



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:41 PM UTC

PDB ID : 6DHQ / pdb_00006dhq
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

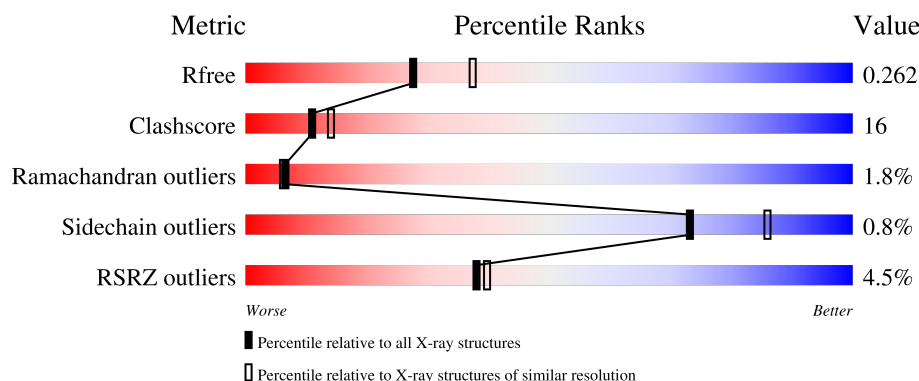
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	501	3% 71% 25% ..
1	B	501	7% 70% 27% ..
1	C	501	4% 70% 26% .
1	D	501	4% 72% 25% .
1	E	501	3% 71% 25% ..

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Mol	Chain	Length	Quality of chain
1	F	501	7% 67% 29% ..

2 Entry composition [i](#)

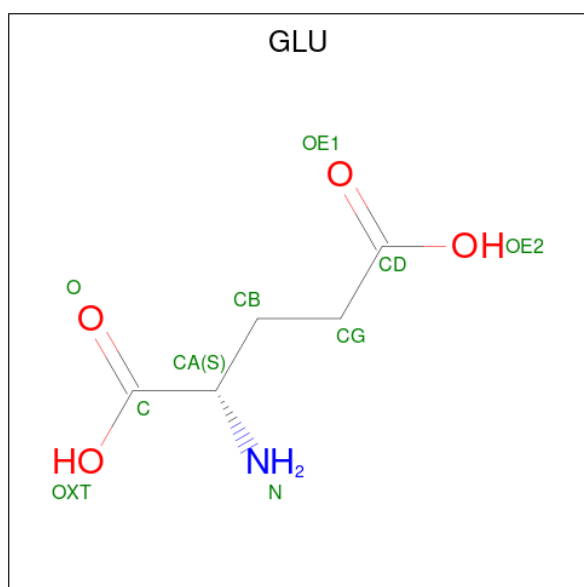
There are 5 unique types of molecules in this entry. The entry contains 24419 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

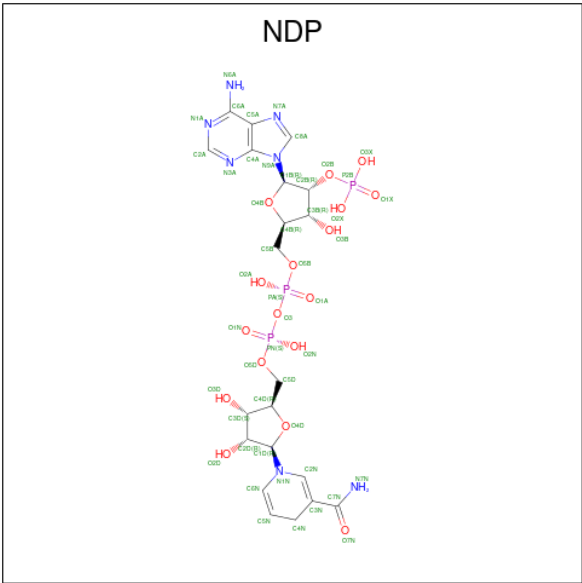
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	B	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	C	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	D	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	E	501	Total	C	N	O	S	0	0	0
			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 (CCD ID: GLU) (formula: C₅H₉NO₄).



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 (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



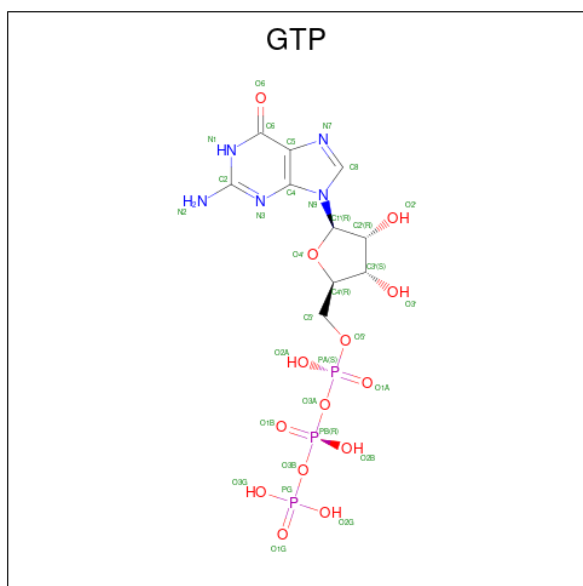
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0

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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 (CCD ID: 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 62 O 62	0	0
5	B	83	Total 83 O 83	0	0

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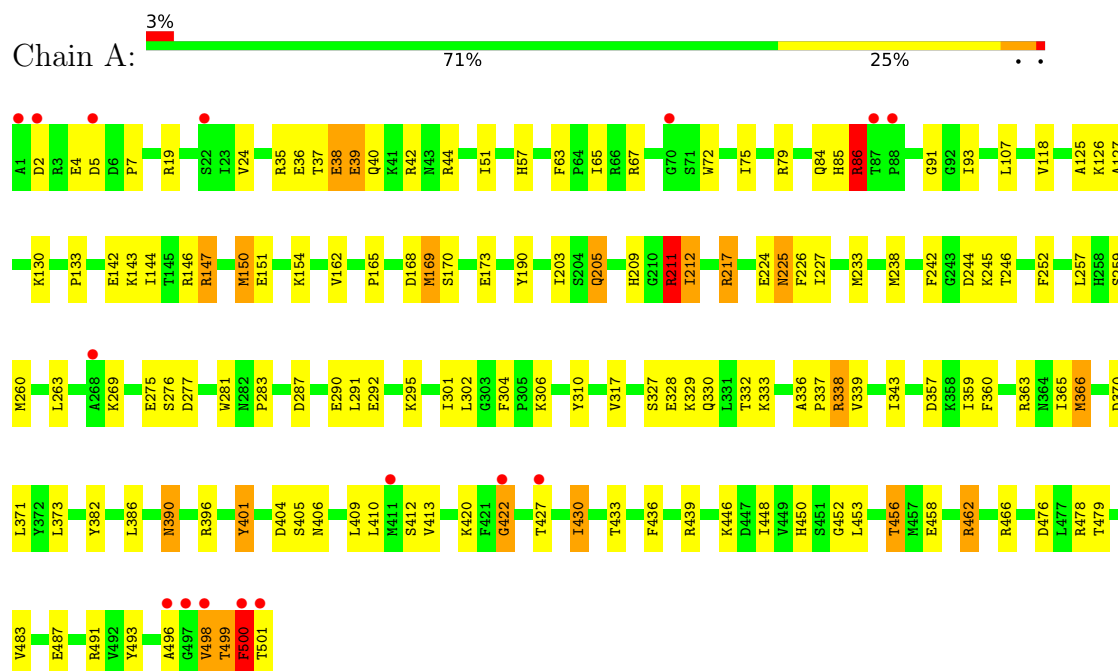
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	50	Total 50	O 50	0	0
5	D	66	Total 66	O 66	0	0
5	E	58	Total 58	O 58	0	0
5	F	64	Total 64	O 64	0	0

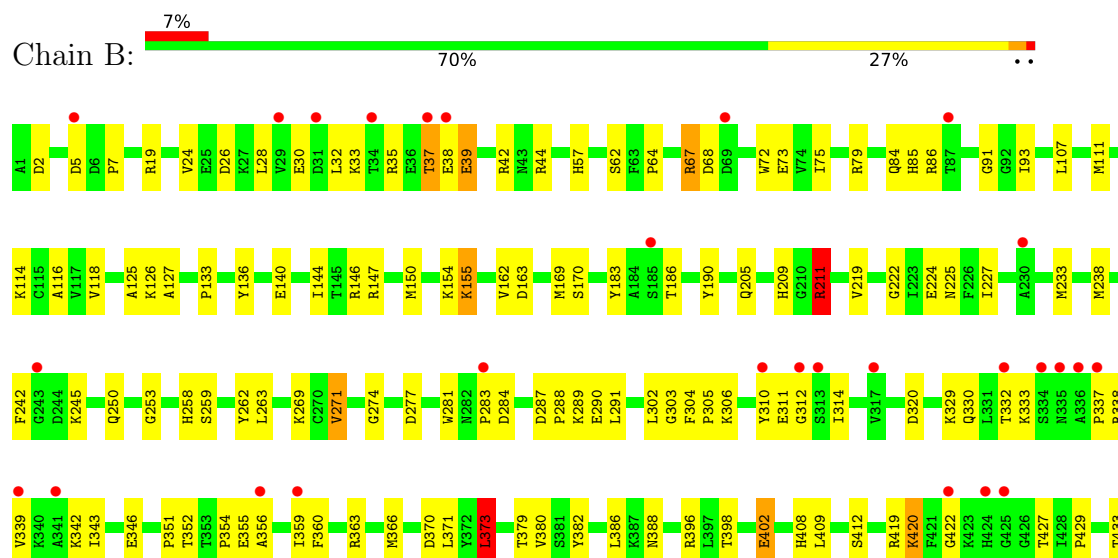
3 Residue-property plots

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

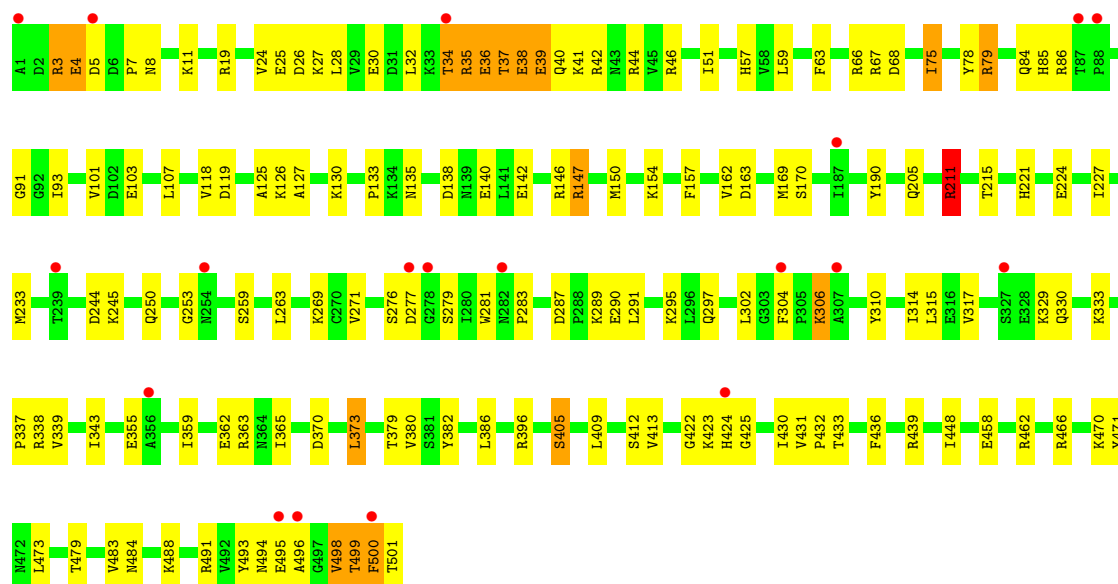


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

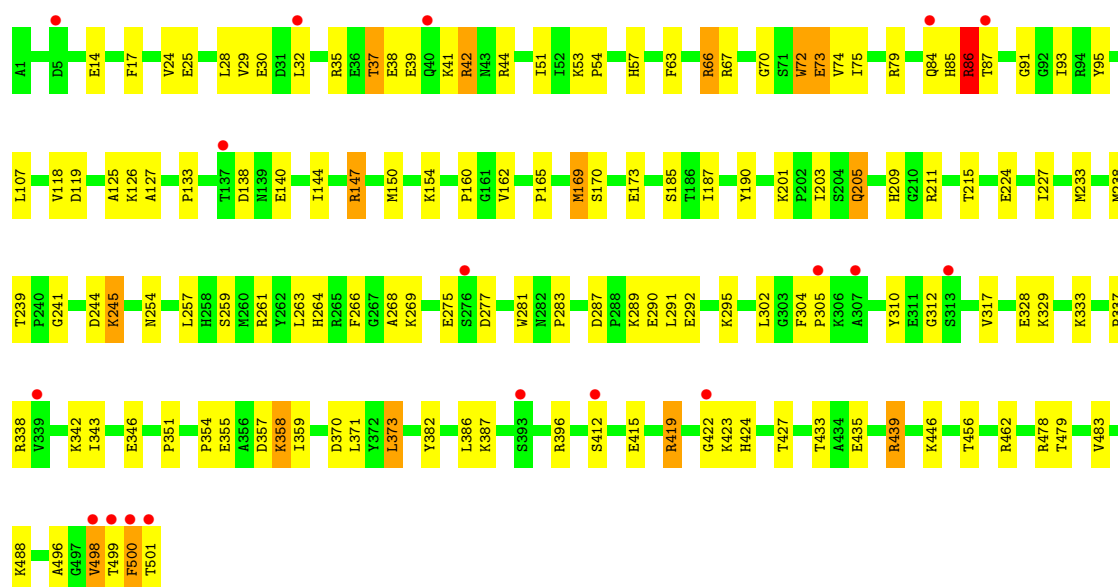
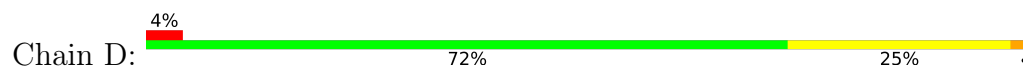




- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

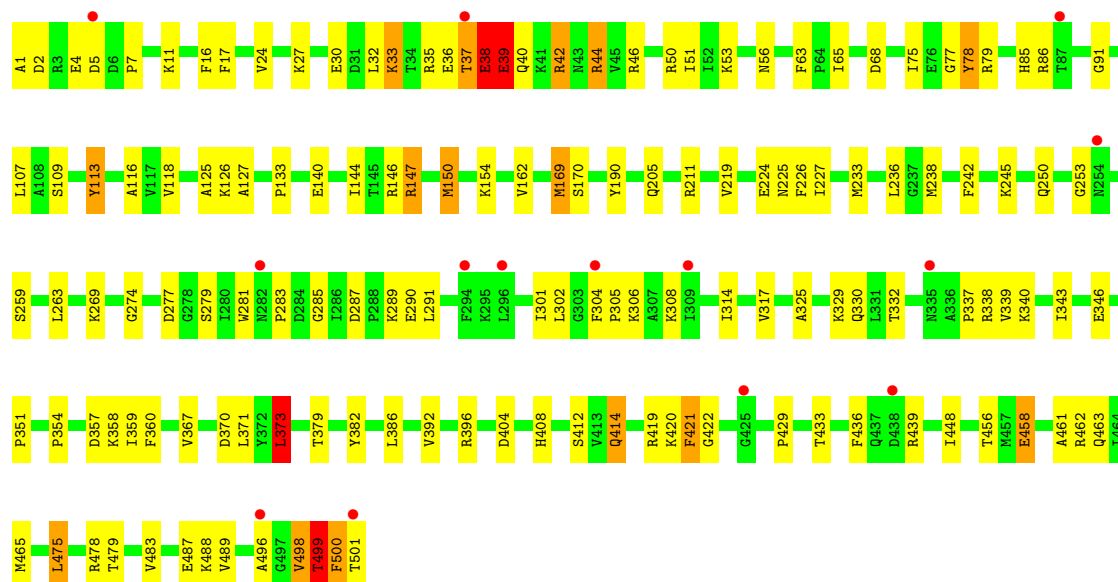


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

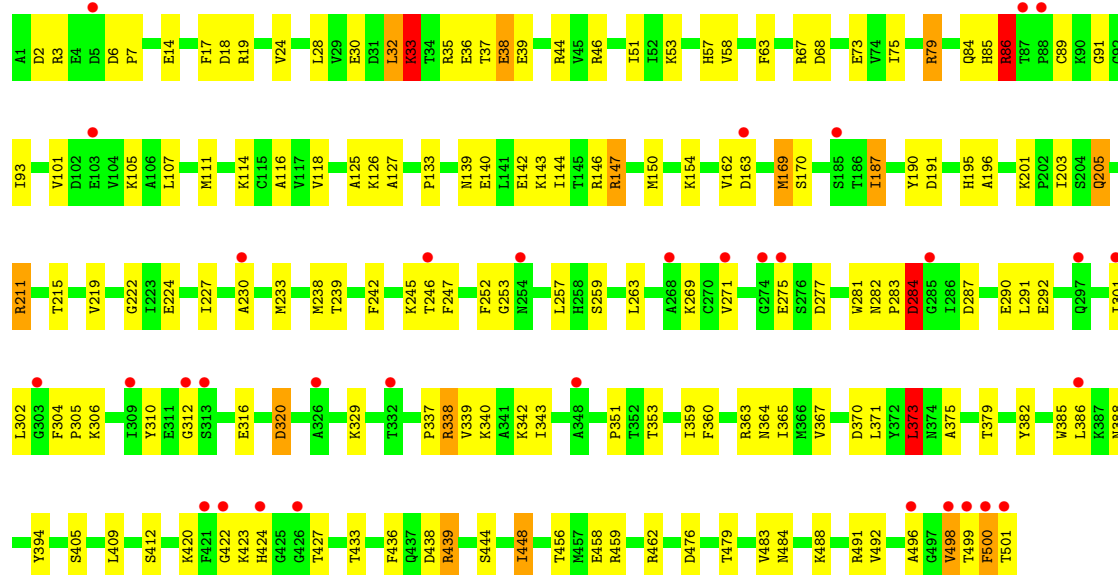


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial





• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	2000 reflections (1.11%)	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)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	17/3999 (0.4%)	1.04	37/5396 (0.7%)
1	B	0.77	9/3999 (0.2%)	0.94	22/5396 (0.4%)
1	C	0.82	15/3999 (0.4%)	1.00	26/5396 (0.5%)
1	D	0.74	13/3999 (0.3%)	0.98	29/5396 (0.5%)
1	E	0.96	27/3999 (0.7%)	1.08	39/5396 (0.7%)
1	F	0.81	18/3999 (0.5%)	1.03	30/5396 (0.6%)
All	All	0.83	99/23994 (0.4%)	1.01	183/32376 (0.6%)

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

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

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	ARG	CB-CG	-13.44	1.12	1.52
1	A	401	TYR	CG-CD1	-12.54	1.13	1.39
1	A	390	ASN	CG-OD1	-12.16	1.00	1.23
1	F	448	ILE	CB-CG2	-12.12	1.12	1.52
1	A	401	TYR	CG-CD2	-12.06	1.14	1.39
1	A	401	TYR	CE2-CZ	-11.45	1.10	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	TYR	CE1-CZ	-11.31	1.11	1.38
1	B	67	ARG	CZ-NH1	-11.27	1.17	1.32
1	C	135	ASN	CG-ND2	-11.20	1.09	1.33
1	D	396	ARG	CZ-NH1	-10.80	1.17	1.32
1	A	390	ASN	CG-ND2	-10.77	1.10	1.33
1	C	373	LEU	CG-CD1	-10.33	1.18	1.52
1	E	414	GLN	CD-NE2	-10.20	1.11	1.33
1	E	78	TYR	CG-CD1	-10.10	1.18	1.39
1	E	78	TYR	CE1-CZ	-10.00	1.14	1.38
1	E	42	ARG	CZ-NH1	-9.82	1.19	1.32
1	E	113	TYR	CG-CD1	-9.65	1.19	1.39
1	E	78	TYR	CG-CD2	-9.64	1.19	1.39
1	E	113	TYR	CE2-CZ	-9.59	1.15	1.38
1	B	408	HIS	CG-ND1	-9.49	1.27	1.38
1	F	439	ARG	CZ-NH1	-9.48	1.19	1.32
1	C	135	ASN	CG-OD1	-9.44	1.05	1.23
1	E	78	TYR	CE2-CZ	-9.28	1.16	1.38
1	E	225	ASN	CG-OD1	-9.27	1.05	1.23
1	D	373	LEU	CG-CD1	-9.25	1.22	1.52
1	E	16	PHE	CE1-CZ	-9.04	1.11	1.38
1	E	113	TYR	CG-CD2	-9.04	1.20	1.39
1	F	439	ARG	CB-CG	-9.04	1.25	1.52
1	B	408	HIS	CE1-NE2	-9.00	1.23	1.32
1	E	16	PHE	CE2-CZ	-9.00	1.11	1.38
1	F	205	GLN	CD-NE2	8.93	1.51	1.33
1	E	56	ASN	CG-ND2	-8.79	1.14	1.33
1	C	75	ILE	CG1-CD1	-8.77	1.17	1.51
1	E	16	PHE	CG-CD1	-8.75	1.20	1.38
1	E	16	PHE	CG-CD2	-8.65	1.20	1.38
1	E	113	TYR	CE1-CZ	-8.64	1.17	1.38
1	E	225	ASN	CG-ND2	-8.44	1.15	1.33
1	E	458	GLU	CD-OE2	-8.28	1.09	1.25
1	E	414	GLN	CD-OE1	-8.10	1.08	1.23
1	E	289	LYS	CG-CD	-7.67	1.29	1.52
1	F	147	ARG	CB-CG	-7.44	1.30	1.52
1	A	225	ASN	CG-ND2	-7.24	1.18	1.33
1	F	484	ASN	CG-ND2	-7.22	1.18	1.33
1	F	147	ARG	CG-CD	-7.11	1.31	1.52
1	B	338	ARG	CB-CG	-6.90	1.31	1.52
1	E	56	ASN	CG-OD1	-6.84	1.10	1.23
1	D	44	ARG	CB-CG	-6.78	1.32	1.52
1	C	297	GLN	CB-CG	-6.75	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	484	ASN	CG-ND2	-6.69	1.19	1.33
1	F	44	ARG	CB-CG	-6.56	1.32	1.52
1	C	44	ARG	CZ-NH1	-6.56	1.23	1.32
1	B	408	HIS	CG-CD2	-6.50	1.28	1.35
1	B	44	ARG	CB-CG	-6.49	1.32	1.52
1	A	169	MET	SD-CE	-6.48	1.63	1.79
1	A	328	GLU	CD-OE2	-6.47	1.13	1.25
1	C	439	ARG	CB-CG	-6.35	1.33	1.52
1	A	328	GLU	CD-OE1	-6.34	1.13	1.25
1	D	328	GLU	CD-OE1	-6.31	1.13	1.25
1	B	289	LYS	CB-CG	-6.27	1.33	1.52
1	A	44	ARG	CB-CG	-6.25	1.33	1.52
1	F	338	ARG	CB-CG	-6.25	1.33	1.52
1	F	484	ASN	CG-OD1	-6.23	1.11	1.23
1	A	373	LEU	CG-CD1	-6.21	1.32	1.52
1	E	42	ARG	CZ-NH2	-6.21	1.25	1.33
1	C	147	ARG	CB-CG	-6.13	1.34	1.52
1	F	195	HIS	CE1-NE2	-6.13	1.26	1.32
1	E	338	ARG	CB-CG	-6.01	1.34	1.52
1	C	338	ARG	CB-CG	-5.99	1.34	1.52
1	D	338	ARG	CB-CG	-5.90	1.34	1.52
1	E	147	ARG	CB-CG	-5.86	1.34	1.52
1	E	373	LEU	CG-CD1	-5.85	1.33	1.52
1	D	138	ASP	CG-OD2	-5.84	1.14	1.25
1	D	147	ARG	CB-CG	-5.83	1.34	1.52
1	F	373	LEU	CG-CD1	-5.82	1.33	1.52
1	F	439	ARG	CD-NE	-5.76	1.38	1.46
1	B	373	LEU	CG-CD1	-5.72	1.33	1.52
1	D	387	LYS	CE-NZ	5.71	1.66	1.49
1	A	366	MET	SD-CE	-5.60	1.65	1.79
1	B	163	ASP	CG-OD2	-5.56	1.14	1.25
1	A	147	ARG	CB-CG	-5.56	1.35	1.52
1	C	44	ARG	CB-CG	-5.56	1.35	1.52
1	F	44	ARG	CZ-NH1	-5.55	1.25	1.32
1	F	195	HIS	CG-ND1	-5.50	1.32	1.38
1	D	138	ASP	CG-OD1	-5.50	1.14	1.25
1	C	484	ASN	CG-OD1	-5.50	1.13	1.23
1	D	338	ARG	CG-CD	-5.43	1.36	1.52
1	F	439	ARG	CG-CD	-5.37	1.36	1.52
1	C	289	LYS	CG-CD	-5.34	1.36	1.52
1	A	67	ARG	CZ-NH1	-5.30	1.25	1.32
1	C	138	ASP	CG-OD1	-5.29	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	ASN	CG-OD1	-5.29	1.13	1.23
1	E	458	GLU	CD-OE1	-5.27	1.15	1.25
1	D	387	LYS	CD-CE	5.24	1.68	1.52
1	D	328	GLU	CD-OE2	-5.23	1.15	1.25
1	A	439	ARG	CZ-NH1	-5.16	1.25	1.32
1	F	169	MET	SD-CE	-5.15	1.66	1.79
1	C	147	ARG	CG-CD	-5.08	1.37	1.52
1	F	205	GLN	CG-CD	5.08	1.64	1.52
1	D	245	LYS	CE-NZ	-5.04	1.34	1.49

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	44	ARG	NE-CZ-NH2	18.14	135.53	119.20
1	E	42	ARG	NE-CZ-NH2	15.63	133.26	119.20
1	F	439	ARG	NE-CZ-NH2	14.10	131.89	119.20
1	B	67	ARG	NE-CZ-NH2	14.03	131.83	119.20
1	F	86	ARG	CB-CG-CD	13.60	142.57	111.30
1	D	396	ARG	NE-CZ-NH1	-12.77	108.73	121.50
1	A	217	ARG	CB-CG-CD	12.72	140.55	111.30
1	A	67	ARG	NE-CZ-NH2	12.21	130.19	119.20
1	F	448	ILE	CA-CB-CG1	12.12	131.00	110.40
1	E	44	ARG	CD-NE-CZ	-12.05	107.53	124.40
1	A	217	ARG	CG-CD-NE	11.92	138.23	112.00
1	C	338	ARG	NE-CZ-NH2	11.74	129.76	119.20
1	D	245	LYS	CD-CE-NZ	11.71	149.36	111.90
1	D	261	ARG	NE-CZ-NH2	11.69	129.72	119.20
1	F	169	MET	CG-SD-CE	11.55	126.32	100.90
1	F	86	ARG	CA-CB-CG	-11.46	91.19	114.10
1	E	11	LYS	CB-CG-CD	11.34	137.38	111.30
1	A	42	ARG	CA-CB-CG	11.28	136.66	114.10
1	D	396	ARG	NE-CZ-NH2	11.24	129.32	119.20
1	E	44	ARG	CG-CD-NE	11.23	136.71	112.00
1	A	169	MET	CG-SD-CE	11.08	125.28	100.90
1	E	16	PHE	CE1-CZ-CE2	-10.64	100.85	120.00
1	C	103	GLU	CA-CB-CG	10.51	135.12	114.10
1	C	79	ARG	NE-CZ-NH2	10.26	128.43	119.20
1	D	261	ARG	NE-CZ-NH1	-10.21	111.30	121.50
1	F	448	ILE	CB-CG1-CD1	-10.15	92.49	113.80
1	E	458	GLU	CB-CG-CD	9.89	129.42	112.60
1	F	79	ARG	NE-CZ-NH2	9.73	127.96	119.20
1	F	187	ILE	CB-CG1-CD1	9.52	133.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	16	PHE	CD1-CG-CD2	-9.46	104.41	118.60
1	F	169	MET	CB-CG-SD	-9.46	84.32	112.70
1	D	211	ARG	NE-CZ-NH2	9.43	127.69	119.20
1	F	86	ARG	CG-CD-NE	9.32	132.51	112.00
1	B	420	LYS	CG-CD-CE	9.26	132.59	111.30
1	C	373	LEU	CB-CG-CD2	9.26	138.47	110.70
1	D	261	ARG	CD-NE-CZ	9.16	137.22	124.40
1	B	146	ARG	NE-CZ-NH2	9.05	127.35	119.20
1	E	11	LYS	CA-CB-CG	-8.97	96.15	114.10
1	C	103	GLU	CB-CG-CD	8.95	127.81	112.60
1	F	439	ARG	NE-CZ-NH1	-8.93	112.57	121.50
1	A	42	ARG	CB-CA-C	-8.92	95.51	110.68
1	B	146	ARG	NE-CZ-NH1	-8.84	112.66	121.50
1	A	401	TYR	CE1-CZ-CE2	-8.78	102.74	120.30
1	A	67	ARG	NE-CZ-NH1	-8.77	112.73	121.50
1	C	373	LEU	CD1-CG-CD2	-8.77	91.51	110.80
1	C	79	ARG	NE-CZ-NH1	-8.74	112.76	121.50
1	E	44	ARG	NH1-CZ-NH2	-8.67	108.03	119.30
1	C	338	ARG	NE-CZ-NH1	-8.63	112.87	121.50
1	F	44	ARG	NE-CZ-NH2	8.60	126.94	119.20
1	A	42	ARG	CG-CD-NE	8.52	130.75	112.00
1	D	338	ARG	NE-CZ-NH2	8.50	126.85	119.20
1	E	289	LYS	CA-CB-CG	-8.21	97.68	114.10
1	A	211	ARG	NE-CZ-NH2	8.15	126.54	119.20
1	F	205	GLN	CA-CB-CG	-8.09	97.93	114.10
1	E	146	ARG	NE-CZ-NH1	-8.08	113.42	121.50
1	C	44	ARG	NE-CZ-NH2	8.04	126.44	119.20
1	F	79	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	A	217	ARG	CA-CB-CG	7.97	130.03	114.10
1	A	211	ARG	NE-CZ-NH1	-7.96	113.53	121.50
1	B	420	LYS	CD-CE-NZ	7.86	137.06	111.90
1	D	373	LEU	CB-CG-CD2	7.75	133.96	110.70
1	F	79	ARG	CB-CG-CD	7.74	129.10	111.30
1	D	373	LEU	CD1-CG-CD2	-7.70	93.85	110.80
1	B	155	LYS	CA-CB-CG	-7.69	98.71	114.10
1	C	297	GLN	CB-CG-CD	7.69	125.67	112.60
1	B	306	LYS	CB-CG-CD	7.65	128.90	111.30
1	D	245	LYS	CG-CD-CE	-7.65	93.71	111.30
1	F	448	ILE	CG1-CB-CG2	-7.64	87.78	110.70
1	E	146	ARG	NE-CZ-NH2	7.59	126.04	119.20
1	E	42	ARG	NH1-CZ-NH2	-7.59	109.43	119.30
1	B	408	HIS	ND1-CG-CD2	-7.55	98.55	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	16	PHE	CZ-CE2-CD2	7.43	133.38	120.00
1	E	16	PHE	CD1-CE1-CZ	7.43	133.38	120.00
1	D	211	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	E	78	TYR	CE1-CZ-CE2	-7.33	105.64	120.30
1	A	401	TYR	CD1-CG-CD2	-7.29	107.16	118.10
1	C	79	ARG	CD-NE-CZ	7.26	134.56	124.40
1	D	44	ARG	NE-CZ-NH2	7.24	125.72	119.20
1	D	211	ARG	CD-NE-CZ	7.14	134.40	124.40
1	C	439	ARG	NE-CZ-NH2	6.99	125.50	119.20
1	F	86	ARG	CD-NE-CZ	-6.82	114.85	124.40
1	B	169	MET	CG-SD-CE	6.81	115.88	100.90
1	B	44	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	E	78	TYR	CD1-CG-CD2	-6.79	107.91	118.10
1	C	130	LYS	CD-CE-NZ	6.79	133.63	111.90
1	E	169	MET	CG-SD-CE	6.74	115.74	100.90
1	B	211	ARG	CB-CG-CD	6.72	126.76	111.30
1	F	147	ARG	CA-CB-CG	-6.72	100.67	114.10
1	A	217	ARG	CD-NE-CZ	6.71	133.80	124.40
1	C	338	ARG	CB-CA-C	-6.67	100.28	111.02
1	D	387	LYS	CD-CE-NZ	-6.66	90.60	111.90
1	B	67	ARG	NH1-CZ-NH2	-6.61	110.71	119.30
1	E	44	ARG	CB-CG-CD	6.60	126.48	111.30
1	E	113	TYR	CD1-CG-CD2	-6.58	108.23	118.10
1	E	113	TYR	CE1-CZ-CE2	-6.57	107.17	120.30
1	D	86	ARG	CA-CB-CG	-6.51	101.08	114.10
1	A	86	ARG	CB-CG-CD	6.51	126.26	111.30
1	C	67	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	E	44	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	E	211	ARG	CB-CG-CD	6.45	126.13	111.30
1	C	211	ARG	CB-CG-CD	6.32	125.85	111.30
1	E	475	LEU	CB-CG-CD1	6.32	129.66	110.70
1	F	211	ARG	CB-CG-CD	6.28	125.73	111.30
1	D	169	MET	CG-SD-CE	6.27	114.69	100.90
1	C	169	MET	CG-SD-CE	6.26	114.67	100.90
1	A	42	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	B	408	HIS	CG-CD2-NE2	6.21	113.41	107.20
1	A	401	TYR	CD1-CE1-CZ	6.21	130.77	119.60
1	C	44	ARG	CG-CD-NE	6.18	125.59	112.00
1	F	147	ARG	CG-CD-NE	-6.16	98.46	112.00
1	D	439	ARG	NE-CZ-NH2	6.15	124.74	119.20
1	D	329	LYS	CG-CD-CE	6.12	125.38	111.30
1	C	458	GLU	CA-CB-CG	-6.08	101.94	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	295	LYS	CG-CD-CE	6.08	125.27	111.30
1	A	328	GLU	OE1-CD-OE2	-6.07	108.33	122.90
1	B	146	ARG	CD-NE-CZ	6.07	132.90	124.40
1	E	499	THR	CA-C-N	6.06	133.11	121.54
1	E	499	THR	C-N-CA	6.06	133.11	121.54
1	A	212	ILE	CG1-CB-CG2	-5.99	92.73	110.70
1	E	458	GLU	OE1-CD-OE2	-5.96	108.60	122.90
1	F	86	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	401	TYR	CZ-CE2-CD2	5.94	130.29	119.60
1	D	138	ASP	OD1-CG-OD2	-5.90	108.75	122.90
1	A	42	ARG	N-CA-CB	5.85	118.83	110.06
1	D	295	LYS	CA-CB-CG	-5.79	102.51	114.10
1	A	42	ARG	NE-CZ-NH1	-5.74	115.77	121.50
1	D	328	GLU	OE1-CD-OE2	-5.73	109.16	122.90
1	A	169	MET	CB-CG-SD	-5.68	95.67	112.70
1	F	284	ASP	CB-CG-OD2	5.66	131.42	118.40
1	C	306	LYS	CB-CG-CD	5.65	124.29	111.30
1	D	329	LYS	CD-CE-NZ	-5.65	93.83	111.90
1	A	205	GLN	CA-CB-CG	-5.62	102.86	114.10
1	A	42	ARG	CD-NE-CZ	-5.58	116.59	124.40
1	F	79	ARG	CG-CD-NE	5.58	124.26	112.00
1	B	402	GLU	CB-CG-CD	5.56	122.05	112.60
1	E	42	ARG	CA-CB-CG	5.53	125.16	114.10
1	C	458	GLU	CG-CD-OE1	-5.49	105.77	118.40
1	C	75	ILE	N-CA-CB	-5.49	103.50	111.52
1	E	306	LYS	CA-CB-CG	-5.49	103.12	114.10
1	B	352	THR	OG1-CB-CG2	5.46	120.22	109.30
1	A	44	ARG	CG-CD-NE	5.44	123.96	112.00
1	A	430	ILE	CG1-CB-CG2	-5.44	94.39	110.70
1	A	462	ARG	CG-CD-NE	5.43	123.94	112.00
1	B	163	ASP	OD1-CG-OD2	-5.41	109.91	122.90
1	F	306	LYS	CA-CB-CG	-5.41	103.29	114.10
1	A	295	LYS	CD-CE-NZ	5.39	129.15	111.90
1	E	289	LYS	CB-CG-CD	5.36	123.64	111.30
1	F	338	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	F	195	HIS	ND1-CG-CD2	-5.35	100.75	106.10
1	F	353	THR	OG1-CB-CG2	5.35	120.00	109.30
1	C	439	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	E	78	TYR	CZ-CE2-CD2	5.29	129.13	119.60
1	E	42	ARG	CG-CD-NE	5.29	123.63	112.00
1	F	79	ARG	CA-CB-CG	5.29	124.67	114.10
1	D	73	GLU	CA-C-N	5.28	128.95	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	GLU	C-N-CA	5.28	128.95	121.66
1	E	421	PHE	CD1-CG-CD2	-5.28	110.68	118.60
1	E	146	ARG	CD-NE-CZ	5.27	131.77	124.40
1	A	500	PHE	CA-C-N	5.26	131.17	121.70
1	A	500	PHE	C-N-CA	5.26	131.17	121.70
1	D	205	GLN	CB-CG-CD	-5.25	103.68	112.60
1	A	366	MET	CG-SD-CE	5.24	112.43	100.90
1	C	295	LYS	CD-CE-NZ	5.23	128.63	111.90
1	B	402	GLU	CA-CB-CG	5.22	124.55	114.10
1	A	439	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	338	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	44	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	E	32	LEU	CA-C-N	5.17	131.41	121.54
1	E	32	LEU	C-N-CA	5.17	131.41	121.54
1	F	79	ARG	CD-NE-CZ	5.16	131.62	124.40
1	A	390	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	C	138	ASP	OD1-CG-OD2	-5.12	110.62	122.90
1	B	439	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	A	211	ARG	CG-CD-NE	5.08	123.16	112.00
1	D	73	GLU	CB-CG-CD	5.08	121.23	112.60
1	E	44	ARG	CA-CB-CG	-5.08	103.95	114.10
1	F	444	SER	CB-CA-C	-5.07	100.62	111.78
1	B	408	HIS	CG-ND1-CE1	5.06	117.91	109.30
1	B	499	THR	CA-C-N	5.03	131.15	121.54
1	B	499	THR	C-N-CA	5.03	131.15	121.54
1	D	42	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	C	373	LEU	CB-CG-CD1	-5.00	95.70	110.70
1	E	338	ARG	NE-CZ-NH2	5.00	123.70	119.20

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

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Mol	Chain	Res	Type	Group
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
1	F	439	ARG	Sidechain
1	F	86	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3916	0	3880	165	0
1	B	3916	0	3880	128	0
1	C	3916	0	3880	142	0
1	D	3916	0	3880	134	0
1	E	3916	0	3880	142	0
1	F	3916	0	3880	139	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	48	0	26	5	0
4	A	32	0	12	0	0
4	B	32	0	12	2	0
4	C	32	0	12	0	0
4	D	32	0	12	1	0
4	E	32	0	12	1	0
4	F	32	0	12	1	0
5	A	62	0	0	10	0
5	B	83	0	0	9	1
5	C	50	0	0	8	0
5	D	66	0	0	17	0
5	E	58	0	0	6	1
5	F	64	0	0	20	0
All	All	24419	0	23538	785	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 (785) 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	1.38
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:E:458:GLU:CD	1:E:462:ARG:NH2	2.12	1.08
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: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:A:130:LYS:NZ	5:A:701:HOH:O	1.86	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:65:ILE:HG22	1:A:143:LYS:HZ2	1.32	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:337:PRO:HD3	1:C:359:ILE:HD13	1.66	0.78
1:A:357:ASP:CG	1:A:478:ARG:HH21	1.91	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:227:ILE:HA	1:B:233:MET:HE3	1.66	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:B:147:ARG:HH22	1:E:499:THR:C	1.94	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:357:ASP:CG	1:D:478:ARG:HH21	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TYR:CD2	1:B:162:VAL:HG21	2.27	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
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:C:24:VAL:CG1	1:C:483:VAL:HG13	2.24	0.68
1:C:36:GLU:HG2	1:C:41:LYS:HZ1	1.57	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:233:MET:HE1	1:B:343:ILE:HD11	1.74	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:B:238:MET:HE3	1:B:342:LYS:HE3	1.76	0.66
1:A:310:TYR:HE2	1:A:317:VAL:CG2	2.05	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:183:TYR:OH	5:B:703:HOH:O	2.11	0.65
1:D:25:GLU:C	1:D:42:ARG:NH2	2.54	0.65
1:D:85:HIS:C	1:D:86:ARG:HG2	2.21	0.65
1:A:238:MET:HE2	1:A:245:LYS:HE3	1.78	0.65
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:B:147:ARG:NH2	1:E:499:THR:C	2.55	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
1:E:224:GLU:HA	1:E:227:ILE:HG22	1.79	0.64
1:E:238:MET:HE2	1:E:245:LYS:HE3	1.77	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:A:233:MET:HE1	1:A:343:ILE:HD11	1.80	0.64
1:D:254:ASN:ND2	5:D:709:HOH:O	2.22	0.64
1:E:458:GLU:CD	1:E:462:ARG:HE	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:186:THR:HG22	1:C:150:MET:HE1	1.80	0.62
1:E:233:MET:HE1	1:E:343:ILE:HD11	1.79	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:F:233:MET:HE1	1:F:343:ILE:HD11	1.83	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:C:3:ARG:C	1:C:5:ASP:H	2.07	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:OD2	1:A:244:ASP:N	2.34	0.60
1:B:238:MET:HE2	1:B:245:LYS:HE3	1.82	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:233:MET:HE1	1:D:343:ILE:HD11	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:C:423:LYS:C	1:C:425:GLY:H	2.10	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: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:A:427:THR:O	1:F:420:LYS:NZ	2.28	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
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:F:499:THR:O	1:F:500:PHE:HB2	2.02	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:CZ	2.76	0.59
1:B:370:ASP:OD1	1:B:371:LEU:N	2.36	0.59
1:C:5:ASP:CG	1:C:333:LYS:HB2	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:58:VAL:C	5:F:713:HOH:O	2.47	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: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:A:211:ARG:HD2	1:A:211:ARG:C	2.30	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
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:E:358:LYS:NZ	5:E:711:HOH:O	2.37	0.57
1:A:147:ARG:NH2	1:D:500:PHE:CD2	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:65:ILE:CG2	1:A:143:LYS:HZ2	2.11	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:A:85:HIS:C	1:A:86:ARG:HG2	2.30	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
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:C:498:VAL:HG12	1:C:499:THR:H	1.71	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:B:37:THR:C	1:B:39:GLU:N	2.65	0.54
1:C:3:ARG:C	1:C:5:ASP:N	2.66	0.54
1:D:87:THR:N	5:D:713:HOH:O	2.40	0.54
1:B:238:MET:SD	1:B:342:LYS:HE3	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:65:ILE:HG22	1:A:143:LYS:NZ	2.14	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:E:51:ILE:HD13	1:E:498:VAL:HG11	1.91	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:226:PHE:HB3	1:A:366:MET:HE1	1.91	0.53
1:A:370:ASP:OD1	1:A:371:LEU:N	2.42	0.53
1:D:85:HIS:O	1:D:86:ARG:HG2	2.07	0.53
1:A:363:ARG:NE	1:A:365:ILE:HD11	2.24	0.52
1:E:458:GLU:CD	1:E:462:ARG:NE	2.66	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:E:238:MET:HE2	1:E:245:LYS:CE	2.39	0.52
1:A:51:ILE:HD13	1:A:498:VAL:HG11	1.91	0.52
3:D:602:NDP:N7N	3:D:602:NDP:O1N	2.43	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:B:224:GLU:HB2	1:B:242:PHE:HE2	1.75	0.52
1:C:233:MET:HE1	1:C:343:ILE:HD11	1.91	0.52
1:E:37:THR:C	1:E:39:GLU:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:GLU:C	1:F:38:GLU:H	2.16	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:E:458:GLU:OE1	1:E:462:ARG:NH2	2.31	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:ARG:NH2	1:F:500:PHE:CG	2.79	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:B:269:LYS:HE3	1:B:284:ASP:C	2.37	0.49
1:C:409:LEU:HD12	1:E:436:PHE:CZ	2.48	0.49
1:F:282:ASN:C	1:F:284:ASP:H	2.19	0.49
1:B:346:GLU:CD	1:B:478:ARG:HH22	2.21	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:F:238:MET:HE2	1:F:245:LYS:HE3	1.95	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:B:262:TYR:OH	4:B:603:GTP:O2G	2.25	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
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:238:MET:HE2	1:A:245:LYS:CE	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:238:MET:HE2	1:F:245:LYS:CE	2.44	0.47
1:A:487:GLU:OE2	5:A:709:HOH:O	2.20	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: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:169:MET:HE1	1:A:327:SER:OG	2.15	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: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:D:25:GLU:C	1:D:42:ARG:HH22	2.21	0.47
1:E:27:LYS:NZ	1:E:487:GLU:OE1	2.47	0.47
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:D:354:PRO:O	1:D:358:LYS:NZ	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:65:ILE:HA	1:A:143:LYS:HZ2	1.79	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:A:118:VAL:HG12	1:A:118:VAL:O	2.15	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:B:154:LYS:C	1:B:155:LYS:HG2	2.41	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HE2	1:A:327:SER:HA	1.98	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
4:B:603:GTP:O2G	4:B:603:GTP:O2'	2.32	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: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: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:65:ILE:HA	1:A:143:LYS:HZ1	1.82	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: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: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:38:GLU:C	1:E:40:GLN:H	2.26	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
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:B:62:SER:OG	5:B:706:HOH:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:GLU:C	1:A:40:GLN:H	2.27	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:F:337:PRO:C	1:F:363:ARG:NH1	2.77	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:D:25:GLU:C	1:D:42:ARG:HH21	2.26	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:OD2	1:C:244:ASP:N	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
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:D:289:LYS:C	1:D:289:LYS:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:ILE:HD12	1:E:65:ILE:C	2.44	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:E:226:PHE:CD2	1:E:465:MET:HE2	2.55	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:C:38:GLU:C	1:C:40:GLN:H	2.27	0.42
1:F:85:HIS:C	1:F:86:ARG:HG3	2.33	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:37:THR:C	1:B:39:GLU:H	2.27	0.41
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:B:222:GLY:HA3	1:B:373:LEU:HD23	2.03	0.41
1:B:269:LYS:HE3	1:B:284:ASP:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:25:GLU:CD	1:C:46:ARG:HE	2.27	0.41
1:C:79:ARG:HH21	1:C:163:ASP:CG	2.27	0.41
1:D:150:MET:HE1	1:D:187:ILE:CD1	2.50	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:F:500:PHE:C	5:F:707:HOH:O	2.62	0.41
1:C:473:LEU:HD23	1:C:473:LEU:HA	1.89	0.41
4:E:603:GTP:O2G	4:E:603:GTP:O2'	2.36	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:D:150:MET:HE1	1:D:187:ILE:HD11	2.02	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:A:226:PHE:HB3	1:A:366:MET:CE	2.51	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:O	1:E:118:VAL:HG12	2.21	0.41
1:F:111:MET:SD	1:F:114:LYS:HE3	2.60	0.41
1:F:203:ILE:C	1:F:205:GLN:H	2.29	0.41
1:F:246:THR:O	1:F:320:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:491:ARG:HG2	5:C:711:HOH:O	2.22	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
1:D:238:MET:HE2	1:D:245:LYS:HD3	2.03	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

5.3.1 Protein backbone

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

of similar resolution.

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

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

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

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Mol	Chain	Res	Type
1	E	499	THR
1	E	500	PHE
1	F	422	GLY
1	F	500	PHE
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 ⓘ

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%)	411 (99%)	6 (1%)	59	76
1	B	417/417 (100%)	414 (99%)	3 (1%)	76	87
1	C	417/417 (100%)	415 (100%)	2 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	417/417 (100%)	414 (99%)	3 (1%)	76	87
1	E	417/417 (100%)	415 (100%)	2 (0%)	81	90
1	F	417/417 (100%)	413 (99%)	4 (1%)	68	82
All	All	2502/2502 (100%)	2482 (99%)	20 (1%)	73	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	MET
1	A	211	ARG
1	A	260	MET
1	A	333	LYS
1	A	405	SER
1	A	456	THR
1	B	211	ARG
1	B	271	VAL
1	B	373	LEU
1	C	211	ARG
1	C	405	SER
1	D	66	ARG
1	D	358	LYS
1	D	419	ARG
1	E	150	MET
1	E	373	LEU
1	F	169	MET
1	F	211	ARG
1	F	373	LEU
1	F	405	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	225	ASN
1	A	254	ASN
1	A	264	HIS
1	A	298	HIS
1	A	390	ASN
1	A	408	HIS
1	A	450	HIS

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Mol	Chain	Res	Type
1	B	221	HIS
1	B	250	GLN
1	B	254	ASN
1	B	264	HIS
1	B	298	HIS
1	C	193	ASN
1	C	205	GLN
1	C	225	ASN
1	C	250	GLN
1	C	254	ASN
1	C	297	GLN
1	C	298	HIS
1	C	408	HIS
1	C	484	ASN
1	C	494	ASN
1	D	193	ASN
1	D	254	ASN
1	D	264	HIS
1	D	298	HIS
1	E	193	ASN
1	E	225	ASN
1	E	250	GLN
1	E	264	HIS
1	E	298	HIS
1	E	414	GLN
1	E	437	GLN
1	F	84	GLN
1	F	193	ASN
1	F	205	GLN
1	F	254	ASN
1	F	264	HIS
1	F	298	HIS
1	F	408	HIS
1	F	484	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	602	-	51,52,52	2.64	12 (23%)	71,80,80	1.42	14 (19%)
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%)
3	NDP	E	602	-	51,52,52	2.93	14 (27%)	71,80,80	1.43	10 (14%)
2	GLU	D	601	-	8,9,9	1.07	0	8,11,11	1.47	1 (12%)
2	GLU	F	601	-	8,9,9	1.05	0	8,11,11	1.76	1 (12%)
3	NDP	C	602	-	51,52,52	2.46	12 (23%)	71,80,80	1.57	16 (22%)
2	GLU	E	601	-	8,9,9	1.24	2 (25%)	8,11,11	1.21	1 (12%)
4	GTP	A	603	-	33,34,34	0.92	1 (3%)	50,54,54	1.67	11 (22%)
4	GTP	B	603	-	33,34,34	1.19	4 (12%)	50,54,54	1.55	9 (18%)
3	NDP	F	602	-	51,52,52	2.45	13 (25%)	71,80,80	1.60	17 (23%)
4	GTP	D	603	-	33,34,34	0.98	1 (3%)	50,54,54	1.57	10 (20%)
4	GTP	F	603	-	33,34,34	0.92	1 (3%)	50,54,54	1.72	12 (24%)
4	GTP	E	603	-	33,34,34	0.77	1 (3%)	50,54,54	1.62	9 (18%)
3	NDP	D	602	-	51,52,52	2.21	13 (25%)	71,80,80	1.66	18 (25%)
4	GTP	C	603	-	33,34,34	1.06	4 (12%)	50,54,54	1.59	12 (24%)
3	NDP	B	602	-	51,52,52	2.47	11 (21%)	71,80,80	1.52	15 (21%)
2	GLU	A	601	-	8,9,9	1.19	2 (25%)	8,11,11	1.27	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	A	602	-	-	3/34/77/77	0/5/5/5
2	GLU	B	601	-	-	2/9/9/9	-
2	GLU	C	601	-	-	2/9/9/9	-
3	NDP	E	602	-	-	11/34/77/77	0/5/5/5
2	GLU	D	601	-	-	4/9/9/9	-
2	GLU	F	601	-	-	2/9/9/9	-
3	NDP	C	602	-	-	6/34/77/77	0/5/5/5
2	GLU	E	601	-	-	4/9/9/9	-
4	GTP	A	603	-	-	2/22/38/38	0/3/3/3
4	GTP	B	603	-	-	2/22/38/38	0/3/3/3
3	NDP	F	602	-	-	5/34/77/77	0/5/5/5
4	GTP	D	603	-	-	2/22/38/38	0/3/3/3
4	GTP	F	603	-	-	5/22/38/38	0/3/3/3
4	GTP	E	603	-	-	4/22/38/38	0/3/3/3
3	NDP	D	602	-	-	10/34/77/77	0/5/5/5
4	GTP	C	603	-	-	2/22/38/38	0/3/3/3
3	NDP	B	602	-	-	6/34/77/77	0/5/5/5
2	GLU	A	601	-	-	4/9/9/9	-

All (92) 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
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	E	602	NDP	PN-O5D	4.80	1.78	1.59
3	B	602	NDP	PN-O5D	4.79	1.78	1.59
3	B	602	NDP	O2B-C2B	-4.01	1.30	1.44
3	A	602	NDP	PN-O5D	3.94	1.74	1.59
3	F	602	NDP	PN-O3	3.79	1.63	1.59
3	B	602	NDP	C2A-N1A	3.77	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	C5A-C4A	3.42	1.45	1.39
3	C	602	NDP	PN-O3	3.24	1.63	1.59
3	B	602	NDP	C5A-C4A	3.09	1.44	1.39
3	E	602	NDP	C8A-N9A	3.01	1.42	1.37
3	E	602	NDP	C4A-N3A	2.97	1.40	1.34
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	A	602	NDP	O2B-C2B	-2.86	1.34	1.44
3	E	602	NDP	C2A-N1A	2.85	1.39	1.33
3	A	602	NDP	C5A-C4A	2.80	1.44	1.39
3	B	602	NDP	C2B-C1B	2.73	1.59	1.53
4	B	603	GTP	PA-O3A	2.72	1.62	1.59
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	B	602	NDP	C4A-N3A	2.62	1.39	1.34
3	E	602	NDP	PN-O3	2.59	1.62	1.59
3	C	602	NDP	C4A-N3A	2.56	1.39	1.34
3	F	602	NDP	C4A-N3A	2.55	1.39	1.34
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	E	602	NDP	C5A-C4A	2.42	1.43	1.39
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	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	F	602	NDP	C5A-C4A	2.35	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	NDP	O4B-C4B	-2.35	1.39	1.45
3	C	602	NDP	C8A-N9A	2.34	1.41	1.37
3	D	602	NDP	C4A-N3A	2.31	1.38	1.34
3	A	602	NDP	C3B-C2B	2.31	1.58	1.53
3	F	602	NDP	C8A-N7A	2.29	1.36	1.31
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	O4B-C1B	2.25	1.47	1.42
3	F	602	NDP	C5A-N7A	2.24	1.43	1.39
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	F	602	NDP	C8A-N9A	2.19	1.41	1.37
3	E	602	NDP	C7N-N7N	2.18	1.39	1.33
3	D	602	NDP	C5A-C4A	2.18	1.43	1.39
4	B	603	GTP	C2-N3	2.17	1.38	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	C	603	GTP	C2-N3	2.14	1.38	1.33
2	E	601	GLU	OE2-CD	-2.13	1.23	1.30
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	B	602	NDP	C8A-N9A	2.10	1.41	1.37
3	A	602	NDP	C4A-N3A	2.10	1.38	1.34
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	2.07	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
3	D	602	NDP	C8A-N9A	2.02	1.41	1.37
3	D	602	NDP	C8A-N7A	2.00	1.35	1.31

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	GTP	C2-N3-C4	4.88	120.70	112.30
4	F	603	GTP	C5-C4-N3	-4.86	120.65	128.39
4	E	603	GTP	C5-C4-N3	-4.76	120.81	128.39
4	B	603	GTP	C5-C4-N3	-4.69	120.93	128.39
4	A	603	GTP	C5-C4-N3	-4.68	120.95	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	603	GTP	C2-N3-C4	4.62	120.26	112.30
4	D	603	GTP	C2-N3-C4	4.56	120.16	112.30
4	D	603	GTP	C5-C4-N3	-4.55	121.16	128.39
4	E	603	GTP	C2-N3-C4	4.52	120.09	112.30
4	C	603	GTP	C5-C4-N3	-4.39	121.41	128.39
4	C	603	GTP	C2-N3-C4	4.21	119.55	112.30
3	F	602	NDP	O2N-PN-O3	4.19	118.59	107.27
4	B	603	GTP	C2-N3-C4	4.02	119.23	112.30
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
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
3	F	602	NDP	O2B-P2B-O1X	-3.61	96.48	109.33
3	C	602	NDP	O2B-P2B-O1X	-3.48	96.93	109.33
3	C	602	NDP	O2N-PN-O3	3.46	116.62	107.27
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
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
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	-3.29	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	C	602	NDP	O4B-C1B-N9A	-3.20	101.95	108.09
4	B	603	GTP	C2-N1-C6	-3.18	119.35	125.11
3	D	602	NDP	C3B-C2B-C1B	-3.17	96.73	102.81
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
2	E	601	GLU	OXT-C-O	-3.05	117.16	124.08
3	B	602	NDP	O4B-C4B-C3B	2.99	111.10	105.15
4	C	603	GTP	N9-C4-N3	2.98	131.91	125.95
2	C	601	GLU	OXT-C-O	-2.96	117.36	124.08
3	D	602	NDP	O3-PA-O1A	-2.92	101.91	110.70
4	A	603	GTP	C5-C6-N1	2.92	120.69	113.25
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
4	D	603	GTP	N9-C8-N7	-2.85	108.12	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	GTP	N9-C4-N3	2.85	131.65	125.95
3	E	602	NDP	P2B-O2B-C2B	-2.84	115.83	123.43
4	A	603	GTP	C2-N1-C6	-2.84	119.97	125.11
4	A	603	GTP	N9-C4-N3	2.83	131.62	125.95
3	E	602	NDP	PA-O5B-C5B	-2.83	105.12	121.35
4	D	603	GTP	C2-N1-C6	-2.82	119.99	125.11
4	F	603	GTP	C8-N7-C5	2.82	109.28	104.26
3	F	602	NDP	PN-O5D-C5D	-2.81	105.24	121.35
4	C	603	GTP	C2-N1-C6	-2.79	120.04	125.11
4	F	603	GTP	N9-C8-N7	-2.79	108.23	113.40
4	E	603	GTP	C2-N1-C6	-2.78	120.06	125.11
4	F	603	GTP	N9-C4-N3	2.77	131.48	125.95
3	A	602	NDP	O2B-P2B-O1X	-2.76	99.48	109.33
4	A	603	GTP	N9-C8-N7	-2.74	108.31	113.40
4	C	603	GTP	O6-C6-C5	-2.74	119.29	126.53
4	C	603	GTP	C2'-C1'-N9	-2.72	105.67	113.25
4	E	603	GTP	N9-C4-N3	2.69	131.33	125.95
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	N3A-C4A-N9A	2.66	131.69	127.17
4	D	603	GTP	N9-C4-N3	2.65	131.26	125.95
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
4	A	603	GTP	O4'-C1'-N9	2.65	114.36	108.36
3	A	602	NDP	PA-O5B-C5B	-2.64	106.21	121.35
4	F	603	GTP	C5-C6-N1	2.63	119.94	113.25
4	B	603	GTP	N9-C8-N7	-2.63	108.53	113.40
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
4	B	603	GTP	C8-N7-C5	2.59	108.87	104.26
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	C	603	GTP	N9-C8-N7	-2.55	108.67	113.40
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
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
4	B	603	GTP	C5-C6-N1	2.53	119.70	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	NDP	O5D-PN-O1N	-2.52	98.94	108.94
3	B	602	NDP	N3A-C4A-N9A	2.52	131.45	127.17
4	F	603	GTP	O6-C6-C5	-2.51	119.91	126.53
3	A	602	NDP	O3X-P2B-O2X	2.50	117.16	107.80
3	C	602	NDP	C2A-N1A-C6A	-2.49	114.64	118.73
4	D	603	GTP	C8-N7-C5	2.48	108.69	104.26
3	D	602	NDP	C3D-C2D-C1D	-2.47	96.78	101.46
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
4	E	603	GTP	C8-N7-C5	2.43	108.59	104.26
4	E	603	GTP	N9-C8-N7	-2.41	108.94	113.40
3	D	602	NDP	C2B-C1B-N9A	2.40	117.70	113.75
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
4	D	603	GTP	O2G-PG-O3B	2.31	112.37	104.64
4	E	603	GTP	C5-C6-N1	2.30	119.11	113.25
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
4	A	603	GTP	C8-N7-C5	2.29	108.34	104.26
3	C	602	NDP	PN-O5D-C5D	-2.29	108.24	121.35
3	F	602	NDP	C2A-N1A-C6A	-2.28	114.99	118.73
3	D	602	NDP	C4A-N9A-C1B	-2.28	121.31	126.63
3	C	602	NDP	C5A-C4A-N3A	-2.27	123.59	126.72
3	E	602	NDP	C3B-C2B-C1B	-2.26	98.48	102.81
3	B	602	NDP	C2A-N1A-C6A	-2.26	115.02	118.73
3	F	602	NDP	O3X-P2B-O2B	-2.25	97.10	105.85
4	C	603	GTP	C8-N7-C5	2.24	108.24	104.26
4	C	603	GTP	C5-C6-N1	2.23	118.94	113.25
3	C	602	NDP	C3B-C2B-C1B	-2.23	98.53	102.81
4	D	603	GTP	C5-C6-N1	2.23	118.93	113.25
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
4	C	603	GTP	N2-C2-N1	2.18	121.36	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
4	A	603	GTP	O6-C6-C5	-2.14	120.89	126.53
4	D	603	GTP	O3'-C3'-C4'	-2.13	104.97	111.08
4	F	603	GTP	C4-C5-N7	-2.12	107.31	110.67
3	E	602	NDP	O7N-C7N-N7N	-2.12	118.14	122.89
4	D	603	GTP	O6-C6-C5	-2.12	120.95	126.53
3	B	602	NDP	C5A-C4A-N3A	-2.11	123.80	126.72
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
4	B	603	GTP	O6-C6-C5	-2.09	121.00	126.53
3	A	602	NDP	N3A-C4A-N9A	2.09	130.72	127.17
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
4	A	603	GTP	C6-C5-N7	2.08	134.07	130.29
3	A	602	NDP	O4B-C1B-N9A	-2.07	104.11	108.09
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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.

16 monomers are involved in 33 short contacts:

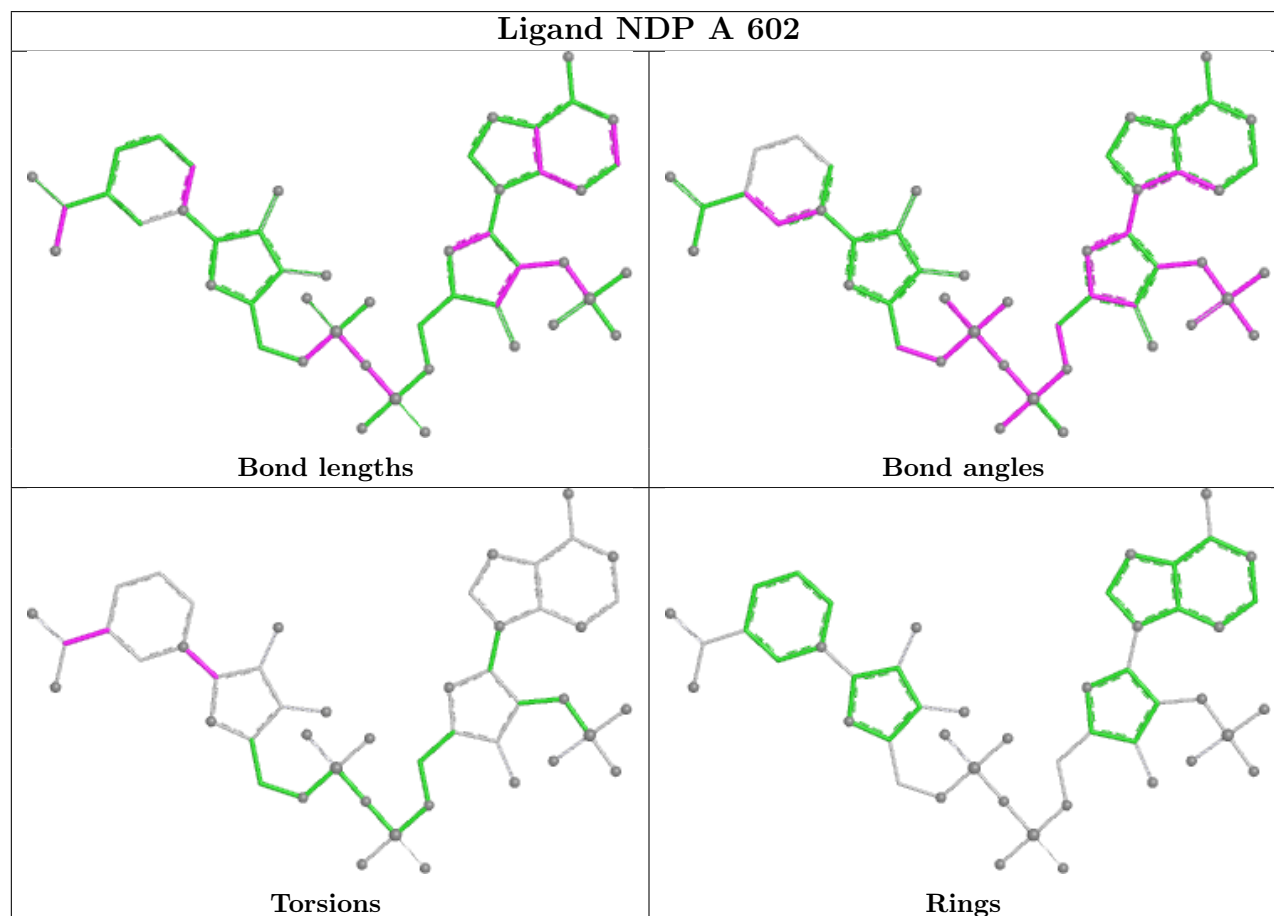
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NDP	4	0
2	B	601	GLU	2	0
2	C	601	GLU	2	0
3	E	602	NDP	4	0
2	D	601	GLU	1	0
2	F	601	GLU	1	0
3	C	602	NDP	4	0
2	E	601	GLU	1	0
4	B	603	GTP	2	0
3	F	602	NDP	5	0

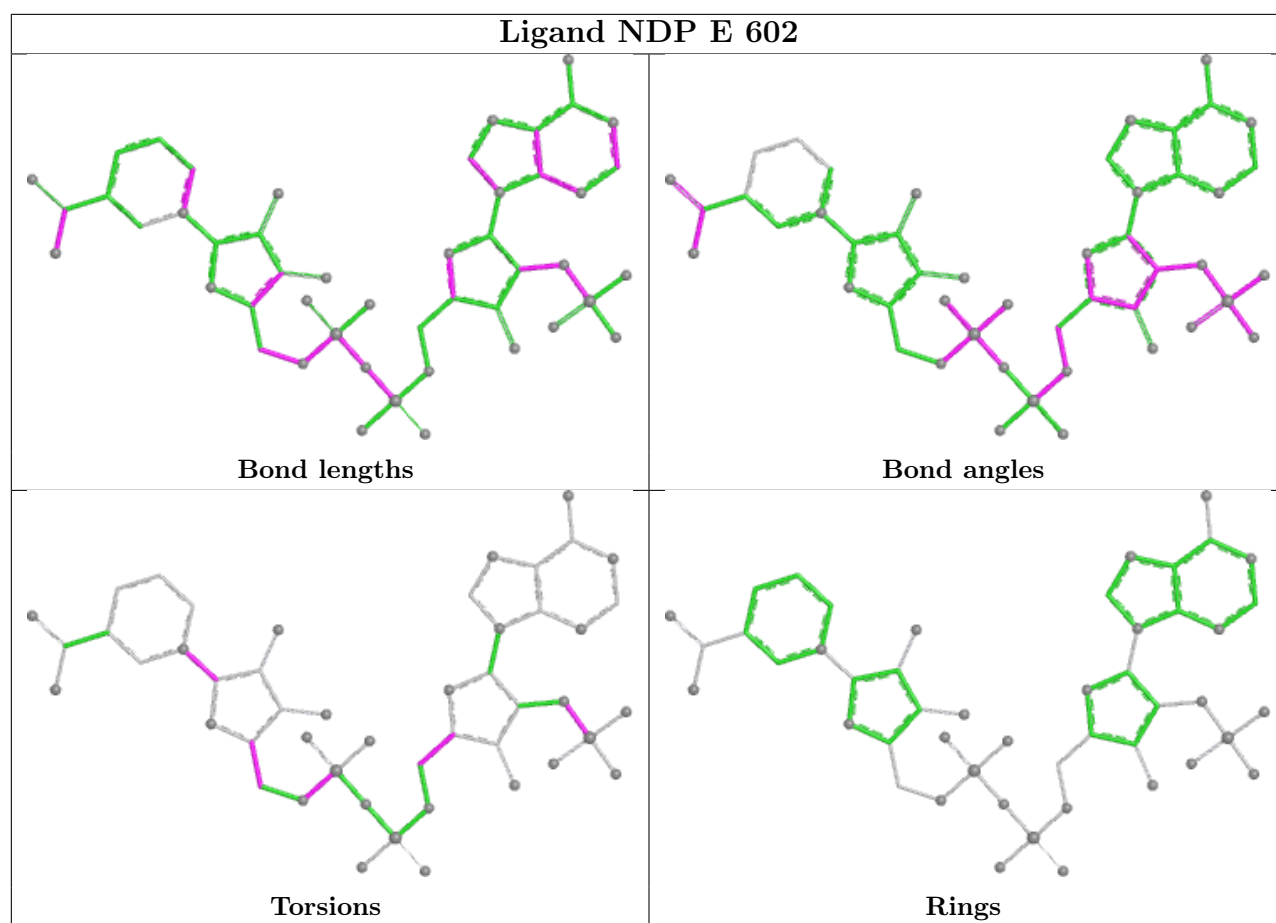
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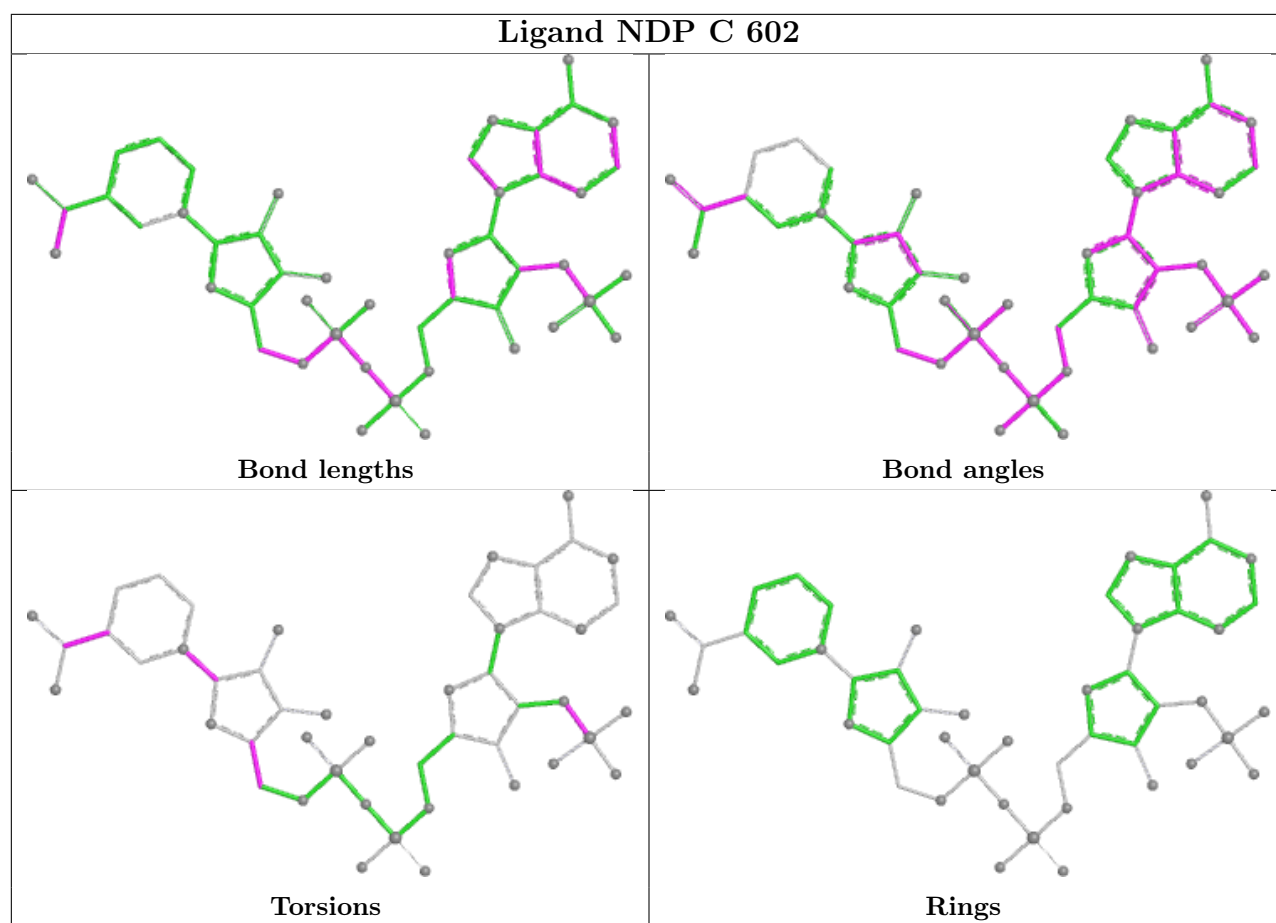
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	GTP	1	0
4	F	603	GTP	1	0
4	E	603	GTP	1	0
3	D	602	NDP	7	0
3	B	602	NDP	3	0
2	A	601	GLU	1	0

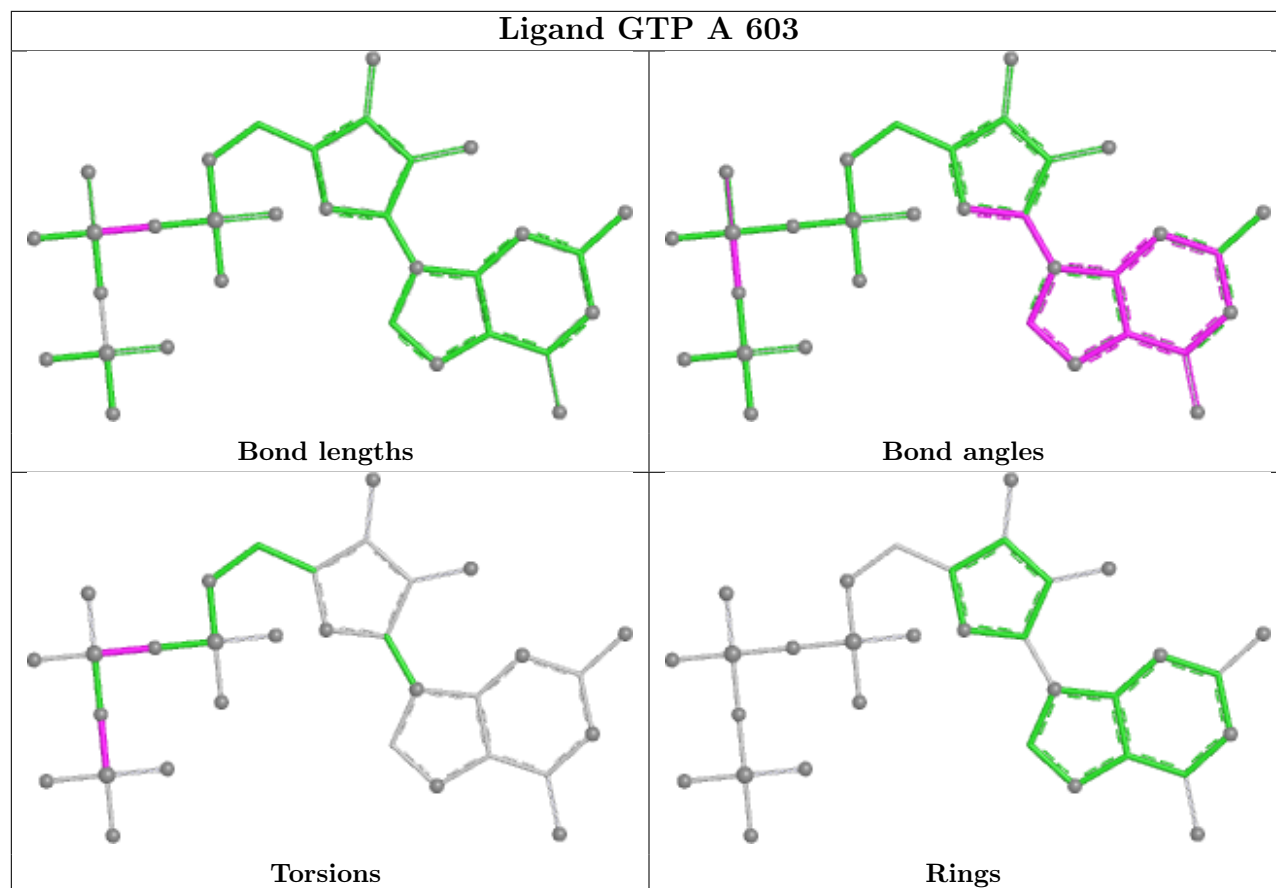
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



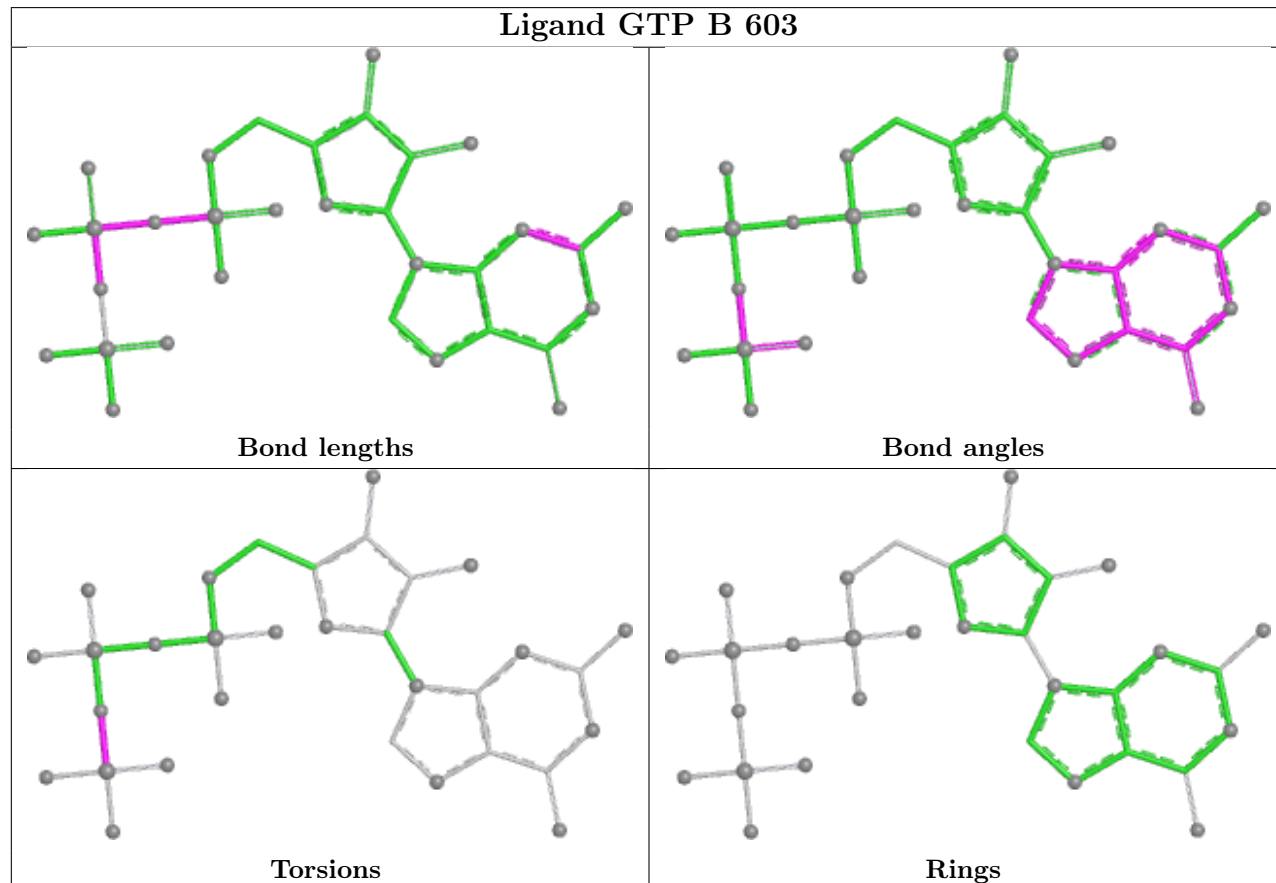


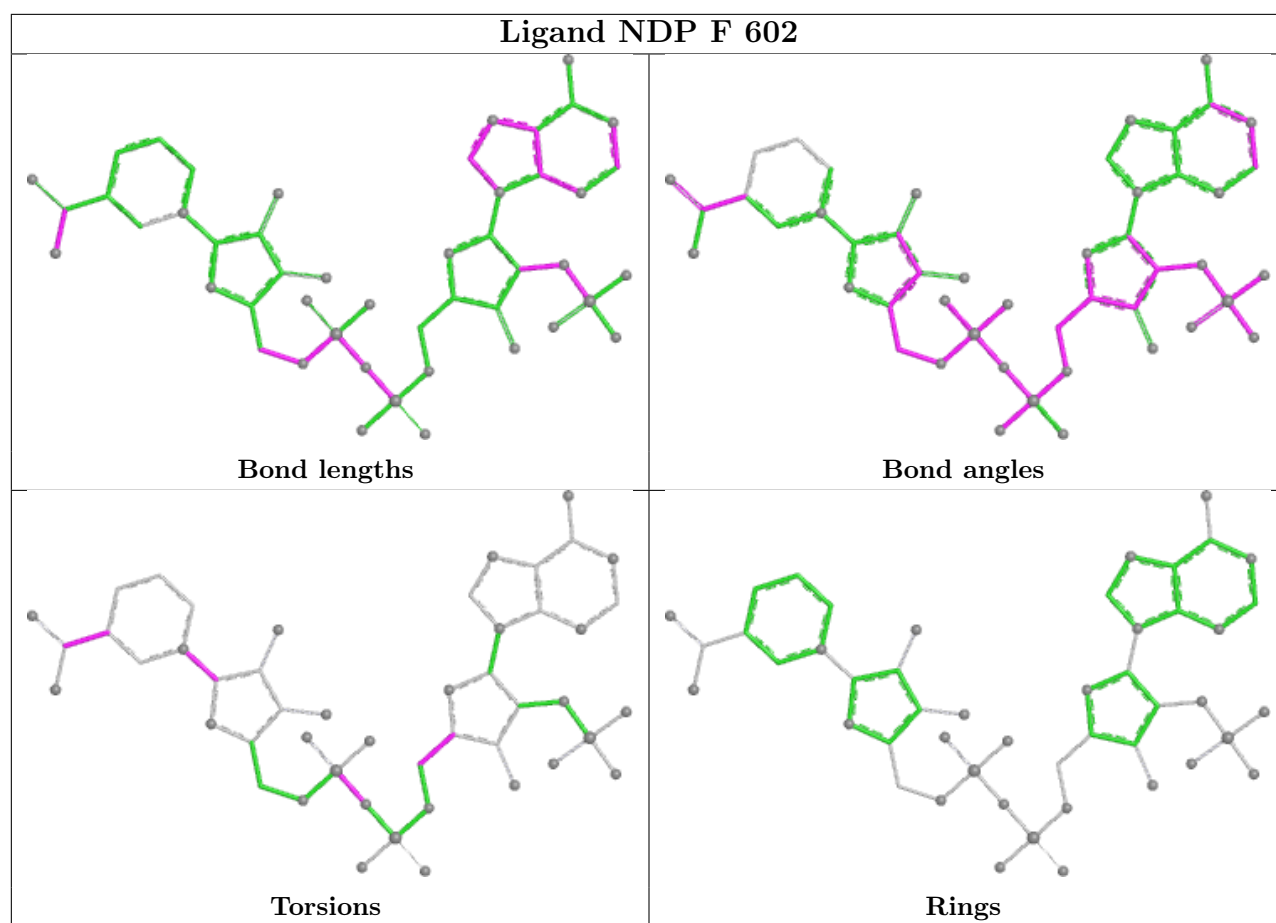


Ligand GTP A 603

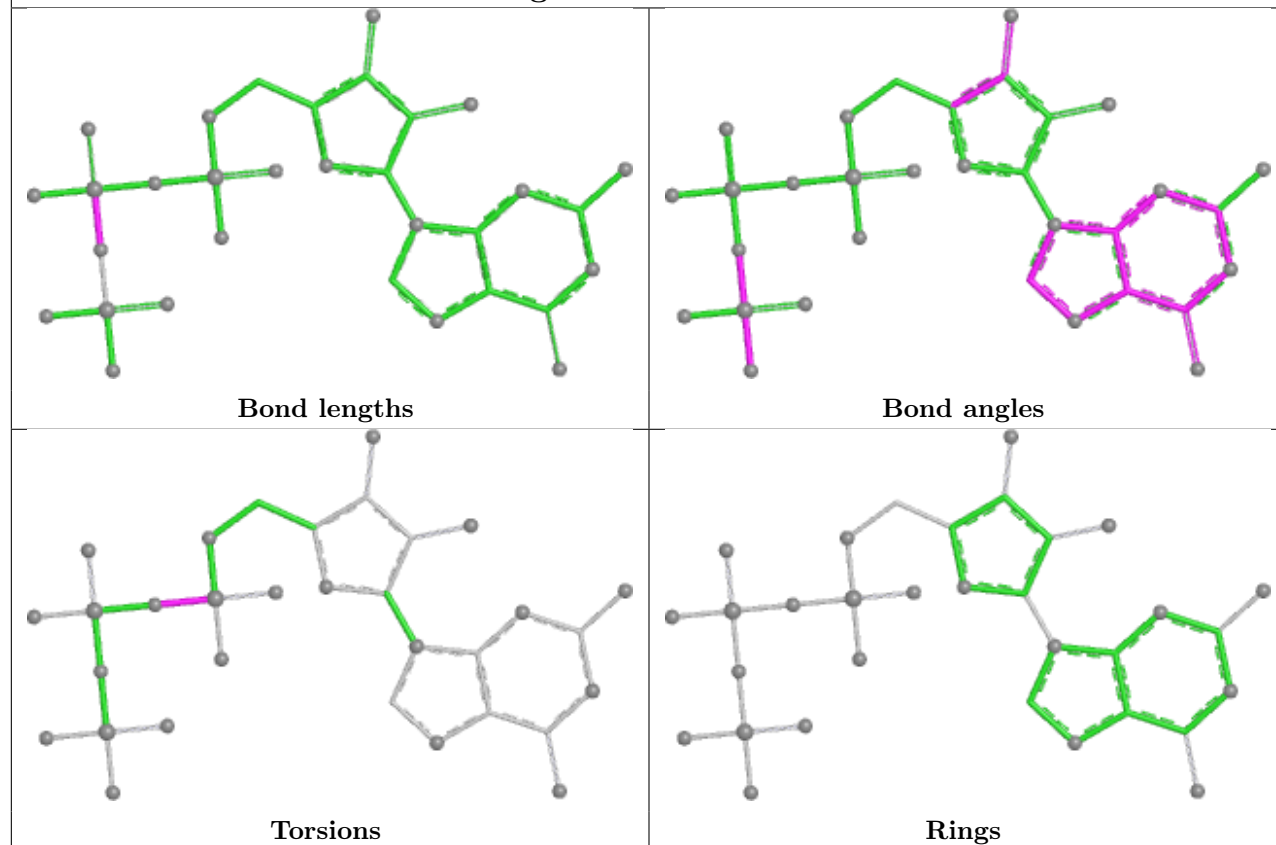


Ligand GTP B 603

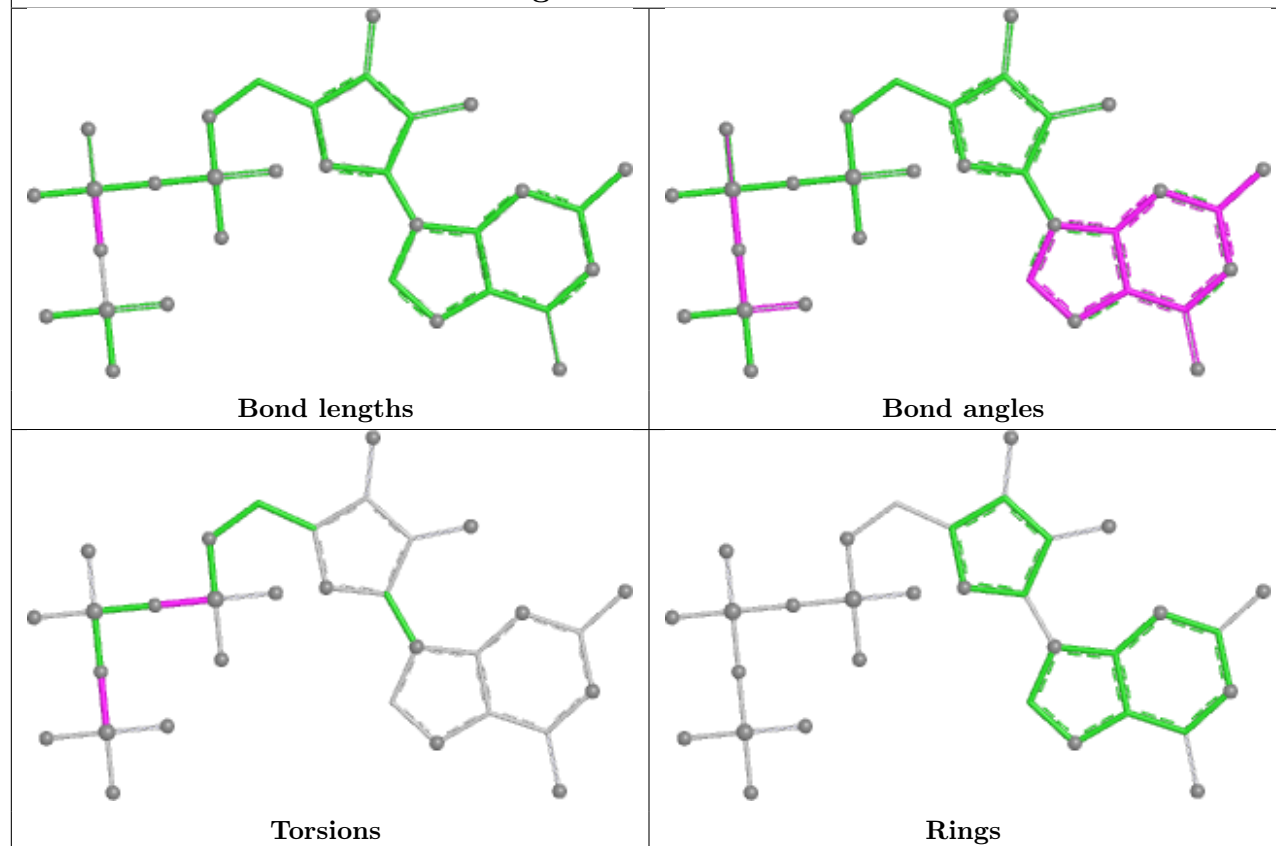


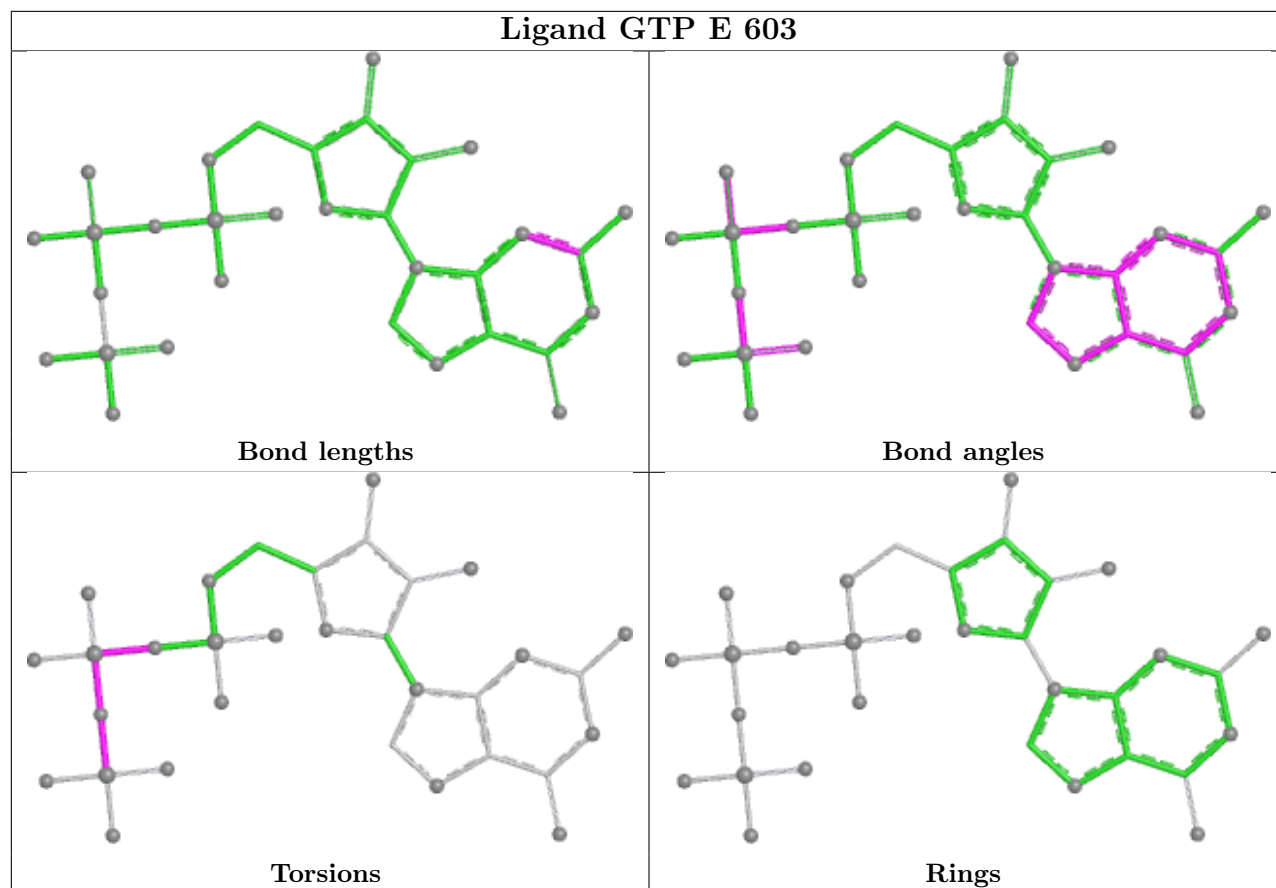


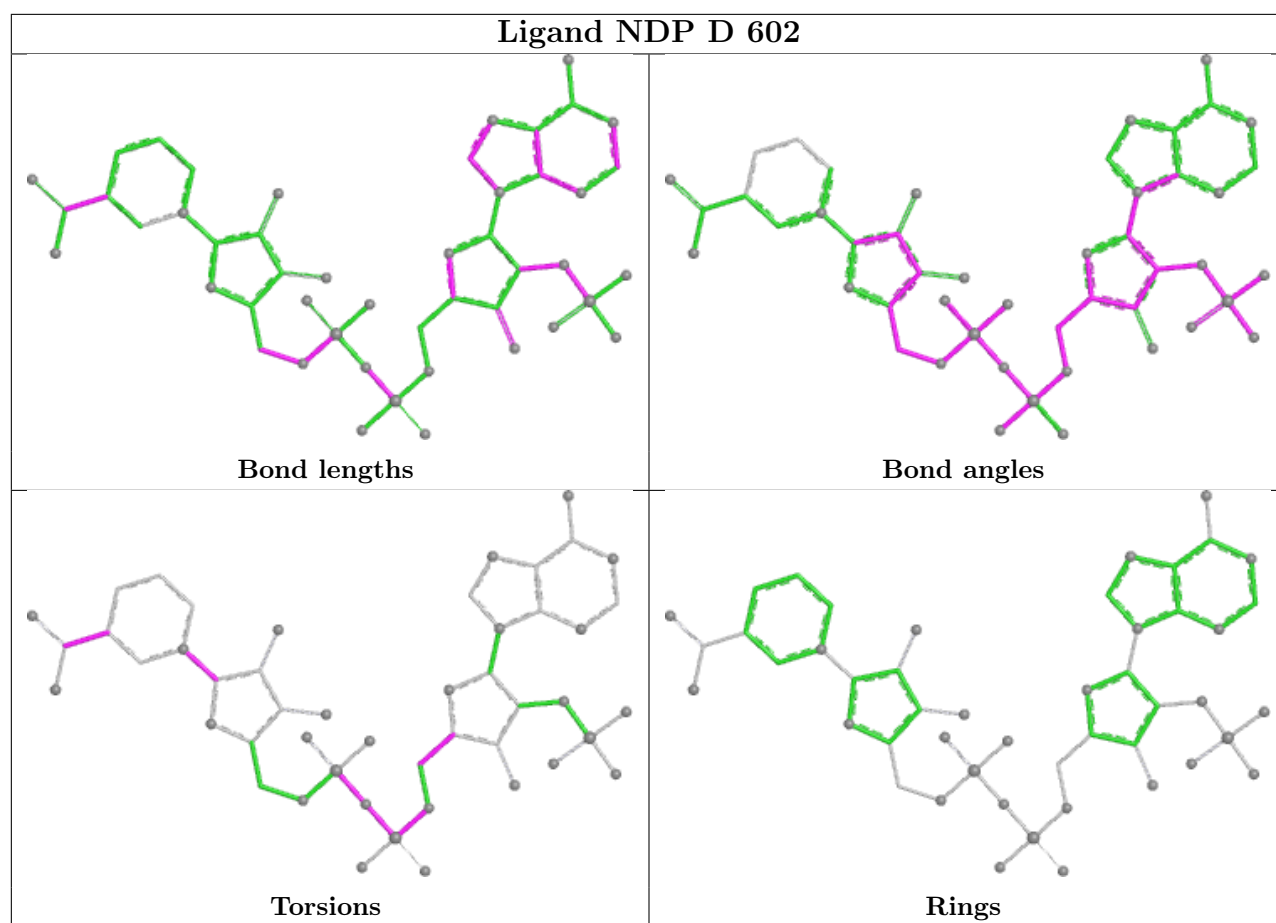
Ligand GTP D 603

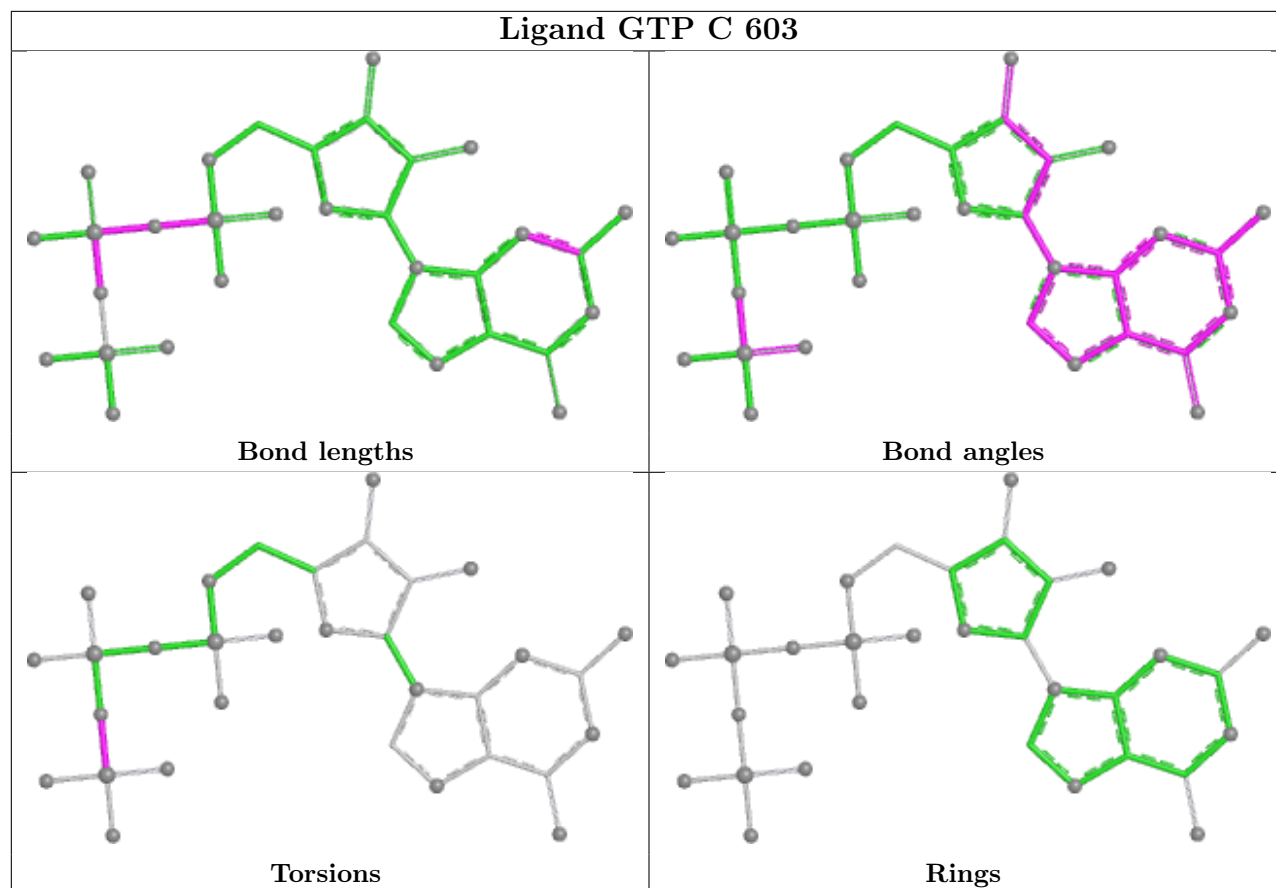


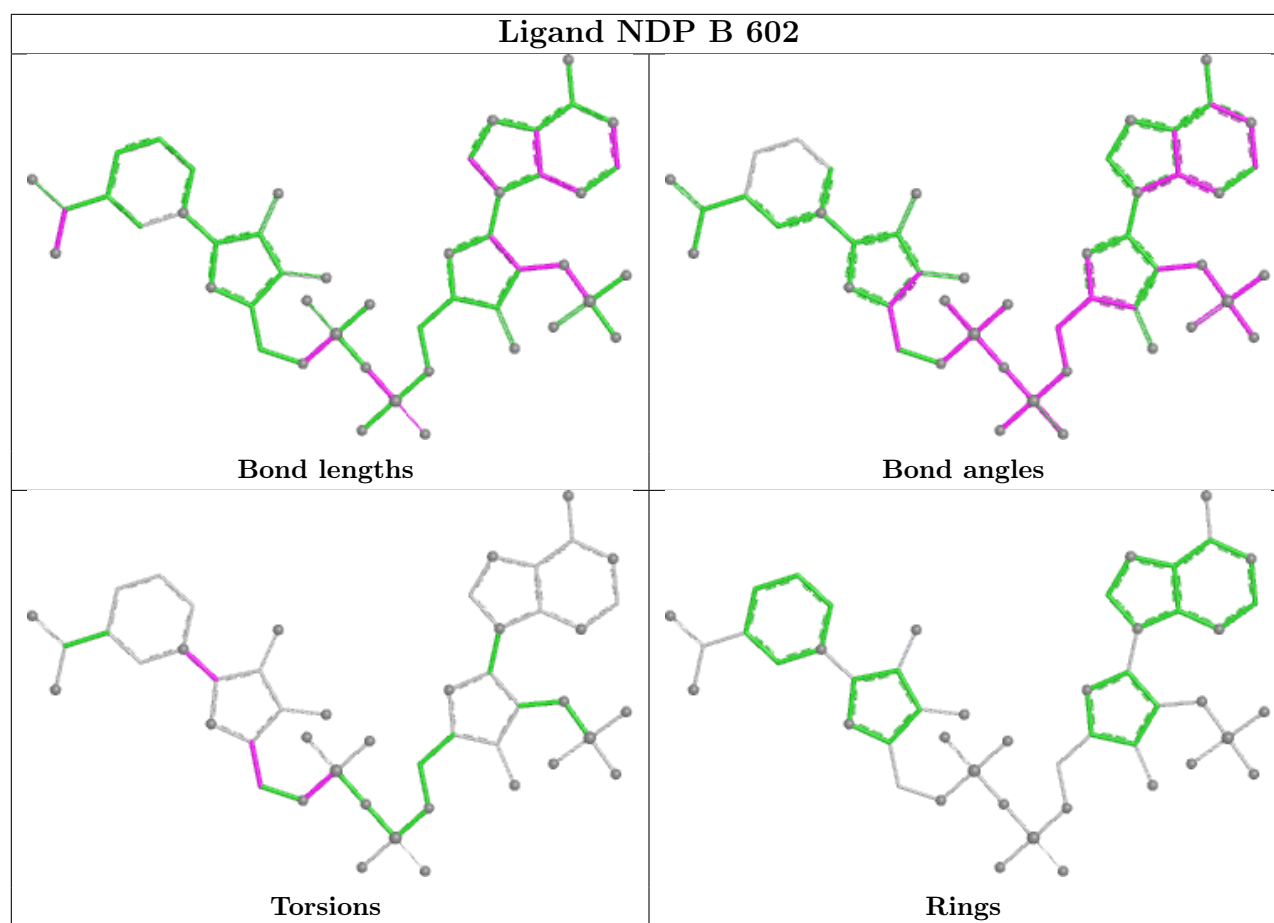
Ligand GTP F 603











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	501/501 (100%)	0.47	16 (3%)	50	52	34, 55, 86, 115	0
1	B	501/501 (100%)	0.57	35 (6%)	22	24	34, 54, 86, 118	0
1	C	501/501 (100%)	0.57	19 (3%)	44	46	40, 57, 88, 112	0
1	D	501/501 (100%)	0.50	18 (3%)	46	48	39, 56, 89, 112	0
1	E	501/501 (100%)	0.60	14 (2%)	55	57	37, 62, 93, 113	0
1	F	501/501 (100%)	0.69	33 (6%)	24	26	38, 60, 90, 117	0
All	All	3006/3006 (100%)	0.57	135 (4%)	38	40	34, 57, 91, 118	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	499	THR	6.4
1	E	425	GLY	5.4
1	E	501	THR	4.4
1	D	87	THR	4.3
1	C	496	ALA	4.2
1	C	88	PRO	4.1
1	E	5	ASP	4.0
1	C	307	ALA	4.0
1	D	500	PHE	4.0
1	D	422	GLY	3.9
1	A	498	VAL	3.8
1	A	87	THR	3.8
1	E	304	PHE	3.8
1	A	22	SER	3.7
1	B	499	THR	3.5
1	B	498	VAL	3.5
1	F	498	VAL	3.4
1	F	268	ALA	3.4
1	D	498	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	339	VAL	3.3
1	F	5	ASP	3.3
1	F	422	GLY	3.2
1	F	500	PHE	3.2
1	B	337	PRO	3.2
1	C	87	THR	3.2
1	D	276	SER	3.1
1	C	5	ASP	3.1
1	B	356	ALA	3.1
1	F	501	THR	3.0
1	F	421	PHE	3.0
1	F	426	GLY	3.0
1	B	341	ALA	3.0
1	C	500	PHE	3.0
1	B	230	ALA	3.0
1	F	348	ALA	3.0
1	F	88	PRO	3.0
1	B	500	PHE	2.9
1	E	438	ASP	2.9
1	A	5	ASP	2.9
1	A	2	ASP	2.9
1	F	87	THR	2.8
1	D	501	THR	2.8
1	A	427	THR	2.7
1	A	88	PRO	2.7
1	D	32	LEU	2.7
1	E	282	ASN	2.7
1	A	500	PHE	2.7
1	B	29	VAL	2.7
1	A	422	GLY	2.7
1	C	282	ASN	2.7
1	D	5	ASP	2.6
1	E	37	THR	2.6
1	D	305	PRO	2.6
1	B	38	GLU	2.6
1	F	326	ALA	2.6
1	A	411	MET	2.6
1	B	317	VAL	2.6
1	E	87	THR	2.6
1	B	313	SER	2.6
1	B	243	GLY	2.6
1	F	499	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	334	SER	2.6
1	F	230	ALA	2.5
1	B	424	HIS	2.5
1	D	137	THR	2.5
1	E	296	LEU	2.5
1	C	34	THR	2.5
1	F	271	VAL	2.5
1	E	496	ALA	2.5
1	F	297	GLN	2.5
1	F	303	GLY	2.5
1	B	480	ALA	2.4
1	B	87	THR	2.4
1	B	185	SER	2.4
1	B	69	ASP	2.4
1	B	335	ASN	2.4
1	C	495	GLU	2.4
1	E	335	ASN	2.4
1	B	425	GLY	2.4
1	C	278	GLY	2.4
1	B	34	THR	2.4
1	F	332	THR	2.4
1	D	393	SER	2.4
1	E	254	ASN	2.3
1	A	268	ALA	2.3
1	C	187	ILE	2.3
1	A	70	GLY	2.3
1	B	496	ALA	2.3
1	F	309	ILE	2.3
1	F	254	ASN	2.3
1	B	497	GLY	2.3
1	A	1	ALA	2.3
1	C	356	ALA	2.3
1	F	386	LEU	2.3
1	F	274	GLY	2.3
1	F	275	GLU	2.3
1	E	309	ILE	2.3
1	E	294	PHE	2.2
1	B	422	GLY	2.2
1	A	501	THR	2.2
1	C	304	PHE	2.2
1	C	277	ASP	2.2
1	A	496	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	501	THR	2.2
1	F	496	ALA	2.2
1	B	312	GLY	2.2
1	F	285	GLY	2.2
1	F	185	SER	2.2
1	B	31	ASP	2.1
1	D	339	VAL	2.1
1	D	84	GLN	2.1
1	B	37	THR	2.1
1	C	327	SER	2.1
1	F	246	THR	2.1
1	B	310	TYR	2.1
1	B	359	ILE	2.1
1	F	163	ASP	2.1
1	B	336	ALA	2.1
1	D	313	SER	2.1
1	F	313	SER	2.1
1	B	5	ASP	2.1
1	D	40	GLN	2.1
1	B	283	PRO	2.1
1	F	103	GLU	2.1
1	C	254	ASN	2.1
1	F	301	ILE	2.1
1	A	497	GLY	2.1
1	C	239	THR	2.0
1	D	412	SER	2.0
1	C	1	ALA	2.0
1	C	424	HIS	2.0
1	F	312	GLY	2.0
1	B	332	THR	2.0
1	D	307	ALA	2.0
1	F	424	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

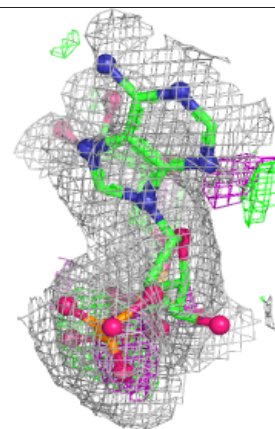
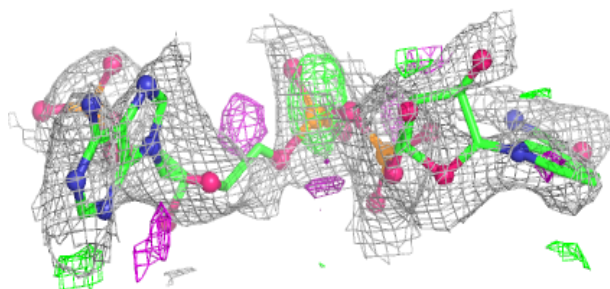
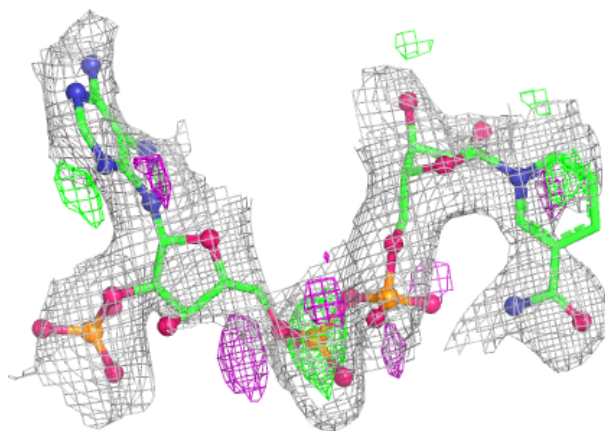
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLU	E	601	10/10	0.88	0.11	50,56,64,67	0
2	GLU	F	601	10/10	0.89	0.10	50,57,65,66	0
3	NDP	F	602	48/48	0.90	0.12	51,68,78,204	0
2	GLU	D	601	10/10	0.91	0.09	48,54,60,62	0
2	GLU	C	601	10/10	0.92	0.10	43,50,63,65	0
4	GTP	A	603	32/32	0.93	0.10	41,53,60,65	0
4	GTP	E	603	32/32	0.93	0.10	55,62,71,76	0
2	GLU	A	601	10/10	0.94	0.08	48,52,60,67	0
3	NDP	C	602	48/48	0.94	0.09	44,54,62,67	0
4	GTP	D	603	32/32	0.94	0.08	46,54,63,66	0
3	NDP	E	602	48/48	0.94	0.10	52,63,74,81	0
3	NDP	B	602	48/48	0.95	0.09	38,50,59,64	0
2	GLU	B	601	10/10	0.95	0.08	42,50,56,57	0
4	GTP	B	603	32/32	0.95	0.08	42,49,59,62	0
4	GTP	C	603	32/32	0.95	0.09	48,56,65,69	0
3	NDP	D	602	48/48	0.95	0.09	38,55,61,67	0
3	NDP	A	602	48/48	0.95	0.09	39,51,60,63	0
4	GTP	F	603	32/32	0.96	0.08	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.

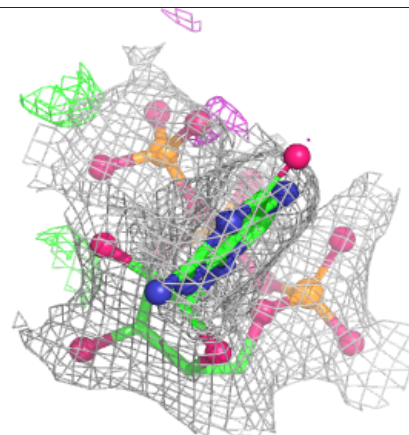
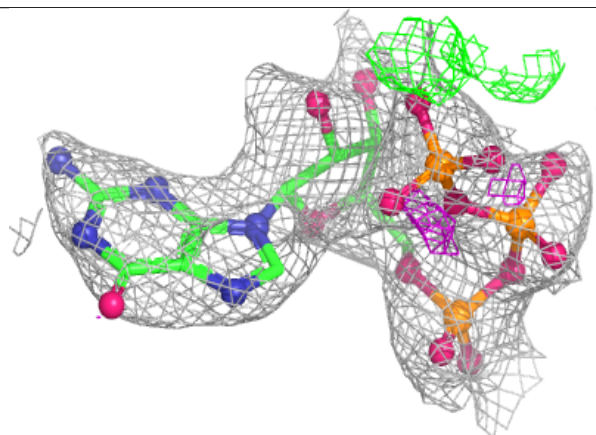
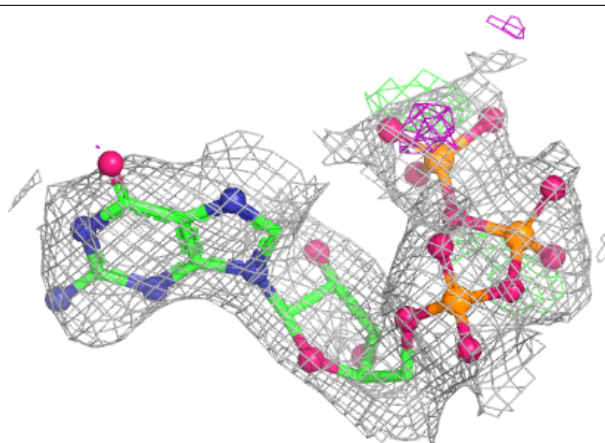
Electron density around NDP F 602:

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

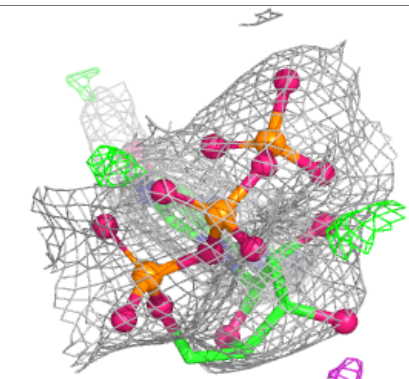
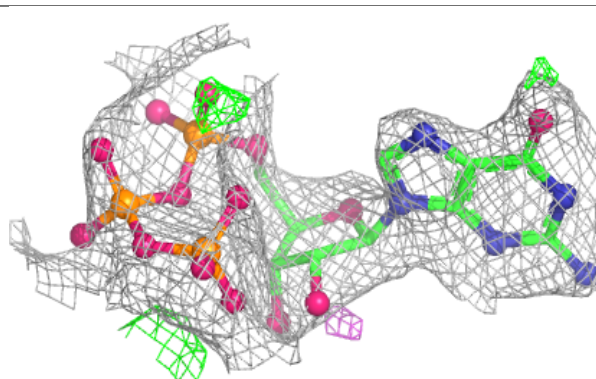
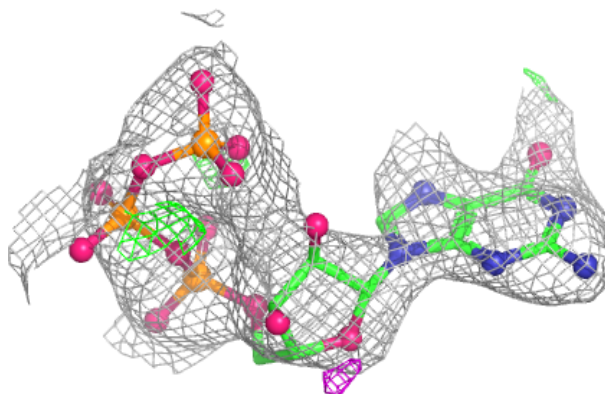


Electron density around GTP A 603:

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

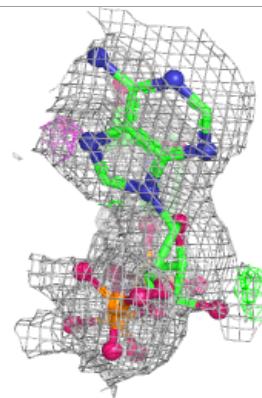
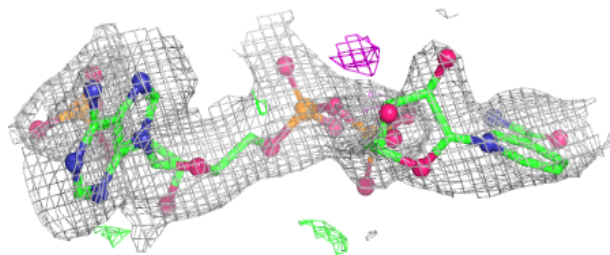
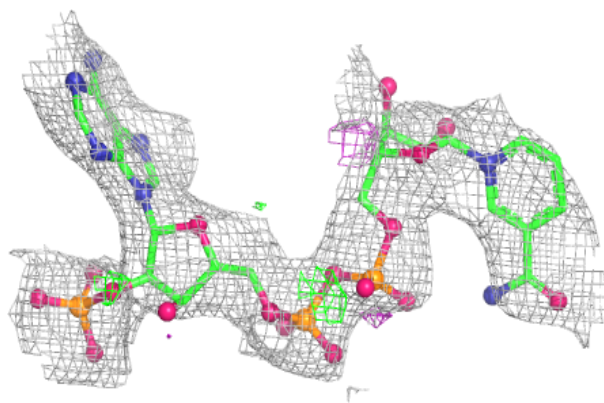
**Electron density around GTP E 603:**

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

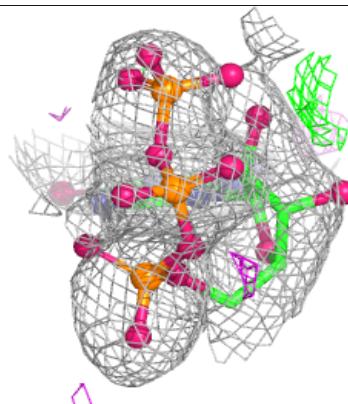
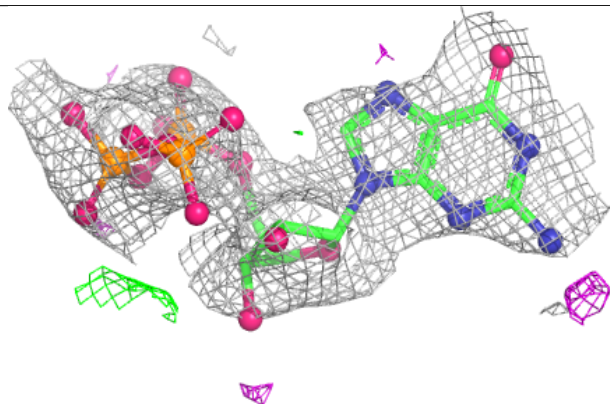
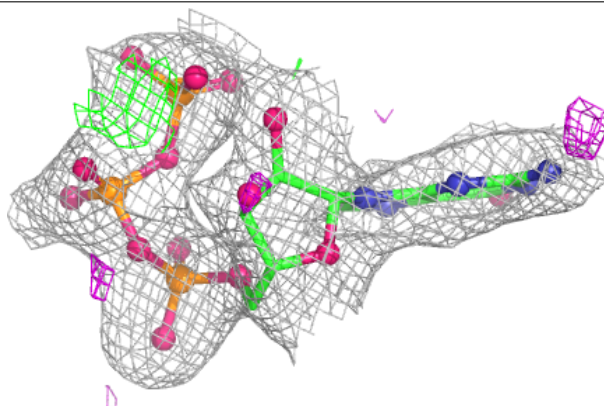


Electron density around NDP C 602:

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

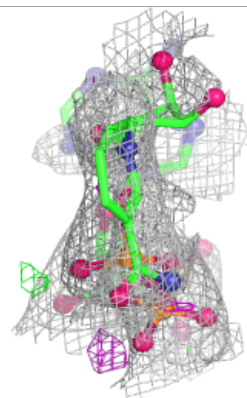
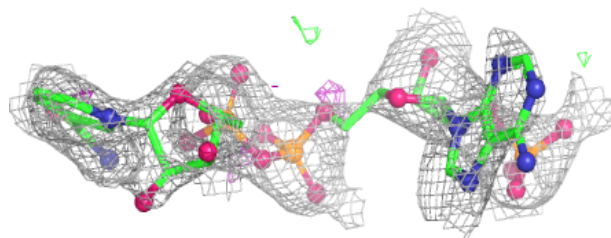
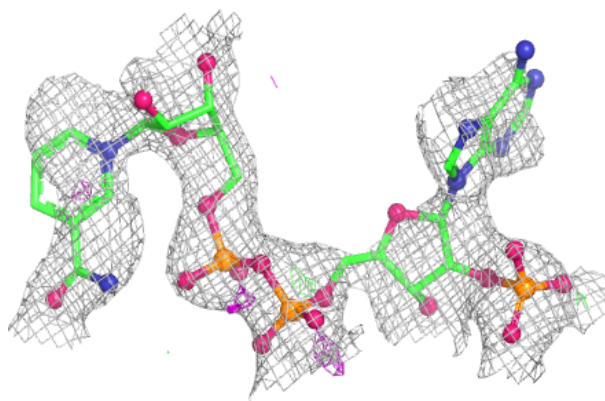
**Electron density around GTP D 603:**

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

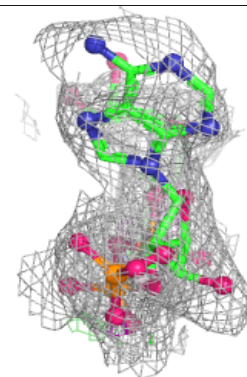
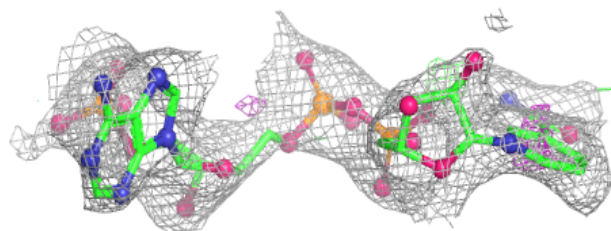
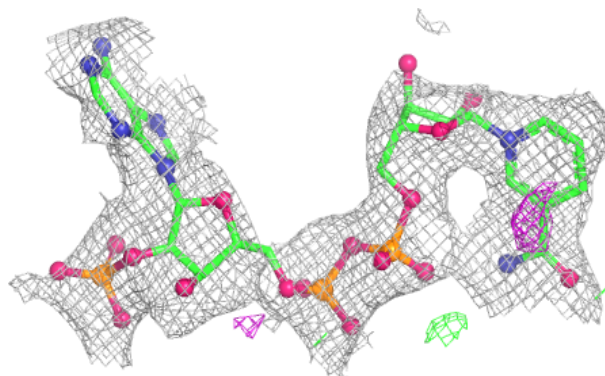


Electron density around NDP E 602:

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

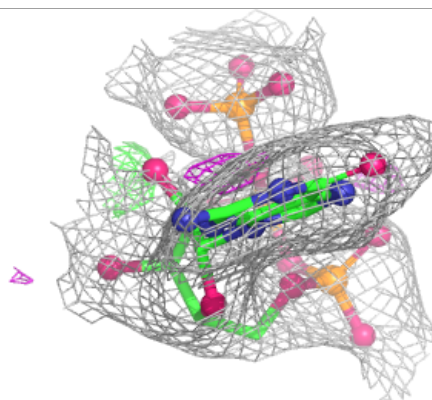
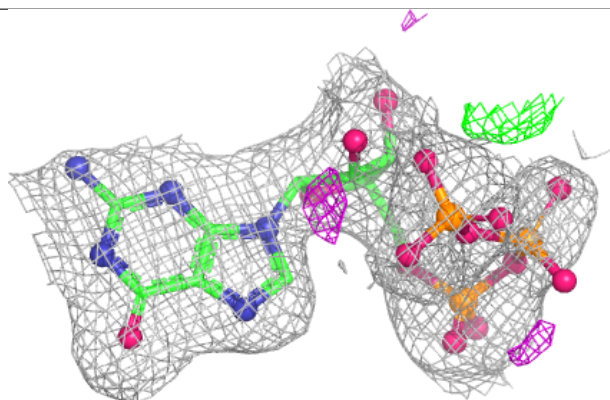
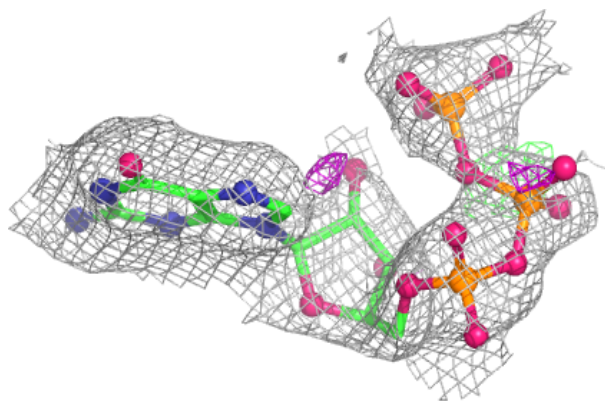
**Electron density around NDP B 602:**

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

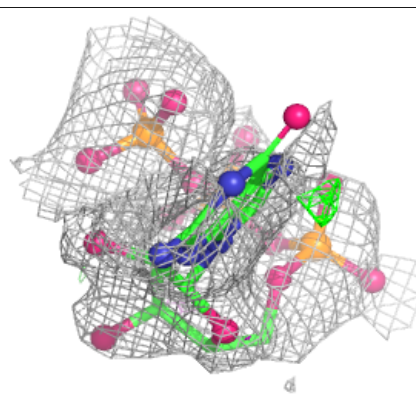
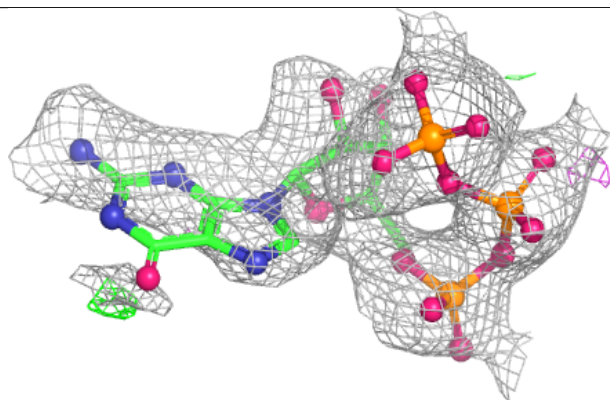
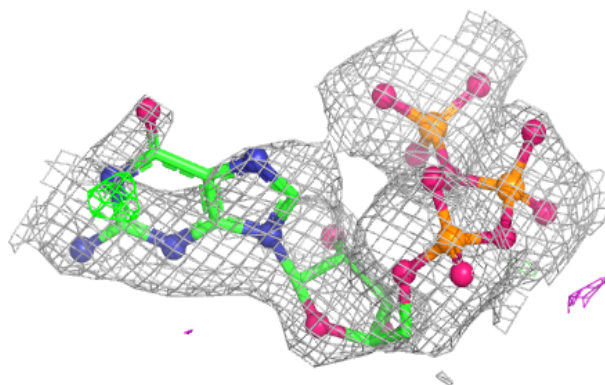


Electron density around GTP B 603:

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

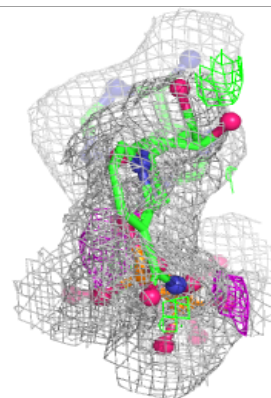
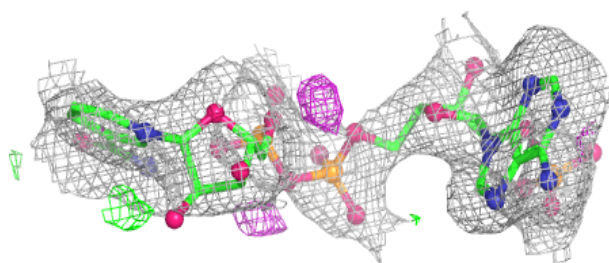
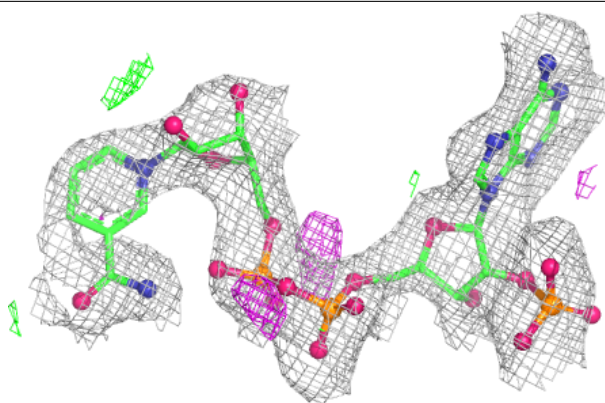
**Electron density around GTP C 603:**

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

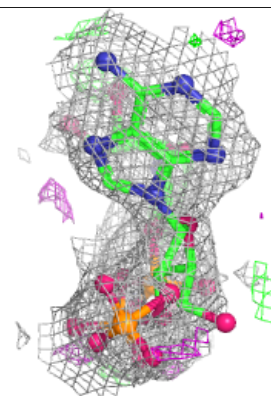
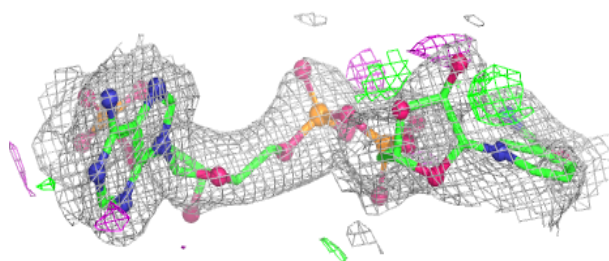
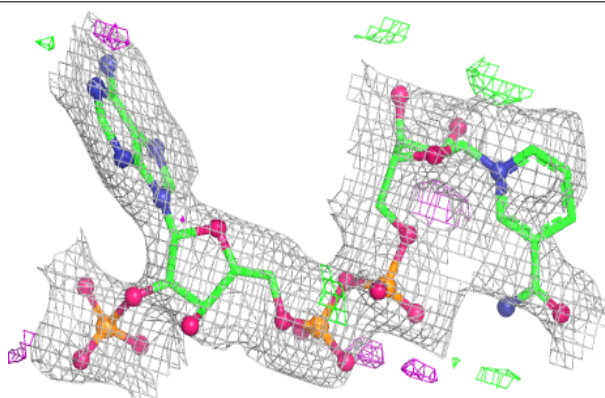


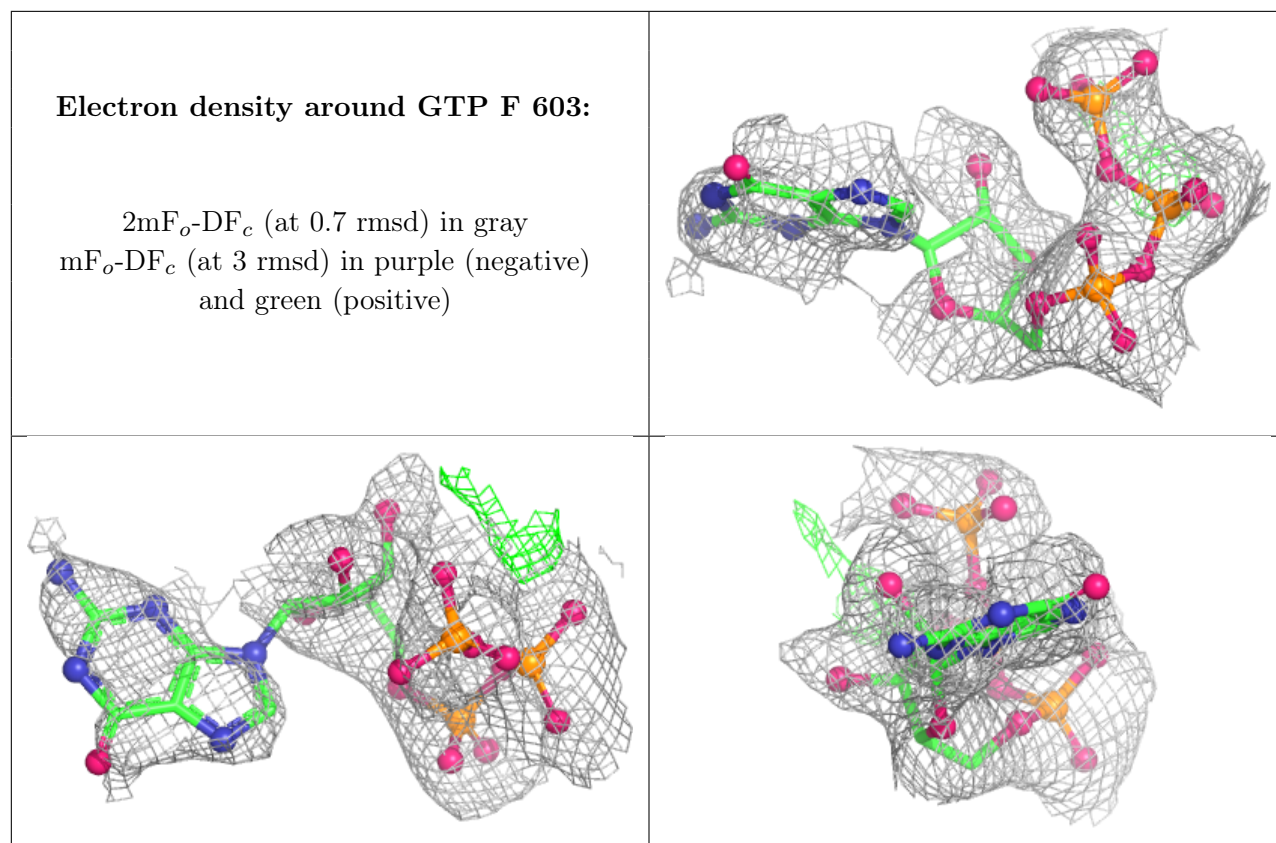
Electron density around NDP D 602:

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

**Electron density around NDP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.