP	C2N-N1N	2.43	1.37	1.35
3	B	502	NAP	C2A-N1A	2.41	1.38	1.33
3	F	502	NAP	C2A-N1A	2.38	1.38	1.33
3	B	502	NAP	PN-O3	2.32	1.62	1.59
3	B	502	NAP	C5A-N7A	-2.30	1.34	1.39
3	D	502	NAP	PA-O3	2.27	1.61	1.59
3	D	502	NAP	PN-O3	2.12	1.61	1.59
3	F	502	NAP	C8A-N7A	2.11	1.35	1.31
3	D	502	NAP	C2N-N1N	2.08	1.37	1.35
3	B	502	NAP	C8A-N7A	2.06	1.35	1.31

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAP	C5A-C4A-N3A	-5.61	118.99	126.72
3	C	502	NAP	C5A-C4A-N3A	-5.58	119.04	126.72
3	F	502	NAP	N3A-C2A-N1A	-5.43	120.37	128.58
3	E	502	NAP	N3A-C2A-N1A	-5.33	120.51	128.58
3	E	502	NAP	C5A-C4A-N3A	-5.18	119.58	126.72
3	A	502	NAP	C5A-C4A-N3A	-5.15	119.62	126.72
3	D	502	NAP	C5A-C4A-N3A	-5.13	119.65	126.72
3	B	502	NAP	N3A-C2A-N1A	-5.05	120.93	128.58
3	A	502	NAP	N3A-C2A-N1A	-5.05	120.94	128.58
3	D	502	NAP	N3A-C2A-N1A	-5.01	121.00	128.58
3	F	502	NAP	C5A-C4A-N3A	-4.85	120.04	126.72
3	C	502	NAP	N3A-C2A-N1A	-4.68	121.49	128.58
3	C	502	NAP	C3N-C7N-N7N	3.70	122.30	117.74
3	E	502	NAP	C2A-N3A-C4A	3.67	120.80	111.83
3	B	502	NAP	C2A-N3A-C4A	3.67	120.79	111.83
3	F	502	NAP	C2A-N3A-C4A	3.64	120.72	111.83
4	E	503	AKG	O1-C1-C2	-3.62	117.31	121.81
3	E	502	NAP	N9A-C8A-N7A	-3.62	108.80	113.94
3	A	502	NAP	C2A-N3A-C4A	3.58	120.58	111.83
3	C	502	NAP	C2A-N3A-C4A	3.52	120.42	111.83
4	F	503	AKG	O1-C1-C2	-3.51	117.44	121.81
3	D	502	NAP	C2A-N3A-C4A	3.50	120.39	111.83
3	B	502	NAP	N3A-C4A-N9A	3.45	133.03	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	AKG	O1-C1-C2	-3.28	117.73	121.81
3	E	502	NAP	C5A-N7A-C8A	3.27	108.59	103.45
3	E	502	NAP	N3A-C4A-N9A	3.25	132.70	127.17
3	A	502	NAP	N3A-C4A-N9A	3.21	132.62	127.17
3	A	502	NAP	N9A-C8A-N7A	-3.17	109.44	113.94
3	C	502	NAP	O2A-PA-O3	3.17	115.83	107.27
4	D	503	AKG	O1-C1-C2	-3.15	117.89	121.81
3	C	502	NAP	N3A-C4A-N9A	3.12	132.47	127.17
3	F	502	NAP	N9A-C8A-N7A	-3.07	109.58	113.94
4	C	503	AKG	O1-C1-C2	-2.98	118.10	121.81
3	D	502	NAP	C4D-O4D-C1D	2.96	112.64	109.92
3	D	502	NAP	O2A-PA-O3	2.92	115.17	107.27
3	A	502	NAP	C5A-N7A-C8A	2.92	108.04	103.45
3	F	502	NAP	C5A-N7A-C8A	2.90	108.00	103.45
3	F	502	NAP	N3A-C4A-N9A	2.85	132.01	127.17
3	A	502	NAP	O2B-C2B-C1B	-2.81	100.17	110.05
3	E	502	NAP	O2B-C2B-C1B	-2.75	100.39	110.05
3	B	502	NAP	C5A-N7A-C8A	2.73	107.75	103.45
4	E	503	AKG	O2-C1-C2	2.72	121.12	113.59
3	C	502	NAP	C5A-N7A-C8A	2.68	107.66	103.45
3	D	502	NAP	N3A-C4A-N9A	2.67	131.71	127.17
3	C	502	NAP	N9A-C8A-N7A	-2.65	110.17	113.94
3	E	502	NAP	C2B-C1B-N9A	-2.65	109.39	113.75
3	D	502	NAP	C5A-N7A-C8A	2.60	107.54	103.45
3	D	502	NAP	C5A-C4A-N9A	2.59	108.63	105.81
4	F	503	AKG	C3-C4-C5	-2.57	106.85	113.67
4	B	503	AKG	O2-C1-C2	2.57	120.71	113.59
3	D	502	NAP	N9A-C8A-N7A	-2.54	110.33	113.94
4	F	503	AKG	O2-C1-C2	2.54	120.62	113.59
4	C	503	AKG	C4-C3-C2	-2.53	108.17	112.91
3	F	502	NAP	O2A-PA-O3	2.51	114.06	107.27
3	E	502	NAP	C4A-C5A-N7A	-2.48	107.74	110.58
4	D	503	AKG	O2-C1-C2	2.47	120.43	113.59
3	C	502	NAP	C4A-C5A-N7A	-2.46	107.76	110.58
3	D	502	NAP	C4A-C5A-N7A	-2.45	107.78	110.58
4	C	503	AKG	C3-C2-C1	2.45	120.03	115.86
3	C	502	NAP	C5A-C4A-N9A	2.45	108.48	105.81
3	D	502	NAP	C6N-N1N-C2N	-2.45	119.79	121.88
3	B	502	NAP	N9A-C8A-N7A	-2.44	110.47	113.94
4	A	503	AKG	O1-C1-C2	-2.40	118.83	121.81
3	D	502	NAP	O4D-C4D-C5D	-2.36	101.78	109.33
4	A	503	AKG	C4-C3-C2	-2.35	108.49	112.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAP	C6N-N1N-C2N	-2.35	119.88	121.88
3	F	502	NAP	C4A-C5A-N7A	-2.34	107.91	110.58
3	C	502	NAP	C4D-O4D-C1D	2.33	112.06	109.92
4	D	503	AKG	C3-C2-C1	2.32	119.80	115.86
3	C	502	NAP	O2B-C2B-C1B	-2.32	101.91	110.05
4	C	503	AKG	O2-C1-C2	2.31	120.00	113.59
4	A	503	AKG	O2-C1-C2	2.28	119.91	113.59
4	A	503	AKG	C3-C2-C1	2.26	119.71	115.86
3	A	502	NAP	C4A-C5A-N7A	-2.26	107.99	110.58
3	B	502	NAP	C6A-C5A-C4A	2.25	120.25	117.18
3	C	502	NAP	C6A-C5A-C4A	2.25	120.24	117.18
3	D	502	NAP	C3N-C7N-N7N	2.24	120.50	117.74
4	D	503	AKG	C4-C3-C2	-2.21	108.75	112.91
3	D	502	NAP	O2B-C2B-C1B	-2.17	102.41	110.05
3	A	502	NAP	O4B-C1B-N9A	2.12	112.16	108.09
3	B	502	NAP	C4A-C5A-N7A	-2.11	108.17	110.58
3	F	502	NAP	C2B-C1B-N9A	-2.04	110.39	113.75
3	C	502	NAP	O7N-C7N-C3N	-2.04	117.11	119.60
3	B	502	NAP	C5N-C4N-C3N	-2.04	118.36	120.36
3	B	502	NAP	C6N-N1N-C2N	-2.02	120.16	121.88
3	C	502	NAP	C2B-C1B-N9A	-2.01	110.45	113.75

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAP	C5D-O5D-PN-O3
3	A	502	NAP	C5D-O5D-PN-O2N
3	A	502	NAP	O4D-C1D-N1N-C2N
3	A	502	NAP	O4D-C1D-N1N-C6N
3	B	502	NAP	C5B-O5B-PA-O1A
3	B	502	NAP	C5B-O5B-PA-O2A
3	B	502	NAP	C5D-O5D-PN-O3
3	B	502	NAP	C5D-O5D-PN-O1N
3	B	502	NAP	C5D-O5D-PN-O2N
3	B	502	NAP	O4D-C1D-N1N-C2N
3	B	502	NAP	O4D-C1D-N1N-C6N
3	B	502	NAP	C2D-C1D-N1N-C2N
3	C	502	NAP	C5B-O5B-PA-O3
3	C	502	NAP	O4D-C1D-N1N-C2N
3	C	502	NAP	O4D-C1D-N1N-C6N
3	C	502	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	C	502	NAP	C2D-C1D-N1N-C6N
3	D	502	NAP	O4B-C4B-C5B-O5B
3	D	502	NAP	O4D-C1D-N1N-C2N
3	D	502	NAP	O4D-C1D-N1N-C6N
3	D	502	NAP	C2D-C1D-N1N-C2N
3	D	502	NAP	C2D-C1D-N1N-C6N
3	E	502	NAP	O4D-C1D-N1N-C2N
3	E	502	NAP	O4D-C1D-N1N-C6N
3	E	502	NAP	C2D-C1D-N1N-C2N
3	F	502	NAP	C5D-O5D-PN-O3
3	F	502	NAP	C5D-O5D-PN-O2N
3	F	502	NAP	O4D-C1D-N1N-C2N
3	F	502	NAP	O4D-C1D-N1N-C6N
3	A	502	NAP	O4B-C4B-C5B-O5B
3	E	502	NAP	O4B-C4B-C5B-O5B
3	D	502	NAP	C3B-C4B-C5B-O5B
3	A	502	NAP	C3B-C2B-O2B-P2B
3	B	502	NAP	C3B-C2B-O2B-P2B
3	E	502	NAP	C3B-C4B-C5B-O5B
3	A	502	NAP	C1B-C2B-O2B-P2B
3	B	502	NAP	C1B-C2B-O2B-P2B
3	D	502	NAP	C1B-C2B-O2B-P2B
3	E	502	NAP	C1B-C2B-O2B-P2B
3	C	502	NAP	C1B-C2B-O2B-P2B
3	B	502	NAP	O4B-C4B-C5B-O5B
3	A	502	NAP	C3B-C4B-C5B-O5B
3	B	502	NAP	PA-O3-PN-O5D
3	D	502	NAP	PA-O3-PN-O5D
3	A	502	NAP	PN-O3-PA-O2A
3	D	502	NAP	PN-O3-PA-O2A
3	E	502	NAP	PN-O3-PA-O2A
3	A	502	NAP	C5D-O5D-PN-O1N
3	B	502	NAP	C5B-O5B-PA-O3
3	C	502	NAP	C5B-O5B-PA-O1A
3	C	502	NAP	C5B-O5B-PA-O2A
3	F	502	NAP	C5B-O5B-PA-O1A
3	F	502	NAP	C5B-O5B-PA-O2A
3	F	502	NAP	C5B-O5B-PA-O3
3	F	502	NAP	C5D-O5D-PN-O1N
3	D	502	NAP	C3B-C2B-O2B-P2B
3	B	502	NAP	PN-O3-PA-O2A
3	F	502	NAP	PN-O3-PA-O1A

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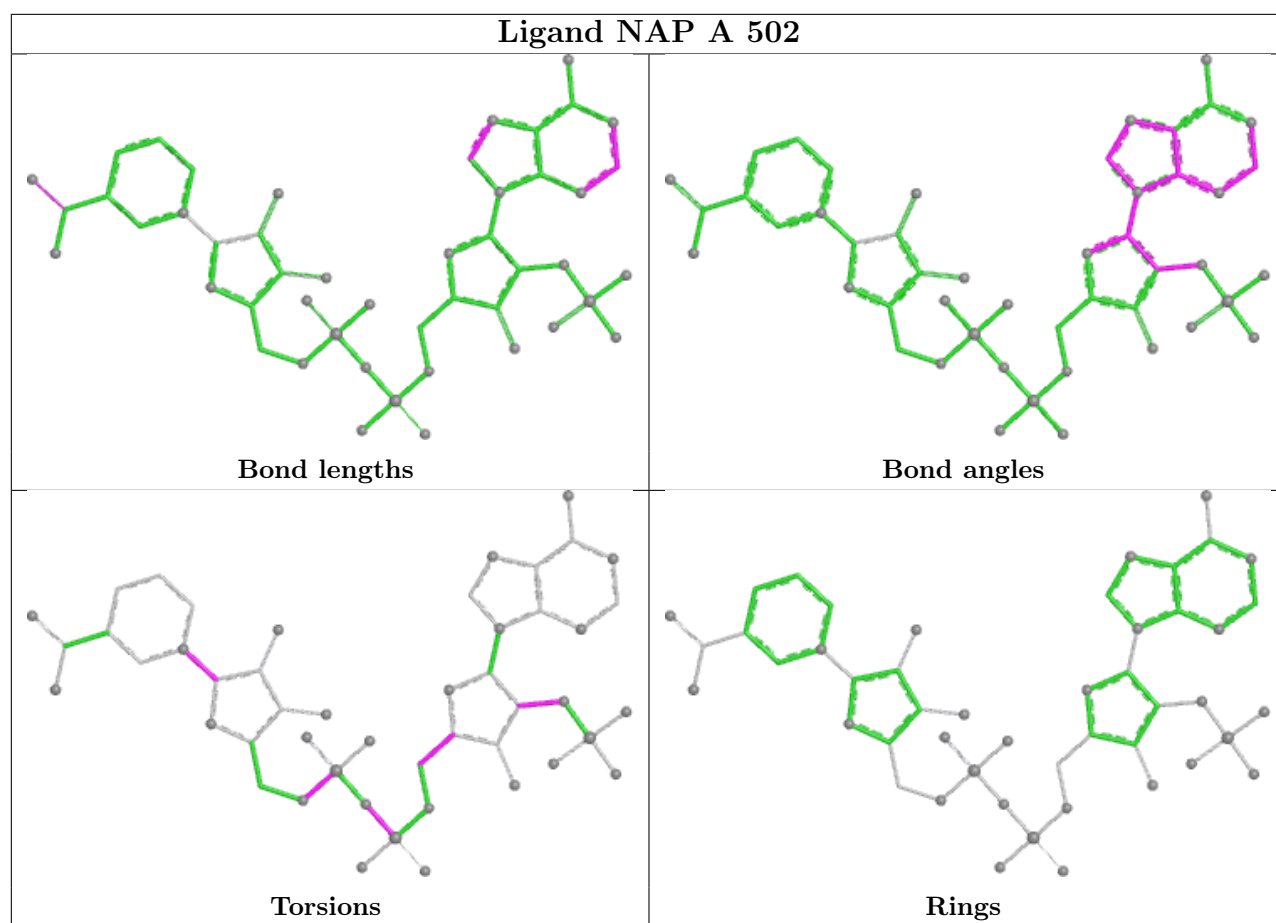
Mol	Chain	Res	Type	Atoms
4	D	503	AKG	C2-C3-C4-C5
3	A	502	NAP	C2D-C1D-N1N-C2N
3	B	502	NAP	C2D-C1D-N1N-C6N
3	E	502	NAP	C2D-C1D-N1N-C6N
3	F	502	NAP	C2D-C1D-N1N-C2N
3	E	502	NAP	C3B-C2B-O2B-P2B
3	C	502	NAP	C3B-C2B-O2B-P2B
3	D	502	NAP	O4D-C4D-C5D-O5D
3	A	502	NAP	PN-O3-PA-O1A
3	B	502	NAP	PN-O3-PA-O1A
3	D	502	NAP	PN-O3-PA-O1A
3	E	502	NAP	PN-O3-PA-O1A
3	D	502	NAP	C3D-C4D-C5D-O5D
3	D	502	NAP	PA-O3-PN-O1N
3	F	502	NAP	PN-O3-PA-O2A

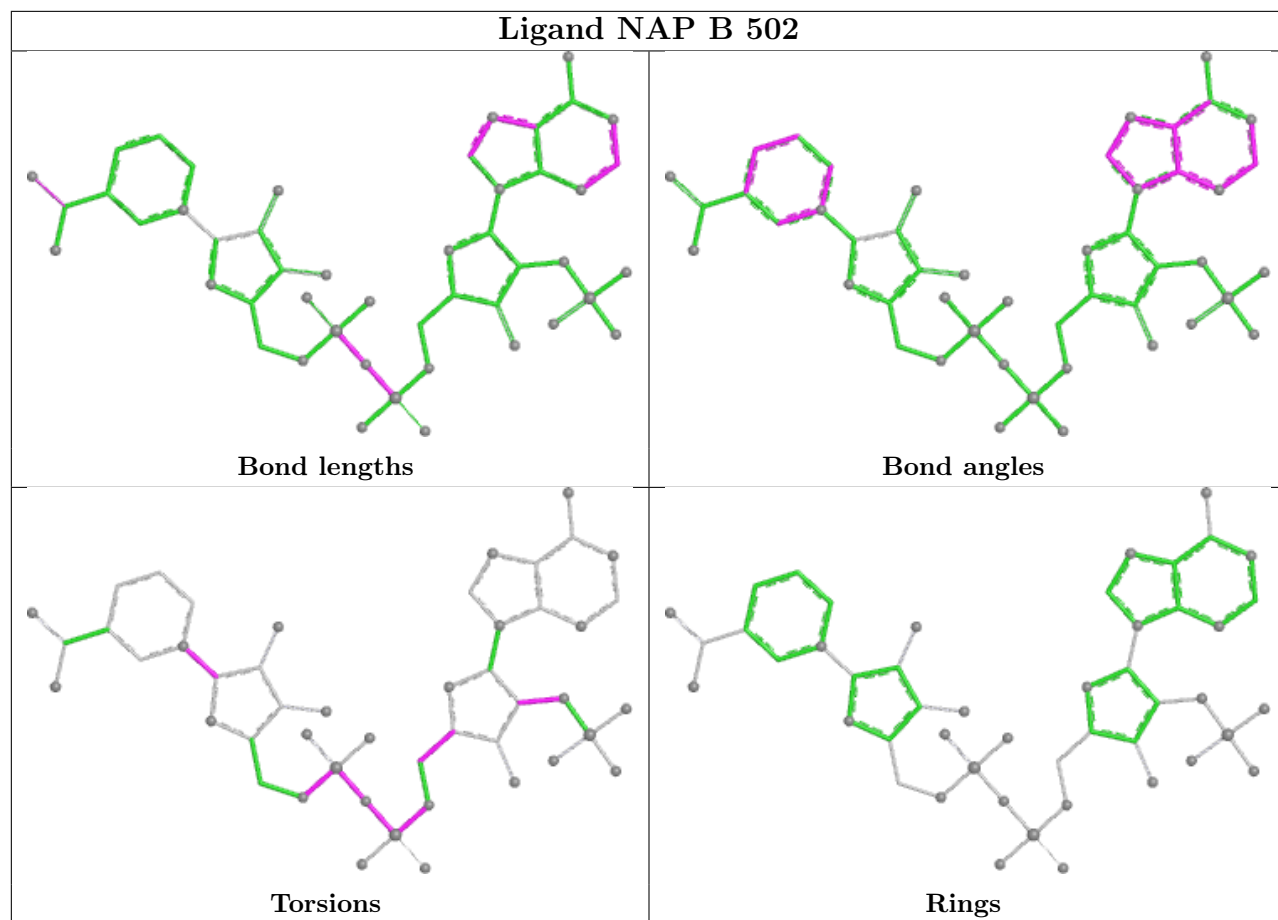
There are no ring outliers.

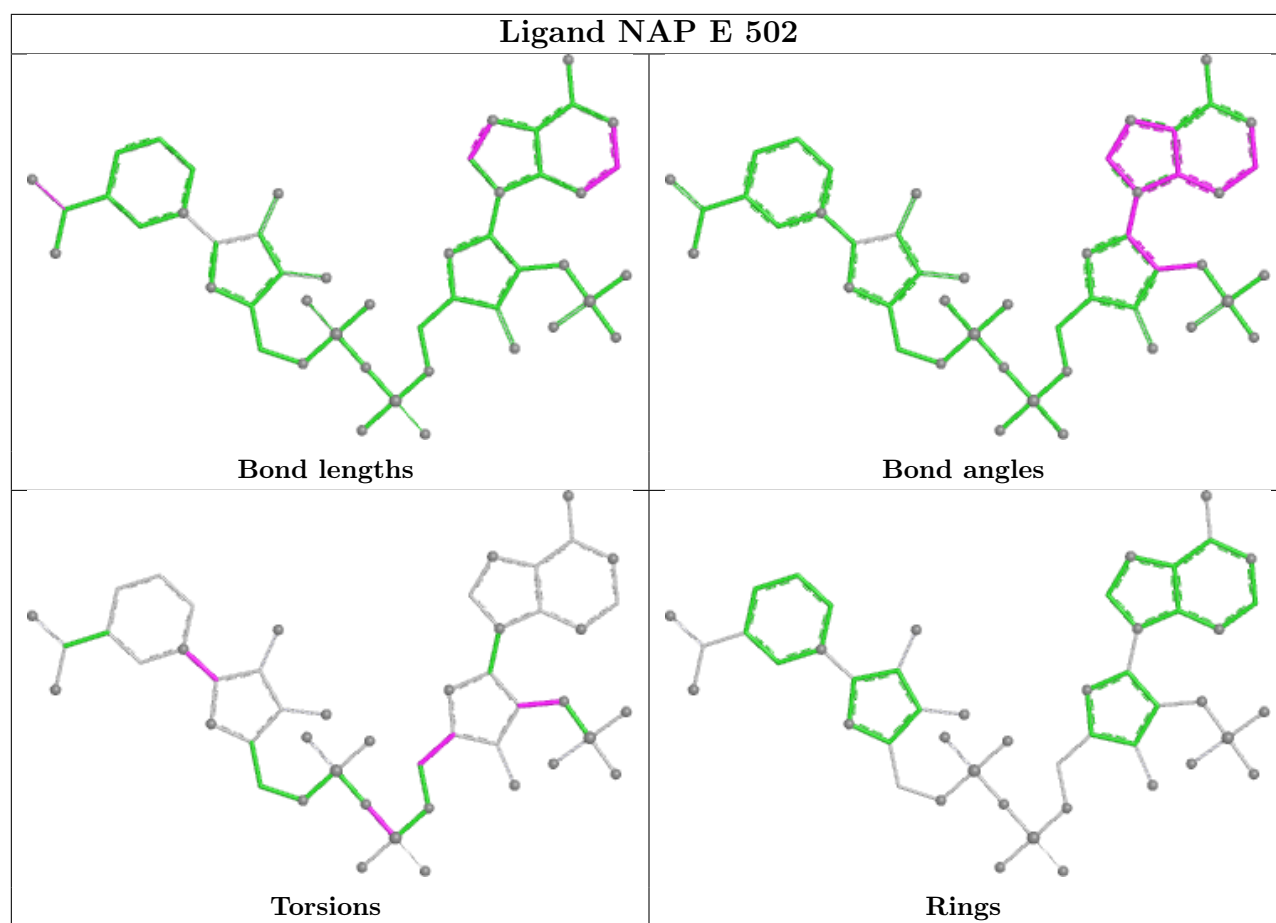
6 monomers are involved in 15 short contacts:

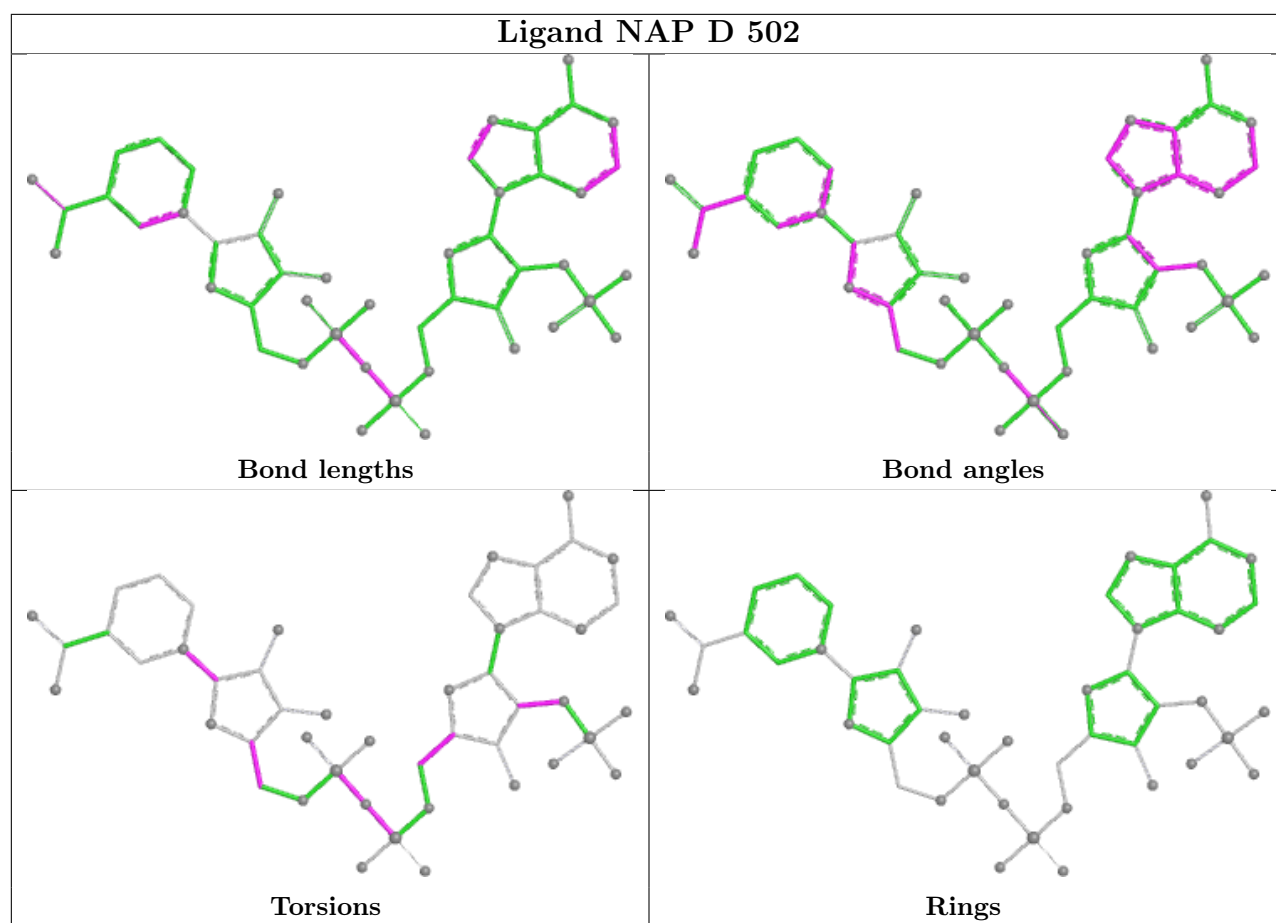
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAP	2	0
3	B	502	NAP	3	0
3	D	502	NAP	6	0
3	F	502	NAP	1	0
3	C	502	NAP	2	0
4	C	503	AKG	1	0

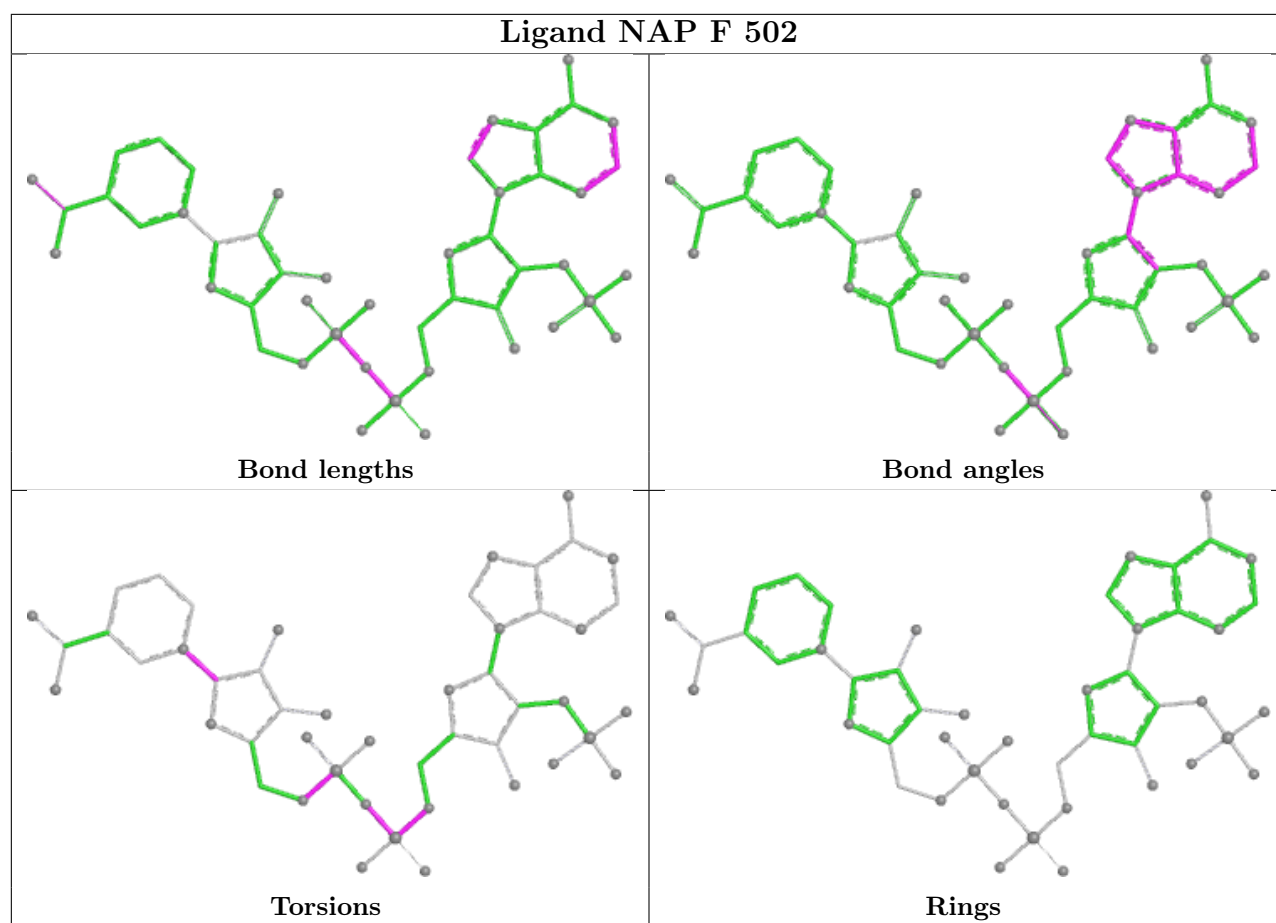
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

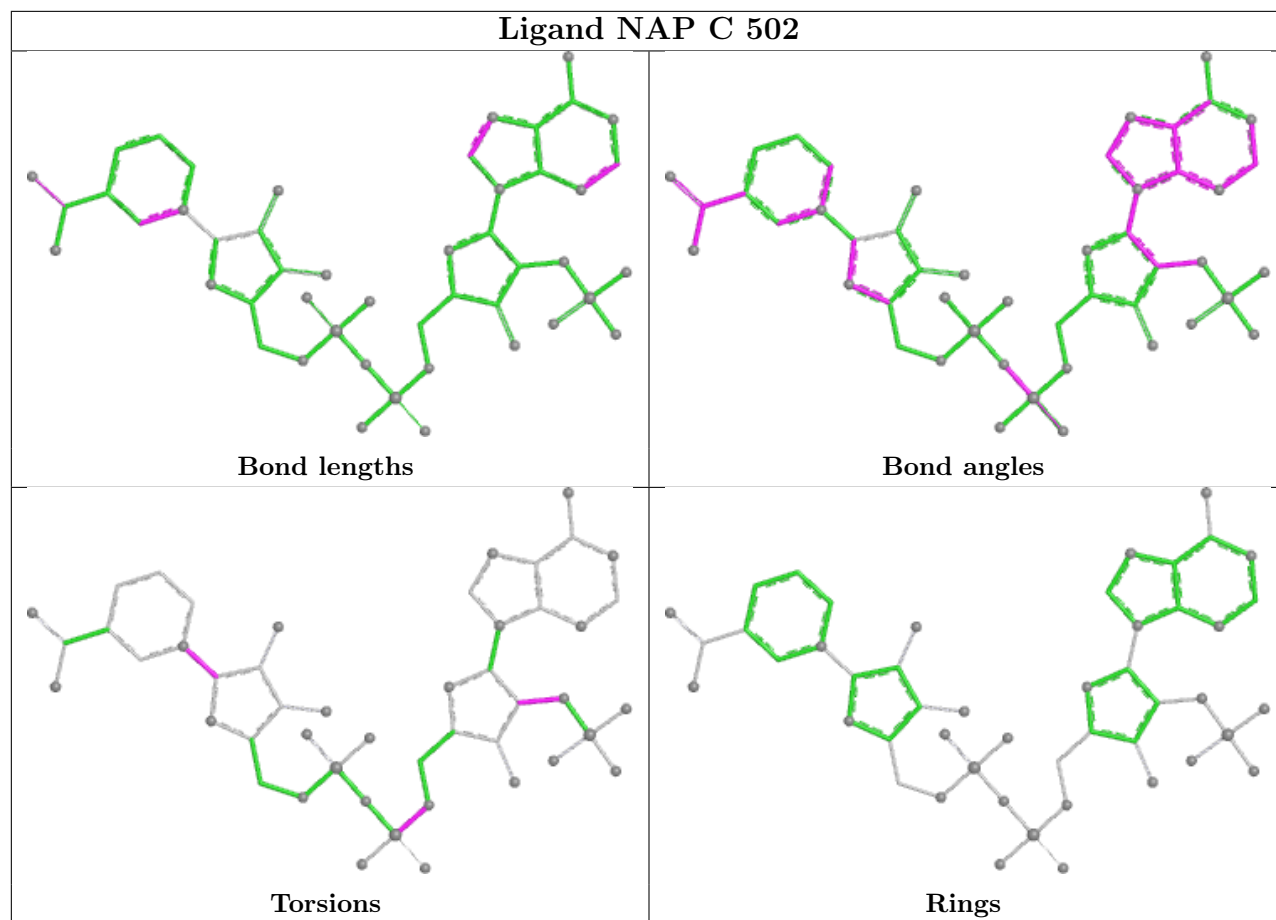












5.7 Other polymers [i](#)

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	413/425 (97%)	-0.16	2 (0%) 87 88	12, 32, 55, 67	1 (0%)
1	B	412/425 (96%)	0.08	6 (1%) 72 73	15, 40, 65, 92	2 (0%)
1	C	411/425 (96%)	-0.15	2 (0%) 87 88	15, 31, 54, 73	0
1	D	411/425 (96%)	0.51	25 (6%) 27 28	18, 45, 77, 96	1 (0%)
1	E	413/425 (97%)	0.00	6 (1%) 72 73	12, 33, 56, 65	1 (0%)
1	F	412/425 (96%)	-0.02	5 (1%) 76 78	12, 35, 58, 80	1 (0%)
All	All	2472/2550 (96%)	0.04	46 (1%) 66 68	12, 36, 62, 96	6 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	414	LEU	4.8
1	B	414	LEU	4.8
1	C	3	LYS	4.5
1	D	319	TYR	4.5
1	E	3	LYS	3.9
1	D	41	SER	3.8
1	F	299	ASP	3.7
1	A	3	LYS	3.5
1	A	415	SER	3.3
1	F	300	GLY	3.2
1	D	50	ASP	3.2
1	D	139	ASP	3.2
1	E	299	ASP	3.1
1	D	4	LYS	3.1
1	D	413	LYS	3.1
1	D	316	TYR	3.0
1	D	36	GLU	3.0
1	E	348	ASN	2.9
1	D	46	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	415	SER	2.7
1	D	18	MET	2.6
1	D	61	ALA	2.6
1	D	318	MET	2.6
1	D	322	GLY	2.5
1	B	19	THR	2.5
1	D	56	VAL	2.5
1	D	10	VAL	2.4
1	F	414	LEU	2.4
1	F	395	PHE	2.4
1	F	412	ALA	2.3
1	B	3	LYS	2.3
1	E	300	GLY	2.3
1	B	413	LYS	2.3
1	D	64	ILE	2.3
1	D	92	TRP	2.2
1	B	412	ALA	2.1
1	C	291	MET	2.1
1	D	8	GLY	2.1
1	D	140	ARG	2.1
1	D	51	ALA	2.1
1	D	5	ILE	2.1
1	E	379	CYS	2.1
1	D	346	LEU	2.1
1	D	86	PHE	2.1
1	B	321	LYS	2.0
1	D	22	ILE	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,

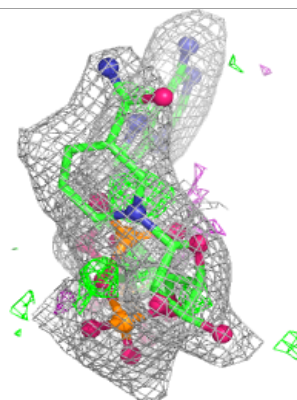
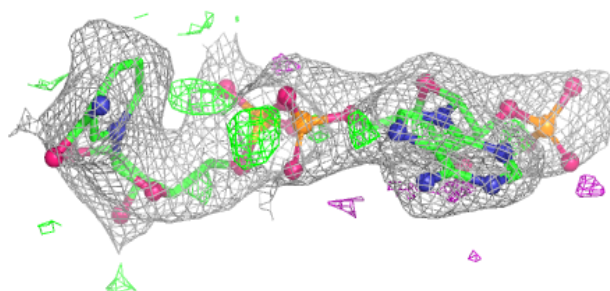
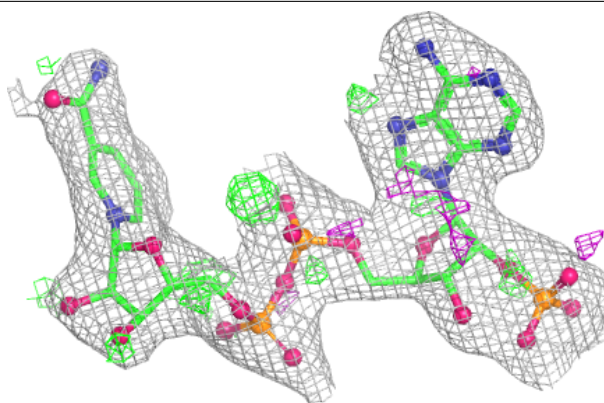
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AKG	D	503	10/10	0.82	0.18	61,69,76,76	0
4	AKG	B	503	10/10	0.85	0.14	70,77,81,82	0
4	AKG	F	503	10/10	0.86	0.12	42,61,75,77	0
4	AKG	E	503	10/10	0.88	0.11	41,51,58,62	0
4	AKG	C	503	10/10	0.89	0.10	42,48,51,52	0
4	AKG	A	503	10/10	0.91	0.08	32,42,45,48	0
3	NAP	D	502	48/48	0.93	0.10	12,35,50,111	0
2	CA	C	501	1/1	0.94	0.09	42,42,42,42	0
3	NAP	B	502	48/48	0.94	0.09	18,44,53,57	0
2	CA	B	501	1/1	0.94	0.07	49,49,49,49	0
2	CA	E	501	1/1	0.96	0.04	35,35,35,35	0
2	CA	F	501	1/1	0.96	0.04	39,39,39,39	0
3	NAP	E	502	48/48	0.96	0.06	7,23,35,74	0
3	NAP	F	502	48/48	0.96	0.07	11,37,47,54	0
3	NAP	A	502	48/48	0.96	0.06	6,20,32,60	0
3	NAP	C	502	48/48	0.97	0.06	5,19,27,41	0
2	CA	A	501	1/1	0.97	0.04	34,34,34,34	0
2	CA	D	501	1/1	0.98	0.08	55,55,55,55	0

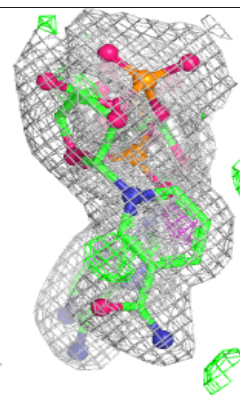
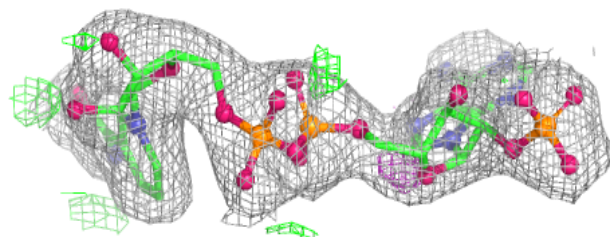
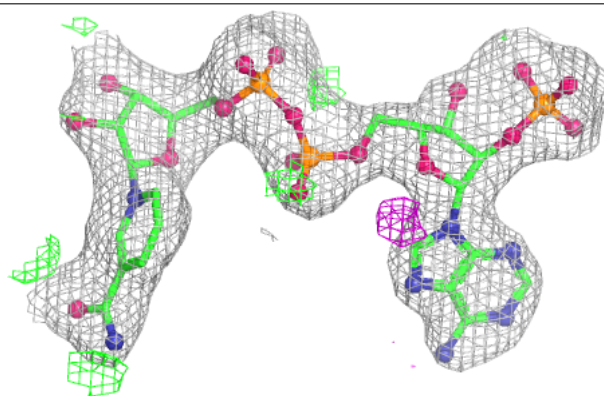
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 502:

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

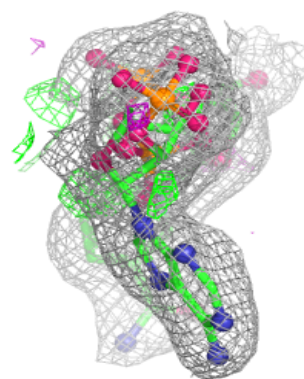
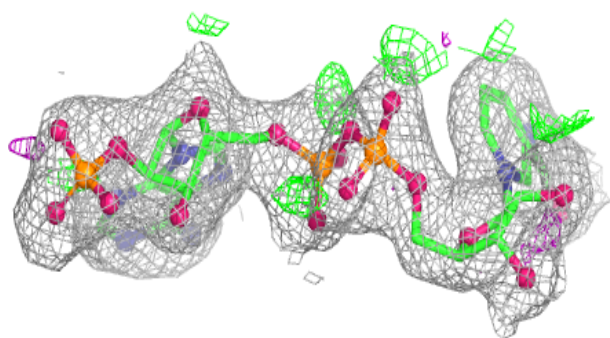
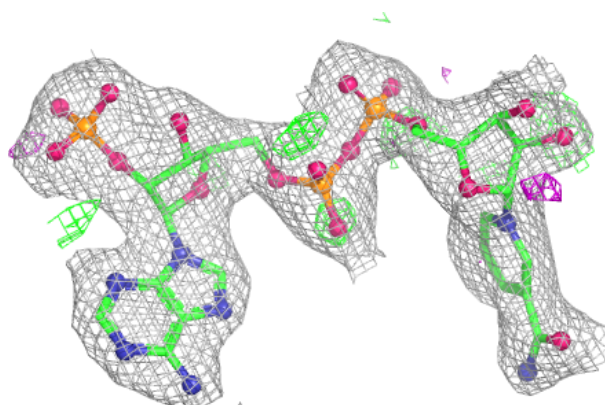
**Electron density around NAP B 502:**

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



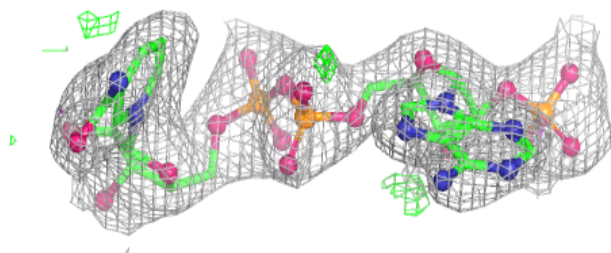
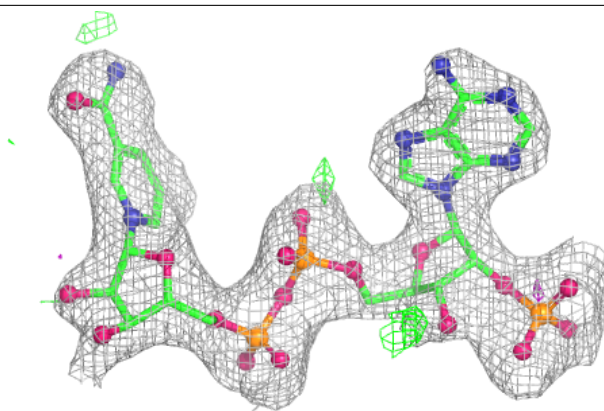
Electron density around NAP E 502:

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

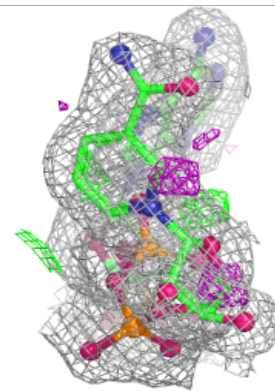
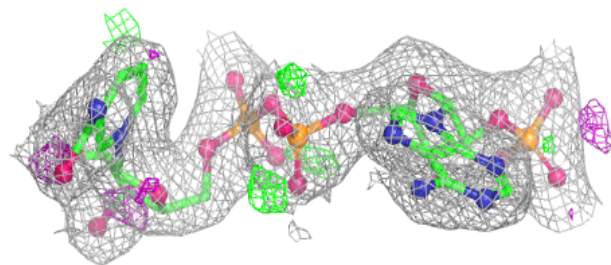
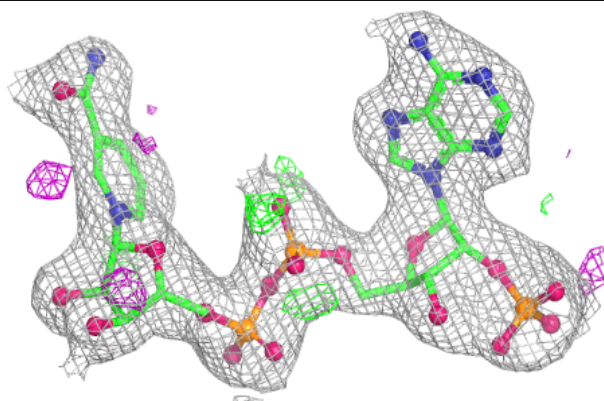


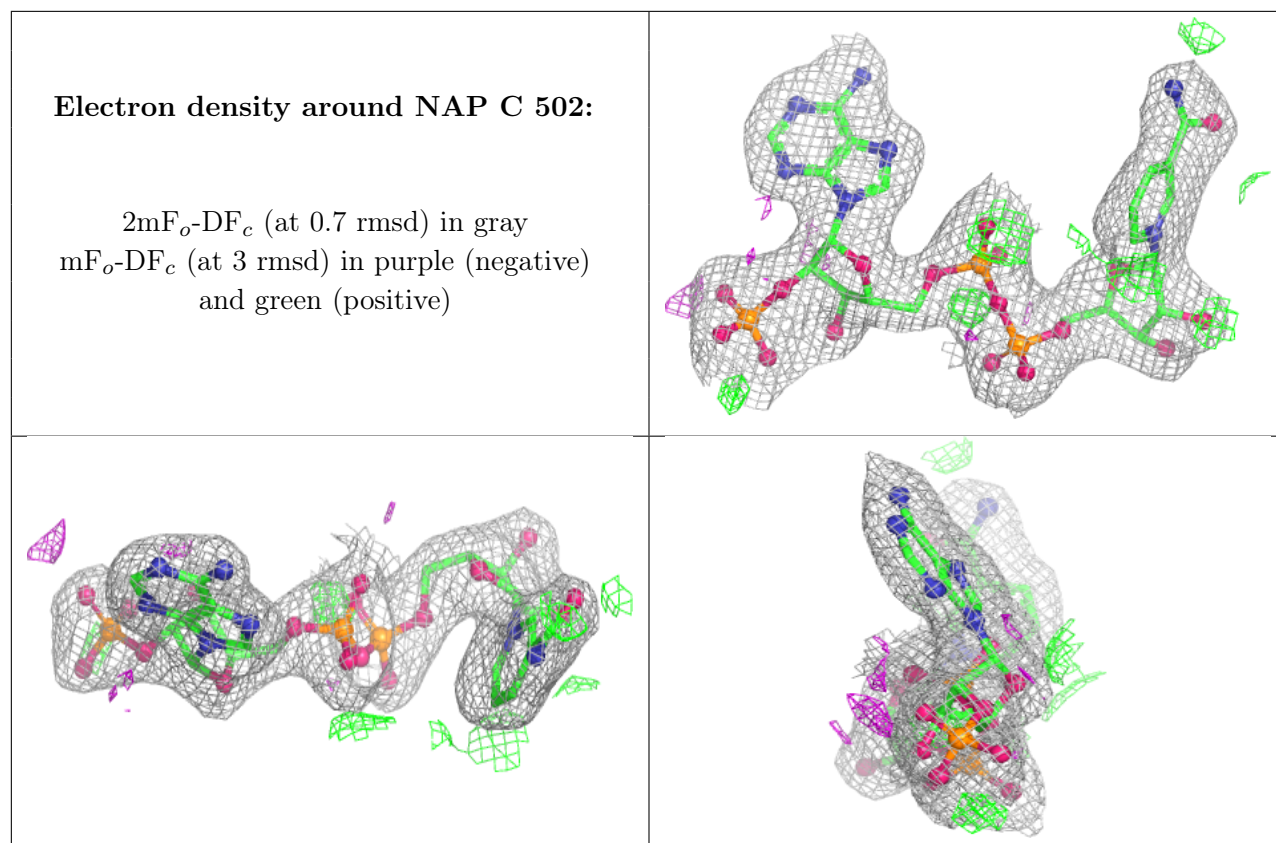
Electron density around NAP F 502:

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

**Electron density around NAP A 502:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.