Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:02 AM EDT

PDB ID	:	6DHQ
Title	:	Bovine glutamate dehydrogenase complexed with NADPH, glutamate, and GTP
Authors	:	Smith, T.J.
Deposited on	:	2018-05-20
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

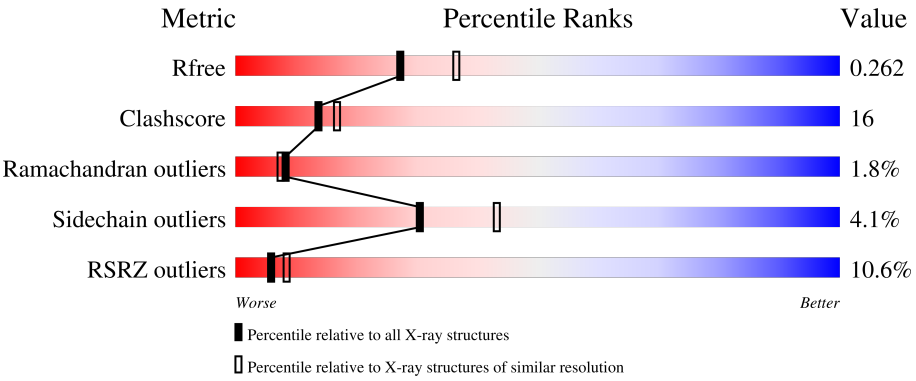
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	501	10% 68% 25% 6% •
1	B	501	9% 69% 27% •
1	C	501	12% 67% 27% 5% •
1	D	501	9% 70% 26% •
1	E	501	12% 70% 24% 5% •

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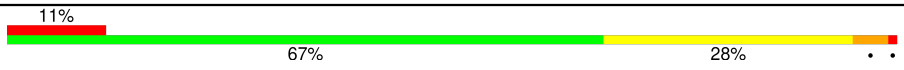
Mol	Chain	Length	Quality of chain
1	F	501	

2 Entry composition (i)

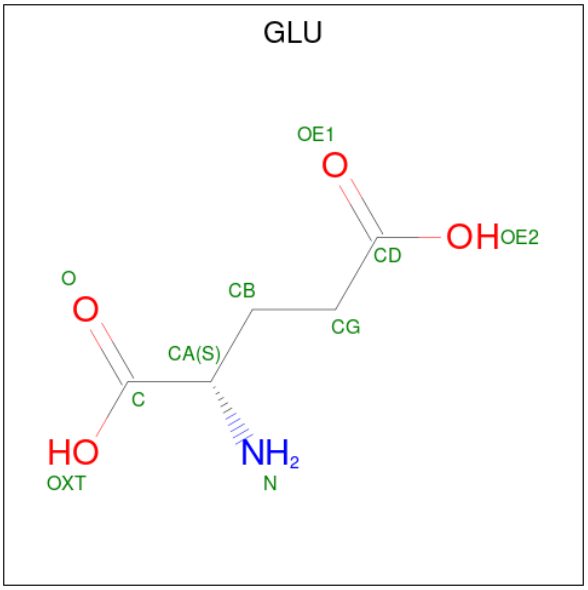
There are 5 unique types of molecules in this entry. The entry contains 24419 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase 1, mitochondrial.

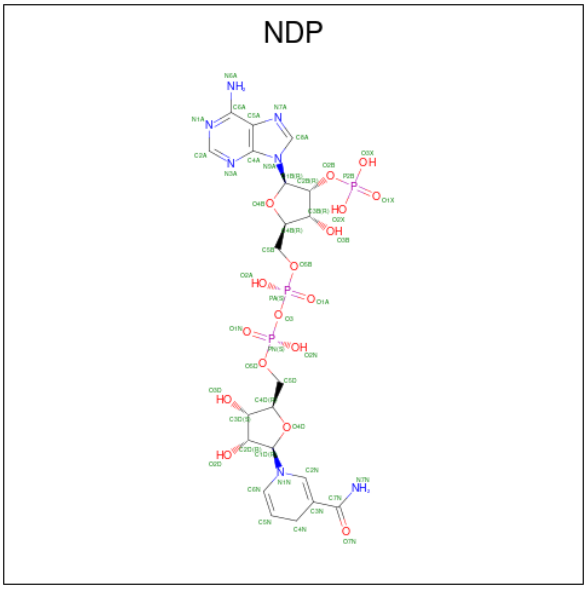
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	B	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	C	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	D	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	E	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	F	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

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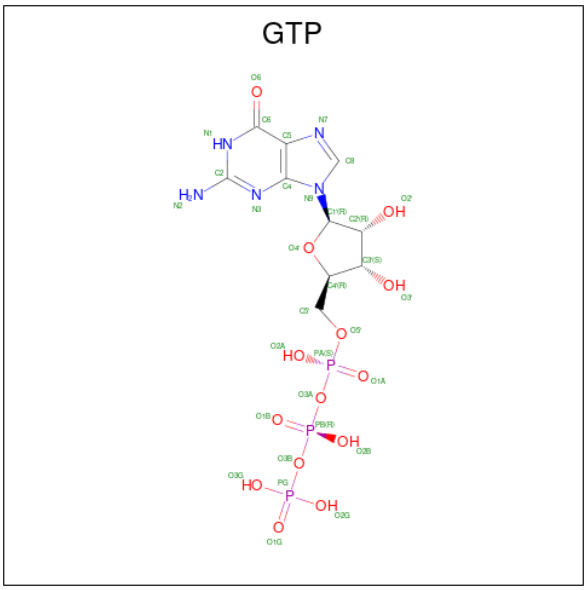
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	83	Total	O	0	0
			83	83		

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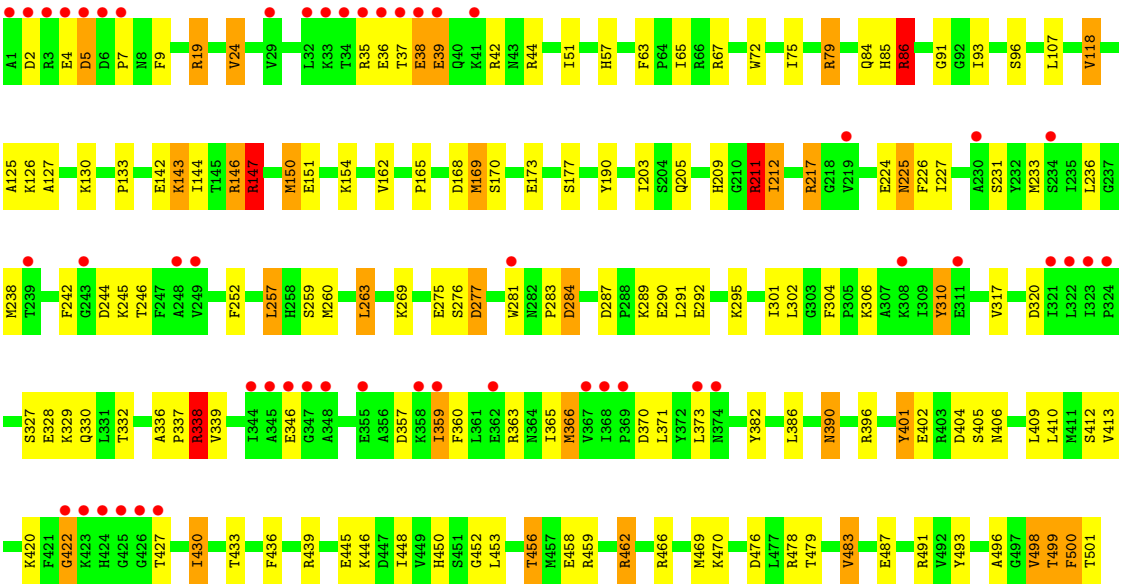
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	50	Total O 50 50	0	0
5	D	66	Total O 66 66	0	0
5	E	58	Total O 58 58	0	0
5	F	64	Total O 64 64	0	0

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.

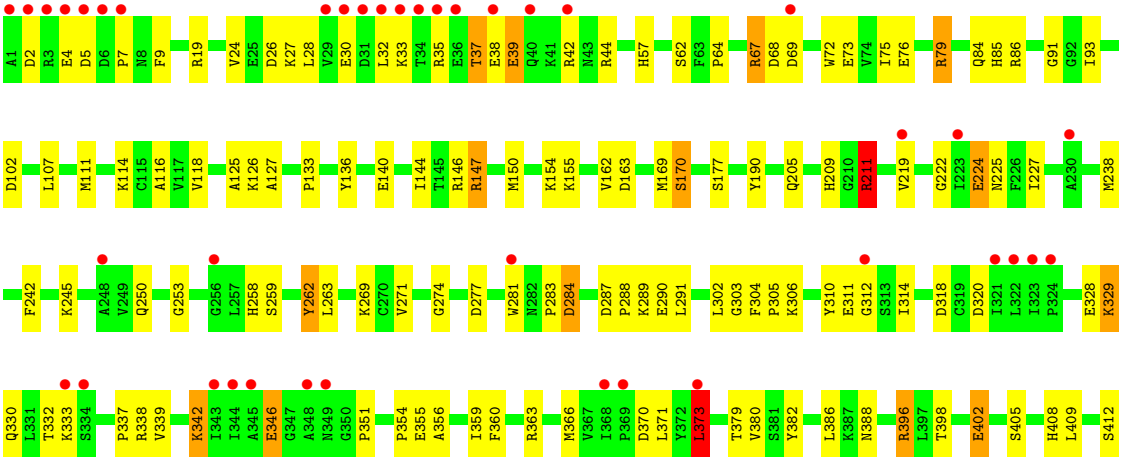
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

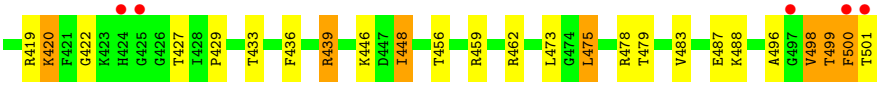
Chain A:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

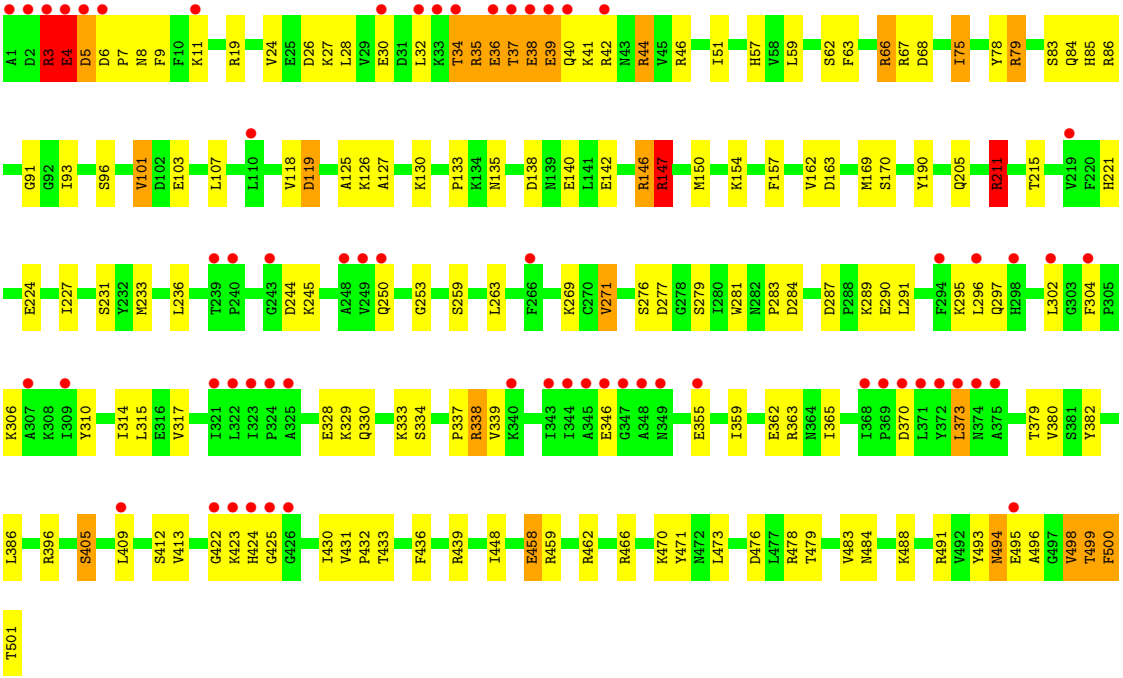
Chain B:





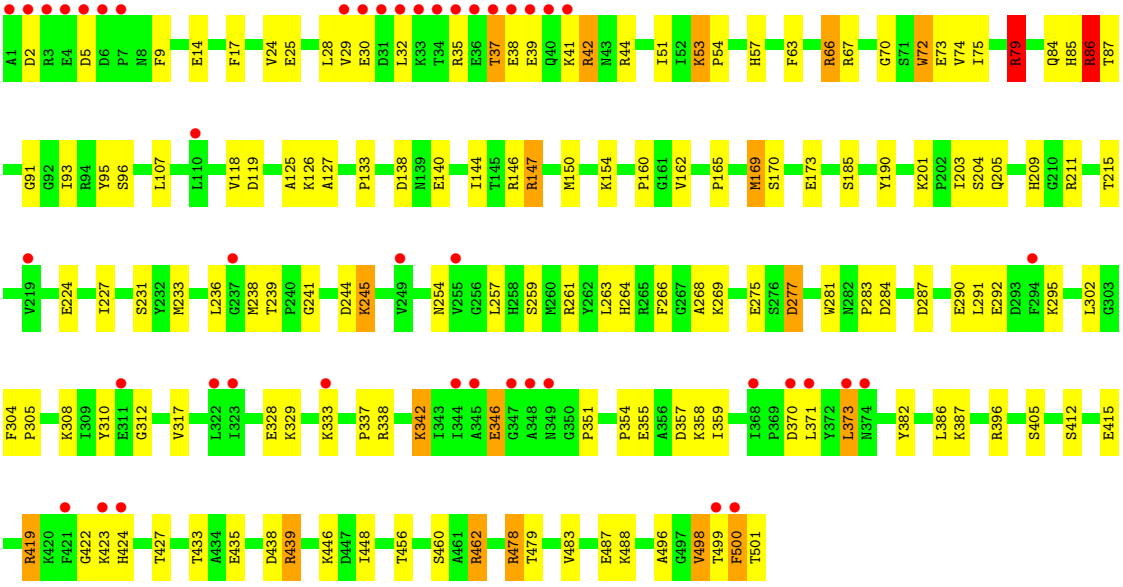
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:



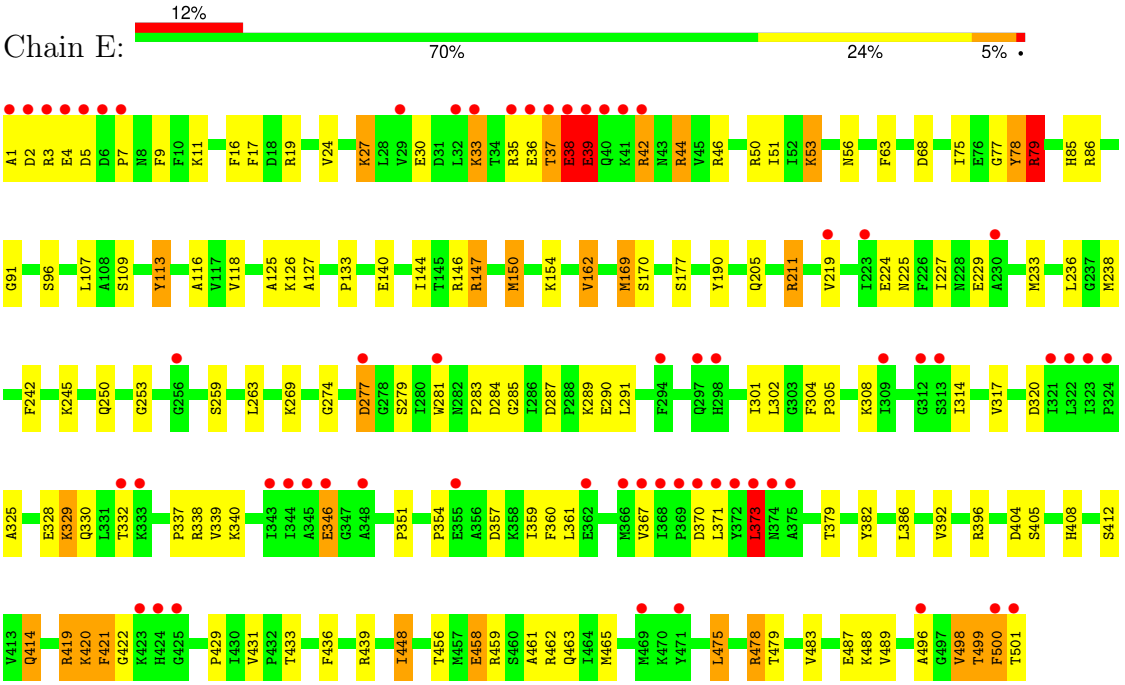
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D:



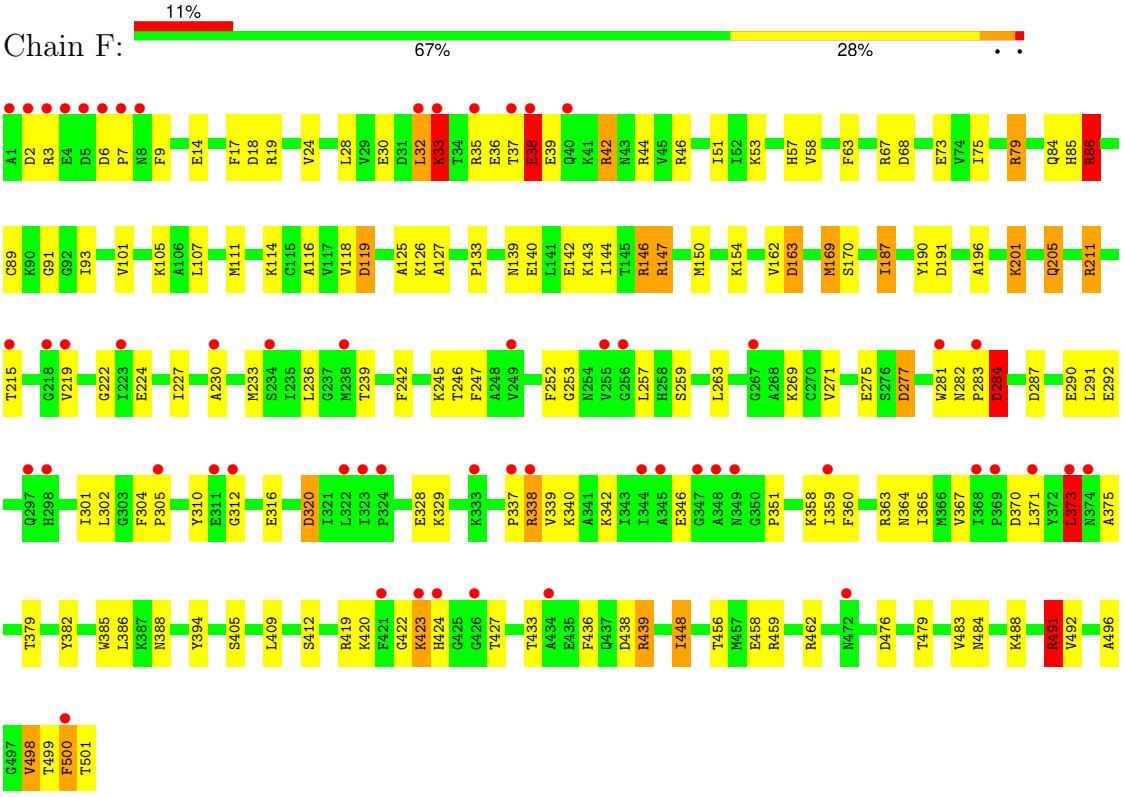
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain E:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	123.25Å 101.75Å 167.85Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	29.55 – 2.30 29.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	60.2 (29.55-2.30) 60.2 (29.55-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.224 , 0.262 0.224 , 0.262	Depositor DCC
R_{free} test set	1998 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.8	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	0.93	EDS
Total number of atoms	24419	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, GTP

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	1.03	19/3999 (0.5%)	1.22	54/5396 (1.0%)
1	B	0.79	10/3999 (0.3%)	1.05	37/5396 (0.7%)
1	C	0.83	17/3999 (0.4%)	1.16	49/5396 (0.9%)
1	D	0.80	12/3999 (0.3%)	1.20	42/5396 (0.8%)
1	E	1.21	34/3999 (0.9%)	1.30	59/5396 (1.1%)
1	F	0.83	16/3999 (0.4%)	1.18	45/5396 (0.8%)
All	All	0.93	108/23994 (0.5%)	1.19	286/32376 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	7
1	D	0	3
1	E	0	4
1	F	0	6
All	All	0	25

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	TYR	CE2-CZ	-21.36	1.10	1.38
1	A	401	TYR	CE1-CZ	-21.11	1.11	1.38
1	A	401	TYR	CG-CD1	-20.11	1.13	1.39
1	A	401	TYR	CG-CD2	-19.33	1.14	1.39
1	E	78	TYR	CE1-CZ	-18.69	1.14	1.38
1	E	113	TYR	CE2-CZ	-17.94	1.15	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	78	TYR	CE2-CZ	-17.36	1.16	1.38
1	E	113	TYR	CE1-CZ	-16.19	1.17	1.38
1	E	78	TYR	CG-CD1	-16.16	1.18	1.39
1	E	113	TYR	CG-CD1	-15.43	1.19	1.39
1	E	78	TYR	CG-CD2	-15.41	1.19	1.39
1	E	44	ARG	CB-CG	-14.97	1.12	1.52
1	E	458	GLU	CD-OE2	-14.58	1.09	1.25
1	E	113	TYR	CG-CD2	-14.45	1.20	1.39
1	E	16	PHE	CE1-CZ	-13.60	1.11	1.37
1	E	16	PHE	CE2-CZ	-13.52	1.11	1.37
1	F	448	ILE	CB-CG2	-12.99	1.12	1.52
1	B	67	ARG	CZ-NH1	-12.37	1.17	1.33
1	E	16	PHE	CG-CD1	-12.18	1.20	1.38
1	E	16	PHE	CG-CD2	-12.04	1.20	1.38
1	D	396	ARG	CZ-NH1	-11.86	1.17	1.33
1	A	328	GLU	CD-OE2	-11.45	1.13	1.25
1	A	328	GLU	CD-OE1	-11.22	1.13	1.25
1	D	328	GLU	CD-OE1	-11.16	1.13	1.25
1	E	42	ARG	CZ-NH1	-10.80	1.19	1.33
1	A	390	ASN	CG-OD1	-10.68	1.00	1.24
1	F	439	ARG	CZ-NH1	-10.44	1.19	1.33
1	F	439	ARG	CB-CG	-10.08	1.25	1.52
1	E	458	GLU	CD-OE1	-9.38	1.15	1.25
1	D	328	GLU	CD-OE2	-9.31	1.15	1.25
1	C	135	ASN	CG-ND2	-9.25	1.09	1.32
1	C	373	LEU	CG-CD1	-9.02	1.18	1.51
1	A	390	ASN	CG-ND2	-8.89	1.10	1.32
1	C	103	GLU	CD-OE1	-8.57	1.16	1.25
1	E	346	GLU	CD-OE2	-8.42	1.16	1.25
1	E	414	GLN	CD-NE2	-8.41	1.11	1.32
1	B	76	GLU	CD-OE2	-8.36	1.16	1.25
1	C	135	ASN	CG-OD1	-8.34	1.05	1.24
1	F	147	ARG	CG-CD	-8.33	1.31	1.51
1	F	147	ARG	CB-CG	-8.30	1.30	1.52
1	E	225	ASN	CG-OD1	-8.19	1.05	1.24
1	D	373	LEU	CG-CD1	-8.06	1.22	1.51
1	B	338	ARG	CB-CG	-7.71	1.31	1.52
1	F	205	GLN	CD-NE2	7.66	1.51	1.32
1	D	44	ARG	CB-CG	-7.57	1.32	1.52
1	C	297	GLN	CB-CG	-7.54	1.32	1.52
1	D	346	GLU	CD-OE2	-7.40	1.17	1.25
1	C	103	GLU	CB-CG	-7.39	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	44	ARG	CB-CG	-7.33	1.32	1.52
1	C	44	ARG	CZ-NH1	-7.29	1.23	1.33
1	B	44	ARG	CB-CG	-7.24	1.32	1.52
1	E	56	ASN	CG-ND2	-7.22	1.14	1.32
1	E	414	GLN	CD-OE1	-7.18	1.08	1.24
1	B	328	GLU	CD-OE2	-7.13	1.17	1.25
1	C	346	GLU	CD-OE2	-7.10	1.17	1.25
1	C	439	ARG	CB-CG	-7.09	1.33	1.52
1	B	289	LYS	CB-CG	-7.00	1.33	1.52
1	A	44	ARG	CB-CG	-6.98	1.33	1.52
1	D	387	LYS	CE-NZ	6.98	1.66	1.49
1	F	338	ARG	CB-CG	-6.98	1.33	1.52
1	E	225	ASN	CG-ND2	-6.93	1.15	1.32
1	E	458	GLU	CG-CD	-6.89	1.41	1.51
1	C	147	ARG	CB-CG	-6.85	1.34	1.52
1	B	346	GLU	CD-OE2	-6.85	1.18	1.25
1	F	346	GLU	CD-OE2	-6.85	1.18	1.25
1	E	289	LYS	CG-CD	-6.77	1.29	1.52
1	D	387	LYS	CD-CE	6.76	1.68	1.51
1	E	338	ARG	CB-CG	-6.71	1.34	1.52
1	C	338	ARG	CB-CG	-6.69	1.34	1.52
1	D	338	ARG	CB-CG	-6.59	1.34	1.52
1	E	147	ARG	CB-CG	-6.55	1.34	1.52
1	D	147	ARG	CB-CG	-6.52	1.34	1.52
1	A	402	GLU	CB-CG	-6.43	1.40	1.52
1	C	328	GLU	CD-OE2	-6.35	1.18	1.25
1	D	338	ARG	CG-CD	-6.32	1.36	1.51
1	A	346	GLU	CD-OE2	-6.26	1.18	1.25
1	F	439	ARG	CG-CD	-6.25	1.36	1.51
1	A	147	ARG	CB-CG	-6.21	1.35	1.52
1	C	44	ARG	CB-CG	-6.21	1.35	1.52
1	F	44	ARG	CZ-NH1	-6.21	1.25	1.33
1	F	328	GLU	CD-OE1	-6.18	1.18	1.25
1	E	56	ASN	CG-OD1	-6.09	1.10	1.24
1	F	205	GLN	CG-CD	5.95	1.64	1.51
1	A	67	ARG	CZ-NH1	-5.94	1.25	1.33
1	D	245	LYS	CE-NZ	-5.93	1.34	1.49
1	A	225	ASN	CG-ND2	-5.92	1.18	1.32
1	E	42	ARG	CZ-NH2	-5.90	1.25	1.33
1	F	484	ASN	CG-ND2	-5.90	1.18	1.32
1	C	147	ARG	CG-CD	-5.89	1.37	1.51
1	B	346	GLU	CD-OE1	-5.87	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	458	GLU	CG-CD	-5.85	1.43	1.51
1	A	439	ARG	CZ-NH1	-5.79	1.25	1.33
1	E	328	GLU	CD-OE1	-5.73	1.19	1.25
1	B	328	GLU	CD-OE1	-5.71	1.19	1.25
1	A	289	LYS	CB-CG	-5.58	1.37	1.52
1	F	484	ASN	CG-OD1	-5.56	1.11	1.24
1	A	147	ARG	CG-CD	-5.55	1.38	1.51
1	A	338	ARG	CB-CG	-5.52	1.37	1.52
1	F	205	GLN	CB-CG	-5.48	1.37	1.52
1	C	484	ASN	CG-ND2	-5.46	1.19	1.32
1	E	289	LYS	CB-CG	-5.36	1.38	1.52
1	A	373	LEU	CG-CD1	-5.35	1.32	1.51
1	E	289	LYS	CD-CE	-5.33	1.38	1.51
1	E	328	GLU	CD-OE2	-5.32	1.19	1.25
1	C	289	LYS	CB-CG	-5.20	1.38	1.52
1	B	487	GLU	CD-OE1	-5.13	1.20	1.25
1	E	373	LEU	CG-CD1	-5.03	1.33	1.51
1	E	338	ARG	CG-CD	-5.02	1.39	1.51

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	44	ARG	NE-CZ-NH2	30.45	135.53	120.30
1	E	42	ARG	NE-CZ-NH2	25.93	133.26	120.30
1	F	439	ARG	NE-CZ-NH2	23.18	131.89	120.30
1	D	396	ARG	NE-CZ-NH1	-23.13	108.73	120.30
1	B	67	ARG	NE-CZ-NH2	23.05	131.83	120.30
1	A	67	ARG	NE-CZ-NH2	19.79	130.19	120.30
1	C	338	ARG	NE-CZ-NH2	18.93	129.76	120.30
1	D	261	ARG	NE-CZ-NH2	18.84	129.72	120.30
1	D	396	ARG	NE-CZ-NH2	18.03	129.32	120.30
1	D	261	ARG	NE-CZ-NH1	-18.01	111.30	120.30
1	D	245	LYS	CD-CE-NZ	16.38	149.36	111.70
1	F	169	MET	CG-SD-CE	16.33	126.32	100.20
1	C	79	ARG	NE-CZ-NH2	16.26	128.43	120.30
1	C	373	LEU	CB-CG-CD2	16.16	138.47	111.00
1	A	169	MET	CG-SD-CE	15.67	125.28	100.20
1	F	439	ARG	NE-CZ-NH1	-15.47	112.57	120.30
1	F	79	ARG	NE-CZ-NH2	15.32	127.96	120.30
1	B	146	ARG	NE-CZ-NH1	-15.29	112.66	120.30
1	A	67	ARG	NE-CZ-NH1	-15.14	112.73	120.30
1	C	79	ARG	NE-CZ-NH1	-15.09	112.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	338	ARG	NE-CZ-NH1	-14.85	112.87	120.30
1	D	211	ARG	NE-CZ-NH2	14.78	127.69	120.30
1	F	284	ASP	CB-CG-OD2	14.58	131.42	118.30
1	B	146	ARG	NE-CZ-NH2	14.09	127.35	120.30
1	E	146	ARG	NE-CZ-NH1	-13.76	113.42	120.30
1	F	79	ARG	NE-CZ-NH1	-13.66	113.47	120.30
1	A	211	ARG	NE-CZ-NH1	-13.53	113.53	120.30
1	D	373	LEU	CB-CG-CD2	13.51	133.96	111.00
1	F	44	ARG	NE-CZ-NH2	13.28	126.94	120.30
1	D	338	ARG	NE-CZ-NH2	13.10	126.85	120.30
1	A	217	ARG	CG-CD-NE	12.59	138.23	111.80
1	F	284	ASP	CB-CG-OD1	-12.54	107.02	118.30
1	A	328	GLU	OE1-CD-OE2	-12.48	108.33	123.30
1	A	211	ARG	NE-CZ-NH2	12.47	126.54	120.30
1	D	211	ARG	NE-CZ-NH1	-12.39	114.11	120.30
1	C	44	ARG	NE-CZ-NH2	12.28	126.44	120.30
1	E	458	GLU	OE1-CD-OE2	-12.25	108.60	123.30
1	A	401	TYR	CD1-CE1-CZ	12.19	130.77	119.80
1	C	5	ASP	CB-CG-OD2	12.06	129.16	118.30
1	F	86	ARG	CB-CG-CD	11.91	142.57	111.60
1	E	44	ARG	CG-CD-NE	11.86	136.71	111.80
1	D	328	GLU	OE1-CD-OE2	-11.79	109.16	123.30
1	A	401	TYR	CZ-CE2-CD2	11.66	130.29	119.80
1	E	44	ARG	CD-NE-CZ	-11.48	107.53	123.60
1	E	146	ARG	NE-CZ-NH2	11.47	126.04	120.30
1	A	217	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	A	217	ARG	CB-CG-CD	11.13	140.55	111.60
1	A	217	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	E	16	PHE	CZ-CE2-CD2	11.07	133.38	120.10
1	E	16	PHE	CD1-CE1-CZ	11.06	133.38	120.10
1	D	284	ASP	CB-CG-OD1	-11.06	108.35	118.30
1	B	420	LYS	CD-CE-NZ	11.03	137.06	111.70
1	E	16	PHE	CB-CG-CD1	11.02	128.52	120.80
1	E	475	LEU	CB-CG-CD1	10.98	129.66	111.00
1	A	462	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	D	44	ARG	NE-CZ-NH2	10.84	125.72	120.30
1	F	448	ILE	CG1-CB-CG2	-10.73	87.78	111.40
1	E	16	PHE	CD1-CG-CD2	-10.69	104.41	118.30
1	A	401	TYR	CE1-CZ-CE2	-10.66	102.74	119.80
1	E	16	PHE	CE1-CZ-CE2	-10.64	100.85	120.00
1	A	42	ARG	CA-CB-CG	10.57	136.66	113.40
1	E	44	ARG	NE-CZ-NH1	-10.54	115.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	448	ILE	CA-CB-CG1	10.53	131.00	111.00
1	E	211	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	C	439	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	E	78	TYR	CZ-CE2-CD2	10.36	129.13	119.80
1	E	44	ARG	NH1-CZ-NH2	-10.34	108.03	119.40
1	F	211	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	F	86	ARG	CA-CB-CG	-10.10	91.19	113.40
1	B	44	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	E	11	LYS	CB-CG-CD	9.91	137.38	111.60
1	E	211	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	C	103	GLU	CA-CB-CG	9.87	135.12	113.40
1	F	86	ARG	CG-CD-NE	9.86	132.51	111.80
1	B	169	MET	CG-SD-CE	9.80	115.88	100.20
1	D	146	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	E	78	TYR	CD1-CE1-CZ	9.77	128.59	119.80
1	A	401	TYR	CD1-CG-CD2	-9.76	107.16	117.90
1	D	261	ARG	CD-NE-CZ	9.73	137.22	123.60
1	E	169	MET	CG-SD-CE	9.71	115.74	100.20
1	B	163	ASP	CB-CG-OD1	9.66	126.99	118.30
1	A	79	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	C	130	LYS	CD-CE-NZ	9.54	133.63	111.70
1	C	67	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	D	284	ASP	CB-CG-OD2	9.48	126.84	118.30
1	F	169	MET	CB-CG-SD	-9.36	84.32	112.40
1	F	491	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	E	113	TYR	CB-CG-CD1	9.19	126.51	121.00
1	D	387	LYS	CD-CE-NZ	-9.18	90.60	111.70
1	A	401	TYR	CB-CG-CD1	9.16	126.49	121.00
1	C	6	ASP	CB-CG-OD2	-9.11	110.11	118.30
1	E	78	TYR	CD1-CG-CD2	-9.09	107.91	117.90
1	E	113	TYR	CD1-CE1-CZ	9.08	127.97	119.80
1	A	42	ARG	NE-CZ-NH1	-9.07	115.77	120.30
1	E	42	ARG	NH1-CZ-NH2	-9.06	109.43	119.40
1	D	169	MET	CG-SD-CE	9.06	114.69	100.20
1	C	169	MET	CG-SD-CE	9.05	114.67	100.20
1	A	42	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	A	42	ARG	CG-CD-NE	9.03	130.75	111.80
1	C	373	LEU	CB-CG-CD1	-9.00	95.70	111.00
1	A	462	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	C	119	ASP	CB-CG-OD2	-8.99	110.20	118.30
1	C	146	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	E	16	PHE	CB-CG-CD2	8.95	127.07	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	401	TYR	CB-CG-CD2	8.91	126.34	121.00
1	F	146	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	D	439	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	C	211	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	E	78	TYR	CE1-CZ-CE2	-8.85	105.64	119.80
1	E	113	TYR	CD1-CG-CD2	-8.79	108.23	117.90
1	F	211	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	D	138	ASP	CB-CG-OD2	8.73	126.15	118.30
1	D	79	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	E	113	TYR	CZ-CE2-CD2	8.62	127.55	119.80
1	D	146	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	284	ASP	CB-CG-OD1	-8.53	110.62	118.30
1	F	86	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	A	212	ILE	CG1-CB-CG2	-8.48	92.73	111.40
1	A	79	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	E	78	TYR	CB-CG-CD2	8.25	125.95	121.00
1	C	439	ARG	NE-CZ-NH1	-8.25	116.18	120.30
1	C	146	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	E	284	ASP	CB-CG-OD1	-8.18	110.94	118.30
1	B	67	ARG	NH1-CZ-NH2	-7.90	110.71	119.40
1	B	211	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	E	113	TYR	CE1-CZ-CE2	-7.89	107.17	119.80
1	B	211	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	F	146	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	E	11	LYS	CA-CB-CG	-7.84	96.15	113.40
1	C	79	ARG	CD-NE-CZ	7.83	134.56	123.60
1	C	119	ASP	CB-CG-OD1	7.80	125.32	118.30
1	E	78	TYR	CB-CG-CD1	7.78	125.67	121.00
1	D	329	LYS	CD-CE-NZ	-7.77	93.83	111.70
1	B	69	ASP	CB-CG-OD2	7.74	125.26	118.30
1	A	430	ILE	CG1-CB-CG2	-7.73	94.39	111.40
1	D	211	ARG	CD-NE-CZ	7.71	134.40	123.60
1	A	146	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	D	138	ASP	OD1-CG-OD2	-7.66	108.75	123.30
1	F	448	ILE	CB-CG1-CD1	-7.65	92.49	113.90
1	A	366	MET	CG-SD-CE	7.64	112.43	100.20
1	A	295	LYS	CD-CE-NZ	7.59	129.15	111.70
1	A	338	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	A	217	ARG	CA-CB-CG	7.56	130.03	113.40
1	C	211	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	439	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	F	338	ARG	NE-CZ-NH2	7.45	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	ARG	CB-CA-C	-7.44	95.51	110.40
1	C	284	ASP	CB-CG-OD2	7.44	125.00	118.30
1	C	138	ASP	CB-CG-OD2	7.43	124.98	118.30
1	D	373	LEU	CB-CG-CD1	-7.40	98.42	111.00
1	C	295	LYS	CD-CE-NZ	7.36	128.63	111.70
1	D	138	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	217	ARG	CD-NE-CZ	7.29	133.80	123.60
1	F	86	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	C	5	ASP	CB-CG-OD1	-7.25	111.78	118.30
1	F	373	LEU	CB-CG-CD2	7.24	123.31	111.00
1	A	146	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	439	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	338	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	D	338	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	B	284	ASP	CB-CG-OD1	-7.15	111.86	118.30
1	E	289	LYS	CA-CB-CG	-7.15	97.68	113.40
1	F	187	ILE	CB-CG1-CD1	7.10	133.79	113.90
1	A	44	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	D	448	ILE	CG1-CB-CG2	-7.10	95.78	111.40
1	B	163	ASP	OD1-CG-OD2	-7.05	109.91	123.30
1	F	205	GLN	CA-CB-CG	-7.03	97.93	113.40
1	B	439	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	F	119	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	B	147	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	B	408	HIS	CG-ND1-CE1	6.93	117.91	108.20
1	E	284	ASP	CB-CG-OD2	6.92	124.53	118.30
1	C	328	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	B	420	LYS	CG-CD-CE	6.90	132.59	111.90
1	D	42	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	E	338	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	D	439	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	F	79	ARG	CB-CG-CD	6.73	129.10	111.60
1	B	155	LYS	CA-CB-CG	-6.68	98.71	113.40
1	C	138	ASP	OD1-CG-OD2	-6.67	110.62	123.30
1	B	306	LYS	CB-CG-CD	6.65	128.90	111.60
1	B	146	ARG	CD-NE-CZ	6.64	132.90	123.60
1	B	373	LEU	CB-CG-CD2	6.63	122.27	111.00
1	F	163	ASP	CB-CG-OD1	6.63	124.27	118.30
1	E	162	VAL	CG1-CB-CG2	6.62	121.49	110.90
1	A	483	VAL	CG1-CB-CG2	-6.61	100.32	110.90
1	C	44	ARG	CG-CD-NE	6.57	125.59	111.80
1	C	289	LYS	CD-CE-NZ	-6.56	96.60	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	346	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	B	76	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	B	306	LYS	CD-CE-NZ	6.50	126.64	111.70
1	B	284	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	6	ASP	CB-CG-OD1	6.40	124.06	118.30
1	F	147	ARG	CG-CD-NE	-6.35	98.46	111.80
1	C	138	ASP	CB-CG-OD1	6.34	124.01	118.30
1	C	373	LEU	CD1-CG-CD2	-6.33	91.51	110.50
1	F	42	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	C	458	GLU	CG-CD-OE1	-6.27	105.77	118.30
1	F	86	ARG	CD-NE-CZ	-6.25	114.85	123.60
1	B	346	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	E	42	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	A	284	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	D	79	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	F	346	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	B	67	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	C	101	VAL	CG1-CB-CG2	6.17	120.77	110.90
1	E	338	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	373	LEU	CB-CG-CD2	6.09	121.36	111.00
1	D	245	LYS	CG-CD-CE	-6.06	93.71	111.90
1	A	346	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	D	86	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	E	373	LEU	CB-CG-CD2	5.96	121.14	111.00
1	D	487	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	F	79	ARG	CG-CD-NE	5.93	124.26	111.80
1	E	328	GLU	OE1-CD-OE2	-5.92	116.20	123.30
1	B	328	GLU	OE1-CD-OE2	-5.87	116.25	123.30
1	E	421	PHE	CD1-CG-CD2	-5.86	110.68	118.30
1	F	328	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	E	146	ARG	CD-NE-CZ	5.84	131.77	123.60
1	B	211	ARG	CB-CG-CD	5.83	126.76	111.60
1	A	44	ARG	CG-CD-NE	5.79	123.96	111.80
1	F	147	ARG	CA-CB-CG	-5.79	100.67	113.40
1	A	462	ARG	CG-CD-NE	5.78	123.94	111.80
1	F	79	ARG	CD-NE-CZ	5.73	131.62	123.60
1	E	44	ARG	CB-CG-CD	5.72	126.48	111.60
1	E	421	PHE	CB-CG-CD2	5.71	124.80	120.80
1	F	201	LYS	CD-CE-NZ	5.71	124.83	111.70
1	D	295	LYS	CD-CE-NZ	-5.67	98.67	111.70
1	B	262	TYR	CB-CG-CD1	5.67	124.40	121.00
1	C	44	ARG	NH1-CZ-NH2	-5.65	113.18	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	44	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	A	86	ARG	CB-CG-CD	5.64	126.26	111.60
1	E	458	GLU	CB-CG-CD	5.64	129.42	114.20
1	E	42	ARG	CG-CD-NE	5.63	123.63	111.80
1	E	458	GLU	CG-CD-OE2	5.62	129.55	118.30
1	D	86	ARG	CA-CB-CG	-5.60	101.08	113.40
1	E	211	ARG	CB-CG-CD	5.59	126.13	111.60
1	A	169	MET	CB-CG-SD	-5.58	95.67	112.40
1	E	346	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	C	75	ILE	CG1-CB-CG2	5.56	123.64	111.40
1	D	373	LEU	CD1-CG-CD2	-5.55	93.85	110.50
1	B	147	ARG	CD-NE-CZ	5.54	131.36	123.60
1	F	169	MET	CA-CB-CG	5.52	122.68	113.30
1	B	475	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	D	86	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	211	ARG	CB-CG-CD	5.48	125.85	111.60
1	F	211	ARG	CB-CG-CD	5.44	125.73	111.60
1	C	346	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	E	113	TYR	CB-CG-CD2	5.43	124.26	121.00
1	F	338	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	C	297	GLN	CB-CG-CD	5.41	125.67	111.60
1	A	211	ARG	CG-CD-NE	5.41	123.16	111.80
1	E	431	VAL	CG1-CB-CG2	5.40	119.54	110.90
1	B	448	ILE	CG1-CB-CG2	-5.39	99.54	111.40
1	E	211	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	284	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	44	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	E	42	ARG	CA-CB-CG	5.34	125.16	113.40
1	B	408	HIS	ND1-CG-CD2	-5.32	98.55	106.00
1	C	67	ARG	CG-CD-NE	5.31	122.95	111.80
1	C	67	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	B	396	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	44	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	F	439	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
1	C	458	GLU	CA-CB-CG	-5.21	101.94	113.40
1	C	271	VAL	CG1-CB-CG2	5.21	119.23	110.90
1	C	296	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	476	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	5	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	D	487	GLU	CG-CD-OE1	5.14	128.58	118.30
1	F	79	ARG	CA-CB-CG	5.12	124.67	113.40
1	E	79	ARG	NE-CZ-NH1	5.11	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	329	LYS	CD-CE-NZ	-5.09	99.98	111.70
1	D	5	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	359	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	B	329	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	A	79	ARG	CD-NE-CZ	5.08	130.71	123.60
1	F	147	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	402	GLU	CA-CB-CG	5.07	124.55	113.40
1	C	338	ARG	CB-CA-C	-5.06	100.28	110.40
1	E	421	PHE	CD1-CE1-CZ	5.05	126.17	120.10
1	A	118	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	C	103	GLU	CB-CG-CD	5.04	127.81	114.20
1	A	24	VAL	CB-CA-C	-5.04	101.83	111.40
1	E	448	ILE	CG1-CB-CG2	-5.03	100.34	111.40
1	A	42	ARG	CD-NE-CZ	-5.01	116.59	123.60

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	GLU	Peptide
1	A	499	THR	Peptide
1	A	86	ARG	Peptide
1	B	37	THR	Peptide
1	B	86	ARG	Peptide
1	C	3	ARG	Peptide
1	C	34	THR	Peptide
1	C	37	THR	Peptide
1	C	370	ASP	Sidechain
1	C	39	GLU	Peptide
1	C	4	GLU	Peptide
1	C	86	ARG	Peptide
1	D	39	GLU	Peptide
1	D	72	TRP	Peptide
1	D	86	ARG	Peptide
1	E	33	LYS	Peptide
1	E	38	GLU	Peptide
1	E	39	GLU	Peptide
1	E	86	ARG	Peptide
1	F	284	ASP	Sidechain
1	F	32	LEU	Peptide
1	F	320	ASP	Sidechain
1	F	33	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	F	439	ARG	Sidechain
1	F	86	ARG	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	3916	0	3880	161	0
1	B	3916	0	3880	120	0
1	C	3916	0	3880	141	0
1	D	3916	0	3880	129	0
1	E	3916	0	3880	137	0
1	F	3916	0	3880	134	0
2	A	10	0	5	1	0
2	B	10	0	5	2	0
2	C	10	0	5	2	0
2	D	10	0	5	1	0
2	E	10	0	5	1	0
2	F	10	0	5	1	0
3	A	48	0	26	4	0
3	B	48	0	26	3	0
3	C	48	0	26	4	0
3	D	48	0	26	7	0
3	E	48	0	26	4	0
3	F	48	0	26	5	0
4	A	32	0	12	0	0
4	B	32	0	12	1	0
4	C	32	0	12	0	0
4	D	32	0	12	1	0
4	E	32	0	12	0	0
4	F	32	0	12	1	0
5	A	62	0	0	10	0
5	B	83	0	0	8	1
5	C	50	0	0	10	0
5	D	66	0	0	17	0
5	E	58	0	0	5	1
5	F	64	0	0	20	0
All	All	24419	0	23538	756	1

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 16.

All (756) 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:A:363:ARG:HH21	1:A:365:ILE:CD1	1.25	1.48
1:A:363:ARG:NH2	1:A:365:ILE:HD11	1.36	1.40
1:E:458:GLU:CD	1:E:462:ARG:HH21	1.31	1.33
1:C:333:LYS:HE2	1:C:355:GLU:CB	1.63	1.26
1:C:333:LYS:HE2	1:C:355:GLU:CG	1.65	1.24
1:A:363:ARG:NH2	1:A:365:ILE:CD1	1.94	1.16
1:A:130:LYS:NZ	5:A:701:HOH:O	1.86	1.09
1:C:333:LYS:HE2	1:C:355:GLU:HG2	1.25	1.08
1:A:339:VAL:HG12	1:A:363:ARG:NH2	1.69	1.07
1:A:339:VAL:HG12	1:A:363:ARG:HH22	0.93	1.04
1:A:310:TYR:HE2	1:A:317:VAL:HG23	1.24	1.03
1:A:86:ARG:NH1	5:A:702:HOH:O	1.90	1.02
1:E:458:GLU:CD	1:E:462:ARG:NH2	2.12	1.02
1:C:333:LYS:HE2	1:C:355:GLU:HB3	1.37	1.02
1:A:496:ALA:HB2	1:F:205:GLN:HE22	1.26	1.00
1:F:46:ARG:NH1	5:F:701:HOH:O	1.85	0.99
1:C:333:LYS:CE	1:C:355:GLU:HG2	1.92	0.99
1:B:147:ARG:HH22	1:E:500:PHE:N	1.62	0.98
1:A:436:PHE:CZ	1:F:409:LEU:HD12	1.98	0.97
1:C:277:ASP:HB3	1:C:302:LEU:HD11	1.47	0.96
1:C:333:LYS:CE	1:C:355:GLU:HB3	1.95	0.96
1:A:337:PRO:HD3	1:A:359:ILE:HD13	1.46	0.95
1:A:151:GLU:OE1	1:A:154:LYS:NZ	1.99	0.95
1:D:73:GLU:HG2	1:D:74:VAL:H	1.30	0.95
1:B:419:ARG:NH2	5:B:701:HOH:O	2.00	0.94
1:A:339:VAL:CG1	1:A:363:ARG:HH22	1.79	0.94
1:A:7:PRO:O	1:A:329:LYS:NZ	2.00	0.94
1:C:333:LYS:CD	1:C:355:GLU:HB3	1.98	0.93
1:E:279:SER:OG	1:E:314:ILE:HG23	1.67	0.92
1:C:126:LYS:NZ	5:C:701:HOH:O	2.03	0.91
1:D:427:THR:O	1:E:420:LYS:NZ	2.03	0.90
1:F:458:GLU:OE1	1:F:462:ARG:NH1	2.04	0.90
1:B:333:LYS:HB2	1:B:355:GLU:HG3	1.54	0.90
1:D:346:GLU:OE1	1:D:478:ARG:NH1	2.06	0.89
1:F:205:GLN:OE1	5:F:702:HOH:O	1.89	0.89
1:A:24:VAL:HG13	1:A:483:VAL:HG13	1.54	0.89
1:C:7:PRO:O	1:C:329:LYS:NZ	2.04	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLU:OE2	1:A:212:ILE:HD11	1.73	0.88
1:F:19:ARG:NH2	1:F:476:ASP:OD1	2.05	0.88
1:F:86:ARG:NH2	5:F:704:HOH:O	2.05	0.88
1:D:268:ALA:O	5:D:701:HOH:O	1.92	0.88
1:E:414:GLN:NE2	1:E:429:PRO:HA	1.89	0.88
1:A:357:ASP:OD1	1:A:478:ARG:NH2	2.06	0.88
1:C:59:LEU:HD12	5:F:713:HOH:O	1.73	0.88
1:A:496:ALA:CB	1:F:205:GLN:HE22	1.88	0.87
1:D:119:ASP:OD2	1:D:488:LYS:NZ	2.07	0.87
1:E:414:GLN:HE22	1:E:429:PRO:HA	1.39	0.87
1:A:401:TYR:CD2	1:B:439:ARG:NH2	2.42	0.86
1:A:496:ALA:HB2	1:F:205:GLN:NE2	1.89	0.86
1:A:310:TYR:CE2	1:A:317:VAL:HG23	2.10	0.86
1:E:7:PRO:O	1:E:329:LYS:NZ	2.08	0.86
1:A:277:ASP:HB3	1:A:302:LEU:HD11	1.57	0.85
1:A:363:ARG:CZ	1:A:365:ILE:HD11	2.06	0.85
1:B:7:PRO:O	1:B:329:LYS:NZ	2.08	0.85
1:F:7:PRO:O	1:F:329:LYS:NZ	2.09	0.84
1:A:65:ILE:HG22	1:A:143:LYS:HZ2	1.42	0.84
1:A:217:ARG:NH1	1:A:450:HIS:CE1	2.44	0.84
1:A:479:THR:O	1:A:483:VAL:HG23	1.77	0.83
1:C:333:LYS:CE	1:C:355:GLU:CG	2.54	0.83
1:F:89:CYS:HB2	1:F:163:ASP:OD2	1.79	0.82
2:B:601:GLU:HA	3:B:602:NDP:H41N	1.61	0.82
1:A:363:ARG:NH2	1:A:365:ILE:HD13	1.94	0.82
1:E:325:ALA:O	5:E:701:HOH:O	1.96	0.82
1:A:252:PHE:CZ	1:A:257:LEU:HD12	2.14	0.82
1:D:239:THR:O	1:D:245:LYS:NZ	2.12	0.82
2:A:601:GLU:HA	3:A:602:NDP:H41N	1.61	0.82
1:D:357:ASP:OD1	1:D:478:ARG:NH2	2.12	0.81
1:A:291:LEU:HD13	1:A:304:PHE:HD2	1.43	0.80
1:D:73:GLU:CG	1:D:74:VAL:H	1.93	0.80
1:C:363:ARG:HH21	1:C:365:ILE:HD11	1.47	0.79
1:F:269:LYS:O	5:F:703:HOH:O	2.00	0.79
1:D:275:GLU:OE1	5:D:702:HOH:O	1.99	0.79
1:F:24:VAL:HG13	1:F:483:VAL:HG13	1.65	0.79
1:C:291:LEU:HD13	1:C:304:PHE:HD2	1.46	0.79
1:E:79:ARG:HD2	1:E:127:ALA:HB2	1.65	0.79
1:A:363:ARG:HH21	1:A:365:ILE:HD11	0.62	0.78
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.66	0.78
1:F:277:ASP:HB3	1:F:302:LEU:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PRO:HD3	1:C:359:ILE:HD13	1.66	0.78
1:C:66:ARG:HD3	1:C:66:ARG:H	1.47	0.77
1:C:250:GLN:OE1	1:C:315:LEU:HD21	1.84	0.77
1:B:79:ARG:HD2	1:B:127:ALA:HB2	1.66	0.77
1:B:147:ARG:HH22	1:E:500:PHE:H	1.31	0.77
1:A:205:GLN:OE1	5:A:703:HOH:O	2.01	0.77
1:B:346:GLU:OE1	1:B:478:ARG:NH2	2.18	0.77
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.14	0.77
1:C:24:VAL:HG13	1:C:483:VAL:HG13	1.67	0.76
1:F:337:PRO:O	1:F:363:ARG:NH1	2.18	0.76
1:D:79:ARG:HD2	1:D:127:ALA:HB2	1.67	0.76
1:B:277:ASP:HB3	1:B:302:LEU:HD11	1.67	0.76
1:A:363:ARG:CZ	1:A:365:ILE:CD1	2.63	0.76
1:B:498:VAL:HG12	1:B:499:THR:N	2.00	0.76
1:B:24:VAL:HG13	1:B:483:VAL:HG13	1.68	0.75
1:A:217:ARG:HH12	1:A:450:HIS:CE1	2.05	0.75
1:F:337:PRO:HD3	1:F:359:ILE:HD13	1.68	0.75
1:F:79:ARG:NH2	1:F:163:ASP:OD1	2.18	0.74
1:E:337:PRO:HD3	1:E:359:ILE:HD13	1.67	0.74
1:B:304:PHE:HD1	1:B:305:PRO:HD2	1.51	0.74
1:A:291:LEU:HD13	1:A:304:PHE:CD2	2.23	0.74
1:F:85:HIS:HA	1:F:501:THR:HG23	1.68	0.74
1:D:337:PRO:HD3	1:D:359:ILE:HD13	1.71	0.73
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.18	0.73
1:E:24:VAL:HG13	1:E:483:VAL:HG13	1.69	0.73
1:C:162:VAL:HG21	1:D:190:TYR:CD2	2.24	0.73
1:F:230:ALA:N	5:F:710:HOH:O	2.21	0.73
1:A:357:ASP:CG	1:A:478:ARG:HH21	1.91	0.73
1:E:382:TYR:CE1	1:E:386:LEU:HD11	2.23	0.73
1:A:422:GLY:O	5:A:704:HOH:O	2.06	0.73
1:D:54:PRO:O	5:D:703:HOH:O	2.07	0.73
1:B:85:HIS:HA	1:B:501:THR:HG23	1.71	0.72
1:B:498:VAL:HG12	1:B:499:THR:H	1.54	0.72
1:C:291:LEU:HD13	1:C:304:PHE:CD2	2.23	0.72
1:E:304:PHE:HD1	1:E:305:PRO:HD2	1.54	0.72
1:C:190:TYR:CD2	1:E:162:VAL:HG21	2.23	0.72
1:C:250:GLN:HB2	1:C:314:ILE:HD12	1.70	0.72
1:F:191:ASP:OD2	5:F:705:HOH:O	2.07	0.72
1:C:500:PHE:CD1	1:F:147:ARG:NH2	2.58	0.72
1:B:147:ARG:NH2	1:E:500:PHE:N	2.36	0.72
1:D:73:GLU:HG2	1:D:74:VAL:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:PHE:HD1	1:F:305:PRO:HD2	1.54	0.71
1:B:190:TYR:CD2	1:F:162:VAL:HG21	2.26	0.71
1:E:44:ARG:NH1	5:E:704:HOH:O	2.23	0.71
1:F:33:LYS:H	1:F:33:LYS:HD3	1.56	0.71
1:D:304:PHE:HD1	1:D:305:PRO:HD2	1.54	0.71
1:A:225:ASN:HD21	1:A:458:GLU:HA	1.55	0.71
1:E:109:SER:O	1:E:113:TYR:HD2	1.73	0.71
1:A:227:ILE:HD11	1:A:245:LYS:HD2	1.71	0.71
1:C:337:PRO:O	1:C:363:ARG:NH1	2.24	0.71
1:D:162:VAL:HG21	1:E:190:TYR:CD2	2.25	0.71
1:C:34:THR:O	1:C:36:GLU:N	2.24	0.71
1:E:116:ALA:HB1	1:E:488:LYS:HD3	1.71	0.71
1:C:396:ARG:HH21	1:E:456:THR:HG21	1.56	0.70
1:D:85:HIS:HA	1:D:501:THR:HG23	1.73	0.70
1:C:250:GLN:HE22	1:C:330:GLN:HG3	1.56	0.70
1:C:333:LYS:CE	1:C:355:GLU:CB	2.51	0.70
1:E:277:ASP:HB3	1:E:302:LEU:HD11	1.73	0.70
1:C:224:GLU:HA	1:C:227:ILE:HG22	1.72	0.70
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.71	0.70
1:D:227:ILE:HD11	1:D:245:LYS:HD2	1.73	0.70
1:A:205:GLN:HE22	1:B:496:ALA:HB2	1.57	0.70
1:A:203:ILE:O	5:A:705:HOH:O	2.09	0.70
1:A:190:TYR:CD2	1:B:162:VAL:HG21	2.27	0.70
1:B:147:ARG:HH22	1:E:499:THR:C	1.94	0.70
2:E:601:GLU:HA	3:E:602:NDP:H41N	1.74	0.70
1:A:24:VAL:HG13	1:A:483:VAL:CG1	2.21	0.69
1:D:238:MET:SD	1:D:342:LYS:HE3	2.31	0.69
1:E:46:ARG:O	1:E:46:ARG:NH1	2.25	0.69
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.22	0.69
1:E:458:GLU:OE2	1:E:462:ARG:NH2	2.23	0.69
1:E:463:GLN:OE1	5:E:702:HOH:O	2.09	0.69
1:D:277:ASP:HB3	1:D:302:LEU:HD11	1.73	0.69
1:A:224:GLU:HA	1:A:227:ILE:HG22	1.75	0.69
1:A:327:SER:HB2	1:A:330:GLN:NE2	2.08	0.69
1:C:333:LYS:CG	1:C:355:GLU:HB3	2.23	0.69
1:E:346:GLU:OE2	1:E:351:PRO:HD2	1.93	0.69
1:F:147:ARG:NH1	5:F:706:HOH:O	2.10	0.69
1:A:162:VAL:HG21	1:F:190:TYR:CD2	2.27	0.69
1:C:205:GLN:HE22	1:E:496:ALA:HB2	1.58	0.69
1:A:205:GLN:NE2	1:B:496:ALA:HB2	2.08	0.68
1:D:173:GLU:OE2	5:D:704:HOH:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:VAL:HA	1:E:373:LEU:HD22	1.73	0.68
1:E:227:ILE:HD11	1:E:245:LYS:HD2	1.75	0.68
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.24	0.68
1:C:227:ILE:HD11	1:C:245:LYS:HD2	1.75	0.68
1:D:357:ASP:CG	1:D:478:ARG:HH21	1.97	0.68
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.24	0.68
1:C:83:SER:OG	5:C:703:HOH:O	2.12	0.68
1:C:291:LEU:HA	1:C:304:PHE:HE2	1.59	0.68
1:C:276:SER:OG	5:C:702:HOH:O	2.11	0.67
1:D:382:TYR:CE1	1:D:386:LEU:HD11	2.29	0.67
1:B:258:HIS:O	1:B:262:TYR:HD1	1.77	0.67
1:E:1:ALA:HB3	1:E:332:THR:HG21	1.76	0.67
1:A:269:LYS:HE3	1:A:283:PRO:O	1.94	0.67
1:B:219:VAL:HA	1:B:373:LEU:HD22	1.77	0.67
1:F:363:ARG:HH21	1:F:365:ILE:HD11	1.59	0.67
1:C:27:LYS:HG3	1:C:471:TYR:OH	1.94	0.67
1:C:287:ASP:HB3	1:C:290:GLU:HG2	1.77	0.67
1:E:116:ALA:CB	1:E:488:LYS:HD3	2.24	0.67
1:B:303:GLY:O	5:B:704:HOH:O	2.11	0.67
1:C:277:ASP:HB3	1:C:302:LEU:CD1	2.21	0.67
1:A:458:GLU:OE1	5:A:707:HOH:O	2.13	0.66
1:A:310:TYR:HE2	1:A:317:VAL:CG2	2.05	0.66
1:B:382:TYR:CE1	1:B:386:LEU:HD11	2.30	0.66
2:C:601:GLU:HA	3:C:602:NDP:H41N	1.78	0.66
1:C:333:LYS:HG2	1:C:355:GLU:HB3	1.77	0.66
1:F:247:PHE:O	5:F:703:HOH:O	2.13	0.66
1:A:85:HIS:HA	1:A:501:THR:HG23	1.78	0.66
1:C:85:HIS:HA	1:C:501:THR:HG23	1.76	0.66
1:A:493:TYR:OH	5:A:706:HOH:O	2.13	0.66
1:E:85:HIS:NE2	1:E:488:LYS:NZ	2.38	0.66
1:C:190:TYR:HD2	1:E:162:VAL:HG21	1.61	0.65
1:D:169:MET:HG2	3:D:602:NDP:H51N	1.78	0.65
1:A:401:TYR:CE2	1:B:439:ARG:NH2	2.64	0.65
1:F:291:LEU:HD13	1:F:304:PHE:CD2	2.32	0.65
1:B:420:LYS:NZ	1:F:427:THR:O	2.27	0.65
1:E:346:GLU:OE1	1:E:478:ARG:NH1	2.27	0.65
1:F:37:THR:O	1:F:39:GLU:N	2.29	0.65
1:A:304:PHE:HD1	1:A:306:LYS:H	1.43	0.65
1:E:269:LYS:HD2	1:E:285:GLY:HA3	1.79	0.65
1:F:91:GLY:HA3	1:F:125:ALA:O	1.97	0.65
1:E:85:HIS:HA	1:E:501:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:GLU:HA	1:E:227:ILE:HG22	1.79	0.64
1:A:147:ARG:HH22	1:D:500:PHE:HA	1.62	0.64
1:A:496:ALA:CA	1:F:205:GLN:HE22	2.11	0.64
1:B:91:GLY:HA3	1:B:125:ALA:O	1.97	0.64
1:C:91:GLY:HA3	1:C:125:ALA:O	1.95	0.64
1:F:500:PHE:O	5:F:707:HOH:O	2.14	0.64
1:F:394:TYR:CE1	1:F:448:ILE:HD11	2.33	0.64
1:D:254:ASN:ND2	5:D:709:HOH:O	2.22	0.64
1:D:29:VAL:HG21	1:D:42:ARG:NE	2.13	0.63
1:B:224:GLU:HA	1:B:227:ILE:HG22	1.80	0.63
1:F:67:ARG:NE	1:F:73:GLU:OE2	2.32	0.63
1:B:67:ARG:NH1	1:B:136:TYR:CE2	2.67	0.63
1:C:19:ARG:NE	5:C:705:HOH:O	2.32	0.63
1:B:277:ASP:HB3	1:B:302:LEU:CD1	2.28	0.63
1:C:79:ARG:HD3	1:C:163:ASP:OD1	1.99	0.63
1:C:304:PHE:HD1	1:C:306:LYS:H	1.46	0.63
1:A:396:ARG:HH21	1:B:456:THR:HG21	1.63	0.63
1:B:205:GLN:HE22	1:F:496:ALA:HB2	1.64	0.63
1:B:238:MET:SD	1:B:342:LYS:HG3	2.38	0.63
1:A:65:ILE:HG22	1:A:143:LYS:NZ	2.14	0.62
1:C:107:LEU:HB3	1:C:126:LYS:HE3	1.81	0.62
1:D:37:THR:HG23	1:D:38:GLU:H	1.62	0.62
1:B:227:ILE:HD11	1:B:245:LYS:HD2	1.82	0.62
1:A:107:LEU:HB3	1:A:126:LYS:HE3	1.81	0.62
1:A:462:ARG:O	1:A:466:ARG:HG2	2.00	0.62
1:C:205:GLN:NE2	1:E:496:ALA:HB2	2.15	0.62
2:D:601:GLU:HA	3:D:602:NDP:H41N	1.81	0.62
1:C:496:ALA:HB2	1:D:205:GLN:HE22	1.64	0.62
1:D:310:TYR:CE2	1:D:317:VAL:HG23	2.35	0.62
1:F:488:LYS:O	1:F:491:ARG:HB2	2.00	0.62
1:A:259:SER:O	1:A:263:LEU:HD12	2.00	0.61
1:B:396:ARG:HH21	1:F:456:THR:HG21	1.65	0.61
1:D:287:ASP:HB3	1:D:290:GLU:HG2	1.82	0.61
1:C:279:SER:OG	1:C:314:ILE:HG23	1.99	0.61
1:C:496:ALA:HB2	1:D:205:GLN:NE2	2.16	0.61
1:C:498:VAL:HG12	1:C:499:THR:N	2.15	0.61
1:E:458:GLU:OE2	1:E:462:ARG:NE	2.33	0.61
1:F:287:ASP:HB3	1:F:290:GLU:HG2	1.81	0.61
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.82	0.61
1:F:57:HIS:CE1	1:F:84:GLN:HE22	2.18	0.61
1:A:277:ASP:HB3	1:A:302:LEU:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:PHE:CG	1:E:147:ARG:NH2	2.69	0.61
1:F:215:THR:HG21	3:F:602:NDP:H42N	1.82	0.61
1:A:65:ILE:HA	1:A:143:LYS:HZ2	1.65	0.61
1:A:287:ASP:HB3	1:A:290:GLU:HG2	1.82	0.61
1:A:142:GLU:O	1:A:146:ARG:HG3	2.01	0.61
1:D:66:ARG:HH11	1:D:70:GLY:HA2	1.66	0.61
1:D:25:GLU:C	1:D:42:ARG:NH2	2.54	0.61
1:C:412:SER:HA	1:E:433:THR:HG23	1.82	0.61
1:E:287:ASP:HB3	1:E:290:GLU:HG2	1.83	0.61
1:B:238:MET:CE	1:B:342:LYS:HE3	2.31	0.61
1:C:291:LEU:HA	1:C:304:PHE:CE2	2.35	0.61
1:E:291:LEU:HD13	1:E:304:PHE:CD2	2.35	0.60
1:F:38:GLU:O	1:F:39:GLU:HB3	2.01	0.60
1:A:244:ASP:OD2	1:A:244:ASP:N	2.34	0.60
1:B:287:ASP:HB3	1:B:290:GLU:HG2	1.83	0.60
1:D:37:THR:HB	1:D:41:LYS:HD2	1.83	0.60
1:D:91:GLY:HA3	1:D:125:ALA:O	2.01	0.60
1:A:65:ILE:HA	1:A:143:LYS:NZ	2.16	0.60
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.36	0.60
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.36	0.60
1:C:5:ASP:OD1	1:C:333:LYS:HB2	2.01	0.60
1:D:496:ALA:HB2	1:E:205:GLN:HE22	1.65	0.60
1:A:91:GLY:HA3	1:A:125:ALA:O	2.02	0.60
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.36	0.60
1:A:63:PHE:CD1	1:A:147:ARG:HG2	2.36	0.60
1:B:147:ARG:NH2	1:E:499:THR:C	2.55	0.60
1:E:37:THR:O	1:E:39:GLU:N	2.33	0.60
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.36	0.60
1:D:85:HIS:C	1:D:86:ARG:HG2	2.21	0.59
2:C:601:GLU:HB3	5:C:701:HOH:O	2.02	0.59
1:D:29:VAL:HG21	1:D:42:ARG:CZ	2.32	0.59
1:F:499:THR:O	1:F:500:PHE:HB2	2.02	0.59
3:D:602:NDP:O2X	5:D:705:HOH:O	2.16	0.59
1:E:107:LEU:HB3	1:E:126:LYS:HE3	1.84	0.59
1:A:339:VAL:CG1	1:A:363:ARG:NH2	2.52	0.59
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.37	0.59
1:E:458:GLU:CD	1:E:462:ARG:HE	2.05	0.59
1:B:370:ASP:OD1	1:B:371:LEU:N	2.36	0.59
1:B:388:ASN:ND2	5:B:712:HOH:O	2.33	0.59
1:C:37:THR:HG23	1:C:38:GLU:CB	2.33	0.59
1:D:73:GLU:HG2	1:D:74:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:LYS:HG3	1:F:424:HIS:N	2.17	0.59
1:C:291:LEU:CD1	1:C:304:PHE:HD2	2.14	0.58
1:C:310:TYR:CE2	1:C:317:VAL:HG23	2.38	0.58
1:D:496:ALA:HB2	1:E:205:GLN:NE2	2.18	0.58
1:F:63:PHE:CD1	1:F:147:ARG:HD3	2.38	0.58
1:B:225:ASN:OD1	5:B:705:HOH:O	2.17	0.58
1:D:73:GLU:CG	1:D:74:VAL:HG22	2.33	0.58
1:E:281:TRP:CE3	1:E:308:LYS:HD3	2.38	0.58
1:C:493:TYR:OH	5:C:703:HOH:O	2.16	0.58
1:C:36:GLU:HG2	1:C:41:LYS:NZ	2.19	0.58
1:C:291:LEU:CA	1:C:304:PHE:HE2	2.17	0.58
1:F:277:ASP:HB3	1:F:302:LEU:CD1	2.33	0.58
1:A:36:GLU:OE2	1:A:36:GLU:HA	2.02	0.58
1:A:277:ASP:CB	1:A:302:LEU:HD11	2.31	0.58
1:C:37:THR:CG2	1:C:40:GLN:HB3	2.34	0.58
1:C:500:PHE:CG	1:F:147:ARG:NH2	2.72	0.58
1:D:66:ARG:NH1	1:D:70:GLY:HA2	2.18	0.58
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.85	0.58
1:F:253:GLY:HA3	3:F:602:NDP:O5B	2.03	0.58
1:F:316:GLU:O	1:F:340:LYS:HG3	2.03	0.58
1:A:436:PHE:CZ	1:F:409:LEU:CD1	2.83	0.58
1:C:37:THR:HG23	1:C:38:GLU:HB3	1.85	0.58
1:A:72:TRP:CH2	1:D:498:VAL:HB	2.39	0.58
1:A:209:HIS:NE2	1:A:446:LYS:HG3	2.18	0.58
1:D:269:LYS:HA	5:D:707:HOH:O	2.03	0.58
1:D:333:LYS:HB2	1:D:355:GLU:HB3	1.86	0.58
1:B:412:SER:HA	1:F:433:THR:HG23	1.86	0.57
1:F:219:VAL:HA	1:F:373:LEU:HD22	1.85	0.57
1:A:37:THR:O	1:A:38:GLU:HB2	2.05	0.57
1:E:2:ASP:HB2	1:E:5:ASP:HB2	1.86	0.57
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.39	0.57
1:D:63:PHE:CE1	1:D:147:ARG:HG2	2.39	0.57
1:A:427:THR:O	1:F:420:LYS:NZ	2.28	0.57
1:D:439:ARG:HH12	1:E:404:ASP:HB2	1.68	0.57
2:F:601:GLU:HA	3:F:602:NDP:H41N	1.86	0.57
1:E:36:GLU:O	1:E:38:GLU:N	2.29	0.57
1:E:314:ILE:O	1:E:317:VAL:HG12	2.05	0.57
1:F:58:VAL:N	5:F:713:HOH:O	2.37	0.57
1:A:211:ARG:HD2	1:A:211:ARG:O	2.04	0.57
1:E:250:GLN:HB2	1:E:314:ILE:HD12	1.87	0.57
1:E:370:ASP:OD1	1:E:371:LEU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HG2	1:A:491:ARG:HH11	1.70	0.57
1:D:291:LEU:HD13	1:D:304:PHE:CD2	2.39	0.57
1:A:147:ARG:NH2	1:D:500:PHE:CD2	2.73	0.56
1:C:3:ARG:C	1:C:5:ASP:H	2.07	0.56
1:C:36:GLU:HG2	1:C:41:LYS:HZ1	1.69	0.56
1:A:65:ILE:CG2	1:A:143:LYS:HZ2	2.16	0.56
1:A:150:MET:O	1:A:154:LYS:HG3	2.05	0.56
1:B:205:GLN:NE2	1:F:496:ALA:HB2	2.19	0.56
1:E:46:ARG:NH1	1:E:50:ARG:HG3	2.20	0.56
1:E:281:TRP:HE3	1:E:308:LYS:HD3	1.70	0.56
1:E:150:MET:O	1:E:154:LYS:HG3	2.06	0.56
1:E:169:MET:HG2	3:E:602:NDP:H52N	1.88	0.56
1:C:63:PHE:O	1:C:75:ILE:HG23	2.05	0.56
1:E:75:ILE:HD13	1:E:144:ILE:HG12	1.88	0.56
1:F:150:MET:O	1:F:154:LYS:HG3	2.05	0.56
1:D:75:ILE:HD13	1:D:144:ILE:HG12	1.87	0.56
1:D:439:ARG:HH12	1:E:404:ASP:CB	2.19	0.56
1:E:91:GLY:HA3	1:E:125:ALA:O	2.05	0.56
1:A:291:LEU:HD11	1:A:301:ILE:HD12	1.88	0.56
1:C:499:THR:O	1:C:500:PHE:HB2	2.06	0.56
1:A:19:ARG:NH2	1:A:476:ASP:OD1	2.39	0.56
1:C:431:VAL:HG22	1:D:419:ARG:HH12	1.71	0.56
1:C:423:LYS:C	1:C:425:GLY:H	2.10	0.55
1:A:225:ASN:ND2	1:A:458:GLU:HA	2.20	0.55
1:E:109:SER:O	1:E:113:TYR:CD2	2.56	0.55
1:C:66:ARG:HD3	1:C:66:ARG:N	2.21	0.55
1:A:169:MET:HG2	3:A:602:NDP:H3D	1.88	0.55
1:D:244:ASP:OD2	1:D:244:ASP:N	2.40	0.55
1:C:162:VAL:HG21	1:D:190:TYR:HD2	1.72	0.55
1:F:107:LEU:HB3	1:F:126:LYS:HE3	1.89	0.55
1:A:433:THR:HG23	1:F:412:SER:HA	1.88	0.55
1:B:291:LEU:HD13	1:B:304:PHE:CD2	2.42	0.55
1:A:37:THR:HG22	1:A:38:GLU:H	1.72	0.55
1:C:150:MET:O	1:C:154:LYS:HG3	2.07	0.55
1:D:415:GLU:O	1:D:419:ARG:HG2	2.06	0.55
1:B:75:ILE:HD11	1:B:144:ILE:HG23	1.88	0.55
1:D:224:GLU:HA	1:D:227:ILE:HG22	1.87	0.55
1:F:33:LYS:H	1:F:33:LYS:CD	2.19	0.55
1:D:118:VAL:HG12	1:D:118:VAL:O	2.07	0.54
1:D:435:GLU:HG2	1:E:408:HIS:NE2	2.22	0.54
1:F:101:VAL:O	1:F:105:LYS:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:ILE:HD11	1:F:245:LYS:HD2	1.88	0.54
1:B:33:LYS:O	1:B:33:LYS:HD3	2.07	0.54
1:C:363:ARG:NH2	1:C:365:ILE:HD11	2.20	0.54
1:E:458:GLU:CD	1:E:462:ARG:CZ	2.76	0.54
1:C:498:VAL:HG12	1:C:499:THR:H	1.71	0.54
1:C:5:ASP:CG	1:C:333:LYS:HB2	2.28	0.54
1:C:462:ARG:O	1:C:466:ARG:HG2	2.07	0.54
1:E:17:PHE:CD1	1:E:113:TYR:HE1	2.26	0.54
1:D:87:THR:N	5:D:713:HOH:O	2.40	0.54
1:A:233:MET:HE1	1:A:236:LEU:HD12	1.89	0.54
1:B:238:MET:SD	1:B:342:LYS:HE3	2.47	0.54
1:B:320:ASP:HA	1:B:342:LYS:HE2	1.90	0.54
1:D:25:GLU:HG3	5:D:720:HOH:O	2.06	0.54
1:B:19:ARG:NH2	5:B:716:HOH:O	2.41	0.54
1:C:433:THR:HG23	1:D:412:SER:HA	1.89	0.54
1:D:354:PRO:O	1:D:358:LYS:NZ	2.35	0.54
1:E:458:GLU:OE2	1:E:462:ARG:CZ	2.56	0.54
1:F:224:GLU:HA	1:F:227:ILE:HG22	1.89	0.54
1:F:2:ASP:O	1:F:6:ASP:HB2	2.08	0.53
1:A:412:SER:HA	1:B:433:THR:HG23	1.90	0.53
1:B:409:LEU:HD11	1:F:409:LEU:HD22	1.89	0.53
1:E:420:LYS:HG3	1:E:421:PHE:CE2	2.44	0.53
1:A:390:ASN:ND2	5:A:711:HOH:O	2.27	0.53
1:D:85:HIS:O	1:D:86:ARG:HG2	2.07	0.53
1:E:51:ILE:HD13	1:E:498:VAL:HG11	1.91	0.53
1:F:58:VAL:C	5:F:713:HOH:O	2.47	0.53
1:E:53:LYS:HE2	1:E:113:TYR:OH	2.08	0.53
1:A:252:PHE:CE1	1:A:257:LEU:HD12	2.44	0.53
1:D:386:LEU:HD21	1:E:392:VAL:CG1	2.39	0.53
1:A:79:ARG:HD2	1:A:127:ALA:HB2	1.91	0.53
1:A:75:ILE:HD11	1:A:144:ILE:HG23	1.91	0.53
1:A:370:ASP:OD1	1:A:371:LEU:N	2.42	0.53
1:C:233:MET:HE1	1:C:236:LEU:HD12	1.90	0.53
1:A:363:ARG:NE	1:A:365:ILE:HD11	2.24	0.52
1:C:250:GLN:NE2	1:C:330:GLN:HG3	2.24	0.52
1:C:314:ILE:HG13	1:C:315:LEU:H	1.75	0.52
1:D:72:TRP:O	1:D:73:GLU:HB2	2.09	0.52
1:E:277:ASP:HB3	1:E:302:LEU:CD1	2.39	0.52
1:B:39:GLU:OE1	1:B:39:GLU:HA	2.09	0.52
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.90	0.52
1:A:51:ILE:HD13	1:A:498:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:602:NDP:N7N	3:D:602:NDP:O1N	2.43	0.52
1:A:211:ARG:HD2	1:A:211:ARG:C	2.30	0.52
1:A:209:HIS:CE1	1:A:446:LYS:HG3	2.44	0.52
1:C:431:VAL:CG2	1:D:419:ARG:HH12	2.22	0.52
1:C:500:PHE:CD2	1:D:185:SER:HB3	2.45	0.52
1:D:238:MET:CG	1:D:342:LYS:HE3	2.40	0.52
1:A:169:MET:HE1	1:A:327:SER:HA	1.91	0.52
1:B:224:GLU:HB2	1:B:242:PHE:HE2	1.75	0.52
1:B:150:MET:O	1:B:154:LYS:HG3	2.09	0.52
1:D:382:TYR:CE1	1:D:386:LEU:CD1	2.93	0.52
1:A:336:ALA:O	1:A:363:ARG:NH1	2.43	0.52
1:E:236:LEU:HD21	1:E:475:LEU:HD13	1.91	0.52
1:D:456:THR:HG21	1:E:396:ARG:HH21	1.74	0.51
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.92	0.51
4:F:603:GTP:N2	5:F:720:HOH:O	2.40	0.51
1:D:277:ASP:HB3	1:D:302:LEU:CD1	2.39	0.51
1:F:394:TYR:CD1	1:F:448:ILE:HD11	2.45	0.51
1:A:291:LEU:HA	1:A:304:PHE:CE2	2.46	0.51
1:D:241:GLY:O	1:D:245:LYS:HE3	2.10	0.51
1:A:363:ARG:NE	1:A:365:ILE:CD1	2.72	0.51
1:A:500:PHE:N	1:D:147:ARG:HH22	2.09	0.51
1:D:25:GLU:O	1:D:42:ARG:NH2	2.42	0.51
1:D:73:GLU:HG2	1:D:74:VAL:CG2	2.40	0.51
1:D:51:ILE:HD13	1:D:498:VAL:HG11	1.92	0.51
1:D:370:ASP:OD1	1:D:371:LEU:N	2.44	0.51
1:D:433:THR:HG23	1:E:412:SER:HA	1.91	0.51
1:A:436:PHE:CE2	1:F:409:LEU:HD12	2.44	0.51
1:B:72:TRP:CH2	1:E:498:VAL:HB	2.46	0.51
1:C:79:ARG:HE	1:C:127:ALA:HB2	1.75	0.51
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.92	0.51
1:C:396:ARG:NH2	1:E:456:THR:HG21	2.24	0.51
1:A:276:SER:OG	3:A:602:NDP:O3X	2.16	0.51
1:A:168:ASP:OD1	3:A:602:NDP:H2D	2.11	0.51
1:D:150:MET:O	1:D:154:LYS:HG3	2.11	0.51
1:F:38:GLU:O	1:F:39:GLU:CB	2.59	0.51
1:F:339:VAL:HG12	1:F:363:ARG:NH2	2.25	0.51
1:A:382:TYR:CE1	1:A:386:LEU:HD11	2.46	0.50
1:E:488:LYS:HE2	1:E:489:VAL:N	2.26	0.50
1:F:233:MET:HE1	1:F:236:LEU:HD12	1.92	0.50
1:B:37:THR:C	1:B:39:GLU:N	2.65	0.50
1:E:458:GLU:OE1	1:E:462:ARG:NH2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:HIS:C	1:A:86:ARG:HG2	2.30	0.50
1:E:279:SER:OG	1:E:314:ILE:CG2	2.52	0.50
1:F:14:GLU:O	1:F:18:ASP:OD2	2.30	0.50
1:D:162:VAL:HG21	1:E:190:TYR:HD2	1.72	0.50
1:E:233:MET:HE1	1:E:236:LEU:HD12	1.92	0.50
1:E:75:ILE:CD1	1:E:144:ILE:HG12	2.42	0.50
1:B:258:HIS:O	1:B:262:TYR:CD1	2.62	0.50
1:D:259:SER:O	1:D:263:LEU:HD12	2.11	0.50
1:A:238:MET:HE1	1:A:320:ASP:HB3	1.94	0.50
1:D:75:ILE:HD11	1:D:144:ILE:HG23	1.92	0.50
1:B:209:HIS:CE1	1:B:446:LYS:HG3	2.47	0.50
1:E:39:GLU:HB3	1:E:42:ARG:HB2	1.94	0.50
1:E:46:ARG:HH12	1:E:50:ARG:HG3	1.77	0.50
1:B:499:THR:O	1:B:500:PHE:HB2	2.11	0.49
1:D:266:PHE:O	5:D:706:HOH:O	2.19	0.49
1:A:456:THR:HG22	5:F:728:HOH:O	2.12	0.49
1:D:238:MET:SD	1:D:342:LYS:HG3	2.52	0.49
1:C:250:GLN:HB2	1:C:314:ILE:CD1	2.38	0.49
1:D:433:THR:HB	5:D:729:HOH:O	2.12	0.49
1:F:85:HIS:CD2	1:F:86:ARG:HD3	2.46	0.49
1:F:370:ASP:OD1	1:F:371:LEU:N	2.43	0.49
1:C:3:ARG:C	1:C:5:ASP:N	2.66	0.49
1:C:147:ARG:NH2	1:F:500:PHE:CG	2.79	0.49
1:B:262:TYR:OH	4:B:603:GTP:O2G	2.25	0.49
1:F:215:THR:CG2	3:F:602:NDP:H42N	2.42	0.49
1:B:67:ARG:NH1	1:B:73:GLU:OE2	2.46	0.49
1:F:93:ILE:HG12	1:F:127:ALA:HB3	1.95	0.49
1:B:2:ASP:OD1	1:B:5:ASP:HB2	2.12	0.49
1:B:498:VAL:CG1	1:B:499:THR:N	2.70	0.49
1:C:34:THR:O	1:C:36:GLU:HG3	2.12	0.49
1:F:459:ARG:HA	1:F:462:ARG:HD2	1.95	0.49
1:C:409:LEU:HD12	1:E:436:PHE:CZ	2.48	0.49
1:E:421:PHE:N	1:E:421:PHE:CD2	2.81	0.49
1:F:259:SER:O	1:F:263:LEU:HD12	2.13	0.49
1:A:363:ARG:HE	1:A:365:ILE:CD1	2.26	0.48
1:D:268:ALA:O	5:D:707:HOH:O	2.20	0.48
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.95	0.48
1:C:26:ASP:OD2	1:C:42:ARG:NH2	2.45	0.48
1:C:271:VAL:CG2	1:C:283:PRO:HA	2.42	0.48
1:F:201:LYS:NZ	1:F:388:ASN:OD1	2.46	0.48
1:C:221:HIS:HE1	5:C:715:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:O	1:C:37:THR:N	2.47	0.48
1:C:373:LEU:HD12	1:C:373:LEU:O	2.13	0.48
1:A:404:ASP:HB2	1:B:439:ARG:HH12	1.79	0.48
1:B:37:THR:O	1:B:39:GLU:N	2.47	0.48
1:C:333:LYS:HD3	1:C:355:GLU:HB3	1.91	0.48
1:E:458:GLU:CD	1:E:462:ARG:NE	2.66	0.48
1:B:259:SER:O	1:B:263:LEU:HD12	2.14	0.48
1:F:51:ILE:HD13	1:F:498:VAL:HG11	1.95	0.48
1:F:86:ARG:NH1	1:F:492:VAL:HG21	2.29	0.48
1:E:259:SER:O	1:E:263:LEU:HD12	2.13	0.48
1:F:271:VAL:N	5:F:703:HOH:O	2.46	0.48
1:D:233:MET:HE1	1:D:236:LEU:HD12	1.95	0.47
1:E:419:ARG:HD3	1:E:420:LYS:N	2.29	0.47
1:E:439:ARG:NH2	5:E:713:HOH:O	2.41	0.47
1:B:500:PHE:CD1	1:E:147:ARG:NH2	2.82	0.47
1:D:95:TYR:O	5:D:708:HOH:O	2.20	0.47
1:E:17:PHE:HD1	1:E:113:TYR:CE1	2.31	0.47
1:A:487:GLU:OE2	5:A:709:HOH:O	2.20	0.47
1:E:238:MET:HE1	1:E:320:ASP:HB3	1.97	0.47
1:B:118:VAL:HG12	1:B:118:VAL:O	2.14	0.47
1:B:253:GLY:HA3	3:B:602:NDP:O5B	2.14	0.47
1:F:304:PHE:HD1	1:F:305:PRO:CD	2.25	0.47
3:F:602:NDP:H52N	3:F:602:NDP:H2N	1.97	0.47
1:C:291:LEU:CD1	1:C:304:PHE:CD2	2.93	0.47
1:E:37:THR:C	1:E:39:GLU:N	2.67	0.47
1:A:162:VAL:HG21	1:F:190:TYR:HD2	1.78	0.47
1:B:64:PRO:HD2	1:B:147:ARG:HH12	1.78	0.47
1:C:271:VAL:HG22	1:C:283:PRO:HA	1.95	0.47
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.97	0.47
1:D:424:HIS:O	1:D:424:HIS:ND1	2.46	0.47
1:F:363:ARG:NH2	1:F:365:ILE:HD11	2.28	0.47
1:A:275:GLU:OE2	1:A:301:ILE:HG12	2.13	0.47
1:A:452:GLY:O	1:A:456:THR:HG23	2.15	0.47
1:C:119:ASP:OD2	1:C:488:LYS:HE2	2.15	0.47
1:C:314:ILE:HG13	1:C:315:LEU:N	2.30	0.47
1:F:36:GLU:C	1:F:38:GLU:H	2.16	0.47
1:F:118:VAL:HG12	1:F:118:VAL:O	2.15	0.47
1:F:367:VAL:HG23	5:F:732:HOH:O	2.14	0.47
1:E:250:GLN:NE2	1:E:330:GLN:HE21	2.12	0.47
1:F:68:ASP:HB2	1:F:140:GLU:OE2	2.15	0.47
1:E:27:LYS:NZ	1:E:487:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:ALA:O	1:F:488:LYS:HD3	2.15	0.47
1:A:35:ARG:HE	1:A:35:ARG:HA	1.80	0.46
1:F:187:ILE:H	1:F:187:ILE:HG12	1.48	0.46
1:C:79:ARG:HG2	1:C:157:PHE:HD2	1.81	0.46
1:C:413:VAL:HG12	1:C:430:ILE:HG13	1.98	0.46
1:A:304:PHE:HE1	1:A:306:LYS:HG3	1.79	0.46
1:D:14:GLU:OE1	1:D:53:LYS:HD3	2.14	0.46
1:C:147:ARG:NH2	1:F:500:PHE:CD2	2.83	0.46
1:C:479:THR:O	1:C:483:VAL:HG23	2.15	0.46
1:D:57:HIS:CE1	1:D:84:GLN:HE22	2.34	0.46
1:E:382:TYR:CE1	1:E:386:LEU:CD1	2.96	0.46
1:B:190:TYR:HD2	1:F:162:VAL:HG21	1.78	0.46
1:C:259:SER:O	1:C:263:LEU:HD12	2.16	0.46
1:D:67:ARG:NH1	1:D:140:GLU:OE1	2.34	0.46
1:E:236:LEU:HD21	1:E:475:LEU:CD1	2.46	0.46
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.98	0.46
1:A:118:VAL:HG12	1:A:118:VAL:O	2.15	0.46
1:A:498:VAL:HB	1:D:72:TRP:CH2	2.50	0.46
1:B:211:ARG:HG2	1:B:380:VAL:HG12	1.98	0.46
1:D:63:PHE:CD1	1:D:147:ARG:HG2	2.51	0.46
1:E:17:PHE:CD1	1:E:113:TYR:CE1	3.04	0.46
1:A:448:ILE:HG23	1:A:448:ILE:HD12	1.56	0.46
1:A:24:VAL:CG1	1:A:483:VAL:CG1	2.93	0.46
1:B:287:ASP:HB3	1:B:290:GLU:CG	2.46	0.46
1:D:386:LEU:HD21	1:E:392:VAL:HG11	1.98	0.46
1:E:274:GLY:HA3	1:E:314:ILE:HG21	1.97	0.45
1:E:367:VAL:O	5:E:703:HOH:O	2.21	0.45
1:F:252:PHE:CZ	1:F:257:LEU:HD12	2.51	0.45
1:C:470:LYS:O	1:C:470:LYS:HG3	2.15	0.45
1:D:215:THR:HG21	3:D:602:NDP:H42N	1.98	0.45
1:B:57:HIS:CE1	1:B:84:GLN:HE22	2.35	0.45
1:D:160:PRO:HD2	5:D:757:HOH:O	2.15	0.45
1:A:291:LEU:HA	1:A:304:PHE:HE2	1.81	0.45
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.98	0.45
1:B:62:SER:OG	5:B:706:HOH:O	2.20	0.45
1:B:304:PHE:CD1	1:B:305:PRO:HD2	2.41	0.45
1:F:79:ARG:HE	1:F:127:ALA:HB2	1.80	0.45
1:F:342:LYS:NZ	1:F:364:ASN:O	2.47	0.45
1:A:406:ASN:O	1:A:410:LEU:HD12	2.17	0.45
1:D:67:ARG:HD2	1:D:140:GLU:OE1	2.17	0.45
1:E:250:GLN:CB	1:E:314:ILE:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PRO:HD3	1:A:359:ILE:CD1	2.33	0.45
1:C:269:LYS:HB3	1:C:269:LYS:HE3	1.67	0.45
1:E:224:GLU:HB2	1:E:242:PHE:HE2	1.82	0.45
1:F:246:THR:HB	1:F:271:VAL:CG2	2.47	0.45
1:B:75:ILE:HD13	1:B:144:ILE:HG12	1.98	0.45
1:C:500:PHE:CE1	1:F:147:ARG:NH2	2.85	0.45
1:D:423:LYS:HE2	1:D:423:LYS:HB2	1.73	0.45
1:D:462:ARG:HE	1:D:462:ARG:HB3	1.61	0.45
1:B:288:PRO:HD2	5:B:710:HOH:O	2.17	0.44
1:E:448:ILE:HD12	1:E:448:ILE:HG23	1.52	0.44
1:A:396:ARG:NH2	1:B:456:THR:HG21	2.31	0.44
1:F:382:TYR:CE1	1:F:386:LEU:HD11	2.52	0.44
1:B:26:ASP:OD2	1:B:42:ARG:NH2	2.51	0.44
1:C:57:HIS:CE1	1:C:84:GLN:HE22	2.34	0.44
1:E:118:VAL:HG11	1:E:379:THR:OG1	2.17	0.44
1:F:282:ASN:C	1:F:284:ASP:H	2.19	0.44
1:A:217:ARG:HG3	1:A:453:LEU:HD23	1.98	0.44
1:A:491:ARG:HH11	1:A:491:ARG:CG	2.30	0.44
1:B:269:LYS:HE3	1:B:284:ASP:C	2.37	0.44
1:C:215:THR:CG2	3:C:602:NDP:H42N	2.47	0.44
1:D:257:LEU:HD11	1:D:292:GLU:HG3	2.00	0.44
1:F:438:ASP:O	5:F:709:HOH:O	2.21	0.44
1:A:339:VAL:HG11	1:A:360:PHE:CE2	2.52	0.44
1:E:304:PHE:HD1	1:E:305:PRO:CD	2.27	0.44
1:F:222:GLY:HA3	1:F:373:LEU:HD23	1.98	0.44
1:A:91:GLY:O	1:A:165:PRO:HA	2.18	0.44
1:B:346:GLU:CD	1:B:478:ARG:HH22	2.21	0.44
1:C:448:ILE:HD12	1:C:448:ILE:HG23	1.62	0.44
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.99	0.44
1:F:292:GLU:OE1	5:F:708:HOH:O	2.21	0.44
1:A:226:PHE:HB3	1:A:366:MET:HE1	2.00	0.44
1:B:19:ARG:NH2	1:B:354:PRO:HB3	2.32	0.44
1:D:264:HIS:CD2	5:D:707:HOH:O	2.69	0.44
1:E:46:ARG:HD2	1:E:46:ARG:HA	1.68	0.44
1:F:75:ILE:HD11	1:F:144:ILE:HG23	2.00	0.44
1:F:118:VAL:HG11	1:F:379:THR:OG1	2.17	0.44
1:A:338:ARG:H	1:A:338:ARG:HG2	1.62	0.44
1:B:473:LEU:HA	1:B:473:LEU:HD23	1.67	0.44
1:F:239:THR:O	1:F:245:LYS:NZ	2.39	0.44
1:A:327:SER:HB2	1:A:330:GLN:HE21	1.82	0.44
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ASN:O	1:F:143:LYS:HG3	2.18	0.44
1:A:224:GLU:HB2	1:A:242:PHE:HE2	1.81	0.43
1:C:68:ASP:HB2	1:C:140:GLU:OE2	2.18	0.43
1:D:310:TYR:CZ	1:D:317:VAL:HG23	2.53	0.43
1:A:281:TRP:HB2	1:A:310:TYR:HD2	1.83	0.43
1:C:85:HIS:HB3	5:C:703:HOH:O	2.17	0.43
1:D:275:GLU:HA	3:D:602:NDP:N3A	2.33	0.43
1:F:339:VAL:HG11	1:F:360:PHE:HE2	1.83	0.43
1:A:291:LEU:CA	1:A:304:PHE:HE2	2.31	0.43
1:C:339:VAL:HG12	1:C:363:ARG:NH2	2.34	0.43
1:E:301:ILE:HD12	1:E:302:LEU:N	2.33	0.43
1:E:421:PHE:H	1:E:421:PHE:HD2	1.66	0.43
1:A:339:VAL:H	1:A:363:ARG:HH12	1.67	0.43
1:A:420:LYS:HD3	5:A:708:HOH:O	2.19	0.43
1:C:28:LEU:O	1:C:32:LEU:HD13	2.18	0.43
1:C:211:ARG:HG2	1:C:380:VAL:HG12	2.01	0.43
1:E:301:ILE:H	1:E:301:ILE:HG13	1.68	0.43
1:B:311:GLU:OE1	1:B:312:GLY:N	2.52	0.43
1:E:5:ASP:HB3	1:E:332:THR:HB	1.99	0.43
1:F:107:LEU:HB2	1:F:126:LYS:HG2	2.01	0.43
1:A:63:PHE:CE1	1:A:147:ARG:HG2	2.52	0.43
1:A:291:LEU:HB2	1:A:304:PHE:HE2	1.83	0.43
1:C:215:THR:HG21	3:C:602:NDP:H42N	2.01	0.43
1:C:333:LYS:HG2	1:C:355:GLU:CB	2.48	0.43
1:D:118:VAL:O	1:D:118:VAL:CG1	2.67	0.43
1:E:291:LEU:HD11	1:E:301:ILE:HG22	2.01	0.43
1:A:57:HIS:CE1	1:A:84:GLN:HE22	2.36	0.43
1:B:366:MET:HB2	1:B:475:LEU:HD13	2.01	0.43
1:F:114:LYS:HG3	1:F:375:ALA:HB2	2.00	0.43
1:A:190:TYR:HD2	1:B:162:VAL:HG21	1.77	0.43
1:A:413:VAL:HG12	1:A:430:ILE:HG13	2.01	0.43
1:B:398:THR:O	1:B:402:GLU:HB2	2.19	0.43
1:C:118:VAL:O	1:C:118:VAL:HG12	2.18	0.43
1:C:244:ASP:N	1:C:244:ASP:OD2	2.52	0.43
1:C:362:GLU:O	1:C:362:GLU:HG3	2.19	0.43
1:D:209:HIS:NE2	1:D:446:LYS:HG3	2.33	0.43
1:B:116:ALA:O	1:B:488:LYS:HD3	2.18	0.43
1:C:310:TYR:CZ	1:C:317:VAL:HG23	2.54	0.43
1:F:28:LEU:O	1:F:32:LEU:HD13	2.19	0.43
1:C:8:ASN:HB3	1:C:11:LYS:HB2	2.01	0.43
1:D:264:HIS:HD2	5:D:707:HOH:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:GLN:HE22	1:E:330:GLN:NE2	2.17	0.43
1:A:304:PHE:HD1	1:A:306:LYS:N	2.15	0.42
1:B:479:THR:O	1:B:483:VAL:HG23	2.18	0.42
1:E:68:ASP:HB2	1:E:140:GLU:OE2	2.18	0.42
1:B:250:GLN:NE2	1:B:330:GLN:HE21	2.17	0.42
1:A:75:ILE:HD13	1:A:144:ILE:HG12	2.01	0.42
1:C:51:ILE:HD13	1:C:498:VAL:HG11	2.01	0.42
1:D:346:GLU:OE2	1:D:351:PRO:HD2	2.19	0.42
1:F:351:PRO:HD2	5:F:747:HOH:O	2.20	0.42
1:C:373:LEU:HD12	1:C:373:LEU:HA	1.55	0.42
1:D:169:MET:SD	3:D:602:NDP:H3D	2.59	0.42
1:E:53:LYS:CE	1:E:113:TYR:OH	2.67	0.42
1:D:373:LEU:O	1:D:373:LEU:HD12	2.20	0.42
1:C:32:LEU:HD11	1:C:494:ASN:HD21	1.84	0.42
1:E:420:LYS:HG3	1:E:421:PHE:CD2	2.54	0.42
1:F:142:GLU:O	1:F:146:ARG:HG3	2.19	0.42
1:B:355:GLU:HG2	1:B:356:ALA:N	2.35	0.42
1:E:479:THR:O	1:E:483:VAL:HG23	2.19	0.42
1:F:275:GLU:HG3	1:F:301:ILE:HD11	2.02	0.42
1:F:339:VAL:HG11	1:F:360:PHE:CE2	2.54	0.42
1:B:133:PRO:HG2	1:B:170:SER:HB3	2.02	0.42
1:B:339:VAL:HG11	1:B:360:PHE:CE2	2.55	0.42
1:C:253:GLY:HA3	3:C:602:NDP:O5B	2.19	0.42
1:D:91:GLY:O	1:D:165:PRO:HA	2.19	0.42
1:D:201:LYS:HB2	1:D:201:LYS:HE2	1.87	0.42
1:A:2:ASP:OD1	1:A:332:THR:HG21	2.19	0.42
1:A:37:THR:HG22	1:A:38:GLU:N	2.35	0.42
1:A:257:LEU:HD11	1:A:292:GLU:HG3	2.02	0.42
1:B:409:LEU:HD12	1:F:436:PHE:CZ	2.55	0.42
1:F:246:THR:HB	1:F:271:VAL:HG21	2.02	0.42
1:F:479:THR:O	1:F:483:VAL:HG23	2.19	0.42
1:A:339:VAL:HG11	1:A:360:PHE:HE2	1.84	0.42
1:D:28:LEU:O	1:D:32:LEU:HD13	2.20	0.42
1:D:257:LEU:CD1	1:D:292:GLU:HG3	2.49	0.42
1:E:147:ARG:O	1:E:147:ARG:HG3	2.19	0.42
1:B:224:GLU:HB2	1:B:242:PHE:CE2	2.55	0.41
1:D:107:LEU:HB2	1:D:126:LYS:HG2	2.03	0.41
1:E:113:TYR:CD2	1:E:113:TYR:N	2.88	0.41
1:E:461:ALA:O	1:E:465:MET:HG3	2.20	0.41
1:A:226:PHE:HB3	1:A:366:MET:CE	2.51	0.41
1:B:222:GLY:HA3	1:B:373:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LYS:HE3	1:B:284:ASP:O	2.19	0.41
1:D:25:GLU:C	1:D:42:ARG:HH22	2.21	0.41
3:E:602:NDP:N7N	3:E:602:NDP:O1N	2.53	0.41
1:B:68:ASP:HB2	1:B:140:GLU:OE2	2.20	0.41
1:D:17:PHE:CD2	1:D:53:LYS:HE3	2.55	0.41
1:E:63:PHE:CE1	1:E:147:ARG:HG2	2.56	0.41
1:F:224:GLU:HB2	1:F:242:PHE:HE2	1.85	0.41
1:D:382:TYR:O	1:D:386:LEU:HD13	2.20	0.41
1:E:339:VAL:HG11	1:E:360:PHE:CE2	2.55	0.41
1:E:354:PRO:O	1:E:357:ASP:HB2	2.21	0.41
1:F:17:PHE:CE2	1:F:53:LYS:HD2	2.55	0.41
1:C:473:LEU:HD23	1:C:473:LEU:HA	1.89	0.41
1:A:409:LEU:HD12	1:B:436:PHE:CZ	2.55	0.41
1:C:78:TYR:CD2	1:C:101:VAL:HG22	2.56	0.41
1:E:253:GLY:HA3	3:E:602:NDP:O5B	2.21	0.41
1:A:147:ARG:HH11	1:A:147:ARG:HD3	1.67	0.41
1:B:28:LEU:O	1:B:32:LEU:HD13	2.20	0.41
1:B:337:PRO:O	1:B:363:ARG:NH1	2.54	0.41
1:B:339:VAL:HG11	1:B:360:PHE:HE2	1.85	0.41
1:B:448:ILE:HD12	1:B:448:ILE:HG23	1.54	0.41
1:C:118:VAL:HG11	1:C:379:THR:OG1	2.21	0.41
1:F:196:ALA:HB1	1:F:385:TRP:CD1	2.56	0.41
1:A:5:ASP:HB3	1:A:332:THR:HB	2.03	0.41
1:B:5:ASP:HB3	1:B:332:THR:HB	2.02	0.41
1:B:118:VAL:HG11	1:B:379:THR:OG1	2.21	0.41
1:C:142:GLU:O	1:C:146:ARG:HG3	2.20	0.41
1:C:279:SER:CB	1:C:314:ILE:HG23	2.50	0.41
1:A:147:ARG:NH2	1:D:500:PHE:HA	2.32	0.41
1:B:274:GLY:N	1:B:314:ILE:HD13	2.36	0.41
1:B:427:THR:HG22	1:B:429:PRO:HD3	2.02	0.41
1:C:382:TYR:CE1	1:C:386:LEU:HD11	2.55	0.41
1:D:119:ASP:OD2	1:D:488:LYS:CE	2.68	0.41
1:E:118:VAL:HG12	1:E:118:VAL:O	2.21	0.41
1:F:111:MET:SD	1:F:114:LYS:HE3	2.60	0.41
1:F:246:THR:O	1:F:320:ASP:HB2	2.21	0.41
1:F:338:ARG:O	1:F:340:LYS:HG2	2.20	0.41
1:A:291:LEU:CD1	1:A:304:PHE:HD2	2.24	0.41
1:A:496:ALA:CA	1:F:205:GLN:NE2	2.82	0.41
2:B:601:GLU:HA	3:B:602:NDP:C4N	2.42	0.41
1:C:495:GLU:HA	5:C:733:HOH:O	2.21	0.41
4:D:603:GTP:O2G	4:D:603:GTP:O2'	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:LYS:HD2	1:E:340:LYS:HA	1.83	0.41
1:E:382:TYR:O	1:E:386:LEU:HD13	2.21	0.41
1:F:281:TRP:HB2	1:F:310:TYR:HB2	2.02	0.41
1:B:271:VAL:HG22	1:B:283:PRO:HA	2.03	0.40
1:D:203:ILE:HG13	5:D:704:HOH:O	2.21	0.40
1:D:479:THR:O	1:D:483:VAL:HG23	2.20	0.40
1:F:227:ILE:HD13	1:F:242:PHE:CE1	2.56	0.40
1:F:448:ILE:HG21	1:F:448:ILE:HD13	1.23	0.40
1:E:77:GLY:O	1:E:78:TYR:CD1	2.74	0.40
1:F:3:ARG:H	1:F:3:ARG:HG2	1.54	0.40
1:A:246:THR:HG22	1:A:269:LYS:HG2	2.03	0.40
1:B:459:ARG:NH2	5:B:702:HOH:O	2.10	0.40
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.86	0.40
1:A:209:HIS:CD2	1:A:446:LYS:HG3	2.56	0.40
1:C:405:SER:N	1:E:439:ARG:NH1	2.69	0.40
1:C:458:GLU:HG2	1:C:459:ARG:N	2.36	0.40
1:C:491:ARG:HG2	5:C:711:HOH:O	2.22	0.40
1:F:53:LYS:NZ	5:F:729:HOH:O	2.53	0.40
1:B:111:MET:SD	1:B:114:LYS:HE3	2.62	0.40
1:B:281:TRP:HB2	1:B:310:TYR:HB2	2.04	0.40
1:B:346:GLU:OE2	1:B:351:PRO:HD2	2.20	0.40
1:B:382:TYR:CE1	1:B:386:LEU:CD1	3.01	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:783:HOH:O	5:E:757:HOH:O[1_655]	1.81	0.39

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	499/501 (100%)	467 (94%)	25 (5%)	7 (1%)	11	11
1	B	499/501 (100%)	468 (94%)	23 (5%)	8 (2%)	9	9
1	C	499/501 (100%)	463 (93%)	25 (5%)	11 (2%)	6	5
1	D	499/501 (100%)	469 (94%)	22 (4%)	8 (2%)	9	9
1	E	499/501 (100%)	464 (93%)	24 (5%)	11 (2%)	6	5
1	F	499/501 (100%)	465 (93%)	26 (5%)	8 (2%)	9	9
All	All	2994/3006 (100%)	2796 (93%)	145 (5%)	53 (2%)	8	7

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	38	GLU
1	A	500	PHE
1	B	35	ARG
1	B	38	GLU
1	C	4	GLU
1	C	35	ARG
1	C	38	GLU
1	C	422	GLY
1	C	500	PHE
1	D	35	ARG
1	E	4	GLU
1	E	35	ARG
1	E	37	THR
1	E	39	GLU
1	F	33	LYS
1	F	38	GLU
1	A	422	GLY
1	A	499	THR
1	B	422	GLY
1	B	500	PHE
1	D	422	GLY
1	D	500	PHE
1	E	33	LYS
1	E	38	GLU
1	E	422	GLY
1	E	499	THR
1	E	500	PHE
1	F	422	GLY
1	F	500	PHE

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Mol	Chain	Res	Type
1	A	39	GLU
1	B	39	GLU
1	C	36	GLU
1	C	424	HIS
1	C	499	THR
1	D	37	THR
1	D	499	THR
1	F	30	GLU
1	A	498	VAL
1	B	30	GLU
1	B	498	VAL
1	B	499	THR
1	C	30	GLU
1	C	498	VAL
1	D	30	GLU
1	D	498	VAL
1	E	30	GLU
1	E	498	VAL
1	F	498	VAL
1	C	39	GLU
1	D	312	GLY
1	F	35	ARG
1	F	312	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	417/417 (100%)	395 (95%)	22 (5%)	22	31
1	B	417/417 (100%)	403 (97%)	14 (3%)	37	51
1	C	417/417 (100%)	401 (96%)	16 (4%)	33	47
1	D	417/417 (100%)	399 (96%)	18 (4%)	29	40
1	E	417/417 (100%)	397 (95%)	20 (5%)	25	36
1	F	417/417 (100%)	404 (97%)	13 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2502/2502 (100%)	2399 (96%)	103 (4%)	30 43

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	19	ARG
1	A	96	SER
1	A	143	LYS
1	A	147	ARG
1	A	150	MET
1	A	177	SER
1	A	211	ARG
1	A	231	SER
1	A	257	LEU
1	A	260	MET
1	A	263	LEU
1	A	277	ASP
1	A	284	ASP
1	A	310	TYR
1	A	338	ARG
1	A	405	SER
1	A	445	GLU
1	A	456	THR
1	A	459	ARG
1	A	469	MET
1	A	470	LYS
1	B	4	GLU
1	B	9	PHE
1	B	27	LYS
1	B	79	ARG
1	B	102	ASP
1	B	170	SER
1	B	177	SER
1	B	211	ARG
1	B	224	GLU
1	B	318	ASP
1	B	342	LYS
1	B	373	LEU
1	B	405	SER
1	B	462	ARG
1	C	3	ARG

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Mol	Chain	Res	Type
1	C	4	GLU
1	C	9	PHE
1	C	44	ARG
1	C	46	ARG
1	C	62	SER
1	C	66	ARG
1	C	96	SER
1	C	147	ARG
1	C	211	ARG
1	C	231	SER
1	C	334	SER
1	C	338	ARG
1	C	405	SER
1	C	478	ARG
1	C	494	ASN
1	D	2	ASP
1	D	9	PHE
1	D	53	LYS
1	D	66	ARG
1	D	79	ARG
1	D	86	ARG
1	D	96	SER
1	D	204	SER
1	D	231	SER
1	D	277	ASP
1	D	308	LYS
1	D	342	LYS
1	D	405	SER
1	D	419	ARG
1	D	438	ASP
1	D	460	SER
1	D	462	ARG
1	D	478	ARG
1	E	3	ARG
1	E	9	PHE
1	E	19	ARG
1	E	27	LYS
1	E	38	GLU
1	E	53	LYS
1	E	79	ARG
1	E	96	SER
1	E	150	MET

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Mol	Chain	Res	Type
1	E	177	SER
1	E	211	ARG
1	E	229	GLU
1	E	277	ASP
1	E	361	LEU
1	E	373	LEU
1	E	405	SER
1	E	419	ARG
1	E	420	LYS
1	E	459	ARG
1	E	478	ARG
1	F	9	PHE
1	F	38	GLU
1	F	42	ARG
1	F	119	ASP
1	F	169	MET
1	F	211	ARG
1	F	277	ASP
1	F	358	LYS
1	F	373	LEU
1	F	405	SER
1	F	419	ARG
1	F	423	LYS
1	F	491	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	450	HIS
1	B	250	GLN
1	C	205	GLN
1	C	250	GLN
1	C	408	HIS
1	C	494	ASN
1	D	205	GLN
1	E	205	GLN
1	E	225	ASN
1	E	250	GLN
1	E	414	GLN
1	F	205	GLN
1	F	484	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	NDP	D	602	-	47,52,52	2.23	10 (21%)	61,80,80	1.81	19 (31%)
3	NDP	B	602	-	47,52,52	2.49	8 (17%)	61,80,80	1.62	13 (21%)
4	GTP	F	603	-	29,34,34	1.21	2 (6%)	35,54,54	1.59	8 (22%)
2	GLU	B	601	-	8,9,9	1.05	1 (12%)	8,11,11	1.76	2 (25%)
2	GLU	C	601	-	8,9,9	1.01	0	8,11,11	1.51	2 (25%)
4	GTP	C	603	-	29,34,34	1.31	5 (17%)	35,54,54	1.42	8 (22%)
2	GLU	E	601	-	8,9,9	1.24	2 (25%)	8,11,11	1.21	1 (12%)
4	GTP	A	603	-	29,34,34	1.20	2 (6%)	35,54,54	1.56	5 (14%)
3	NDP	A	602	-	47,52,52	2.78	11 (23%)	61,80,80	1.55	14 (22%)
2	GLU	A	601	-	8,9,9	1.19	2 (25%)	8,11,11	1.27	1 (12%)
4	GTP	B	603	-	29,34,34	1.46	5 (17%)	35,54,54	1.41	5 (14%)
4	GTP	E	603	-	29,34,34	1.06	2 (6%)	35,54,54	1.39	5 (14%)
3	NDP	C	602	-	47,52,52	2.53	13 (27%)	61,80,80	1.69	14 (22%)
3	NDP	E	602	-	47,52,52	2.98	12 (25%)	61,80,80	1.55	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NDP	F	602	-	47,52,52	2.49	10 (21%)	61,80,80	1.70	18 (29%)
2	GLU	F	601	-	8,9,9	1.05	0	8,11,11	1.76	1 (12%)
4	GTP	D	603	-	29,34,34	1.30	2 (6%)	35,54,54	1.49	7 (20%)
2	GLU	D	601	-	8,9,9	1.07	0	8,11,11	1.47	1 (12%)

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	NDP	D	602	-	-	10/30/77/77	0/5/5/5
3	NDP	B	602	-	-	6/30/77/77	0/5/5/5
4	GTP	F	603	-	-	5/18/38/38	0/3/3/3
2	GLU	B	601	-	-	2/9/9/9	-
2	GLU	C	601	-	-	2/9/9/9	-
4	GTP	C	603	-	-	2/18/38/38	0/3/3/3
2	GLU	E	601	-	-	4/9/9/9	-
4	GTP	A	603	-	-	2/18/38/38	0/3/3/3
3	NDP	A	602	-	-	3/30/77/77	0/5/5/5
2	GLU	A	601	-	-	4/9/9/9	-
4	GTP	B	603	-	-	2/18/38/38	0/3/3/3
4	GTP	E	603	-	-	4/18/38/38	0/3/3/3
3	NDP	C	602	-	-	6/30/77/77	0/5/5/5
3	NDP	E	602	-	-	11/30/77/77	0/5/5/5
3	NDP	F	602	-	-	5/30/77/77	0/5/5/5
2	GLU	F	601	-	-	2/9/9/9	-
4	GTP	D	603	-	-	2/18/38/38	0/3/3/3
2	GLU	D	601	-	-	4/9/9/9	-

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NDP	P2B-O2B	13.88	1.83	1.59
3	E	602	NDP	P2B-O2B	13.25	1.82	1.59
3	F	602	NDP	P2B-O2B	12.94	1.82	1.59
3	C	602	NDP	P2B-O2B	11.87	1.80	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NDP	P2B-O2B	11.64	1.79	1.59
3	E	602	NDP	PA-O3	11.18	1.71	1.59
3	B	602	NDP	P2B-O2B	10.07	1.77	1.59
3	B	602	NDP	PA-O3	9.02	1.69	1.59
3	C	602	NDP	PA-O3	6.82	1.66	1.59
3	A	602	NDP	PA-O3	6.57	1.66	1.59
3	F	602	NDP	PA-O3	5.08	1.65	1.59
3	A	602	NDP	O4B-C1B	4.81	1.47	1.40
3	E	602	NDP	PN-O5D	4.80	1.78	1.59
3	B	602	NDP	PN-O5D	4.79	1.78	1.59
4	B	603	GTP	C5-C6	-4.43	1.38	1.47
4	D	603	GTP	C5-C6	-4.14	1.39	1.47
3	B	602	NDP	O2B-C2B	-4.01	1.30	1.44
3	A	602	NDP	PN-O5D	3.94	1.74	1.59
4	A	603	GTP	C5-C6	-3.92	1.39	1.47
4	F	603	GTP	C5-C6	-3.92	1.39	1.47
4	C	603	GTP	C5-C6	-3.80	1.39	1.47
3	F	602	NDP	PN-O3	3.79	1.63	1.59
3	B	602	NDP	C2A-N1A	3.77	1.40	1.33
4	E	603	GTP	C5-C6	-3.77	1.40	1.47
3	D	602	NDP	PN-O5D	3.65	1.73	1.59
3	D	602	NDP	O2B-C2B	-3.63	1.31	1.44
3	A	602	NDP	PN-O3	3.61	1.63	1.59
3	D	602	NDP	PA-O3	3.61	1.63	1.59
3	C	602	NDP	O2B-C2B	-3.59	1.31	1.44
3	E	602	NDP	O2B-C2B	-3.56	1.31	1.44
4	B	603	GTP	PB-O3B	3.44	1.63	1.59
3	F	602	NDP	PN-O5D	3.43	1.72	1.59
3	C	602	NDP	PN-O3	3.24	1.63	1.59
3	E	602	NDP	C4A-N3A	3.21	1.40	1.35
3	C	602	NDP	C2A-N3A	2.99	1.36	1.32
3	F	602	NDP	O2B-C2B	-2.97	1.34	1.44
3	B	602	NDP	C7N-N7N	2.96	1.42	1.33
3	C	602	NDP	PN-O5D	2.94	1.70	1.59
3	F	602	NDP	C2A-N1A	2.91	1.39	1.33
4	D	603	GTP	PB-O3B	2.89	1.62	1.59
3	C	602	NDP	C2A-N1A	2.87	1.39	1.33
3	C	602	NDP	O4B-C1B	2.86	1.44	1.40
3	A	602	NDP	O2B-C2B	-2.86	1.34	1.44
3	E	602	NDP	C2A-N1A	2.85	1.39	1.33
4	B	603	GTP	PA-O3A	2.72	1.62	1.59
3	B	602	NDP	C4A-N3A	2.71	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	GTP	PB-O3A	2.70	1.62	1.59
3	A	602	NDP	C2A-N1A	2.64	1.38	1.33
3	C	602	NDP	C4A-N3A	2.63	1.39	1.35
3	F	602	NDP	C4A-N3A	2.62	1.39	1.35
3	E	602	NDP	PN-O3	2.59	1.62	1.59
4	C	603	GTP	PA-O3A	2.55	1.62	1.59
4	A	603	GTP	PB-O3A	2.48	1.62	1.59
3	A	602	NDP	C6N-N1N	2.47	1.43	1.37
4	F	603	GTP	PB-O3B	2.47	1.62	1.59
3	D	602	NDP	O5D-C5D	-2.42	1.35	1.44
3	E	602	NDP	O5D-C5D	-2.42	1.35	1.44
3	E	602	NDP	C6N-N1N	2.41	1.43	1.37
3	A	602	NDP	C1B-N9A	-2.40	1.44	1.49
3	C	602	NDP	O5D-C5D	-2.39	1.35	1.44
3	D	602	NDP	O4B-C4B	-2.39	1.39	1.45
3	C	602	NDP	O4B-C4B	-2.37	1.39	1.45
3	E	602	NDP	O4B-C4B	-2.35	1.39	1.45
3	C	602	NDP	C1B-N9A	-2.33	1.44	1.49
3	A	602	NDP	C3B-C2B	2.31	1.58	1.53
3	D	602	NDP	C4A-N3A	2.29	1.38	1.35
3	F	602	NDP	O5D-C5D	-2.29	1.35	1.44
3	D	602	NDP	C2A-N1A	2.26	1.37	1.33
3	A	602	NDP	C7N-N7N	2.23	1.39	1.33
3	F	602	NDP	C7N-N7N	2.21	1.39	1.33
3	E	602	NDP	C7N-N7N	2.18	1.39	1.33
3	B	602	NDP	PA-O2A	-2.16	1.45	1.55
2	A	601	GLU	OXT-C	-2.15	1.23	1.30
4	B	603	GTP	C2-N3	2.15	1.38	1.33
2	E	601	GLU	OE2-CD	-2.13	1.23	1.30
4	C	603	GTP	C2-N3	2.12	1.38	1.33
3	D	602	NDP	C7N-C3N	-2.12	1.44	1.48
3	C	602	NDP	C7N-N7N	2.11	1.39	1.33
4	C	603	GTP	PB-O3B	2.10	1.61	1.59
3	F	602	NDP	C2A-N3A	2.09	1.35	1.32
2	E	601	GLU	OXT-C	-2.09	1.24	1.30
2	B	601	GLU	OXT-C	-2.09	1.24	1.30
4	C	603	GTP	PB-O3A	2.08	1.61	1.59
4	E	603	GTP	C2-N3	2.05	1.38	1.33
2	A	601	GLU	OE2-CD	-2.03	1.24	1.30
3	E	602	NDP	C3D-C4D	2.02	1.58	1.53
3	D	602	NDP	O3B-C3B	-2.02	1.38	1.43

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	NDP	O4B-C1B-N9A	-5.13	101.95	108.75
3	B	602	NDP	C4B-O4B-C1B	-4.36	105.93	109.92
4	A	603	GTP	O4'-C1'-N9	4.23	114.36	108.75
3	F	602	NDP	O2N-PN-O3	4.19	118.59	107.27
3	D	602	NDP	P2B-O2B-C2B	-4.02	112.69	123.43
3	D	602	NDP	O2B-P2B-O1X	-3.99	95.10	109.33
4	F	603	GTP	C8-N7-C5	3.96	109.28	102.55
3	B	602	NDP	O2B-P2B-O1X	-3.93	95.31	109.33
3	F	602	NDP	P2B-O2B-C2B	-3.85	113.16	123.43
3	E	602	NDP	O2B-P2B-O1X	-3.84	95.66	109.33
4	F	603	GTP	O2B-PB-O3B	3.73	117.36	107.27
4	B	603	GTP	C8-N7-C5	3.71	108.87	102.55
3	F	602	NDP	O2B-P2B-O1X	-3.61	96.48	109.33
4	D	603	GTP	C8-N7-C5	3.61	108.69	102.55
4	D	603	GTP	O4'-C1'-N9	-3.60	103.97	108.75
4	E	603	GTP	C8-N7-C5	3.55	108.59	102.55
3	A	602	NDP	O4B-C1B-N9A	-3.50	104.11	108.75
3	C	602	NDP	O2B-P2B-O1X	-3.48	96.93	109.33
4	A	603	GTP	C5-C6-N1	3.47	120.69	114.07
3	C	602	NDP	O2N-PN-O3	3.46	116.62	107.27
3	D	602	NDP	C4B-O4B-C1B	-3.44	106.77	109.92
3	D	602	NDP	O2N-PN-O3	3.42	116.52	107.27
2	F	601	GLU	OXT-C-O	-3.40	116.36	124.08
4	A	603	GTP	C8-N7-C5	3.40	108.34	102.55
2	B	601	GLU	OXT-C-O	-3.39	116.40	124.08
3	B	602	NDP	PA-O5B-C5B	-3.38	101.96	121.35
2	D	601	GLU	OXT-C-O	-3.36	116.45	124.08
4	C	603	GTP	C8-N7-C5	3.34	108.24	102.55
3	D	602	NDP	O5D-PN-O1N	-3.32	95.77	108.94
2	A	601	GLU	OXT-C-O	-3.31	116.58	124.08
4	F	603	GTP	C2-N1-C6	-3.26	119.14	125.11
3	C	602	NDP	P2B-O2B-C2B	-3.26	114.73	123.43
3	A	602	NDP	O2N-PN-O3	3.26	116.07	107.27
3	D	602	NDP	PN-O5D-C5D	-3.21	102.97	121.35
3	D	602	NDP	C3B-C2B-C1B	-3.17	96.73	102.81
3	E	602	NDP	C4B-O4B-C1B	-3.17	107.02	109.92
4	B	603	GTP	C2-N1-C6	-3.15	119.35	125.11
3	B	602	NDP	O2N-PN-O3	3.10	115.64	107.27
3	B	602	NDP	P2B-O2B-C2B	-3.09	115.18	123.43
3	A	602	NDP	C4B-O4B-C1B	-3.08	107.11	109.92
4	F	603	GTP	C5-C6-N1	3.08	119.94	114.07
2	E	601	GLU	OXT-C-O	-3.05	117.16	124.08
3	D	602	NDP	C1B-N9A-C4A	-3.03	121.31	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	NDP	C4B-O4B-C1B	-3.02	107.16	109.92
3	B	602	NDP	O4B-C4B-C3B	2.99	111.10	105.15
2	C	601	GLU	OXT-C-O	-2.96	117.36	124.08
4	B	603	GTP	C5-C6-N1	2.95	119.70	114.07
3	D	602	NDP	O3-PA-O1A	-2.92	101.91	110.70
4	B	603	GTP	C4'-O4'-C1'	2.92	112.59	109.92
3	A	602	NDP	PN-O5D-C5D	-2.88	104.83	121.35
3	D	602	NDP	PA-O5B-C5B	-2.86	104.96	121.35
3	E	602	NDP	P2B-O2B-C2B	-2.84	115.83	123.43
3	E	602	NDP	PA-O5B-C5B	-2.83	105.12	121.35
3	F	602	NDP	PN-O5D-C5D	-2.81	105.24	121.35
4	A	603	GTP	C2-N1-C6	-2.81	119.97	125.11
4	D	603	GTP	C2-N1-C6	-2.80	119.99	125.11
4	C	603	GTP	C2-N1-C6	-2.77	120.04	125.11
3	A	602	NDP	O2B-P2B-O1X	-2.76	99.48	109.33
4	E	603	GTP	C2-N1-C6	-2.76	120.06	125.11
3	E	602	NDP	O3X-P2B-O2X	2.68	117.86	107.80
3	F	602	NDP	O5D-PN-O1N	-2.68	98.30	108.94
3	F	602	NDP	O3X-P2B-O2X	2.68	117.85	107.80
3	E	602	NDP	O2N-PN-O3	2.68	114.51	107.27
3	C	602	NDP	C4B-O4B-C1B	-2.66	107.49	109.92
3	A	602	NDP	P2B-O2B-C2B	-2.65	116.36	123.43
3	F	602	NDP	PA-O5B-C5B	-2.65	106.18	121.35
3	A	602	NDP	PA-O5B-C5B	-2.64	106.21	121.35
4	E	603	GTP	C5-C6-N1	2.64	119.11	114.07
3	A	602	NDP	O3X-P2B-O2B	-2.59	95.75	105.85
3	E	602	NDP	O4B-C4B-C3B	2.59	110.30	105.15
3	D	602	NDP	C5B-C4B-C3B	-2.58	105.91	115.21
3	D	602	NDP	O3X-P2B-O2X	2.58	117.48	107.80
3	C	602	NDP	PA-O5B-C5B	-2.58	106.58	121.35
3	A	602	NDP	C3N-C2N-N1N	-2.58	119.42	123.20
4	D	603	GTP	C4'-O4'-C1'	2.56	112.27	109.92
4	C	603	GTP	C5-C6-N1	2.55	118.94	114.07
4	D	603	GTP	C5-C6-N1	2.55	118.93	114.07
3	A	602	NDP	O3-PA-O1A	-2.54	103.05	110.70
3	F	602	NDP	C3B-C2B-C1B	-2.54	97.94	102.81
4	C	603	GTP	O6-C6-C5	-2.54	119.29	124.32
3	C	602	NDP	O3X-P2B-O2X	2.54	117.31	107.80
3	B	602	NDP	O3X-P2B-O2X	2.53	117.30	107.80
3	C	602	NDP	O5D-PN-O1N	-2.52	98.94	108.94
3	A	602	NDP	O3X-P2B-O2X	2.50	117.16	107.80
3	D	602	NDP	C3D-C2D-C1D	-2.47	96.78	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	603	GTP	O3G-PG-O3B	2.47	112.92	104.64
3	C	602	NDP	C3D-C2D-C1D	-2.47	96.80	101.46
3	B	602	NDP	O2A-PA-O1A	2.45	123.85	112.44
3	E	602	NDP	C1B-N9A-C4A	-2.40	122.42	126.64
4	A	603	GTP	O2B-PB-O3B	2.40	113.76	107.27
4	C	603	GTP	O3G-PG-O3B	2.40	112.67	104.64
3	B	602	NDP	O5D-PN-O1N	-2.39	99.45	108.94
3	F	602	NDP	O7N-C7N-C3N	2.37	125.36	120.90
3	C	602	NDP	O3B-C3B-C2B	-2.36	104.59	111.19
3	C	602	NDP	O3-PA-O1A	-2.35	103.64	110.70
3	F	602	NDP	C5D-C4D-C3D	-2.34	106.79	115.21
3	A	602	NDP	O2N-PN-O1N	2.32	123.25	112.44
3	D	602	NDP	C2B-C1B-N9A	2.32	117.70	112.56
4	D	603	GTP	O2G-PG-O3B	2.31	112.37	104.64
3	F	602	NDP	O3-PA-O1A	-2.30	103.79	110.70
3	A	602	NDP	O5D-PN-O1N	-2.29	99.86	108.94
3	C	602	NDP	PN-O5D-C5D	-2.29	108.24	121.35
3	E	602	NDP	C3B-C2B-C1B	-2.26	98.48	102.81
3	F	602	NDP	O3X-P2B-O2B	-2.25	97.10	105.85
3	C	602	NDP	C3B-C2B-C1B	-2.23	98.53	102.81
4	F	603	GTP	O4'-C1'-N9	2.23	111.70	108.75
4	F	603	GTP	O6-C6-C5	-2.22	119.91	124.32
4	B	603	GTP	O3G-PG-O3B	2.22	112.09	104.64
2	B	601	GLU	CG-CB-CA	2.21	118.93	113.86
3	F	602	NDP	C5B-C4B-C3B	-2.21	107.26	115.21
3	D	602	NDP	C2D-C3D-C4D	-2.20	98.37	102.61
3	E	602	NDP	O4B-C1B-N9A	-2.19	105.84	108.75
4	C	603	GTP	N2-C2-N1	2.18	121.36	116.76
3	D	602	NDP	C5D-C4D-C3D	-2.17	107.39	115.21
4	F	603	GTP	O3G-PG-O3B	2.17	111.90	104.64
4	C	603	GTP	O3'-C3'-C2'	-2.16	104.89	111.82
3	F	602	NDP	O2N-PN-O1N	2.16	122.48	112.44
3	B	602	NDP	C5B-C4B-C3B	-2.15	107.47	115.21
3	D	602	NDP	O2N-PN-O1N	2.15	122.45	112.44
3	D	602	NDP	O3X-P2B-O2B	-2.14	97.51	105.85
3	F	602	NDP	C1B-N9A-C4A	-2.14	122.89	126.64
4	D	603	GTP	O3'-C3'-C4'	-2.13	104.97	111.08
4	C	603	GTP	O4'-C1'-N9	2.13	111.56	108.75
3	E	602	NDP	O7N-C7N-N7N	-2.12	118.14	122.89
4	F	603	GTP	N2-C2-N1	2.10	121.20	116.76
3	F	602	NDP	O4B-C4B-C3B	2.10	109.32	105.15
4	E	603	GTP	O2B-PB-O3A	2.10	112.95	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	NDP	O4B-C4B-C3B	2.08	109.29	105.15
3	F	602	NDP	C2D-C3D-C4D	-2.08	98.59	102.61
3	E	602	NDP	O2N-PN-O1N	2.08	122.12	112.44
3	B	602	NDP	O2N-PN-O1N	2.07	122.06	112.44
3	E	602	NDP	O5D-PN-O1N	-2.06	100.77	108.94
3	B	602	NDP	O3-PA-O1A	-2.03	104.59	110.70
2	C	601	GLU	OE2-CD-CG	2.03	120.40	114.00
3	D	602	NDP	O4B-C4B-C3B	2.01	109.15	105.15
3	C	602	NDP	O7N-C7N-C3N	2.01	124.69	120.90
3	B	602	NDP	C5D-C4D-C3D	-2.01	107.97	115.21

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	NDP	C5D-O5D-PN-O3
3	B	602	NDP	C5D-O5D-PN-O2N
3	B	602	NDP	O4D-C4D-C5D-O5D
3	C	602	NDP	O4D-C4D-C5D-O5D
3	D	602	NDP	C5B-O5B-PA-O1A
3	D	602	NDP	C5B-O5B-PA-O2A
3	D	602	NDP	C5B-O5B-PA-O3
3	D	602	NDP	PN-O3-PA-O5B
3	D	602	NDP	C3B-C4B-C5B-O5B
3	E	602	NDP	C5D-O5D-PN-O2N
3	E	602	NDP	O4D-C4D-C5D-O5D
4	B	603	GTP	PB-O3B-PG-O3G
4	C	603	GTP	PB-O3B-PG-O3G
4	F	603	GTP	PB-O3B-PG-O2G
4	F	603	GTP	PB-O3B-PG-O3G
3	D	602	NDP	O4B-C4B-C5B-O5B
3	E	602	NDP	C3D-C4D-C5D-O5D
3	B	602	NDP	C3D-C4D-C5D-O5D
3	C	602	NDP	C3D-C4D-C5D-O5D
4	E	603	GTP	PG-O3B-PB-O1B
4	A	603	GTP	PB-O3B-PG-O3G
4	F	603	GTP	PB-O3A-PA-O1A
3	E	602	NDP	C5D-O5D-PN-O3
3	E	602	NDP	C5D-O5D-PN-O1N
4	D	603	GTP	PB-O3A-PA-O2A
3	E	602	NDP	C2B-O2B-P2B-O3X
2	A	601	GLU	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	A	601	GLU	OXT-C-CA-CB
2	D	601	GLU	O-C-CA-CB
2	D	601	GLU	OXT-C-CA-CB
3	D	602	NDP	O4D-C1D-N1N-C6N
3	E	602	NDP	O4D-C1D-N1N-C6N
3	F	602	NDP	O4D-C1D-N1N-C6N
3	A	602	NDP	C2D-C1D-N1N-C6N
3	A	602	NDP	O4D-C1D-N1N-C6N
2	B	601	GLU	OE1-CD-CG-CB
4	F	603	GTP	PB-O3B-PG-O1G
2	C	601	GLU	OE1-CD-CG-CB
3	C	602	NDP	C2D-C1D-N1N-C6N
2	B	601	GLU	OE2-CD-CG-CB
2	D	601	GLU	OE1-CD-CG-CB
3	B	602	NDP	O4D-C1D-N1N-C6N
3	C	602	NDP	O4D-C1D-N1N-C6N
3	C	602	NDP	C2N-C3N-C7N-N7N
3	D	602	NDP	C2N-C3N-C7N-N7N
3	F	602	NDP	C2N-C3N-C7N-N7N
2	A	601	GLU	OE2-CD-CG-CB
3	C	602	NDP	C2B-O2B-P2B-O1X
3	E	602	NDP	C2B-O2B-P2B-O1X
2	E	601	GLU	O-C-CA-CB
2	E	601	GLU	OXT-C-CA-CB
3	D	602	NDP	PA-O3-PN-O2N
4	A	603	GTP	PA-O3A-PB-O1B
4	E	603	GTP	PA-O3A-PB-O2B
2	F	601	GLU	OE2-CD-CG-CB
3	B	602	NDP	C2D-C1D-N1N-C6N
2	C	601	GLU	OE2-CD-CG-CB
2	F	601	GLU	OE1-CD-CG-CB
4	B	603	GTP	PB-O3B-PG-O1G
4	C	603	GTP	PB-O3B-PG-O1G
2	A	601	GLU	OE1-CD-CG-CB
2	D	601	GLU	OE2-CD-CG-CB
2	E	601	GLU	OE2-CD-CG-CB
2	E	601	GLU	OE1-CD-CG-CB
3	E	602	NDP	C2D-C1D-N1N-C6N
4	E	603	GTP	PA-O3A-PB-O1B
3	E	602	NDP	O4B-C4B-C5B-O5B
3	E	602	NDP	C2B-O2B-P2B-O2X
4	E	603	GTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
3	F	602	NDP	C2D-C1D-N1N-C6N
3	F	602	NDP	O4B-C4B-C5B-O5B
3	A	602	NDP	C2N-C3N-C7N-O7N
3	D	602	NDP	C2D-C1D-N1N-C6N
3	F	602	NDP	PA-O3-PN-O1N
4	D	603	GTP	PB-O3A-PA-O1A
4	F	603	GTP	PB-O3A-PA-O2A

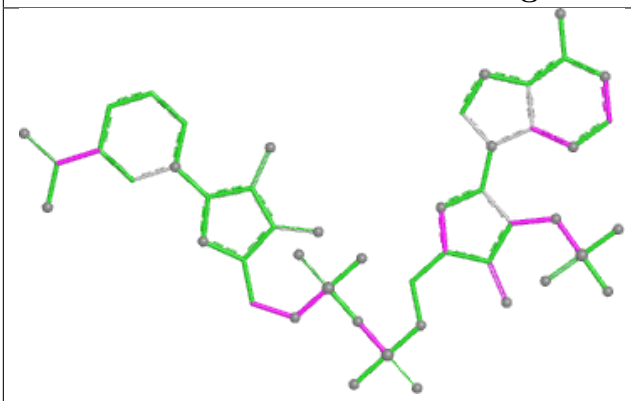
There are no ring outliers.

15 monomers are involved in 31 short contacts:

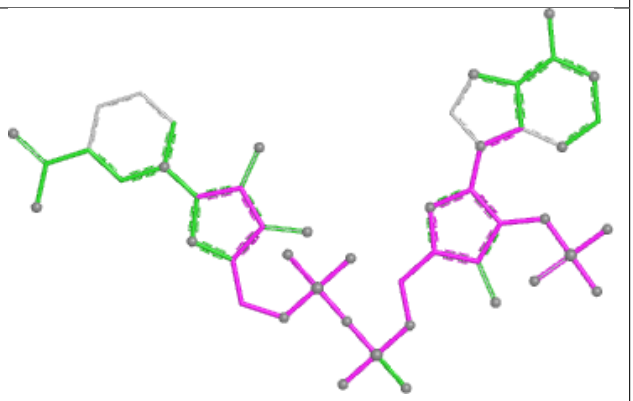
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	NDP	7	0
3	B	602	NDP	3	0
4	F	603	GTP	1	0
2	B	601	GLU	2	0
2	C	601	GLU	2	0
2	E	601	GLU	1	0
3	A	602	NDP	4	0
2	A	601	GLU	1	0
4	B	603	GTP	1	0
3	C	602	NDP	4	0
3	E	602	NDP	4	0
3	F	602	NDP	5	0
2	F	601	GLU	1	0
4	D	603	GTP	1	0
2	D	601	GLU	1	0

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.

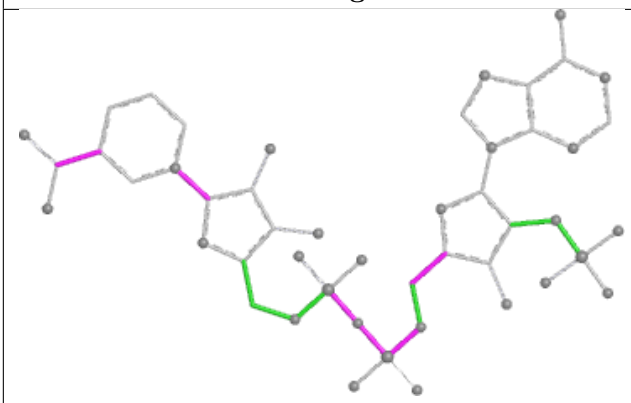
Ligand NDP D 602



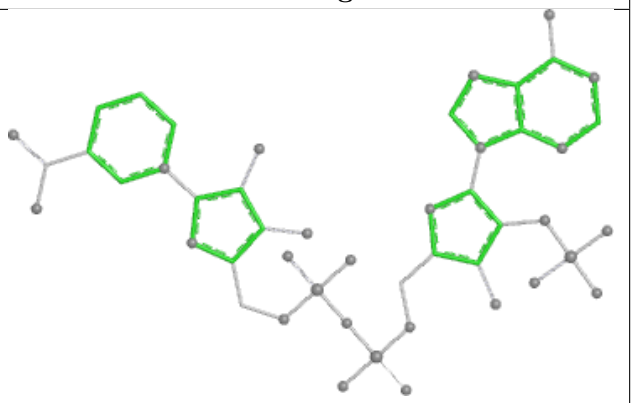
Bond lengths



Bond angles

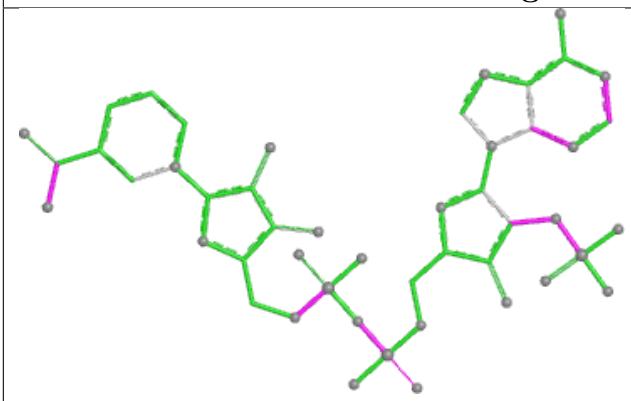


Torsions

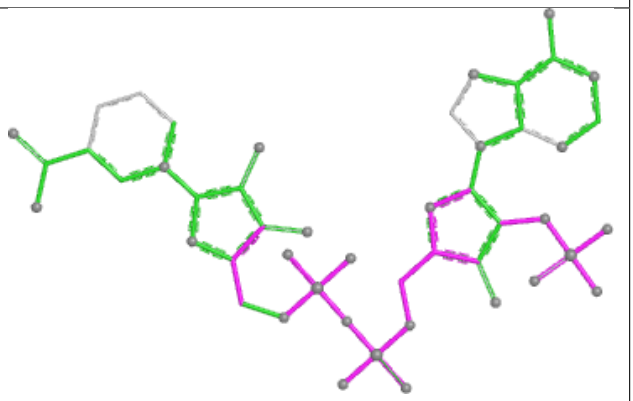


Rings

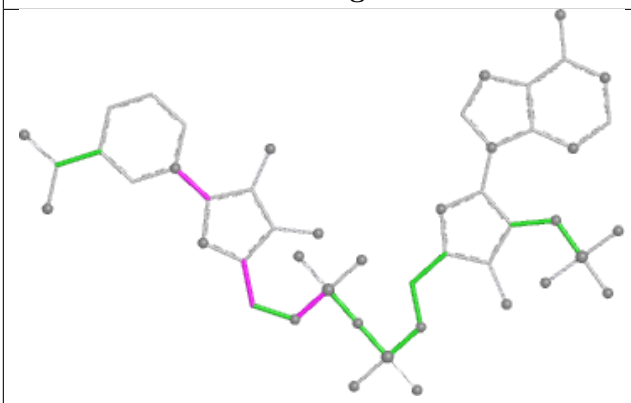
Ligand NDP B 602



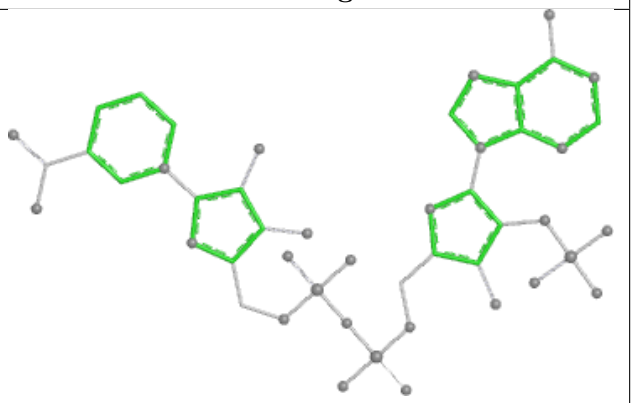
Bond lengths



Bond angles

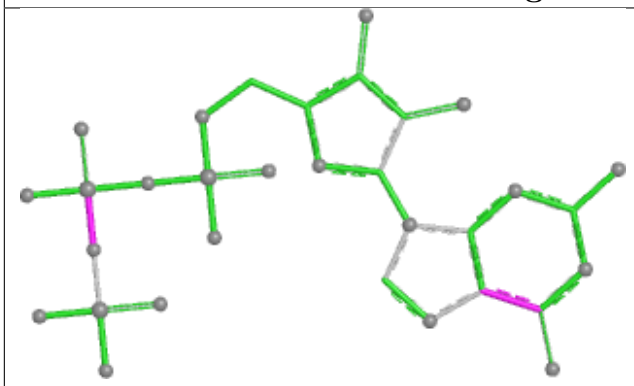


Torsions

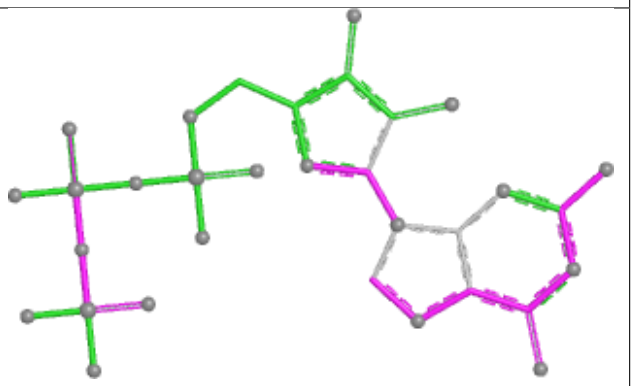


Rings

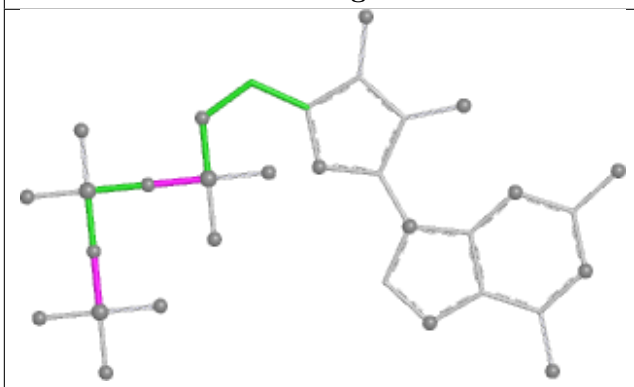
Ligand GTP F 603



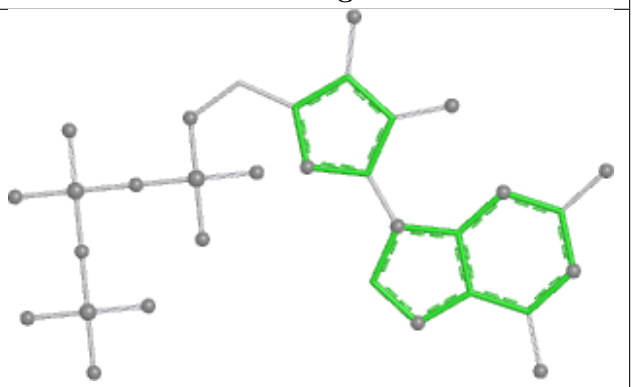
Bond lengths



Bond angles

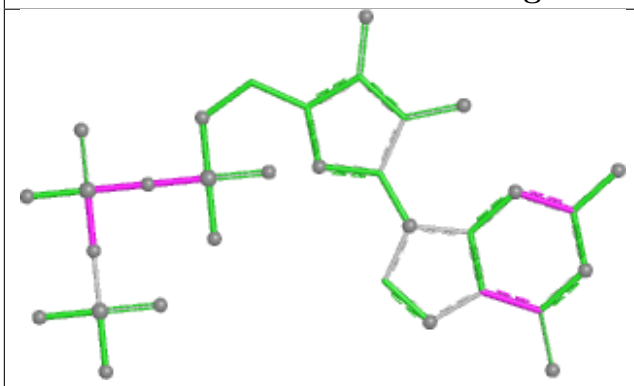


Torsions

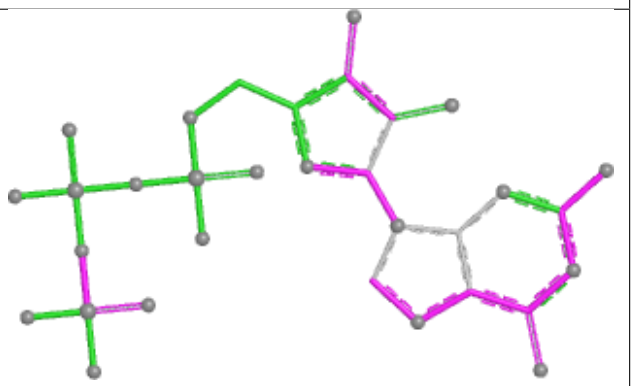


Rings

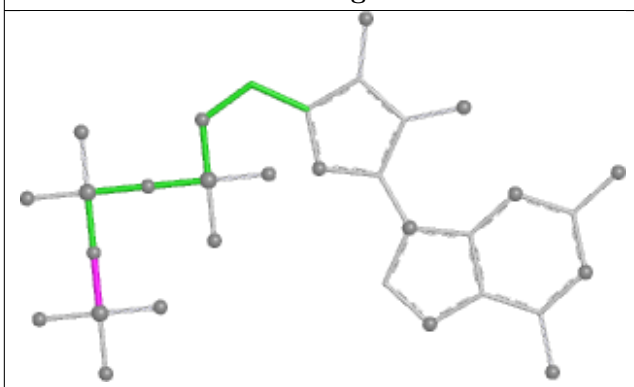
Ligand GTP C 603



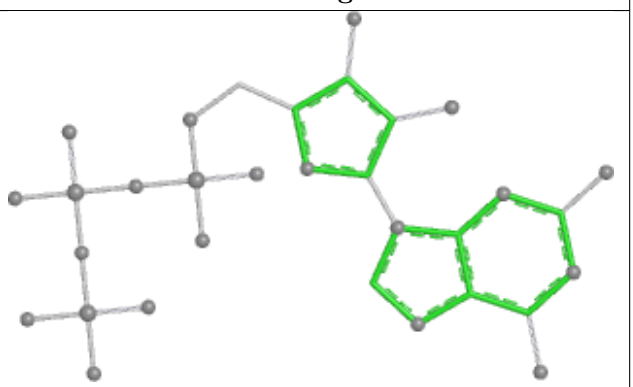
Bond lengths



Bond angles

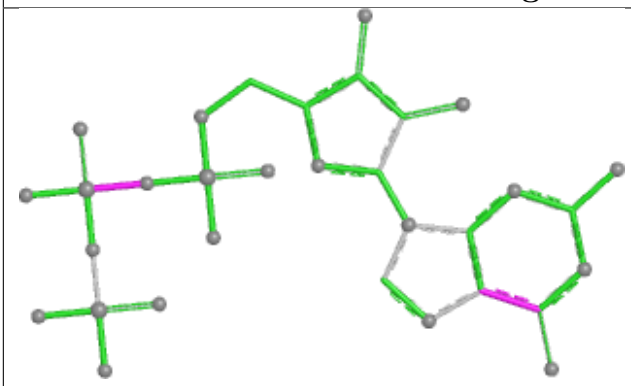


Torsions

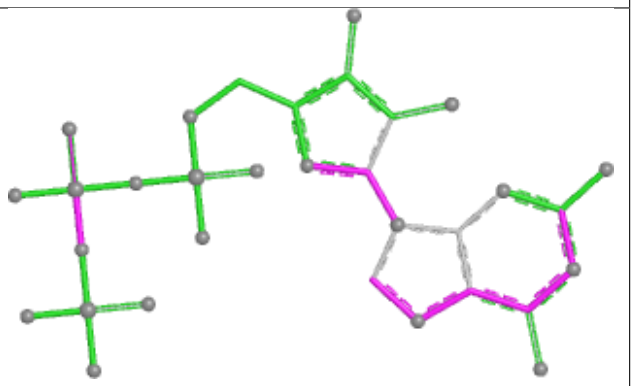


Rings

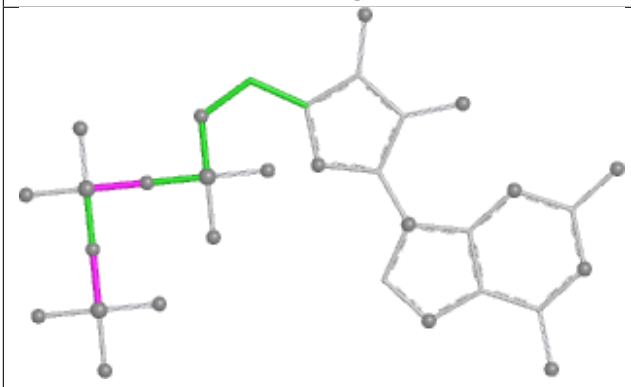
Ligand GTP A 603



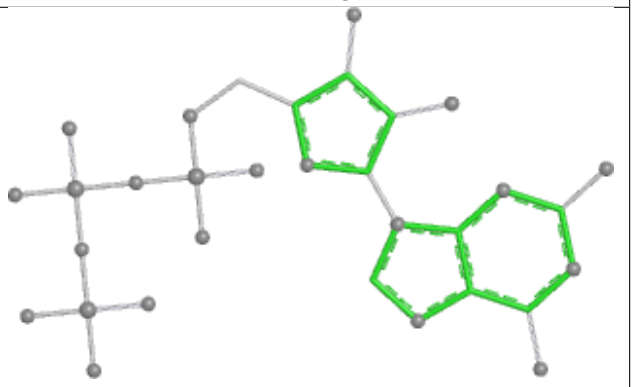
Bond lengths



Bond angles

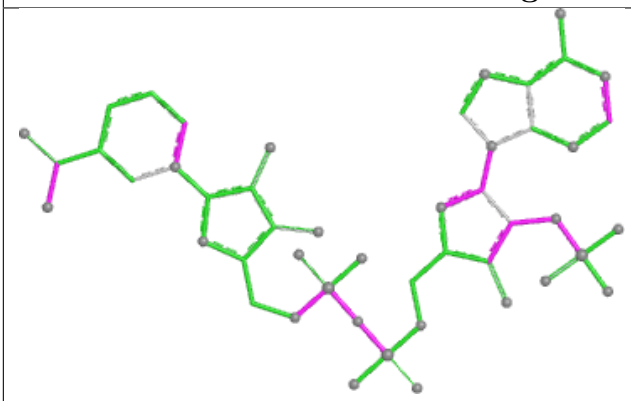


Torsions

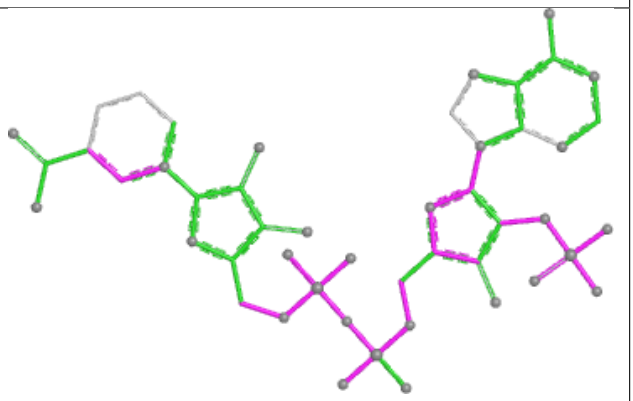


Rings

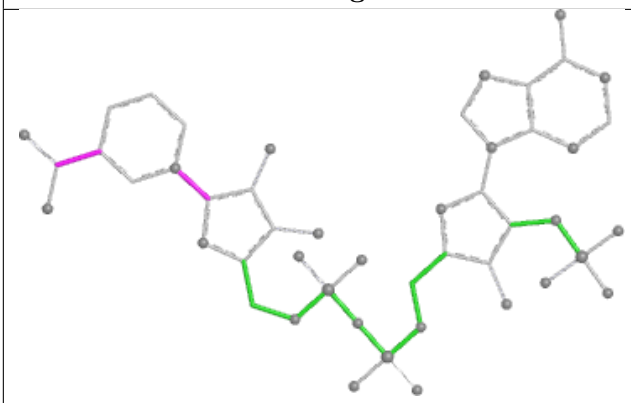
Ligand NDP A 602



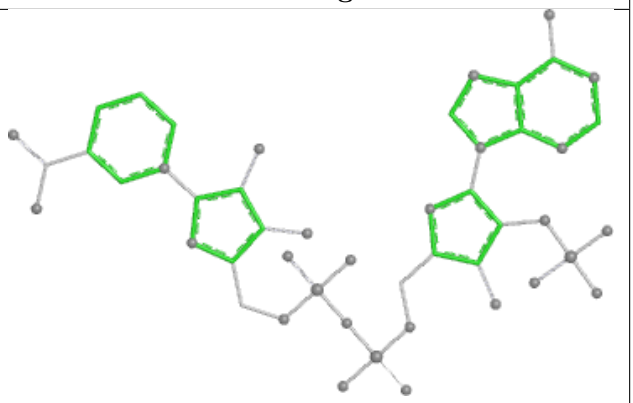
Bond lengths



Bond angles

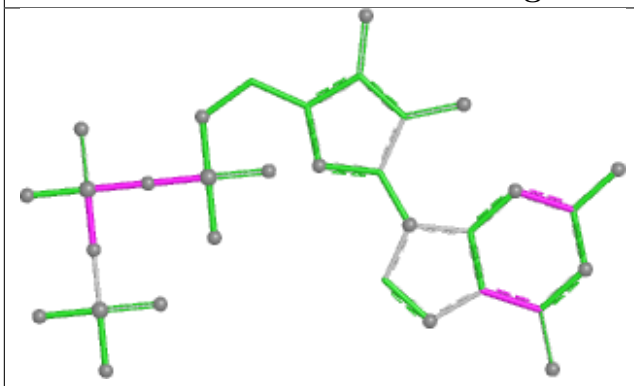


Torsions

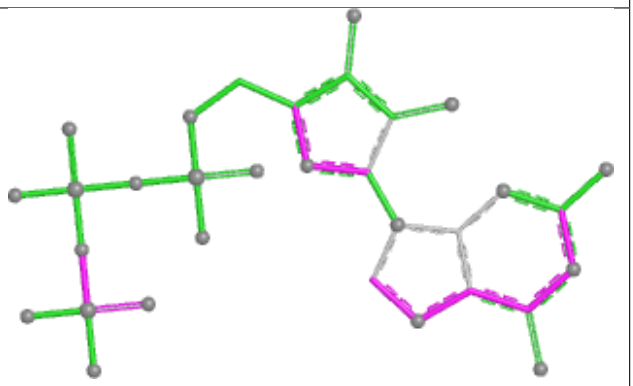


Rings

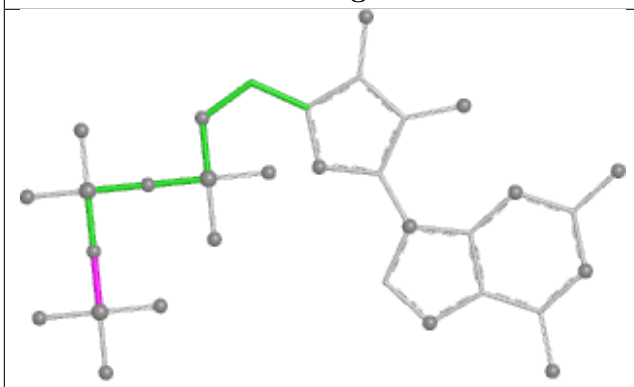
Ligand GTP B 603



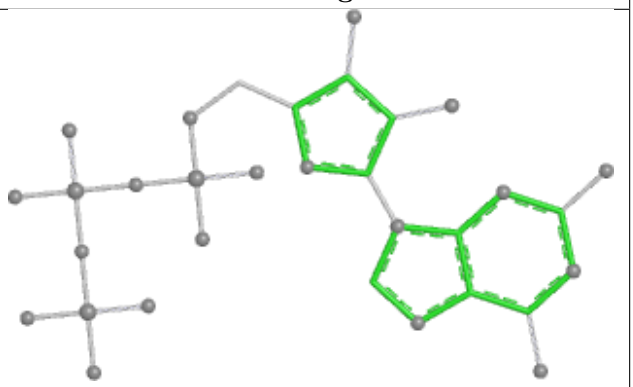
Bond lengths



Bond angles

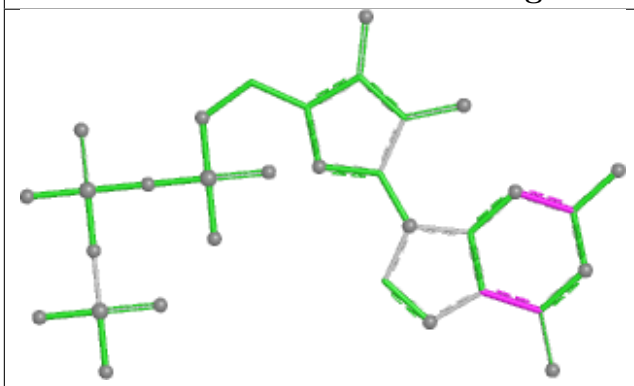


Torsions

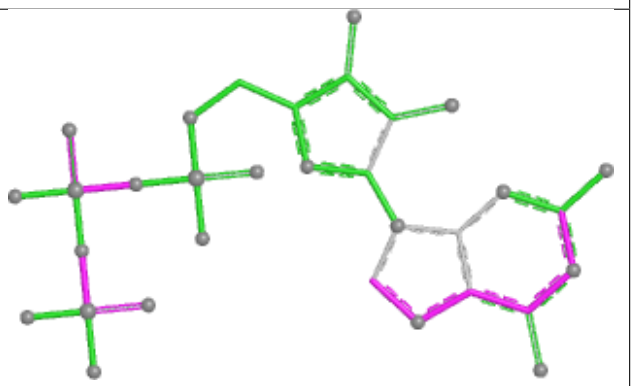


Rings

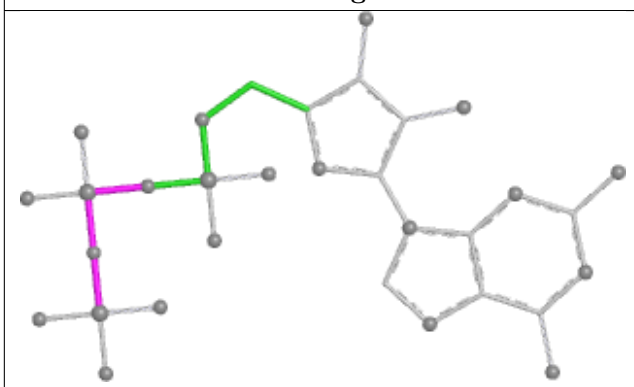
Ligand GTP E 603



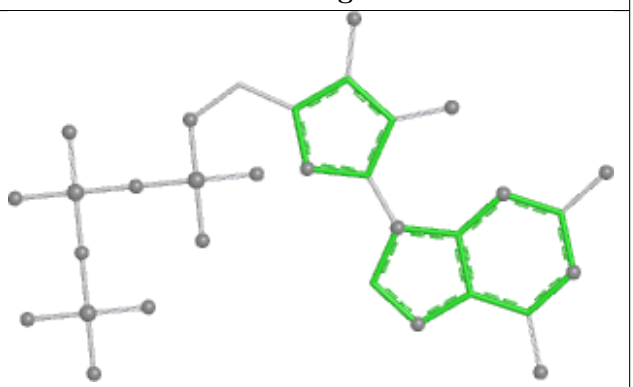
Bond lengths



Bond angles

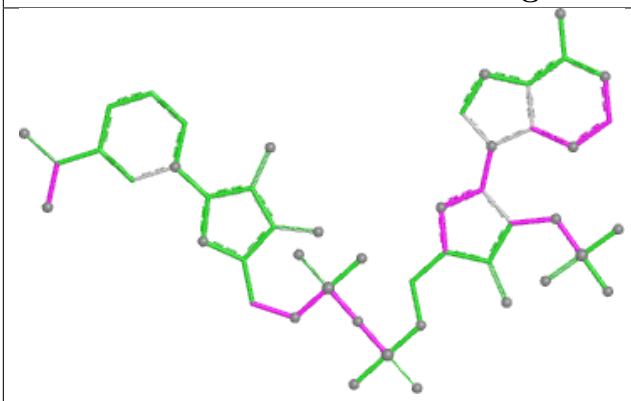


Torsions

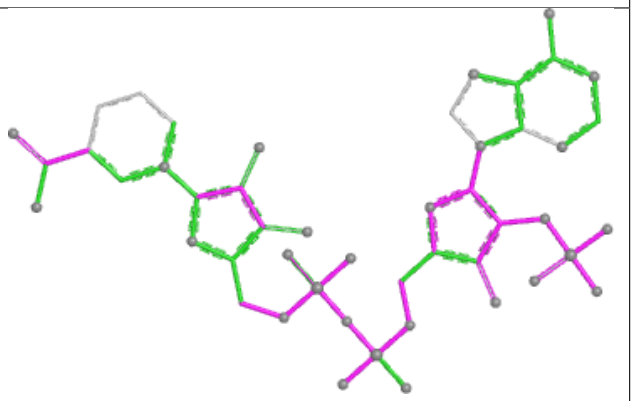


Rings

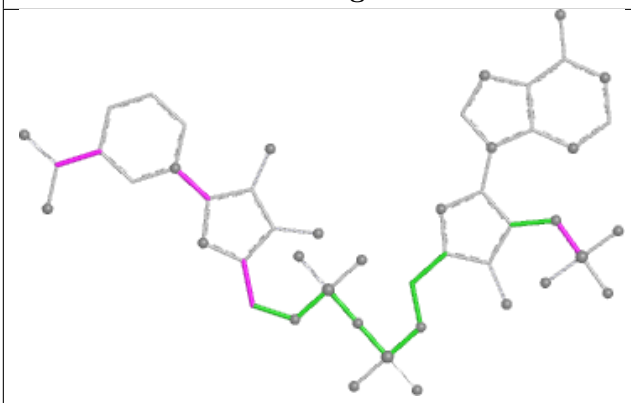
Ligand NDP C 602



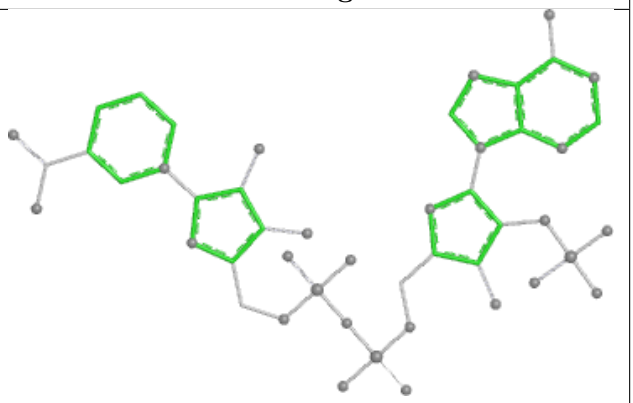
Bond lengths



Bond angles

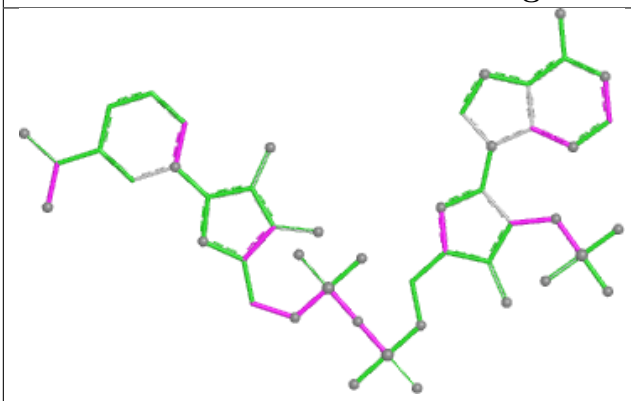


Torsions

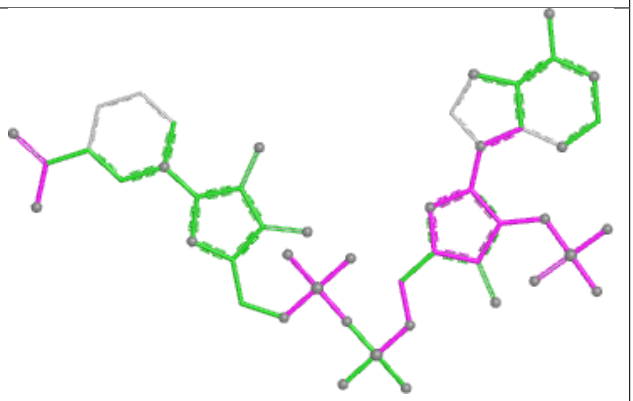


Rings

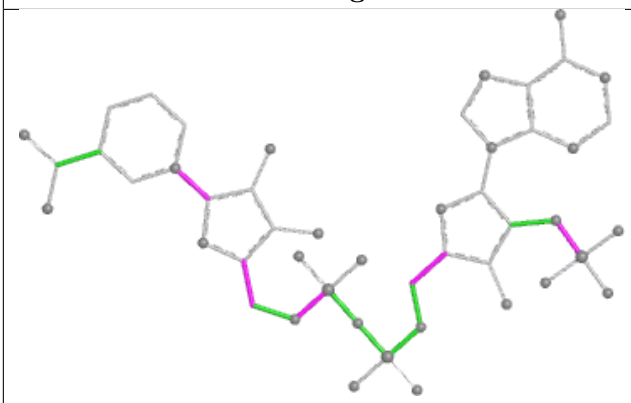
Ligand NDP E 602



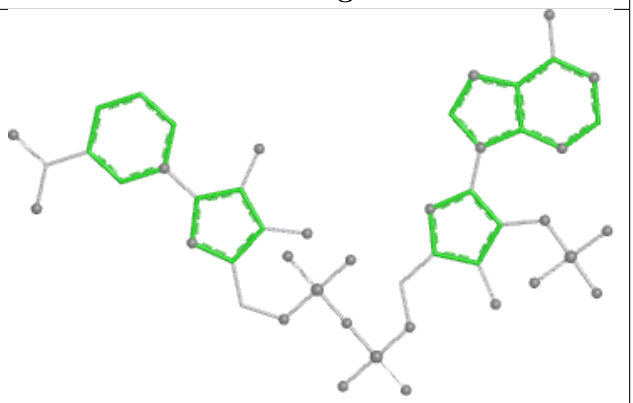
Bond lengths



Bond angles

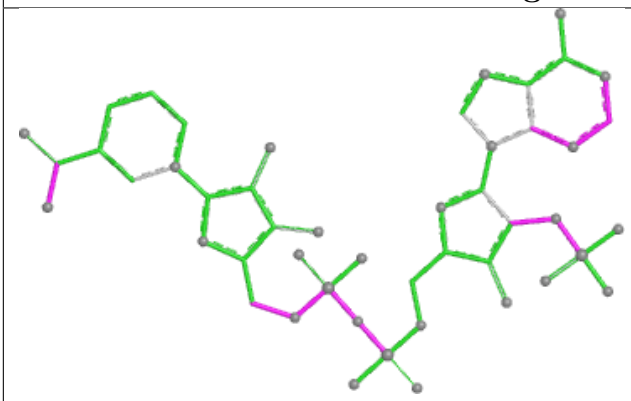


Torsions

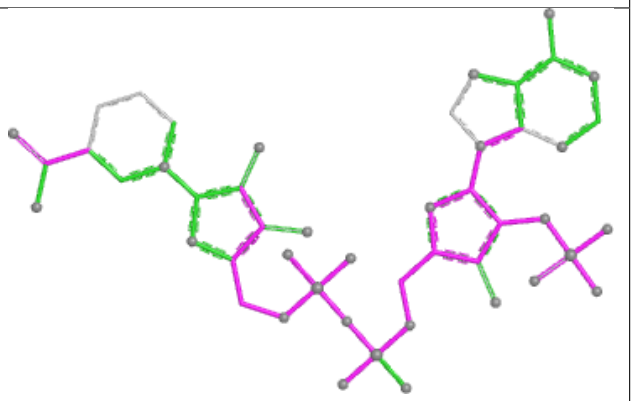


Rings

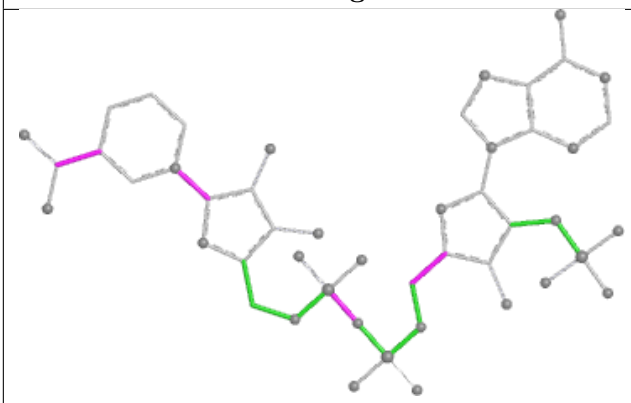
Ligand NDP F 602



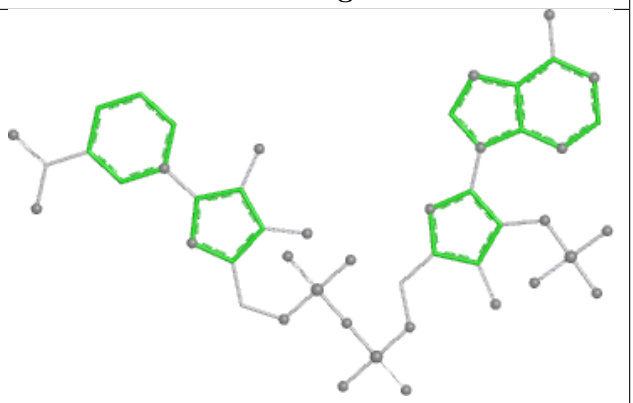
Bond lengths



Bond angles

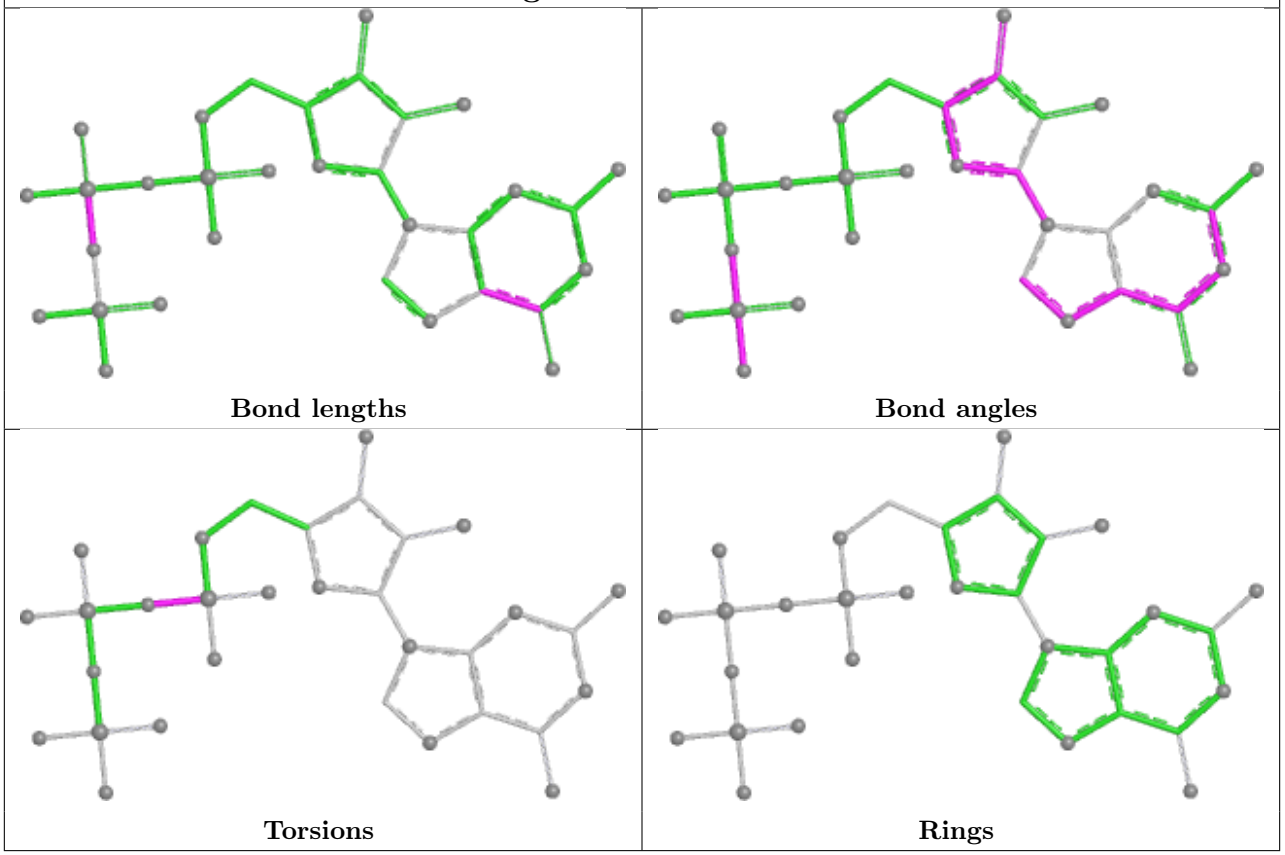


Torsions



Rings

Ligand GTP D 603



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	501/501 (100%)	0.48	51 (10%) 6 9	34, 55, 86, 115	0
1	B	501/501 (100%)	0.49	45 (8%) 9 12	34, 54, 86, 118	0
1	C	501/501 (100%)	0.53	62 (12%) 4 5	40, 57, 88, 112	0
1	D	501/501 (100%)	0.45	45 (8%) 9 12	39, 56, 89, 112	0
1	E	501/501 (100%)	0.63	61 (12%) 4 6	37, 62, 93, 113	0
1	F	501/501 (100%)	0.57	56 (11%) 5 7	38, 60, 90, 117	0
All	All	3006/3006 (100%)	0.52	320 (10%) 6 8	34, 57, 91, 118	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	8.4
1	F	1	ALA	8.3
1	B	1	ALA	8.0
1	B	3	ARG	7.6
1	F	5	ASP	6.6
1	A	424	HIS	6.6
1	A	1	ALA	6.5
1	E	345	ALA	6.1
1	A	38	GLU	5.7
1	D	37	THR	5.6
1	E	368	ILE	5.6
1	D	423	LYS	5.5
1	F	3	ARG	5.4
1	D	424	HIS	5.3
1	A	2	ASP	5.3
1	E	37	THR	5.1
1	D	33	LYS	5.1
1	A	3	ARG	5.1
1	F	4	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	1	ALA	5.1
1	C	345	ALA	5.1
1	A	323	ILE	5.0
1	A	35	ARG	4.9
1	A	345	ALA	4.9
1	B	323	ILE	4.9
1	F	423	LYS	4.9
1	C	368	ILE	4.8
1	B	424	HIS	4.8
1	C	323	ILE	4.8
1	A	32	LEU	4.7
1	D	35	ARG	4.7
1	E	312	GLY	4.7
1	D	1	ALA	4.7
1	E	323	ILE	4.7
1	C	424	HIS	4.7
1	D	5	ASP	4.6
1	B	345	ALA	4.6
1	A	4	GLU	4.5
1	E	5	ASP	4.5
1	B	4	GLU	4.5
1	F	373	LEU	4.5
1	F	424	HIS	4.5
1	D	2	ASP	4.5
1	E	343	ILE	4.5
1	F	37	THR	4.4
1	E	3	ARG	4.4
1	F	323	ILE	4.4
1	D	4	GLU	4.4
1	E	373	LEU	4.4
1	F	2	ASP	4.3
1	E	6	ASP	4.3
1	B	34	THR	4.3
1	A	6	ASP	4.3
1	C	5	ASP	4.3
1	C	423	LYS	4.3
1	E	298	HIS	4.2
1	A	423	LYS	4.2
1	F	40	GLN	4.2
1	A	368	ILE	4.2
1	C	2	ASP	4.2
1	A	7	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	321	ILE	4.1
1	A	34	THR	4.1
1	B	322	LEU	4.1
1	B	5	ASP	4.0
1	E	371	LEU	4.0
1	C	32	LEU	3.9
1	C	425	GLY	3.9
1	B	29	VAL	3.9
1	F	345	ALA	3.9
1	A	426	GLY	3.8
1	D	3	ARG	3.8
1	B	368	ILE	3.8
1	A	36	GLU	3.8
1	D	30	GLU	3.8
1	E	281	TRP	3.8
1	E	425	GLY	3.8
1	D	38	GLU	3.7
1	E	369	PRO	3.7
1	A	33	LYS	3.7
1	D	29	VAL	3.7
1	C	369	PRO	3.7
1	C	38	GLU	3.6
1	F	38	GLU	3.6
1	B	344	ILE	3.6
1	C	348	ALA	3.6
1	B	2	ASP	3.6
1	E	322	LEU	3.6
1	C	33	LYS	3.5
1	E	367	VAL	3.5
1	E	38	GLU	3.5
1	D	34	THR	3.5
1	D	345	ALA	3.5
1	C	3	ARG	3.5
1	A	324	PRO	3.5
1	E	344	ILE	3.4
1	F	219	VAL	3.4
1	C	373	LEU	3.4
1	B	373	LEU	3.4
1	A	230	ALA	3.3
1	C	40	GLN	3.3
1	B	223	ILE	3.3
1	A	322	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	283	PRO	3.3
1	A	37	THR	3.3
1	A	5	ASP	3.3
1	C	30	GLU	3.3
1	D	40	GLN	3.2
1	F	324	PRO	3.2
1	A	29	VAL	3.2
1	D	373	LEU	3.2
1	F	359	ILE	3.2
1	B	324	PRO	3.2
1	A	373	LEU	3.2
1	B	321	ILE	3.2
1	E	230	ALA	3.2
1	D	500	PHE	3.2
1	F	348	ALA	3.2
1	B	38	GLU	3.2
1	D	347	GLY	3.2
1	E	469	MET	3.2
1	A	39	GLU	3.1
1	E	35	ARG	3.1
1	F	421	PHE	3.1
1	F	6	ASP	3.1
1	B	31	ASP	3.0
1	A	239	THR	3.0
1	C	426	GLY	3.0
1	F	32	LEU	3.0
1	F	347	GLY	3.0
1	B	40	GLN	3.0
1	F	33	LYS	3.0
1	F	281	TRP	3.0
1	F	298	HIS	2.9
1	B	219	VAL	2.9
1	B	35	ARG	2.9
1	E	2	ASP	2.9
1	F	338	ARG	2.9
1	B	333	LYS	2.9
1	D	348	ALA	2.9
1	F	230	ALA	2.9
1	D	323	ILE	2.8
1	D	32	LEU	2.8
1	A	427	THR	2.8
1	F	249	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	32	LEU	2.8
1	C	37	THR	2.8
1	F	426	GLY	2.8
1	C	374	ASN	2.8
1	F	311	GLU	2.8
1	C	248	ALA	2.7
1	E	36	GLU	2.8
1	E	324	PRO	2.7
1	C	249	VAL	2.7
1	C	347	GLY	2.7
1	A	344	ILE	2.7
1	E	346	GLU	2.7
1	F	312	GLY	2.7
1	A	249	VAL	2.7
1	E	309	ILE	2.7
1	C	324	PRO	2.7
1	E	297	GLN	2.7
1	E	39	GLU	2.7
1	F	35	ARG	2.7
1	A	362	GLU	2.7
1	A	321	ILE	2.7
1	C	110	LEU	2.7
1	C	219	VAL	2.7
1	E	29	VAL	2.7
1	E	294	PHE	2.7
1	A	281	TRP	2.6
1	B	334	SER	2.6
1	B	312	GLY	2.6
1	D	7	PRO	2.6
1	D	36	GLU	2.6
1	E	41	LYS	2.6
1	C	309	ILE	2.6
1	A	348	ALA	2.6
1	D	368	ILE	2.6
1	C	239	THR	2.6
1	C	4	GLU	2.6
1	A	243	GLY	2.6
1	B	230	ALA	2.6
1	E	40	GLN	2.6
1	F	368	ILE	2.6
1	C	302	LEU	2.6
1	E	7	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	248	ALA	2.6
1	B	348	ALA	2.6
1	B	36	GLU	2.6
1	E	362	GLU	2.6
1	C	11	LYS	2.6
1	C	243	GLY	2.5
1	A	358	LYS	2.5
1	C	375	ALA	2.5
1	D	39	GLU	2.5
1	F	322	LEU	2.5
1	F	371	LEU	2.5
1	C	304	PHE	2.5
1	D	333	LYS	2.5
1	F	333	LYS	2.5
1	B	343	ILE	2.5
1	E	355	GLU	2.5
1	F	297	GLN	2.5
1	E	33	LYS	2.5
1	F	234	SER	2.5
1	D	499	THR	2.5
1	E	223	ILE	2.5
1	F	7	PRO	2.5
1	B	425	GLY	2.5
1	C	298	HIS	2.5
1	C	355	GLU	2.5
1	C	344	ILE	2.5
1	D	219	VAL	2.4
1	E	219	VAL	2.4
1	C	34	THR	2.4
1	B	256	GLY	2.4
1	E	370	ASP	2.4
1	A	346	GLU	2.4
1	E	496	ALA	2.4
1	C	346	GLU	2.4
1	C	340	LYS	2.4
1	C	266	PHE	2.4
1	D	31	ASP	2.4
1	D	311	GLU	2.4
1	F	344	ILE	2.4
1	D	349	ASN	2.4
1	B	500	PHE	2.4
1	E	372	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	495	GLU	2.4
1	C	240	PRO	2.4
1	F	369	PRO	2.4
1	C	349	ASN	2.4
1	E	4	GLU	2.4
1	A	41	LYS	2.3
1	D	374	ASN	2.3
1	B	497	GLY	2.3
1	A	248	ALA	2.3
1	B	42	ARG	2.3
1	F	218	GLY	2.3
1	A	369	PRO	2.3
1	B	69	ASP	2.3
1	C	322	LEU	2.3
1	D	110	LEU	2.3
1	D	371	LEU	2.3
1	E	423	LYS	2.3
1	A	425	GLY	2.3
1	E	256	GLY	2.3
1	F	255	VAL	2.3
1	E	375	ALA	2.3
1	C	372	TYR	2.3
1	E	471	TYR	2.3
1	E	424	HIS	2.3
1	E	313	SER	2.3
1	F	434	ALA	2.3
1	C	294	PHE	2.2
1	C	371	LEU	2.2
1	F	8	ASN	2.2
1	E	501	THR	2.2
1	C	409	LEU	2.2
1	D	370	ASP	2.2
1	F	374	ASN	2.2
1	F	238	MET	2.2
1	F	337	PRO	2.2
1	D	249	VAL	2.2
1	A	355	GLU	2.2
1	C	39	GLU	2.2
1	C	325	ALA	2.2
1	F	349	ASN	2.2
1	C	42	ARG	2.2
1	B	369	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	422	GLY	2.2
1	F	500	PHE	2.2
1	A	308	LYS	2.2
1	C	296	LEU	2.2
1	E	32	LEU	2.2
1	C	36	GLU	2.2
1	A	347	GLY	2.2
1	B	33	LYS	2.1
1	B	349	ASN	2.1
1	E	374	ASN	2.1
1	D	255	VAL	2.1
1	A	311	GLU	2.1
1	D	344	ILE	2.1
1	F	223	ILE	2.1
1	D	6	ASP	2.1
1	D	421	PHE	2.1
1	E	332	THR	2.1
1	F	215	THR	2.1
1	A	367	VAL	2.1
1	B	501	THR	2.1
1	C	307	ALA	2.1
1	C	6	ASP	2.1
1	C	250	GLN	2.1
1	E	500	PHE	2.1
1	F	472	ASN	2.1
1	D	322	LEU	2.1
1	E	366	MET	2.1
1	E	348	ALA	2.1
1	D	294	PHE	2.1
1	A	422	GLY	2.1
1	B	7	PRO	2.1
1	D	237	GLY	2.1
1	F	267	GLY	2.1
1	C	321	ILE	2.1
1	C	370	ASP	2.1
1	B	30	GLU	2.1
1	A	219	VAL	2.1
1	F	256	GLY	2.1
1	F	305	PRO	2.1
1	C	343	ILE	2.1
1	A	374	ASN	2.1
1	D	41	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	234	SER	2.1
1	B	6	ASP	2.0
1	B	281	TRP	2.0
1	E	333	LYS	2.0
1	E	42	ARG	2.0
1	E	277	ASP	2.0
1	A	359	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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	NDP	F	602	48/48	0.92	0.16	51,68,78,204	0
2	GLU	D	601	10/10	0.95	0.19	48,54,60,62	0
2	GLU	E	601	10/10	0.95	0.14	50,56,64,67	0
2	GLU	F	601	10/10	0.95	0.18	50,57,65,66	0
2	GLU	C	601	10/10	0.95	0.20	43,50,63,65	0
3	NDP	D	602	48/48	0.96	0.13	38,55,61,67	0
3	NDP	E	602	48/48	0.96	0.10	52,63,74,81	0
3	NDP	C	602	48/48	0.96	0.13	44,54,62,67	0
2	GLU	A	601	10/10	0.97	0.16	48,52,60,67	0
2	GLU	B	601	10/10	0.97	0.17	42,50,56,57	0
3	NDP	A	602	48/48	0.97	0.13	39,51,60,63	0
3	NDP	B	602	48/48	0.97	0.13	38,50,59,64	0
4	GTP	A	603	32/32	0.97	0.12	41,53,60,65	0
4	GTP	C	603	32/32	0.97	0.12	48,56,65,69	0
4	GTP	E	603	32/32	0.97	0.15	55,62,71,76	0
4	GTP	D	603	32/32	0.98	0.10	46,54,63,66	0

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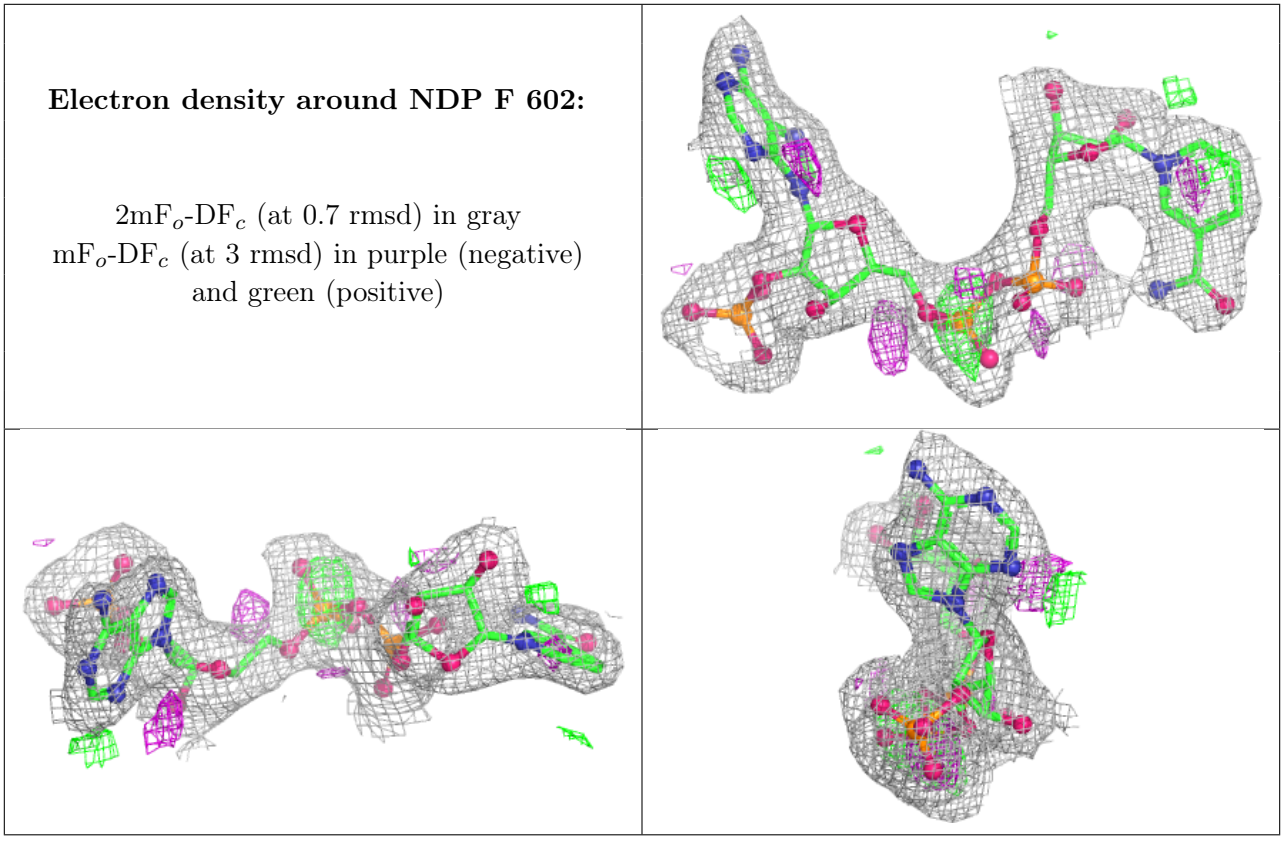
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GTP	B	603	32/32	0.98	0.11	42,49,59,62	0
4	GTP	F	603	32/32	0.98	0.12	53,60,67,73	0

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

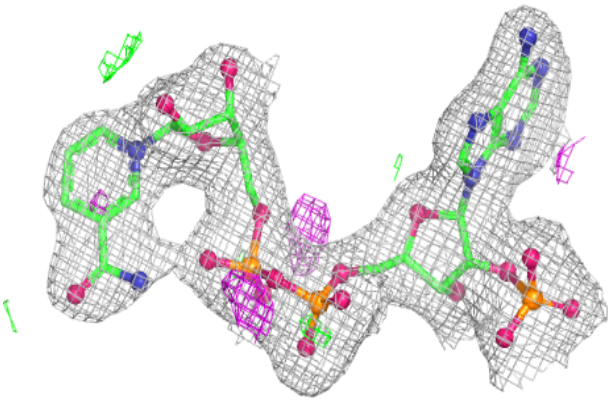
Electron density around NDP F 602:

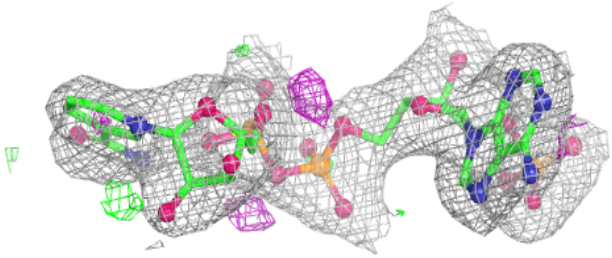
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

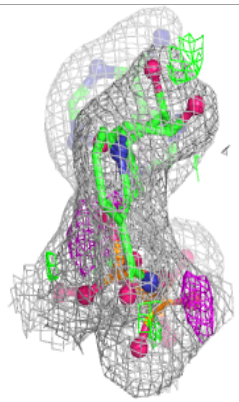


Electron density around NDP D 602:

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

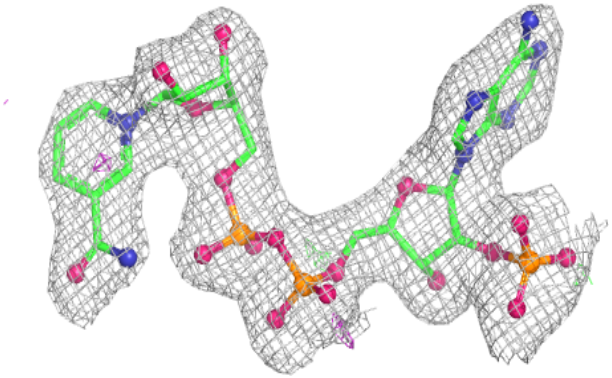


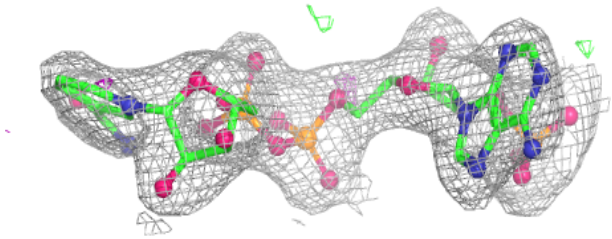


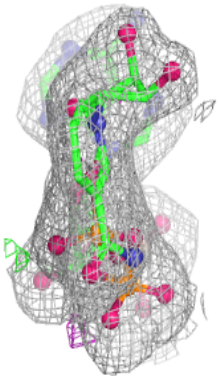


Electron density around NDP E 602:

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

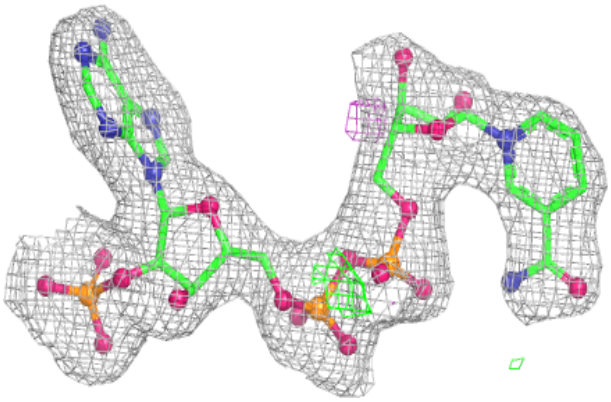


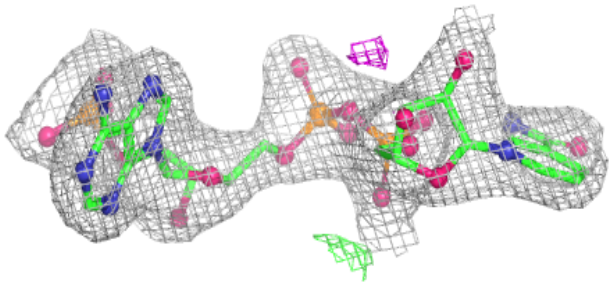


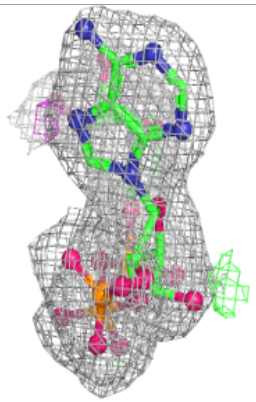


Electron density around NDP C 602:

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

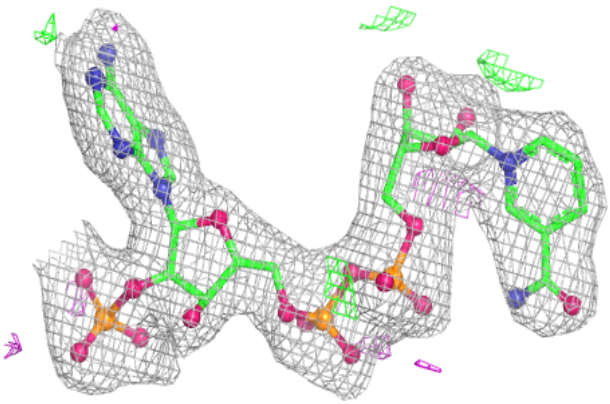


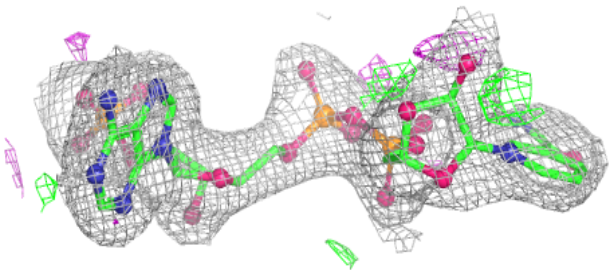


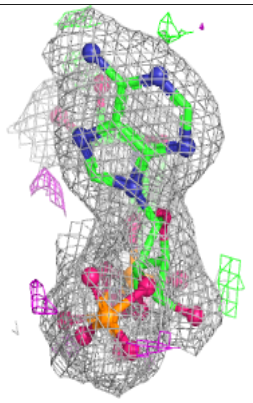


Electron density around NDP A 602:

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

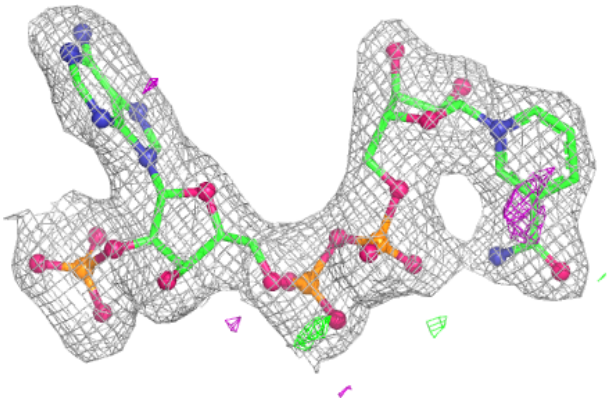


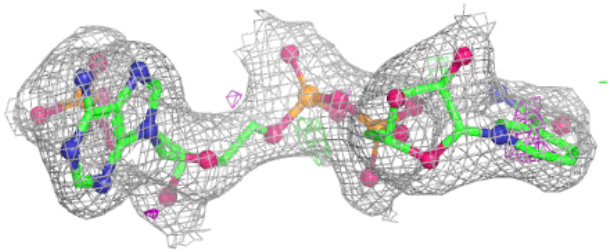


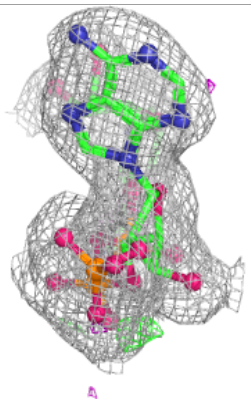


Electron density around NDP B 602:

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

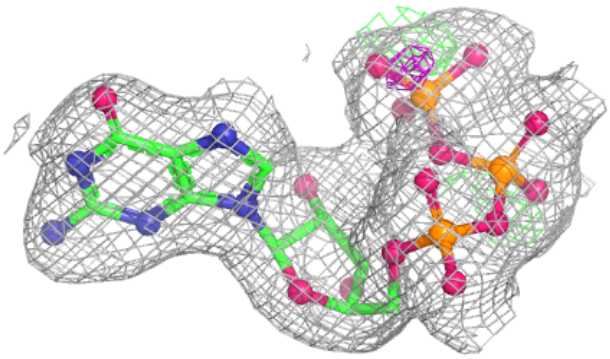


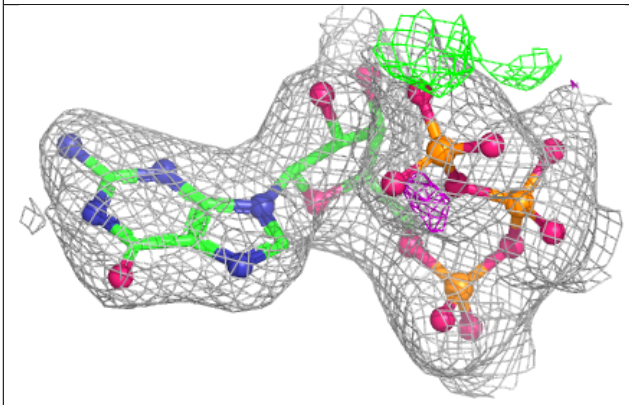


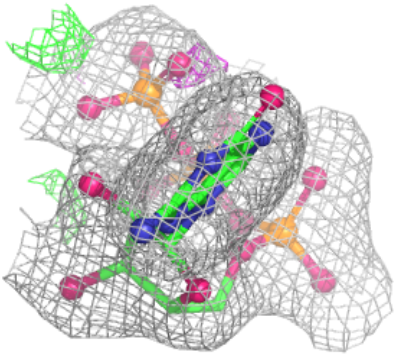


Electron density around GTP A 603:

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

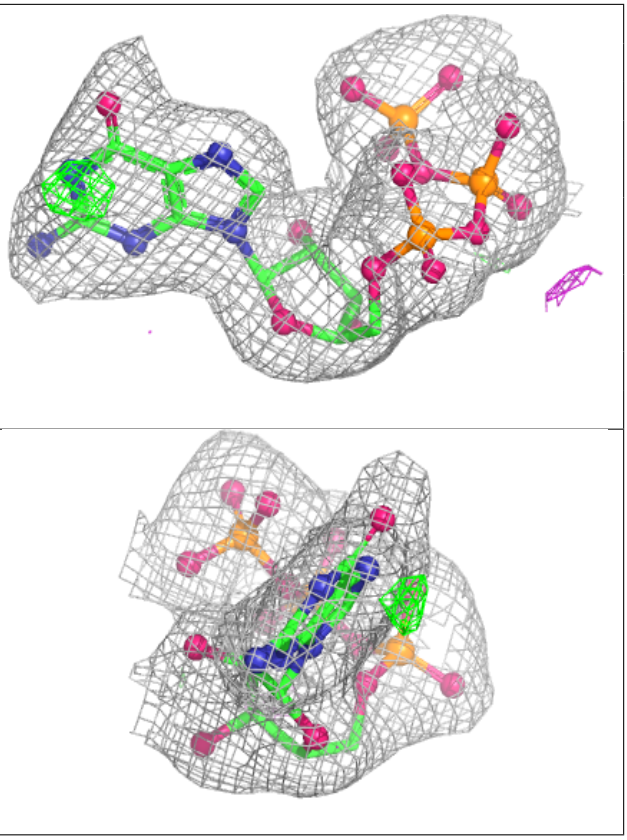






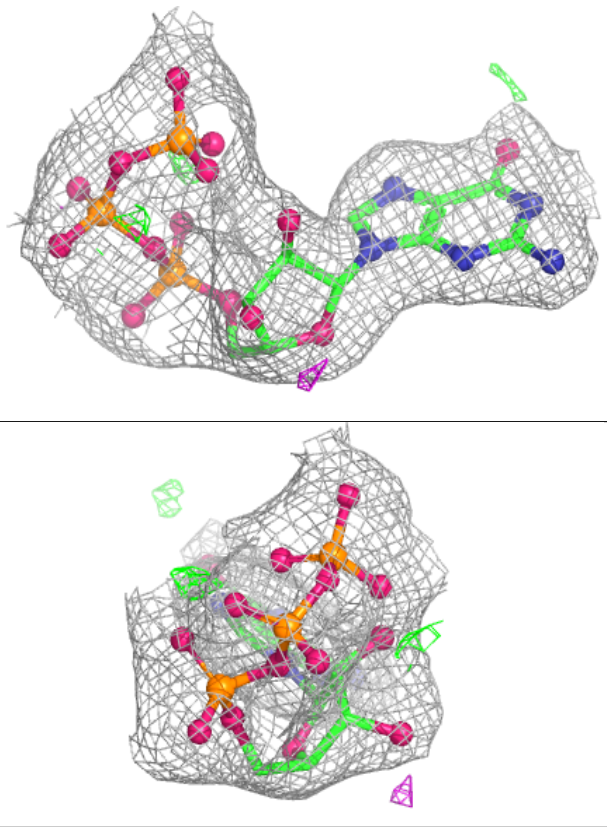
Electron density around GTP C 603:

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



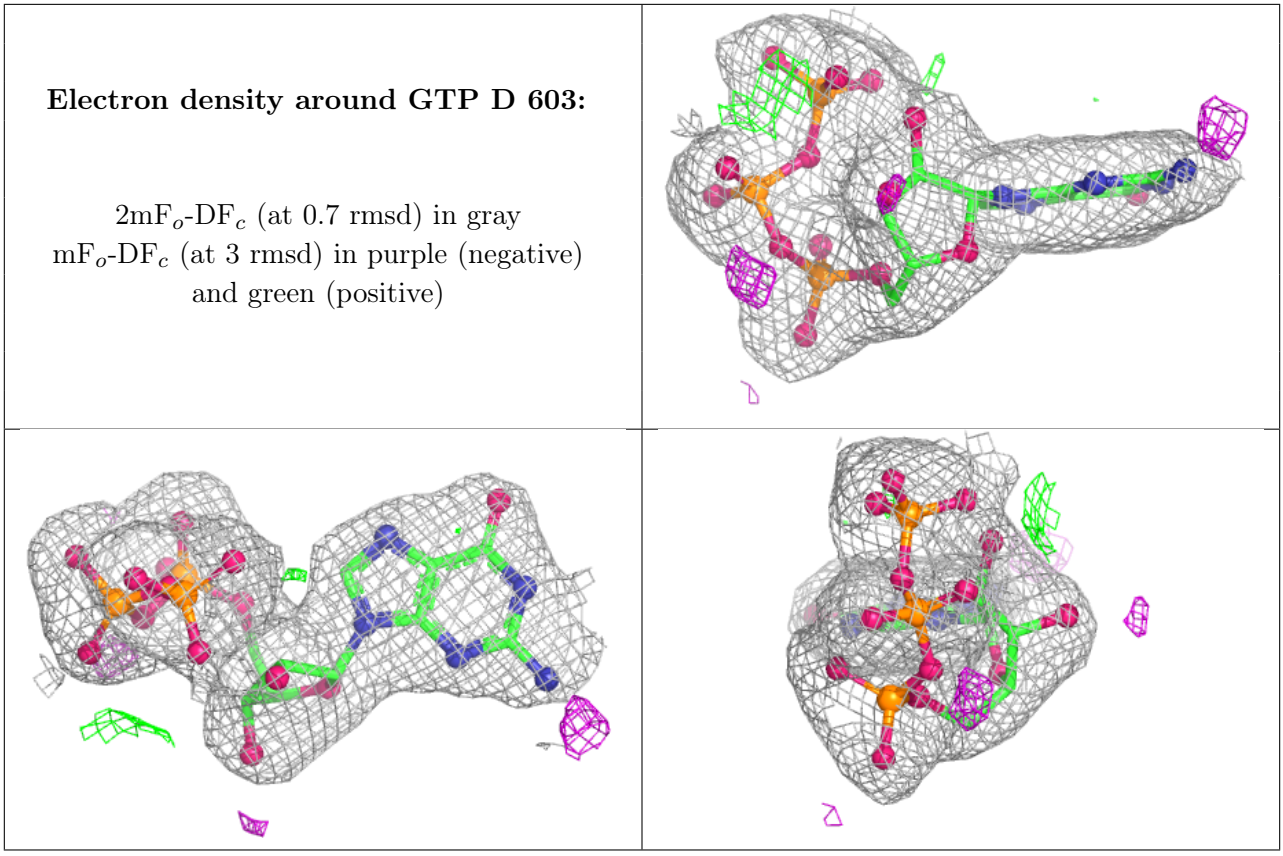
Electron density around GTP E 603:

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



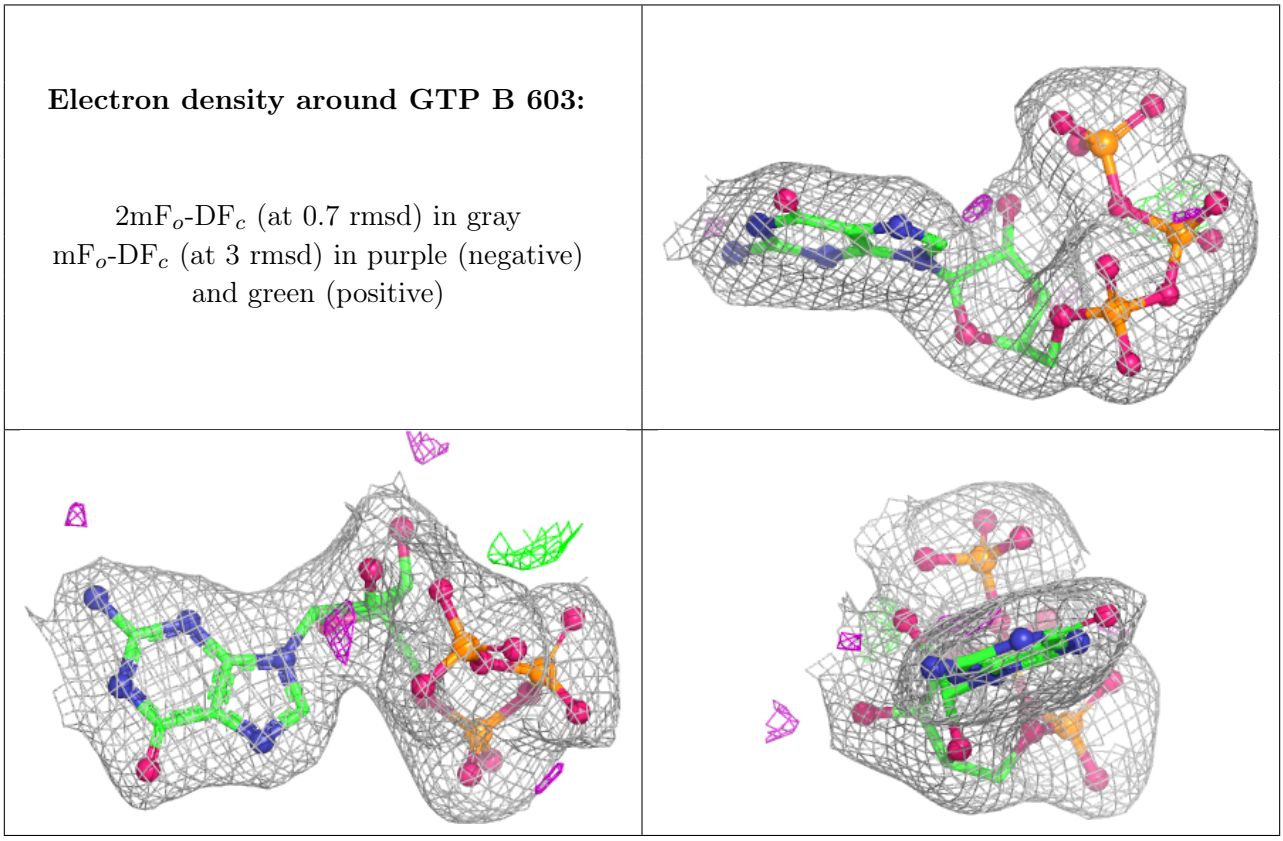
Electron density around GTP D 603:

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



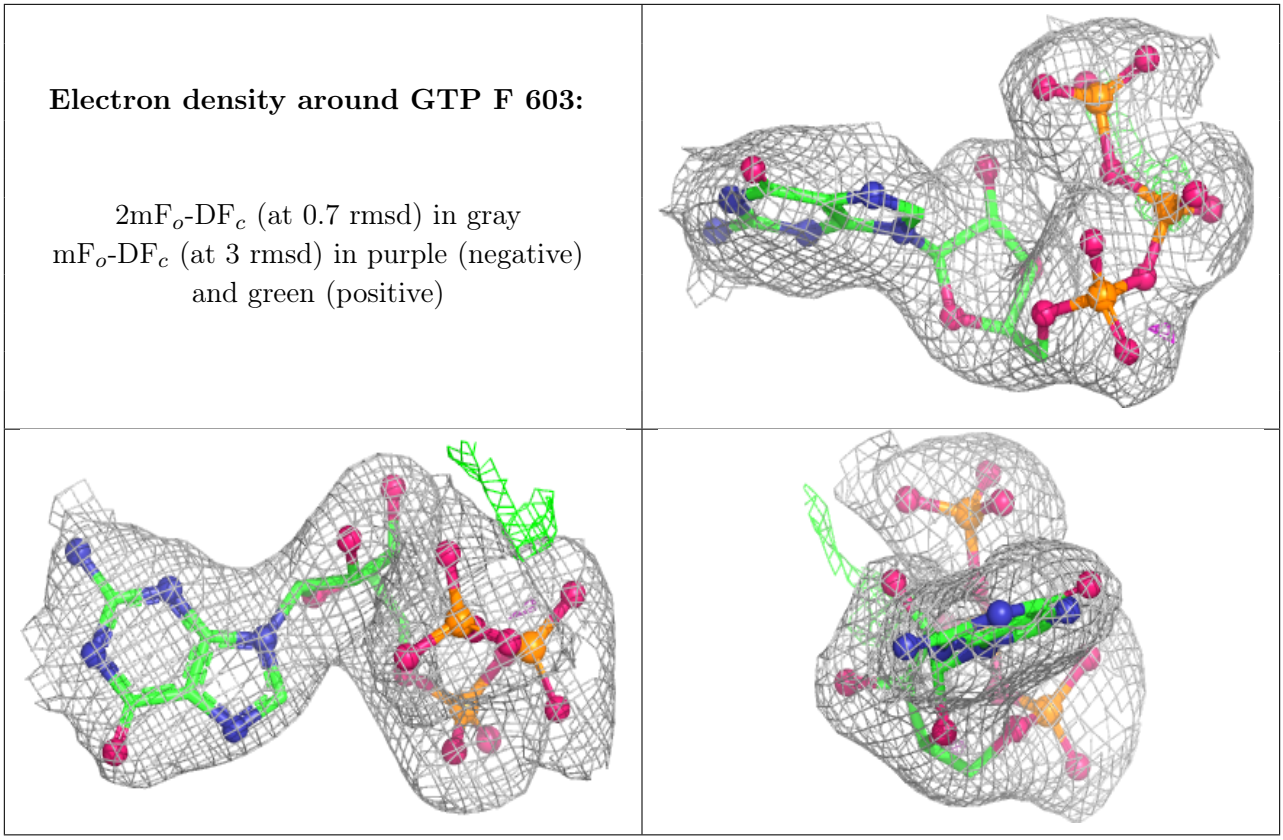
Electron density around GTP B 603:

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



Electron density around GTP F 603:

$2mF_o$-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.