Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 01:46 PM JST

PDB ID	:	5IJZ
Title	:	Crystal structure of glutamate dehydrogenase(GDH) from Corynebacterium glutamicum
Authors	:	Son, H.-F.; Kim, K.-J.
Deposited on	:	2016-03-03
Resolution	:	2.29 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 (i) 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 (i)) were used in the production of this report:

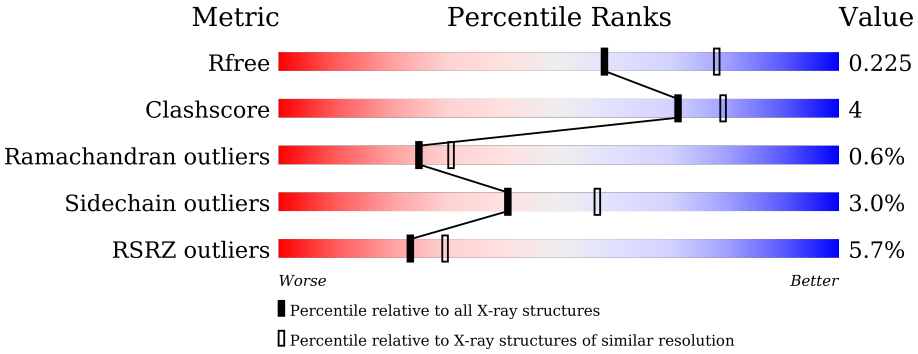
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	447	%, 90%, 10%
1	B	447	89%, 10%, •
1	C	447	89%, 9%, •
1	D	447	%, 90%, 9%, •
1	E	447	%, 91%, 9%
1	F	447	%, 89%, 10%

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Mol	Chain	Length	Quality of chain
1	G	447	%, 93%, 7%
1	H	447	3%, 91%, 8%
1	I	447	10%, 83%, 15%, •
1	J	447	33%, 85%, 13%, •
1	K	447	11%, 63%, 5%, 32%
1	L	447	5%, 86%, 13%, •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AKG	A	502	-	X	-	-
3	AKG	B	502	-	X	-	-
3	AKG	C	502	-	X	-	-
3	AKG	E	502	-	X	-	-
3	AKG	F	502	-	X	-	-
3	AKG	G	502	-	X	-	-
3	AKG	H	502	-	X	-	-
3	AKG	J	502	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 42426 atoms, of which 0 are hydrogens and 0 are deuteriums.

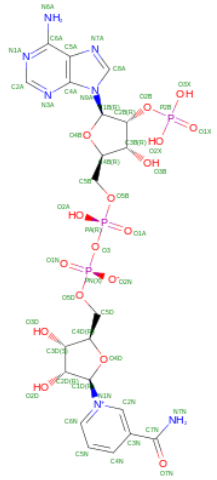
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADP-specific glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3447	2166	605	659	17	0	0	0
1	B	447	3447	2166	605	659	17	0	0	0
1	C	447	3447	2166	605	659	17	0	0	0
1	D	447	3447	2166	605	659	17	0	0	0
1	E	447	3447	2166	605	659	17	0	0	0
1	F	447	3447	2166	605	659	17	0	0	0
1	G	447	3447	2166	605	659	17	0	0	0
1	H	447	3447	2166	605	659	17	0	0	0
1	I	447	3447	2166	605	659	17	0	0	0
1	J	447	3447	2166	605	659	17	0	0	0
1	K	304	2358	1495	413	437	13	0	0	0
1	L	447	3447	2166	605	659	17	0	0	0

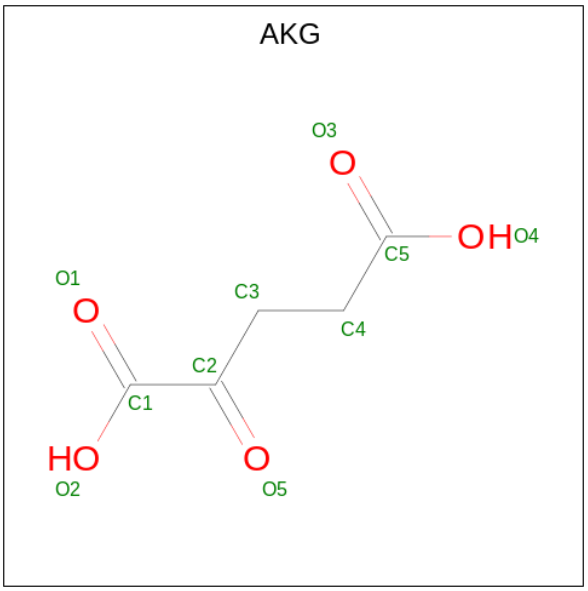
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP



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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0
3	E	1	Total C O 10 5 5	0	0
3	F	1	Total C O 10 5 5	0	0
3	G	1	Total C O 10 5 5	0	0
3	H	1	Total C O 10 5 5	0	0
3	J	1	Total C O 10 5 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	169	Total O 169 169	0	0
4	B	172	Total O 172 172	0	0
4	C	161	Total O 161 161	0	0

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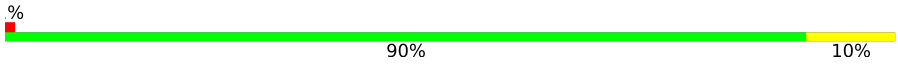
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	172	172	172	0	0
			Total	O		
4	E	160	160	160	0	0
			Total	O		
4	F	162	162	162	0	0
			Total	O		
4	G	149	149	149	0	0
			Total	O		
4	H	111	111	111	0	0
			Total	O		
4	I	107	107	107	0	0
			Total	O		
4	J	68	68	68	0	0
			Total	O		
4	K	66	66	66	0	0
			Total	O		
4	L	132	132	132	0	0

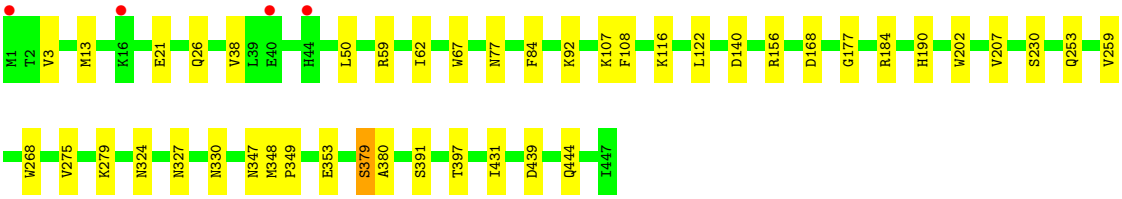
3 Residue-property plots (i)

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

• Molecule 1: NADP-specific glutamate dehydrogenase

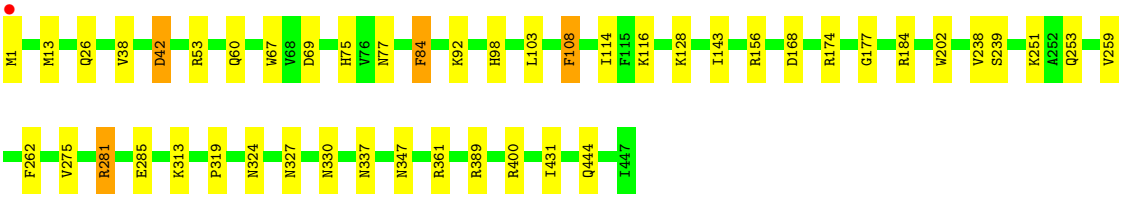
Chain A:





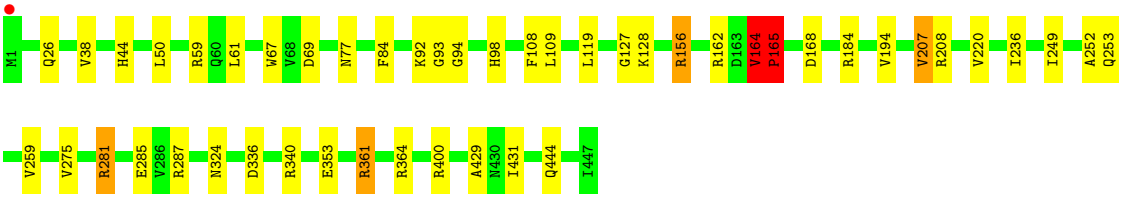
• Molecule 1: NADP-specific glutamate dehydrogenase

Chain B:



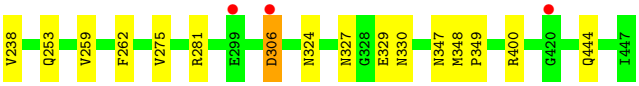
• Molecule 1: NADP-specific glutamate dehydrogenase

Chain C:



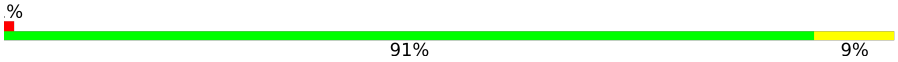
• Molecule 1: NADP-specific glutamate dehydrogenase

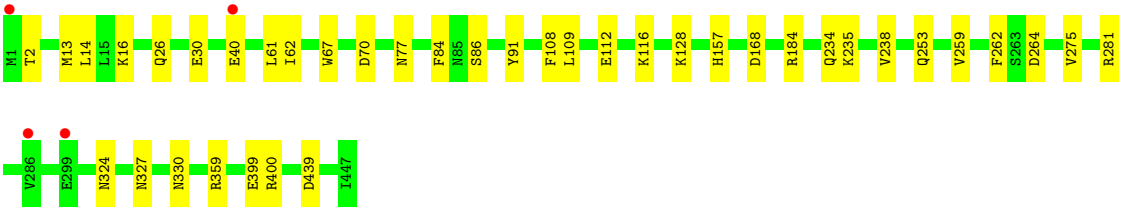
Chain D:



• Molecule 1: NADP-specific glutamate dehydrogenase

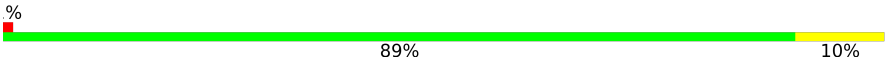
Chain E:

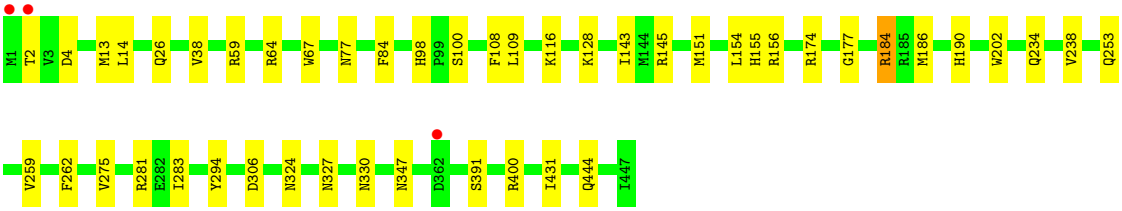




• Molecule 1: NADP-specific glutamate dehydrogenase

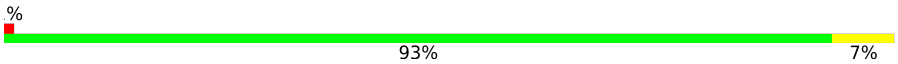
Chain F:

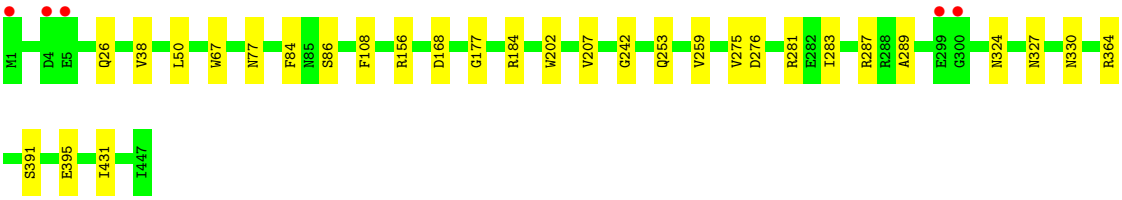




• Molecule 1: NADP-specific glutamate dehydrogenase

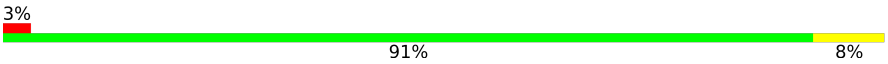
Chain G:

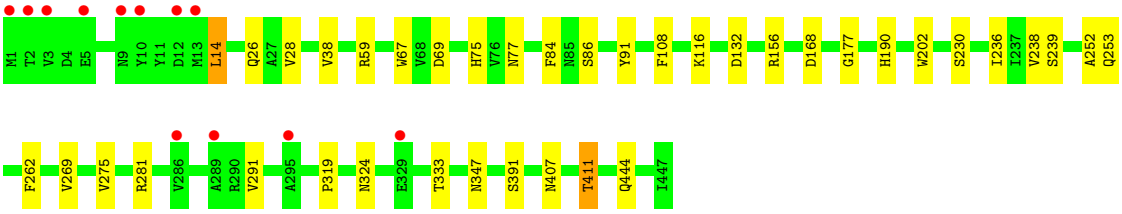




• Molecule 1: NADP-specific glutamate dehydrogenase

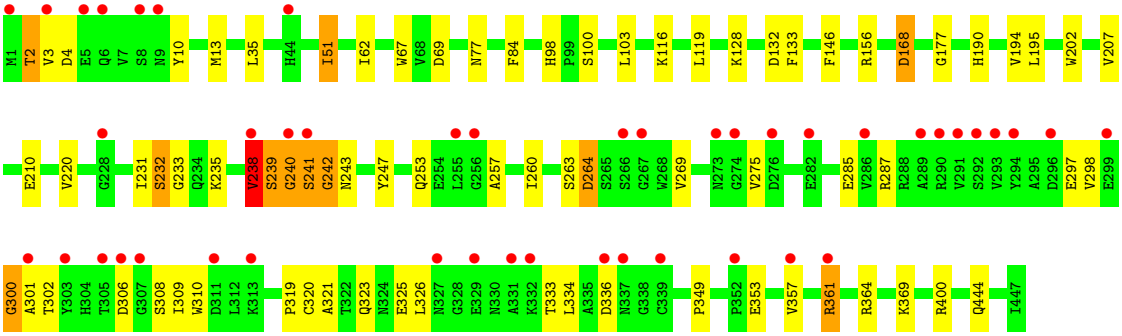
Chain H:





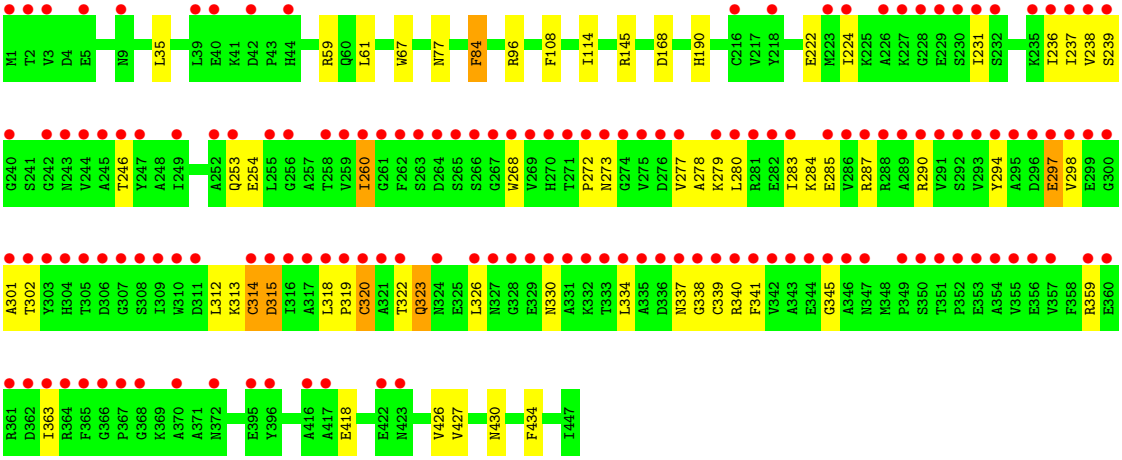
• Molecule 1: NADP-specific glutamate dehydrogenase

Chain I:



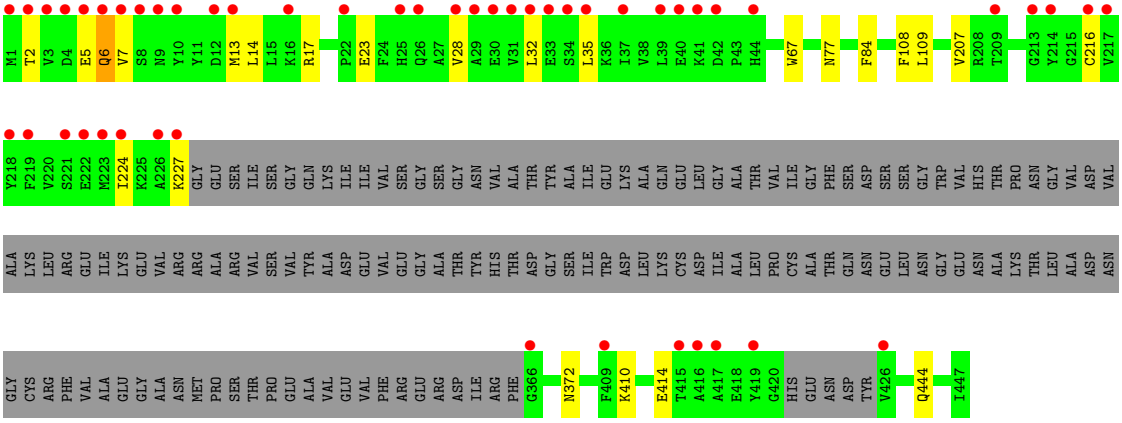
- Molecule 1: NADP-specific glutamate dehydrogenase

Chain J:



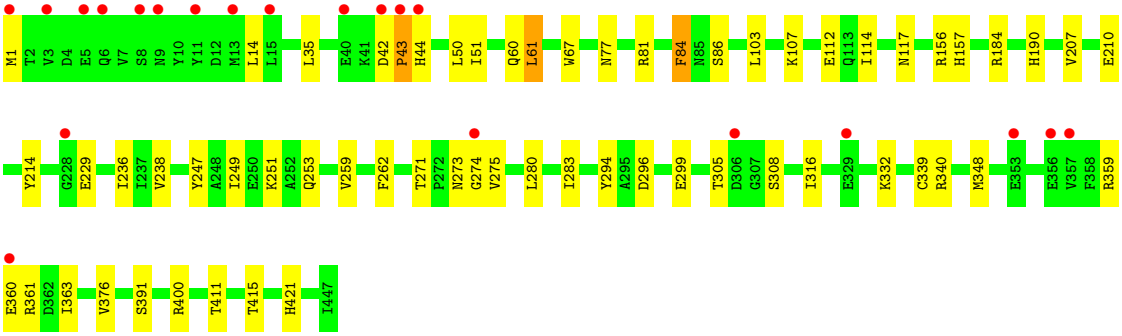
- Molecule 1: NADP-specific glutamate dehydrogenase

Chain K:



- Molecule 1: NADP-specific glutamate dehydrogenase

Chain L:


M1
T2
V3
D4
E5
Q6
V7
S8
N9
Y10
Y11
D12
M13
L14
L15
L35
E40
K41
D42
P43
H44
L50
I51
Q60
L61
W67
N77
R81
F84
N85
S86
L103
K107
E112
Q113
I114
N117
R156
H157
R184
H190
V207
E210
Y214
G228
E229
I236
I237
V238
Y247
A248
I249
E250
K251
A252
Q253
V259
F262
T271
P272
N273
G274
V275
L280
I283
Y294
A295
D296
E299
T305
D306
G307
S308
I316
E329
K332
C339
R340
M348
E353
E356
V357
F358
R359
E360
R361
D362
I363
V376
S391
R400
T411
T415
H421
I447

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	171.22Å 93.03Å 187.88Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	34.37 – 2.29 34.37 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.37-2.29) 97.8 (34.37-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.20 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.165 , 0.222 0.173 , 0.225	Depositor DCC
R_{free} test set	12145 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	42426	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.82	2/3517 (0.1%)	0.88	4/4748 (0.1%)
1	B	0.81	1/3517 (0.0%)	0.92	10/4748 (0.2%)
1	C	0.83	1/3517 (0.0%)	0.95	17/4748 (0.4%)
1	D	0.82	1/3517 (0.0%)	0.90	8/4748 (0.2%)
1	E	0.81	0/3517	0.85	6/4748 (0.1%)
1	F	0.78	0/3517	0.89	9/4748 (0.2%)
1	G	0.77	0/3517	0.88	9/4748 (0.2%)
1	H	0.77	0/3517	0.87	5/4748 (0.1%)
1	I	0.78	1/3517 (0.0%)	0.91	9/4748 (0.2%)
1	J	0.74	0/3517	0.85	2/4748 (0.0%)
1	K	0.72	0/2407	0.84	1/3239 (0.0%)
1	L	0.74	1/3517 (0.0%)	0.87	4/4748 (0.1%)
All	All	0.79	7/41094 (0.0%)	0.89	84/55467 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	1
1	I	0	2
1	J	0	1
1	L	0	2
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	353	GLU	CD-OE1	9.24	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	206	LEU	C-O	6.53	1.35	1.23
1	A	353	GLU	CD-OE2	5.53	1.31	1.25
1	A	268	TRP	CE3-CZ3	5.50	1.47	1.38
1	L	112	GLU	CG-CD	5.46	1.60	1.51
1	I	242	GLY	N-CA	-5.18	1.38	1.46
1	B	42	ASP	CB-CG	5.04	1.62	1.51

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	164	VAL	CB-CA-C	11.65	133.53	111.40
1	G	276	ASP	CB-CG-OD1	8.98	126.38	118.30
1	C	361	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	D	164	VAL	C-N-CD	-8.15	102.67	120.60
1	I	361	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	281	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	C	164	VAL	C-N-CD	-7.73	103.60	120.60
1	B	281	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	D	281	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	H	59	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	281	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	G	281	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	L	156	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	G	281	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	F	59	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	H	132	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	156	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	D	164	VAL	CA-C-N	6.88	136.35	117.10
1	H	281	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	C	69	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	162	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	400	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	389	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	281	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	J	59	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	F	400	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	281	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	361	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	140	ASP	CB-CG-OD1	6.28	123.96	118.30
1	C	208	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	53	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	281	ARG	NE-CZ-NH2	-6.22	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	81	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	L	400	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	G	287	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	G	287	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	I	69	ASP	CB-CG-OD1	6.02	123.72	118.30
1	I	156	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	K	17	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	J	145	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	439	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	400	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	F	156	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	I	232	SER	N-CA-C	5.70	126.39	111.00
1	B	156	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	L	156	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	361	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	F	156	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	C	364	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	156	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	C	400	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	E	439	ASP	CB-CG-OD1	5.51	123.26	118.30
1	G	276	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	361	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	I	264	ASP	CB-CG-OD1	5.39	123.15	118.30
1	E	264	ASP	CB-CG-OD1	5.39	123.15	118.30
1	I	132	ASP	CB-CG-OD1	5.37	123.13	118.30
1	F	64	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	F	281	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	53	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	E	264	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	F	145	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	H	156	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	281	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	164	VAL	O-C-N	-5.22	111.18	121.10
1	G	364	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	287	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	G	156	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	G	156	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	156	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	400	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	400	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	I	69	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	H	281	ARG	NE-CZ-NH1	5.12	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	I	361	ARG	CG-CD-NE	5.12	122.55	111.80
1	A	59	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	59	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	165	PRO	N-CA-C	5.09	125.33	112.10
1	E	70	ASP	CB-CG-OD1	5.09	122.88	118.30
1	I	156	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	47	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	156	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	F	184	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	164	VAL	Mainchain,Peptide
1	D	306	ASP	Peptide
1	I	238	VAL	Peptide
1	I	301	ALA	Peptide
1	J	314	CYS	Peptide
1	L	273	ASN	Peptide
1	L	421	HIS	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	3447	0	3356	24	0
1	B	3447	0	3356	25	0
1	C	3447	0	3356	26	0
1	D	3447	0	3356	38	0
1	E	3447	0	3356	16	0
1	F	3447	0	3356	29	0
1	G	3447	0	3356	13	0
1	H	3447	0	3356	22	0
1	I	3447	0	3356	37	0
1	J	3447	0	3356	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2358	0	2313	13	0
1	L	3447	0	3356	32	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	2	0
2	H	48	0	25	0	0
2	J	48	0	25	0	0
3	A	10	0	4	0	0
3	B	10	0	4	2	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
3	E	10	0	4	1	0
3	F	10	0	4	0	0
3	G	10	0	4	0	0
3	H	10	0	4	0	0
3	J	10	0	4	1	0
4	A	169	0	0	1	0
4	B	172	0	0	1	0
4	C	161	0	0	6	0
4	D	172	0	0	7	0
4	E	160	0	0	1	0
4	F	162	0	0	2	0
4	G	149	0	0	1	0
4	H	111	0	0	0	0
4	I	107	0	0	1	0
4	J	68	0	0	0	0
4	K	66	0	0	0	0
4	L	132	0	0	1	0
All	All	42426	0	39490	282	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (282) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:O	1:C:194:VAL:O	1.65	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:PRO:HA	4:D:601:HOH:O	1.52	1.09
1:D:164:VAL:CA	4:D:601:HOH:O	2.18	0.90
1:C:165:PRO:N	4:C:601:HOH:O	2.08	0.86
1:D:165:PRO:CA	4:D:601:HOH:O	2.17	0.83
1:C:164:VAL:C	4:C:601:HOH:O	2.18	0.82
1:H:269:VAL:HG23	1:H:291:VAL:CG1	2.10	0.81
1:J:297:GLU:HB3	1:J:298:VAL:HA	1.60	0.81
1:D:253:GLN:HE22	1:D:275:VAL:H	1.31	0.77
1:B:26:GLN:HE22	1:B:324:ASN:HD21	1.32	0.77
1:I:239:SER:OG	1:I:320:CYS:C	2.24	0.76
1:G:253:GLN:HE22	1:G:275:VAL:H	1.30	0.76
1:G:327:ASN:H	1:G:330:ASN:HD22	1.32	0.75
1:C:164:VAL:CA	4:C:601:HOH:O	2.35	0.74
1:F:67:TRP:HE1	1:F:77:ASN:HD22	1.36	0.74
1:G:395:GLU:HG2	4:G:709:HOH:O	1.87	0.74
1:G:67:TRP:HE1	1:G:77:ASN:HD22	1.35	0.73
1:F:253:GLN:HE22	1:F:275:VAL:H	1.34	0.73
1:I:353:GLU:O	1:I:357:VAL:HG23	1.89	0.72
1:J:96:ARG:HH12	1:J:323:GLN:HE22	1.34	0.72
1:F:26:GLN:HE22	1:F:324:ASN:HD21	1.36	0.70
1:E:253:GLN:HE22	1:E:275:VAL:H	1.39	0.70
1:D:26:GLN:HE22	1:D:324:ASN:HD21	1.39	0.69
1:E:26:GLN:HE22	1:E:324:ASN:HD21	1.39	0.69
1:F:151:MET:CE	1:F:155:HIS:N	2.55	0.69
1:F:151:MET:HE2	1:F:155:HIS:N	2.07	0.69
1:G:26:GLN:HE22	1:G:324:ASN:HD21	1.40	0.68
1:C:253:GLN:HE22	1:C:275:VAL:H	1.41	0.68
1:C:165:PRO:CA	4:C:601:HOH:O	2.40	0.68
1:I:67:TRP:HE1	1:I:77:ASN:HD22	1.42	0.68
1:C:165:PRO:HA	4:C:601:HOH:O	1.94	0.68
1:B:253:GLN:HE22	1:B:275:VAL:H	1.41	0.68
1:D:164:VAL:C	4:D:601:HOH:O	2.32	0.68
1:K:410:LYS:O	1:K:414:GLU:HG2	1.94	0.67
1:E:253:GLN:HE21	1:E:259:VAL:H	1.43	0.66
1:H:69:ASP:OD2	1:H:75:HIS:HE1	1.79	0.66
1:H:67:TRP:HE1	1:H:77:ASN:HD22	1.41	0.66
1:L:271:THR:HG21	1:L:275:VAL:HG22	1.77	0.66
1:L:271:THR:OG1	1:L:274:GLY:HA3	1.96	0.66
1:I:238:VAL:HG21	1:I:325:GLU:OE1	1.96	0.66
1:A:67:TRP:HE1	1:A:77:ASN:HD22	1.42	0.65
1:A:253:GLN:HE21	1:A:259:VAL:H	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:TRP:HE1	1:L:77:ASN:HD22	1.44	0.65
1:F:151:MET:HE2	1:F:155:HIS:CA	2.27	0.65
1:A:253:GLN:HE22	1:A:275:VAL:H	1.44	0.64
1:I:242:GLY:HA2	1:I:243:ASN:C	2.18	0.63
1:E:67:TRP:HE1	1:E:77:ASN:HD22	1.47	0.62
1:I:238:VAL:HG22	1:I:319:PRO:HA	1.81	0.62
1:C:26:GLN:HE22	1:C:324:ASN:HD21	1.47	0.62
1:D:151:MET:HE1	1:D:155:HIS:HA	1.81	0.62
1:B:253:GLN:HE21	1:B:259:VAL:H	1.48	0.62
1:F:151:MET:HE3	1:F:154:LEU:HB3	1.82	0.61
1:G:253:GLN:HE21	1:G:259:VAL:H	1.48	0.61
1:A:26:GLN:HE22	1:A:324:ASN:HD21	1.48	0.61
1:H:269:VAL:HG23	1:H:291:VAL:HG12	1.83	0.60
1:H:26:GLN:HE22	1:H:324:ASN:HD21	1.50	0.60
1:J:298:VAL:O	1:J:298:VAL:HG13	2.02	0.60
1:B:327:ASN:H	1:B:330:ASN:HD22	1.49	0.60
1:D:190:HIS:HE1	4:D:640:HOH:O	1.84	0.59
1:L:253:GLN:HE22	1:L:275:VAL:H	1.50	0.59
1:A:327:ASN:H	1:A:330:ASN:HD22	1.48	0.59
1:L:190:HIS:HE1	4:L:506:HOH:O	1.86	0.59
1:B:128:LYS:NZ	3:B:502:AKG:O5	2.33	0.59
1:D:165:PRO:N	4:D:601:HOH:O	2.29	0.59
1:J:67:TRP:HE1	1:J:77:ASN:HD22	1.52	0.58
1:J:320:CYS:SG	1:J:345:GLY:HA3	2.43	0.58
1:K:23:GLU:O	1:K:108:PHE:CD1	2.56	0.58
1:D:151:MET:CE	1:D:155:HIS:CA	2.81	0.58
1:I:98:HIS:HD2	1:I:100:SER:H	1.51	0.58
1:C:67:TRP:HE1	1:C:77:ASN:HD22	1.52	0.58
1:K:28:VAL:O	1:K:32:LEU:HB2	2.03	0.57
1:B:67:TRP:HE1	1:B:77:ASN:HD22	1.53	0.57
1:F:253:GLN:HE21	1:F:259:VAL:H	1.51	0.57
1:C:253:GLN:HE21	1:C:259:VAL:H	1.53	0.57
1:I:10:TYR:O	1:I:13:MET:HB3	2.04	0.57
1:I:241:SER:OG	1:I:242:GLY:N	2.34	0.56
1:J:236:ILE:HB	1:J:318:LEU:HD23	1.88	0.55
1:H:253:GLN:HE22	1:H:275:VAL:H	1.53	0.55
1:D:30:GLU:OE2	1:D:112:GLU:OE2	2.24	0.55
1:L:253:GLN:HE22	1:L:275:VAL:N	2.04	0.55
1:A:184:ARG:HE	1:H:444:GLN:HE22	1.55	0.55
1:K:67:TRP:HE1	1:K:77:ASN:HD22	1.54	0.54
1:J:298:VAL:HG12	1:J:301:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:269:VAL:HG23	1:H:291:VAL:HG13	1.88	0.54
1:B:60:GLN:HE21	1:B:103:LEU:HD11	1.73	0.54
1:F:151:MET:HE3	1:F:151:MET:HA	1.88	0.54
1:K:224:ILE:HA	1:K:227:LYS:HE2	1.89	0.54
1:I:190:HIS:HE1	4:I:501:HOH:O	1.91	0.54
1:K:7:VAL:HG13	1:K:32:LEU:HD23	1.89	0.54
1:I:238:VAL:HG13	1:I:310:TRP:CH2	2.43	0.53
1:E:116:LYS:HZ2	3:E:502:AKG:C1	2.22	0.53
1:I:239:SER:HB3	1:I:321:ALA:HA	1.90	0.53
1:L:42:ASP:O	1:L:44:HIS:N	2.42	0.53
1:I:35:LEU:HD22	1:I:51:ILE:HG21	1.91	0.53
1:L:411:THR:O	1:L:415:THR:HG23	2.09	0.53
1:H:269:VAL:CG2	1:H:291:VAL:HG13	2.39	0.52
1:L:359:ARG:O	1:L:361:ARG:O	2.28	0.52
1:C:336:ASP:OD1	1:C:361:ARG:NH2	2.34	0.52
1:I:231:ILE:O	1:I:233:GLY:N	2.43	0.52
1:L:61:LEU:HD21	1:L:157:HIS:NE2	2.25	0.52
1:D:67:TRP:HE1	1:D:77:ASN:HD22	1.57	0.51
1:D:92:LYS:HD2	1:D:164:VAL:HB	1.93	0.51
1:L:271:THR:HG21	1:L:275:VAL:CG2	2.40	0.51
1:F:327:ASN:H	1:F:330:ASN:HD22	1.59	0.51
1:D:151:MET:HE2	1:D:155:HIS:HB3	1.92	0.51
1:E:109:LEU:HB3	1:E:128:LYS:HG3	1.93	0.51
1:L:35:LEU:HD13	1:L:51:ILE:HD11	1.92	0.51
1:E:327:ASN:H	1:E:330:ASN:HD22	1.59	0.51
1:I:239:SER:O	1:I:240:GLY:C	2.48	0.50
1:I:287:ARG:NH2	1:I:297:GLU:OE2	2.32	0.50
1:J:297:GLU:N	1:J:297:GLU:OE2	2.44	0.50
1:E:184:ARG:HE	1:F:444:GLN:HE22	1.59	0.50
3:J:502:AKG:O2	3:J:502:AKG:H41	2.11	0.50
1:D:116:LYS:NZ	1:D:347:ASN:HD21	2.09	0.50
1:L:271:THR:HG23	1:L:271:THR:O	2.10	0.50
1:D:151:MET:HE3	1:D:155:HIS:N	2.27	0.50
1:I:239:SER:HB3	1:I:321:ALA:CA	2.41	0.50
1:I:128:LYS:NZ	1:I:168:ASP:OD2	2.45	0.50
1:I:207:VAL:O	1:I:207:VAL:HG12	2.12	0.50
1:I:238:VAL:HG12	1:I:309:ILE:HG21	1.93	0.50
1:A:62:ILE:HB	1:L:60:GLN:HB2	1.94	0.49
1:A:67:TRP:HE1	1:A:77:ASN:ND2	2.08	0.49
1:I:238:VAL:O	1:I:263:SER:N	2.45	0.49
1:J:246:THR:HG23	1:J:280:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ARG:HH21	1:I:444:GLN:NE2	2.10	0.49
1:L:60:GLN:NE2	1:L:107:LYS:HD2	2.28	0.49
1:J:35:LEU:HD21	1:J:434:PHE:CE1	2.47	0.49
1:L:238:VAL:O	1:L:262:PHE:HA	2.11	0.49
1:B:92:LYS:NZ	3:B:502:AKG:O3	2.36	0.49
1:J:277:VAL:O	1:J:278:ALA:C	2.49	0.49
1:A:444:GLN:NE2	1:G:184:ARG:HH21	2.11	0.49
1:D:151:MET:CE	1:D:155:HIS:HA	2.41	0.49
1:D:151:MET:CE	1:D:155:HIS:N	2.76	0.49
1:H:14:LEU:HD22	1:H:28:VAL:HG11	1.92	0.49
1:D:238:VAL:O	1:D:262:PHE:HA	2.13	0.49
1:I:235:LYS:NZ	1:I:257:ALA:HB1	2.27	0.49
1:I:239:SER:HG	1:I:320:CYS:HB2	1.78	0.49
1:I:323:GLN:HA	1:I:349:PRO:HA	1.95	0.48
1:D:151:MET:CE	1:D:155:HIS:HB3	2.44	0.48
1:D:253:GLN:HE21	1:D:259:VAL:H	1.62	0.48
1:K:224:ILE:HA	1:K:227:LYS:CE	2.43	0.48
1:B:69:ASP:OD2	1:B:75:HIS:HE1	1.96	0.48
1:B:38:VAL:HG23	1:B:431:ILE:HG12	1.96	0.48
1:C:281:ARG:HD2	1:C:285:GLU:OE2	2.14	0.48
1:F:190:HIS:HE1	4:F:616:HOH:O	1.97	0.48
1:K:32:LEU:HD12	1:K:35:LEU:HD22	1.95	0.48
1:J:190:HIS:CD2	1:L:86:SER:O	2.67	0.47
1:C:38:VAL:HG23	1:C:431:ILE:HG12	1.96	0.47
1:F:238:VAL:O	1:F:262:PHE:HA	2.15	0.47
1:A:190:HIS:CD2	1:H:86:SER:O	2.68	0.47
1:A:207:VAL:HG12	1:A:207:VAL:O	2.14	0.47
1:B:313:LYS:HG3	1:B:337:ASN:HB3	1.97	0.47
1:B:444:GLN:HE22	1:D:184:ARG:HE	1.62	0.47
1:D:151:MET:HE1	1:D:155:HIS:CA	2.44	0.47
1:B:98:HIS:HE1	4:B:609:HOH:O	1.98	0.47
1:J:84:PHE:CD1	1:J:114:ILE:HD11	2.50	0.46
1:J:297:GLU:CB	1:J:298:VAL:HA	2.37	0.46
1:J:238:VAL:HA	1:J:318:LEU:O	2.15	0.46
1:H:238:VAL:O	1:H:262:PHE:HA	2.16	0.46
1:L:42:ASP:N	1:L:43:PRO:CD	2.79	0.46
1:E:184:ARG:HE	1:F:444:GLN:NE2	2.14	0.46
1:E:184:ARG:HH21	1:F:444:GLN:NE2	2.14	0.46
1:G:283:ILE:HG23	1:G:289:ALA:HB3	1.96	0.46
1:K:108:PHE:CD2	1:K:109:LEU:HD23	2.50	0.46
1:L:61:LEU:HD21	1:L:157:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:VAL:HG13	1:I:195:LEU:HG	1.98	0.46
1:B:143:ILE:HD13	1:B:174:ARG:NH2	2.31	0.46
1:L:253:GLN:HE21	1:L:259:VAL:H	1.64	0.46
1:D:151:MET:HE3	1:D:151:MET:O	2.16	0.46
1:H:236:ILE:HD12	1:H:252:ALA:HB1	1.98	0.45
1:A:177:GLY:HA2	1:A:202:TRP:CH2	2.51	0.45
1:J:314:CYS:HB3	1:J:315:ASP:HA	1.97	0.45
1:C:119:LEU:HD11	1:C:429:ALA:HB1	1.97	0.45
1:D:10:TYR:CZ	1:D:14:LEU:HD13	2.51	0.45
1:D:164:VAL:O	1:D:194:VAL:O	2.34	0.45
1:I:133:PHE:HB2	1:I:146:PHE:CZ	2.51	0.45
1:B:60:GLN:HB2	1:E:62:ILE:HB	1.99	0.45
1:D:14:LEU:HD23	1:D:28:VAL:HG11	1.99	0.45
1:L:339:CYS:O	1:L:363:ILE:HD12	2.17	0.45
1:J:298:VAL:HG12	1:J:301:ALA:CB	2.47	0.45
1:K:28:VAL:O	1:K:32:LEU:HD13	2.17	0.45
1:B:444:GLN:NE2	1:D:184:ARG:HH21	2.15	0.45
1:C:92:LYS:HD2	1:C:164:VAL:HB	1.99	0.45
1:H:177:GLY:HA2	1:H:202:TRP:CH2	2.52	0.45
1:L:117:ASN:OD1	1:L:376:VAL:HG21	2.17	0.45
1:L:229:GLU:OE2	1:L:340:ARG:NH1	2.50	0.45
1:A:38:VAL:HG23	1:A:431:ILE:HG12	1.98	0.44
1:F:177:GLY:HA2	1:F:202:TRP:CH2	2.52	0.44
1:I:238:VAL:CG1	1:I:310:TRP:CZ2	3.00	0.44
1:A:92:LYS:HE3	1:A:379:SER:HB3	1.99	0.44
1:D:164:VAL:CB	4:D:601:HOH:O	2.58	0.44
1:D:327:ASN:H	1:D:330:ASN:HD22	1.64	0.44
1:I:298:VAL:O	1:I:300:GLY:N	2.50	0.44
1:I:2:THR:OG1	1:I:3:VAL:N	2.51	0.44
1:E:400:ARG:NH1	4:E:607:HOH:O	2.49	0.44
1:A:444:GLN:HE22	1:G:184:ARG:HE	1.66	0.44
1:C:184:ARG:HE	1:D:444:GLN:HE22	1.65	0.44
1:J:323:GLN:H	1:J:323:GLN:HE21	1.63	0.44
1:J:330:ASN:O	1:J:334:LEU:N	2.51	0.44
1:C:98:HIS:HE1	4:C:668:HOH:O	2.00	0.44
1:A:190:HIS:HD2	1:H:86:SER:O	1.99	0.43
1:D:151:MET:HE2	1:D:155:HIS:CB	2.48	0.43
1:E:61:LEU:HD22	1:E:157:HIS:CD2	2.53	0.43
1:F:151:MET:HE2	1:F:155:HIS:HB3	1.99	0.43
1:G:242:GLY:HA3	2:G:501:NAP:O5B	2.18	0.43
1:I:253:GLN:HE22	1:I:275:VAL:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:HIS:HE1	4:F:641:HOH:O	2.00	0.43
1:F:151:MET:CE	1:F:155:HIS:CA	2.94	0.43
1:G:38:VAL:HG23	1:G:431:ILE:HG12	2.00	0.43
1:I:210:GLU:HG3	1:I:247:TYR:CD1	2.53	0.43
1:K:444:GLN:NE2	1:L:184:ARG:HE	2.16	0.43
1:B:84:PHE:CD1	1:B:114:ILE:HD11	2.54	0.43
1:E:30:GLU:OE2	1:E:112:GLU:OE2	2.37	0.43
1:A:207:VAL:HG23	1:A:397:THR:HB	2.00	0.43
1:D:151:MET:CE	1:D:155:HIS:CB	2.96	0.43
1:F:38:VAL:HG23	1:F:431:ILE:HG12	2.00	0.43
1:C:184:ARG:HE	1:D:444:GLN:NE2	2.17	0.43
1:G:177:GLY:HA2	1:G:202:TRP:CH2	2.54	0.43
1:H:269:VAL:CG2	1:H:291:VAL:CG1	2.87	0.43
1:H:407:ASN:O	1:H:411:THR:HG23	2.19	0.43
1:J:268:TRP:CZ3	1:J:312:LEU:HD11	2.54	0.43
1:L:84:PHE:CD1	1:L:114:ILE:HD11	2.54	0.43
1:H:116:LYS:NZ	1:H:347:ASN:HD21	2.17	0.42
1:L:60:GLN:HE21	1:L:103:LEU:HD11	1.84	0.42
1:D:177:GLY:HA2	1:D:202:TRP:CH2	2.54	0.42
1:F:98:HIS:HD2	1:F:100:SER:H	1.67	0.42
1:H:239:SER:OG	1:H:319:PRO:HA	2.20	0.42
1:C:207:VAL:HG12	1:C:207:VAL:O	2.20	0.42
1:E:238:VAL:O	1:E:262:PHE:HA	2.19	0.42
1:A:184:ARG:HE	1:H:444:GLN:NE2	2.16	0.42
1:C:156:ARG:NH2	1:F:186:MET:O	2.52	0.42
1:F:143:ILE:HD13	1:F:174:ARG:NH2	2.34	0.42
1:F:283:ILE:CD1	1:F:294:TYR:HA	2.49	0.42
1:L:249:ILE:HG12	1:L:259:VAL:HG11	2.02	0.42
1:B:281:ARG:HD2	1:B:285:GLU:OE2	2.20	0.42
2:G:501:NAP:O2A	2:G:501:NAP:O1N	2.27	0.42
1:I:177:GLY:HA2	1:I:202:TRP:CH2	2.55	0.42
1:L:214:TYR:CD1	1:L:251:LYS:HB2	2.55	0.42
1:E:86:SER:HB3	1:E:91:TYR:CE1	2.55	0.42
1:J:224:ILE:HG23	1:J:341:PHE:CE2	2.55	0.42
1:B:177:GLY:HA2	1:B:202:TRP:CH2	2.55	0.42
1:C:94:GLY:O	1:C:128:LYS:HD3	2.20	0.42
1:C:236:ILE:HD12	1:C:252:ALA:HB1	2.02	0.42
1:J:314:CYS:CB	1:J:315:ASP:HA	2.50	0.42
1:J:426:VAL:O	1:J:430:ASN:HB2	2.20	0.42
1:K:5:GLU:O	1:K:6:GLN:C	2.58	0.42
1:A:190:HIS:HE1	4:A:611:HOH:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TRP:HE1	1:B:77:ASN:ND2	2.16	0.42
1:F:109:LEU:HB3	1:F:128:LYS:HG3	2.02	0.42
1:J:340:ARG:O	1:J:363:ILE:HG23	2.20	0.42
1:L:262:PHE:CE2	1:L:280:LEU:HD13	2.55	0.42
1:B:239:SER:OG	1:B:319:PRO:HA	2.20	0.41
1:I:116:LYS:HG3	1:I:369:LYS:O	2.19	0.41
1:H:86:SER:HB3	1:H:91:TYR:CE1	2.56	0.41
1:K:14:LEU:HD13	1:K:28:VAL:HG11	2.02	0.41
1:L:236:ILE:HG12	1:L:316:ILE:HB	2.02	0.41
1:A:116:LYS:NZ	1:A:347:ASN:HD21	2.19	0.41
1:J:314:CYS:HB3	1:J:315:ASP:CA	2.51	0.41
1:C:93:GLY:HA3	1:C:127:GLY:O	2.20	0.41
1:C:109:LEU:HB3	1:C:128:LYS:HG3	2.03	0.41
1:D:165:PRO:HB2	1:D:166:ALA:H	1.64	0.41
1:F:2:THR:HG22	1:F:4:ASP:N	2.36	0.41
1:D:116:LYS:HZ1	1:D:347:ASN:HD21	1.67	0.41
1:B:108:PHE:CD1	1:B:108:PHE:C	2.93	0.41
1:B:238:VAL:O	1:B:262:PHE:HA	2.21	0.41
1:D:348:MET:N	1:D:349:PRO:CD	2.84	0.41
1:I:239:SER:HB3	1:I:321:ALA:HB2	2.03	0.41
1:A:21:GLU:CD	1:A:107:LYS:HZ3	2.24	0.41
1:A:122:LEU:HD13	1:A:380:ALA:HB3	2.03	0.41
1:A:348:MET:N	1:A:349:PRO:CD	2.84	0.41
1:B:116:LYS:NZ	1:B:347:ASN:HD21	2.19	0.41
1:B:184:ARG:HH21	1:C:444:GLN:NE2	2.19	0.41
1:C:249:ILE:HG12	1:C:259:VAL:HG11	2.03	0.41
1:J:237:ILE:HG22	1:J:260:ILE:HD12	2.01	0.41
1:A:38:VAL:CG2	1:A:431:ILE:HG12	2.51	0.40
1:G:86:SER:O	1:H:190:HIS:CD2	2.75	0.40
1:F:151:MET:CE	1:F:155:HIS:HA	2.51	0.40
1:I:62:ILE:HD11	1:I:103:LEU:HD22	2.03	0.40
1:F:116:LYS:NZ	1:F:347:ASN:HD21	2.19	0.40
1:I:238:VAL:HG11	1:I:310:TRP:CZ2	2.56	0.40
1:L:283:ILE:HD13	1:L:294:TYR:HA	2.04	0.40
1:L:210:GLU:HG3	1:L:247:TYR:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/447 (100%)	435 (98%)	8 (2%)	2 (0%)	34	42
1	B	445/447 (100%)	434 (98%)	10 (2%)	1 (0%)	47	58
1	C	445/447 (100%)	433 (97%)	9 (2%)	3 (1%)	22	26
1	D	445/447 (100%)	435 (98%)	7 (2%)	3 (1%)	22	26
1	E	445/447 (100%)	436 (98%)	8 (2%)	1 (0%)	47	58
1	F	445/447 (100%)	434 (98%)	11 (2%)	0	100	100
1	G	445/447 (100%)	435 (98%)	8 (2%)	2 (0%)	34	42
1	H	445/447 (100%)	437 (98%)	7 (2%)	1 (0%)	47	58
1	I	445/447 (100%)	420 (94%)	19 (4%)	6 (1%)	12	12
1	J	445/447 (100%)	390 (88%)	45 (10%)	10 (2%)	6	5
1	K	298/447 (67%)	283 (95%)	13 (4%)	2 (1%)	22	26
1	L	445/447 (100%)	429 (96%)	14 (3%)	2 (0%)	34	42
All	All	5193/5364 (97%)	5001 (96%)	159 (3%)	33 (1%)	25	31

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	PRO
1	C	207	VAL
1	D	164	VAL
1	D	165	PRO
1	G	207	VAL
1	I	232	SER
1	J	272	PRO
1	J	319	PRO
1	J	337	ASN
1	K	207	VAL
1	L	43	PRO
1	L	207	VAL

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Mol	Chain	Res	Type
1	G	168	ASP
1	I	240	GLY
1	I	300	GLY
1	J	253	GLN
1	E	168	ASP
1	H	168	ASP
1	I	241	SER
1	J	320	CYS
1	K	6	GLN
1	A	168	ASP
1	B	168	ASP
1	J	297	GLU
1	J	338	GLY
1	J	418	GLU
1	C	168	ASP
1	D	168	ASP
1	I	168	ASP
1	J	168	ASP
1	A	3	VAL
1	I	238	VAL
1	J	231	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	358/358 (100%)	350 (98%)	8 (2%)	52	69
1	B	358/358 (100%)	352 (98%)	6 (2%)	60	76
1	C	358/358 (100%)	352 (98%)	6 (2%)	60	76
1	D	358/358 (100%)	348 (97%)	10 (3%)	43	60
1	E	358/358 (100%)	347 (97%)	11 (3%)	40	55
1	F	358/358 (100%)	351 (98%)	7 (2%)	55	72
1	G	358/358 (100%)	354 (99%)	4 (1%)	73	86
1	H	358/358 (100%)	350 (98%)	8 (2%)	52	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	358/358 (100%)	336 (94%)	22 (6%)	18	25
1	J	358/358 (100%)	334 (93%)	24 (7%)	16	21
1	K	243/358 (68%)	238 (98%)	5 (2%)	53	70
1	L	358/358 (100%)	345 (96%)	13 (4%)	35	49
All	All	4181/4296 (97%)	4057 (97%)	124 (3%)	41	57

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	50	LEU
1	A	84	PHE
1	A	108	PHE
1	A	230	SER
1	A	279	LYS
1	A	379	SER
1	A	391	SER
1	B	1	MET
1	B	13	MET
1	B	42	ASP
1	B	84	PHE
1	B	108	PHE
1	B	251	LYS
1	C	44	HIS
1	C	50	LEU
1	C	61	LEU
1	C	84	PHE
1	C	108	PHE
1	C	220	VAL
1	D	2	THR
1	D	6	GLN
1	D	13	MET
1	D	35	LEU
1	D	61	LEU
1	D	84	PHE
1	D	108	PHE
1	D	202	TRP
1	D	306	ASP
1	D	329	GLU
1	E	2	THR
1	E	13	MET

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Mol	Chain	Res	Type
1	E	14	LEU
1	E	16	LYS
1	E	40	GLU
1	E	84	PHE
1	E	108	PHE
1	E	234	GLN
1	E	235	LYS
1	E	359	ARG
1	E	399	GLU
1	F	13	MET
1	F	14	LEU
1	F	84	PHE
1	F	108	PHE
1	F	234	GLN
1	F	306	ASP
1	F	391	SER
1	G	50	LEU
1	G	84	PHE
1	G	108	PHE
1	G	391	SER
1	H	14	LEU
1	H	38	VAL
1	H	84	PHE
1	H	108	PHE
1	H	230	SER
1	H	333	THR
1	H	391	SER
1	H	411	THR
1	I	2	THR
1	I	4	ASP
1	I	51	ILE
1	I	84	PHE
1	I	119	LEU
1	I	220	VAL
1	I	238	VAL
1	I	239	SER
1	I	260	ILE
1	I	264	ASP
1	I	269	VAL
1	I	285	GLU
1	I	302	THR
1	I	306	ASP

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Mol	Chain	Res	Type
1	I	308	SER
1	I	326	LEU
1	I	333	THR
1	I	334	LEU
1	I	336	ASP
1	I	361	ARG
1	I	364	ARG
1	I	400	ARG
1	J	61	LEU
1	J	84	PHE
1	J	108	PHE
1	J	222	GLU
1	J	239	SER
1	J	254	GLU
1	J	260	ILE
1	J	273	ASN
1	J	279	LYS
1	J	283	ILE
1	J	284	LYS
1	J	285	GLU
1	J	287	ARG
1	J	290	ARG
1	J	294	TYR
1	J	302	THR
1	J	313	LYS
1	J	315	ASP
1	J	322	THR
1	J	323	GLN
1	J	326	LEU
1	J	339	CYS
1	J	359	ARG
1	J	427	VAL
1	K	2	THR
1	K	13	MET
1	K	84	PHE
1	K	216	CYS
1	K	372	ASN
1	L	1	MET
1	L	14	LEU
1	L	50	LEU
1	L	61	LEU
1	L	84	PHE

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Mol	Chain	Res	Type
1	L	296	ASP
1	L	299	GLU
1	L	305	THR
1	L	308	SER
1	L	332	LYS
1	L	348	MET
1	L	360	GLU
1	L	391	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	75	HIS
1	A	77	ASN
1	A	155	HIS
1	A	190	HIS
1	A	234	GLN
1	A	253	GLN
1	A	324	ASN
1	A	330	ASN
1	A	347	ASN
1	A	384	GLN
1	A	423	ASN
1	A	444	GLN
1	B	60	GLN
1	B	75	HIS
1	B	77	ASN
1	B	98	HIS
1	B	190	HIS
1	B	253	GLN
1	B	324	ASN
1	B	330	ASN
1	B	347	ASN
1	B	384	GLN
1	B	444	GLN
1	C	60	GLN
1	C	75	HIS
1	C	77	ASN
1	C	98	HIS
1	C	190	HIS
1	C	253	GLN

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Mol	Chain	Res	Type
1	C	270	HIS
1	C	324	ASN
1	C	330	ASN
1	C	347	ASN
1	C	444	GLN
1	D	60	GLN
1	D	71	GLN
1	D	75	HIS
1	D	77	ASN
1	D	98	HIS
1	D	190	HIS
1	D	253	GLN
1	D	324	ASN
1	D	330	ASN
1	D	347	ASN
1	D	384	GLN
1	D	444	GLN
1	E	75	HIS
1	E	77	ASN
1	E	98	HIS
1	E	190	HIS
1	E	234	GLN
1	E	253	GLN
1	E	324	ASN
1	E	330	ASN
1	E	347	ASN
1	E	384	GLN
1	E	423	ASN
1	E	444	GLN
1	F	60	GLN
1	F	75	HIS
1	F	77	ASN
1	F	98	HIS
1	F	155	HIS
1	F	190	HIS
1	F	234	GLN
1	F	253	GLN
1	F	324	ASN
1	F	330	ASN
1	F	347	ASN
1	F	384	GLN
1	F	444	GLN

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Mol	Chain	Res	Type
1	G	75	HIS
1	G	77	ASN
1	G	98	HIS
1	G	253	GLN
1	G	324	ASN
1	G	330	ASN
1	G	347	ASN
1	G	423	ASN
1	G	444	GLN
1	H	75	HIS
1	H	77	ASN
1	H	98	HIS
1	H	190	HIS
1	H	234	GLN
1	H	253	GLN
1	H	324	ASN
1	H	330	ASN
1	H	347	ASN
1	H	423	ASN
1	H	444	GLN
1	I	60	GLN
1	I	75	HIS
1	I	77	ASN
1	I	98	HIS
1	I	190	HIS
1	I	253	GLN
1	I	384	GLN
1	I	444	GLN
1	J	26	GLN
1	J	60	GLN
1	J	77	ASN
1	J	98	HIS
1	J	155	HIS
1	J	190	HIS
1	J	323	GLN
1	J	324	ASN
1	J	423	ASN
1	J	444	GLN
1	K	60	GLN
1	K	75	HIS
1	K	77	ASN
1	K	98	HIS

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Mol	Chain	Res	Type
1	K	190	HIS
1	K	384	GLN
1	K	444	GLN
1	L	60	GLN
1	L	75	HIS
1	L	77	ASN
1	L	98	HIS
1	L	190	HIS
1	L	253	GLN
1	L	444	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AKG	C	502	-	9,9,9	2.04	2 (22%)	11,11,11	2.45	4 (36%)
3	AKG	A	502	-	9,9,9	2.35	2 (22%)	11,11,11	3.36	5 (45%)
3	AKG	J	502	-	9,9,9	1.69	2 (22%)	11,11,11	1.95	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	E	501	-	45,52,52	1.79	5 (11%)	56,80,80	1.63	9 (16%)
2	NAP	J	501	-	45,52,52	1.71	8 (17%)	56,80,80	1.59	5 (8%)
3	AKG	B	502	-	9,9,9	2.36	4 (44%)	11,11,11	2.07	4 (36%)
2	NAP	D	501	-	45,52,52	1.68	6 (13%)	56,80,80	1.91	8 (14%)
2	NAP	B	501	-	45,52,52	1.59	6 (13%)	56,80,80	1.71	8 (14%)
2	NAP	F	501	-	45,52,52	1.67	7 (15%)	56,80,80	1.89	10 (17%)
2	NAP	G	501	-	45,52,52	1.72	5 (11%)	56,80,80	2.12	14 (25%)
2	NAP	H	501	-	45,52,52	1.65	7 (15%)	56,80,80	1.87	12 (21%)
3	AKG	D	502	-	9,9,9	1.86	1 (11%)	11,11,11	2.14	4 (36%)
3	AKG	H	502	-	9,9,9	2.41	1 (11%)	11,11,11	3.56	7 (63%)
3	AKG	G	502	-	9,9,9	2.58	2 (22%)	11,11,11	1.83	4 (36%)
2	NAP	A	501	-	45,52,52	1.47	4 (8%)	56,80,80	1.77	9 (16%)
2	NAP	C	501	-	45,52,52	1.59	5 (11%)	56,80,80	1.97	11 (19%)
3	AKG	E	502	-	9,9,9	2.35	1 (11%)	11,11,11	2.63	6 (54%)
3	AKG	F	502	-	9,9,9	1.71	1 (11%)	11,11,11	3.13	8 (72%)

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	AKG	C	502	-	-	7/9/9/9	-
3	AKG	A	502	-	-	6/9/9/9	-
3	AKG	J	502	-	-	7/9/9/9	-
2	NAP	E	501	-	-	6/31/67/67	0/5/5/5
2	NAP	J	501	-	-	9/31/67/67	0/5/5/5
3	AKG	B	502	-	-	4/9/9/9	-
2	NAP	D	501	-	-	5/31/67/67	0/5/5/5
2	NAP	B	501	-	-	5/31/67/67	0/5/5/5
2	NAP	F	501	-	-	6/31/67/67	0/5/5/5
2	NAP	G	501	-	-	7/31/67/67	0/5/5/5
2	NAP	H	501	-	-	6/31/67/67	0/5/5/5
3	AKG	D	502	-	-	2/9/9/9	-
3	AKG	H	502	-	-	4/9/9/9	-
3	AKG	G	502	-	-	6/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	501	-	-	5/31/67/67	0/5/5/5
2	NAP	C	501	-	-	4/31/67/67	0/5/5/5
3	AKG	E	502	-	-	6/9/9/9	-
3	AKG	F	502	-	-	8/9/9/9	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	NAP	C4N-C3N	8.66	1.54	1.39
2	F	501	NAP	C4N-C3N	7.94	1.52	1.39
2	H	501	NAP	C4N-C3N	7.71	1.52	1.39
2	J	501	NAP	C4N-C3N	7.71	1.52	1.39
2	B	501	NAP	C4N-C3N	7.58	1.52	1.39
2	D	501	NAP	C4N-C3N	7.52	1.52	1.39
2	G	501	NAP	C4N-C3N	7.24	1.51	1.39
2	C	501	NAP	C4N-C3N	6.98	1.51	1.39
3	G	502	AKG	C2-C1	-6.91	1.44	1.53
2	A	501	NAP	C4N-C3N	6.78	1.50	1.39
3	H	502	AKG	C2-C1	-6.50	1.44	1.53
3	E	502	AKG	C2-C1	-6.13	1.45	1.53
3	A	502	AKG	C2-C1	-6.03	1.45	1.53
3	B	502	AKG	C2-C1	-5.44	1.46	1.53
3	D	502	AKG	C2-C1	-4.95	1.46	1.53
3	C	502	AKG	C2-C1	-4.86	1.47	1.53
3	F	502	AKG	C2-C1	-3.96	1.48	1.53
2	G	501	NAP	O4D-C1D	3.94	1.46	1.41
2	H	501	NAP	C5N-C4N	3.63	1.46	1.38
2	C	501	NAP	C2A-N3A	3.58	1.37	1.32
2	G	501	NAP	C5N-C4N	3.56	1.46	1.38
2	C	501	NAP	C5N-C4N	3.54	1.46	1.38
2	J	501	NAP	C5N-C4N	3.47	1.46	1.38
3	J	502	AKG	C2-C1	-3.42	1.49	1.53
2	D	501	NAP	P2B-O2B	3.31	1.65	1.59
2	E	501	NAP	C5N-C4N	3.31	1.45	1.38
2	J	501	NAP	O4B-C1B	3.26	1.45	1.41
2	D	501	NAP	C5N-C4N	3.25	1.45	1.38
2	A	501	NAP	C5N-C4N	3.14	1.45	1.38
2	B	501	NAP	C2A-N3A	3.03	1.37	1.32
2	G	501	NAP	C2A-N3A	3.03	1.37	1.32
2	J	501	NAP	C5A-C4A	3.02	1.48	1.40
2	H	501	NAP	C4A-N3A	2.98	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAP	C2A-N1A	2.90	1.39	1.33
2	B	501	NAP	C5N-C4N	2.87	1.45	1.38
2	F	501	NAP	C5N-C4N	2.82	1.44	1.38
2	F	501	NAP	C2A-N3A	2.77	1.36	1.32
2	J	501	NAP	C2A-N3A	2.75	1.36	1.32
2	E	501	NAP	P2B-O2B	2.71	1.64	1.59
2	A	501	NAP	C2A-N3A	2.68	1.36	1.32
2	F	501	NAP	C5A-C4A	2.67	1.48	1.40
2	F	501	NAP	O4D-C1D	2.65	1.44	1.41
3	A	502	AKG	C3-C2	-2.64	1.48	1.51
2	D	501	NAP	C4A-N3A	2.61	1.39	1.35
2	G	501	NAP	C5A-C4A	2.36	1.47	1.40
3	G	502	AKG	O4-C5	-2.35	1.22	1.30
2	E	501	NAP	C5A-C4A	2.33	1.47	1.40
2	D	501	NAP	C2A-N3A	2.32	1.35	1.32
2	H	501	NAP	C2A-N3A	2.28	1.35	1.32
2	B	501	NAP	C2N-N1N	-2.27	1.32	1.35
2	C	501	NAP	C5A-C4A	2.26	1.46	1.40
3	B	502	AKG	C4-C5	-2.25	1.45	1.50
2	H	501	NAP	C5A-C4A	2.25	1.46	1.40
2	J	501	NAP	P2B-O2B	2.24	1.63	1.59
2	B	501	NAP	C5A-C4A	2.24	1.46	1.40
3	B	502	AKG	O4-C5	-2.22	1.23	1.30
3	C	502	AKG	O1-C1	2.20	1.28	1.22
2	B	501	NAP	O4B-C1B	2.19	1.44	1.41
3	B	502	AKG	O1-C1	2.18	1.28	1.22
2	D	501	NAP	C8A-N7A	2.15	1.38	1.34
2	F	501	NAP	C2N-N1N	-2.13	1.32	1.35
2	E	501	NAP	C2A-N3A	2.08	1.35	1.32
2	J	501	NAP	O4D-C1D	2.08	1.44	1.41
3	J	502	AKG	O4-C5	-2.06	1.23	1.30
2	J	501	NAP	C6A-C5A	2.05	1.50	1.43
2	F	501	NAP	C4A-N3A	-2.05	1.32	1.35
2	H	501	NAP	C2A-N1A	2.05	1.37	1.33
2	A	501	NAP	C3N-C7N	-2.04	1.47	1.50
2	H	501	NAP	C6A-C5A	2.00	1.50	1.43

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	AKG	O1-C1-C2	-7.81	111.30	121.72
3	H	502	AKG	O1-C1-C2	-7.38	111.86	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAP	C5N-C4N-C3N	-7.36	111.63	120.34
2	J	501	NAP	C5N-C4N-C3N	-7.18	111.85	120.34
2	F	501	NAP	C5N-C4N-C3N	-7.07	111.97	120.34
2	C	501	NAP	C5N-C4N-C3N	-6.92	112.15	120.34
3	H	502	AKG	C3-C4-C5	-6.76	99.05	113.60
2	D	501	NAP	C1B-N9A-C4A	-6.47	115.28	126.64
2	G	501	NAP	C5N-C4N-C3N	-6.43	112.73	120.34
2	D	501	NAP	N3A-C2A-N1A	-6.25	118.91	128.68
2	C	501	NAP	N6A-C6A-N1A	6.16	131.37	118.57
2	D	501	NAP	C5N-C4N-C3N	-6.03	113.21	120.34
3	F	502	AKG	O1-C1-C2	-5.98	113.74	121.72
2	E	501	NAP	C5N-C4N-C3N	-5.94	113.31	120.34
2	A	501	NAP	C5N-C4N-C3N	-5.84	113.43	120.34
2	C	501	NAP	C5A-C6A-N6A	-5.80	111.54	120.35
2	H	501	NAP	C5N-C4N-C3N	-5.63	113.68	120.34
2	H	501	NAP	C1B-N9A-C4A	-5.63	116.75	126.64
3	A	502	AKG	C3-C4-C5	-5.42	101.94	113.60
3	C	502	AKG	C3-C4-C5	-5.19	102.44	113.60
2	G	501	NAP	N3A-C2A-N1A	-5.11	120.69	128.68
2	G	501	NAP	C5A-C6A-N6A	-5.03	112.71	120.35
2	H	501	NAP	N3A-C2A-N1A	-4.96	120.93	128.68
2	G	501	NAP	N6A-C6A-N1A	4.90	128.74	118.57
2	C	501	NAP	N3A-C2A-N1A	-4.86	121.09	128.68
3	F	502	AKG	C4-C3-C2	-4.72	104.14	113.03
2	A	501	NAP	C3N-C7N-N7N	4.66	123.35	117.75
2	F	501	NAP	C3N-C7N-N7N	4.62	123.30	117.75
3	C	502	AKG	O5-C2-C1	4.52	125.98	119.43
2	F	501	NAP	N3A-C2A-N1A	-4.48	121.67	128.68
2	A	501	NAP	N6A-C6A-N1A	4.48	127.88	118.57
3	E	502	AKG	C3-C4-C5	-4.43	104.07	113.60
3	D	502	AKG	O1-C1-C2	-4.42	115.81	121.72
2	A	501	NAP	N3A-C2A-N1A	-4.42	121.77	128.68
2	B	501	NAP	N3A-C2A-N1A	-4.32	121.92	128.68
2	E	501	NAP	N3A-C2A-N1A	-4.14	122.20	128.68
2	E	501	NAP	C3N-C7N-N7N	4.14	122.72	117.75
2	J	501	NAP	N3A-C2A-N1A	-4.14	122.22	128.68
3	B	502	AKG	C4-C3-C2	-4.10	105.31	113.03
2	E	501	NAP	O7N-C7N-N7N	-4.08	116.78	122.58
2	G	501	NAP	C3N-C7N-N7N	4.02	122.58	117.75
2	H	501	NAP	C3N-C7N-N7N	4.02	122.57	117.75
2	B	501	NAP	N6A-C6A-N1A	3.93	126.74	118.57
3	D	502	AKG	C3-C2-C1	3.92	123.26	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	501	NAP	PN-O3-PA	-3.88	119.50	132.83
2	G	501	NAP	O5D-PN-O1N	-3.86	93.97	109.07
3	J	502	AKG	C3-C2-C1	3.76	122.95	115.97
3	E	502	AKG	O3-C5-C4	-3.69	111.24	123.08
2	A	501	NAP	C5A-C6A-N6A	-3.69	114.75	120.35
2	B	501	NAP	C5A-C6A-N6A	-3.61	114.87	120.35
3	F	502	AKG	O5-C2-C1	3.57	124.61	119.43
2	B	501	NAP	C2N-C3N-C4N	3.53	122.26	118.26
2	F	501	NAP	C3D-C2D-C1D	-3.52	95.68	100.98
2	B	501	NAP	PN-O3-PA	-3.46	120.94	132.83
3	A	502	AKG	O2-C1-C2	3.40	123.28	113.97
2	F	501	NAP	PN-O3-PA	-3.37	121.25	132.83
3	E	502	AKG	O5-C2-C1	3.34	124.26	119.43
2	A	501	NAP	O7N-C7N-C3N	-3.27	115.71	119.63
3	F	502	AKG	O2-C1-C2	3.27	122.91	113.97
2	F	501	NAP	N6A-C6A-N1A	3.25	125.33	118.57
2	J	501	NAP	C4A-C5A-N7A	-3.19	106.07	109.40
2	D	501	NAP	O7N-C7N-C3N	3.19	123.45	119.63
2	D	501	NAP	C5A-C6A-N6A	-3.15	115.56	120.35
2	D	501	NAP	O7N-C7N-N7N	-3.15	118.11	122.58
3	H	502	AKG	O5-C2-C1	3.12	123.95	119.43
2	F	501	NAP	C2A-N1A-C6A	3.11	124.08	118.75
2	J	501	NAP	O4B-C1B-C2B	-3.08	101.24	106.59
2	D	501	NAP	PN-O3-PA	-3.07	122.28	132.83
3	H	502	AKG	O2-C1-C2	3.06	122.35	113.97
2	F	501	NAP	O7N-C7N-C3N	-3.03	116.00	119.63
3	E	502	AKG	O4-C5-O3	3.01	130.80	123.30
2	H	501	NAP	C3D-C2D-C1D	-3.00	96.47	100.98
3	J	502	AKG	C4-C3-C2	2.97	118.64	113.03
2	G	501	NAP	O7N-C7N-C3N	-2.94	116.11	119.63
2	C	501	NAP	C4A-C5A-N7A	2.92	112.44	109.40
3	B	502	AKG	C3-C4-C5	-2.89	107.39	113.60
3	E	502	AKG	C3-C2-C1	-2.78	110.82	115.97
2	J	501	NAP	C2N-C3N-C4N	2.77	121.40	118.26
2	E	501	NAP	O4B-C1B-C2B	-2.73	101.85	106.59
3	E	502	AKG	O1-C1-C2	-2.71	118.11	121.72
2	D	501	NAP	C3D-C2D-C1D	-2.69	96.93	100.98
2	H	501	NAP	PN-O3-PA	-2.68	123.62	132.83
3	G	502	AKG	O3-C5-C4	-2.68	114.47	123.08
3	B	502	AKG	O3-C5-C4	-2.68	114.47	123.08
3	A	502	AKG	O5-C2-C1	2.67	123.30	119.43
2	G	501	NAP	O3X-P2B-O2X	2.65	117.76	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	502	AKG	O1-C1-C2	-2.62	118.22	121.72
2	C	501	NAP	C2A-N1A-C6A	2.62	123.23	118.75
3	F	502	AKG	O5-C2-C3	-2.61	115.42	121.20
2	H	501	NAP	O3X-P2B-O2X	2.60	117.57	107.64
3	F	502	AKG	O3-C5-C4	-2.59	114.76	123.08
3	H	502	AKG	O3-C5-C4	-2.57	114.81	123.08
2	C	501	NAP	O7N-C7N-C3N	2.55	122.69	119.63
2	E	501	NAP	C4A-C5A-N7A	-2.54	106.75	109.40
3	C	502	AKG	C3-C2-C1	-2.52	111.30	115.97
2	C	501	NAP	O3X-P2B-O2X	2.51	117.22	107.64
2	A	501	NAP	PN-O3-PA	-2.50	124.24	132.83
2	A	501	NAP	O2N-PN-O1N	2.45	124.34	112.24
3	A	502	AKG	O3-C5-C4	-2.42	115.31	123.08
2	C	501	NAP	C2N-C3N-C4N	2.39	120.97	118.26
2	F	501	NAP	C1B-N9A-C4A	-2.38	122.47	126.64
2	H	501	NAP	C2A-N1A-C6A	2.36	122.80	118.75
2	A	501	NAP	C3D-C2D-C1D	-2.35	97.43	100.98
3	D	502	AKG	O2-C1-C2	2.35	120.39	113.97
2	C	501	NAP	O7N-C7N-N7N	-2.32	119.28	122.58
2	G	501	NAP	O2B-P2B-O1X	-2.32	100.44	109.39
3	B	502	AKG	O4-C5-C4	2.30	121.42	114.03
3	H	502	AKG	O4-C5-O3	2.28	128.99	123.30
3	J	502	AKG	O2-C1-C2	2.26	120.17	113.97
2	G	501	NAP	O2N-PN-O1N	-2.24	101.15	112.24
3	G	502	AKG	C3-C4-C5	-2.24	108.79	113.60
2	E	501	NAP	O3X-P2B-O2X	2.22	116.13	107.64
3	D	502	AKG	O5-C2-C1	-2.21	116.23	119.43
2	E	501	NAP	PN-O3-PA	-2.20	125.27	132.83
2	E	501	NAP	O2X-P2B-O2B	-2.19	96.16	105.99
2	B	501	NAP	C4A-C5A-N7A	2.19	111.68	109.40
2	G	501	NAP	C5N-C6N-N1N	2.16	123.50	120.40
3	F	502	AKG	C3-C2-C1	2.14	119.95	115.97
2	G	501	NAP	C6N-N1N-C2N	-2.13	120.03	121.97
3	J	502	AKG	O5-C2-C3	-2.11	116.53	121.20
2	H	501	NAP	O3D-C3D-C4D	-2.09	105.00	111.05
2	F	501	NAP	O2B-P2B-O1X	-2.09	101.34	109.39
3	H	502	AKG	C4-C3-C2	-2.07	109.14	113.03
3	G	502	AKG	C3-C2-C1	-2.06	112.16	115.97
3	J	502	AKG	O2-C1-O1	-2.05	118.91	123.61
3	F	502	AKG	C3-C4-C5	-2.05	109.20	113.60
2	B	501	NAP	C2A-N1A-C6A	2.03	122.23	118.75
2	H	501	NAP	C4A-C5A-N7A	-2.02	107.29	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	501	NAP	O7N-C7N-N7N	-2.02	119.71	122.58
2	G	501	NAP	C4N-C3N-C7N	-2.01	115.66	121.04
2	H	501	NAP	O5D-PN-O1N	2.01	116.92	109.07
2	C	501	NAP	C6N-C5N-C4N	2.00	122.35	119.44
3	C	502	AKG	O4-C5-O3	2.00	128.29	123.30

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	C2B-O2B-P2B-O1X
2	A	501	NAP	O4D-C1D-N1N-C2N
2	A	501	NAP	O4D-C1D-N1N-C6N
2	B	501	NAP	C2B-O2B-P2B-O1X
2	B	501	NAP	C2B-O2B-P2B-O3X
2	B	501	NAP	O4D-C1D-N1N-C2N
2	B	501	NAP	O4D-C1D-N1N-C6N
2	C	501	NAP	O4D-C1D-N1N-C2N
2	D	501	NAP	O4D-C1D-N1N-C2N
2	E	501	NAP	C5D-O5D-PN-O2N
2	E	501	NAP	O4D-C1D-N1N-C2N
2	E	501	NAP	O4D-C1D-N1N-C6N
2	F	501	NAP	O4D-C1D-N1N-C2N
2	F	501	NAP	O4D-C1D-N1N-C6N
2	G	501	NAP	C2B-O2B-P2B-O2X
2	G	501	NAP	C5D-O5D-PN-O3
2	G	501	NAP	O4D-C1D-N1N-C2N
2	H	501	NAP	O4D-C1D-N1N-C2N
2	J	501	NAP	C5D-O5D-PN-O1N
3	A	502	AKG	O1-C1-C2-O5
3	A	502	AKG	O1-C1-C2-C3
3	A	502	AKG	O2-C1-C2-C3
3	A	502	AKG	C2-C3-C4-C5
3	B	502	AKG	O2-C1-C2-C3
3	C	502	AKG	O1-C1-C2-C3
3	C	502	AKG	O2-C1-C2-O5
3	C	502	AKG	O2-C1-C2-C3
3	C	502	AKG	C2-C3-C4-C5
3	D	502	AKG	C1-C2-C3-C4
3	E	502	AKG	O1-C1-C2-O5
3	E	502	AKG	O1-C1-C2-C3
3	E	502	AKG	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	E	502	AKG	C2-C3-C4-C5
3	F	502	AKG	O1-C1-C2-O5
3	F	502	AKG	O1-C1-C2-C3
3	F	502	AKG	O2-C1-C2-C3
3	F	502	AKG	C2-C3-C4-C5
3	G	502	AKG	O1-C1-C2-C3
3	G	502	AKG	O2-C1-C2-C3
3	H	502	AKG	O2-C1-C2-C3
3	J	502	AKG	C1-C2-C3-C4
3	J	502	AKG	O5-C2-C3-C4
3	J	502	AKG	C2-C3-C4-C5
2	F	501	NAP	O4B-C4B-C5B-O5B
3	G	502	AKG	C2-C3-C4-C5
2	G	501	NAP	O4D-C4D-C5D-O5D
3	D	502	AKG	C2-C3-C4-C5
3	H	502	AKG	C2-C3-C4-C5
2	F	501	NAP	C3B-C4B-C5B-O5B
2	J	501	NAP	C2N-C3N-C7N-N7N
2	J	501	NAP	C2N-C3N-C7N-O7N
2	C	501	NAP	C2B-O2B-P2B-O2X
2	D	501	NAP	C2B-O2B-P2B-O2X
2	E	501	NAP	C5D-O5D-PN-O3
2	J	501	NAP	C5B-O5B-PA-O3
2	J	501	NAP	C5D-O5D-PN-O3
2	J	501	NAP	C5D-O5D-PN-O2N
3	B	502	AKG	O1-C1-C2-O5
3	C	502	AKG	O1-C1-C2-O5
3	G	502	AKG	O1-C1-C2-O5
3	J	502	AKG	O1-C1-C2-O5
3	B	502	AKG	O1-C1-C2-C3
3	J	502	AKG	O1-C1-C2-C3
2	H	501	NAP	O4D-C4D-C5D-O5D
2	J	501	NAP	C4N-C3N-C7N-N7N
3	B	502	AKG	O2-C1-C2-O5
3	F	502	AKG	O2-C1-C2-O5
3	J	502	AKG	O2-C1-C2-O5
2	J	501	NAP	C4N-C3N-C7N-O7N
2	D	501	NAP	O4B-C4B-C5B-O5B
2	E	501	NAP	O4B-C4B-C5B-O5B
2	A	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	O4B-C4B-C5B-O5B
3	G	502	AKG	C3-C4-C5-O4

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Mol	Chain	Res	Type	Atoms
3	G	502	AKG	C3-C4-C5-O3
3	F	502	AKG	C3-C4-C5-O4
3	C	502	AKG	C3-C4-C5-O4
3	E	502	AKG	C3-C4-C5-O3
2	J	501	NAP	O4B-C4B-C5B-O5B
3	C	502	AKG	C3-C4-C5-O3
3	E	502	AKG	C3-C4-C5-O4
3	F	502	AKG	C3-C4-C5-O3
3	H	502	AKG	C3-C4-C5-O4
3	H	502	AKG	C3-C4-C5-O3
2	H	501	NAP	C2B-O2B-P2B-O1X
3	J	502	AKG	O2-C1-C2-C3
3	A	502	AKG	C3-C4-C5-O3
2	G	501	NAP	O4B-C4B-C5B-O5B
3	A	502	AKG	C3-C4-C5-O4
2	A	501	NAP	C2B-O2B-P2B-O2X
2	C	501	NAP	C2B-O2B-P2B-O3X
2	D	501	NAP	C2B-O2B-P2B-O3X
2	D	501	NAP	C5D-O5D-PN-O3
2	E	501	NAP	C2D-C1D-N1N-C6N
2	F	501	NAP	C2B-O2B-P2B-O2X
2	F	501	NAP	C2D-C1D-N1N-C6N
2	H	501	NAP	C2B-O2B-P2B-O2X
2	C	501	NAP	O4B-C4B-C5B-O5B
2	G	501	NAP	C3D-C4D-C5D-O5D
2	H	501	NAP	C3D-C4D-C5D-O5D
2	G	501	NAP	C5D-O5D-PN-O1N
3	F	502	AKG	C1-C2-C3-C4
2	H	501	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

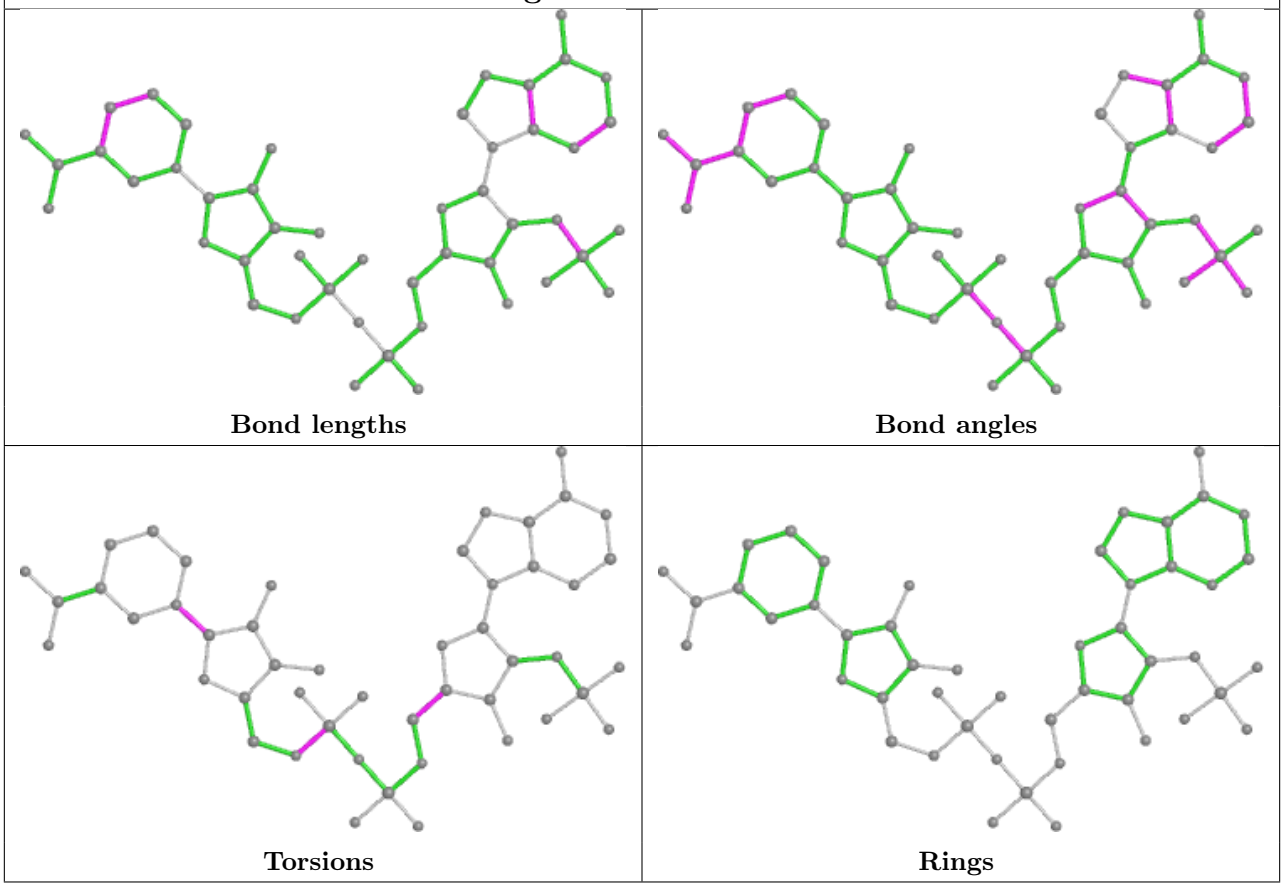
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	502	AKG	1	0
3	B	502	AKG	2	0
2	G	501	NAP	2	0
3	E	502	AKG	1	0

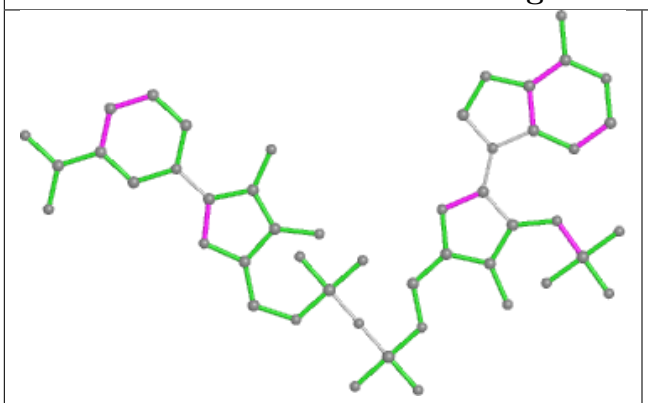
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

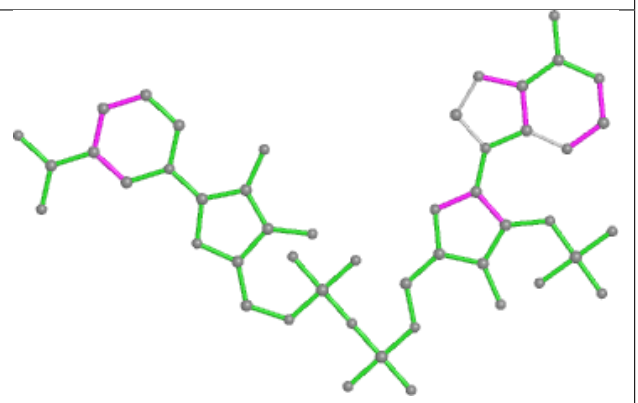
Ligand NAP E 501



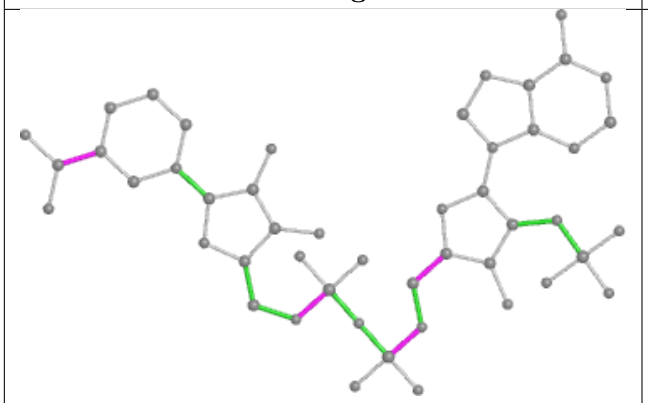
Ligand NAP J 501



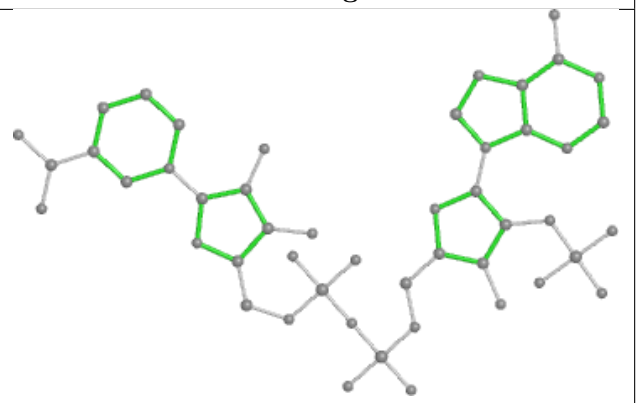
Bond lengths



Bond angles

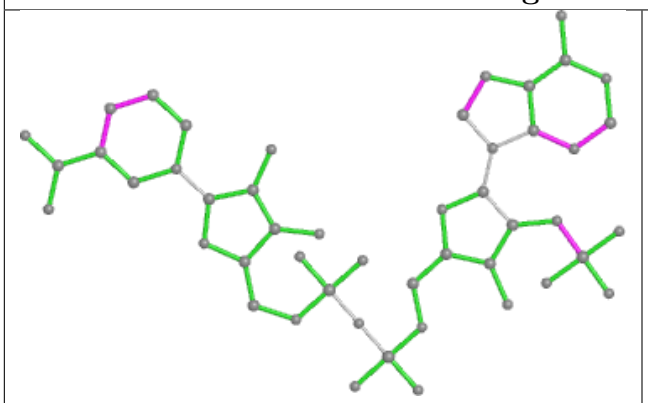


Torsions



Rings

Ligand NAP D 501



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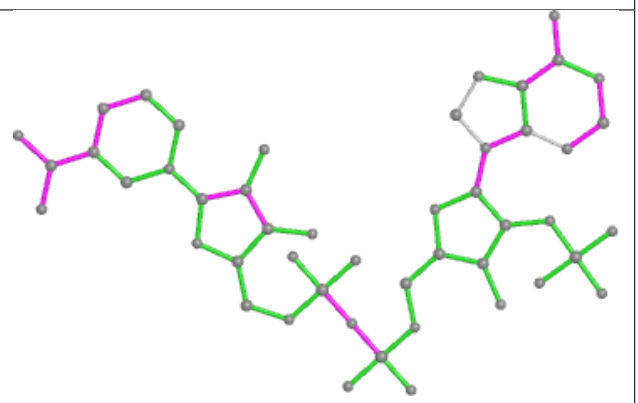
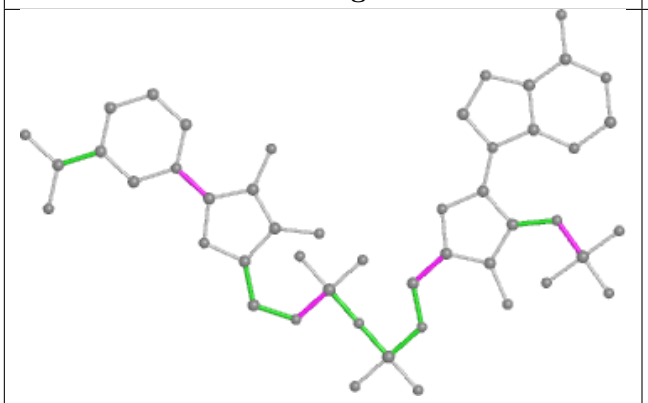
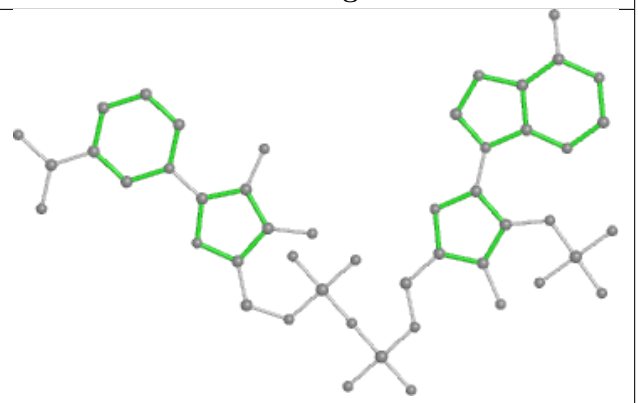


Bond angles

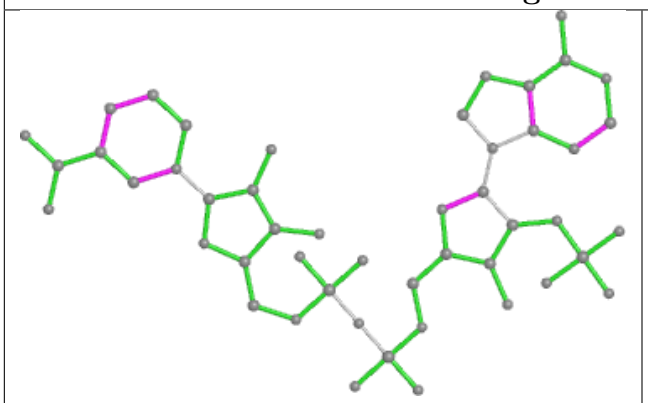


Torsions

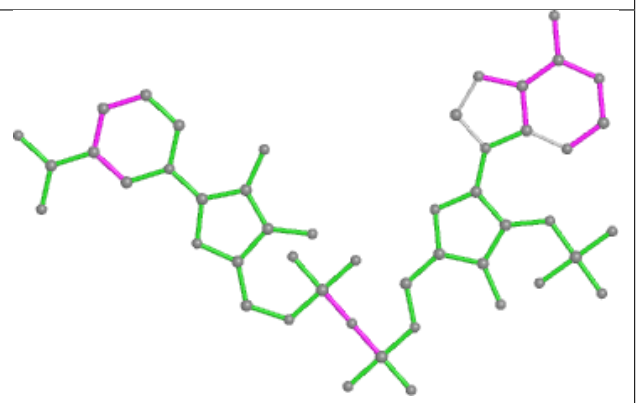


Rings

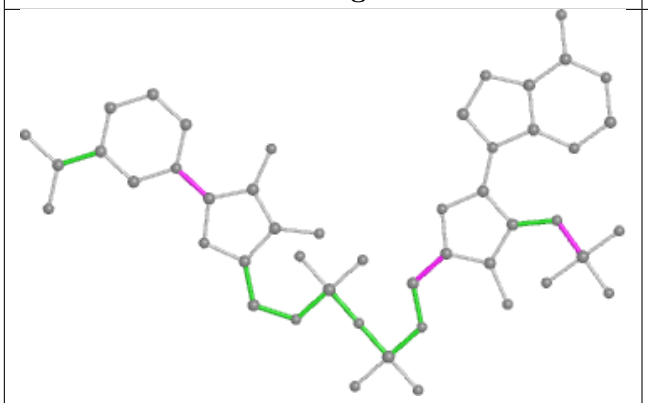
Ligand NAP B 501



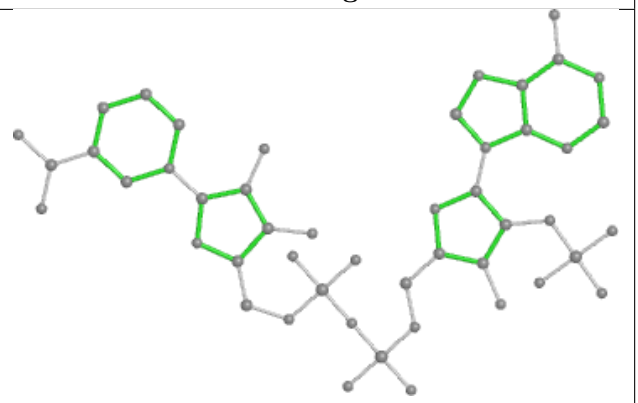
Bond lengths



Bond angles

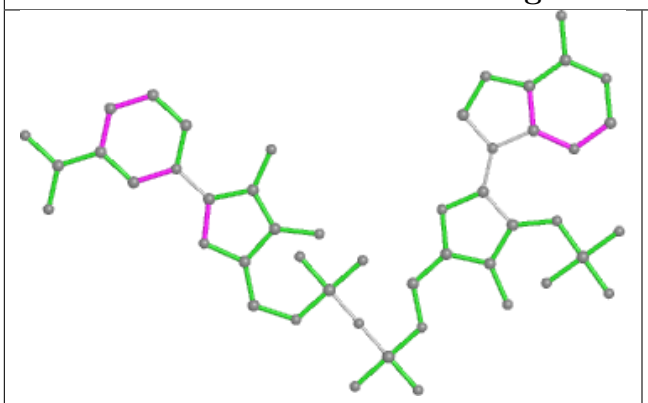


Torsions

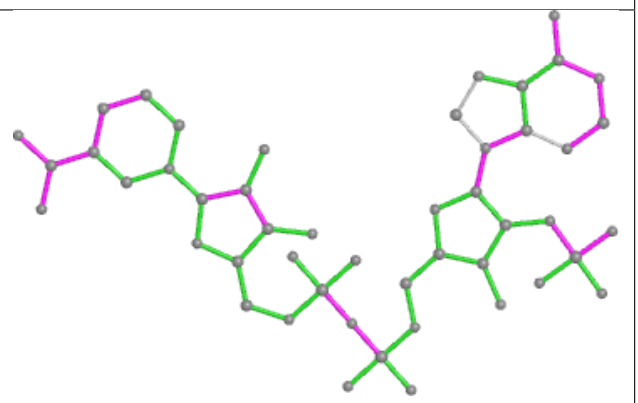


Rings

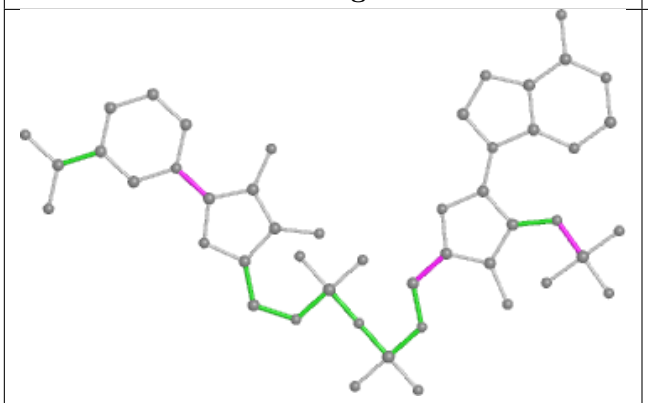
Ligand NAP F 501



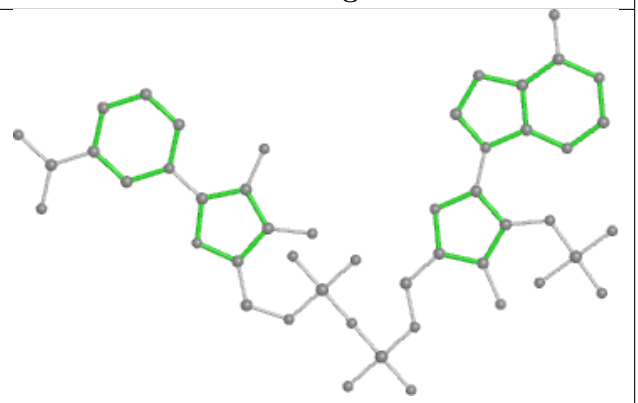
Bond lengths



Bond angles

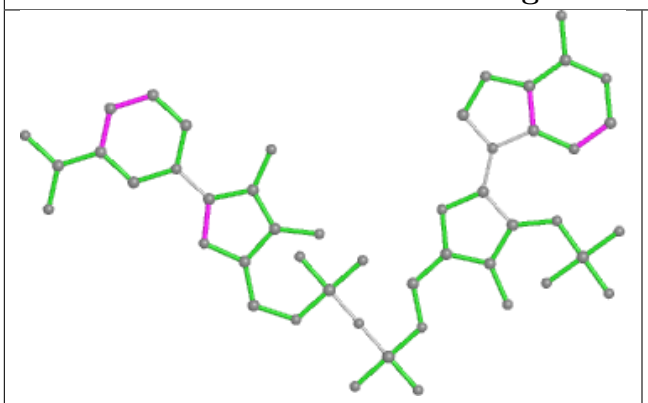


Torsions



Rings

Ligand NAP G 501



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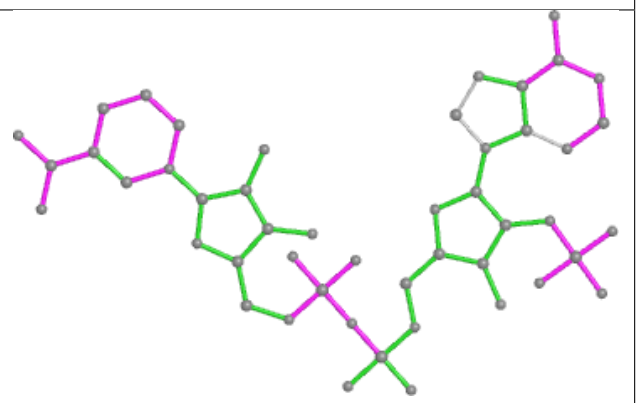

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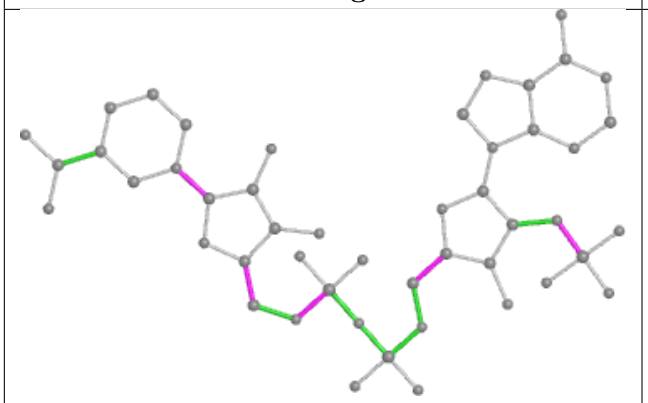

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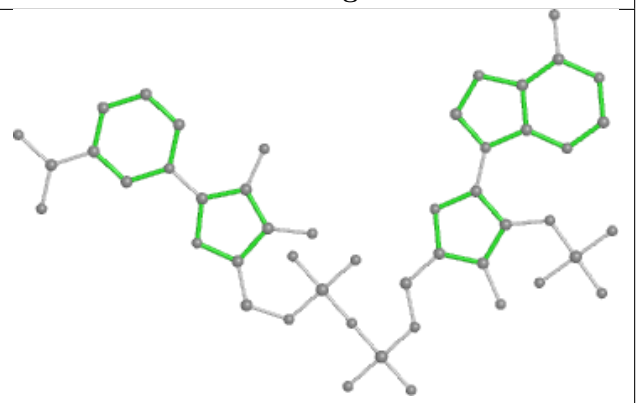
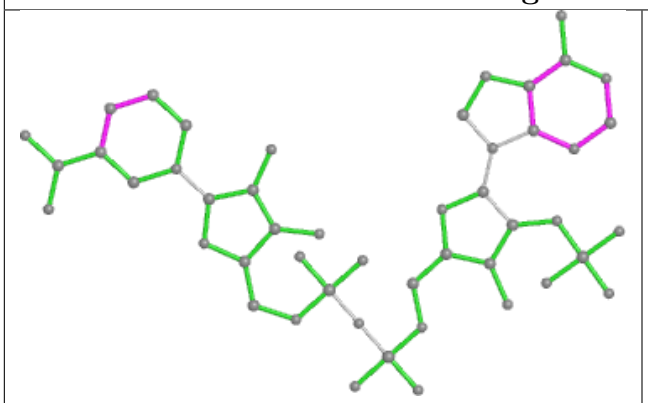


Rings

Ligand NAP H 501



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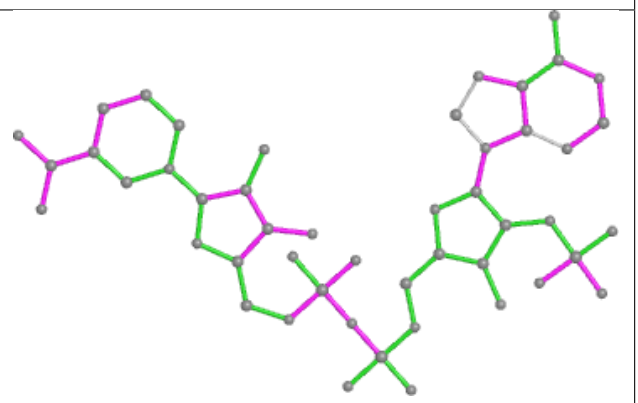
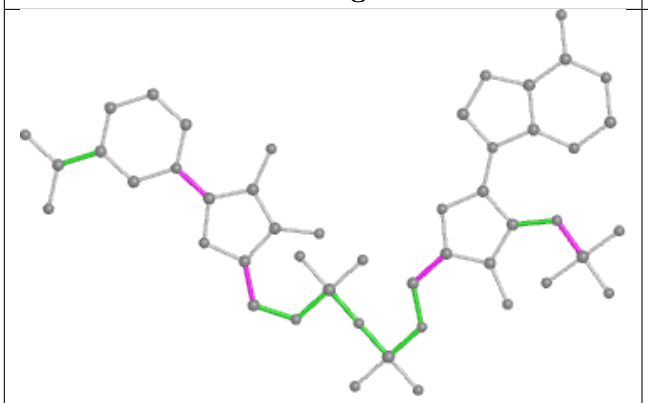


Bond angles



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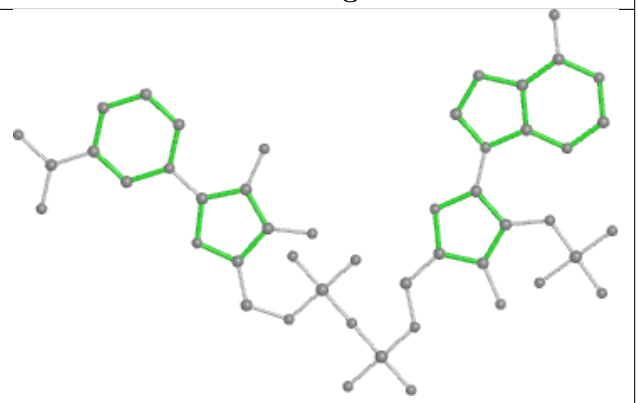
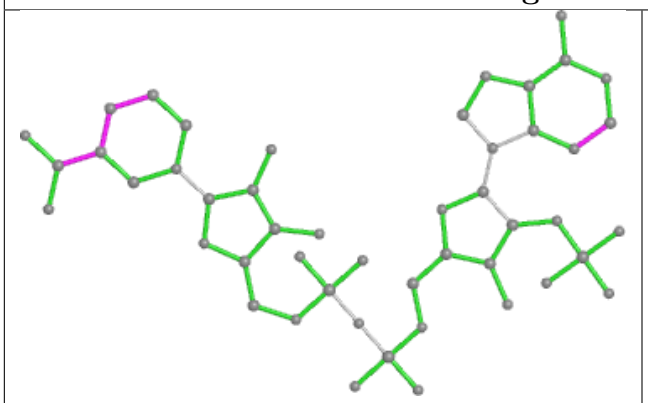
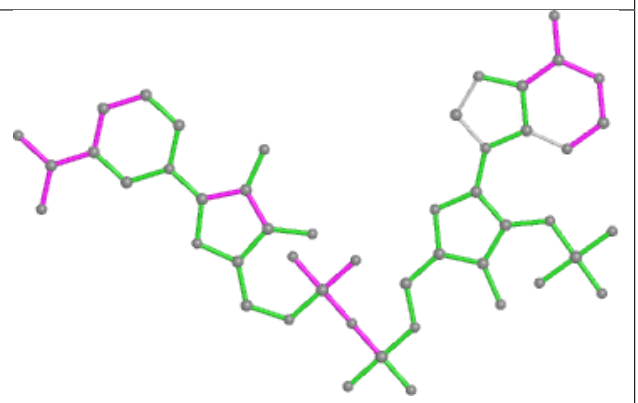


Rings

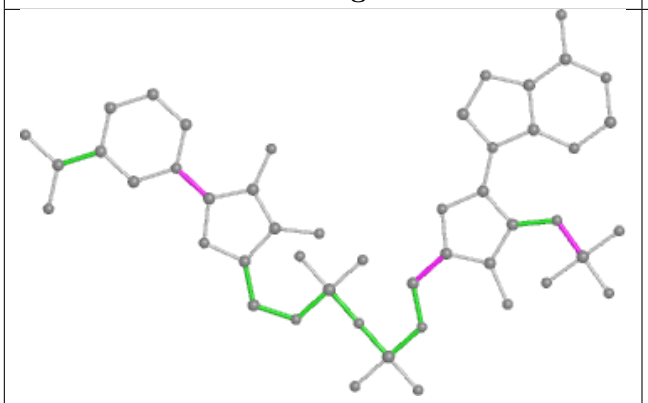
Ligand NAP A 501



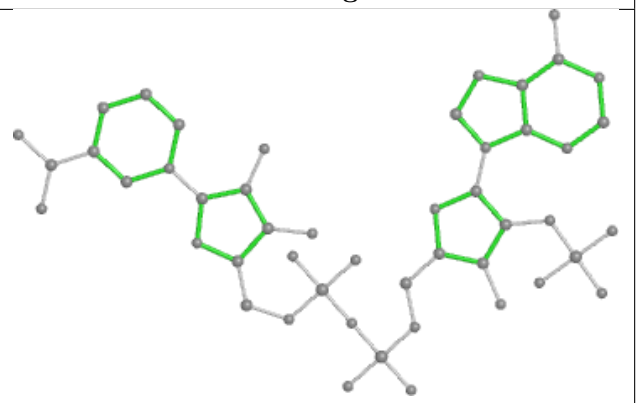
Bond lengths



Bond angles

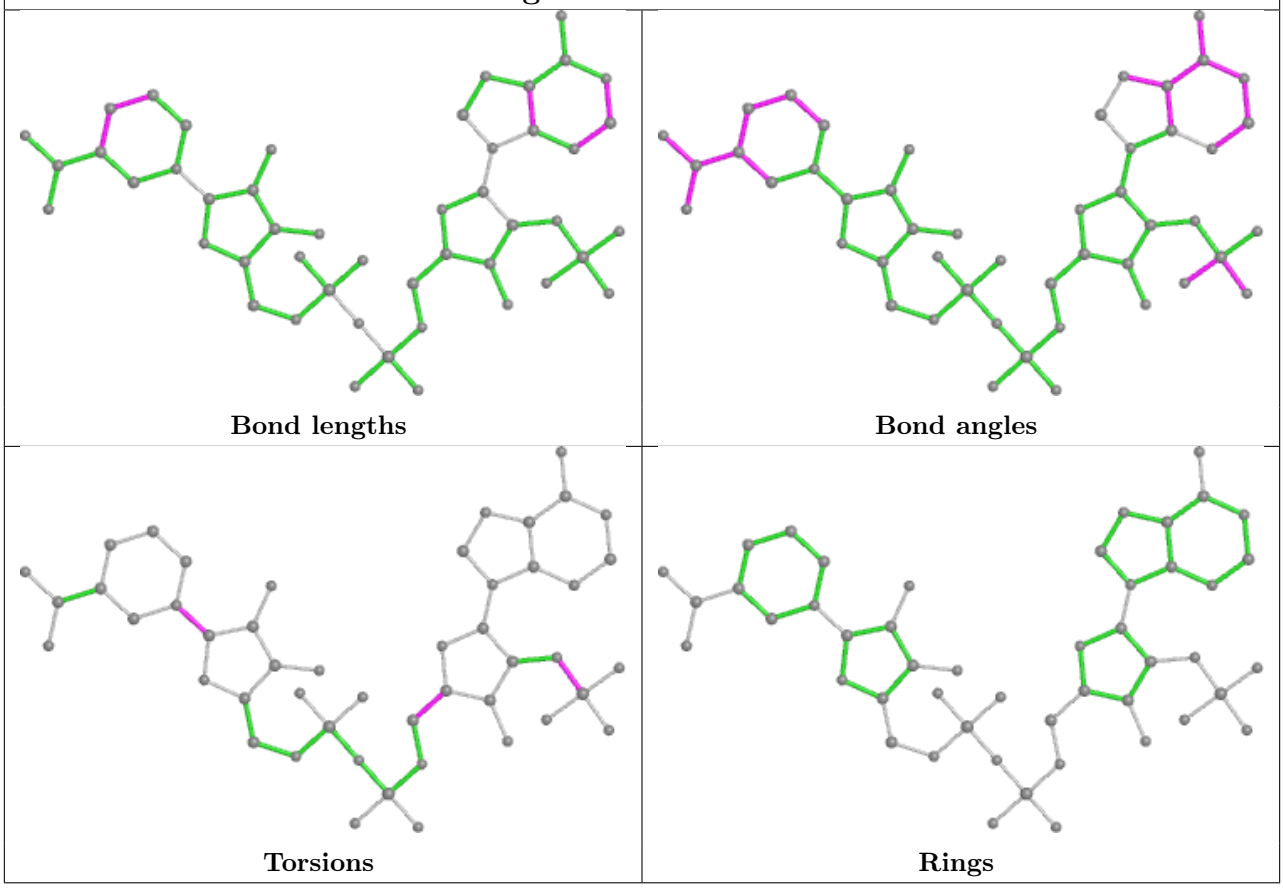


Torsions



Rings

Ligand NAP C 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	447/447 (100%)	-0.27	4 (0%)	84	88	10, 16, 33, 63	0
1	B	447/447 (100%)	-0.37	1 (0%)	95	96	8, 15, 31, 61	0
1	C	447/447 (100%)	-0.35	1 (0%)	95	96	8, 15, 33, 67	0
1	D	447/447 (100%)	-0.23	6 (1%)	77	81	9, 16, 36, 70	0
1	E	447/447 (100%)	-0.25	4 (0%)	84	88	8, 17, 34, 76	0
1	F	447/447 (100%)	-0.19	3 (0%)	87	91	9, 18, 37, 53	0
1	G	447/447 (100%)	-0.29	5 (1%)	80	85	11, 19, 38, 77	0
1	H	447/447 (100%)	-0.10	12 (2%)	54	62	12, 22, 45, 66	0
1	I	447/447 (100%)	0.20	45 (10%)	7	9	8, 23, 69, 91	0
1	J	447/447 (100%)	1.73	148 (33%)	0	0	13, 45, 117, 146	0
1	K	304/447 (68%)	0.57	50 (16%)	1	2	17, 30, 75, 99	0
1	L	447/447 (100%)	-0.01	21 (4%)	31	38	12, 26, 54, 96	0
All	All	5221/5364 (97%)	0.02	300 (5%)	23	30	8, 20, 65, 146	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	314	CYS	15.3
1	J	328	GLY	13.8
1	J	320	CYS	12.2
1	J	277	VAL	10.8
1	J	274	GLY	10.5
1	J	343	ALA	10.3
1	J	319	PRO	10.1
1	J	300	GLY	9.7
1	J	340	ARG	9.7
1	I	1	MET	8.9
1	J	266	SER	8.5

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Mol	Chain	Res	Type	RSRZ
1	J	342	VAL	8.3
1	I	266	SER	8.2
1	J	306	ASP	8.1
1	J	296	ASP	7.9
1	J	272	PRO	7.8
1	J	307	GLY	7.8
1	J	230	SER	7.7
1	J	303	TYR	7.7
1	J	345	GLY	7.6
1	J	276	ASP	7.5
1	J	275	VAL	7.4
1	J	321	ALA	7.3
1	K	1	MET	7.3
1	J	286	VAL	7.2
1	J	353	GLU	7.2
1	I	307	GLY	7.2
1	J	341	PHE	7.1
1	J	346	ALA	7.1
1	J	315	ASP	7.1
1	J	309	ILE	6.9
1	J	361	ARG	6.9
1	J	259	VAL	6.9
1	J	244	VAL	6.9
1	J	237	ILE	6.8
1	L	3	VAL	6.8
1	J	311	ASP	6.8
1	J	329	GLU	6.8
1	J	308	SER	6.8
1	J	293	VAL	6.8
1	J	302	THR	6.7
1	L	1	MET	6.7
1	J	260	ILE	6.6
1	J	226	ALA	6.6
1	J	228	GLY	6.5
1	J	223	MET	6.3
1	J	366	GLY	6.3
1	J	351	THR	6.3
1	J	318	LEU	6.3
1	J	327	ASN	6.2
1	J	344	GLU	6.1
1	J	337	ASN	6.0
1	J	349	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
1	J	339	CYS	5.8
1	J	247	TYR	5.7
1	J	290	ARG	5.7
1	J	359	ARG	5.6
1	J	1	MET	5.6
1	J	289	ALA	5.4
1	J	352	PRO	5.4
1	J	316	ILE	5.4
1	J	263	SER	5.3
1	L	44	HIS	5.2
1	J	326	LEU	5.1
1	J	231	ILE	5.1
1	G	1	MET	5.1
1	J	287	ARG	5.0
1	K	417	ALA	5.0
1	I	336	ASP	5.0
1	J	304	HIS	5.0
1	J	264	ASP	4.9
1	J	357	VAL	4.9
1	I	306	ASP	4.9
1	J	238	VAL	4.9
1	J	324	ASN	4.9
1	K	216	CYS	4.9
1	J	218	TYR	4.8
1	J	365	PHE	4.8
1	J	283	ILE	4.8
1	J	317	ALA	4.8
1	E	1	MET	4.8
1	K	218	TYR	4.8
1	J	268	TRP	4.8
1	J	294	TYR	4.7
1	K	223	MET	4.7
1	J	292	SER	4.7
1	J	350	SER	4.7
1	J	240	GLY	4.7
1	K	3	VAL	4.7
1	K	13	MET	4.6
1	J	305	THR	4.6
1	J	288	ARG	4.6
1	J	269	VAL	4.6
1	J	301	ALA	4.5
1	J	216	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	1	MET	4.5
1	J	279	LYS	4.5
1	K	2	THR	4.4
1	J	224	ILE	4.4
1	B	1	MET	4.4
1	J	360	GLU	4.4
1	I	3	VAL	4.4
1	I	228	GLY	4.4
1	J	291	VAL	4.4
1	J	295	ALA	4.4
1	J	262	PHE	4.3
1	J	333	THR	4.3
1	J	299	GLU	4.3
1	I	286	VAL	4.3
1	K	226	ALA	4.2
1	L	13	MET	4.2
1	J	297	GLU	4.2
1	J	282	GLU	4.2
1	K	217	VAL	4.2
1	K	9	ASN	4.1
1	K	31	VAL	4.1
1	J	368	GLY	4.1
1	D	1	MET	4.1
1	K	39	LEU	4.1
1	J	347	ASN	4.0
1	J	256	GLY	4.0
1	I	329	GLU	3.9
1	H	9	ASN	3.9
1	I	256	GLY	3.9
1	I	282	GLU	3.9
1	J	331	ALA	3.9
1	K	227	LYS	3.8
1	J	227	LYS	3.8
1	K	22	PRO	3.8
1	J	253	GLN	3.7
1	I	296	ASP	3.7
1	K	219	PHE	3.7
1	J	336	ASP	3.7
1	I	293	VAL	3.7
1	K	41	LYS	3.7
1	K	7	VAL	3.7
1	K	6	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.6
1	I	327	ASN	3.6
1	J	265	SER	3.6
1	J	3	VAL	3.6
1	J	356	GLU	3.6
1	K	29	ALA	3.6
1	K	5	GLU	3.5
1	L	6	GLN	3.5
1	K	40	GLU	3.5
1	J	235	LYS	3.5
1	J	246	THR	3.5
1	K	214	TYR	3.5
1	J	273	ASN	3.4
1	J	285	GLU	3.4
1	L	360	GLU	3.4
1	I	238	VAL	3.4
1	I	305	THR	3.4
1	J	239	SER	3.4
1	K	4	ASP	3.4
1	L	43	PRO	3.4
1	K	12	ASP	3.3
1	J	355	VAL	3.3
1	J	5	GLU	3.2
1	K	213	GLY	3.2
1	J	281	ARG	3.2
1	L	9	ASN	3.2
1	J	258	THR	3.2
1	K	44	HIS	3.2
1	H	3	VAL	3.1
1	I	9	ASN	3.1
1	J	232	SER	3.1
1	E	299	GLU	3.1
1	J	417	ALA	3.1
1	K	42	ASP	3.0
1	J	335	ALA	3.0
1	I	240	GLY	3.0
1	K	366	GLY	3.0
1	J	363	ILE	3.0
1	J	229	GLU	3.0
1	I	311	ASP	2.9
1	K	33	GLU	2.9
1	E	40	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	271	THR	2.9
1	K	419	TYR	2.9
1	J	261	GLY	2.9
1	L	329	GLU	2.9
1	J	298	VAL	2.9
1	H	13	MET	2.8
1	J	334	LEU	2.8
1	J	242	GLY	2.8
1	J	245	ALA	2.8
1	K	221	SER	2.8
1	J	422	GLU	2.8
1	I	299	GLU	2.8
1	J	236	ILE	2.8
1	K	26	GLN	2.8
1	J	330	ASN	2.8
1	J	367	PRO	2.8
1	J	338	GLY	2.7
1	L	228	GLY	2.7
1	J	255	LEU	2.7
1	H	5	GLU	2.7
1	J	243	ASN	2.7
1	J	39	LEU	2.7
1	J	332	LYS	2.7
1	K	426	VAL	2.7
1	A	40	GLU	2.7
1	A	44	HIS	2.7
1	K	34	SER	2.7
1	J	310	TRP	2.6
1	J	249	ILE	2.6
1	G	299	GLU	2.6
1	J	280	LEU	2.6
1	J	372	ASN	2.6
1	J	423	ASN	2.6
1	G	5	GLU	2.6
1	L	353	GLU	2.6
1	J	267	GLY	2.6
1	F	1	MET	2.5
1	K	25	HIS	2.5
1	J	40	GLU	2.5
1	L	274	GLY	2.5
1	I	241	SER	2.5
1	H	12	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	362	ASP	2.5
1	H	2	THR	2.5
1	I	267	GLY	2.5
1	L	5	GLU	2.5
1	L	15	LEU	2.5
1	K	28	VAL	2.5
1	J	322	THR	2.5
1	I	337	ASN	2.5
1	K	224	ILE	2.5
1	L	306	ASP	2.5
1	I	301	ALA	2.4
1	I	273	ASN	2.4
1	D	306	ASP	2.4
1	C	1	MET	2.4
1	I	5	GLU	2.4
1	J	395	GLU	2.4
1	J	44	HIS	2.4
1	L	11	TYR	2.4
1	I	332	LYS	2.3
1	I	361	ARG	2.3
1	K	10	TYR	2.3
1	I	289	ALA	2.3
1	I	339	CYS	2.3
1	K	37	ILE	2.3
1	I	294	TYR	2.3
1	J	364	ARG	2.3
1	H	286	VAL	2.3
1	D	420	GLY	2.3
1	J	416	ALA	2.3
1	I	276	ASP	2.3
1	I	274	GLY	2.3
1	G	4	ASP	2.3
1	I	255	LEU	2.3
1	I	352	PRO	2.3
1	H	289	ALA	2.3
1	L	40	GLU	2.3
1	H	295	ALA	2.3
1	J	252	ALA	2.3
1	K	8	SER	2.3
1	K	30	GLU	2.2
1	D	299	GLU	2.2
1	J	42	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	6	GLN	2.2
1	I	44	HIS	2.2
1	G	300	GLY	2.2
1	K	32	LEU	2.2
1	E	286	VAL	2.2
1	D	4	ASP	2.2
1	J	396	TYR	2.2
1	K	16	LYS	2.2
1	H	10	TYR	2.1
1	I	357	VAL	2.1
1	J	2	THR	2.1
1	K	415	THR	2.1
1	K	222	GLU	2.1
1	H	329	GLU	2.1
1	F	2	THR	2.1
1	J	9	ASN	2.1
1	I	290	ARG	2.1
1	I	8	SER	2.1
1	J	270	HIS	2.1
1	K	416	ALA	2.1
1	I	313	LYS	2.1
1	J	370	ALA	2.1
1	A	16	LYS	2.1
1	I	303	TYR	2.1
1	D	5	GLU	2.1
1	L	42	ASP	2.1
1	I	331	ALA	2.1
1	I	291	VAL	2.1
1	L	8	SER	2.1
1	L	357	VAL	2.1
1	K	209	THR	2.0
1	J	354	ALA	2.0
1	I	292	SER	2.0
1	K	35	LEU	2.0
1	K	409	PHE	2.0
1	L	356	GLU	2.0
1	F	362	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

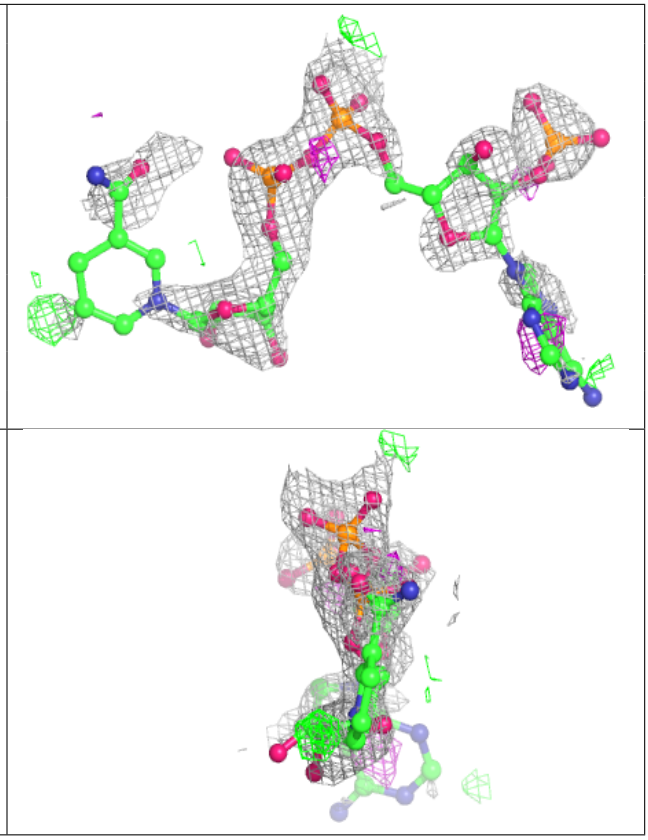
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	J	501	48/48	0.76	0.31	69,96,113,116	0
3	AKG	J	502	10/10	0.83	0.27	40,58,69,71	0
3	AKG	E	502	10/10	0.91	0.20	24,35,41,43	0
3	AKG	B	502	10/10	0.91	0.21	30,33,41,43	0
3	AKG	A	502	10/10	0.92	0.19	23,31,36,39	0
3	AKG	D	502	10/10	0.92	0.22	22,28,42,56	0
3	AKG	H	502	10/10	0.93	0.16	25,33,38,39	0
3	AKG	G	502	10/10	0.94	0.19	21,32,44,48	0
3	AKG	C	502	10/10	0.94	0.14	21,30,35,35	0
3	AKG	F	502	10/10	0.94	0.19	21,32,40,43	0
2	NAP	F	501	48/48	0.96	0.13	11,16,25,27	0
2	NAP	G	501	48/48	0.97	0.12	14,18,31,36	0
2	NAP	H	501	48/48	0.97	0.11	17,24,43,50	0
2	NAP	C	501	48/48	0.97	0.10	12,16,27,32	0
2	NAP	D	501	48/48	0.97	0.14	12,17,29,32	0
2	NAP	E	501	48/48	0.97	0.13	13,18,37,42	0
2	NAP	A	501	48/48	0.97	0.11	12,16,28,32	0
2	NAP	B	501	48/48	0.98	0.10	9,11,21,22	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.

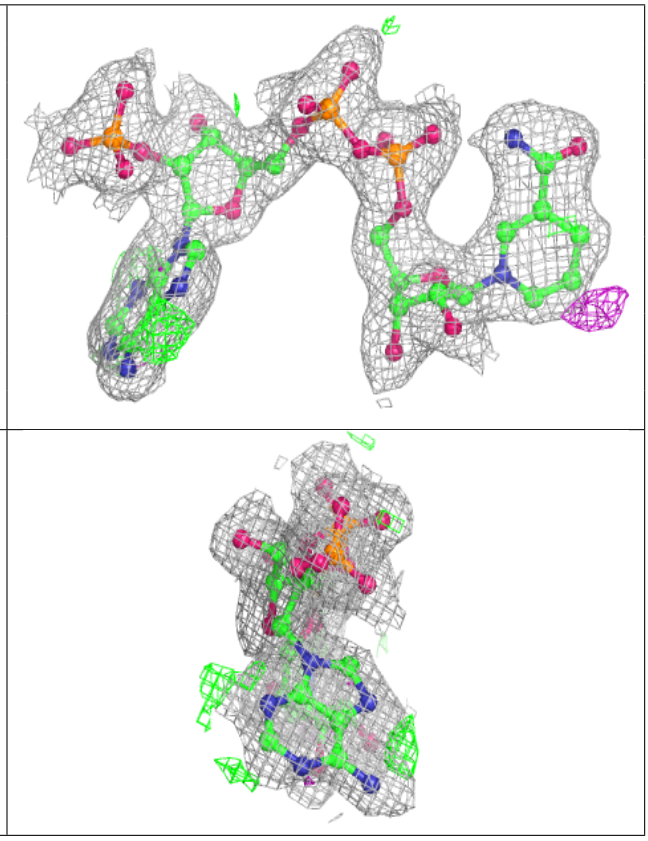
Electron density around NAP J 501:

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



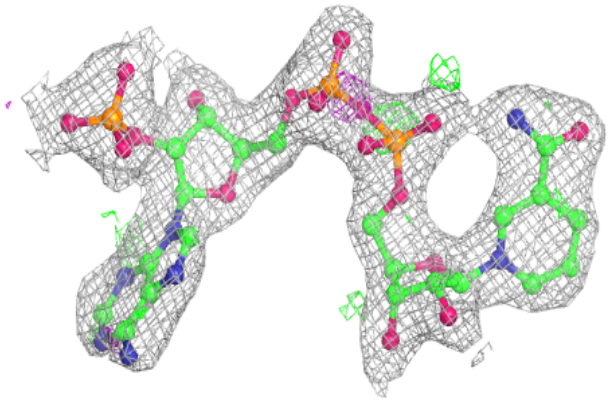
Electron density around NAP F 501:

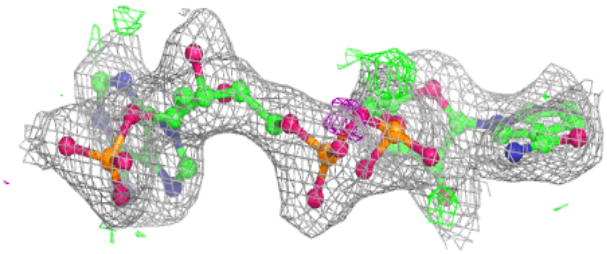
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

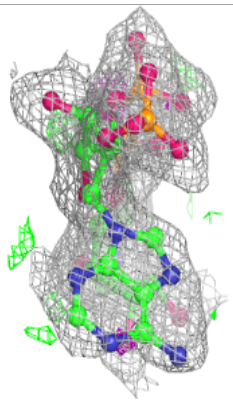


Electron density around NAP G 501:

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

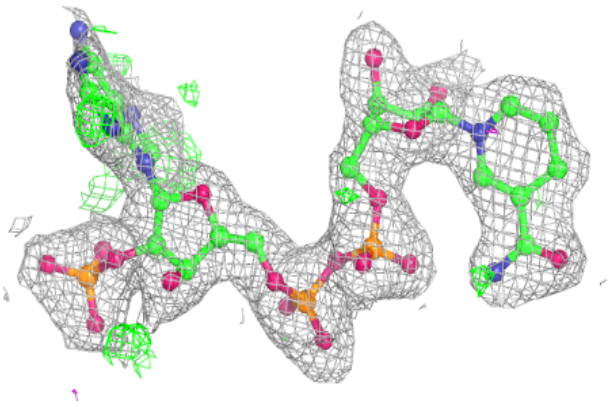


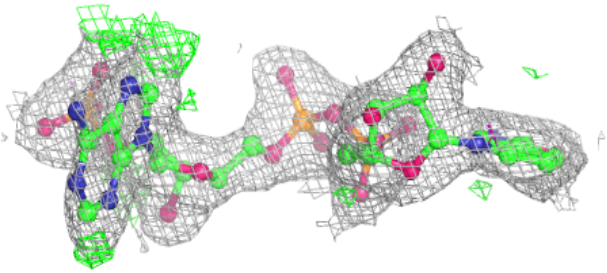




Electron density around NAP H 501:

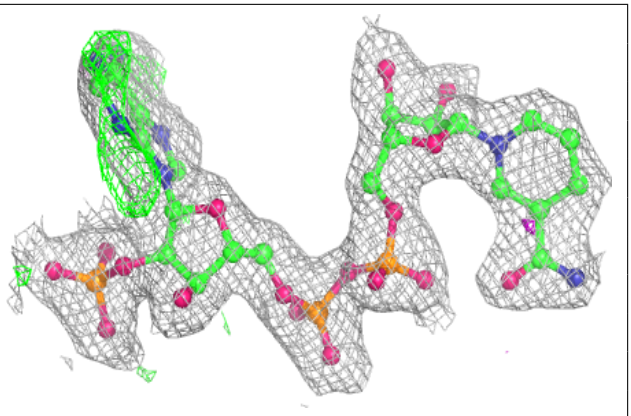
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

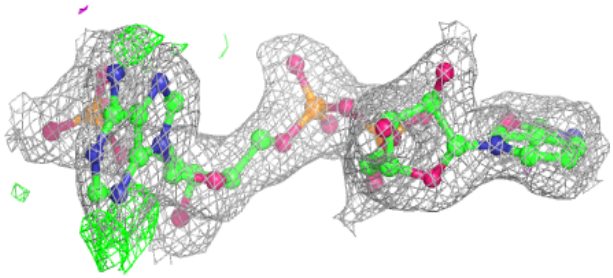


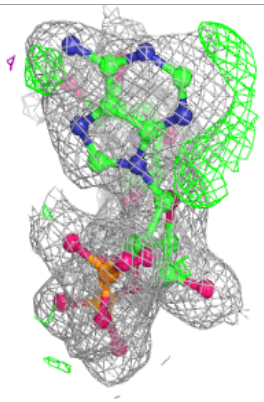


Electron density around NAP C 501:

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

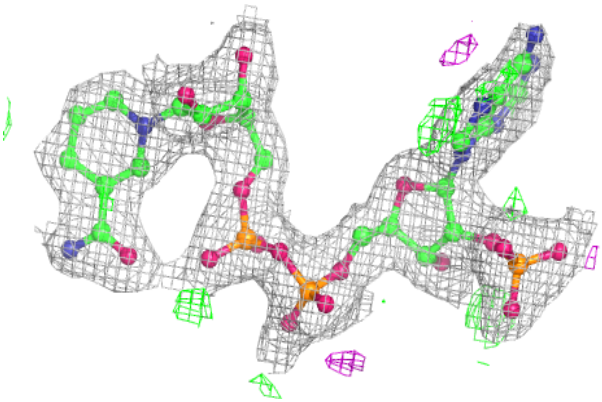


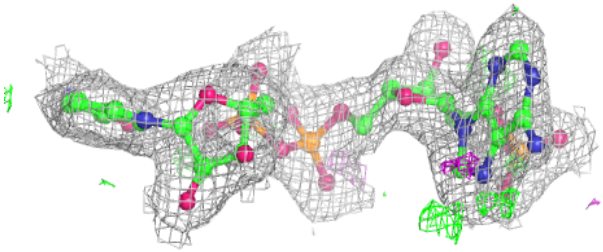


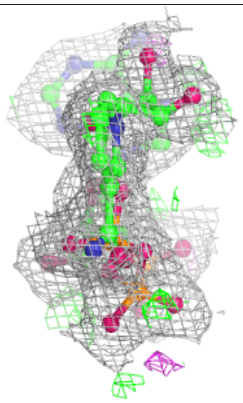


Electron density around NAP D 501:

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

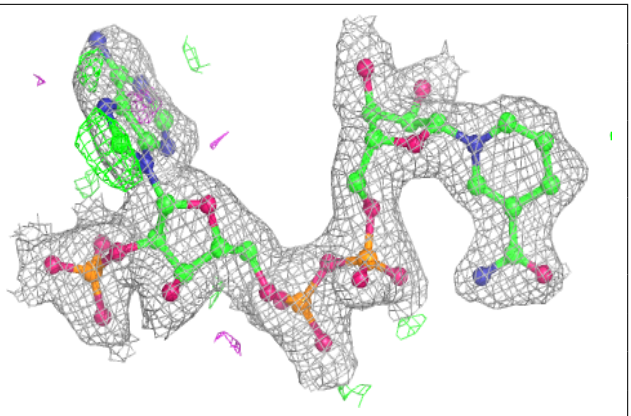


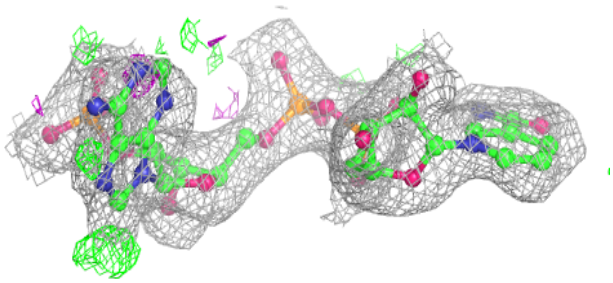


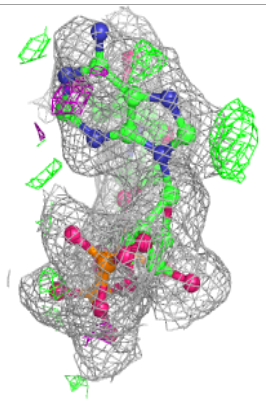


Electron density around NAP E 501:

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

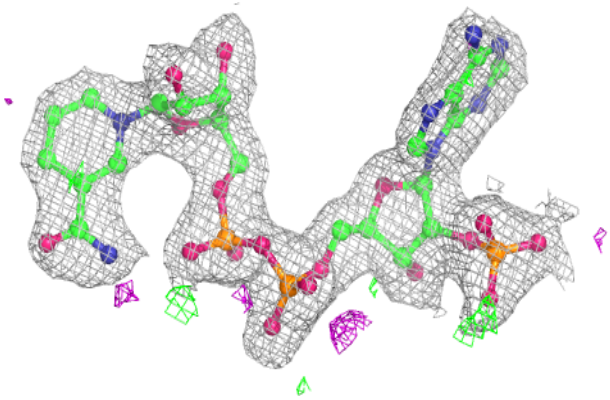


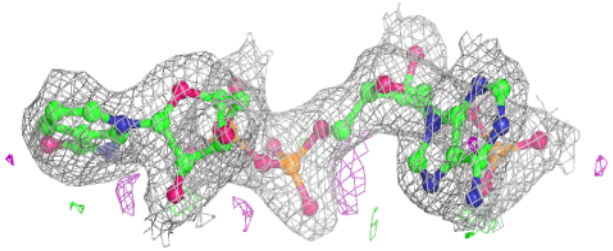


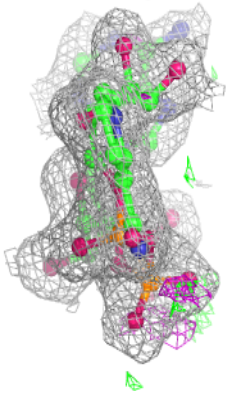


Electron density around NAP A 501:

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

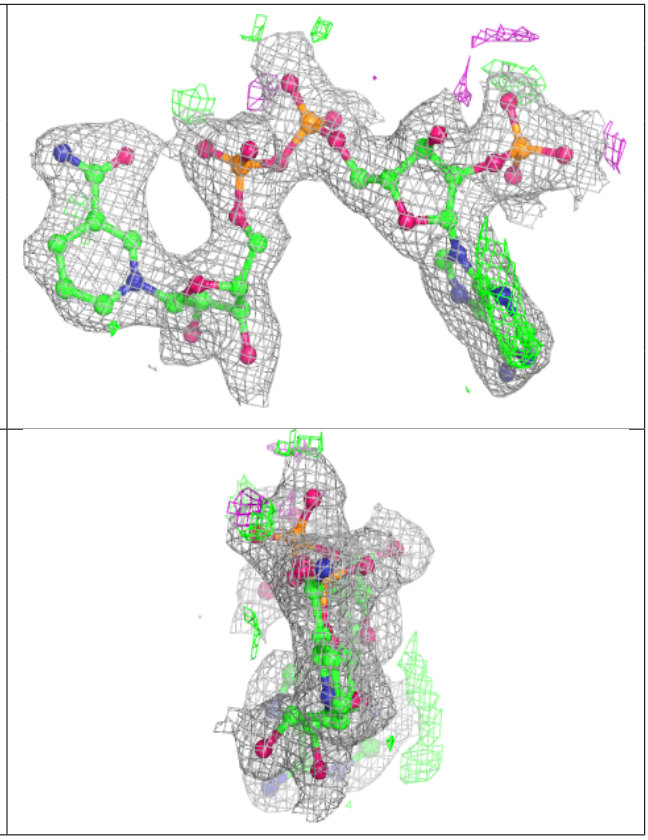






Electron density around NAP B 501:

$2mF_o$-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.