



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:51 PM UTC

PDB ID : 9L6F / pdb_00009L6f
Title : Crystal structure of KRas G12D (GDP) in complex with ASP3082
Authors : Amano, Y.; Tateishi, Y.
Deposited on : 2024-12-24
Resolution : 3.18 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

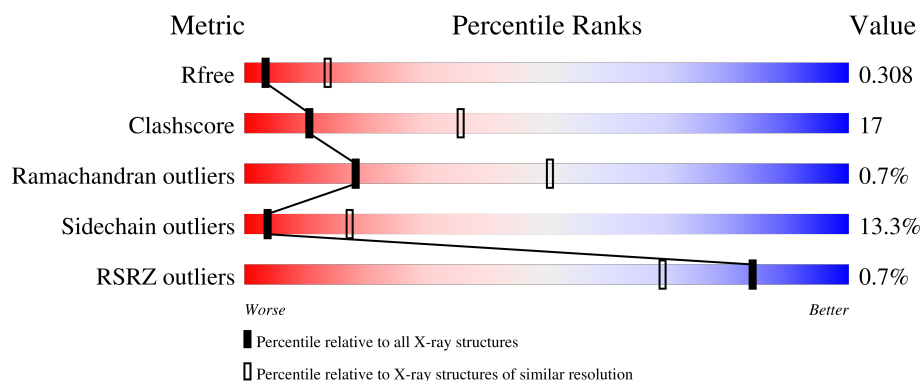
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	163	
1	E	163	
1	I	163	
1	M	163	
2	B	96	

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Mol	Chain	Length	Quality of chain
2	F	96	
2	J	96	
2	N	96	
3	C	118	
3	G	118	
3	K	118	
3	O	118	
4	D	170	
4	H	170	
4	L	170	
4	P	170	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16509 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 von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1207	766	227	212	2			
1	E	149	Total	C	N	O	S	0	0	0
			1203	764	226	211	2			
1	I	149	Total	C	N	O	S	0	0	0
			1203	764	226	211	2			
1	M	149	Total	C	N	O	S	0	0	0
			1203	764	226	211	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP P40337
A	52	SER	-	expression tag	UNP P40337
A	53	HIS	-	expression tag	UNP P40337
E	51	GLY	-	expression tag	UNP P40337
E	52	SER	-	expression tag	UNP P40337
E	53	HIS	-	expression tag	UNP P40337
I	51	GLY	-	expression tag	UNP P40337
I	52	SER	-	expression tag	UNP P40337
I	53	HIS	-	expression tag	UNP P40337
M	51	GLY	-	expression tag	UNP P40337
M	52	SER	-	expression tag	UNP P40337
M	53	HIS	-	expression tag	UNP P40337

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			689	445	109	130	5			
2	F	86	Total	C	N	O	S	0	0	0
			678	438	107	128	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	88	Total	C	N	O	S	0	0	0
			689	445	109	130	5			
2	N	86	Total	C	N	O	S	0	0	0
			678	438	107	128	5			

- Molecule 3 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	0	0	0
			779	493	129	152	5			
3	G	105	Total	C	N	O	S	0	0	0
			826	524	139	158	5			
3	K	101	Total	C	N	O	S	0	0	0
			792	504	129	154	5			
3	O	105	Total	C	N	O	S	0	0	0
			826	524	139	158	5			

- Molecule 4 is a protein called Isoform 2B of GTPase KRas.

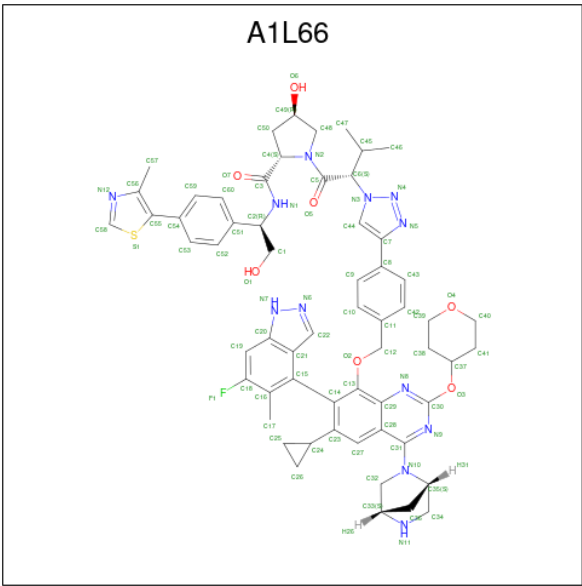
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1328	831	228	263	6			
4	H	164	Total	C	N	O	S	0	0	0
			1312	819	226	261	6			
4	L	166	Total	C	N	O	S	0	0	0
			1328	831	228	263	6			
4	P	166	Total	C	N	O	S	0	0	0
			1328	831	228	263	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP P01116
D	12	ASP	GLY	engineered mutation	UNP P01116
H	0	GLY	-	expression tag	UNP P01116
H	12	ASP	GLY	engineered mutation	UNP P01116
L	0	GLY	-	expression tag	UNP P01116
L	12	ASP	GLY	engineered mutation	UNP P01116
P	0	GLY	-	expression tag	UNP P01116
P	12	ASP	GLY	engineered mutation	UNP P01116

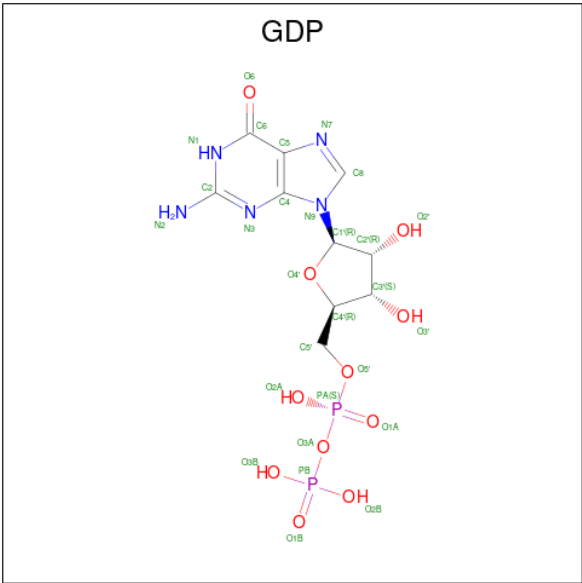
- Molecule 5 is ASP3082 (CCD ID: A1L66) (formula: C₆₀H₆₅FN₁₂O₇S) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	S	0	0
			81	60	1	12	7	1		
5	H	1	Total	C	F	N	O	S	0	0
			81	60	1	12	7	1		
5	L	1	Total	C	F	N	O	S	0	0
			81	60	1	12	7	1		
5	P	1	Total	C	F	N	O	S	0	0
			81	60	1	12	7	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	H	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	L	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	P	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

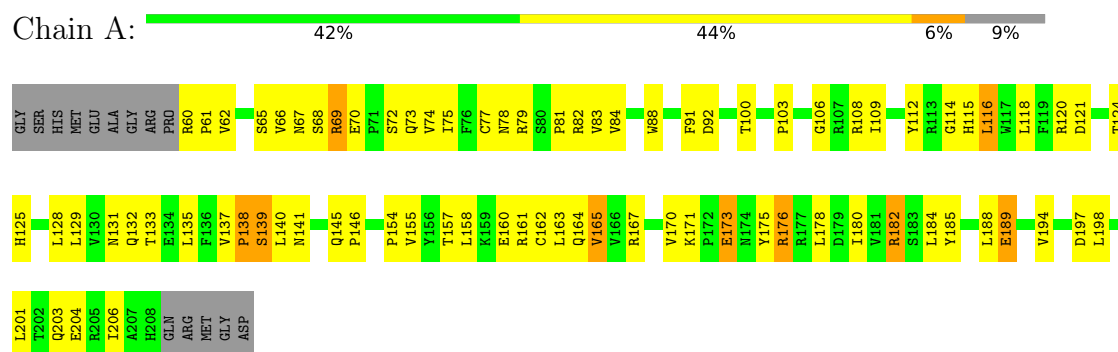
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	H	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		
7	P	1	Total	Mg	0	0
			1	1		

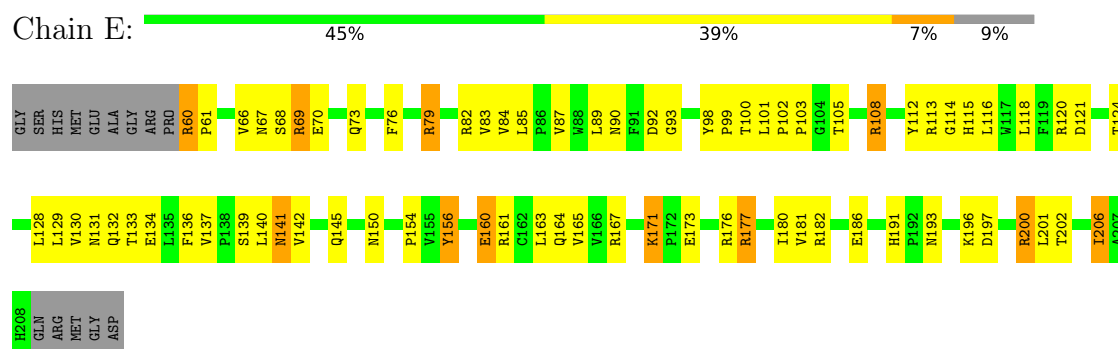
3 Residue-property plots [i](#)

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

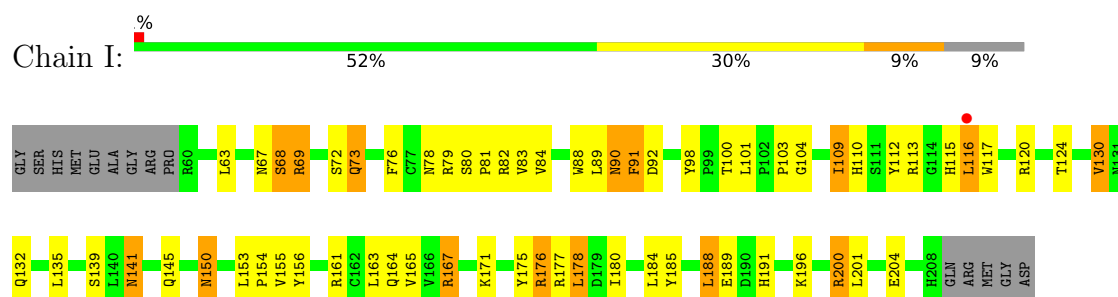
- Molecule 1: von Hippel-Lindau disease tumor suppressor



- Molecule 1: von Hippel-Lindau disease tumor suppressor

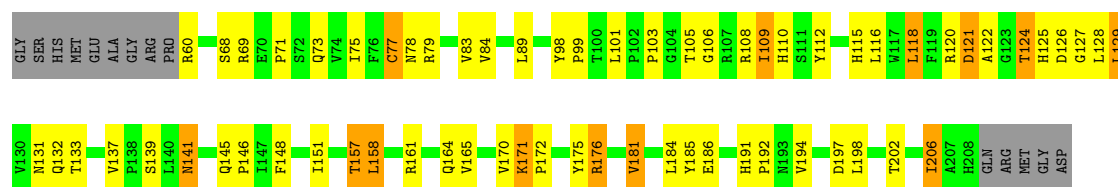


- Molecule 1: von Hippel-Lindau disease tumor suppressor



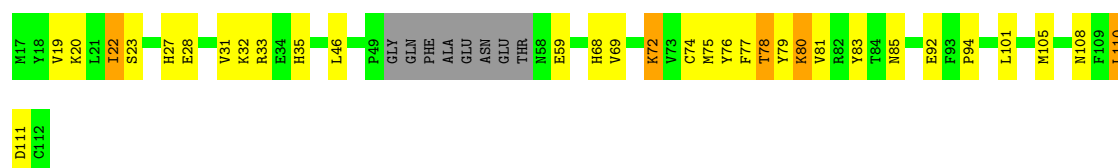
- Molecule 1: von Hippel-Lindau disease tumor suppressor

Chain M: 



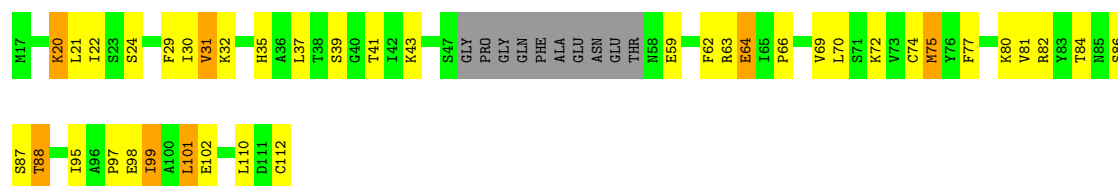
• Molecule 2: Elongin-C

Chain B: 

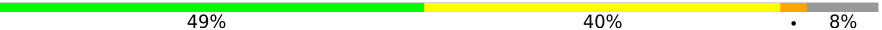


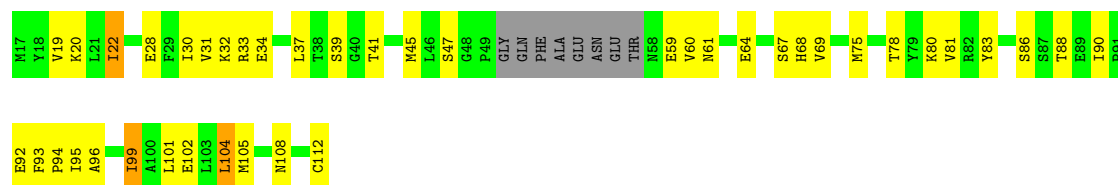
• Molecule 2: Elongin-C

Chain F: 



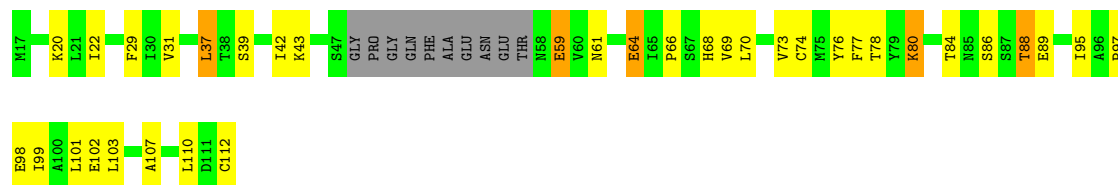
• Molecule 2: Elongin-C

Chain J: 



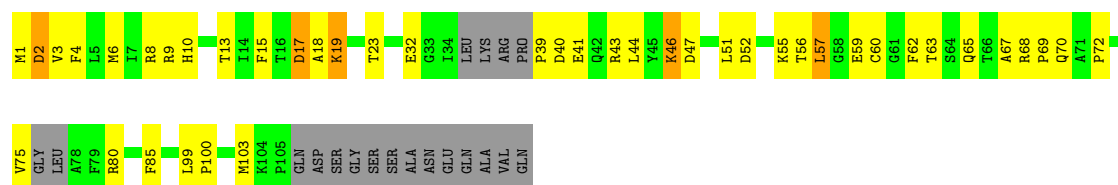
• Molecule 2: Elongin-C

Chain N: 

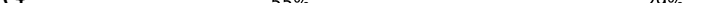


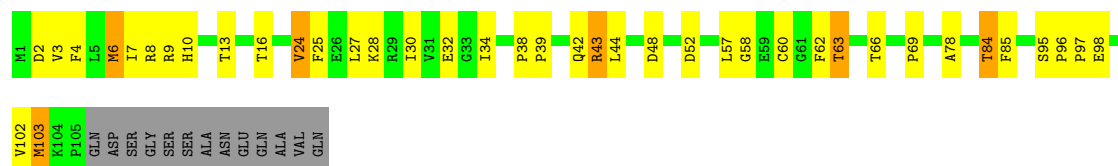
• Molecule 3: Elongin-B

Chain C: 47% 32% . 16%

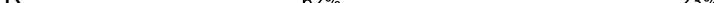


- Molecule 3: Elongin-B

Chain G:  55% 29% 5% 11%

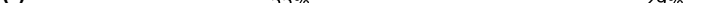


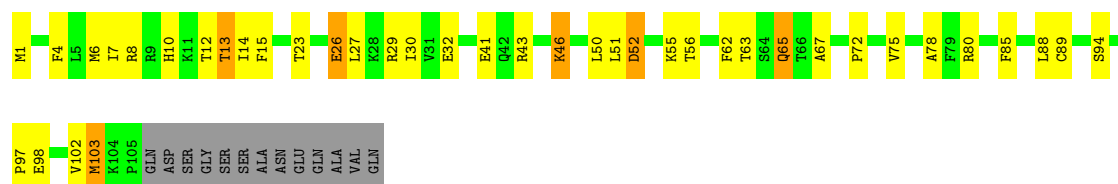
- Molecule 3: Elongin-B

Chain K:  62% 23% 14%

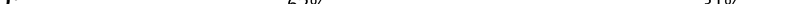


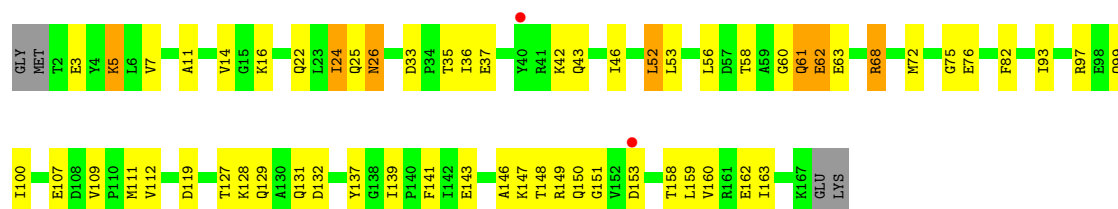
- Molecule 3: Elongin-B

Chain O:  55% 29% 5% 11%

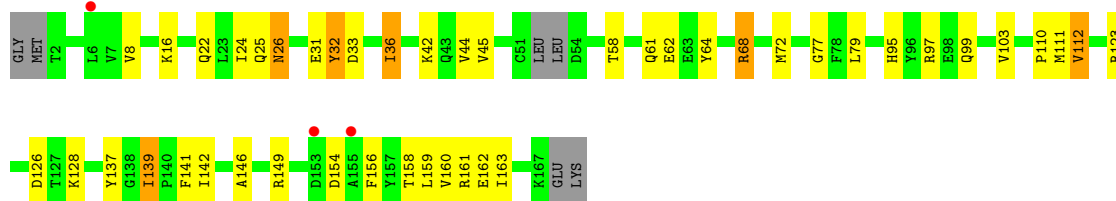


- Molecule 4: Isoform 2B of GTPase KRas

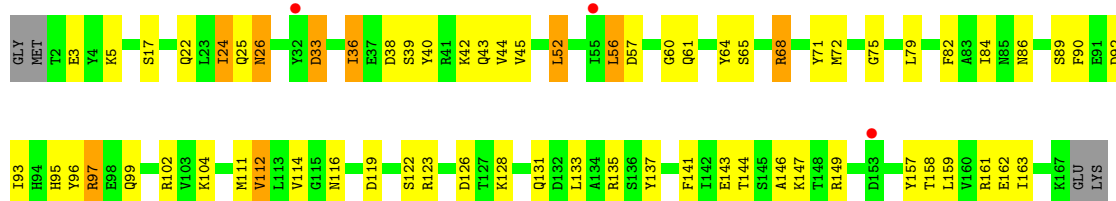
Chain D:  %



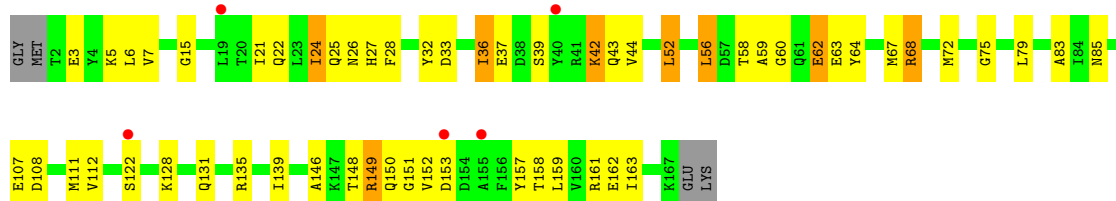
- Molecule 4: Isoform 2B of GTPase KRas



• Molecule 4: Isoform 2B of GTPase KRas



• Molecule 4: Isoform 2B of GTPase KRas



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.35Å 58.91Å 165.98Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	48.76 – 3.18 48.76 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.76-3.18) 99.9 (48.76-3.18)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.241 , 0.305 0.248 , 0.308	Depositor DCC
R_{free} test set	2333 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	82.6	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 104.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16509	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0448e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1L66, MG, GDP

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	0.46	0/1239	0.97	0/1691
1	E	0.49	0/1235	1.00	1/1686 (0.1%)
1	I	0.47	0/1235	1.00	1/1686 (0.1%)
1	M	0.50	0/1235	1.04	0/1686
2	B	0.44	0/704	0.96	0/952
2	F	0.48	0/692	1.02	0/935
2	J	0.43	0/704	1.00	0/952
2	N	0.48	0/692	1.04	0/935
3	C	0.44	0/793	0.94	0/1069
3	G	0.46	0/843	1.05	0/1140
3	K	0.48	0/807	1.01	1/1090 (0.1%)
3	O	0.48	0/843	1.04	0/1140
4	D	0.41	0/1349	0.98	0/1821
4	H	0.43	0/1332	0.99	0/1796
4	L	0.41	0/1349	0.96	0/1821
4	P	0.41	0/1349	0.97	0/1821
All	All	0.45	0/16401	1.00	3/22221 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	38	PRO	N-CA-C	5.87	116.10	110.47
1	I	91	PHE	CB-CA-C	-5.79	101.14	110.74
1	E	156	TYR	CB-CA-C	-5.74	98.98	109.54

There are no chirality outliers.

There are no planarity outliers.

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	1207	0	1198	72	0
1	E	1203	0	1192	56	0
1	I	1203	0	1192	50	0
1	M	1203	0	1192	56	0
2	B	689	0	680	27	0
2	F	678	0	670	26	0
2	J	689	0	680	30	0
2	N	678	0	670	23	0
3	C	779	0	770	35	0
3	G	826	0	829	25	0
3	K	792	0	787	25	0
3	O	826	0	829	26	0
4	D	1328	0	1303	43	0
4	H	1312	0	1281	30	0
4	L	1328	0	1303	46	0
4	P	1328	0	1303	42	0
5	A	81	0	0	2	0
5	H	81	0	0	3	0
5	L	81	0	0	5	0
5	P	81	0	0	10	0
6	D	28	0	12	2	0
6	H	28	0	12	1	0
6	L	28	0	12	2	0
6	P	28	0	12	1	0
7	D	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
7	P	1	0	0	0	0
All	All	16509	0	15927	543	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (543) 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)
3:K:41:GLU:HB2	3:K:79:PHE:CE1	1.35	1.59
3:K:41:GLU:CB	3:K:79:PHE:HE1	1.37	1.34
2:J:101:LEU:HD22	3:K:103:MET:SD	1.90	1.12
1:E:69:ARG:HG3	4:H:62:GLU:HB2	1.39	1.02
4:D:149:ARG:HD3	4:P:148:THR:O	1.60	1.00
1:A:184:LEU:HD21	2:B:108:ASN:ND2	1.81	0.96
3:K:41:GLU:CB	3:K:79:PHE:CE1	2.25	0.94
4:D:153:ASP:OD2	4:P:150:GLN:HG3	1.68	0.93
3:G:7:ILE:HD11	3:G:27:LEU:HD11	1.49	0.93
1:M:69:ARG:HD2	4:P:62:GLU:HG3	1.51	0.91
4:D:148:THR:O	4:P:149:ARG:HD3	1.71	0.91
1:A:180:ILE:O	1:A:182:ARG:NH1	2.04	0.90
3:K:37:ARG:HB3	3:K:79:PHE:CE2	2.07	0.89
1:M:121:ASP:OD2	1:M:124:THR:HG23	1.71	0.89
1:M:141:ASN:HB3	1:M:145:GLN:O	1.74	0.88
4:D:153:ASP:OD2	4:P:150:GLN:CG	2.23	0.86
1:E:167:ARG:HD3	1:E:191:HIS:CD2	2.11	0.86
1:I:167:ARG:HG3	1:I:167:ARG:HH11	1.39	0.85
2:N:102:GLU:OE1	3:O:97:PRO:HD2	1.76	0.85
3:C:9:ARG:HH11	3:C:9:ARG:HG2	1.39	0.85
1:E:69:ARG:HB2	4:H:62:GLU:O	1.77	0.84
1:M:73:GLN:HG2	1:M:110:HIS:CD2	2.13	0.84
1:A:69:ARG:O	1:A:69:ARG:HG2	1.76	0.83
3:C:2:ASP:OD2	3:C:19:LYS:HE2	1.77	0.83
2:F:82:ARG:HG3	2:F:82:ARG:O	1.76	0.83
1:A:184:LEU:HD21	2:B:108:ASN:HD22	1.40	0.83
1:E:167:ARG:HD3	1:E:191:HIS:HD2	1.41	0.82
3:O:8:ARG:HG2	3:O:13:THR:HG23	1.61	0.82
2:J:75:MET:HE2	3:K:72:PRO:HD2	1.61	0.81
1:I:167:ARG:HH11	1:I:167:ARG:CG	1.92	0.81
1:M:176:ARG:HH11	1:M:176:ARG:CG	1.92	0.81
1:M:73:GLN:HG2	1:M:110:HIS:HD2	1.44	0.81
2:B:31:VAL:HG12	3:C:15:PHE:HB2	1.62	0.79
3:K:37:ARG:HB3	3:K:79:PHE:CZ	2.18	0.79
4:D:37:GLU:HG3	4:D:58:THR:HA	1.66	0.78
4:L:17:SER:HA	4:L:57:ASP:OD2	1.85	0.77
4:D:153:ASP:OD2	4:P:150:GLN:CB	2.33	0.77
4:H:111:MET:HB3	4:H:139:ILE:HG21	1.65	0.77
4:L:75:GLY:O	4:L:104:LYS:NZ	2.18	0.76
1:I:68:SER:O	1:I:69:ARG:HG3	1.87	0.74
2:N:29:PHE:HD2	2:N:70:LEU:HD23	1.52	0.74
2:B:22:ILE:HG23	2:B:28:GLU:HG2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:SER:HA	2:F:112:CYS:HB3	1.68	0.74
1:I:76:PHE:HB3	1:I:101:LEU:HD11	1.71	0.73
1:E:98:TYR:HD1	1:E:99:PRO:HD2	1.51	0.73
4:H:79:LEU:HD23	4:H:112:VAL:HG13	1.70	0.72
1:A:141:ASN:HB3	1:A:145:GLN:O	1.90	0.72
1:A:160:GLU:HA	1:A:163:LEU:HB2	1.71	0.71
1:E:130:VAL:HG11	1:E:136:PHE:HB2	1.71	0.71
2:N:20:LYS:HB3	2:N:59:GLU:HG2	1.72	0.71
2:F:20:LYS:HD3	2:F:22:ILE:HD11	1.72	0.71
3:C:44:LEU:HD22	3:C:75:VAL:HG12	1.72	0.71
3:G:6:MET:HE3	3:G:8:ARG:HD2	1.71	0.71
5:A:301:A1L66:N11	4:D:60:GLY:O	2.24	0.70
1:E:79:ARG:HH11	1:E:79:ARG:CG	2.04	0.70
1:A:141:ASN:HD22	1:A:146:PRO:HA	1.56	0.70
1:A:138:PRO:O	1:A:139:SER:HB3	1.90	0.70
4:D:25:GLN:O	4:D:26:ASN:HB2	1.91	0.69
4:L:25:GLN:O	4:L:26:ASN:HB2	1.91	0.69
1:M:176:ARG:HH11	1:M:176:ARG:HG2	1.56	0.69
4:D:22:GLN:OE1	4:D:149:ARG:HD2	1.93	0.69
1:E:76:PHE:HB3	1:E:101:LEU:HD11	1.73	0.69
1:E:177:ARG:HH11	1:E:177:ARG:HG3	1.57	0.69
1:A:170:VAL:HG21	1:A:178:LEU:HD21	1.74	0.69
1:I:161:ARG:NH2	2:J:93:PHE:O	2.22	0.69
2:J:101:LEU:CD2	3:K:100:PRO:HG2	2.22	0.69
1:A:72:SER:O	1:A:74:VAL:HG23	1.93	0.68
3:O:7:ILE:HD11	3:O:27:LEU:HD11	1.75	0.68
1:A:67:ASN:HA	1:A:91:PHE:CE1	2.28	0.68
1:A:185:TYR:O	1:A:189:GLU:HB2	1.93	0.68
1:M:176:ARG:HA	1:M:185:TYR:CE1	2.28	0.68
1:I:175:TYR:CE2	1:I:188:LEU:HB3	2.28	0.68
3:K:42:GLN:HB3	3:K:79:PHE:CE2	2.28	0.68
1:A:184:LEU:CD2	2:B:108:ASN:ND2	2.57	0.68
1:E:69:ARG:HG3	4:H:62:GLU:CB	2.21	0.68
1:M:69:ARG:HB2	4:P:62:GLU:HB2	1.75	0.67
3:C:9:ARG:HG2	3:C:9:ARG:NH1	2.10	0.67
1:E:177:ARG:HG3	1:E:177:ARG:NH1	2.10	0.67
2:N:29:PHE:CD2	2:N:70:LEU:HD23	2.29	0.67
4:H:25:GLN:O	4:H:26:ASN:HB2	1.94	0.67
3:C:23:THR:HA	3:C:56:THR:HA	1.76	0.67
1:E:98:TYR:CD1	1:E:99:PRO:HD2	2.30	0.67
5:L:203:A1L66:C32	5:L:203:A1L66:C27	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:44:VAL:HG21	4:L:157:TYR:OH	1.96	0.66
1:M:131:ASN:O	1:M:132:GLN:HB2	1.96	0.66
4:P:159:LEU:O	4:P:163:ILE:HG13	1.94	0.66
3:G:7:ILE:CD1	3:G:27:LEU:HD11	2.22	0.66
1:M:98:TYR:HD2	5:P:203:A1L66:C53	2.08	0.66
3:G:27:LEU:HA	3:G:30:ILE:HD12	1.77	0.66
1:I:132:GLN:HE22	1:M:108:ARG:HD2	1.59	0.66
4:D:150:GLN:HB2	4:P:153:ASP:OD2	1.96	0.65
1:M:68:SER:O	1:M:69:ARG:HG2	1.95	0.65
1:M:141:ASN:HD22	1:M:146:PRO:HA	1.60	0.65
1:A:69:ARG:HG3	4:D:62:GLU:O	1.97	0.65
2:J:101:LEU:CD2	3:K:103:MET:SD	2.77	0.65
4:D:82:PHE:HB3	4:D:93:ILE:HD11	1.79	0.65
4:H:16:LYS:N	6:H:201:GDP:O1B	2.29	0.65
4:L:119:ASP:OD2	4:L:147:LYS:HB3	1.96	0.65
1:M:120:ARG:HH22	1:M:197:ASP:CG	2.04	0.65
4:P:60:GLY:O	5:P:203:A1L66:N11	2.29	0.65
1:A:67:ASN:HA	1:A:91:PHE:HE1	1.63	0.64
2:J:19:VAL:HG13	2:J:33:ARG:HG3	1.80	0.64
1:A:116:LEU:CD1	1:A:137:VAL:HG22	2.27	0.64
4:L:97:ARG:HD3	4:L:137:TYR:CD1	2.33	0.64
3:C:55:LYS:HD3	3:C:59:GLU:HB3	1.78	0.64
2:B:75:MET:HE2	3:C:72:PRO:HD2	1.80	0.64
4:L:97:ARG:HD3	4:L:137:TYR:CE1	2.33	0.64
1:M:161:ARG:HD2	1:M:164:GLN:NE2	2.13	0.63
1:A:132:GLN:HE22	1:E:108:ARG:HD2	1.63	0.63
3:K:37:ARG:CB	3:K:79:PHE:CE2	2.81	0.63
1:A:60:ARG:N	1:A:61:PRO:CD	2.62	0.63
2:J:20:LYS:HB3	2:J:59:GLU:HG2	1.81	0.63
1:M:170:VAL:O	1:M:175:TYR:HE1	1.81	0.63
4:L:64:TYR:HA	5:L:203:A1L66:N6	2.14	0.63
1:E:112:TYR:HB2	1:E:115:HIS:CD2	2.35	0.62
1:A:75:ILE:HG21	2:F:87:SER:HB2	1.81	0.62
1:A:176:ARG:HH21	1:A:185:TYR:CB	2.12	0.62
2:J:101:LEU:HD23	3:K:100:PRO:HG2	1.81	0.62
1:M:161:ARG:HD2	1:M:164:GLN:HE21	1.65	0.62
4:H:68:ARG:O	4:H:72:MET:HG2	2.00	0.62
1:A:79:ARG:NH2	1:E:150:ASN:OD1	2.33	0.62
1:I:78:ASN:O	1:I:104:GLY:HA2	2.00	0.62
2:N:73:VAL:HG11	2:N:110:LEU:HD13	1.82	0.61
4:H:112:VAL:HG12	4:H:159:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:46:LYS:HB2	3:O:51:LEU:HD21	1.82	0.61
4:P:158:THR:O	4:P:162:GLU:HG2	2.01	0.60
3:G:84:THR:HG22	3:G:85:PHE:H	1.66	0.60
4:L:3:GLU:HA	4:L:52:LEU:O	2.02	0.60
1:M:121:ASP:HB3	1:M:126:ASP:HB2	1.81	0.60
3:C:43:ARG:HG3	3:C:85:PHE:CE1	2.37	0.60
1:E:73:GLN:H	1:E:141:ASN:HD21	1.50	0.59
1:A:114:GLY:HA2	1:A:137:VAL:CG1	2.31	0.59
1:I:150:ASN:HB2	1:M:148:PHE:CE2	2.36	0.59
1:M:112:TYR:HB2	1:M:115:HIS:CD2	2.37	0.59
1:E:102:PRO:HG2	1:E:105:THR:HG21	1.84	0.59
1:M:127:GLY:O	1:M:128:LEU:HD23	2.02	0.59
4:L:44:VAL:HG22	4:L:45:VAL:H	1.68	0.59
5:A:301:A1L66:C27	5:A:301:A1L66:C32	2.80	0.59
1:E:154:PRO:HG2	1:E:156:TYR:CE1	2.38	0.59
4:L:65:SER:OG	4:L:68:ARG:HB2	2.03	0.59
1:A:78:ASN:ND2	1:A:103:PRO:HA	2.18	0.58
1:E:177:ARG:HH11	1:E:177:ARG:CG	2.17	0.58
1:A:73:GLN:OE1	1:A:108:ARG:NH2	2.36	0.58
4:D:22:GLN:NE2	4:D:146:ALA:O	2.33	0.58
1:A:75:ILE:CG2	2:F:87:SER:HB2	2.34	0.58
1:I:112:TYR:OH	4:L:99:GLN:NE2	2.36	0.58
1:A:197:ASP:O	1:A:201:LEU:HD13	2.04	0.58
5:P:203:A1L66:C27	5:P:203:A1L66:C32	2.82	0.58
1:E:82:ARG:HD2	1:E:121:ASP:OD2	2.03	0.58
2:F:37:LEU:HD22	2:F:43:LYS:HG3	1.86	0.58
2:F:82:ARG:O	2:F:82:ARG:CG	2.50	0.58
4:L:68:ARG:O	4:L:72:MET:HG2	2.03	0.58
4:D:153:ASP:OD2	4:P:150:GLN:HB2	2.02	0.58
1:A:129:LEU:HG	1:A:154:PRO:HG3	1.86	0.57
3:C:41:GLU:CB	3:C:80:ARG:HB3	2.34	0.57
2:F:102:GLU:OE1	3:G:97:PRO:HD2	2.04	0.57
1:I:80:SER:HB2	1:I:153:LEU:HG	1.86	0.57
2:B:94:PRO:HD3	3:C:70:GLN:HG3	1.86	0.57
4:L:17:SER:HB2	6:L:201:GDP:O1A	2.03	0.57
3:O:80:ARG:HA	3:O:85:PHE:HA	1.86	0.57
4:P:37:GLU:HG3	4:P:58:THR:HA	1.87	0.57
1:A:163:LEU:O	1:A:167:ARG:HG3	2.05	0.57
1:E:160:GLU:HA	1:E:163:LEU:HB2	1.86	0.57
4:D:46:ILE:HD13	4:D:160:VAL:HG21	1.87	0.57
3:K:37:ARG:NH2	3:K:79:PHE:CD1	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:ARG:NH2	4:P:62:GLU:OE1	2.38	0.57
4:L:146:ALA:N	6:L:201:GDP:O6	2.38	0.56
1:M:176:ARG:HH11	1:M:176:ARG:HG3	1.71	0.56
1:I:175:TYR:CD2	1:I:188:LEU:HB3	2.39	0.56
4:L:82:PHE:HB3	4:L:93:ILE:HD11	1.86	0.56
1:I:81:PRO:HD2	1:I:153:LEU:HD11	1.86	0.56
1:M:103:PRO:O	1:M:105:THR:HG23	2.06	0.56
3:C:44:LEU:HD22	3:C:75:VAL:CG1	2.35	0.56
1:I:178:LEU:HD23	2:J:101:LEU:HD21	1.87	0.56
3:C:3:VAL:HG22	3:C:18:ALA:O	2.05	0.56
4:D:111:MET:HG2	4:D:139:ILE:HD13	1.88	0.56
1:I:196:LYS:O	1:I:200:ARG:HB2	2.06	0.56
4:D:141:PHE:CZ	4:D:143:GLU:HG2	2.40	0.55
2:B:33:ARG:HH22	2:B:46:LEU:HB3	1.71	0.55
1:I:141:ASN:HB3	1:I:145:GLN:O	2.06	0.55
2:J:34:GLU:HA	2:J:37:LEU:HD12	1.88	0.55
3:K:80:ARG:HA	3:K:85:PHE:HA	1.89	0.55
4:H:158:THR:O	4:H:162:GLU:HG2	2.06	0.55
1:I:109:ILE:HG13	5:L:203:A1L66:C59	2.37	0.55
3:O:43:ARG:HB2	3:O:78:ALA:HB3	1.89	0.55
1:I:67:ASN:HA	1:I:91:PHE:CE1	2.41	0.55
1:A:139:SER:OG	1:A:140:LEU:N	2.40	0.54
1:M:78:ASN:ND2	1:M:84:VAL:HG23	2.22	0.54
1:M:161:ARG:O	1:M:164:GLN:HB2	2.07	0.54
1:I:112:TYR:OH	4:L:95:HIS:HE1	1.90	0.54
4:D:119:ASP:OD2	4:D:147:LYS:HB3	2.08	0.54
3:K:41:GLU:C	3:K:79:PHE:CE1	2.86	0.54
4:L:149:ARG:O	4:L:149:ARG:HG2	2.08	0.54
4:P:37:GLU:HB2	4:P:59:ALA:HB3	1.89	0.54
1:E:165:VAL:HG21	2:F:95:ILE:HB	1.88	0.54
2:J:19:VAL:O	2:J:30:ILE:HA	2.07	0.54
4:L:158:THR:O	4:L:162:GLU:HG2	2.08	0.54
1:A:170:VAL:HG23	3:C:103:MET:HG3	1.88	0.54
1:A:83:VAL:HG12	1:A:100:THR:OG1	2.08	0.54
1:A:176:ARG:HH21	1:A:185:TYR:HB3	1.73	0.54
2:B:27:HIS:HE1	3:C:8:ARG:HH22	1.57	0.53
2:B:35:HIS:CD2	2:B:78:THR:HA	2.43	0.53
2:J:94:PRO:HD3	3:K:70:GLN:HG3	1.90	0.53
2:B:83:TYR:OH	3:C:68:ARG:NH1	2.41	0.53
4:P:6:LEU:HD22	4:P:159:LEU:HD23	1.90	0.53
2:F:97:PRO:O	3:G:103:MET:HE3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:VAL:HG22	1:E:103:PRO:HD3	1.90	0.53
1:A:141:ASN:ND2	1:A:146:PRO:HA	2.22	0.53
4:P:111:MET:HB3	4:P:139:ILE:HG21	1.90	0.53
4:H:99:GLN:O	4:H:103:VAL:HG23	2.09	0.53
1:I:130:VAL:HA	1:I:150:ASN:O	2.08	0.53
1:E:141:ASN:HB3	1:E:145:GLN:O	2.07	0.53
4:D:24:ILE:HA	4:D:42:LYS:HD2	1.91	0.53
1:E:99:PRO:HG2	5:H:203:A1L66:C56	2.39	0.53
1:A:145:GLN:HE22	1:E:137:VAL:H	1.56	0.52
2:F:30:ILE:HG21	3:G:34:ILE:HG21	1.91	0.52
1:I:90:ASN:HD21	1:I:92:ASP:HB2	1.74	0.52
3:O:29:ARG:O	3:O:32:GLU:HB3	2.08	0.52
3:C:41:GLU:HB3	3:C:80:ARG:HB3	1.91	0.52
4:D:159:LEU:O	4:D:163:ILE:HG13	2.10	0.52
3:O:43:ARG:HD2	3:O:50:LEU:HD11	1.90	0.52
1:E:79:ARG:HH11	1:E:79:ARG:HG2	1.74	0.52
1:I:163:LEU:HB3	1:I:167:ARG:NH1	2.24	0.52
1:M:157:THR:HA	2:N:76:TYR:OH	2.10	0.52
2:J:39:SER:HA	2:J:112:CYS:HB3	1.91	0.52
4:L:141:PHE:CZ	4:L:143:GLU:HG2	2.45	0.52
3:O:52:ASP:OD1	3:O:52:ASP:C	2.53	0.52
4:L:79:LEU:HD23	4:L:112:VAL:HG13	1.91	0.52
1:M:172:PRO:HA	1:M:175:TYR:CE1	2.45	0.52
1:A:115:HIS:O	1:A:137:VAL:HG13	2.10	0.52
2:B:20:LYS:HB3	2:B:59:GLU:HG3	1.91	0.52
4:D:111:MET:HB3	4:D:139:ILE:HG21	1.92	0.52
4:P:3:GLU:HG3	4:P:52:LEU:HB3	1.91	0.52
3:G:43:ARG:HB2	3:G:78:ALA:HB3	1.92	0.52
4:D:127:THR:O	4:D:131:GLN:HG3	2.09	0.51
3:O:6:MET:HG3	3:O:72:PRO:HB2	1.91	0.51
4:D:160:VAL:HA	4:D:163:ILE:HD12	1.92	0.51
1:I:184:LEU:HD21	2:J:108:ASN:CG	2.35	0.51
2:N:95:ILE:HD13	2:N:103:LEU:HD23	1.92	0.51
1:A:132:GLN:HE22	1:E:108:ARG:CD	2.23	0.51
3:G:4:PHE:CE2	3:G:69:PRO:HG3	2.45	0.51
2:F:35:HIS:CE1	2:F:81:VAL:HG11	2.46	0.51
1:I:98:TYR:OH	5:L:203:A1L66:O7	2.19	0.51
1:M:202:THR:O	1:M:206:ILE:HB	2.11	0.51
2:J:31:VAL:HG12	3:K:15:PHE:HB2	1.91	0.51
1:M:89:LEU:HD11	1:M:198:LEU:HD21	1.93	0.51
1:A:158:LEU:O	1:A:162:CYS:SG	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:THR:O	4:D:162:GLU:HG2	2.10	0.51
3:G:9:ARG:HG3	3:G:10:HIS:ND1	2.25	0.51
1:A:116:LEU:HD13	1:A:137:VAL:HG22	1.93	0.51
2:B:22:ILE:HA	2:B:27:HIS:O	2.11	0.50
3:C:8:ARG:HG2	3:C:13:THR:HG23	1.94	0.50
4:D:7:VAL:HG23	4:D:75:GLY:HA3	1.93	0.50
2:B:101:LEU:HD12	3:C:100:PRO:HG2	1.93	0.50
1:A:201:LEU:HA	1:A:204:GLU:HB2	1.93	0.50
1:E:167:ARG:CD	1:E:191:HIS:HD2	2.21	0.50
1:I:184:LEU:HD21	2:J:108:ASN:ND2	2.27	0.50
2:N:39:SER:HA	2:N:112:CYS:HB3	1.93	0.50
2:N:39:SER:HB3	2:N:42:ILE:HD12	1.94	0.50
1:A:137:VAL:HG12	1:A:138:PRO:HD2	1.94	0.50
4:L:123:ARG:HE	4:L:126:ASP:HA	1.77	0.50
1:E:60:ARG:N	1:E:61:PRO:HD2	2.27	0.49
2:J:22:ILE:HD12	2:J:28:GLU:HG2	1.94	0.49
4:P:112:VAL:HG12	4:P:159:LEU:HD13	1.94	0.49
3:C:80:ARG:HB2	3:C:85:PHE:CE1	2.46	0.49
1:E:66:VAL:HG23	1:E:68:SER:HB2	1.94	0.49
4:L:56:LEU:C	4:L:56:LEU:HD22	2.37	0.49
4:L:114:VAL:HG13	4:L:144:THR:HG23	1.94	0.49
4:P:131:GLN:O	4:P:135:ARG:HG3	2.12	0.49
1:E:176:ARG:HH12	1:E:182:ARG:NH2	2.10	0.49
1:I:112:TYR:OH	4:L:95:HIS:CE1	2.66	0.49
1:I:88:TRP:HB2	1:I:117:TRP:CZ3	2.47	0.49
3:K:10:HIS:O	3:K:91:GLU:HB3	2.12	0.49
1:A:77:CYS:SG	1:A:79:ARG:CZ	3.01	0.49
1:E:87:VAL:HB	1:E:118:LEU:HG	1.93	0.49
4:H:77:GLY:HA2	4:H:110:PRO:HB2	1.95	0.49
1:A:173:GLU:CD	1:A:173:GLU:H	2.21	0.49
1:A:131:ASN:O	1:A:132:GLN:HB2	2.11	0.49
2:F:21:LEU:HB3	2:F:62:PHE:HE2	1.78	0.48
3:O:26:GLU:O	3:O:29:ARG:HB2	2.13	0.48
4:P:68:ARG:O	4:P:72:MET:HG2	2.13	0.48
1:M:79:ARG:HB3	2:N:89:GLU:HG3	1.95	0.48
4:P:22:GLN:CG	4:P:149:ARG:HG3	2.42	0.48
4:D:3:GLU:HA	4:D:52:LEU:O	2.13	0.48
1:E:84:VAL:HG22	1:E:128:LEU:CD1	2.43	0.48
1:I:155:VAL:HG11	2:J:83:TYR:HB2	1.94	0.48
2:N:73:VAL:HG11	2:N:110:LEU:CD1	2.42	0.48
3:O:8:ARG:CG	3:O:13:THR:HG23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:99:GLN:OE1	4:L:102:ARG:NH2	2.45	0.48
2:J:86:SER:OG	2:J:88:THR:HG22	2.14	0.48
2:F:29:PHE:HD2	2:F:70:LEU:HD23	1.79	0.48
2:F:72:LYS:HA	2:F:75:MET:HG3	1.94	0.48
1:A:60:ARG:HG2	1:A:61:PRO:HD3	1.95	0.48
3:C:56:THR:HG22	3:C:59:GLU:CD	2.39	0.48
1:M:176:ARG:HA	1:M:185:TYR:CD1	2.49	0.48
3:G:32:GLU:OE2	3:G:38:PRO:HA	2.14	0.48
1:I:68:SER:C	1:I:69:ARG:HG3	2.38	0.48
2:J:94:PRO:O	2:J:95:ILE:HG13	2.14	0.48
3:K:41:GLU:CA	3:K:79:PHE:CE1	2.93	0.48
1:M:129:LEU:HD13	1:M:132:GLN:O	2.14	0.48
2:N:80:LYS:HE2	2:N:84:THR:OG1	2.14	0.48
2:F:64:GLU:CD	2:F:64:GLU:N	2.72	0.47
3:K:10:HIS:CE1	3:K:89:CYS:HB2	2.49	0.47
4:L:112:VAL:HG12	4:L:159:LEU:HD13	1.96	0.47
4:H:159:LEU:O	4:H:163:ILE:HG13	2.14	0.47
1:M:158:LEU:HG	2:N:76:TYR:CG	2.50	0.47
4:P:32:TYR:CE2	4:P:36:ILE:HD11	2.50	0.47
1:A:176:ARG:HH21	1:A:185:TYR:HB2	1.77	0.47
4:H:156:PHE:O	4:H:160:VAL:HG23	2.13	0.47
5:H:203:A1L66:C27	5:H:203:A1L66:C32	2.92	0.47
1:I:163:LEU:O	1:I:167:ARG:HG2	2.14	0.47
4:D:100:ILE:HG22	4:D:109:VAL:HG11	1.96	0.47
2:F:99:ILE:O	2:F:99:ILE:HG12	2.15	0.47
1:M:109:ILE:HG12	5:P:203:A1L66:C59	2.45	0.47
4:L:71:TYR:O	4:L:72:MET:HE2	2.15	0.47
4:L:86:ASN:OD1	4:L:89:SER:HB3	2.14	0.47
2:J:69:VAL:HG21	2:J:102:GLU:HB3	1.95	0.47
3:O:4:PHE:HB2	3:O:67:ALA:O	2.14	0.47
3:C:63:THR:C	3:C:65:GLN:H	2.23	0.47
3:G:57:LEU:O	3:G:62:PHE:HB2	2.14	0.47
4:P:64:TYR:HB2	5:P:203:A1L66:C9	2.45	0.47
4:P:150:GLN:O	4:P:152:VAL:N	2.47	0.47
3:C:3:VAL:HG21	3:C:57:LEU:HD22	1.96	0.47
1:I:73:GLN:HE22	1:I:110:HIS:HD2	1.63	0.47
4:D:68:ARG:O	4:D:72:MET:HG2	2.15	0.46
4:H:22:GLN:CG	4:H:149:ARG:HG3	2.45	0.46
1:M:98:TYR:HB3	1:M:99:PRO:HD2	1.97	0.46
2:B:72:LYS:HA	2:B:75:MET:SD	2.55	0.46
4:L:96:TYR:O	4:L:97:ARG:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:37:LEU:HD13	2:N:43:LYS:HG3	1.98	0.46
2:N:68:HIS:HB3	3:O:94:SER:O	2.15	0.46
2:F:66:PRO:HG2	2:F:69:VAL:HG23	1.97	0.46
2:F:74:CYS:O	2:F:77:PHE:N	2.48	0.46
3:G:24:VAL:HG21	3:G:52:ASP:O	2.15	0.46
2:J:67:SER:C	2:J:69:VAL:H	2.23	0.46
4:L:17:SER:CA	4:L:57:ASP:OD2	2.60	0.46
2:N:97:PRO:O	3:O:103:MET:HE2	2.15	0.46
1:E:89:LEU:HD12	1:E:116:LEU:HD23	1.98	0.46
1:E:90:ASN:OD1	1:E:93:GLY:N	2.43	0.46
3:G:24:VAL:HG12	3:G:44:LEU:HD12	1.97	0.46
1:I:89:LEU:HD12	1:I:116:LEU:HG	1.98	0.46
4:D:150:GLN:CG	4:P:153:ASP:OD2	2.63	0.46
1:E:89:LEU:HD12	1:E:116:LEU:CD2	2.46	0.46
4:L:22:GLN:CG	4:L:149:ARG:HG3	2.45	0.46
4:P:15:GLY:HA2	6:P:201:GDP:PA	2.55	0.46
3:C:63:THR:C	3:C:65:GLN:N	2.74	0.46
4:D:111:MET:CG	4:D:139:ILE:HD13	2.45	0.46
1:E:79:ARG:HH11	1:E:79:ARG:HG3	1.80	0.46
3:G:38:PRO:O	3:G:42:GLN:HG3	2.16	0.46
2:N:66:PRO:HG2	2:N:69:VAL:HG23	1.98	0.46
1:A:66:VAL:HG23	1:A:68:SER:HB2	1.97	0.46
1:A:157:THR:HA	2:B:76:TYR:OH	2.15	0.46
1:E:112:TYR:OH	4:H:95:HIS:HE1	1.99	0.46
1:E:129:LEU:HG	1:E:154:PRO:HB3	1.98	0.46
2:F:41:THR:HB	2:F:110:LEU:HA	1.98	0.46
4:L:133:LEU:HG	4:L:137:TYR:CE2	2.51	0.46
2:N:31:VAL:HG12	3:O:15:PHE:HB2	1.97	0.46
4:P:7:VAL:HG23	4:P:75:GLY:HA3	1.98	0.46
1:A:118:LEU:HB3	1:A:135:LEU:HD23	1.97	0.45
1:E:61:PRO:HG3	1:E:92:ASP:O	2.16	0.45
1:I:112:TYR:HB2	1:I:115:HIS:CE1	2.50	0.45
1:I:141:ASN:OD1	1:I:141:ASN:N	2.48	0.45
2:J:68:HIS:CD2	2:J:69:VAL:HG23	2.51	0.45
1:M:73:GLN:OE1	1:M:108:ARG:NH2	2.48	0.45
2:J:101:LEU:HA	2:J:101:LEU:HD12	1.77	0.45
2:N:64:GLU:N	2:N:64:GLU:CD	2.74	0.45
4:P:22:GLN:HA	4:P:27:HIS:H	1.80	0.45
1:A:121:ASP:C	1:A:121:ASP:OD1	2.60	0.45
1:E:161:ARG:HH11	1:E:164:GLN:HE21	1.63	0.45
3:C:4:PHE:H	3:C:67:ALA:HB1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG22	1:A:128:LEU:CD1	2.46	0.45
4:H:36:ILE:H	4:H:36:ILE:HG13	1.59	0.45
1:A:77:CYS:HA	1:A:106:GLY:HA3	1.99	0.45
3:C:3:VAL:O	3:C:17:ASP:HB2	2.16	0.45
1:E:180:ILE:CG2	2:F:101:LEU:HD13	2.47	0.45
1:M:158:LEU:HD21	2:N:103:LEU:HD21	1.98	0.45
4:P:39:SER:HB3	4:P:56:LEU:HD23	1.98	0.45
4:P:64:TYR:HB2	5:P:203:A1L66:C10	2.46	0.45
5:P:203:A1L66:C41	5:P:203:A1L66:N9	2.80	0.45
3:G:84:THR:HG22	3:G:85:PHE:N	2.32	0.45
4:H:8:VAL:O	4:H:58:THR:HG23	2.17	0.45
1:M:131:ASN:O	1:M:132:GLN:CB	2.63	0.45
3:O:23:THR:HA	3:O:56:THR:HA	1.98	0.45
4:P:83:ALA:HB1	4:P:85:ASN:OD1	2.17	0.45
1:A:176:ARG:HE	1:A:185:TYR:HB3	1.82	0.45
1:A:82:ARG:HH22	1:A:164:GLN:HE22	1.65	0.45
4:D:151:GLY:C	4:D:153:ASP:H	2.25	0.45
1:M:71:PRO:HA	1:M:112:TYR:HA	1.99	0.45
2:N:86:SER:OG	2:N:88:THR:HG22	2.16	0.45
3:C:32:GLU:CD	3:C:39:PRO:HG3	2.43	0.44
1:E:131:ASN:O	1:E:132:GLN:HB2	2.17	0.44
1:E:202:THR:O	1:E:206:ILE:HB	2.18	0.44
1:I:163:LEU:HB3	1:I:167:ARG:HH12	1.81	0.44
1:A:161:ARG:O	1:A:165:VAL:HG23	2.17	0.44
4:H:123:ARG:HE	4:H:126:ASP:HA	1.80	0.44
4:L:159:LEU:O	4:L:163:ILE:HG13	2.17	0.44
1:M:176:ARG:CG	1:M:176:ARG:NH1	2.62	0.44
1:E:67:ASN:OD1	4:H:64:TYR:HB3	2.17	0.44
2:B:76:TYR:O	2:B:80:LYS:HB3	2.17	0.44
2:F:62:PHE:CE1	2:F:110:LEU:HD21	2.53	0.44
3:K:23:THR:HA	3:K:56:THR:HA	1.99	0.44
4:L:25:GLN:O	4:L:26:ASN:CB	2.60	0.44
1:M:84:VAL:HG21	1:M:151:ILE:HG21	1.99	0.44
2:B:110:LEU:HD13	2:B:110:LEU:HA	1.83	0.44
1:E:118:LEU:CD1	1:E:120:ARG:HD3	2.47	0.44
1:I:161:ARG:O	1:I:164:GLN:HB2	2.17	0.44
4:P:28:PHE:HB2	4:P:146:ALA:O	2.18	0.44
1:I:116:LEU:HD11	1:I:135:LEU:HB3	1.99	0.44
2:J:41:THR:O	2:J:45:MET:HG3	2.18	0.44
1:A:160:GLU:HA	1:A:163:LEU:HD12	2.00	0.44
1:I:184:LEU:HD13	2:J:104:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:77:CYS:HA	1:M:106:GLY:HA2	1.99	0.44
2:N:74:CYS:HA	2:N:77:PHE:CD2	2.53	0.44
4:D:61:GLN:HE21	4:D:61:GLN:HB3	1.62	0.44
4:H:79:LEU:CD2	4:H:112:VAL:HG13	2.43	0.44
4:L:90:PHE:CE1	4:L:133:LEU:HD22	2.52	0.44
4:P:60:GLY:HA3	4:P:68:ARG:HH12	1.83	0.44
2:B:19:VAL:HG13	2:B:33:ARG:HG3	2.00	0.43
3:C:6:MET:HG2	3:C:13:THR:HG22	2.01	0.43
4:D:11:ALA:O	4:D:14:VAL:HG22	2.18	0.43
1:M:98:TYR:CD2	5:P:203:A1L66:C53	2.96	0.43
3:O:43:ARG:HD2	3:O:50:LEU:CD1	2.47	0.43
4:D:97:ARG:HD3	4:D:137:TYR:CD1	2.53	0.43
1:E:120:ARG:HH22	1:E:197:ASP:CG	2.25	0.43
1:I:188:LEU:HD13	1:I:188:LEU:HA	1.85	0.43
2:J:32:LYS:HE3	2:J:32:LYS:HB2	1.86	0.43
1:M:181:VAL:HG13	1:M:184:LEU:HD12	1.99	0.43
4:D:33:ASP:HB3	4:D:35:THR:OG1	2.18	0.43
2:J:96:ALA:H	2:J:99:ILE:HD11	1.83	0.43
3:K:24:VAL:HG13	3:K:44:LEU:HD12	2.01	0.43
4:L:33:ASP:HB3	4:L:36:ILE:HG13	2.01	0.43
4:L:97:ARG:CD	4:L:137:TYR:CD1	3.01	0.43
4:P:79:LEU:HG	4:P:159:LEU:HD22	2.00	0.43
1:E:118:LEU:HD12	1:E:120:ARG:HD3	2.00	0.43
1:E:120:ARG:HA	1:E:120:ARG:HD2	1.95	0.43
1:E:193:ASN:HB3	1:E:196:LYS:HG3	2.01	0.43
2:F:63:ARG:N	2:F:64:GLU:OE2	2.52	0.43
1:I:73:GLN:N	1:I:141:ASN:HD21	2.17	0.43
1:M:125:HIS:O	1:M:192:PRO:HB2	2.18	0.43
3:G:58:GLY:C	3:G:60:CYS:H	2.26	0.43
4:L:60:GLY:O	5:L:203:A1L66:N11	2.51	0.43
1:M:171:LYS:H	1:M:171:LYS:HG2	1.43	0.43
1:A:112:TYR:HB2	1:A:115:HIS:CE1	2.53	0.43
3:G:63:THR:HG23	3:G:66:THR:H	1.83	0.43
3:O:41:GLU:HG2	3:O:80:ARG:NH1	2.34	0.43
1:A:81:PRO:HG2	2:B:92:GLU:HB2	2.00	0.43
1:A:114:GLY:HA2	1:A:137:VAL:HG12	1.99	0.43
3:G:32:GLU:CD	3:G:39:PRO:HD3	2.44	0.43
1:M:75:ILE:HG12	1:M:108:ARG:HB3	2.01	0.43
3:C:57:LEU:HD23	3:C:62:PHE:CD2	2.53	0.42
4:D:150:GLN:CB	4:P:153:ASP:OD2	2.64	0.42
3:K:42:GLN:HB3	3:K:79:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:43:ARG:HG3	3:O:85:PHE:CD2	2.54	0.42
1:A:68:SER:O	1:A:70:GLU:HG3	2.19	0.42
4:H:154:ASP:O	4:H:158:THR:OG1	2.36	0.42
1:I:81:PRO:O	1:I:103:PRO:HB3	2.19	0.42
1:I:82:ARG:HH22	1:I:164:GLN:NE2	2.17	0.42
3:K:41:GLU:HA	3:K:80:ARG:HG2	2.01	0.42
3:O:43:ARG:HG3	3:O:85:PHE:CE2	2.53	0.42
3:O:62:PHE:CZ	3:O:75:VAL:HG22	2.54	0.42
1:A:116:LEU:CD1	1:A:137:VAL:CG2	2.96	0.42
2:B:33:ARG:NH2	2:B:46:LEU:HB3	2.33	0.42
4:H:44:VAL:HG22	4:H:45:VAL:H	1.84	0.42
4:L:111:MET:HE2	4:L:111:MET:HB2	1.82	0.42
1:A:160:GLU:O	1:A:164:GLN:HG3	2.19	0.42
3:G:25:PHE:HA	3:G:28:LYS:HB2	2.00	0.42
1:I:164:GLN:O	1:I:167:ARG:HB2	2.20	0.42
4:L:3:GLU:HG3	4:L:52:LEU:HB3	2.02	0.42
1:M:158:LEU:HD13	2:N:107:ALA:HB2	2.00	0.42
3:O:6:MET:HA	3:O:14:ILE:O	2.19	0.42
1:E:68:SER:O	1:E:70:GLU:HG3	2.19	0.42
4:L:84:ILE:HG23	4:L:116:ASN:O	2.20	0.42
5:P:203:A1L66:N8	5:P:203:A1L66:C12	2.81	0.42
4:D:151:GLY:C	4:D:153:ASP:N	2.76	0.42
4:H:22:GLN:HG3	4:H:149:ARG:HG3	2.01	0.42
1:M:116:LEU:HD13	1:M:137:VAL:CG2	2.50	0.42
3:G:3:VAL:HG11	3:G:62:PHE:O	2.20	0.42
1:E:134:GLU:CD	1:E:200:ARG:HH22	2.27	0.42
2:B:23:SER:OG	2:B:27:HIS:HB2	2.19	0.42
2:B:85:ASN:HD22	2:B:85:ASN:HA	1.67	0.42
3:G:95:SER:HA	3:G:96:PRO:HD3	1.88	0.42
4:H:141:PHE:C	4:H:142:ILE:HG13	2.44	0.42
4:P:44:VAL:HG21	4:P:157:TYR:OH	2.20	0.42
3:C:4:PHE:CE1	3:C:69:PRO:HG3	2.55	0.41
2:J:80:LYS:O	2:J:80:LYS:HG3	2.19	0.41
4:D:129:GLN:O	4:D:132:ASP:HB2	2.20	0.41
1:E:66:VAL:HG22	1:E:114:GLY:HA3	2.02	0.41
3:G:6:MET:CE	3:G:8:ARG:HD2	2.46	0.41
1:I:154:PRO:HD2	1:I:156:TYR:CZ	2.56	0.41
1:I:167:ARG:HG3	1:I:167:ARG:NH1	2.18	0.41
4:L:24:ILE:HD11	4:L:40:TYR:HD2	1.85	0.41
4:L:86:ASN:HB3	4:L:89:SER:OG	2.20	0.41
1:A:124:THR:O	1:A:125:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.91	0.41
1:M:118:LEU:CD1	1:M:120:ARG:HD3	2.50	0.41
3:O:7:ILE:HA	3:O:75:VAL:O	2.20	0.41
4:P:24:ILE:HA	4:P:42:LYS:HD2	2.03	0.41
1:A:66:VAL:HG22	1:A:114:GLY:O	2.21	0.41
4:H:64:TYR:HA	5:H:203:A1L66:N6	2.35	0.41
3:O:65:GLN:O	3:O:65:GLN:CG	2.69	0.41
1:A:118:LEU:HD12	1:A:120:ARG:HD3	2.02	0.41
1:A:138:PRO:O	1:A:139:SER:CB	2.64	0.41
4:H:97:ARG:CZ	4:H:137:TYR:HB3	2.51	0.41
1:I:79:ARG:NH2	1:M:79:ARG:HD2	2.35	0.41
1:A:65:SER:OG	1:A:88:TRP:NE1	2.53	0.41
1:A:62:VAL:O	1:A:62:VAL:HG13	2.20	0.41
1:A:112:TYR:OH	4:D:99:GLN:NE2	2.54	0.41
4:H:22:GLN:NE2	4:H:146:ALA:O	2.46	0.41
1:A:178:LEU:HD22	2:B:101:LEU:HD11	2.03	0.41
2:B:68:HIS:CD2	2:B:69:VAL:HG23	2.55	0.41
2:B:101:LEU:HG	3:C:103:MET:SD	2.61	0.41
4:D:16:LYS:N	6:D:201:GDP:O1B	2.54	0.41
4:D:146:ALA:N	6:D:201:GDP:O6	2.54	0.41
4:H:32:TYR:HD1	4:H:32:TYR:HA	1.75	0.41
1:I:82:ARG:NE	2:J:92:GLU:OE1	2.54	0.41
1:I:90:ASN:O	1:I:91:PHE:C	2.63	0.41
4:L:56:LEU:C	4:L:56:LEU:CD2	2.94	0.41
1:M:99:PRO:HG2	5:P:203:A1L66:C56	2.51	0.41
1:M:172:PRO:HA	1:M:175:TYR:CZ	2.55	0.41
4:P:25:GLN:O	4:P:27:HIS:HD2	2.03	0.41
4:D:26:ASN:OD1	4:P:148:THR:HG22	2.21	0.40
2:F:86:SER:OG	2:F:88:THR:HG23	2.21	0.40
1:I:176:ARG:HA	1:I:185:TYR:CD2	2.57	0.40
1:A:175:TYR:CE2	1:A:188:LEU:HB3	2.56	0.40
2:B:74:CYS:HA	2:B:77:PHE:CD2	2.56	0.40
3:C:4:PHE:CD1	3:C:69:PRO:HG3	2.55	0.40
3:C:46:LYS:HD2	3:C:60:CYS:O	2.22	0.40
3:C:68:ARG:HE	3:C:68:ARG:HA	1.86	0.40
4:D:5:LYS:HG3	4:D:76:GLU:OE2	2.21	0.40
2:F:31:VAL:HG11	2:F:74:CYS:SG	2.61	0.40
4:P:67:MET:HE3	4:P:67:MET:HB3	1.90	0.40
3:C:9:ARG:NH1	3:C:9:ARG:CG	2.77	0.40
1:E:171:LYS:HB2	1:E:173:GLU:OE1	2.22	0.40
2:F:29:PHE:CD1	3:G:13:THR:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:ASN:ND2	1:I:103:PRO:HA	2.36	0.40
1:M:83:VAL:HG12	1:M:122:ALA:HB3	2.04	0.40
3:O:6:MET:HE3	3:O:8:ARG:HD2	2.03	0.40
1:E:128:LEU:HA	1:E:154:PRO:HD3	2.02	0.40
4:H:111:MET:CG	4:H:139:ILE:HD13	2.52	0.40
3:K:41:GLU:HB2	3:K:79:PHE:HE1	0.43	0.40
4:L:131:GLN:O	4:L:135:ARG:HB2	2.22	0.40
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.76	0.40
4:P:25:GLN:O	4:P:27:HIS:CD2	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	147/163 (90%)	131 (89%)	13 (9%)	3 (2%)	6	28
1	E	147/163 (90%)	137 (93%)	9 (6%)	1 (1%)	18	50
1	I	147/163 (90%)	132 (90%)	15 (10%)	0	100	100
1	M	147/163 (90%)	138 (94%)	9 (6%)	0	100	100
2	B	84/96 (88%)	78 (93%)	5 (6%)	1 (1%)	10	39
2	F	82/96 (85%)	75 (92%)	6 (7%)	1 (1%)	10	39
2	J	84/96 (88%)	77 (92%)	7 (8%)	0	100	100
2	N	82/96 (85%)	79 (96%)	2 (2%)	1 (1%)	10	39
3	C	93/118 (79%)	81 (87%)	11 (12%)	1 (1%)	11	41
3	G	103/118 (87%)	92 (89%)	11 (11%)	0	100	100
3	K	95/118 (80%)	84 (88%)	10 (10%)	1 (1%)	11	41
3	O	103/118 (87%)	95 (92%)	8 (8%)	0	100	100
4	D	164/170 (96%)	145 (88%)	18 (11%)	1 (1%)	21	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	160/170 (94%)	147 (92%)	12 (8%)	1 (1%)	21	53
4	L	164/170 (96%)	148 (90%)	15 (9%)	1 (1%)	21	53
4	P	164/170 (96%)	147 (90%)	15 (9%)	2 (1%)	10	39
All	All	1966/2188 (90%)	1786 (91%)	166 (8%)	14 (1%)	18	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	26	ASN
4	H	26	ASN
4	L	26	ASN
1	A	139	SER
2	N	59	GLU
3	C	47	ASP
2	F	59	GLU
4	P	149	ARG
1	A	138	PRO
2	B	111	ASP
3	K	82	ASP
1	A	155	VAL
4	P	151	GLY
1	E	142	VAL

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	134/149 (90%)	119 (89%)	15 (11%)	6	23
1	E	133/149 (89%)	113 (85%)	20 (15%)	3	13
1	I	133/149 (89%)	102 (77%)	31 (23%)	1	4
1	M	133/149 (89%)	112 (84%)	21 (16%)	2	12
2	B	77/85 (91%)	68 (88%)	9 (12%)	5	21
2	F	76/85 (89%)	64 (84%)	12 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	77/85 (91%)	66 (86%)	11 (14%)	3	15
2	N	76/85 (89%)	66 (87%)	10 (13%)	4	17
3	C	87/103 (84%)	76 (87%)	11 (13%)	4	19
3	G	92/103 (89%)	81 (88%)	11 (12%)	5	20
3	K	89/103 (86%)	80 (90%)	9 (10%)	7	27
3	O	92/103 (89%)	76 (83%)	16 (17%)	2	9
4	D	147/150 (98%)	133 (90%)	14 (10%)	8	30
4	H	145/150 (97%)	133 (92%)	12 (8%)	10	35
4	L	147/150 (98%)	129 (88%)	18 (12%)	5	20
4	P	147/150 (98%)	129 (88%)	18 (12%)	5	20
All	All	1785/1948 (92%)	1547 (87%)	238 (13%)	4	17

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	92	ASP
1	A	109	ILE
1	A	116	LEU
1	A	133	THR
1	A	165	VAL
1	A	171	LYS
1	A	173	GLU
1	A	176	ARG
1	A	182	ARG
1	A	189	GLU
1	A	194	VAL
1	A	198	LEU
1	A	203	GLN
1	A	206	ILE
2	B	22	ILE
2	B	32	LYS
2	B	72	LYS
2	B	78	THR
2	B	79	TYR
2	B	80	LYS
2	B	81	VAL
2	B	105	MET

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Mol	Chain	Res	Type
2	B	110	LEU
3	C	1	MET
3	C	2	ASP
3	C	10	HIS
3	C	17	ASP
3	C	19	LYS
3	C	40	ASP
3	C	46	LYS
3	C	51	LEU
3	C	52	ASP
3	C	57	LEU
3	C	99	LEU
4	D	5	LYS
4	D	24	ILE
4	D	36	ILE
4	D	43	GLN
4	D	52	LEU
4	D	53	LEU
4	D	56	LEU
4	D	61	GLN
4	D	62	GLU
4	D	63	GLU
4	D	68	ARG
4	D	107	GLU
4	D	112	VAL
4	D	128	LYS
1	E	60	ARG
1	E	69	ARG
1	E	79	ARG
1	E	85	LEU
1	E	100	THR
1	E	108	ARG
1	E	113	ARG
1	E	124	THR
1	E	133	THR
1	E	139	SER
1	E	140	LEU
1	E	141	ASN
1	E	160	GLU
1	E	171	LYS
1	E	177	ARG
1	E	181	VAL

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Mol	Chain	Res	Type
1	E	186	GLU
1	E	200	ARG
1	E	201	LEU
1	E	206	ILE
2	F	20	LYS
2	F	24	SER
2	F	31	VAL
2	F	32	LYS
2	F	64	GLU
2	F	75	MET
2	F	80	LYS
2	F	84	THR
2	F	88	THR
2	F	98	GLU
2	F	99	ILE
2	F	101	LEU
3	G	2	ASP
3	G	6	MET
3	G	16	THR
3	G	24	VAL
3	G	43	ARG
3	G	48	ASP
3	G	63	THR
3	G	84	THR
3	G	98	GLU
3	G	102	VAL
3	G	103	MET
4	H	24	ILE
4	H	31	GLU
4	H	32	TYR
4	H	33	ASP
4	H	36	ILE
4	H	42	LYS
4	H	61	GLN
4	H	68	ARG
4	H	112	VAL
4	H	128	LYS
4	H	139	ILE
4	H	161	ARG
1	I	63	LEU
1	I	68	SER
1	I	69	ARG

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Mol	Chain	Res	Type
1	I	72	SER
1	I	73	GLN
1	I	83	VAL
1	I	84	VAL
1	I	90	ASN
1	I	100	THR
1	I	109	ILE
1	I	113	ARG
1	I	116	LEU
1	I	120	ARG
1	I	124	THR
1	I	130	VAL
1	I	139	SER
1	I	141	ASN
1	I	150	ASN
1	I	165	VAL
1	I	167	ARG
1	I	171	LYS
1	I	176	ARG
1	I	177	ARG
1	I	178	LEU
1	I	180	ILE
1	I	188	LEU
1	I	189	GLU
1	I	191	HIS
1	I	200	ARG
1	I	201	LEU
1	I	204	GLU
2	J	22	ILE
2	J	47	SER
2	J	60	VAL
2	J	61	ASN
2	J	64	GLU
2	J	78	THR
2	J	81	VAL
2	J	90	ILE
2	J	99	ILE
2	J	104	LEU
2	J	105	MET
3	K	1	MET
3	K	12	THR
3	K	14	ILE

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Mol	Chain	Res	Type
3	K	47	ASP
3	K	50	LEU
3	K	79	PHE
3	K	86	GLU
3	K	88	LEU
3	K	90	ILE
4	L	5	LYS
4	L	24	ILE
4	L	33	ASP
4	L	36	ILE
4	L	38	ASP
4	L	39	SER
4	L	42	LYS
4	L	43	GLN
4	L	52	LEU
4	L	56	LEU
4	L	61	GLN
4	L	68	ARG
4	L	92	ASP
4	L	97	ARG
4	L	112	VAL
4	L	122	SER
4	L	128	LYS
4	L	161	ARG
1	M	60	ARG
1	M	77	CYS
1	M	101	LEU
1	M	109	ILE
1	M	118	LEU
1	M	121	ASP
1	M	124	THR
1	M	129	LEU
1	M	133	THR
1	M	139	SER
1	M	141	ASN
1	M	157	THR
1	M	158	LEU
1	M	165	VAL
1	M	171	LYS
1	M	176	ARG
1	M	181	VAL
1	M	186	GLU

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Mol	Chain	Res	Type
1	M	191	HIS
1	M	194	VAL
1	M	206	ILE
2	N	22	ILE
2	N	37	LEU
2	N	61	ASN
2	N	64	GLU
2	N	78	THR
2	N	80	LYS
2	N	88	THR
2	N	98	GLU
2	N	99	ILE
2	N	101	LEU
3	O	1	MET
3	O	10	HIS
3	O	12	THR
3	O	13	THR
3	O	26	GLU
3	O	30	ILE
3	O	46	LYS
3	O	52	ASP
3	O	55	LYS
3	O	63	THR
3	O	65	GLN
3	O	88	LEU
3	O	89	CYS
3	O	98	GLU
3	O	102	VAL
3	O	103	MET
4	P	5	LYS
4	P	21	ILE
4	P	24	ILE
4	P	26	ASN
4	P	33	ASP
4	P	36	ILE
4	P	42	LYS
4	P	43	GLN
4	P	52	LEU
4	P	56	LEU
4	P	62	GLU
4	P	63	GLU
4	P	68	ARG

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Mol	Chain	Res	Type
4	P	107	GLU
4	P	108	ASP
4	P	122	SER
4	P	128	LYS
4	P	161	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	145	GLN
1	A	164	GLN
1	A	174	ASN
1	A	191	HIS
1	A	203	GLN
2	B	27	HIS
2	B	35	HIS
2	B	85	ASN
2	B	108	ASN
4	D	25	GLN
4	D	61	GLN
1	E	110	HIS
1	E	115	HIS
1	E	164	GLN
1	E	191	HIS
2	F	27	HIS
4	H	95	HIS
4	H	129	GLN
4	H	131	GLN
4	H	150	GLN
1	I	73	GLN
1	I	90	ASN
1	I	115	HIS
1	I	132	GLN
1	I	164	GLN
1	I	203	GLN
2	J	108	ASN
3	K	10	HIS
4	L	22	GLN
4	L	25	GLN
4	L	27	HIS
4	L	70	GLN

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Mol	Chain	Res	Type
4	L	95	HIS
4	L	166	HIS
1	M	110	HIS
1	M	164	GLN
1	M	191	HIS
4	P	27	HIS
4	P	129	GLN
4	P	131	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	A1L66	P	203	-	89,93,93	1.33	14 (15%)	115,138,138	2.11	22 (19%)
5	A1L66	A	301	-	89,93,93	1.25	13 (14%)	115,138,138	1.81	20 (17%)
6	GDP	P	201	7	29,30,30	1.01	1 (3%)	45,47,47	1.15	2 (4%)
6	GDP	D	201	7	29,30,30	1.06	1 (3%)	45,47,47	1.10	3 (6%)
6	GDP	H	201	7	29,30,30	0.94	1 (3%)	45,47,47	1.14	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1L66	H	203	-	89,93,93	1.23	10 (11%)	115,138,138	1.50	16 (13%)
5	A1L66	L	203	-	89,93,93	1.44	15 (16%)	115,138,138	1.72	19 (16%)
6	GDP	L	201	7	29,30,30	1.07	1 (3%)	45,47,47	1.31	4 (8%)

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
5	A1L66	P	203	-	-	10/57/98/98	0/13/13/13
5	A1L66	A	301	-	-	8/57/98/98	0/13/13/13
6	GDP	P	201	7	-	0/16/32/32	0/3/3/3
6	GDP	D	201	7	-	0/16/32/32	0/3/3/3
6	GDP	H	201	7	-	0/16/32/32	0/3/3/3
5	A1L66	H	203	-	-	8/57/98/98	0/13/13/13
5	A1L66	L	203	-	-	3/57/98/98	0/13/13/13
6	GDP	L	201	7	-	5/16/32/32	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	201	GDP	PA-O3A	4.52	1.64	1.59
6	D	201	GDP	PA-O3A	4.51	1.64	1.59
5	L	203	A1L66	O3-C30	4.31	1.39	1.33
5	H	203	A1L66	O3-C30	4.15	1.39	1.33
5	P	203	A1L66	C13-C29	-3.87	1.37	1.42
6	P	201	GDP	PA-O3A	3.82	1.63	1.59
5	L	203	A1L66	C21-C20	-3.56	1.38	1.41
6	H	201	GDP	PA-O3A	3.53	1.63	1.59
5	P	203	A1L66	O3-C30	3.43	1.38	1.33
5	L	203	A1L66	C13-C29	-3.36	1.38	1.42
5	L	203	A1L66	C14-C23	-3.30	1.37	1.41
5	L	203	A1L66	N7-N6	-3.25	1.34	1.36
5	A	301	A1L66	O3-C30	3.07	1.38	1.33
5	H	203	A1L66	N7-N6	-3.05	1.34	1.36
5	L	203	A1L66	C31-C28	-3.02	1.38	1.43
5	A	301	A1L66	N7-N6	-3.00	1.34	1.36
5	A	301	A1L66	C21-C20	-2.96	1.38	1.41
5	P	203	A1L66	N7-N6	-2.93	1.34	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	203	A1L66	C8-C7	-2.90	1.43	1.47
5	L	203	A1L66	C15-C14	-2.86	1.44	1.50
5	P	203	A1L66	C21-C20	-2.86	1.38	1.41
5	A	301	A1L66	C13-C29	-2.85	1.38	1.42
5	H	203	A1L66	C21-C20	-2.76	1.38	1.41
5	A	301	A1L66	C31-C28	-2.74	1.38	1.43
5	L	203	A1L66	C23-C24	-2.74	1.47	1.52
5	A	301	A1L66	C22-N6	2.68	1.34	1.32
5	P	203	A1L66	C15-C14	-2.64	1.44	1.50
5	H	203	A1L66	C22-N6	2.64	1.34	1.32
5	P	203	A1L66	C31-C28	-2.62	1.38	1.43
5	H	203	A1L66	C8-C7	-2.57	1.43	1.47
5	L	203	A1L66	C8-C7	-2.54	1.43	1.47
5	A	301	A1L66	C14-C23	-2.49	1.38	1.41
5	H	203	A1L66	C13-C29	-2.48	1.39	1.42
5	L	203	A1L66	C48-N2	-2.45	1.43	1.47
5	A	301	A1L66	C8-C7	-2.39	1.44	1.47
5	P	203	A1L66	C5-N2	2.38	1.39	1.34
5	L	203	A1L66	C35-N10	-2.33	1.44	1.47
5	P	203	A1L66	C14-C23	-2.29	1.38	1.41
5	P	203	A1L66	C22-N6	2.29	1.33	1.32
5	H	203	A1L66	C31-C28	-2.28	1.39	1.43
5	A	301	A1L66	C3-N1	2.26	1.38	1.34
5	H	203	A1L66	C14-C23	-2.25	1.38	1.41
5	P	203	A1L66	C23-C24	-2.20	1.48	1.52
5	P	203	A1L66	C51-C2	-2.17	1.49	1.52
5	L	203	A1L66	C27-C28	-2.17	1.37	1.42
5	H	203	A1L66	C5-N2	2.16	1.39	1.34
5	L	203	A1L66	C21-C15	-2.15	1.38	1.42
5	A	301	A1L66	C21-C15	-2.13	1.38	1.42
5	A	301	A1L66	C15-C14	-2.08	1.45	1.50
5	P	203	A1L66	C21-C15	-2.06	1.38	1.42
5	A	301	A1L66	C27-C28	-2.04	1.38	1.42
5	L	203	A1L66	C22-N6	2.04	1.33	1.32
5	H	203	A1L66	C31-N10	2.03	1.42	1.36
5	A	301	A1L66	C48-N2	-2.03	1.44	1.47
5	L	203	A1L66	C2-N1	-2.03	1.44	1.46
5	P	203	A1L66	C3-N1	2.02	1.38	1.34

All (89) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	203	A1L66	C30-O3-C37	-14.42	101.52	118.83
5	A	301	A1L66	C30-O3-C37	-7.44	109.90	118.83
5	A	301	A1L66	C40-C41-C37	6.48	117.93	109.89
5	H	203	A1L66	C30-O3-C37	-6.28	111.29	118.83
5	L	203	A1L66	C20-N7-N6	6.06	114.49	111.52
5	L	203	A1L66	C30-O3-C37	-5.95	111.69	118.83
5	L	203	A1L66	C22-N6-N7	-5.95	102.92	106.02
5	A	301	A1L66	C1-C2-N1	5.72	116.78	109.01
5	P	203	A1L66	C36-C35-N10	-5.52	95.60	102.18
5	L	203	A1L66	C40-C41-C37	5.52	116.74	109.89
5	P	203	A1L66	C1-C2-N1	4.48	115.10	109.01
5	A	301	A1L66	C22-N6-N7	-4.43	103.71	106.02
5	A	301	A1L66	C8-C7-C44	-4.33	123.03	129.65
5	H	203	A1L66	C22-N6-N7	-4.16	103.86	106.02
5	P	203	A1L66	C12-O2-C13	-4.11	98.07	114.25
5	A	301	A1L66	C20-N7-N6	4.09	113.53	111.52
5	P	203	A1L66	C20-N7-N6	4.09	113.53	111.52
5	P	203	A1L66	C14-C13-C29	4.01	123.62	121.00
5	H	203	A1L66	C20-N7-N6	3.94	113.45	111.52
5	L	203	A1L66	C21-C22-N6	3.69	112.89	111.34
5	P	203	A1L66	C8-C7-C44	-3.65	124.07	129.65
5	P	203	A1L66	C43-C8-C7	-3.53	116.91	120.87
5	H	203	A1L66	C3-C4-N2	-3.45	103.09	112.50
5	L	203	A1L66	C50-C4-N2	3.42	107.25	103.17
5	L	203	A1L66	C4-C3-N1	-3.41	109.05	116.52
5	L	203	A1L66	C49-C48-N2	3.39	106.27	103.00
5	P	203	A1L66	C22-N6-N7	-3.37	104.27	106.02
5	P	203	A1L66	C3-C4-N2	-3.37	103.31	112.50
5	A	301	A1L66	C8-C7-N5	3.35	127.43	122.05
6	P	201	GDP	O6-C6-N1	3.29	126.30	120.11
6	H	201	GDP	O6-C6-N1	3.26	126.25	120.11
5	L	203	A1L66	C3-C4-N2	-3.21	103.73	112.50
5	H	203	A1L66	C14-C13-C29	3.17	123.07	121.00
5	A	301	A1L66	C58-S1-C55	3.16	90.62	88.96
6	L	201	GDP	O6-C6-N1	3.11	125.97	120.11
5	H	203	A1L66	C36-C35-C34	-3.11	97.30	101.94
5	L	203	A1L66	C50-C49-C48	3.07	106.61	103.18
5	H	203	A1L66	N9-C31-N10	-3.00	111.09	116.75
5	H	203	A1L66	C49-C48-N2	2.98	105.87	103.00
5	L	203	A1L66	C19-C18-C16	-2.95	122.21	124.52
5	A	301	A1L66	C21-C22-N6	2.93	112.57	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	203	A1L66	C21-C22-N6	2.93	112.57	111.34
5	A	301	A1L66	C2-N1-C3	-2.80	119.08	122.98
5	H	203	A1L66	C8-C7-C44	-2.79	125.39	129.65
5	A	301	A1L66	C14-C13-C29	2.78	122.82	121.00
5	L	203	A1L66	O7-C3-N1	2.66	127.72	122.96
5	H	203	A1L66	C28-C31-N10	2.64	125.69	121.18
5	L	203	A1L66	C8-C7-C44	-2.62	125.65	129.65
5	P	203	A1L66	C15-C14-C23	2.62	124.28	120.43
5	H	203	A1L66	C19-C18-C16	-2.56	122.51	124.52
5	A	301	A1L66	C3-C4-N2	-2.56	105.51	112.50
6	D	201	GDP	O6-C6-N1	2.53	124.87	120.11
6	L	201	GDP	N2-C2-N3	2.52	124.59	119.67
6	D	201	GDP	N2-C2-N3	2.49	124.54	119.67
5	A	301	A1L66	C56-C55-S1	-2.47	108.12	109.64
5	A	301	A1L66	C12-O2-C13	-2.47	104.55	114.25
5	P	203	A1L66	C2-N1-C3	-2.46	119.56	122.98
5	P	203	A1L66	C8-C7-N5	2.43	125.96	122.05
6	L	201	GDP	C3'-C2'-C1'	2.43	106.06	101.46
5	H	203	A1L66	C2-N1-C3	-2.43	119.61	122.98
5	P	203	A1L66	O4-C40-C41	-2.43	107.55	111.74
5	A	301	A1L66	C36-C35-N10	-2.39	99.33	102.18
5	H	203	A1L66	C4-C3-N1	-2.37	111.33	116.52
5	A	301	A1L66	C39-C38-C37	2.35	112.81	109.89
5	A	301	A1L66	C49-C50-C4	-2.35	101.01	103.75
5	A	301	A1L66	O5-C5-N2	2.34	125.59	121.38
5	H	203	A1L66	C7-C44-N3	-2.30	103.11	105.31
5	L	203	A1L66	C36-C35-N10	-2.29	99.45	102.18
5	L	203	A1L66	C54-C55-C56	-2.26	127.75	130.81
5	L	203	A1L66	C39-C38-C37	2.24	112.67	109.89
5	L	203	A1L66	C50-C4-C3	-2.21	107.13	111.36
6	H	201	GDP	O3B-PB-O2B	2.18	115.97	107.80
6	L	201	GDP	C5'-C4'-C3'	-2.18	107.38	115.21
5	L	203	A1L66	C48-N2-C4	-2.17	108.95	111.83
6	P	201	GDP	N2-C2-N3	2.17	123.91	119.67
5	P	203	A1L66	C44-C7-N5	2.17	109.94	107.85
5	A	301	A1L66	C19-C18-C16	-2.16	122.83	124.52
6	H	201	GDP	N2-C2-N3	2.16	123.88	119.67
5	A	301	A1L66	N9-C31-N10	-2.15	112.70	116.75
5	L	203	A1L66	C7-C44-N3	-2.15	103.26	105.31
5	P	203	A1L66	C4-C3-N1	-2.13	111.85	116.52
5	P	203	A1L66	C19-C18-C16	-2.13	122.85	124.52
5	P	203	A1L66	C59-C54-C55	2.11	124.20	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	203	A1L66	O5-C5-N2	2.10	125.15	121.38
6	D	201	GDP	C3'-C2'-C1'	2.09	105.41	101.46
5	H	203	A1L66	C50-C4-N2	2.07	105.63	103.17
5	P	203	A1L66	C7-N5-N4	-2.04	107.05	109.23
5	P	203	A1L66	C7-C44-N3	-2.03	103.37	105.31
5	P	203	A1L66	C49-C50-C4	2.00	106.09	103.75

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	A1L66	O1-C1-C2-N1
5	A	301	A1L66	O1-C1-C2-C51
5	H	203	A1L66	N8-C30-O3-C37
5	H	203	A1L66	N9-C30-O3-C37
5	P	203	A1L66	C27-C23-C24-C25
5	P	203	A1L66	N8-C30-O3-C37
5	P	203	A1L66	N9-C30-O3-C37
6	L	201	GDP	PA-O3A-PB-O2B
5	H	203	A1L66	C1-C2-C51-C52
5	H	203	A1L66	C1-C2-C51-C60
5	P	203	A1L66	O1-C1-C2-C51
6	L	201	GDP	O4'-C4'-C5'-O5'
5	P	203	A1L66	C59-C54-C55-C56
6	L	201	GDP	C3'-C4'-C5'-O5'
5	P	203	A1L66	C53-C54-C55-C56
5	L	203	A1L66	O1-C1-C2-N1
5	A	301	A1L66	O5-C5-N2-C48
6	L	201	GDP	PA-O3A-PB-O3B
5	L	203	A1L66	O5-C5-N2-C48
5	A	301	A1L66	N1-C2-C51-C52
5	A	301	A1L66	N1-C2-C51-C60
5	P	203	A1L66	C14-C23-C24-C25
5	H	203	A1L66	C41-C37-O3-C30
5	A	301	A1L66	C1-C2-C51-C60
5	A	301	A1L66	C6-C5-N2-C48
5	P	203	A1L66	C53-C54-C55-S1
5	P	203	A1L66	C59-C54-C55-S1
5	H	203	A1L66	C38-C37-O3-C30
5	H	203	A1L66	C53-C54-C55-C56
5	H	203	A1L66	C59-C54-C55-C56
5	A	301	A1L66	C1-C2-C51-C52

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Mol	Chain	Res	Type	Atoms
5	P	203	A1L66	O1-C1-C2-N1
6	L	201	GDP	PA-O3A-PB-O1B
5	L	203	A1L66	C6-C5-N2-C48

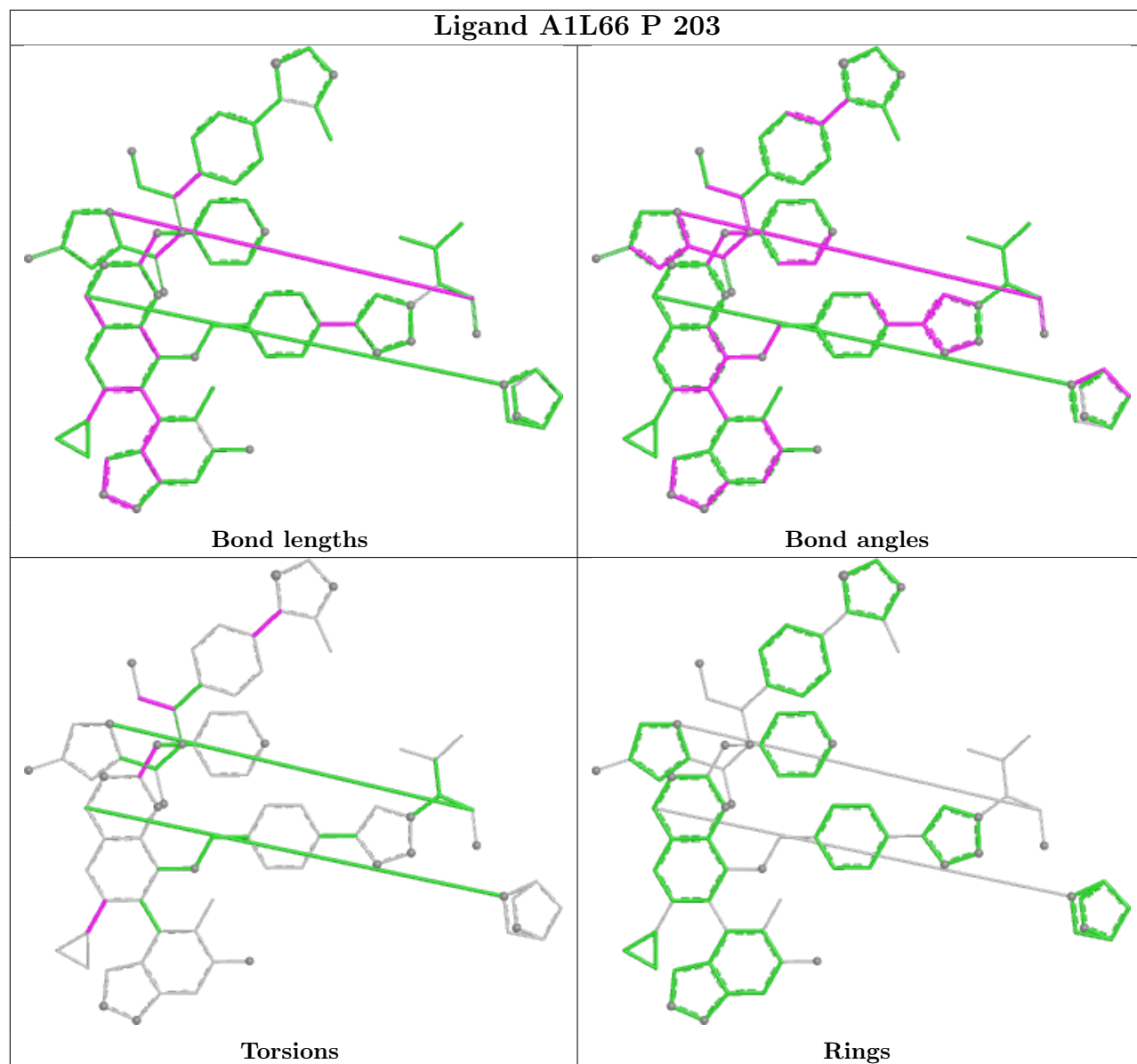
There are no ring outliers.

8 monomers are involved in 26 short contacts:

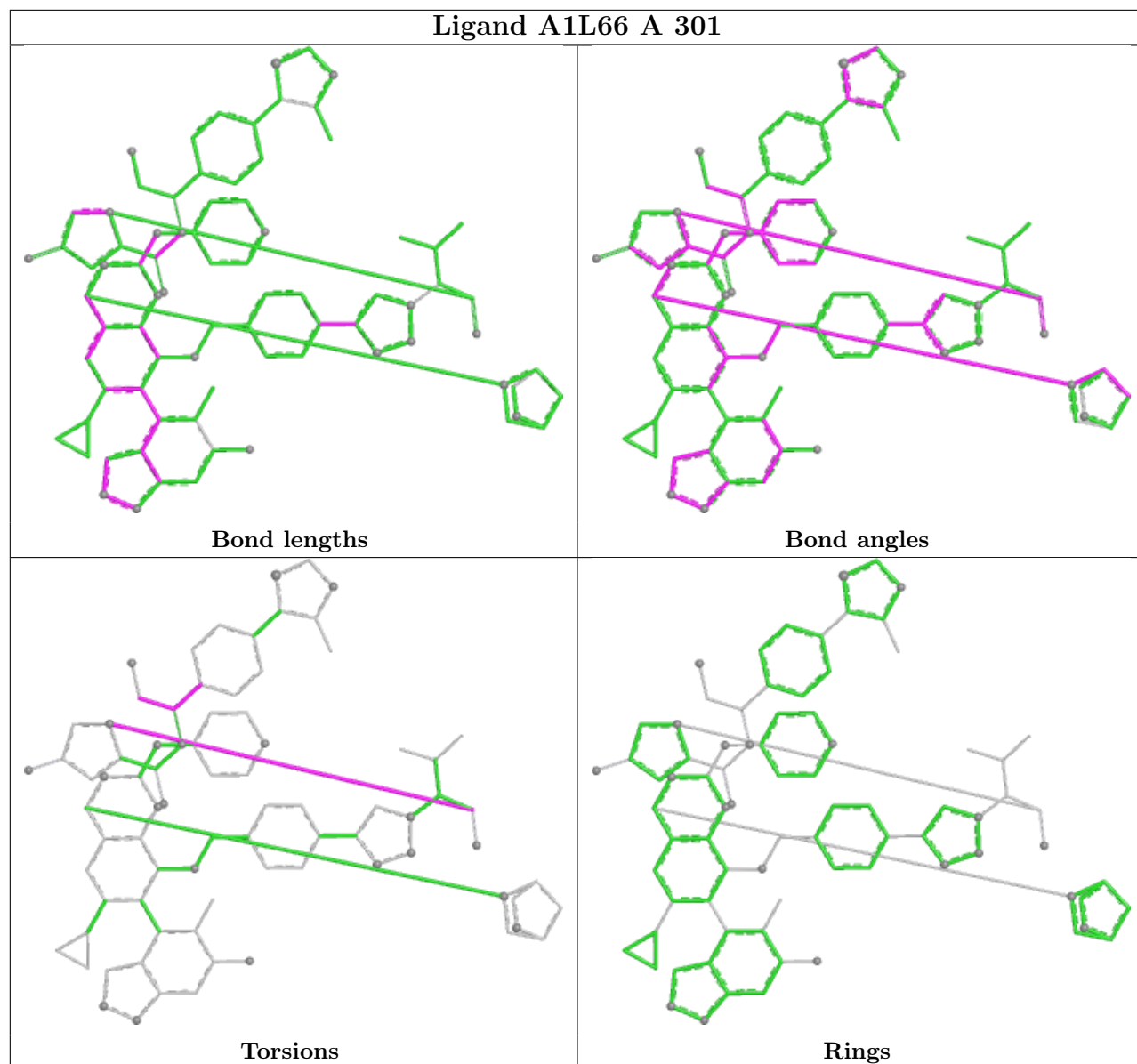
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	203	A1L66	10	0
5	A	301	A1L66	2	0
6	P	201	GDP	1	0
6	D	201	GDP	2	0
6	H	201	GDP	1	0
5	H	203	A1L66	3	0
5	L	203	A1L66	5	0
6	L	201	GDP	2	0

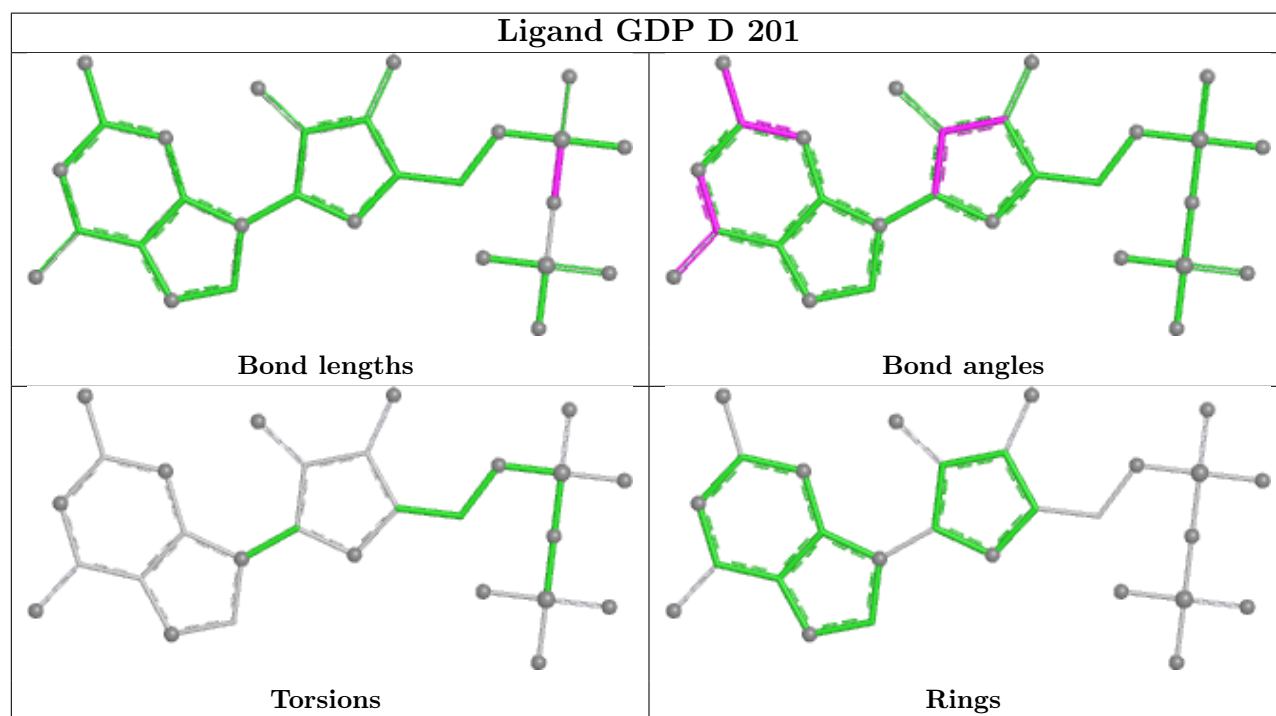
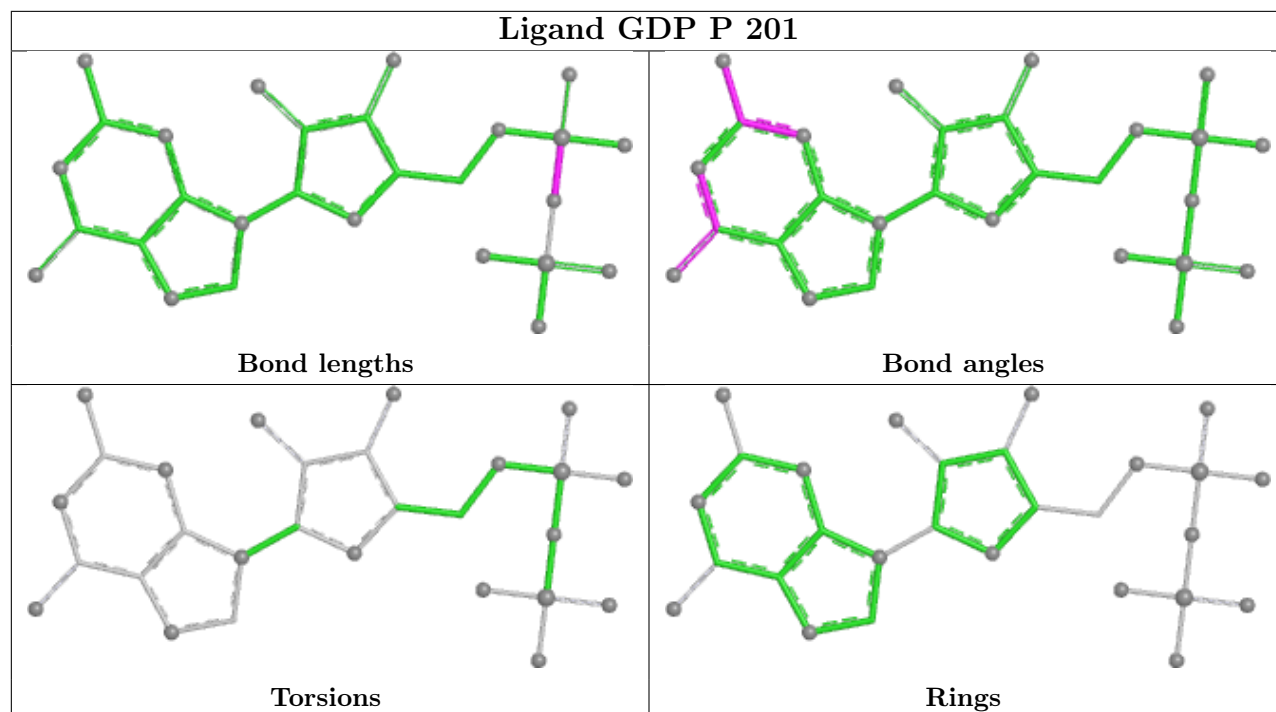
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

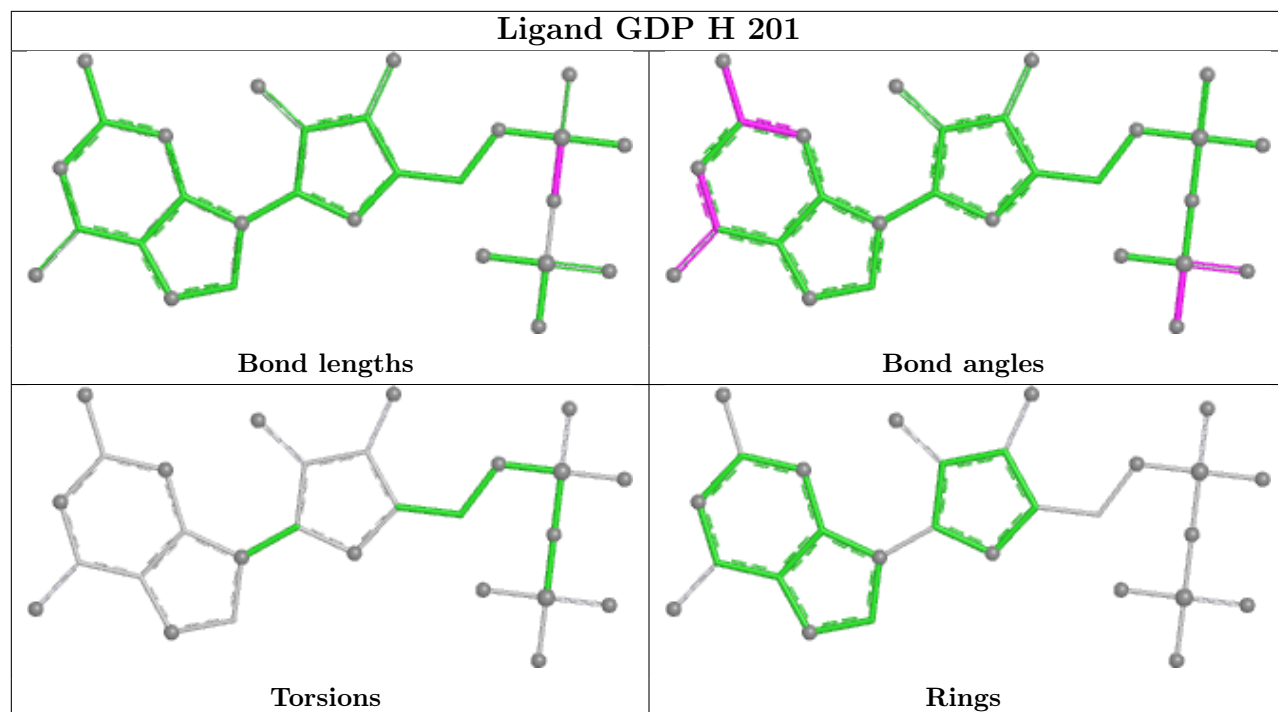
Ligand A1L66 P 203



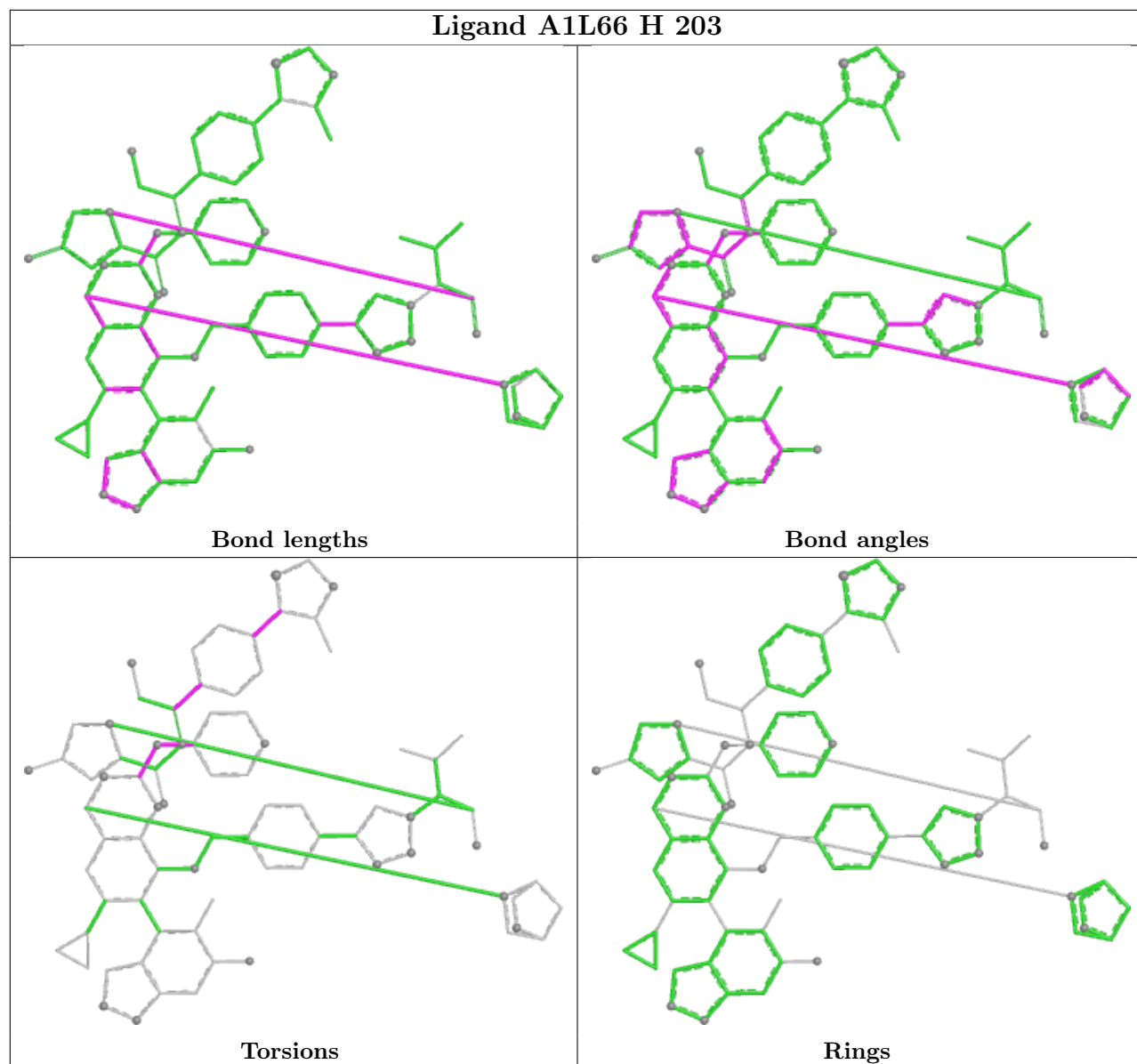
Ligand A1L66 A 301



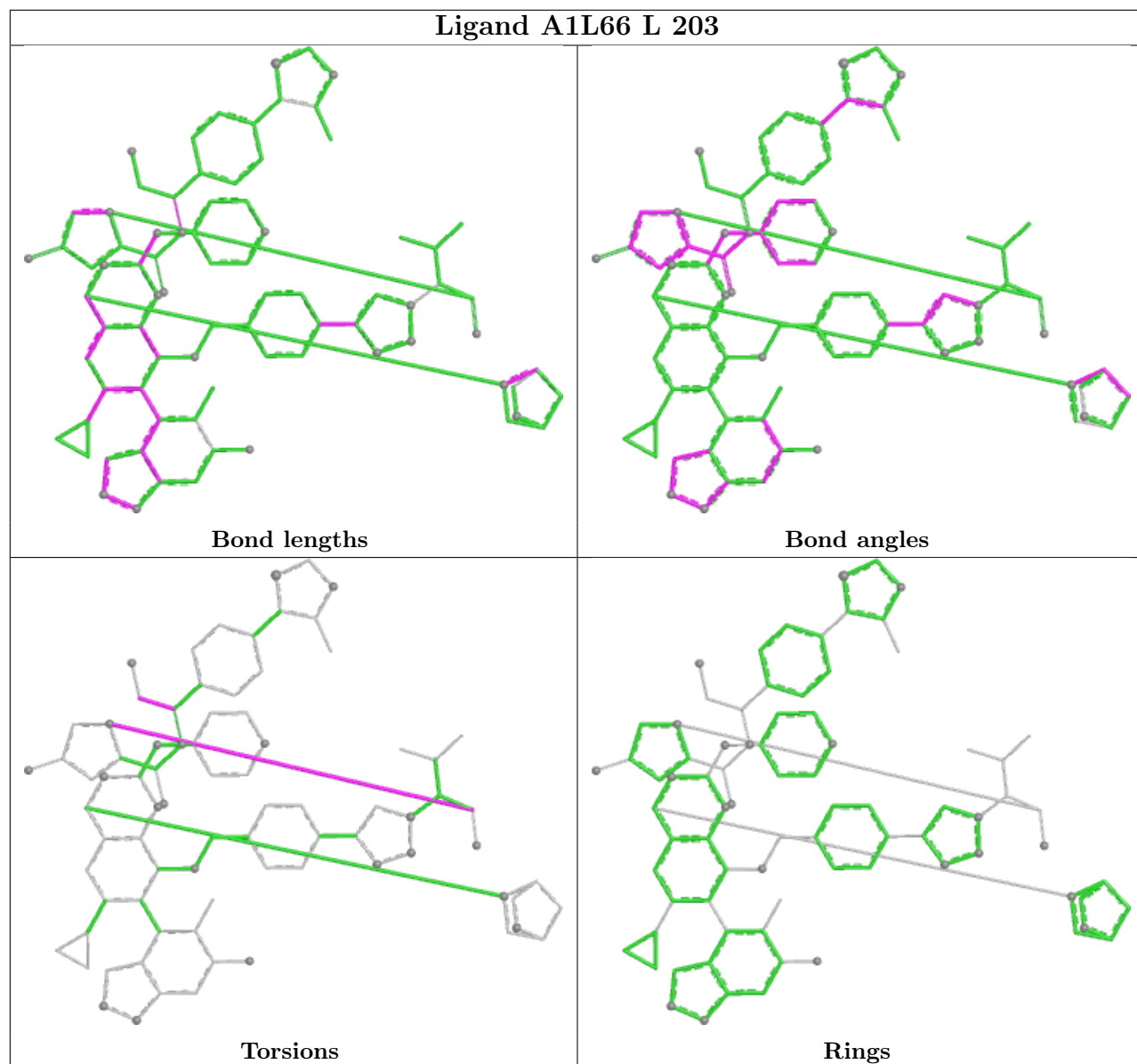


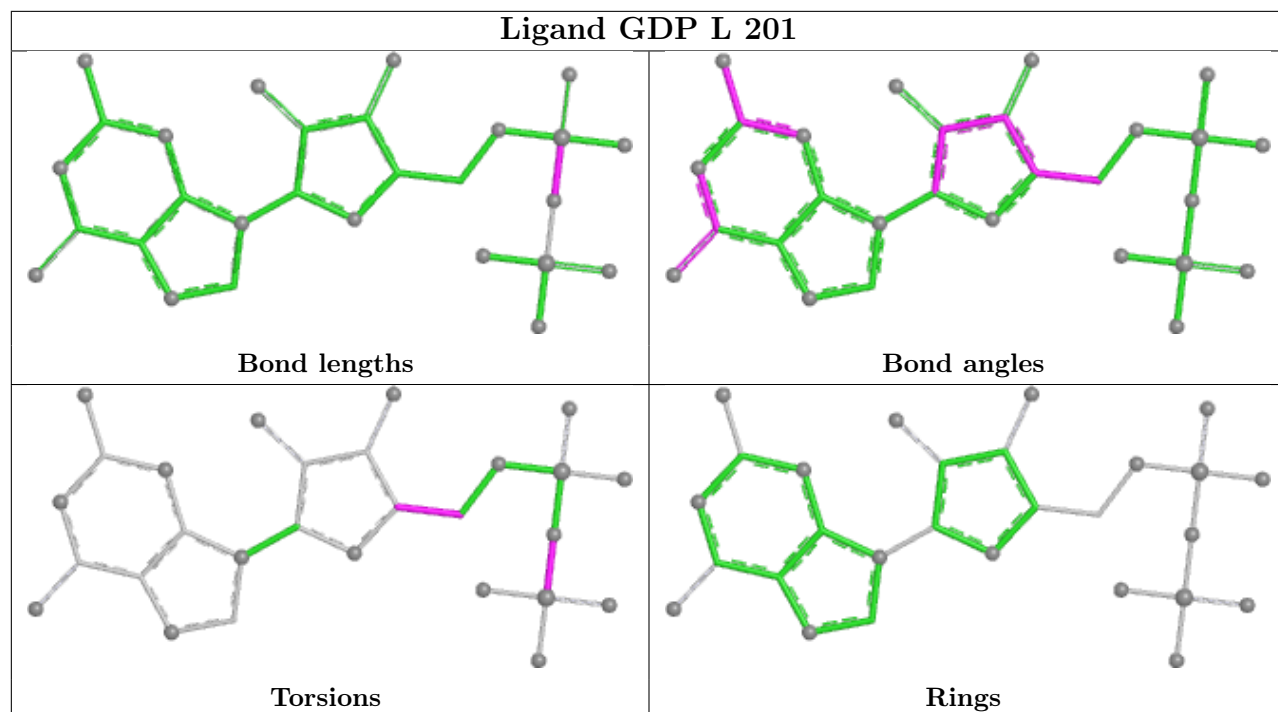


Ligand A1L66 H 203



Ligand A1L66 L 203





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	149/163 (91%)	-0.44	0 100 100	85, 130, 201, 250	0
1	E	149/163 (91%)	-0.63	0 100 100	72, 105, 150, 195	0
1	I	149/163 (91%)	-0.41	1 (0%) 84 69	78, 123, 204, 284	0
1	M	149/163 (91%)	-0.67	0 100 100	66, 100, 151, 219	0
2	B	88/96 (91%)	-0.32	0 100 100	126, 182, 217, 264	0
2	F	86/96 (89%)	-0.64	0 100 100	67, 93, 132, 158	0
2	J	88/96 (91%)	-0.41	0 100 100	136, 186, 227, 262	0
2	N	86/96 (89%)	-0.68	0 100 100	68, 90, 125, 142	0
3	C	99/118 (83%)	-0.47	0 100 100	150, 194, 241, 262	0
3	G	105/118 (88%)	-0.65	0 100 100	67, 90, 124, 144	0
3	K	101/118 (85%)	-0.47	0 100 100	146, 204, 244, 267	0
3	O	105/118 (88%)	-0.78	0 100 100	67, 87, 123, 141	0
4	D	166/170 (97%)	-0.44	2 (1%) 76 57	82, 139, 177, 214	0
4	H	164/170 (96%)	-0.22	3 (1%) 67 47	105, 163, 216, 244	0
4	L	166/170 (97%)	-0.38	3 (1%) 67 47	87, 142, 183, 211	0
4	P	166/170 (97%)	-0.13	5 (3%) 52 32	113, 179, 237, 291	0
All	All	2016/2188 (92%)	-0.46	14 (0%) 84 69	66, 137, 217, 291	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	P	153	ASP	4.5
4	H	155	ALA	3.5
4	D	153	ASP	3.2
4	L	153	ASP	3.2
4	H	153	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
4	P	19	LEU	2.9
4	P	40	TYR	2.9
4	P	122	SER	2.9
4	H	6	LEU	2.9
4	P	155	ALA	2.8
1	I	116	LEU	2.8
4	L	55	ILE	2.7
4	L	32	TYR	2.2
4	D	40	TYR	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

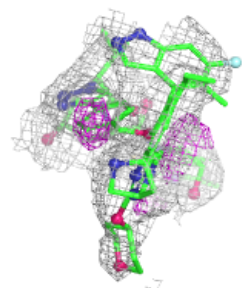
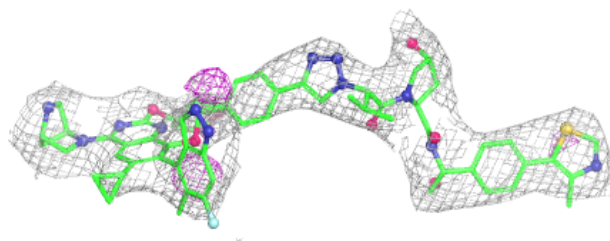
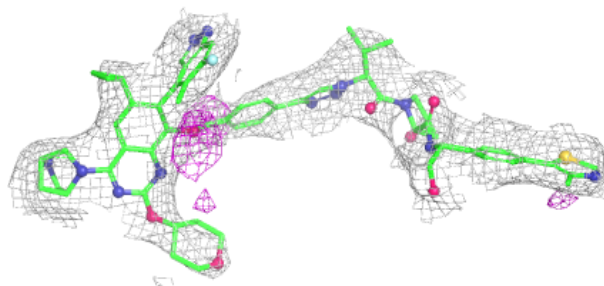
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	A1L66	H	203	81/81	0.90	0.08	94,122,144,151	0
5	A1L66	P	203	81/81	0.90	0.09	104,124,171,185	0
6	GDP	H	201	28/28	0.92	0.06	154,173,197,203	0
6	GDP	P	201	28/28	0.92	0.06	148,168,182,188	0
7	MG	L	202	1/1	0.92	0.14	96,96,96,96	0
5	A1L66	A	301	81/81	0.94	0.07	94,114,137,139	0
5	A1L66	L	203	81/81	0.94	0.07	85,102,120,140	0
7	MG	H	202	1/1	0.95	0.08	117,117,117,117	0
6	GDP	L	201	28/28	0.96	0.05	99,125,145,149	0
6	GDP	D	201	28/28	0.96	0.06	113,135,172,180	0
7	MG	D	202	1/1	0.97	0.09	103,103,103,103	0
7	MG	P	202	1/1	0.98	0.09	99,99,99,99	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.

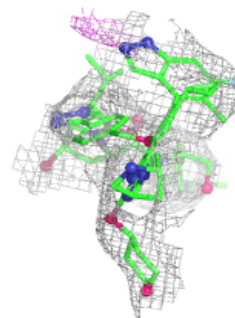
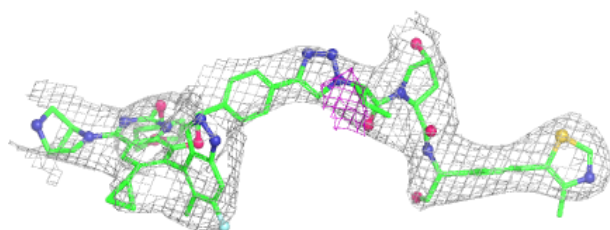
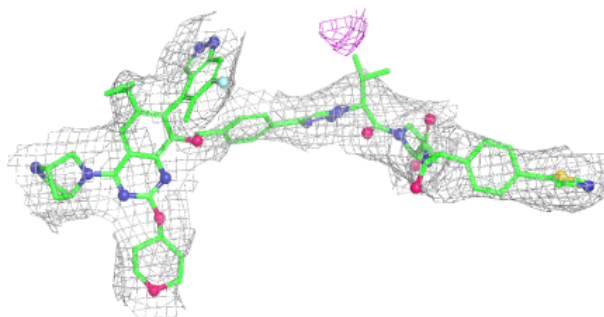
Electron density around A1L66 H 203:

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

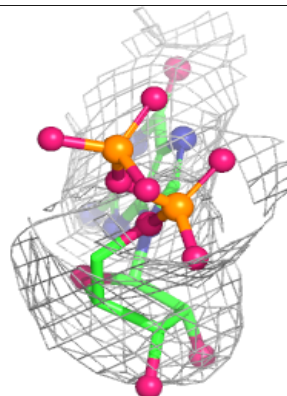
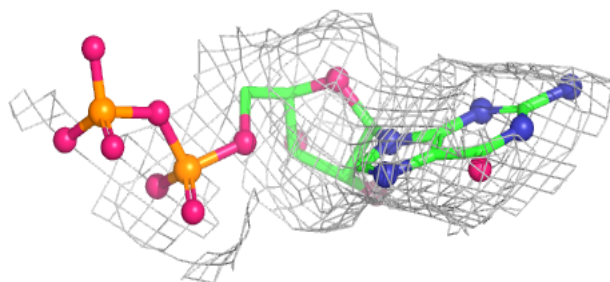
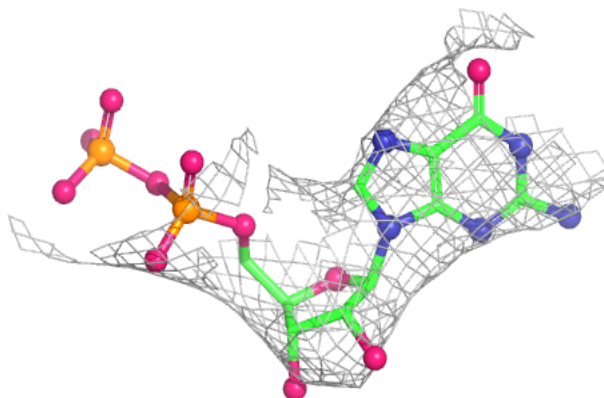


Electron density around A1L66 P 203:

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

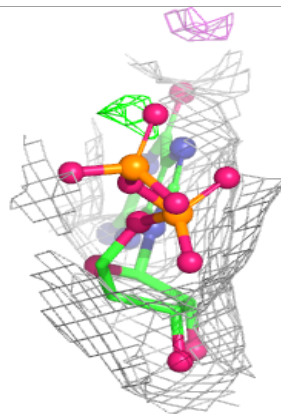
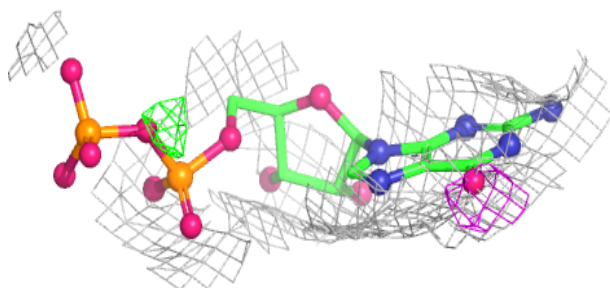
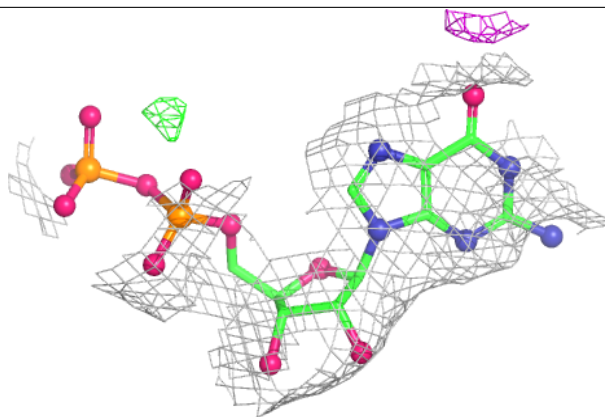
**Electron density around GDP H 201:**

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

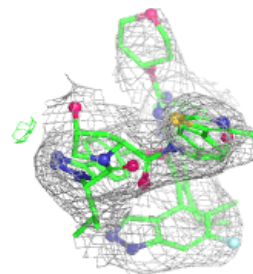
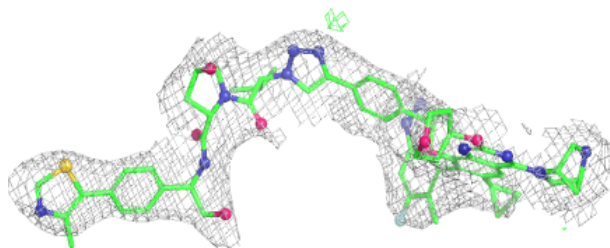
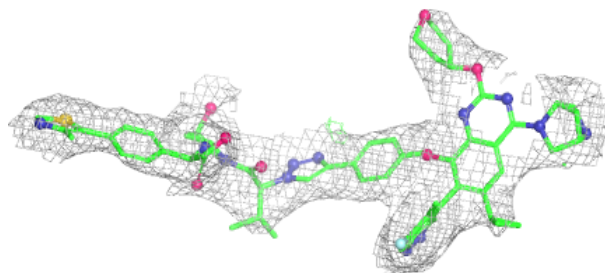


Electron density around GDP P 201:

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

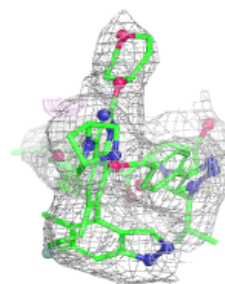
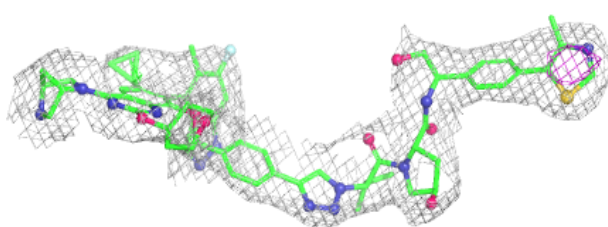
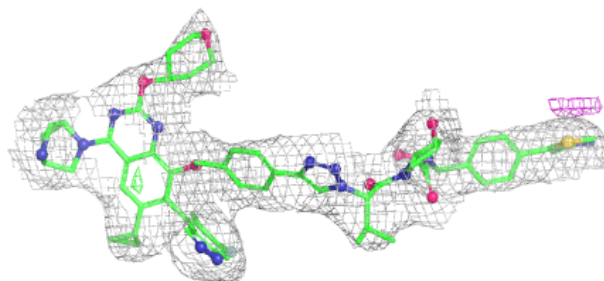
**Electron density around A1L66 A 301:**

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

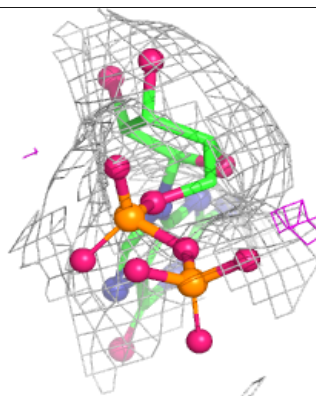
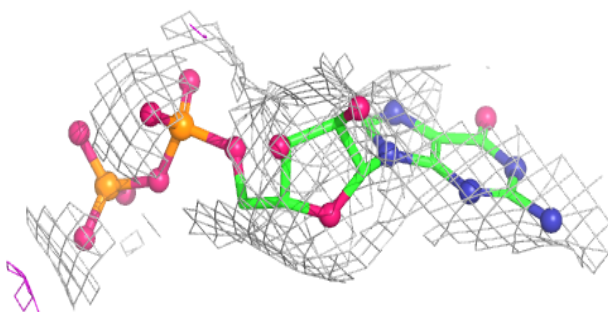
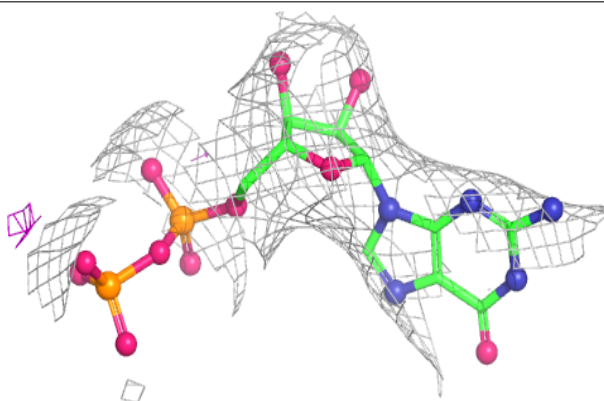


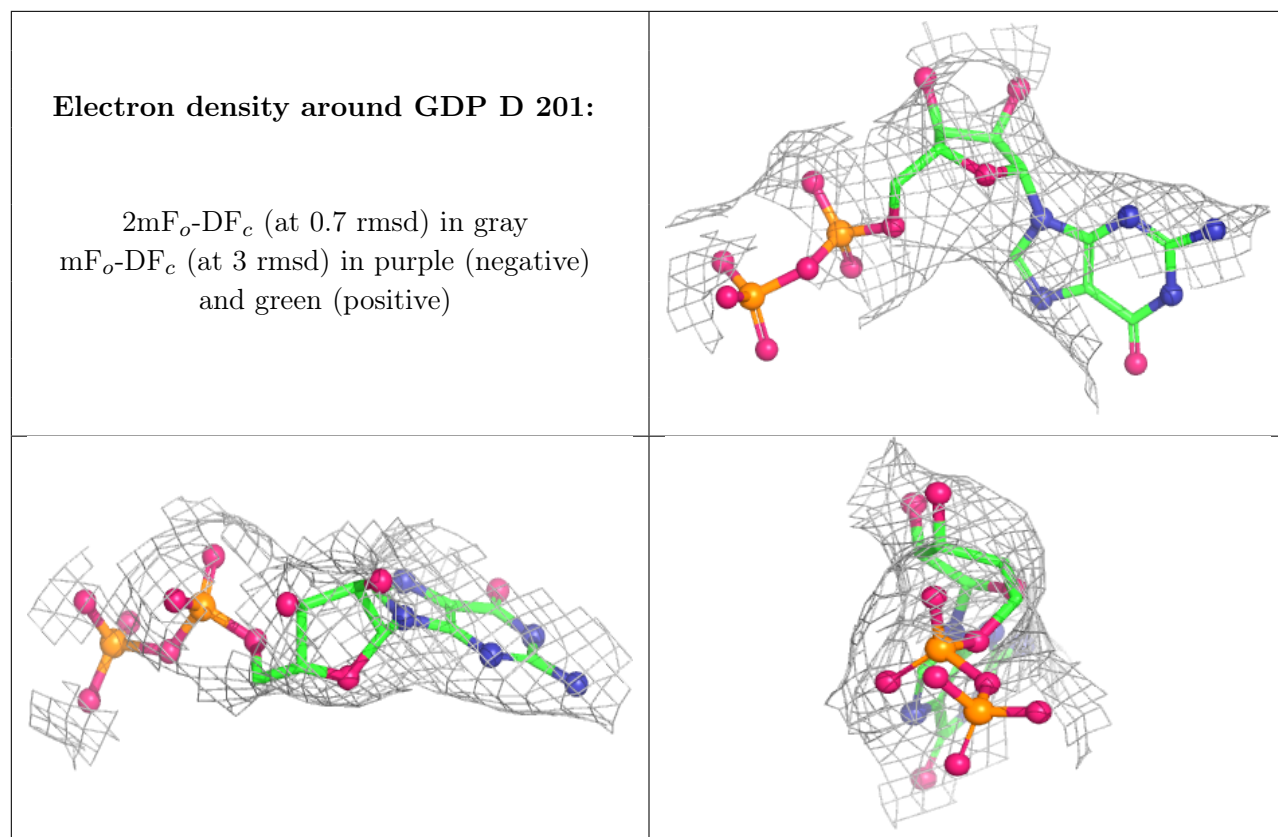
Electron density around A1L66 L 203:

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

**Electron density around GDP L 201:**

$2mF_o-DF_c$ (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.