Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 12:11 AM EDT

PDB ID	:	3GR6
Title	:	Crystal structure of the staphylococcus aureus enoyl-acyl carrier protein reductase (fabI) in complex with NADP and triclosan
Authors	:	Priyadarshi, A.; Hwang, K.Y.
Deposited on	:	2009-03-25
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 (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:

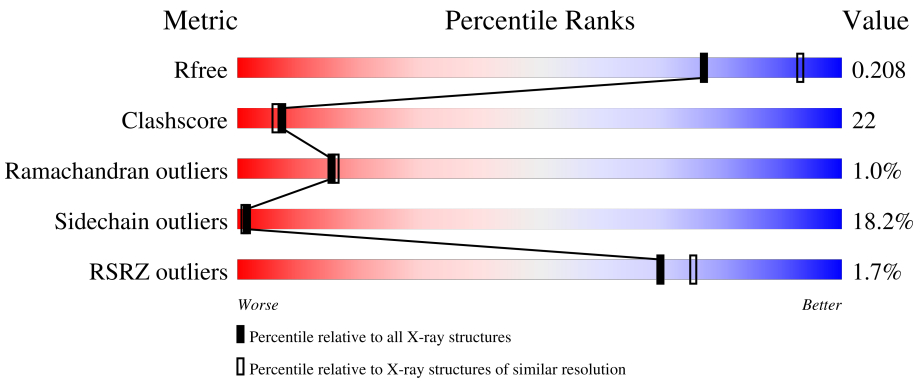
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.28 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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (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 <=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	260	.% 65% 23% 7% • •
1	D	260	.% 63% 23% 9% 5%
1	G	260	.% 61% 25% 8% • •
1	J	260	3% 63% 25% 10% •

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	TCL	A	371	-	-	X	-
3	TCL	D	258	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8334 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

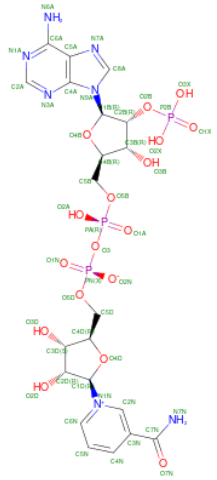
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	1963	1238	339	382	4	0	0	0
1	D	260	1994	1258	344	387	5	0	0	0
1	G	254	1955	1232	338	381	4	0	0	0
1	J	260	1994	1258	344	387	5	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	LEU	-	expression tag	UNP Q6GI75
A	-2	ALA	-	expression tag	UNP Q6GI75
A	-1	ALA	-	expression tag	UNP Q6GI75
A	0	ALA	-	expression tag	UNP Q6GI75
D	-3	LEU	-	expression tag	UNP Q6GI75
D	-2	ALA	-	expression tag	UNP Q6GI75
D	-1	ALA	-	expression tag	UNP Q6GI75
D	0	ALA	-	expression tag	UNP Q6GI75
G	-3	LEU	-	expression tag	UNP Q6GI75
G	-2	ALA	-	expression tag	UNP Q6GI75
G	-1	ALA	-	expression tag	UNP Q6GI75
G	0	ALA	-	expression tag	UNP Q6GI75
J	-3	LEU	-	expression tag	UNP Q6GI75
J	-2	ALA	-	expression tag	UNP Q6GI75
J	-1	ALA	-	expression tag	UNP Q6GI75
J	0	ALA	-	expression tag	UNP Q6GI75

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

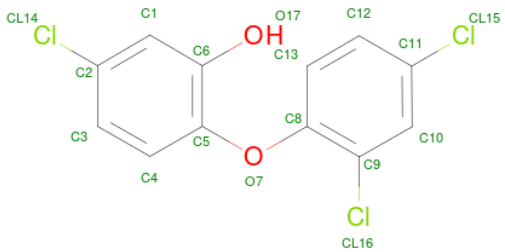
NAP



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

- Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).

TCL



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
3	A	1	17	12	3	2	0	0
3	D	1	17	12	3	2	0	0
3	G	1	17	12	3	2	0	0
3	J	1	17	12	3	2	0	0

- Molecule 4 is water.

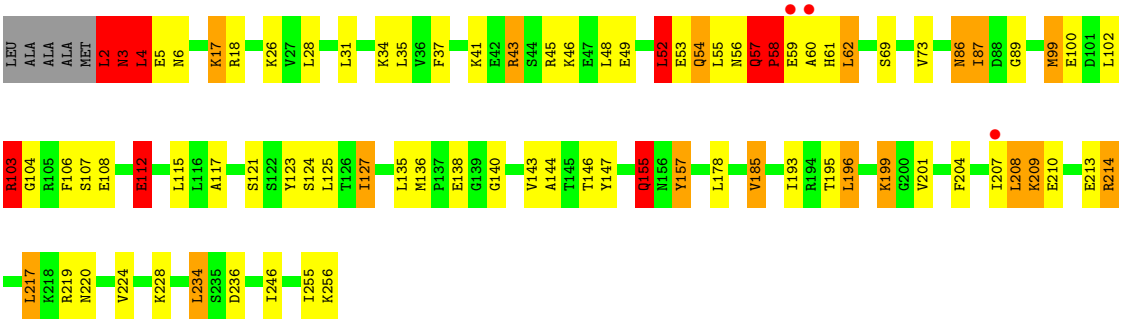
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	41	41	41	0	0
4	D	49	49	49	0	0
4	G	42	42	42	0	0
4	J	36	36	36	0	0

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.

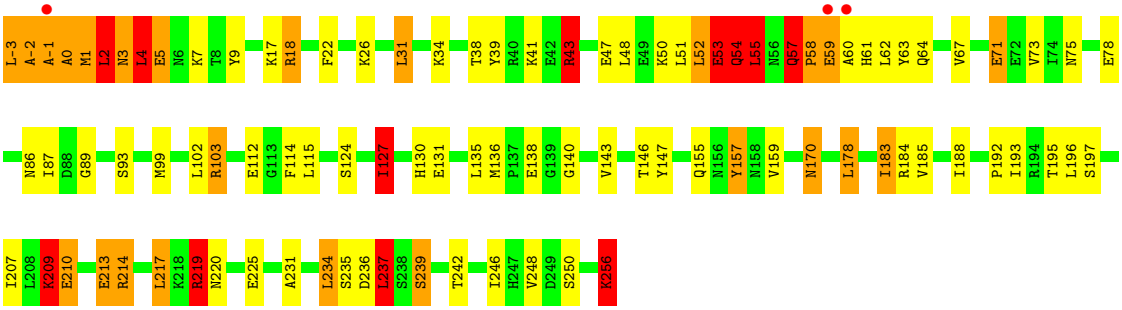
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



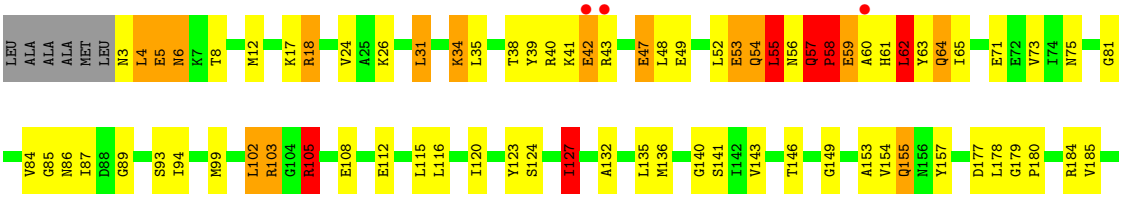
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

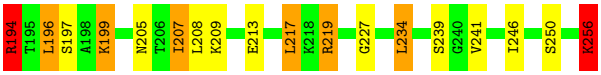
Chain D:



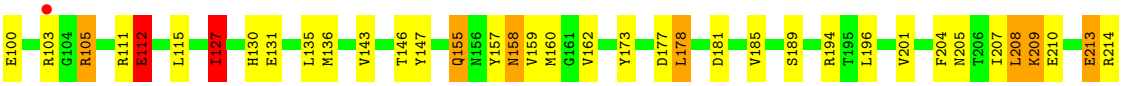
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain G:





• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.56Å 118.44Å 149.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.28 46.46 – 2.28	Depositor EDS
% Data completeness (in resolution range)	90.9 (47.09-2.28) 90.9 (46.46-2.28)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.28	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.264 0.209 , 0.208	Depositor DCC
R_{free} test set	2895 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8334	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: TCL, 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	1.22	6/1990 (0.3%)	1.22	14/2682 (0.5%)
1	D	1.33	12/2021 (0.6%)	1.26	17/2724 (0.6%)
1	G	1.20	3/1982 (0.2%)	1.25	18/2671 (0.7%)
1	J	1.14	6/2021 (0.3%)	1.18	14/2724 (0.5%)
All	All	1.22	27/8014 (0.3%)	1.23	63/10801 (0.6%)

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	3
1	D	1	4
1	G	0	3
1	J	0	6
All	All	1	16

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	210	GLU	CD-OE1	-22.28	1.01	1.25
1	D	-1	ALA	C-N	8.31	1.53	1.34
1	D	59	GLU	CG-CD	7.37	1.63	1.51
1	J	47	GLU	C-N	7.24	1.50	1.34
1	D	112	GLU	CG-CD	6.78	1.62	1.51
1	D	239	SER	CB-OG	-6.30	1.34	1.42
1	A	53	GLU	CB-CG	6.15	1.63	1.52
1	J	112	GLU	CB-CG	6.08	1.63	1.52
1	A	157	TYR	CD2-CE2	-6.04	1.30	1.39
1	D	157	TYR	CD2-CE2	-6.04	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	59	GLU	CG-CD	6.03	1.61	1.51
1	A	108	GLU	CD-OE1	5.79	1.32	1.25
1	D	210	GLU	CD-OE2	5.70	1.31	1.25
1	A	112	GLU	CG-CD	5.64	1.60	1.51
1	A	53	GLU	CG-CD	5.59	1.60	1.51
1	D	5	GLU	CB-CG	5.57	1.62	1.52
1	D	71	GLU	CG-CD	5.57	1.60	1.51
1	G	155	GLN	C-O	5.54	1.33	1.23
1	D	47	GLU	C-N	5.53	1.46	1.34
1	J	100	GLU	CG-CD	5.46	1.60	1.51
1	D	59	GLU	CB-CG	5.36	1.62	1.52
1	J	34	LYS	CD-CE	5.35	1.64	1.51
1	G	155	GLN	CG-CD	5.35	1.63	1.51
1	J	3	ASN	C-N	5.16	1.46	1.34
1	D	209	LYS	C-N	5.08	1.45	1.34
1	J	162	VAL	CA-CB	5.07	1.65	1.54
1	A	155	GLN	CG-CD	5.05	1.62	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	0	ALA	CB-CA-C	-10.88	93.78	110.10
1	G	194	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	D	210	GLU	OE1-CD-OE2	9.34	134.51	123.30
1	A	214	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	D	54	GLN	N-CA-C	8.72	134.56	111.00
1	D	210	GLU	CG-CD-OE1	-8.53	101.23	118.30
1	J	0	ALA	N-CA-C	8.52	134.01	111.00
1	J	54	GLN	N-CA-C	8.50	133.94	111.00
1	D	4	LEU	CA-CB-CG	8.37	134.56	115.30
1	D	237	LEU	CA-CB-CG	8.32	134.43	115.30
1	A	54	GLN	N-CA-C	8.17	133.05	111.00
1	A	86	ASN	CB-CA-C	7.85	126.11	110.40
1	D	55	LEU	CA-CB-CG	7.58	132.73	115.30
1	D	219	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	104	GLY	N-CA-C	-7.40	94.61	113.10
1	D	52	LEU	CA-CB-CG	7.21	131.89	115.30
1	J	219	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	G	102	LEU	CA-CB-CG	6.65	130.60	115.30
1	G	194	ARG	CG-CD-NE	-6.54	98.07	111.80
1	G	54	GLN	N-CA-CB	-6.49	98.92	110.60
1	A	4	LEU	N-CA-C	6.49	128.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	LEU	CA-CB-CG	6.49	130.22	115.30
1	D	43	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	G	219	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	J	219	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	214	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	J	61	HIS	N-CA-C	6.43	128.37	111.00
1	G	105	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	J	0	ALA	C-N-CA	6.38	137.65	121.70
1	J	239	SER	N-CA-CB	-6.37	100.95	110.50
1	A	52	LEU	CA-CB-CG	-6.29	100.83	115.30
1	J	18	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	G	54	GLN	CB-CA-C	6.28	122.95	110.40
1	A	53	GLU	C-N-CA	6.26	137.35	121.70
1	D	2	LEU	CA-CB-CG	6.10	129.32	115.30
1	D	157	TYR	CB-CA-C	6.07	122.54	110.40
1	D	256	LYS	CA-C-O	6.07	132.84	120.10
1	G	47	GLU	O-C-N	6.04	132.37	122.70
1	D	127	ILE	CB-CA-C	-5.88	99.84	111.60
1	D	219	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	G	256	LYS	CA-C-O	5.86	132.40	120.10
1	J	5	GLU	C-N-CA	-5.77	107.26	121.70
1	G	54	GLN	N-CA-C	5.76	126.55	111.00
1	D	155	GLN	C-N-CA	-5.66	107.55	121.70
1	A	53	GLU	CA-C-N	5.66	129.65	117.20
1	G	256	LYS	N-CA-C	5.59	126.10	111.00
1	D	31	LEU	CA-CB-CG	5.58	128.14	115.30
1	G	18	ARG	CB-CA-C	5.54	121.48	110.40
1	G	105	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	185	VAL	CG1-CB-CG2	5.45	119.61	110.90
1	G	47	GLU	CA-C-N	-5.40	105.32	117.20
1	G	4	LEU	N-CA-C	5.36	125.47	111.00
1	J	160	MET	CG-SD-CE	-5.33	91.67	100.20
1	A	43	ARG	CA-CB-CG	5.32	125.10	113.40
1	G	55	LEU	N-CA-CB	5.30	120.99	110.40
1	J	127	ILE	CB-CA-C	-5.29	101.03	111.60
1	J	42	GLU	N-CA-C	5.23	125.12	111.00
1	J	18	ARG	CB-CA-C	5.20	120.81	110.40
1	A	57	GLN	N-CA-C	5.15	124.91	111.00
1	G	127	ILE	CB-CA-C	-5.15	101.30	111.60
1	D	53	GLU	C-N-CA	5.09	134.42	121.70
1	G	62	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	102	LEU	CA-CB-CG	5.01	126.82	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	86	ASN	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Peptide
1	A	2	LEU	Peptide
1	A	58	PRO	Peptide
1	D	-2	ALA	Peptide
1	D	0	ALA	Peptide
1	D	57	GLN	Peptide
1	D	58	PRO	Peptide
1	G	103	ARG	Peptide
1	G	57	GLN	Peptide
1	G	58	PRO	Peptide
1	J	-1	ALA	Peptide
1	J	-2	ALA	Peptide
1	J	-3	LEU	Peptide
1	J	0	ALA	Peptide
1	J	41	LYS	Peptide
1	J	58	PRO	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	1963	0	1979	103	0
1	D	1994	0	2017	91	0
1	G	1955	0	1968	86	0
1	J	1994	0	2017	101	0
2	A	48	0	23	7	0
2	D	48	0	23	10	0
2	G	48	0	23	3	0
2	J	48	0	23	7	0
3	A	17	0	6	6	0
3	D	17	0	6	6	0
3	G	17	0	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	17	0	6	3	0
4	A	41	0	0	0	0
4	D	49	0	0	1	0
4	G	42	0	0	0	0
4	J	36	0	0	1	0
All	All	8334	0	8097	363	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 22.

All (363) 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:59:GLU:HB3	1:D:61:HIS:N	1.48	1.27
1:G:59:GLU:N	1:G:60:ALA:HA	1.45	1.24
1:G:59:GLU:CB	1:G:61:HIS:H	1.53	1.21
1:A:59:GLU:CB	1:A:61:HIS:H	1.52	1.20
1:D:59:GLU:CB	1:D:61:HIS:H	1.53	1.19
1:A:57:GLN:H	1:A:57:GLN:NE2	1.41	1.19
1:G:59:GLU:HB3	1:G:61:HIS:N	1.61	1.16
1:A:59:GLU:N	1:A:60:ALA:HA	1.61	1.16
1:D:59:GLU:N	1:D:60:ALA:HA	1.61	1.11
1:A:59:GLU:HB3	1:A:61:HIS:N	1.67	1.10
1:D:1:MET:HE3	1:G:31:LEU:HD11	1.22	1.10
1:A:256:LYS:HG3	1:A:256:LYS:OXT	1.52	1.09
1:D:59:GLU:HB3	1:D:61:HIS:H	0.97	1.06
1:G:59:GLU:N	1:G:60:ALA:CA	2.19	1.06
1:J:59:GLU:N	1:J:60:ALA:HA	1.69	1.06
1:J:59:GLU:HB3	1:J:61:HIS:N	1.72	1.05
1:D:41:LYS:HD2	1:D:43:ARG:HD2	1.38	1.04
1:A:59:GLU:HB3	1:A:61:HIS:H	1.21	1.03
1:J:58:PRO:C	1:J:60:ALA:HA	1.81	1.00
1:J:59:GLU:CB	1:J:61:HIS:H	1.77	0.97
1:A:57:GLN:H	1:A:57:GLN:CD	1.67	0.97
1:A:57:GLN:NE2	1:A:57:GLN:N	2.13	0.95
1:A:89:GLY:HA2	1:A:136:MET:HE3	1.47	0.94
1:D:59:GLU:N	1:D:60:ALA:CA	2.31	0.94
1:D:1:MET:HE3	1:G:31:LEU:CD1	1.98	0.94
1:G:59:GLU:CB	1:G:61:HIS:N	2.26	0.94
1:J:59:GLU:N	1:J:60:ALA:CA	2.31	0.94
1:J:59:GLU:CB	1:J:61:HIS:N	2.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:GLU:O	1:G:6:ASN:HB2	1.65	0.93
1:J:-1:ALA:HA	1:J:1:MET:H	1.31	0.93
1:A:59:GLU:N	1:A:60:ALA:CA	2.30	0.93
1:G:124:SER:HA	1:G:127:ILE:HD11	1.49	0.93
1:D:1:MET:CE	1:G:31:LEU:HD11	2.00	0.91
1:G:157:TYR:OH	3:G:258:TCL:CL16	2.24	0.90
1:J:58:PRO:O	1:J:60:ALA:HA	1.70	0.90
1:A:59:GLU:CB	1:A:61:HIS:N	2.28	0.89
1:G:59:GLU:H	1:G:60:ALA:CA	1.79	0.89
1:G:59:GLU:HB3	1:G:61:HIS:H	1.21	0.88
1:A:5:GLU:O	1:A:6:ASN:HB2	1.71	0.88
1:G:59:GLU:H	1:G:60:ALA:HA	1.06	0.86
1:D:59:GLU:H	1:D:60:ALA:HA	1.39	0.85
1:G:136:MET:HE2	1:G:140:GLY:HA3	1.59	0.84
1:J:57:GLN:HB2	1:J:58:PRO:CD	2.07	0.84
1:J:57:GLN:HB2	1:J:58:PRO:HD3	1.57	0.84
1:A:52:LEU:CD2	1:A:60:ALA:H	1.90	0.84
1:D:89:GLY:HA2	1:D:136:MET:HE3	1.59	0.84
1:A:59:GLU:HB2	1:A:61:HIS:H	1.41	0.83
1:J:86:ASN:HB2	1:J:135:LEU:O	1.78	0.83
1:A:204:PHE:HA	1:A:207:ILE:HG12	1.61	0.83
1:G:59:GLU:HB2	1:G:61:HIS:H	1.43	0.83
1:D:59:GLU:HB3	1:D:61:HIS:CA	2.09	0.82
1:G:57:GLN:H	1:G:57:GLN:NE2	1.78	0.82
1:A:52:LEU:HD22	1:A:60:ALA:H	1.45	0.82
1:J:58:PRO:O	1:J:60:ALA:CA	2.29	0.81
1:D:-3:LEU:H3	1:D:-1:ALA:H	1.28	0.80
1:D:147:TYR:CD1	2:D:257:NAP:H5N	2.16	0.80
1:A:147:TYR:CD1	2:A:361:NAP:H5N	2.16	0.80
1:D:124:SER:HA	1:D:127:ILE:HD11	1.63	0.80
1:D:136:MET:CE	1:D:140:GLY:HA3	2.12	0.79
1:G:86:ASN:HB2	1:G:135:LEU:O	1.83	0.79
1:J:157:TYR:OH	3:J:258:TCL:CL16	2.38	0.78
1:D:246:ILE:HD12	1:G:246:ILE:HD12	1.66	0.78
1:D:157:TYR:OH	3:D:258:TCL:CL16	2.38	0.78
1:A:209:LYS:O	1:A:213:GLU:HG3	1.85	0.77
1:D:136:MET:HE1	1:D:140:GLY:HA3	1.65	0.77
1:D:86:ASN:HB2	1:D:135:LEU:O	1.84	0.77
1:G:58:PRO:C	1:G:60:ALA:HA	2.04	0.77
1:D:256:LYS:NZ	1:J:207:ILE:HG22	2.00	0.77
1:D:1:MET:CE	1:G:31:LEU:CD1	2.60	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:PRO:HA	2:D:257:NAP:O7N	1.86	0.75
1:A:58:PRO:C	1:A:60:ALA:HA	2.06	0.74
1:D:58:PRO:C	1:D:60:ALA:HA	2.07	0.74
1:G:146:THR:O	2:G:257:NAP:H6N	1.88	0.74
1:D:59:GLU:CA	1:D:61:HIS:H	1.99	0.74
1:A:46:LYS:HE3	1:A:49:GLU:OE1	1.89	0.72
1:J:155:GLN:CD	1:J:155:GLN:H	1.92	0.72
1:A:204:PHE:HA	1:A:207:ILE:CD1	2.19	0.72
1:A:59:GLU:H	1:A:60:ALA:HA	1.49	0.72
1:G:5:GLU:O	1:G:6:ASN:CB	2.36	0.72
1:J:45:ARG:NH2	1:J:59:GLU:OE1	2.23	0.71
1:A:60:ALA:O	1:A:61:HIS:C	2.27	0.71
1:A:204:PHE:CD1	1:A:207:ILE:HD11	2.26	0.71
1:D:209:LYS:O	1:D:213:GLU:HG2	1.91	0.70
1:G:35:LEU:H	1:G:56:ASN:HD21	1.37	0.70
1:J:57:GLN:CD	1:J:57:GLN:H	1.94	0.70
1:G:136:MET:CE	1:G:140:GLY:HA3	2.21	0.70
1:D:59:GLU:H	1:D:60:ALA:CA	2.00	0.69
1:J:58:PRO:C	1:J:60:ALA:CA	2.59	0.69
1:A:204:PHE:HA	1:A:207:ILE:CG1	2.22	0.69
1:D:124:SER:HA	1:D:127:ILE:CD1	2.23	0.69
1:D:39:TYR:CE1	1:D:64:GLN:HG3	2.28	0.69
1:J:219:ARG:HD3	4:J:266:HOH:O	1.91	0.69
1:A:204:PHE:O	1:A:207:ILE:HG12	1.93	0.68
1:G:57:GLN:NE2	1:G:57:GLN:N	2.39	0.68
1:J:209:LYS:O	1:J:213:GLU:HG3	1.93	0.68
1:A:210:GLU:OE2	1:G:256:LYS:HE3	1.93	0.68
1:A:146:THR:O	2:A:361:NAP:H6N	1.94	0.68
1:A:2:LEU:HA	1:A:3:ASN:HB2	1.75	0.67
1:A:4:LEU:HG	1:A:5:GLU:HG3	1.76	0.67
1:G:57:GLN:H	1:G:57:GLN:CD	1.97	0.67
1:G:124:SER:HA	1:G:127:ILE:CD1	2.24	0.67
1:A:201:VAL:CG2	3:A:371:TCL:O17	2.43	0.66
1:J:146:THR:O	2:J:257:NAP:H6N	1.95	0.66
1:A:99:MET:HE2	1:A:103:ARG:HG3	1.77	0.66
1:J:204:PHE:O	1:J:207:ILE:HG12	1.96	0.66
1:J:59:GLU:HB2	1:J:61:HIS:H	1.59	0.66
1:A:204:PHE:CA	1:A:207:ILE:HG12	2.25	0.65
1:J:57:GLN:H	1:J:57:GLN:NE2	1.93	0.65
1:J:-2:ALA:HA	1:J:-1:ALA:O	1.96	0.65
1:D:147:TYR:HD1	2:D:257:NAP:H5N	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:LYS:OXT	1:G:256:LYS:HG3	1.94	0.65
1:A:155:GLN:CD	1:A:155:GLN:H	1.98	0.65
1:D:59:GLU:H	1:D:61:HIS:N	1.94	0.65
1:D:256:LYS:OXT	1:D:256:LYS:HG3	1.97	0.65
1:A:124:SER:HA	1:A:127:ILE:HD11	1.79	0.64
1:D:146:THR:O	2:D:257:NAP:H6N	1.97	0.64
1:A:35:LEU:H	1:A:56:ASN:HD21	1.45	0.64
1:A:143:VAL:HG23	1:A:234:LEU:HD13	1.79	0.64
1:A:204:PHE:CE2	1:A:208:LEU:HD22	2.33	0.64
1:J:210:GLU:OE2	1:J:214:ARG:NH1	2.30	0.64
1:A:35:LEU:H	1:A:56:ASN:ND2	1.96	0.63
1:J:112:GLU:H	1:J:112:GLU:CD	2.00	0.63
1:D:-2:ALA:HB1	1:D:0:ALA:H	1.62	0.63
2:D:257:NAP:C4N	3:D:258:TCL:C11	2.76	0.63
1:A:99:MET:CE	1:A:103:ARG:HG3	2.29	0.63
1:A:2:LEU:C	1:A:2:LEU:HD23	2.19	0.63
1:A:54:GLN:HG3	1:A:55:LEU:H	1.62	0.63
1:J:217:LEU:O	1:J:219:ARG:HG2	1.99	0.62
1:D:256:LYS:HE2	1:J:155:GLN:OE1	1.99	0.62
1:J:204:PHE:CE2	1:J:208:LEU:HD22	2.34	0.62
1:J:57:GLN:OE1	1:J:58:PRO:HD2	1.99	0.62
1:J:-1:ALA:HA	1:J:1:MET:N	2.10	0.62
1:J:-1:ALA:HB1	1:J:2:LEU:H	1.65	0.62
1:A:4:LEU:HG	1:A:5:GLU:H	1.64	0.62
1:G:57:GLN:N	1:G:57:GLN:CD	2.52	0.62
1:J:52:LEU:HD21	1:J:60:ALA:HB3	1.81	0.62
1:A:136:MET:HE2	1:A:140:GLY:HA3	1.82	0.61
1:A:204:PHE:C	1:A:207:ILE:HG12	2.21	0.61
1:J:42:GLU:OE1	1:J:42:GLU:HA	2.00	0.61
1:J:44:SER:O	1:J:48:LEU:HB2	2.01	0.61
1:D:188:ILE:HG23	1:D:248:VAL:HG23	1.83	0.61
1:G:194:ARG:NH2	1:G:205:ASN:OD1	2.30	0.60
1:A:214:ARG:HH22	1:A:256:LYS:HB3	1.67	0.60
1:D:256:LYS:HZ1	1:J:207:ILE:HG22	1.67	0.60
1:A:136:MET:CE	1:A:140:GLY:HA3	2.32	0.60
1:J:59:GLU:H	1:J:61:HIS:H	1.50	0.60
1:A:41:LYS:HE2	2:A:361:NAP:O3X	2.02	0.59
3:G:258:TCL:C8	3:G:258:TCL:O17	2.50	0.59
3:J:258:TCL:C8	3:J:258:TCL:O17	2.51	0.59
1:D:59:GLU:HB3	1:D:61:HIS:HA	1.85	0.59
3:D:258:TCL:C8	3:D:258:TCL:O17	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:O	1:A:61:HIS:O	2.21	0.58
1:D:2:LEU:HD13	1:D:237:LEU:HD22	1.84	0.57
2:A:361:NAP:C3N	3:A:371:TCL:C13	2.82	0.57
1:A:157:TYR:OH	3:A:371:TCL:CL16	2.51	0.57
3:A:371:TCL:O17	3:A:371:TCL:C8	2.52	0.57
1:J:130:HIS:HD2	1:J:131:GLU:OE1	1.87	0.57
1:A:124:SER:HA	1:A:127:ILE:CD1	2.34	0.57
1:A:58:PRO:O	1:A:60:ALA:HA	2.05	0.57
1:D:210:GLU:OE1	1:J:256:LYS:NZ	2.36	0.56
1:A:123:TYR:CE2	1:A:127:ILE:HG12	2.40	0.56
1:A:193:ILE:N	2:A:361:NAP:O7N	2.32	0.56
1:D:136:MET:HE2	1:D:140:GLY:HA3	1.86	0.56
1:A:210:GLU:OE2	1:G:256:LYS:CE	2.53	0.56
1:J:59:GLU:N	1:J:61:HIS:H	2.02	0.56
1:J:209:LYS:O	1:J:213:GLU:CG	2.54	0.56
1:J:59:GLU:CA	1:J:61:HIS:H	2.19	0.56
1:D:22:PHE:CZ	1:D:51:LEU:HD22	2.41	0.56
1:J:143:VAL:HG23	1:J:234:LEU:HD13	1.87	0.55
1:G:197:SER:HB3	3:G:258:TCL:C4	2.36	0.55
1:A:155:GLN:CD	1:A:155:GLN:N	2.60	0.55
1:D:-3:LEU:H2	1:D:-2:ALA:HA	1.72	0.55
1:J:57:GLN:CD	1:J:57:GLN:N	2.60	0.55
1:J:57:GLN:CB	1:J:58:PRO:CD	2.83	0.54
1:J:194:ARG:HH11	1:J:194:ARG:HG2	1.72	0.54
1:D:59:GLU:CB	1:D:61:HIS:N	2.29	0.54
1:D:136:MET:HE1	1:D:140:GLY:CA	2.36	0.54
1:D:256:LYS:HZ3	1:J:207:ILE:HG22	1.72	0.54
1:A:106:PHE:HE1	1:D:170:ASN:ND2	2.06	0.54
1:A:201:VAL:HG23	3:A:371:TCL:O17	2.07	0.54
1:D:57:GLN:H	1:D:57:GLN:CD	2.11	0.54
1:J:5:GLU:O	1:J:32:GLY:O	2.26	0.54
1:G:35:LEU:H	1:G:56:ASN:ND2	2.06	0.53
1:D:1:MET:HE1	1:G:31:LEU:HD13	1.90	0.53
1:J:205:ASN:O	1:J:209:LYS:CD	2.57	0.53
1:A:2:LEU:CA	1:A:3:ASN:HB2	2.39	0.53
1:D:3:ASN:O	1:D:7:LYS:CD	2.57	0.53
1:D:219:ARG:NH2	1:D:225:GLU:OE1	2.42	0.53
2:D:257:NAP:O2D	3:D:258:TCL:CL16	2.54	0.53
1:D:59:GLU:N	1:D:61:HIS:H	2.06	0.52
1:A:246:ILE:HD12	1:J:246:ILE:HD12	1.92	0.52
1:G:132:ALA:O	1:G:136:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:PHE:HB2	1:J:62:LEU:HD12	1.92	0.52
1:G:116:LEU:HD11	1:G:120:ILE:HD11	1.92	0.52
1:D:58:PRO:O	1:D:60:ALA:HA	2.09	0.52
1:G:4:LEU:HG	1:G:5:GLU:H	1.74	0.52
1:G:58:PRO:O	1:G:60:ALA:HA	2.09	0.52
1:D:1:MET:CE	1:G:31:LEU:HD13	2.38	0.52
1:D:210:GLU:O	1:D:214:ARG:HB2	2.09	0.52
1:D:102:LEU:HD23	1:D:157:TYR:O	2.10	0.52
1:J:37:PHE:CE2	1:J:52:LEU:HD11	2.45	0.52
1:G:40:ARG:HD3	2:G:257:NAP:C5A	2.40	0.52
1:G:89:GLY:HA2	1:G:141:SER:O	2.09	0.51
1:D:59:GLU:H	1:D:61:HIS:H	1.57	0.51
1:D:124:SER:O	1:D:127:ILE:HD12	2.11	0.51
1:D:210:GLU:CD	1:J:256:LYS:NZ	2.64	0.51
1:G:24:VAL:HG22	1:G:227:GLY:HA2	1.93	0.51
1:J:67:VAL:HG22	2:J:257:NAP:N1A	2.26	0.51
2:D:257:NAP:C4N	3:D:258:TCL:C10	2.88	0.51
1:J:17:LYS:HB3	1:J:51:LEU:HD21	1.93	0.51
1:D:71:GLU:HG3	1:D:75:ASN:ND2	2.26	0.51
1:G:42:GLU:O	1:G:42:GLU:HG3	2.11	0.50
1:J:59:GLU:CA	1:J:61:HIS:N	2.75	0.50
1:G:194:ARG:NH1	1:G:208:LEU:CD1	2.75	0.50
1:J:52:LEU:HD23	1:J:60:ALA:H	1.77	0.50
1:J:155:GLN:CD	1:J:155:GLN:N	2.64	0.50
1:J:205:ASN:O	1:J:209:LYS:HD3	2.11	0.50
1:A:56:ASN:HA	1:A:57:GLN:NE2	2.26	0.50
1:J:44:SER:HA	1:J:47:GLU:HB2	1.93	0.50
1:G:4:LEU:HG	1:G:5:GLU:HG3	1.94	0.50
1:A:35:LEU:O	1:A:60:ALA:HB1	2.12	0.49
1:D:114:PHE:HA	1:D:159:VAL:HG21	1.94	0.49
1:J:59:GLU:N	1:J:61:HIS:N	2.60	0.49
1:A:5:GLU:O	1:A:6:ASN:CB	2.43	0.49
1:D:-3:LEU:N	1:D:-2:ALA:HA	2.27	0.49
1:D:41:LYS:CD	1:D:43:ARG:HD2	2.26	0.49
1:G:59:GLU:CA	1:G:61:HIS:H	2.22	0.49
1:A:54:GLN:HG3	1:A:55:LEU:N	2.27	0.49
1:G:3:ASN:O	1:G:4:LEU:HB2	2.13	0.49
1:J:59:GLU:HB3	1:J:61:HIS:CA	2.41	0.49
1:D:103:ARG:NH2	4:D:409:HOH:O	2.46	0.49
1:A:57:GLN:CD	1:A:57:GLN:N	2.37	0.49
1:A:123:TYR:CE2	1:A:127:ILE:CG1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:HG22	1:A:136:MET:HG3	1.95	0.48
2:A:361:NAP:C3N	3:A:371:TCL:C12	2.90	0.48
1:G:49:GLU:HG2	1:G:62:LEU:HD21	1.94	0.48
1:A:18:ARG:HG3	1:A:195:THR:HA	1.96	0.48
1:A:204:PHE:HA	1:A:207:ILE:HD11	1.96	0.48
1:D:217:LEU:O	1:D:219:ARG:HG2	2.13	0.48
1:J:54:GLN:HE21	1:J:54:GLN:HB3	1.42	0.48
1:A:199:LYS:NZ	1:A:199:LYS:CB	2.76	0.48
1:A:217:LEU:HD13	1:J:242:THR:HG21	1.94	0.48
1:G:209:LYS:O	1:G:213:GLU:HG3	2.13	0.48
1:G:48:LEU:O	1:G:52:LEU:HG	2.12	0.48
1:D:-3:LEU:N	1:D:-1:ALA:H	2.03	0.48
1:G:71:GLU:HG3	1:G:75:ASN:ND2	2.28	0.48
1:G:59:GLU:H	1:G:61:HIS:N	2.12	0.48
1:A:214:ARG:NH2	1:A:256:LYS:HB3	2.28	0.48
1:D:256:LYS:OXT	1:D:256:LYS:CG	2.60	0.48
1:G:177:ASP:OD1	1:J:105:ARG:NH1	2.46	0.48
1:A:107:SER:O	1:D:130:HIS:HB2	2.14	0.48
1:D:54:GLN:HG3	1:D:55:LEU:H	1.79	0.48
1:D:59:GLU:N	1:D:61:HIS:N	2.62	0.48
1:A:59:GLU:CA	1:A:61:HIS:H	2.20	0.47
1:D:197:SER:HB3	3:D:258:TCL:C4	2.44	0.47
1:A:86:ASN:HB2	1:A:135:LEU:O	2.14	0.47
1:G:39:TYR:CE1	1:G:64:GLN:HG3	2.50	0.47
1:J:59:GLU:H	1:J:61:HIS:N	2.12	0.47
1:J:249:ASP:O	1:J:250:SER:HB2	2.14	0.47
1:J:42:GLU:OE1	1:J:42:GLU:CA	2.62	0.47
1:J:201:VAL:CG2	3:J:258:TCL:O17	2.62	0.47
1:A:256:LYS:HB2	1:G:154:VAL:HG22	1.96	0.47
1:D:219:ARG:HH22	1:D:225:GLU:CD	2.18	0.47
1:G:184:ARG:HD2	1:G:241:VAL:O	2.14	0.47
1:A:228:LYS:HZ2	1:J:239:SER:HB2	1.77	0.47
1:J:39:TYR:CE1	1:J:64:GLN:HG3	2.49	0.47
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.78	0.47
1:A:37:PHE:CE2	1:A:60:ALA:HB3	2.50	0.47
1:A:204:PHE:O	1:A:207:ILE:CG1	2.61	0.47
1:J:58:PRO:O	1:J:60:ALA:N	2.48	0.46
1:D:217:LEU:HB2	1:D:250:SER:HB3	1.96	0.46
1:G:81:GLY:HA2	1:G:85:GLY:O	2.15	0.46
1:J:52:LEU:CD2	1:J:60:ALA:H	2.27	0.46
1:J:63:TYR:N	1:J:63:TYR:CD2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:HE2	1:A:60:ALA:HB3	1.80	0.46
1:A:4:LEU:CG	1:A:5:GLU:H	2.26	0.46
1:D:57:GLN:CD	1:D:57:GLN:N	2.69	0.46
1:J:-2:ALA:HB1	1:J:0:ALA:HB3	1.97	0.46
1:G:8:THR:HA	1:G:34:LYS:O	2.16	0.46
1:J:67:VAL:HG22	2:J:257:NAP:C6A	2.46	0.46
1:D:-3:LEU:HD23	1:D:-1:ALA:HB2	1.98	0.46
1:G:179:GLY:N	1:G:180:PRO:CD	2.79	0.46
1:A:52:LEU:HD21	1:A:60:ALA:H	1.77	0.46
1:G:123:TYR:CE2	1:J:111:ARG:HB2	2.51	0.46
1:G:124:SER:O	1:G:127:ILE:HD12	2.16	0.46
1:J:46:LYS:HA	1:J:46:LYS:HD3	1.70	0.46
1:J:178:LEU:O	1:J:181:ASP:HB2	2.16	0.45
1:J:236:ASP:O	1:J:239:SER:HB2	2.16	0.45
1:A:89:GLY:CA	1:A:136:MET:HE3	2.32	0.45
1:D:-3:LEU:H3	1:D:-1:ALA:N	2.06	0.45
1:A:52:LEU:HD22	1:A:60:ALA:N	2.23	0.45
1:J:213:GLU:O	1:J:218:LYS:HE3	2.16	0.45
1:D:193:ILE:H	2:D:257:NAP:C7N	2.28	0.45
1:G:217:LEU:HB2	1:G:250:SER:HB3	1.98	0.45
1:D:143:VAL:CG2	1:D:234:LEU:HD13	2.47	0.45
1:G:12:MET:HB3	1:G:94:ILE:HD11	1.97	0.45
1:G:81:GLY:HA3	1:G:135:LEU:HD21	1.97	0.45
1:A:125:LEU:HD13	1:A:144:ALA:HB2	1.99	0.45
1:J:57:GLN:NE2	1:J:57:GLN:N	2.62	0.45
1:D:53:GLU:H	1:D:53:GLU:HG3	1.61	0.44
1:D:59:GLU:CA	1:D:61:HIS:N	2.74	0.44
1:D:178:LEU:HB3	1:D:183:ILE:HB	1.99	0.44
1:J:205:ASN:O	1:J:209:LYS:HD2	2.16	0.44
1:G:40:ARG:HD3	2:G:257:NAP:C6A	2.48	0.44
1:G:217:LEU:HD22	1:G:250:SER:HA	1.98	0.44
1:D:67:VAL:HG22	2:D:257:NAP:N1A	2.32	0.44
1:D:38:THR:HA	1:D:63:TYR:O	2.18	0.44
1:J:127:ILE:H	1:J:127:ILE:HG13	1.61	0.44
1:A:147:TYR:HB2	2:A:361:NAP:C6N	2.48	0.44
1:G:143:VAL:HG23	1:G:234:LEU:HD13	1.99	0.44
1:J:-2:ALA:HA	1:J:-1:ALA:C	2.37	0.44
1:G:59:GLU:HB3	1:G:61:HIS:CA	2.43	0.44
1:A:228:LYS:NZ	1:J:239:SER:CB	2.81	0.43
1:A:246:ILE:HD12	1:J:246:ILE:CD1	2.48	0.43
1:G:155:GLN:CD	1:G:155:GLN:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:GLU:H	1:G:53:GLU:HG3	1.62	0.43
1:D:59:GLU:H	1:D:60:ALA:C	2.22	0.43
1:J:58:PRO:C	1:J:60:ALA:N	2.71	0.43
1:G:38:THR:HG21	1:G:65:ILE:HD12	2.00	0.43
1:G:105:ARG:HD3	1:J:177:ASP:OD1	2.18	0.43
1:A:34:LYS:HA	1:A:56:ASN:HD21	1.84	0.43
1:D:184:ARG:HG2	1:D:242:THR:HB	2.01	0.43
1:J:204:PHE:HA	1:J:207:ILE:CD1	2.49	0.43
1:J:214:ARG:NH2	1:J:256:LYS:HB3	2.35	0.42
1:G:5:GLU:H	1:G:5:GLU:HG3	1.57	0.42
1:G:38:THR:HA	1:G:63:TYR:O	2.20	0.42
1:G:54:GLN:HG3	1:G:55:LEU:H	1.84	0.42
1:A:17:LYS:HE3	1:A:18:ARG:NH1	2.35	0.42
1:A:28:LEU:HD11	1:A:234:LEU:HD23	2.01	0.42
1:G:112:GLU:CD	1:G:112:GLU:H	2.23	0.42
1:G:153:ALA:HA	1:J:173:TYR:CZ	2.55	0.42
1:A:3:ASN:O	1:A:4:LEU:HB2	2.19	0.42
1:A:209:LYS:O	1:A:213:GLU:CG	2.64	0.42
1:G:105:ARG:HB2	1:G:108:GLU:OE1	2.20	0.42
1:A:196:LEU:O	1:A:199:LYS:HG2	2.20	0.41
1:A:45:ARG:NE	1:A:49:GLU:OE2	2.53	0.41
1:A:204:PHE:HD1	1:A:207:ILE:HD11	1.80	0.41
1:D:18:ARG:O	1:D:195:THR:HG22	2.20	0.41
1:D:193:ILE:N	2:D:257:NAP:O7N	2.50	0.41
1:J:89:GLY:HA2	1:J:136:MET:CE	2.50	0.41
1:G:42:GLU:O	1:G:42:GLU:CG	2.69	0.41
1:J:214:ARG:HH21	1:J:256:LYS:HB3	1.86	0.41
1:D:4:LEU:HB2	1:D:9:TYR:OH	2.21	0.41
1:J:147:TYR:HB2	2:J:257:NAP:C6N	2.51	0.41
1:D:130:HIS:HD2	1:D:131:GLU:OE1	2.03	0.41
1:D:231:ALA:O	1:D:235:SER:HB3	2.21	0.41
1:G:196:LEU:O	1:G:199:LYS:HG2	2.21	0.41
1:J:65:ILE:O	2:J:257:NAP:H2A	2.21	0.41
1:G:31:LEU:HD12	1:G:31:LEU:HA	1.93	0.41
1:G:141:SER:HB3	1:G:234:LEU:HD12	2.03	0.41
1:A:18:ARG:O	1:A:195:THR:HG22	2.21	0.41
1:A:106:PHE:CE1	1:D:170:ASN:ND2	2.88	0.41
1:A:256:LYS:OXT	1:A:256:LYS:CG	2.34	0.41
1:G:207:ILE:HD12	1:G:207:ILE:HG21	1.74	0.41
1:J:158:ASN:HB3	1:J:159:VAL:H	1.20	0.41
1:J:66:ASP:HA	2:J:257:NAP:N1A	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:204:PHE:HA	1:J:207:ILE:HD11	2.03	0.40
1:A:3:ASN:HD22	1:A:3:ASN:HA	1.70	0.40
1:A:112:GLU:CD	1:A:112:GLU:H	2.23	0.40
1:G:40:ARG:HE	1:G:40:ARG:HB3	1.55	0.40
2:J:257:NAP:H2D	2:J:257:NAP:H2N	1.64	0.40
1:A:117:ALA:O	1:A:121:SER:HB2	2.21	0.40
1:J:189:SER:HB2	1:J:245:ASN:OD1	2.22	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	253/260 (97%)	230 (91%)	20 (8%)	3 (1%)	13	12
1	D	258/260 (99%)	236 (92%)	21 (8%)	1 (0%)	34	40
1	G	252/260 (97%)	229 (91%)	20 (8%)	3 (1%)	13	12
1	J	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	13	12
All	All	1021/1040 (98%)	932 (91%)	79 (8%)	10 (1%)	15	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	58	PRO
1	J	54	GLN
1	A	52	LEU
1	G	58	PRO
1	D	54	GLN
1	G	42	GLU
1	J	43	ARG

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Mol	Chain	Res	Type
1	J	60	ALA
1	G	149	GLY

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	209/211 (99%)	174 (83%)	35 (17%)	2	1
1	D	211/211 (100%)	165 (78%)	46 (22%)	1	0
1	G	208/211 (99%)	172 (83%)	36 (17%)	2	1
1	J	211/211 (100%)	175 (83%)	36 (17%)	2	1
All	All	839/844 (99%)	686 (82%)	153 (18%)	1	1

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	ASN
1	A	4	LEU
1	A	17	LYS
1	A	26	LYS
1	A	31	LEU
1	A	43	ARG
1	A	48	LEU
1	A	52	LEU
1	A	57	GLN
1	A	62	LEU
1	A	69	SER
1	A	73	VAL
1	A	87	ILE
1	A	99	MET
1	A	100	GLU
1	A	103	ARG
1	A	112	GLU
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	127	ILE
1	A	138	GLU
1	A	155	GLN
1	A	178	LEU
1	A	185	VAL
1	A	196	LEU
1	A	199	LYS
1	A	208	LEU
1	A	209	LYS
1	A	217	LEU
1	A	219	ARG
1	A	220	ASN
1	A	224	VAL
1	A	234	LEU
1	A	236	ASP
1	A	255	ILE
1	D	-3	LEU
1	D	1	MET
1	D	2	LEU
1	D	3	ASN
1	D	4	LEU
1	D	5	GLU
1	D	17	LYS
1	D	18	ARG
1	D	26	LYS
1	D	31	LEU
1	D	34	LYS
1	D	43	ARG
1	D	48	LEU
1	D	50	LYS
1	D	52	LEU
1	D	53	GLU
1	D	54	GLN
1	D	55	LEU
1	D	57	GLN
1	D	62	LEU
1	D	73	VAL
1	D	78	GLU
1	D	87	ILE
1	D	93	SER
1	D	99	MET
1	D	103	ARG

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Mol	Chain	Res	Type
1	D	115	LEU
1	D	127	ILE
1	D	138	GLU
1	D	170	ASN
1	D	178	LEU
1	D	183	ILE
1	D	185	VAL
1	D	196	LEU
1	D	207	ILE
1	D	209	LYS
1	D	213	GLU
1	D	214	ARG
1	D	217	LEU
1	D	219	ARG
1	D	220	ASN
1	D	234	LEU
1	D	236	ASP
1	D	237	LEU
1	D	239	SER
1	D	256	LYS
1	G	5	GLU
1	G	6	ASN
1	G	17	LYS
1	G	18	ARG
1	G	26	LYS
1	G	31	LEU
1	G	34	LYS
1	G	41	LYS
1	G	43	ARG
1	G	47	GLU
1	G	53	GLU
1	G	55	LEU
1	G	57	GLN
1	G	62	LEU
1	G	64	GLN
1	G	73	VAL
1	G	84	VAL
1	G	87	ILE
1	G	93	SER
1	G	99	MET
1	G	102	LEU
1	G	103	ARG

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Mol	Chain	Res	Type
1	G	105	ARG
1	G	115	LEU
1	G	127	ILE
1	G	178	LEU
1	G	185	VAL
1	G	194	ARG
1	G	196	LEU
1	G	199	LYS
1	G	207	ILE
1	G	217	LEU
1	G	219	ARG
1	G	234	LEU
1	G	239	SER
1	G	256	LYS
1	J	5	GLU
1	J	11	ILE
1	J	17	LYS
1	J	31	LEU
1	J	43	ARG
1	J	45	ARG
1	J	48	LEU
1	J	52	LEU
1	J	53	GLU
1	J	54	GLN
1	J	55	LEU
1	J	56	ASN
1	J	57	GLN
1	J	62	LEU
1	J	73	VAL
1	J	84	VAL
1	J	87	ILE
1	J	103	ARG
1	J	105	ARG
1	J	112	GLU
1	J	115	LEU
1	J	127	ILE
1	J	155	GLN
1	J	158	ASN
1	J	178	LEU
1	J	185	VAL
1	J	196	LEU
1	J	208	LEU

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Mol	Chain	Res	Type
1	J	209	LYS
1	J	213	GLU
1	J	217	LEU
1	J	219	ARG
1	J	224	VAL
1	J	234	LEU
1	J	250	SER
1	J	255	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	6	ASN
1	A	56	ASN
1	A	57	GLN
1	A	130	HIS
1	A	220	ASN
1	D	3	ASN
1	D	54	GLN
1	D	56	ASN
1	D	75	ASN
1	D	130	HIS
1	D	170	ASN
1	G	6	ASN
1	G	54	GLN
1	G	56	ASN
1	G	57	GLN
1	G	75	ASN
1	G	220	ASN
1	J	3	ASN
1	J	54	GLN
1	J	56	ASN
1	J	130	HIS

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)

8 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	TCL	G	258	-	18,18,18	2.04	5 (27%)	25,25,25	0.94	1 (4%)
3	TCL	A	371	-	18,18,18	2.05	5 (27%)	25,25,25	0.94	1 (4%)
3	TCL	D	258	-	18,18,18	2.05	5 (27%)	25,25,25	0.94	1 (4%)
2	NAP	A	361	-	45,52,52	4.86	13 (28%)	56,80,80	3.58	21 (37%)
2	NAP	D	257	-	45,52,52	5.53	11 (24%)	56,80,80	5.18	22 (39%)
2	NAP	G	257	-	45,52,52	5.26	9 (20%)	56,80,80	3.43	19 (33%)
3	TCL	J	258	-	18,18,18	2.05	5 (27%)	25,25,25	0.94	1 (4%)
2	NAP	J	257	-	45,52,52	4.45	13 (28%)	56,80,80	4.15	23 (41%)

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	TCL	G	258	-	-	2/4/4/4	0/2/2/2
3	TCL	A	371	-	-	2/4/4/4	0/2/2/2
3	TCL	D	258	-	-	2/4/4/4	0/2/2/2
2	NAP	A	361	-	-	6/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	257	-	-	6/31/67/67	0/5/5/5
2	NAP	G	257	-	-	7/31/67/67	0/5/5/5
3	TCL	J	258	-	-	2/4/4/4	0/2/2/2
2	NAP	J	257	-	-	5/31/67/67	0/5/5/5

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	257	NAP	C2N-N1N	23.57	1.63	1.35
2	D	257	NAP	C2N-N1N	22.87	1.62	1.35
2	A	361	NAP	C2N-N1N	20.94	1.60	1.35
2	D	257	NAP	C7N-N7N	-17.19	1.00	1.33
2	G	257	NAP	C2N-C3N	15.04	1.62	1.39
2	A	361	NAP	C2N-C3N	14.04	1.60	1.39
2	J	257	NAP	C4N-C3N	13.82	1.63	1.39
2	G	257	NAP	C3N-C7N	-13.62	1.30	1.50
2	J	257	NAP	C2N-C3N	13.43	1.59	1.39
2	D	257	NAP	C2N-C3N	12.66	1.58	1.39
2	D	257	NAP	C4N-C3N	11.83	1.59	1.39
2	J	257	NAP	C7N-N7N	-11.48	1.11	1.33
2	J	257	NAP	C6N-C5N	11.31	1.63	1.38
2	J	257	NAP	O7N-C7N	10.55	1.44	1.24
2	A	361	NAP	C6N-N1N	9.96	1.59	1.35
2	A	361	NAP	C7N-N7N	-9.88	1.14	1.33
2	G	257	NAP	C6N-C5N	9.47	1.59	1.38
2	A	361	NAP	C5N-C4N	8.80	1.57	1.38
2	J	257	NAP	C2N-N1N	8.15	1.44	1.35
2	A	361	NAP	C6N-C5N	8.03	1.56	1.38
2	D	257	NAP	C6N-C5N	8.02	1.56	1.38
2	D	257	NAP	C6N-N1N	7.83	1.54	1.35
2	D	257	NAP	C5N-C4N	7.38	1.54	1.38
2	G	257	NAP	C7N-N7N	-6.29	1.21	1.33
2	G	257	NAP	C6N-N1N	6.28	1.50	1.35
2	G	257	NAP	O4D-C1D	6.17	1.49	1.41
3	A	371	TCL	C8-C9	5.31	1.48	1.39
3	J	258	TCL	C8-C9	5.30	1.48	1.39
3	G	258	TCL	C8-C9	5.28	1.48	1.39
3	D	258	TCL	C8-C9	5.25	1.48	1.39
3	D	258	TCL	C6-C5	4.76	1.48	1.40
3	J	258	TCL	C6-C5	4.74	1.48	1.40
3	A	371	TCL	C6-C5	4.71	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	258	TCL	C6-C5	4.69	1.48	1.40
2	D	257	NAP	O4D-C1D	4.31	1.47	1.41
2	D	257	NAP	C2D-C1D	4.30	1.60	1.53
2	G	257	NAP	O7N-C7N	4.06	1.31	1.24
2	A	361	NAP	C2A-N3A	3.85	1.38	1.32
2	J	257	NAP	C2A-N3A	3.79	1.38	1.32
2	D	257	NAP	C2A-N1A	3.52	1.40	1.33
2	A	361	NAP	O4D-C1D	3.47	1.45	1.41
2	J	257	NAP	O4D-C1D	3.15	1.45	1.41
2	A	361	NAP	O7N-C7N	-3.09	1.18	1.24
2	A	361	NAP	C2A-N1A	3.03	1.39	1.33
2	J	257	NAP	P2B-O2B	2.73	1.64	1.59
3	D	258	TCL	C9-CL16	2.70	1.80	1.73
3	A	371	TCL	C9-CL16	2.68	1.80	1.73
3	J	258	TCL	C9-CL16	2.67	1.80	1.73
3	G	258	TCL	C9-CL16	2.67	1.80	1.73
3	D	258	TCL	C11-CL15	2.54	1.80	1.74
2	A	361	NAP	O4B-C4B	-2.54	1.39	1.45
3	J	258	TCL	C11-CL15	2.53	1.80	1.74
3	A	371	TCL	C2-CL14	2.53	1.80	1.74
3	J	258	TCL	C2-CL14	2.51	1.80	1.74
3	D	258	TCL	C2-CL14	2.51	1.80	1.74
3	A	371	TCL	C11-CL15	2.49	1.79	1.74
3	G	258	TCL	C2-CL14	2.49	1.79	1.74
3	G	258	TCL	C11-CL15	2.49	1.79	1.74
2	A	361	NAP	P2B-O2B	2.46	1.64	1.59
2	G	257	NAP	C2A-N3A	2.41	1.36	1.32
2	D	257	NAP	C2A-N3A	2.35	1.35	1.32
2	J	257	NAP	C5N-C4N	-2.21	1.34	1.38
2	A	361	NAP	C2D-C1D	2.09	1.56	1.53
2	J	257	NAP	C3D-C4D	-2.06	1.47	1.53
2	J	257	NAP	C8A-N7A	2.04	1.38	1.34
2	J	257	NAP	O3B-C3B	-2.02	1.38	1.43

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	257	NAP	O7N-C7N-N7N	22.52	154.56	122.58
2	D	257	NAP	O7N-C7N-C3N	-18.79	97.14	119.63
2	A	361	NAP	C2N-C3N-C4N	-15.16	101.07	118.26
2	A	361	NAP	O4D-C1D-C2D	-12.69	88.37	106.93
2	J	257	NAP	O7N-C7N-C3N	-12.57	104.59	119.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	257	NAP	C2N-N1N-C1D	-12.50	91.29	119.14
2	G	257	NAP	C2N-N1N-C1D	-10.71	95.27	119.14
2	J	257	NAP	O7N-C7N-N7N	10.60	137.63	122.58
2	J	257	NAP	C2N-C3N-C7N	10.58	150.18	119.46
2	D	257	NAP	O4D-C1D-C2D	-10.43	91.69	106.93
2	D	257	NAP	C6N-C5N-C4N	9.48	133.21	119.44
2	G	257	NAP	O4D-C1D-C2D	-9.20	93.48	106.93
2	J	257	NAP	O4D-C1D-C2D	-9.11	93.62	106.93
2	A	361	NAP	C4N-C3N-C7N	-8.62	97.96	121.04
2	J	257	NAP	C4N-C3N-C7N	-8.60	98.01	121.04
2	D	257	NAP	C5N-C6N-N1N	-8.38	108.38	120.40
2	G	257	NAP	C2N-C3N-C7N	8.11	142.99	119.46
2	G	257	NAP	C4N-C3N-C7N	-7.95	99.75	121.04
2	D	257	NAP	C3N-C7N-N7N	-7.88	108.29	117.75
2	G	257	NAP	C5N-C4N-C3N	7.60	129.34	120.34
2	G	257	NAP	N3A-C2A-N1A	-7.53	116.91	128.68
2	J	257	NAP	C3D-C2D-C1D	7.15	111.75	100.98
2	A	361	NAP	C5N-C6N-N1N	-6.67	110.83	120.40
2	D	257	NAP	C4N-C3N-C7N	-6.43	103.83	121.04
2	D	257	NAP	C2N-C3N-C4N	-5.93	111.54	118.26
2	J	257	NAP	C2N-C3N-C4N	-5.76	111.73	118.26
2	J	257	NAP	N3A-C2A-N1A	-5.73	119.72	128.68
2	A	361	NAP	N3A-C2A-N1A	-5.63	119.88	128.68
2	G	257	NAP	C3D-C2D-C1D	5.44	109.16	100.98
2	G	257	NAP	C3N-C2N-N1N	-5.42	115.13	120.43
2	D	257	NAP	C3N-C2N-N1N	5.32	125.63	120.43
2	D	257	NAP	C3D-C2D-C1D	5.31	108.98	100.98
2	D	257	NAP	C2N-C3N-C7N	5.02	134.03	119.46
2	A	361	NAP	C3D-C2D-C1D	4.93	108.40	100.98
2	D	257	NAP	N3A-C2A-N1A	-4.48	121.68	128.68
2	D	257	NAP	O4B-C1B-C2B	-4.27	99.18	106.59
2	D	257	NAP	C2N-N1N-C1D	-4.24	109.69	119.14
2	G	257	NAP	C3N-C7N-N7N	4.22	122.82	117.75
2	J	257	NAP	C6N-N1N-C2N	4.17	125.78	121.97
2	A	361	NAP	C2N-N1N-C1D	-3.92	110.42	119.14
2	D	257	NAP	O2D-C2D-C3D	-3.90	99.22	111.82
2	G	257	NAP	C6N-N1N-C2N	-3.70	118.60	121.97
2	G	257	NAP	C2A-N1A-C6A	3.58	124.88	118.75
2	A	361	NAP	C5A-C6A-N6A	3.41	125.53	120.35
2	J	257	NAP	O4B-C1B-C2B	-3.37	100.74	106.59
2	D	257	NAP	PN-O3-PA	3.33	144.27	132.83
2	G	257	NAP	C5N-C6N-N1N	-3.25	115.75	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	361	NAP	C1B-N9A-C4A	-3.19	121.04	126.64
2	J	257	NAP	O5D-C5D-C4D	3.17	119.91	108.99
2	A	361	NAP	C4A-C5A-N7A	-3.17	106.09	109.40
2	A	361	NAP	C6N-C5N-C4N	-3.16	114.85	119.44
2	J	257	NAP	O2D-C2D-C3D	-3.14	101.66	111.82
2	G	257	NAP	O3D-C3D-C4D	-3.12	102.03	111.05
2	G	257	NAP	O4D-C4D-C5D	3.11	119.59	109.37
2	J	257	NAP	O4D-C4D-C5D	3.08	119.50	109.37
2	J	257	NAP	O3D-C3D-C4D	-3.05	102.24	111.05
2	G	257	NAP	C2N-C3N-C4N	-2.97	114.89	118.26
2	A	361	NAP	O2D-C2D-C1D	2.91	121.59	110.85
2	J	257	NAP	C3B-C2B-C1B	-2.87	97.50	102.89
2	D	257	NAP	O2D-C2D-C1D	2.86	121.43	110.85
2	A	361	NAP	C6N-N1N-C2N	-2.81	119.41	121.97
2	A	361	NAP	O4B-C1B-C2B	-2.73	101.85	106.59
2	J	257	NAP	C4A-C5A-N7A	-2.73	106.56	109.40
2	D	257	NAP	O3D-C3D-C4D	-2.66	103.36	111.05
2	A	361	NAP	O2N-PN-O1N	2.58	125.00	112.24
2	G	257	NAP	O4B-C1B-C2B	-2.56	102.15	106.59
2	D	257	NAP	O4D-C4D-C5D	2.51	117.63	109.37
2	A	361	NAP	O4D-C4D-C3D	-2.47	100.23	105.11
2	J	257	NAP	O5B-C5B-C4B	-2.46	100.51	108.99
2	J	257	NAP	O2D-C2D-C1D	2.43	119.81	110.85
2	J	257	NAP	C3N-C7N-N7N	-2.41	114.86	117.75
2	A	361	NAP	C5N-C4N-C3N	2.40	123.19	120.34
2	A	361	NAP	C2N-C3N-C7N	2.40	126.43	119.46
2	J	257	NAP	C5N-C6N-N1N	-2.37	117.01	120.40
2	G	257	NAP	C5B-C4B-C3B	-2.36	106.34	115.18
3	A	371	TCL	O7-C5-C6	2.32	120.56	116.22
3	J	258	TCL	O7-C5-C6	2.31	120.54	116.22
3	G	258	TCL	O7-C5-C6	2.30	120.53	116.22
3	D	258	TCL	O7-C5-C6	2.30	120.52	116.22
2	J	257	NAP	O3D-C3D-C2D	-2.24	104.58	111.82
2	D	257	NAP	C5D-C4D-C3D	-2.20	106.94	115.18
2	D	257	NAP	O2N-PN-O1N	2.20	123.10	112.24
2	G	257	NAP	O7N-C7N-N7N	-2.16	119.51	122.58
2	D	257	NAP	O2B-P2B-O1X	-2.14	101.11	109.39
2	A	361	NAP	O2D-C2D-C3D	-2.14	104.91	111.82
2	G	257	NAP	O2N-PN-O1N	2.13	122.77	112.24
2	A	361	NAP	C2A-N1A-C6A	2.08	122.31	118.75
2	A	361	NAP	O5B-C5B-C4B	-2.07	101.87	108.99
2	J	257	NAP	C1B-N9A-C4A	-2.06	123.03	126.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	361	NAP	C5D-O5D-PN-O3
2	A	361	NAP	C5D-O5D-PN-O1N
2	D	257	NAP	C5D-O5D-PN-O1N
2	D	257	NAP	C5D-O5D-PN-O2N
2	G	257	NAP	C2B-O2B-P2B-O1X
2	G	257	NAP	C5D-O5D-PN-O1N
2	G	257	NAP	C5D-O5D-PN-O2N
2	G	257	NAP	O4D-C1D-N1N-C6N
2	G	257	NAP	C2D-C1D-N1N-C6N
2	J	257	NAP	C2B-O2B-P2B-O3X
2	J	257	NAP	C5D-O5D-PN-O3
3	A	371	TCL	C6-C5-O7-C8
3	D	258	TCL	C6-C5-O7-C8
3	D	258	TCL	C4-C5-O7-C8
3	G	258	TCL	C6-C5-O7-C8
3	G	258	TCL	C4-C5-O7-C8
3	J	258	TCL	C6-C5-O7-C8
3	A	371	TCL	C4-C5-O7-C8
3	J	258	TCL	C4-C5-O7-C8
2	A	361	NAP	C2N-C3N-C7N-O7N
2	A	361	NAP	PA-O3-PN-O2N
2	J	257	NAP	C5D-O5D-PN-O1N
2	D	257	NAP	O4B-C4B-C5B-O5B
2	A	361	NAP	PA-O3-PN-O1N
2	D	257	NAP	C5D-O5D-PN-O3
2	G	257	NAP	C5D-O5D-PN-O3
2	J	257	NAP	C2D-C1D-N1N-C6N
2	G	257	NAP	O4B-C4B-C5B-O5B
2	J	257	NAP	O4B-C4B-C5B-O5B
2	D	257	NAP	PA-O3-PN-O2N
2	D	257	NAP	C5B-O5B-PA-O1A
2	A	361	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	258	TCL	3	0
3	A	371	TCL	6	0
3	D	258	TCL	6	0

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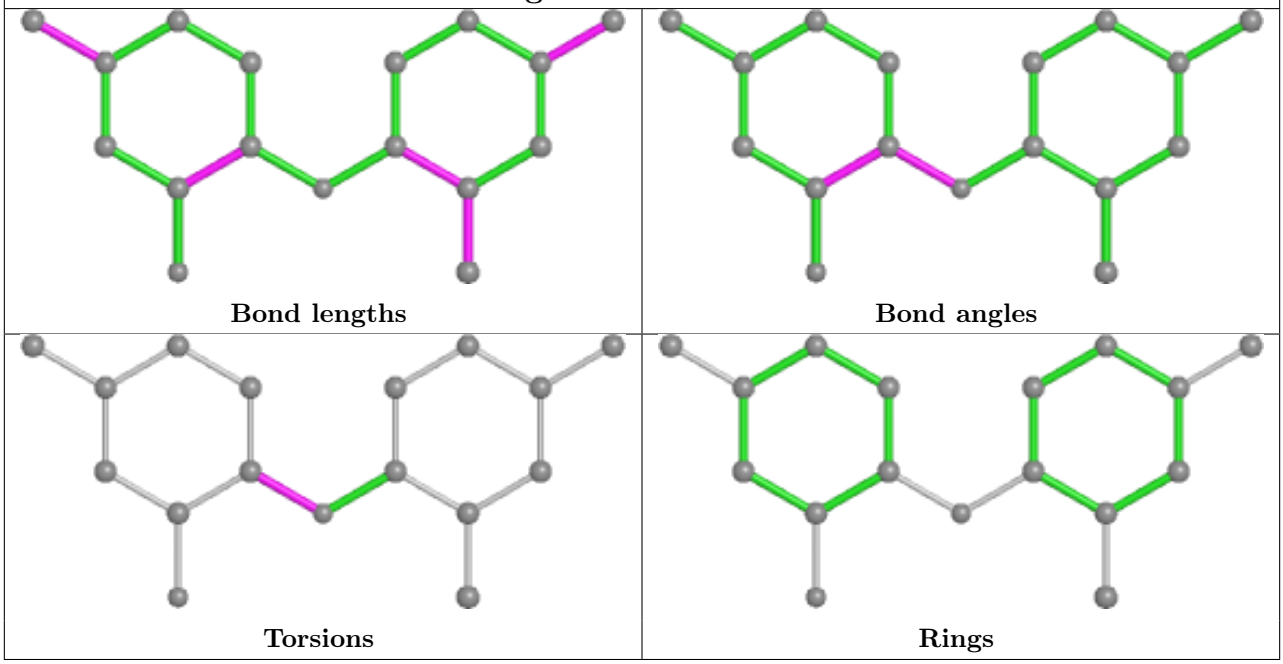
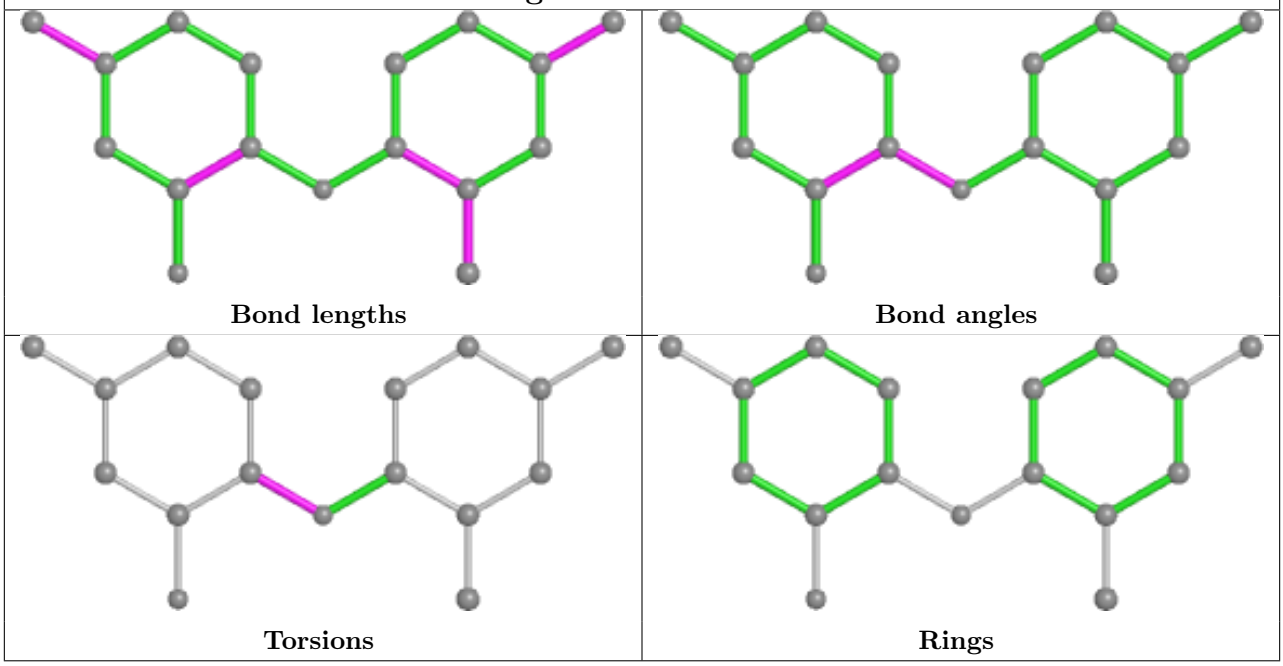
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	NAP	7	0
2	D	257	NAP	10	0
2	G	257	NAP	3	0
3	J	258	TCL	3	0
2	J	257	NAP	7	0

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.

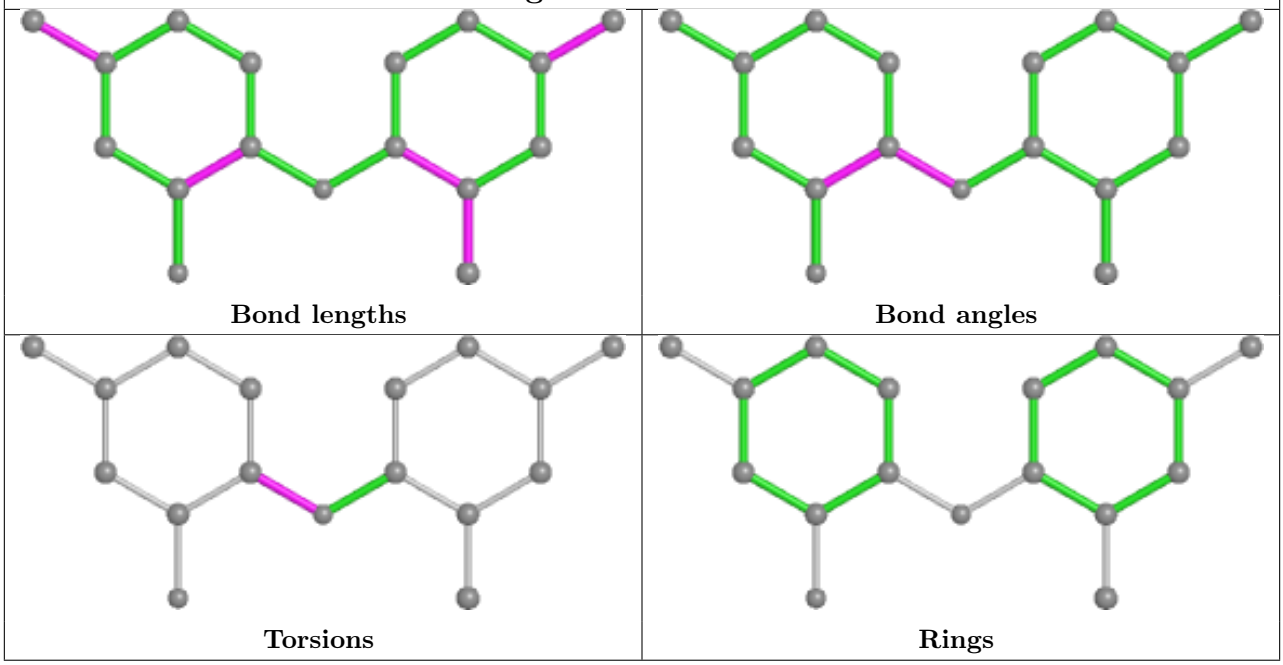
Ligand TCL G 258



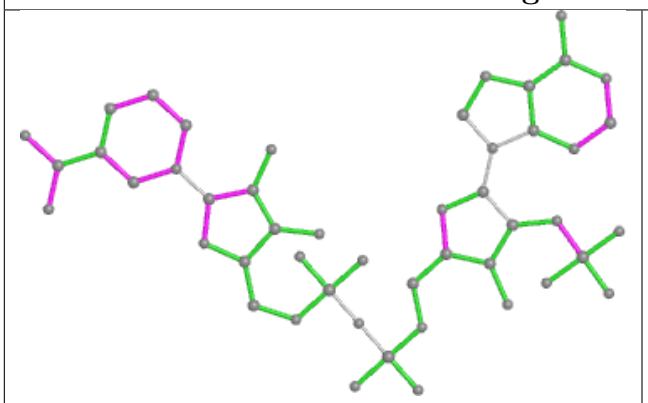
Ligand TCL A 371



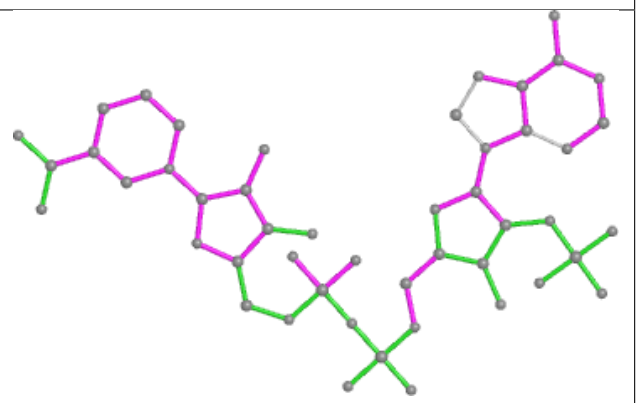
Ligand TCL D 258



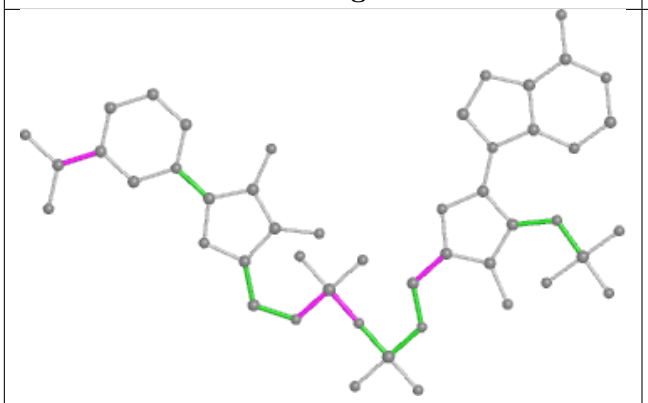
Ligand NAP A 361



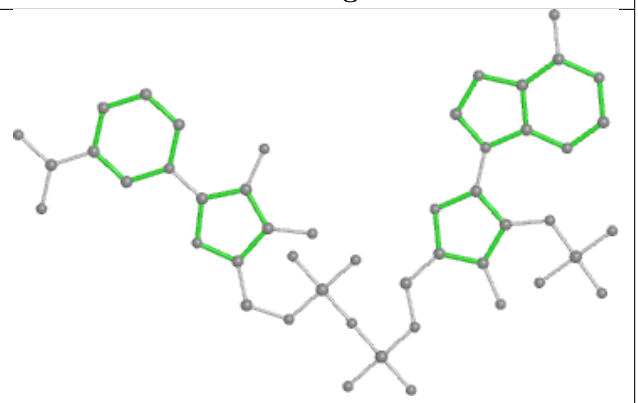
Bond lengths



Bond angles

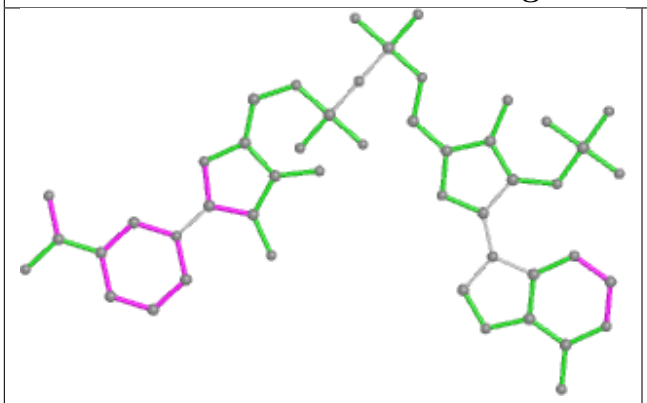


Torsions



Rings

Ligand NAP D 257



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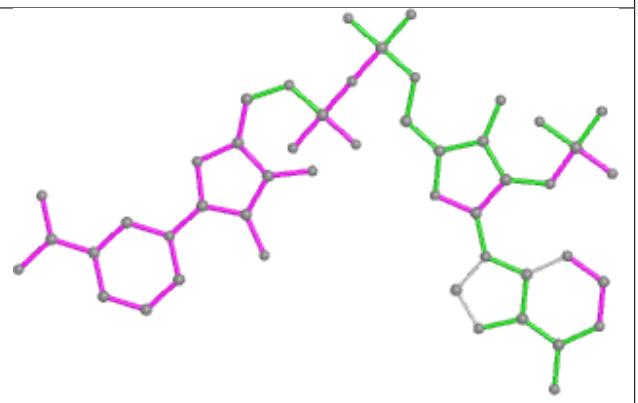

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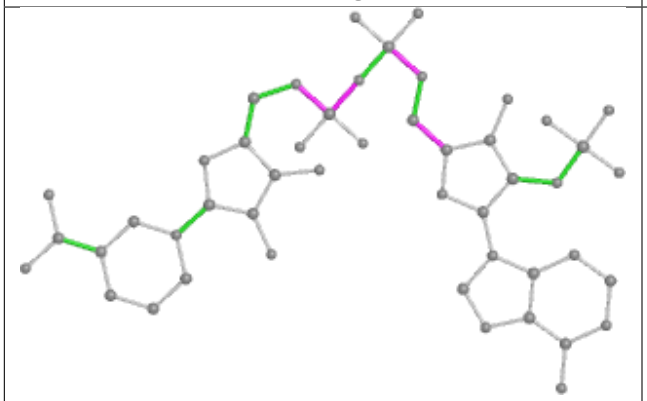

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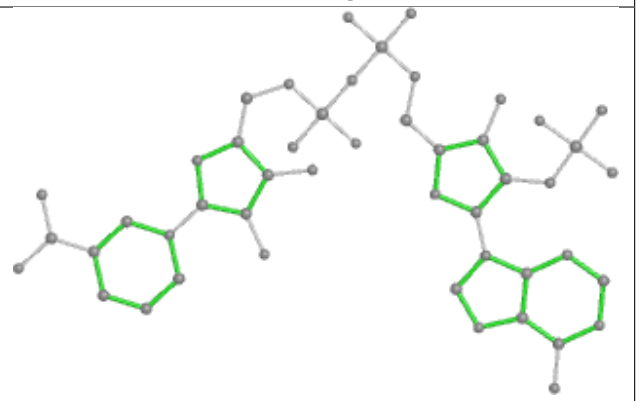
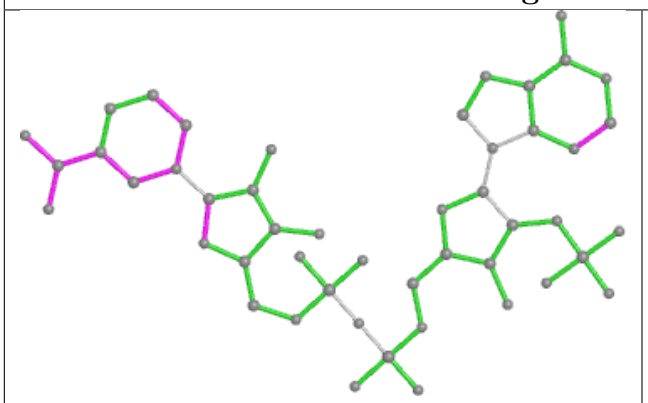
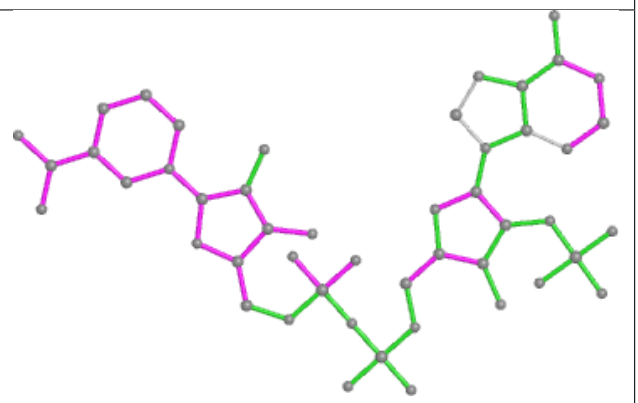


Rings

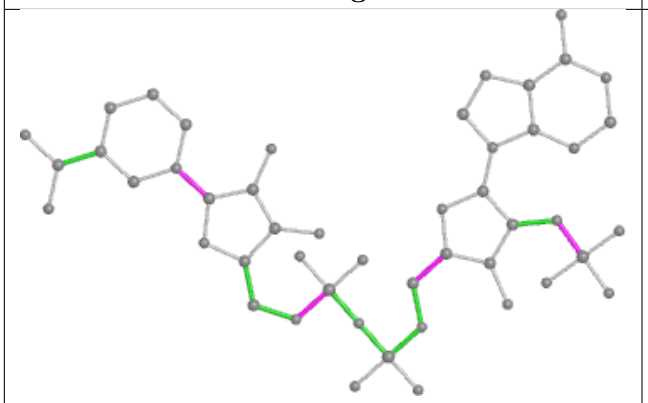
Ligand NAP G 257



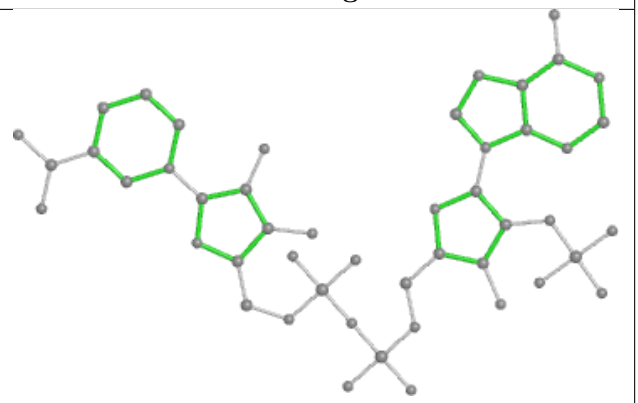
Bond lengths



Bond angles

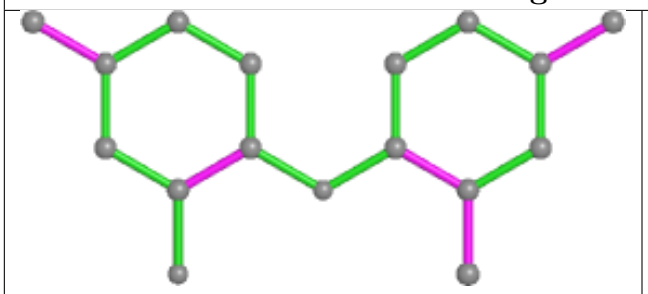


Torsions

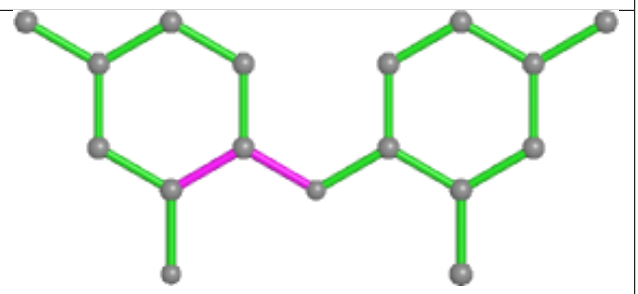


Rings

Ligand TCL J 258



Bond lengths



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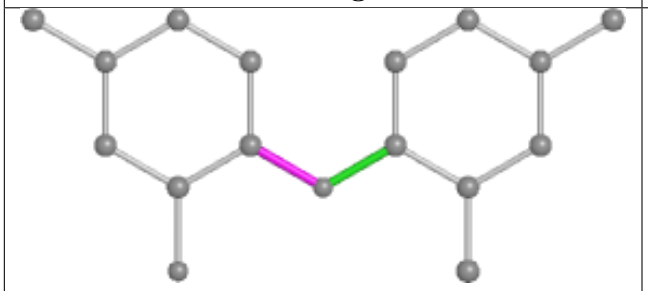

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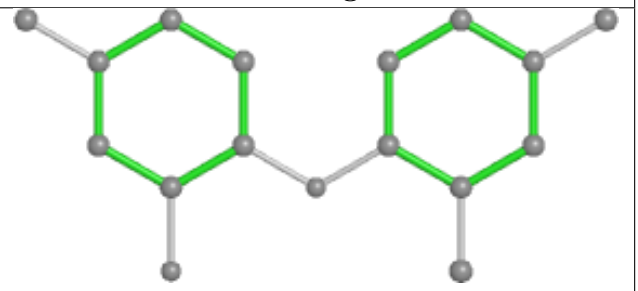
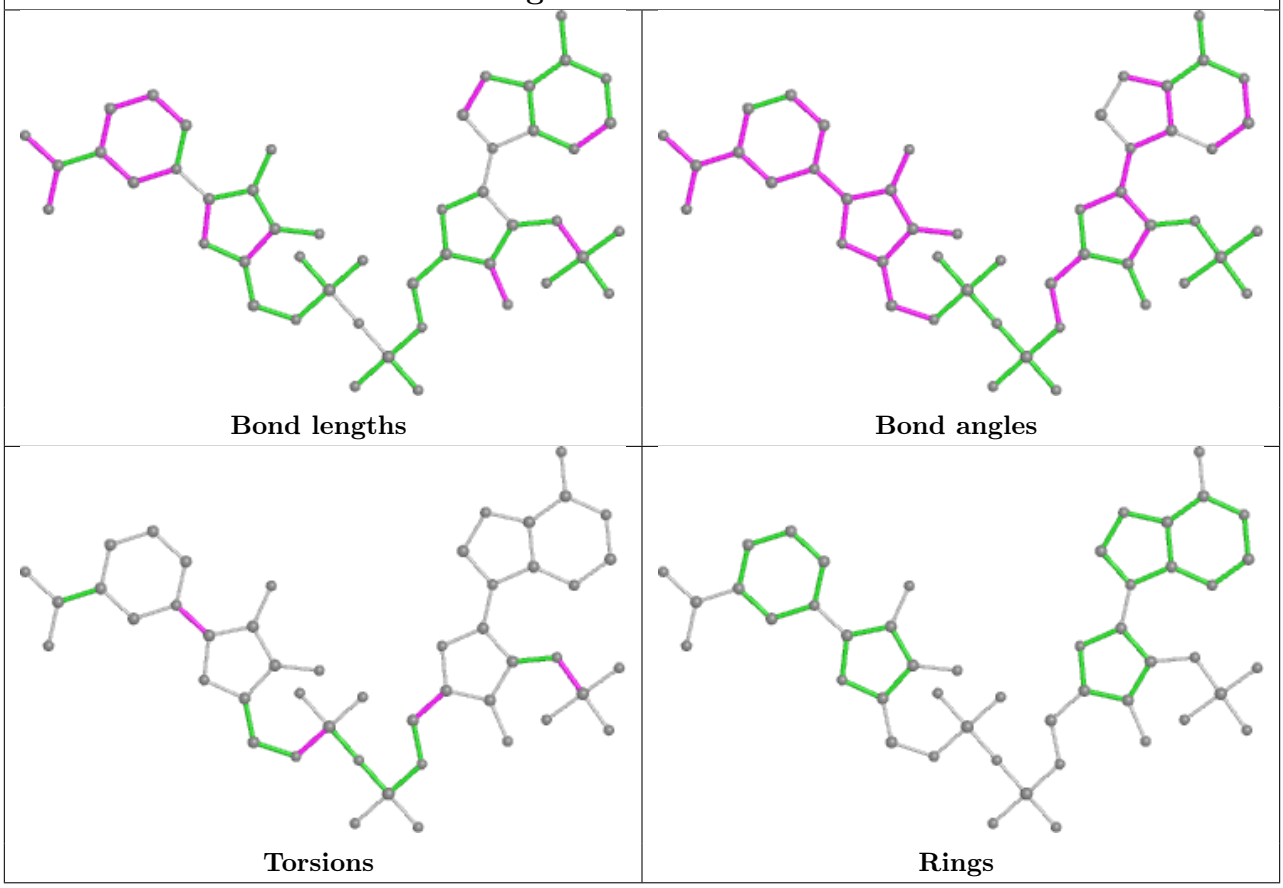


Rings

Ligand NAP J 257



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	255/260 (98%)	-0.45	3 (1%)	79	82	6, 16, 31, 50	0
1	D	260/260 (100%)	-0.38	3 (1%)	79	82	8, 19, 40, 52	0
1	G	254/260 (97%)	-0.34	3 (1%)	79	82	8, 18, 40, 60	0
1	J	260/260 (100%)	-0.19	9 (3%)	44	49	7, 19, 48, 60	0
All	All	1029/1040 (98%)	-0.34	18 (1%)	70	75	6, 18, 41, 60	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	60	ALA	9.8
1	J	60	ALA	6.9
1	A	60	ALA	5.7
1	J	103	ARG	5.4
1	G	60	ALA	4.5
1	G	43	ARG	4.4
1	J	59	GLU	3.4
1	J	43	ARG	2.7
1	G	42	GLU	2.5
1	J	58	PRO	2.5
1	J	-2	ALA	2.4
1	J	57	GLN	2.3
1	J	44	SER	2.2
1	D	59	GLU	2.2
1	J	55	LEU	2.2
1	A	207	ILE	2.2
1	A	59	GLU	2.1
1	D	-1	ALA	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)

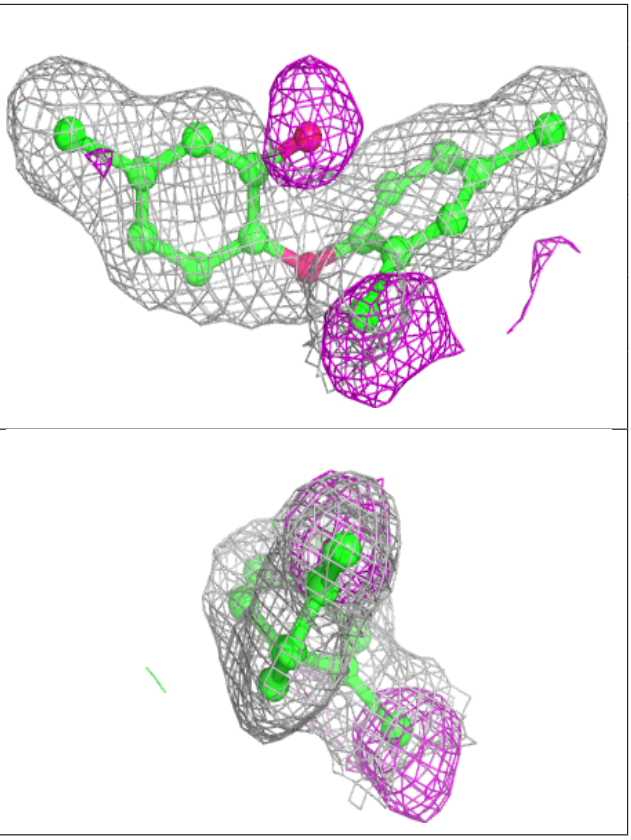
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TCL	D	258	17/17	0.82	0.17	25,29,35,42	0
3	TCL	J	258	17/17	0.87	0.17	19,25,34,39	0
3	TCL	A	371	17/17	0.88	0.16	16,21,28,32	0
3	TCL	G	258	17/17	0.92	0.15	18,20,26,32	0
2	NAP	J	257	48/48	0.93	0.13	14,20,32,33	0
2	NAP	G	257	48/48	0.94	0.12	9,16,33,41	0
2	NAP	D	257	48/48	0.94	0.12	5,16,24,30	0
2	NAP	A	361	48/48	0.97	0.09	6,14,24,27	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.

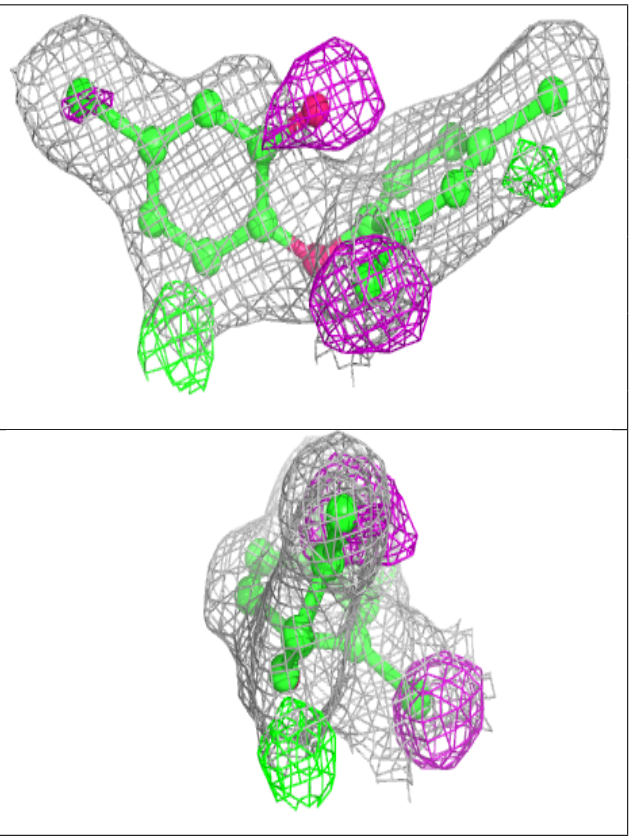
Electron density around TCL D 258:

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



Electron density around TCL J 258:

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



Electron density around TCL A 371:

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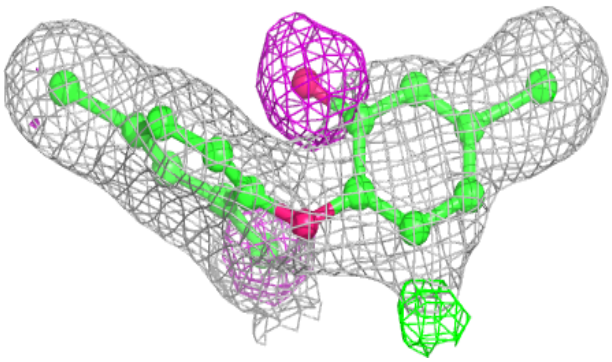
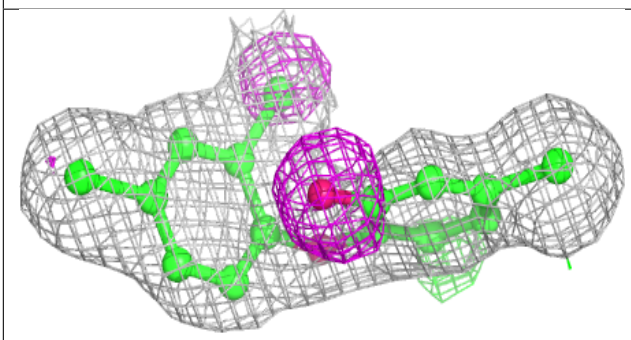
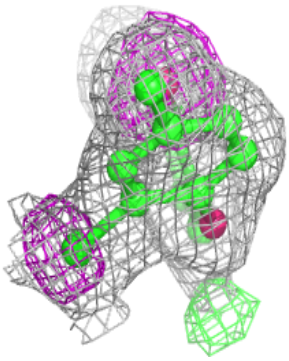
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around TCL G 258:

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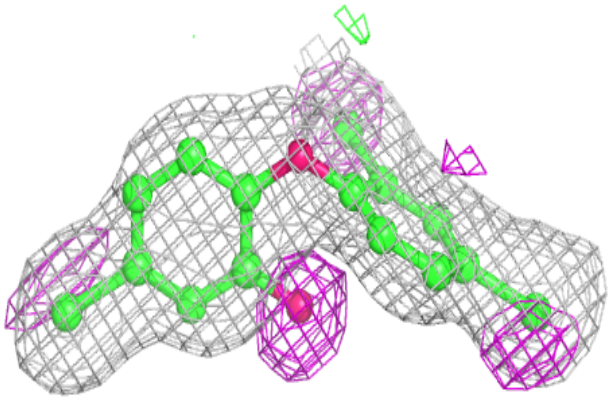
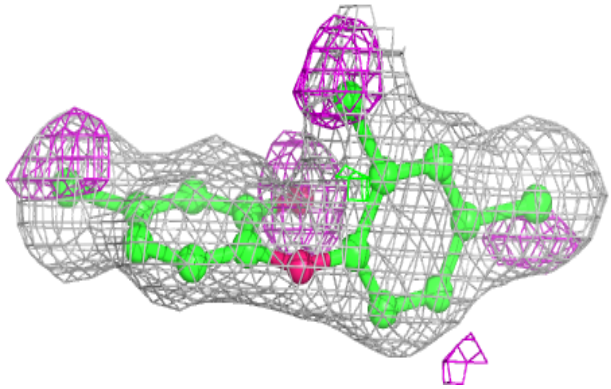
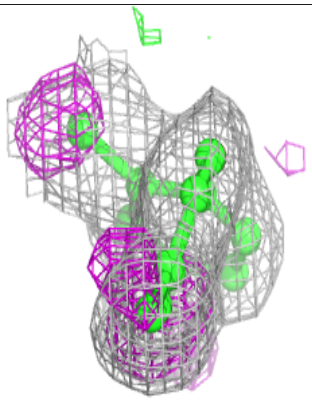
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAP J 257:

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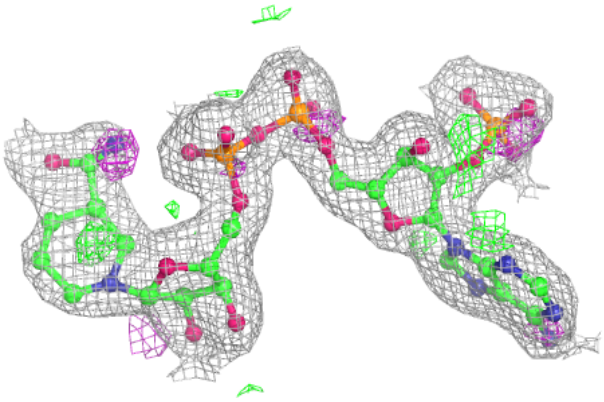
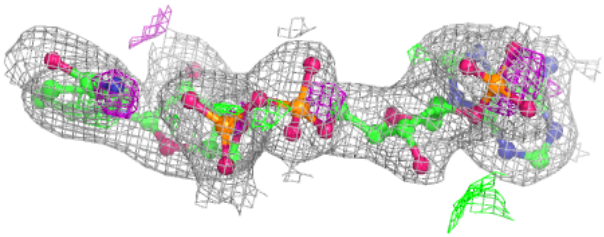
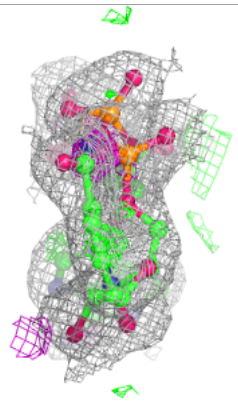
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

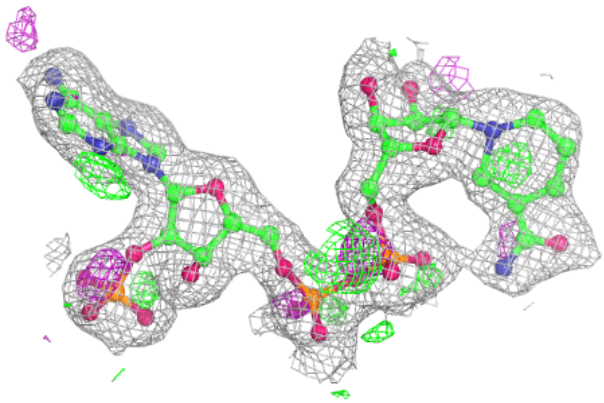


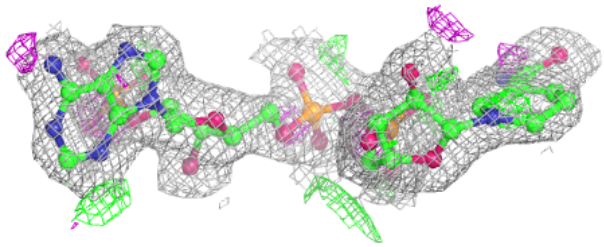


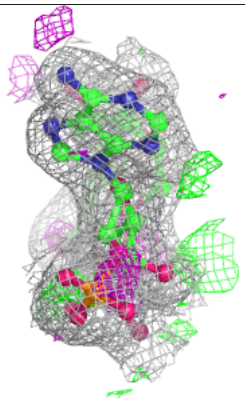


Electron density around NAP G 257:

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

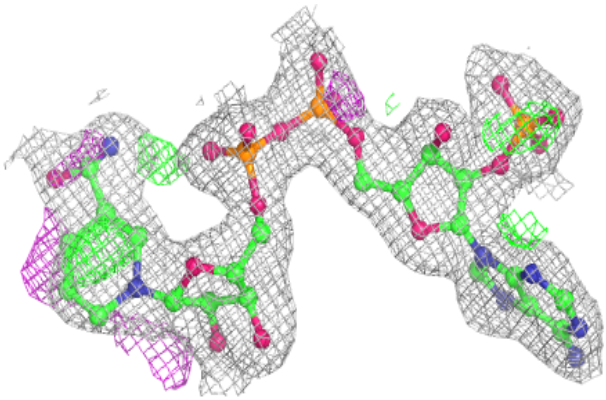


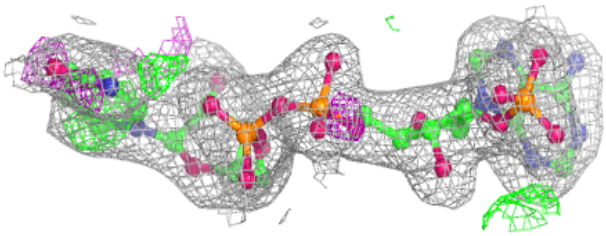


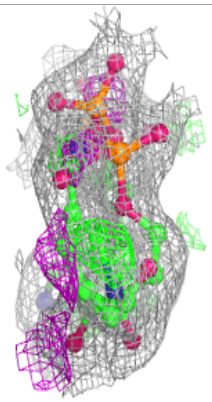


Electron density around NAP D 257:

$2mF_o$-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 361:

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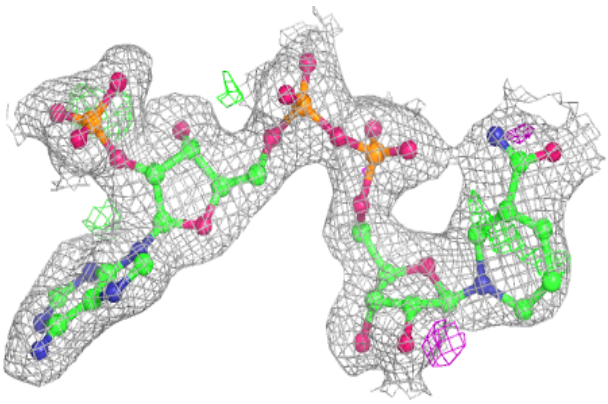
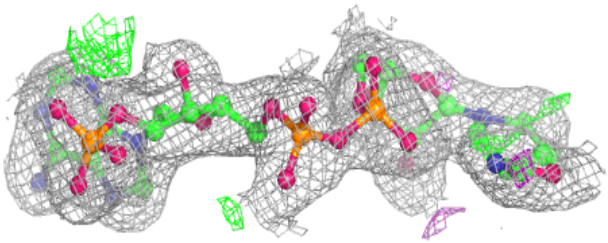
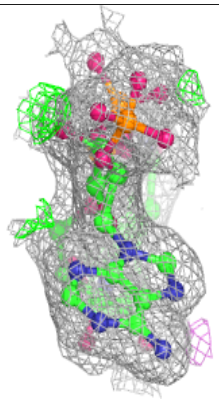
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.