Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 04:22 PM EDT

PDB ID	:	8VGB
Title	:	Crystal Structure of Guanine Nucleotide-Binding Protein Alpha Subunit (G Protein) from Oryza sativa in complex with GDP
Authors	:	Lee, S.G.; Jez, J.M.
Deposited on	:	2023-12-27
Resolution	:	2.99 Å(reported)

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

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

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

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

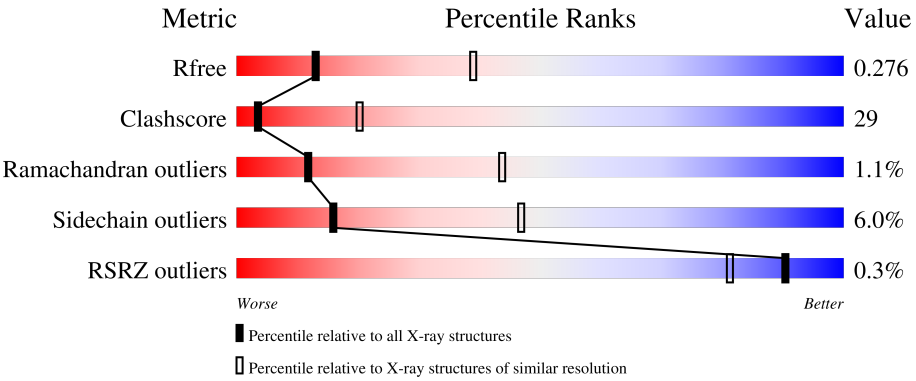
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	383	34% 37% • • 25%
1	B	383	37% 37% • 23%
1	C	383	% 35% 37% • • 23%
1	D	383	39% 36% • 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9917 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.

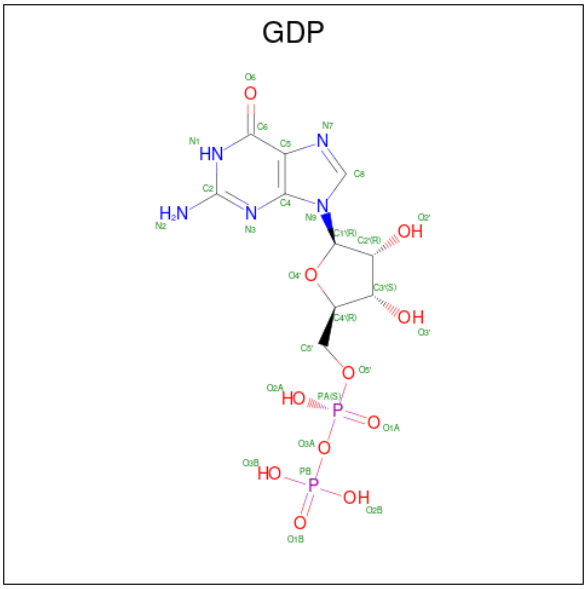
- Molecule 1 is a protein called Guanine nucleotide-binding protein alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2398	1553	390	445	10			
1	B	296	Total	C	N	O	S	0	0	0
			2468	1597	411	450	10			
1	C	293	Total	C	N	O	S	0	0	0
			2428	1576	397	445	10			
1	D	299	Total	C	N	O	S	0	0	0
			2507	1624	417	456	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A2Y3B5
A	-1	ALA	-	expression tag	UNP A2Y3B5
A	0	SER	-	expression tag	UNP A2Y3B5
A	173	VAL	ASP	conflict	UNP A2Y3B5
A	293	CYS	PHE	conflict	UNP A2Y3B5
B	-2	MET	-	initiating methionine	UNP A2Y3B5
B	-1	ALA	-	expression tag	UNP A2Y3B5
B	0	SER	-	expression tag	UNP A2Y3B5
B	173	VAL	ASP	conflict	UNP A2Y3B5
B	293	CYS	PHE	conflict	UNP A2Y3B5
C	-2	MET	-	initiating methionine	UNP A2Y3B5
C	-1	ALA	-	expression tag	UNP A2Y3B5
C	0	SER	-	expression tag	UNP A2Y3B5
C	173	VAL	ASP	conflict	UNP A2Y3B5
C	293	CYS	PHE	conflict	UNP A2Y3B5
D	-2	MET	-	initiating methionine	UNP A2Y3B5
D	-1	ALA	-	expression tag	UNP A2Y3B5
D	0	SER	-	expression tag	UNP A2Y3B5
D	173	VAL	ASP	conflict	UNP A2Y3B5
D	293	CYS	PHE	conflict	UNP A2Y3B5

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

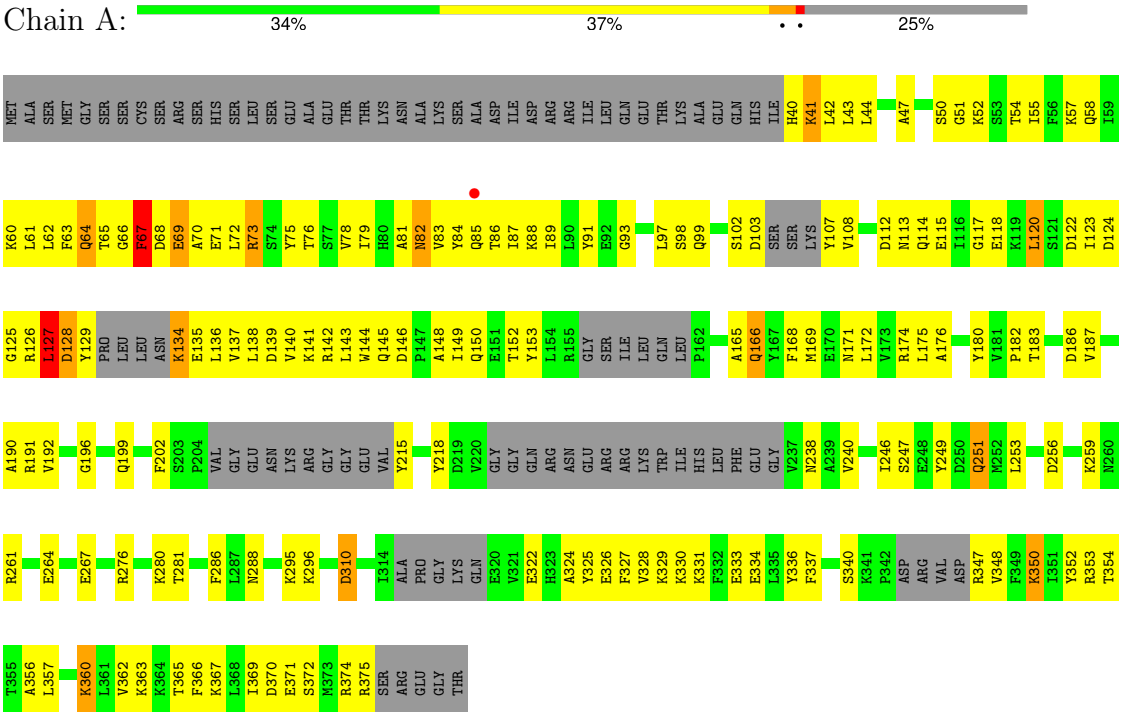
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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.

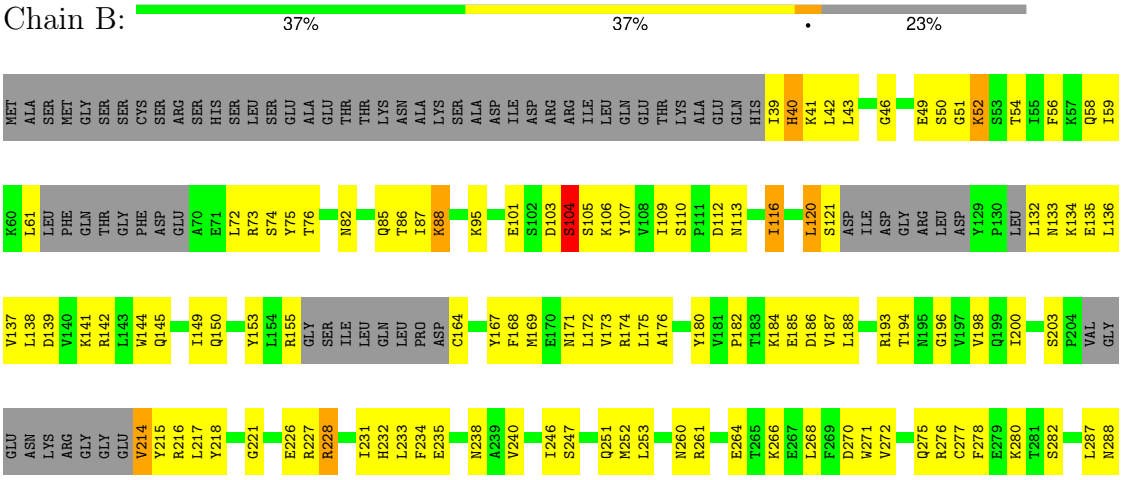
• Molecule 1: Guanine nucleotide-binding protein alpha-1 subunit

Chain A:



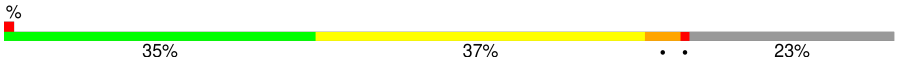
• Molecule 1: Guanine nucleotide-binding protein alpha-1 subunit

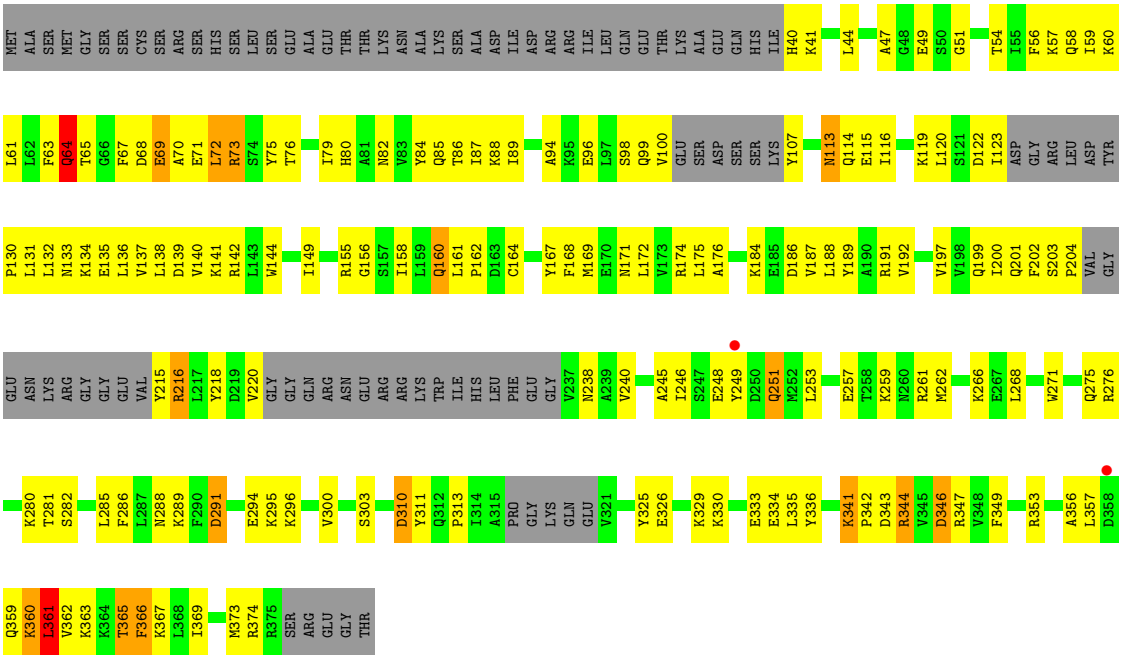
Chain B:



• Molecule 1: Guanine nucleotide-binding protein alpha-1 subunit

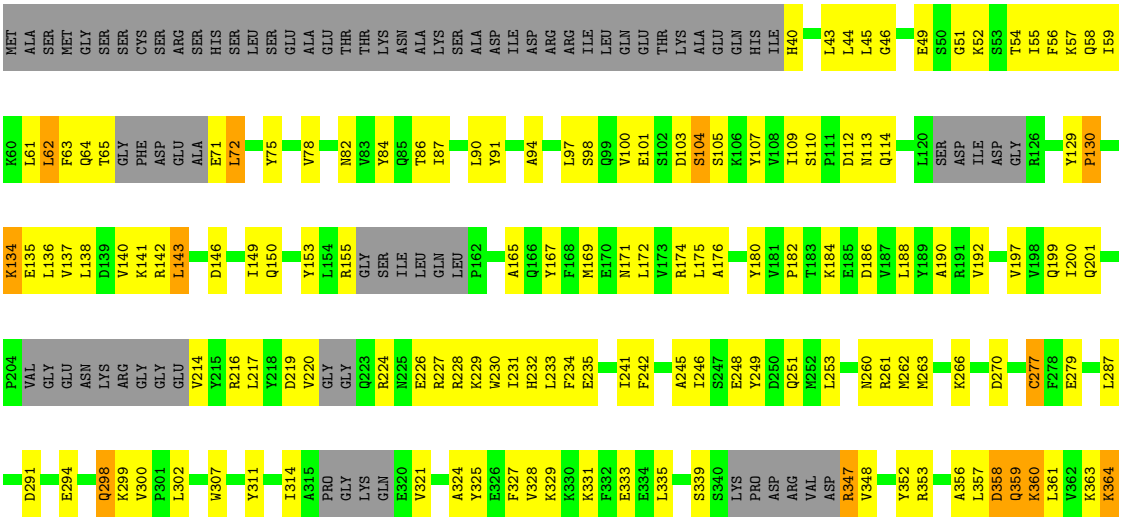
Chain C:





• Molecule 1: Guanine nucleotide-binding protein alpha-1 subunit

Chain D:




T365
F366
K367
L368
I369
D370
E371
S372
M373
R374
R375
SER
ARG
GLU
GLY
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.39Å 68.42Å 167.98Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	48.37 – 2.99 48.37 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.37-2.99) 95.1 (48.37-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.266 , 0.306 0.243 , 0.276	Depositor DCC
R_{free} test set	28282 reflections (6.39%)	wwPDB-VP
Wilson B-factor (Å^2)	85.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 111.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.468 for k,h,-l 0.468 for -k,-h,-l 0.470 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9917	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/2441	0.67	5/3276 (0.2%)
1	B	0.29	0/2513	0.58	3/3371 (0.1%)
1	C	0.33	0/2473	0.66	4/3325 (0.1%)
1	D	0.28	0/2553	0.63	3/3426 (0.1%)
All	All	0.30	0/9980	0.64	15/13398 (0.1%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	62	LEU	CA-CB-CG	10.74	140.01	115.30
1	A	69	GLU	C-N-CA	8.74	143.55	121.70
1	C	69	GLU	C-N-CA	8.63	143.26	121.70
1	C	360	LYS	C-N-CA	7.01	139.24	121.70
1	D	360	LYS	C-N-CA	6.64	138.30	121.70
1	C	361	LEU	CA-CB-CG	6.49	130.22	115.30
1	C	64	GLN	C-N-CA	6.05	136.83	121.70
1	B	227	ARG	C-N-CA	5.82	136.25	121.70
1	B	104	SER	C-N-CA	5.69	135.92	121.70
1	A	120	LEU	CA-CB-CG	5.53	128.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	104	SER	C-N-CA	5.45	135.33	121.70
1	B	357	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	64	GLN	C-N-CA	5.34	135.06	121.70
1	A	127	LEU	CA-CB-CG	5.21	127.27	115.30
1	A	67	PHE	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	LYS	Peptide
1	C	361	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2398	0	2404	152	0
1	B	2468	0	2490	145	0
1	C	2428	0	2460	157	0
1	D	2507	0	2530	129	0
2	A	28	0	12	4	0
2	B	28	0	12	5	0
2	C	28	0	12	3	0
2	D	28	0	12	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	9917	0	9932	575	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 29.

All (575) 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:B:58:GLN:HE22	1:B:188:LEU:HD11	1.27	0.96
1:D:231:ILE:HG22	1:D:233:LEU:H	1.30	0.94
1:C:87:ILE:HD11	1:C:120:LEU:HD11	1.55	0.88
1:C:363:LYS:O	1:C:367:LYS:N	2.09	0.84
1:B:59:ILE:HD13	1:B:217:LEU:HD22	1.58	0.84
1:C:72:LEU:HB2	1:C:187:VAL:HG21	1.60	0.83
1:D:298:GLN:HG2	1:D:300:VAL:HG12	1.61	0.83
1:C:201:GLN:HB2	1:C:216:ARG:HD3	1.61	0.82
1:D:329:LYS:NZ	1:D:333:GLU:OE2	2.12	0.81
1:B:203:SER:HB2	1:B:214:VAL:HA	1.61	0.80
1:A:61:LEU:HD11	1:A:187:VAL:HG11	1.63	0.80
1:A:117:GLY:HA2	1:A:143:LEU:HD21	1.62	0.79
1:A:144:TRP:HE3	1:A:145:GLN:HA	1.48	0.78
1:A:251:GLN:HB2	1:A:261:ARG:HD2	1.64	0.78
1:A:91:TYR:OH	1:A:114:GLN:NE2	2.15	0.78
1:C:69:GLU:H	1:C:70:ALA:HB3	1.51	0.76
1:A:122:ASP:O	1:A:126:ARG:NH1	2.19	0.76
1:A:57:LYS:NZ	1:A:190:ALA:O	2.19	0.75
1:B:298:GLN:HG3	1:B:300:VAL:H	1.49	0.75
1:A:280:LYS:HA	1:A:347:ARG:HH12	1.52	0.74
1:B:103:ASP:HB2	1:B:106:LYS:H	1.52	0.74
1:D:91:TYR:HE1	1:D:109:ILE:HD13	1.53	0.74
1:A:72:LEU:HB3	1:A:182:PRO:HG2	1.69	0.74
1:A:62:LEU:HD11	1:A:363:LYS:HB2	1.71	0.73
1:B:50:SER:O	1:B:288:ASN:ND2	2.21	0.73
1:B:251:GLN:OE1	1:B:261:ARG:NH1	2.22	0.72
1:B:226:GLU:HG2	1:B:228:ARG:HH11	1.52	0.72
1:C:79:ILE:HG23	1:C:168:PHE:HE1	1.54	0.72
1:C:133:ASN:OD1	1:C:136:LEU:N	2.22	0.72
1:C:167:TYR:O	1:C:171:ASN:ND2	2.17	0.72
1:C:40:HIS:N	1:C:238:ASN:OD1	2.23	0.72
1:A:150:GLN:HA	1:A:153:TYR:HB3	1.71	0.71
1:C:116:ILE:HA	1:C:119:LYS:HB3	1.72	0.71
1:C:40:HIS:HB3	1:C:215:TYR:HA	1.72	0.71
1:B:226:GLU:HB3	1:B:228:ARG:HD3	1.73	0.71
1:A:120:LEU:HA	1:A:123:ILE:HD12	1.73	0.70
1:B:356:ALA:HB3	2:B:401:GDP:N7	2.06	0.70
1:D:107:TYR:OH	1:D:155:ARG:NH1	2.24	0.70
1:D:78:VAL:O	1:D:82:ASN:ND2	2.23	0.70
1:C:123:ILE:HD12	1:C:123:ILE:H	1.57	0.70
1:C:58:GLN:HG2	1:C:61:LEU:HD12	1.73	0.70
1:C:251:GLN:HB2	1:C:261:ARG:HE	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:OE2	1:B:233:LEU:N	2.25	0.69
1:A:72:LEU:H	1:A:72:LEU:HD12	1.56	0.69
1:D:359:GLN:HB2	1:D:363:LYS:HE3	1.75	0.69
1:B:329:LYS:NZ	1:B:333:GLU:OE1	2.26	0.69
1:A:141:LYS:HG2	1:A:172:LEU:HD22	1.73	0.69
1:C:138:LEU:HD12	1:C:141:LYS:NZ	2.07	0.69
1:A:144:TRP:CE3	1:A:145:GLN:HA	2.27	0.69
1:A:68:ASP:HA	1:A:71:GLU:HB2	1.74	0.68
1:D:294:GLU:HG3	1:D:321:VAL:HG21	1.74	0.68
1:A:330:LYS:O	1:A:334:GLU:HG3	1.94	0.68
1:B:238:ASN:O	1:B:282:SER:N	2.27	0.67
1:C:240:VAL:HG23	1:C:281:THR:HG21	1.76	0.67
1:B:42:LEU:HD21	1:B:373:MET:HE1	1.76	0.67
1:C:133:ASN:HD21	1:C:136:LEU:HD13	1.58	0.67
1:B:141:LYS:HE2	1:B:145:GLN:HE21	1.59	0.67
1:D:226:GLU:HB2	1:D:228:ARG:HG2	1.76	0.67
1:D:234:PHE:HD2	1:D:277:CYS:HB3	1.60	0.67
1:D:358:ASP:HB3	1:D:361:LEU:HG	1.75	0.67
1:C:326:GLU:O	1:C:330:LYS:HG2	1.94	0.66
1:D:110:SER:OG	1:D:112:ASP:OD1	2.12	0.66
1:A:78:VAL:HG11	1:A:192:VAL:HG22	1.76	0.66
1:B:184:LYS:O	1:B:188:LEU:HD13	1.95	0.66
1:D:279:GLU:HA	1:D:347:ARG:HH21	1.61	0.66
1:A:91:TYR:HD2	1:A:120:LEU:HD22	1.60	0.66
1:D:302:LEU:HD23	1:D:302:LEU:H	1.59	0.66
1:A:240:VAL:HG23	1:A:281:THR:HG21	1.78	0.66
1:B:235:GLU:N	1:B:235:GLU:OE2	2.29	0.66
1:D:58:GLN:NE2	1:D:356:ALA:O	2.29	0.65
1:A:64:GLN:HB3	1:A:66:GLY:HA2	1.79	0.65
1:C:329:LYS:NZ	1:C:333:GLU:OE2	2.29	0.65
1:C:138:LEU:HD12	1:C:141:LYS:HZ3	1.60	0.65
1:C:160:GLN:HG3	1:C:162:PRO:HD2	1.79	0.65
1:C:119:LYS:HG3	1:C:120:LEU:H	1.61	0.64
1:D:174:ARG:NH2	1:D:186:ASP:OD1	2.30	0.64
1:B:357:LEU:HA	1:B:359:GLN:HE22	1.63	0.64
1:C:359:GLN:HG2	1:C:362:VAL:HG22	1.79	0.64
1:D:188:LEU:HB3	1:D:357:LEU:HD22	1.80	0.64
1:B:107:TYR:OH	1:B:155:ARG:NH1	2.30	0.64
1:D:138:LEU:HD12	1:D:141:LYS:HD3	1.80	0.64
1:C:116:ILE:HA	1:C:119:LYS:CB	2.28	0.64
1:D:150:GLN:HA	1:D:153:TYR:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ILE:HD12	1:C:119:LYS:HD3	1.81	0.63
1:D:62:LEU:HD12	1:D:363:LYS:HG2	1.81	0.63
1:A:253:LEU:HD11	1:A:264:GLU:HG3	1.79	0.63
1:B:61:LEU:HD21	1:B:184:LYS:HB2	1.81	0.63
1:D:201:GLN:HB2	1:D:216:ARG:HG2	1.81	0.62
1:C:67:PHE:O	1:C:71:GLU:HB2	1.99	0.62
1:C:356:ALA:N	2:C:401:GDP:O6	2.31	0.62
1:C:58:GLN:HG3	1:C:188:LEU:HD11	1.80	0.62
1:B:270:ASP:OD1	1:B:339:SER:OG	2.15	0.62
1:A:98:SER:OG	1:A:99:GLN:NE2	2.33	0.62
1:C:253:LEU:HD12	1:C:259:LYS:HB3	1.80	0.62
1:B:76:THR:HG22	1:B:182:PRO:HD3	1.82	0.62
1:A:88:LYS:HA	1:A:120:LEU:HD21	1.81	0.62
1:C:59:ILE:HG13	1:C:202:PHE:HZ	1.65	0.62
1:A:137:VAL:HG11	1:A:176:ALA:HB2	1.80	0.61
1:D:137:VAL:HG21	1:D:176:ALA:HB1	1.82	0.61
1:D:235:GLU:OE2	1:D:235:GLU:N	2.25	0.61
1:C:288:ASN:HD21	1:C:356:ALA:HB2	1.65	0.61
1:B:364:LYS:O	1:B:368:LEU:HG	2.00	0.61
1:D:146:ASP:N	1:D:146:ASP:OD1	2.32	0.61
1:C:356:ALA:HB3	2:C:401:GDP:N7	2.16	0.61
1:A:356:ALA:N	2:A:500:GDP:O6	2.33	0.60
1:B:110:SER:OG	1:B:112:ASP:OD1	2.17	0.60
1:D:367:LYS:O	1:D:371:GLU:HG2	2.01	0.60
1:B:167:TYR:O	1:B:171:ASN:ND2	2.34	0.60
1:C:87:ILE:HD12	1:C:88:LYS:N	2.16	0.60
1:C:360:LYS:H	1:C:361:LEU:HB3	1.66	0.60
1:A:253:LEU:HD23	1:A:261:ARG:HG2	1.83	0.60
1:B:101:GLU:OE2	1:B:155:ARG:NH2	2.34	0.60
1:D:51:GLY:O	1:D:54:THR:OG1	2.18	0.60
1:B:133:ASN:OD1	1:B:136:LEU:N	2.35	0.60
1:C:119:LYS:O	1:C:120:LEU:HG	2.00	0.60
1:C:201:GLN:HB2	1:C:216:ARG:CD	2.32	0.59
1:C:59:ILE:HD11	1:C:366:PHE:CE1	2.36	0.59
1:A:144:TRP:HA	1:A:149:ILE:HD11	1.84	0.59
1:A:202:PHE:HE2	1:A:366:PHE:HE2	1.51	0.59
1:C:59:ILE:HD11	1:C:366:PHE:CD1	2.38	0.59
1:D:101:GLU:OE1	1:D:155:ARG:NH2	2.35	0.59
1:C:266:LYS:HG3	1:C:335:LEU:HD11	1.85	0.59
1:A:150:GLN:HG3	1:A:153:TYR:CD2	2.38	0.59
1:D:169:MET:HA	1:D:172:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:THR:O	1:D:369:ILE:HD12	2.03	0.59
1:D:365:THR:O	1:D:368:LEU:N	2.36	0.58
1:A:82:ASN:ND2	1:A:191:ARG:H	2.00	0.58
1:A:69:GLU:HG3	1:A:70:ALA:HB3	1.85	0.58
1:C:114:GLN:O	1:C:116:ILE:N	2.29	0.58
1:C:326:GLU:HA	1:C:329:LYS:HB3	1.84	0.58
1:C:114:GLN:C	1:C:116:ILE:H	2.07	0.58
1:B:112:ASP:OD1	1:B:113:ASN:ND2	2.36	0.58
1:B:167:TYR:OH	1:B:186:ASP:OD1	2.14	0.58
1:C:330:LYS:O	1:C:334:GLU:HG3	2.04	0.58
1:C:136:LEU:O	1:C:140:VAL:HG23	2.04	0.57
1:A:41:LYS:HB2	1:A:238:ASN:H	1.70	0.57
1:D:134:LYS:HG3	1:D:135:GLU:H	1.69	0.57
1:A:70:ALA:HB1	1:A:73:ARG:HB2	1.87	0.57
1:A:82:ASN:HD21	1:A:191:ARG:H	1.51	0.57
1:A:137:VAL:O	1:A:141:LYS:HG3	2.04	0.57
1:A:62:LEU:HD22	1:A:63:PHE:CE2	2.40	0.57
1:B:216:ARG:NH2	1:B:218:TYR:OH	2.38	0.57
1:C:56:PHE:O	1:C:59:ILE:HG22	2.05	0.57
1:C:341:LYS:HE2	1:C:343:ASP:HB3	1.86	0.57
1:C:69:GLU:N	1:C:70:ALA:HB3	2.20	0.57
1:B:363:LYS:HA	1:B:366:PHE:HD2	1.68	0.57
1:C:191:ARG:NH1	1:C:192:VAL:O	2.38	0.57
1:D:167:TYR:OH	1:D:186:ASP:OD1	2.20	0.57
1:D:270:ASP:OD1	1:D:339:SER:OG	2.18	0.56
1:D:231:ILE:HB	1:D:234:PHE:CE1	2.40	0.56
1:B:358:ASP:OD1	1:B:360:LYS:HG2	2.05	0.56
1:D:104:SER:N	1:D:105:SER:HA	2.20	0.56
1:B:366:PHE:HA	1:B:369:ILE:HD12	1.87	0.56
1:D:40:HIS:HB3	1:D:214:VAL:O	2.06	0.56
1:C:86:THR:HG23	1:C:160:GLN:HE22	1.70	0.56
1:D:227:ARG:C	1:D:227:ARG:HD2	2.26	0.56
1:D:369:ILE:O	1:D:373:MET:HG2	2.05	0.56
1:C:116:ILE:HD11	1:C:139:ASP:CG	2.26	0.56
1:A:63:PHE:HE2	1:A:366:PHE:CD2	2.24	0.56
1:A:370:ASP:OD2	1:A:371:GLU:N	2.38	0.56
1:B:360:LYS:O	1:B:361:LEU:HB2	2.05	0.56
1:C:98:SER:OG	1:C:99:GLN:NE2	2.39	0.56
1:C:156:GLY:O	1:C:158:ILE:N	2.37	0.56
1:D:227:ARG:HE	1:D:231:ILE:HA	1.69	0.56
1:D:266:LYS:HG3	1:D:335:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLY:O	1:A:97:LEU:HG	2.06	0.55
1:D:109:ILE:HD11	1:D:114:GLN:HA	1.88	0.55
1:C:85:GLN:O	1:C:89:ILE:HG13	2.06	0.55
1:D:246:ILE:HD13	1:D:287:LEU:HB3	1.88	0.55
1:B:72:LEU:HD12	1:B:72:LEU:H	1.72	0.55
1:A:183:THR:N	1:A:186:ASP:OD2	2.33	0.55
1:B:226:GLU:N	1:B:226:GLU:OE1	2.39	0.55
1:C:347:ARG:HG3	1:C:347:ARG:HH11	1.70	0.55
1:D:298:GLN:HG3	1:D:299:LYS:H	1.72	0.55
1:C:79:ILE:HG23	1:C:168:PHE:CE1	2.38	0.55
1:D:251:GLN:OE1	1:D:261:ARG:NH1	2.39	0.55
1:A:139:ASP:O	1:A:143:LEU:N	2.40	0.55
1:B:355:THR:HB	1:B:358:ASP:HB3	1.88	0.55
1:C:360:LYS:N	1:C:361:LEU:HB3	2.21	0.55
1:D:298:GLN:CG	1:D:300:VAL:HG12	2.36	0.55
1:A:67:PHE:HA	1:A:68:ASP:C	2.28	0.54
1:A:202:PHE:CE2	1:A:366:PHE:HE2	2.24	0.54
1:B:144:TRP:HA	1:B:149:ILE:HG21	1.90	0.54
1:A:76:THR:HG22	1:A:182:PRO:HD3	1.88	0.54
1:B:247:SER:O	1:B:296:LYS:NZ	2.40	0.54
1:A:325:TYR:CZ	1:A:329:LYS:HE2	2.43	0.54
1:C:47:ALA:HB2	1:C:268:LEU:HD23	1.88	0.54
1:B:40:HIS:HD2	1:B:41:LYS:HE3	1.71	0.54
1:B:174:ARG:NH2	1:B:186:ASP:OD1	2.41	0.54
1:D:103:ASP:C	1:D:105:SER:HA	2.27	0.54
1:C:336:TYR:O	1:C:344:ARG:NH2	2.41	0.54
1:D:130:PRO:HB2	1:D:136:LEU:HD21	1.90	0.54
1:C:251:GLN:OE1	1:C:261:ARG:NH2	2.41	0.54
1:C:257:GLU:OE1	1:C:257:GLU:N	2.40	0.54
1:C:329:LYS:O	1:C:333:GLU:HG3	2.07	0.54
1:A:73:ARG:NH1	1:A:180:TYR:O	2.41	0.53
1:D:113:ASN:HD21	1:D:142:ARG:HG2	1.73	0.53
1:A:123:ILE:HG22	1:A:125:GLY:H	1.72	0.53
1:C:59:ILE:HG13	1:C:202:PHE:CZ	2.42	0.53
1:C:310:ASP:N	1:C:310:ASP:OD1	2.42	0.53
1:A:333:GLU:HB3	1:A:337:PHE:HE1	1.72	0.53
1:A:43:LEU:HD12	1:A:44:LEU:H	1.74	0.53
1:A:113:ASN:O	1:A:117:GLY:N	2.41	0.53
1:B:141:LYS:O	1:B:145:GLN:HG2	2.09	0.53
1:C:174:ARG:HH22	1:C:186:ASP:CG	2.10	0.53
1:A:288:ASN:HD21	1:A:356:ALA:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:O	1:A:83:VAL:HG23	2.09	0.53
1:B:103:ASP:CB	1:B:106:LYS:H	2.22	0.53
1:B:138:LEU:O	1:B:142:ARG:HG3	2.08	0.53
1:A:107:TYR:HA	1:A:148:ALA:HB1	1.90	0.53
1:B:75:TYR:CD2	1:B:187:VAL:HG13	2.44	0.52
1:A:366:PHE:CE1	1:A:370:ASP:HB3	2.45	0.52
1:B:58:GLN:HG2	1:B:359:GLN:OE1	2.09	0.52
1:B:41:LYS:H	1:B:41:LYS:HD2	1.73	0.52
1:C:363:LYS:HA	1:C:366:PHE:HB3	1.92	0.52
1:D:46:GLY:N	1:D:52:LYS:HD3	2.24	0.52
1:A:142:ARG:O	1:A:145:GLN:NE2	2.42	0.52
1:A:325:TYR:OH	1:A:353:ARG:HB2	2.10	0.52
1:B:357:LEU:HA	1:B:359:GLN:NE2	2.24	0.52
1:C:75:TYR:O	1:C:79:ILE:HG13	2.09	0.52
1:A:259:LYS:NZ	1:A:267:GLU:OE2	2.43	0.52
1:C:135:GLU:OE2	1:C:135:GLU:N	2.40	0.52
1:D:249:TYR:HA	1:D:262:MET:HB2	1.91	0.52
1:C:215:TYR:CZ	1:C:366:PHE:HZ	2.27	0.52
1:D:227:ARG:HD2	1:D:227:ARG:O	2.08	0.52
1:B:56:PHE:CZ	1:B:200:ILE:HD11	2.45	0.52
1:C:58:GLN:HB3	1:C:359:GLN:HG3	1.91	0.52
1:C:171:ASN:O	1:C:175:LEU:HG	2.09	0.52
1:A:87:ILE:O	1:A:120:LEU:HD11	2.10	0.52
1:A:144:TRP:HZ2	1:A:150:GLN:CD	2.13	0.52
1:A:374:ARG:HH11	1:A:375:ARG:HH12	1.57	0.52
1:B:169:MET:HA	1:B:172:LEU:HG	1.91	0.52
1:D:253:LEU:HD23	1:D:261:ARG:HG2	1.92	0.52
1:A:68:ASP:HA	1:A:71:GLU:CB	2.40	0.51
1:D:56:PHE:CZ	1:D:200:ILE:HG13	2.45	0.51
1:A:51:GLY:O	1:A:54:THR:OG1	2.26	0.51
1:A:135:GLU:OE1	1:A:135:GLU:N	2.44	0.51
1:C:86:THR:HG23	1:C:160:GLN:NE2	2.25	0.51
1:A:69:GLU:HB3	1:A:70:ALA:C	2.29	0.51
1:A:153:TYR:HE1	1:A:166:GLN:HG2	1.75	0.51
1:C:58:GLN:CG	1:C:188:LEU:HD21	2.41	0.51
1:A:103:ASP:OD2	1:A:108:VAL:N	2.44	0.51
1:B:138:LEU:HA	1:B:141:LYS:HG2	1.93	0.51
1:A:165:ALA:HA	1:A:168:PHE:HD2	1.75	0.51
1:A:372:SER:O	1:A:374:ARG:NH1	2.44	0.51
1:D:199:GLN:OE1	1:D:216:ARG:NH2	2.34	0.51
1:C:138:LEU:HA	1:C:141:LYS:HZ3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ILE:HD11	1:D:366:PHE:CE2	2.46	0.51
1:D:227:ARG:N	1:D:228:ARG:HA	2.25	0.51
1:A:67:PHE:HD1	1:A:67:PHE:H	1.59	0.51
1:A:374:ARG:HD2	1:A:375:ARG:HH22	1.76	0.51
1:B:86:THR:HG21	1:B:168:PHE:HD1	1.76	0.51
1:C:72:LEU:HD23	1:C:73:ARG:N	2.25	0.50
1:D:57:LYS:NZ	1:D:190:ALA:O	2.44	0.50
1:A:44:LEU:HD13	1:A:52:LYS:HB2	1.93	0.50
1:A:322:GLU:OE1	1:A:353:ARG:NH2	2.34	0.50
1:C:134:LYS:O	1:C:138:LEU:HD13	2.11	0.50
1:B:188:LEU:CD2	1:B:359:GLN:HE21	2.24	0.50
1:C:134:LYS:HA	1:C:137:VAL:HG22	1.92	0.50
1:B:135:GLU:HG2	1:B:136:LEU:HD22	1.93	0.50
1:C:360:LYS:HB2	1:C:361:LEU:HB3	1.94	0.50
1:D:63:PHE:O	1:D:65:THR:OG1	2.24	0.50
1:A:40:HIS:HB3	1:A:215:TYR:N	2.27	0.50
1:A:325:TYR:CE2	1:A:329:LYS:HE2	2.46	0.50
1:C:120:LEU:HB3	1:C:136:LEU:HG	1.93	0.50
1:A:73:ARG:HD2	1:B:228:ARG:HD2	1.94	0.50
1:C:41:LYS:HB2	1:C:238:ASN:H	1.77	0.50
1:A:85:GLN:HA	1:A:88:LYS:HB3	1.94	0.50
1:C:374:ARG:HB3	1:C:374:ARG:NH1	2.27	0.50
1:D:360:LYS:HB2	1:D:363:LYS:HD2	1.94	0.50
1:A:363:LYS:O	1:A:367:LYS:HG3	2.11	0.49
1:C:271:TRP:O	1:C:275:GLN:HG2	2.12	0.49
1:C:341:LYS:HG2	1:C:342:PRO:HD2	1.94	0.49
1:B:104:SER:N	1:B:105:SER:HA	2.27	0.49
1:C:49:GLU:OE2	1:C:261:ARG:NH1	2.44	0.49
1:C:63:PHE:O	1:C:65:THR:OG1	2.20	0.49
1:C:291:ASP:O	1:C:294:GLU:HG2	2.11	0.49
1:D:231:ILE:HB	1:D:234:PHE:HE1	1.76	0.49
1:B:133:ASN:HD21	1:B:136:LEU:HB2	1.77	0.49
1:B:171:ASN:O	1:B:175:LEU:HG	2.12	0.49
1:C:266:LYS:HG3	1:C:335:LEU:CD1	2.41	0.49
1:A:47:ALA:N	1:A:50:SER:OG	2.44	0.49
1:B:73:ARG:O	1:B:76:THR:HG23	2.13	0.49
1:C:184:LYS:O	1:C:188:LEU:HD23	2.13	0.49
1:D:59:ILE:HD12	1:D:217:LEU:HD22	1.94	0.49
1:D:329:LYS:O	1:D:333:GLU:HG3	2.12	0.49
1:A:374:ARG:HD2	1:A:375:ARG:NH2	2.27	0.49
1:C:68:ASP:H	1:C:71:GLU:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ARG:O	1:C:76:THR:HG23	2.13	0.49
1:D:143:LEU:HD13	1:D:149:ILE:HD13	1.95	0.49
1:A:329:LYS:O	1:A:333:GLU:HG3	2.13	0.49
1:B:231:ILE:HG22	1:B:233:LEU:H	1.77	0.49
1:B:253:LEU:HD23	1:B:261:ARG:HG2	1.95	0.49
1:C:246:ILE:O	1:C:249:TYR:HD2	1.95	0.49
1:B:365:THR:O	1:B:369:ILE:N	2.40	0.49
1:C:365:THR:O	1:C:369:ILE:HG13	2.13	0.49
1:A:82:ASN:OD1	1:A:82:ASN:N	2.45	0.48
1:C:63:PHE:CD1	1:C:202:PHE:HB2	2.48	0.48
1:A:67:PHE:CD1	1:A:67:PHE:N	2.80	0.48
1:A:68:ASP:CA	1:A:71:GLU:HB2	2.43	0.48
1:B:365:THR:O	1:B:369:ILE:HD12	2.13	0.48
1:B:50:SER:N	2:B:401:GDP:O3B	2.47	0.48
1:C:311:TYR:OH	1:C:313:PRO:HB3	2.14	0.48
1:A:86:THR:O	1:A:89:ILE:HG13	2.14	0.48
1:A:360:LYS:HE2	1:A:363:LYS:HD3	1.96	0.48
1:A:84:TYR:CE1	1:A:136:LEU:HD13	2.49	0.48
1:B:87:ILE:HD12	1:B:88:LYS:N	2.28	0.48
1:B:88:LYS:HD2	1:B:120:LEU:HD13	1.95	0.48
1:C:51:GLY:O	1:C:54:THR:OG1	2.28	0.48
1:B:133:ASN:CG	1:B:137:VAL:HG23	2.34	0.48
1:D:75:TYR:CE2	1:D:192:VAL:HG21	2.48	0.48
1:B:82:ASN:O	1:B:86:THR:HG23	2.14	0.48
1:B:185:GLU:HA	1:B:188:LEU:HD22	1.95	0.48
1:B:268:LEU:O	1:B:272:VAL:HG23	2.13	0.48
1:D:54:THR:HG23	2:D:401:GDP:O2A	2.13	0.48
1:D:84:TYR:CE2	1:D:130:PRO:HD2	2.49	0.48
1:D:352:TYR:HE2	1:D:368:LEU:HD12	1.78	0.48
1:A:67:PHE:CE2	1:B:233:LEU:HD23	2.49	0.47
1:D:359:GLN:HB2	1:D:363:LYS:CE	2.43	0.47
1:B:298:GLN:HG3	1:B:299:LYS:N	2.30	0.47
1:D:356:ALA:HB3	2:D:401:GDP:N7	2.29	0.47
1:A:357:LEU:HB2	2:A:500:GDP:C6	2.49	0.47
1:B:103:ASP:HB2	1:B:106:LYS:N	2.26	0.47
1:A:366:PHE:HD1	1:A:369:ILE:CD1	2.27	0.47
1:C:168:PHE:HE2	1:C:189:TYR:HB3	1.79	0.47
1:D:86:THR:HG21	1:D:165:ALA:HB1	1.95	0.47
1:B:43:LEU:HB3	1:B:240:VAL:HG22	1.97	0.47
1:C:203:SER:HA	1:C:215:TYR:CE2	2.49	0.47
1:B:333:GLU:O	1:B:337:PHE:HD1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HA	1:A:60:LYS:HD3	1.68	0.47
1:A:127:LEU:O	1:A:129:TYR:N	2.47	0.47
1:A:357:LEU:HD12	1:A:357:LEU:HA	1.78	0.47
1:B:294:GLU:CG	1:B:321:VAL:HG21	2.44	0.47
1:C:325:TYR:CZ	1:C:353:ARG:HB2	2.50	0.47
1:A:169:MET:HA	1:A:172:LEU:HD11	1.96	0.47
1:C:96:GLU:O	1:C:100:VAL:HG22	2.15	0.47
1:A:64:GLN:HE22	1:A:68:ASP:CB	2.27	0.47
1:B:252:MET:O	1:B:261:ARG:NE	2.48	0.47
1:D:44:LEU:HD12	1:D:241:ILE:HB	1.97	0.47
1:D:143:LEU:CD1	1:D:149:ILE:HD13	2.45	0.47
1:A:174:ARG:HH22	1:A:186:ASP:CG	2.18	0.46
1:B:253:LEU:HA	1:B:261:ARG:HE	1.80	0.46
1:C:288:ASN:OD1	1:C:289:LYS:N	2.46	0.46
1:A:62:LEU:HD22	1:A:63:PHE:CD2	2.50	0.46
1:C:245:ALA:O	1:C:248:GLU:HG2	2.15	0.46
1:C:137:VAL:HG23	1:C:138:LEU:N	2.30	0.46
1:C:168:PHE:CE2	1:C:189:TYR:HB3	2.50	0.46
1:A:63:PHE:CE2	1:A:366:PHE:CD2	3.04	0.46
1:B:116:ILE:HD11	1:B:139:ASP:O	2.16	0.46
1:A:63:PHE:HE2	1:A:366:PHE:HD2	1.62	0.46
1:B:194:THR:O	1:B:221:GLY:HA3	2.15	0.46
1:D:97:LEU:HA	1:D:100:VAL:HG12	1.97	0.46
1:A:69:GLU:H	1:A:71:GLU:N	2.13	0.46
1:A:117:GLY:O	1:A:120:LEU:HB3	2.16	0.46
1:A:253:LEU:HB2	1:A:256:ASP:O	2.15	0.46
1:B:82:ASN:HA	1:B:85:GLN:OE1	2.16	0.46
1:C:44:LEU:HB2	1:C:218:TYR:O	2.14	0.46
1:D:43:LEU:HD12	1:D:44:LEU:H	1.81	0.46
1:D:62:LEU:HD23	1:D:63:PHE:CG	2.51	0.46
1:D:325:TYR:CZ	1:D:353:ARG:HB2	2.50	0.46
1:A:363:LYS:CE	1:A:367:LYS:HD2	2.46	0.46
1:B:138:LEU:HG	1:B:142:ARG:HE	1.81	0.46
1:C:94:ALA:O	1:C:98:SER:N	2.48	0.46
1:A:75:TYR:HE2	1:B:196:GLY:HA3	1.79	0.45
1:A:123:ILE:O	1:A:126:ARG:HG3	2.16	0.45
1:A:196:GLY:HA2	1:B:74:SER:HB2	1.97	0.45
1:B:365:THR:C	1:B:369:ILE:HD12	2.36	0.45
1:C:54:THR:HA	1:C:57:LYS:HE2	1.98	0.45
1:C:141:LYS:O	1:C:144:TRP:N	2.49	0.45
1:C:359:GLN:O	1:C:360:LYS:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:O	1:A:371:GLU:HG2	2.16	0.45
1:C:144:TRP:HA	1:C:149:ILE:HD11	1.98	0.45
1:A:58:GLN:OE1	1:A:362:VAL:HG21	2.16	0.45
1:A:352:TYR:CE1	1:A:369:ILE:HG23	2.51	0.45
1:B:173:VAL:HG21	1:C:303:SER:OG	2.16	0.45
1:B:360:LYS:HD3	1:B:360:LYS:N	2.32	0.45
1:C:197:VAL:HG23	1:C:220:VAL:HG12	1.97	0.45
1:A:69:GLU:N	1:A:71:GLU:H	2.13	0.45
1:C:347:ARG:HG3	1:C:347:ARG:NH1	2.31	0.45
1:D:137:VAL:O	1:D:141:LYS:HG2	2.17	0.45
1:A:175:LEU:HD22	1:A:180:TYR:CZ	2.51	0.45
1:B:133:ASN:ND2	1:B:136:LEU:HB2	2.32	0.45
1:B:360:LYS:HD3	1:B:360:LYS:H	1.82	0.45
1:C:132:LEU:HD11	1:C:176:ALA:O	2.17	0.45
1:D:175:LEU:HD22	1:D:180:TYR:CZ	2.52	0.45
1:B:200:ILE:O	1:B:216:ARG:HA	2.17	0.45
1:B:278:PHE:O	1:B:347:ARG:NH1	2.49	0.45
1:C:70:ALA:HA	1:C:72:LEU:HD22	1.99	0.45
1:C:113:ASN:HA	1:C:116:ILE:CG2	2.47	0.45
1:D:360:LYS:N	1:D:361:LEU:HB2	2.32	0.45
1:B:103:ASP:OD1	1:B:103:ASP:N	2.50	0.45
1:D:227:ARG:HH21	1:D:231:ILE:HA	1.82	0.45
1:A:117:GLY:HA2	1:A:143:LEU:CD2	2.40	0.45
1:B:136:LEU:HD13	1:B:139:ASP:OD2	2.17	0.45
1:C:60:LYS:HG2	1:C:200:ILE:HD13	1.98	0.45
1:C:107:TYR:OH	1:C:155:ARG:NH2	2.50	0.45
1:C:285:LEU:HD12	1:C:286:PHE:N	2.32	0.45
1:D:311:TYR:HB2	1:D:327:PHE:CZ	2.52	0.45
1:A:87:ILE:HG21	1:A:140:VAL:HG13	1.98	0.45
1:A:191:ARG:HD3	1:A:191:ARG:HA	1.84	0.45
1:A:369:ILE:HD12	1:A:370:ASP:N	2.33	0.44
1:B:59:ILE:CD1	1:B:217:LEU:HD22	2.40	0.44
1:B:103:ASP:HB2	1:B:106:LYS:CB	2.47	0.44
1:D:357:LEU:HD23	1:D:357:LEU:HA	1.82	0.44
1:B:226:GLU:CB	1:B:228:ARG:HD3	2.46	0.44
1:B:311:TYR:HB2	1:B:327:PHE:CZ	2.52	0.44
1:C:174:ARG:NH2	1:C:186:ASP:OD1	2.50	0.44
1:D:43:LEU:HD12	1:D:44:LEU:N	2.31	0.44
1:D:44:LEU:HD13	1:D:217:LEU:HD11	2.00	0.44
1:A:88:LYS:HA	1:A:120:LEU:HD11	1.99	0.44
1:D:231:ILE:CG2	1:D:233:LEU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ARG:HH21	1:D:232:HIS:H	1.65	0.44
1:D:357:LEU:HD11	2:D:401:GDP:O2'	2.17	0.44
1:A:199:GLN:HG2	1:A:218:TYR:CE1	2.52	0.44
1:B:137:VAL:HG21	1:B:176:ALA:CB	2.47	0.44
1:B:150:GLN:HA	1:B:153:TYR:HB3	2.00	0.44
1:C:89:ILE:HB	1:C:160:GLN:OE1	2.17	0.44
1:C:188:LEU:HD12	1:C:357:LEU:HD23	1.99	0.44
1:D:61:LEU:HD13	1:D:184:LYS:HB3	1.98	0.44
1:C:114:GLN:C	1:C:116:ILE:N	2.69	0.44
1:C:296:LYS:HG3	1:C:300:VAL:CG1	2.48	0.44
1:C:336:TYR:CZ	1:C:349:PHE:HB2	2.52	0.44
1:D:231:ILE:HG22	1:D:233:LEU:N	2.14	0.44
1:B:40:HIS:HA	1:B:215:TYR:CD1	2.53	0.44
1:A:70:ALA:CB	1:A:73:ARG:HB2	2.47	0.44
1:B:175:LEU:HD22	1:B:180:TYR:CZ	2.53	0.44
1:B:266:LYS:HB2	1:B:307:TRP:CZ3	2.53	0.44
1:D:327:PHE:O	1:D:331:LYS:HG2	2.17	0.44
1:D:364:LYS:HD2	1:D:365:THR:N	2.33	0.44
1:A:365:THR:O	1:A:369:ILE:HG13	2.17	0.44
1:B:49:GLU:HB3	2:B:401:GDP:H5'	2.00	0.44
1:B:88:LYS:HD2	1:B:120:LEU:HD22	1.99	0.44
1:B:184:LYS:HG3	1:B:185:GLU:N	2.32	0.44
1:D:49:GLU:HA	2:D:401:GDP:O1B	2.17	0.44
1:D:298:GLN:HG3	1:D:299:LYS:N	2.33	0.44
1:A:81:ALA:O	1:A:85:GLN:HG2	2.18	0.43
1:A:83:VAL:O	1:A:87:ILE:HG13	2.18	0.43
1:C:132:LEU:HD21	1:C:176:ALA:HA	1.99	0.43
1:C:140:VAL:CG1	1:C:172:LEU:HD21	2.48	0.43
1:D:137:VAL:HA	1:D:140:VAL:HG12	2.00	0.43
1:D:226:GLU:O	1:D:226:GLU:HG2	2.17	0.43
1:A:327:PHE:CE2	1:A:331:LYS:HD2	2.53	0.43
1:B:352:TYR:HE1	1:B:368:LEU:HD12	1.83	0.43
1:C:58:GLN:HG3	1:C:188:LEU:HD21	2.00	0.43
1:C:360:LYS:O	1:C:363:LYS:HD2	2.19	0.43
1:B:298:GLN:HG2	1:B:300:VAL:HG12	2.00	0.43
1:C:191:ARG:HD2	1:C:192:VAL:N	2.33	0.43
1:D:197:VAL:HA	1:D:219:ASP:O	2.17	0.43
1:B:40:HIS:CD2	1:B:41:LYS:HE3	2.51	0.43
1:B:294:GLU:HG2	1:B:321:VAL:HG21	2.01	0.43
1:C:76:THR:HA	1:C:79:ILE:HB	1.99	0.43
1:C:295:LYS:O	1:C:295:LYS:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ASN:HD22	1:D:82:ASN:H	1.66	0.43
1:D:87:ILE:HG13	1:D:143:LEU:HD12	2.00	0.43
1:A:310:ASP:OD1	1:A:310:ASP:N	2.50	0.43
1:B:54:THR:HG21	2:B:401:GDP:H2'	2.00	0.43
1:D:56:PHE:CD2	1:D:217:LEU:HD23	2.54	0.43
1:D:231:ILE:CG2	1:D:233:LEU:H	2.15	0.43
1:D:356:ALA:N	2:D:401:GDP:O6	2.49	0.43
1:A:112:ASP:OD2	1:A:112:ASP:N	2.51	0.43
1:B:132:LEU:HA	1:B:133:ASN:HA	1.67	0.43
1:C:82:ASN:H	1:C:82:ASN:HD22	1.67	0.43
1:D:266:LYS:HB2	1:D:307:TRP:CZ3	2.54	0.43
1:C:67:PHE:HA	1:C:68:ASP:HA	1.90	0.43
1:D:171:ASN:O	1:D:175:LEU:HG	2.19	0.43
1:A:196:GLY:HA3	1:B:75:TYR:HE1	1.84	0.43
1:B:138:LEU:HG	1:B:142:ARG:NE	2.34	0.43
1:B:350:LYS:HE3	1:B:350:LYS:HB3	1.72	0.43
1:B:39:ILE:HG13	1:B:40:HIS:CE1	2.54	0.43
1:B:109:ILE:H	1:B:109:ILE:HD12	1.84	0.43
1:C:144:TRP:CE2	1:C:169:MET:HB3	2.54	0.43
1:D:71:GLU:N	1:D:71:GLU:OE1	2.52	0.43
1:D:167:TYR:O	1:D:171:ASN:ND2	2.46	0.43
1:A:91:TYR:CD2	1:A:120:LEU:HD22	2.48	0.42
1:B:134:LYS:HB3	1:B:134:LYS:HE2	1.70	0.42
1:A:75:TYR:CE2	1:B:196:GLY:HA3	2.53	0.42
1:B:87:ILE:HG23	1:B:169:MET:CE	2.49	0.42
1:B:271:TRP:O	1:B:275:GLN:HG2	2.18	0.42
1:D:55:ILE:HA	1:D:58:GLN:OE1	2.19	0.42
1:D:356:ALA:HB3	2:D:401:GDP:C5	2.54	0.42
1:D:365:THR:C	1:D:369:ILE:HD12	2.39	0.42
1:C:346:ASP:OD2	1:C:346:ASP:N	2.52	0.42
1:D:94:ALA:O	1:D:98:SER:OG	2.29	0.42
1:A:86:THR:HG21	1:A:165:ALA:HB1	2.00	0.42
1:C:80:HIS:HB3	1:C:84:TYR:CE1	2.53	0.42
1:C:164:CYS:HB2	1:C:189:TYR:CD2	2.55	0.42
1:A:246:ILE:O	1:A:249:TYR:HD1	2.03	0.42
1:A:247:SER:O	1:A:296:LYS:NZ	2.51	0.42
1:C:122:ASP:HB2	1:C:130:PRO:HD3	2.01	0.42
1:D:260:ASN:HB3	1:D:263:MET:HG2	2.01	0.42
1:A:54:THR:HG23	2:A:500:GDP:O2A	2.20	0.42
1:B:137:VAL:HG21	1:B:176:ALA:HB2	2.01	0.42
1:C:54:THR:HG23	2:C:401:GDP:O1A	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLU:O	1:C:119:LYS:N	2.53	0.42
1:C:202:PHE:CZ	1:C:215:TYR:HE1	2.37	0.42
1:D:45:LEU:O	1:D:242:PHE:HA	2.19	0.42
1:B:144:TRP:CE3	1:B:169:MET:HG3	2.55	0.42
1:C:59:ILE:CG1	1:C:202:PHE:HZ	2.31	0.42
1:C:138:LEU:HD12	1:C:141:LYS:HZ1	1.84	0.42
1:C:199:GLN:OE1	1:C:216:ARG:NE	2.34	0.42
1:D:359:GLN:C	1:D:361:LEU:HB2	2.40	0.42
1:A:286:PHE:CG	1:A:354:THR:HG21	2.55	0.42
1:A:360:LYS:HE2	1:A:363:LYS:CD	2.50	0.42
1:C:80:HIS:ND1	1:C:131:LEU:O	2.43	0.42
1:D:245:ALA:O	1:D:248:GLU:HG2	2.20	0.42
1:D:130:PRO:HB2	1:D:136:LEU:CD2	2.49	0.42
1:B:51:GLY:N	2:B:401:GDP:O3B	2.47	0.41
1:D:58:GLN:HE21	1:D:188:LEU:HD13	1.85	0.41
1:A:41:LYS:O	1:A:42:LEU:HD12	2.20	0.41
1:A:55:ILE:HD13	1:A:55:ILE:HA	1.88	0.41
1:A:97:LEU:HD12	1:A:152:THR:HG22	2.02	0.41
1:A:326:GLU:O	1:A:330:LYS:HG3	2.19	0.41
1:D:72:LEU:O	1:D:182:PRO:HD2	2.19	0.41
1:A:134:LYS:O	1:A:137:VAL:HG22	2.20	0.41
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.86	0.41
1:A:356:ALA:HB3	2:A:500:GDP:N7	2.35	0.41
1:A:363:LYS:HE3	1:A:367:LYS:HD2	2.02	0.41
1:B:41:LYS:O	1:B:42:LEU:HD23	2.21	0.41
1:B:110:SER:OG	1:B:113:ASN:ND2	2.32	0.41
1:B:120:LEU:HD12	1:B:121:SER:N	2.35	0.41
1:C:184:LYS:HB2	1:C:184:LYS:HE2	1.85	0.41
1:C:296:LYS:O	1:C:300:VAL:HG12	2.20	0.41
1:D:59:ILE:CD1	1:D:217:LEU:HD22	2.50	0.41
1:A:57:LYS:O	1:A:60:LYS:HB2	2.19	0.41
1:A:337:PHE:O	1:A:340:SER:HB3	2.21	0.41
1:B:246:ILE:HD13	1:B:287:LEU:HB3	2.01	0.41
1:C:132:LEU:HD22	1:C:133:ASN:N	2.35	0.41
1:C:168:PHE:O	1:C:172:LEU:HD12	2.21	0.41
1:C:203:SER:HA	1:C:204:PRO:HD3	1.92	0.41
1:D:91:TYR:CE1	1:D:109:ILE:HD13	2.44	0.41
1:D:311:TYR:HB2	1:D:327:PHE:CE2	2.55	0.41
1:A:138:LEU:HD12	1:A:139:ASP:N	2.35	0.41
1:B:302:LEU:HD21	1:B:328:VAL:CG2	2.51	0.41
1:D:324:ALA:O	1:D:328:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:O	1:A:65:THR:OG1	2.38	0.41
1:C:64:GLN:HA	1:C:65:THR:OG1	2.21	0.41
1:C:359:GLN:HG2	1:C:362:VAL:CG2	2.47	0.41
1:D:59:ILE:HA	1:D:62:LEU:HD22	2.03	0.41
1:A:103:ASP:OD2	1:A:107:TYR:N	2.53	0.41
1:A:333:GLU:O	1:A:336:TYR:N	2.53	0.41
1:B:234:PHE:CG	1:B:277:CYS:HB3	2.55	0.41
1:C:282:SER:HA	1:C:347:ARG:HB2	2.01	0.41
1:B:46:GLY:N	1:B:52:LYS:HD3	2.36	0.41
1:B:144:TRP:CD2	1:B:169:MET:HG3	2.56	0.41
1:B:358:ASP:O	1:B:362:VAL:HG23	2.21	0.41
1:C:98:SER:HG	1:C:99:GLN:NE2	2.18	0.41
1:C:336:TYR:OH	1:C:347:ARG:NH1	2.53	0.41
1:D:90:LEU:HB3	1:D:149:ILE:HG13	2.03	0.41
1:D:228:ARG:O	1:D:229:LYS:HG2	2.21	0.41
1:B:40:HIS:HB3	1:B:214:VAL:O	2.21	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD12	1.90	0.41
1:B:226:GLU:HG2	1:B:228:ARG:NH1	2.28	0.41
1:B:360:LYS:H	1:B:360:LYS:CD	2.33	0.41
1:C:353:ARG:HE	1:C:353:ARG:HB3	1.59	0.41
1:D:291:ASP:OD1	1:D:291:ASP:N	2.54	0.41
1:B:40:HIS:HB2	1:B:216:ARG:HG3	2.03	0.40
1:B:246:ILE:H	1:B:246:ILE:HG12	1.76	0.40
1:B:260:ASN:O	1:B:264:GLU:HG2	2.21	0.40
1:D:129:TYR:CE2	1:D:130:PRO:HB3	2.56	0.40
1:D:138:LEU:O	1:D:142:ARG:HB2	2.21	0.40
1:A:166:GLN:H	1:A:166:GLN:HG3	1.48	0.40
1:B:311:TYR:HB2	1:B:327:PHE:CE2	2.56	0.40
1:B:133:ASN:HD21	1:B:136:LEU:CB	2.35	0.40
1:C:82:ASN:HD22	1:C:82:ASN:N	2.19	0.40
1:C:246:ILE:HA	1:C:262:MET:HE1	2.04	0.40
1:D:75:TYR:O	1:D:78:VAL:HG22	2.21	0.40
1:B:41:LYS:C	1:B:42:LEU:HD23	2.42	0.40
1:B:329:LYS:O	1:B:333:GLU:HG3	2.21	0.40
1:D:64:GLN:HA	1:D:65:THR:OG1	2.22	0.40
1:A:66:GLY:O	1:A:68:ASP:HB3	2.22	0.40
1:A:171:ASN:O	1:A:175:LEU:HG	2.22	0.40
1:A:324:ALA:O	1:A:328:VAL:HG23	2.20	0.40
1:B:291:ASP:OD1	1:B:291:ASP:N	2.55	0.40
1:B:325:TYR:CZ	1:B:353:ARG:HB2	2.57	0.40
1:D:137:VAL:HG21	1:D:176:ALA:CB	2.50	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	272/383 (71%)	258 (95%)	13 (5%)	1 (0%)	30	66
1	B	280/383 (73%)	272 (97%)	6 (2%)	2 (1%)	19	54
1	C	281/383 (73%)	258 (92%)	20 (7%)	3 (1%)	12	44
1	D	283/383 (74%)	264 (93%)	13 (5%)	6 (2%)	5	28
All	All	1116/1532 (73%)	1052 (94%)	52 (5%)	12 (1%)	12	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ASP
1	B	361	LEU
1	D	134	LYS
1	D	348	VAL
1	C	361	LEU
1	D	314	ILE
1	C	160	GLN
1	D	72	LEU
1	B	341	LYS
1	D	298	GLN
1	C	161	LEU
1	D	130	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/344 (77%)	246 (93%)	19 (7%)	12	39
1	B	272/344 (79%)	252 (93%)	20 (7%)	11	38
1	C	269/344 (78%)	252 (94%)	17 (6%)	15	45
1	D	277/344 (80%)	268 (97%)	9 (3%)	34	67
All	All	1083/1376 (79%)	1018 (94%)	65 (6%)	16	47

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	67	PHE
1	A	73	ARG
1	A	82	ASN
1	A	102	SER
1	A	115	GLU
1	A	118	GLU
1	A	124	ASP
1	A	127	LEU
1	A	128	ASP
1	A	134	LYS
1	A	146	ASP
1	A	166	GLN
1	A	251	GLN
1	A	276	ARG
1	A	295	LYS
1	A	310	ASP
1	A	348	VAL
1	A	350	LYS
1	B	40	HIS
1	B	52	LYS
1	B	88	LYS
1	B	95	LYS
1	B	104	SER
1	B	116	ILE
1	B	120	LEU
1	B	164	CYS
1	B	193	ARG
1	B	198	VAL
1	B	214	VAL
1	B	228	ARG

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Mol	Chain	Res	Type
1	B	232	HIS
1	B	276	ARG
1	B	280	LYS
1	B	350	LYS
1	B	358	ASP
1	B	360	LYS
1	B	371	GLU
1	B	375	ARG
1	C	64	GLN
1	C	72	LEU
1	C	73	ARG
1	C	113	ASN
1	C	142	ARG
1	C	216	ARG
1	C	251	GLN
1	C	276	ARG
1	C	280	LYS
1	C	291	ASP
1	C	310	ASP
1	C	341	LYS
1	C	344	ARG
1	C	346	ASP
1	C	365	THR
1	C	366	PHE
1	C	373	MET
1	D	143	LEU
1	D	220	VAL
1	D	224	ARG
1	D	230	TRP
1	D	277	CYS
1	D	347	ARG
1	D	358	ASP
1	D	359	GLN
1	D	364	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	99	GLN
1	A	114	GLN
1	A	338	GLN

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Mol	Chain	Res	Type
1	B	40	HIS
1	B	58	GLN
1	B	145	GLN
1	B	199	GLN
1	B	359	GLN
1	C	99	GLN
1	D	113	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	GDP	A	500	3	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
2	GDP	D	401	3	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
2	GDP	B	401	3	25,30,30	0.98	1 (4%)	30,47,47	1.15	2 (6%)
2	GDP	C	401	3	25,30,30	0.98	1 (4%)	30,47,47	1.03	2 (6%)

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
2	GDP	A	500	3	-	4/12/32/32	0/3/3/3
2	GDP	D	401	3	-	5/12/32/32	0/3/3/3
2	GDP	B	401	3	-	6/12/32/32	0/3/3/3
2	GDP	C	401	3	-	3/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	GDP	C6-N1	-2.42	1.34	1.37
2	C	401	GDP	C6-N1	-2.41	1.34	1.37
2	D	401	GDP	C6-N1	-2.38	1.34	1.37
2	B	401	GDP	C6-N1	-2.25	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GDP	C8-N7-C5	3.42	108.38	102.55
2	D	401	GDP	C8-N7-C5	3.39	108.32	102.55
2	C	401	GDP	C8-N7-C5	3.21	108.01	102.55
2	A	500	GDP	C8-N7-C5	2.91	107.51	102.55
2	A	500	GDP	C5-C6-N1	2.20	118.27	114.07
2	B	401	GDP	O2A-PA-O3A	2.17	113.13	107.27
2	C	401	GDP	C5-C6-N1	2.12	118.11	114.07
2	D	401	GDP	C5-C6-N1	2.05	117.99	114.07

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	GDP	C5'-O5'-PA-O3A
2	B	401	GDP	C5'-O5'-PA-O3A
2	B	401	GDP	C5'-O5'-PA-O2A
2	C	401	GDP	C5'-O5'-PA-O3A
2	C	401	GDP	C5'-O5'-PA-O2A
2	D	401	GDP	PA-O3A-PB-O3B
2	D	401	GDP	C5'-O5'-PA-O3A
2	D	401	GDP	C5'-O5'-PA-O1A
2	A	500	GDP	O4'-C4'-C5'-O5'

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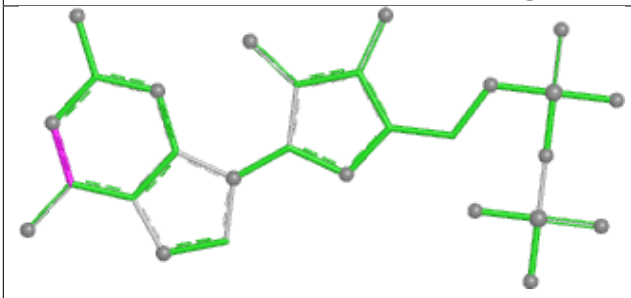
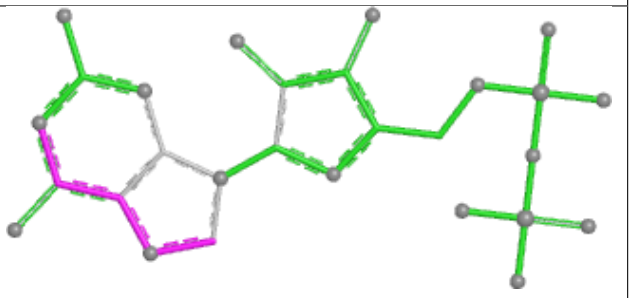
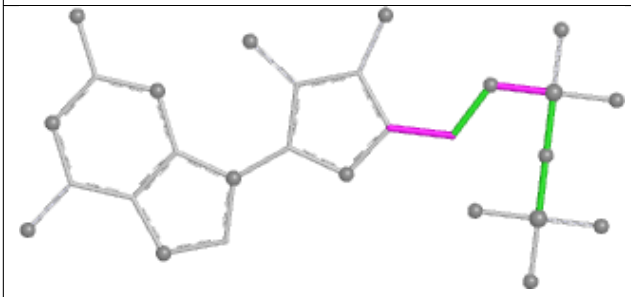
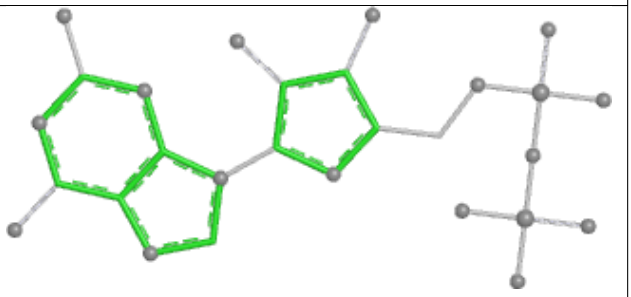
Mol	Chain	Res	Type	Atoms
2	A	500	GDP	C3'-C4'-C5'-O5'
2	D	401	GDP	PA-O3A-PB-O1B
2	B	401	GDP	PB-O3A-PA-O2A
2	A	500	GDP	C5'-O5'-PA-O2A
2	B	401	GDP	C5'-O5'-PA-O1A
2	C	401	GDP	C5'-O5'-PA-O1A
2	D	401	GDP	C5'-O5'-PA-O2A
2	B	401	GDP	O4'-C4'-C5'-O5'
2	B	401	GDP	C3'-C4'-C5'-O5'

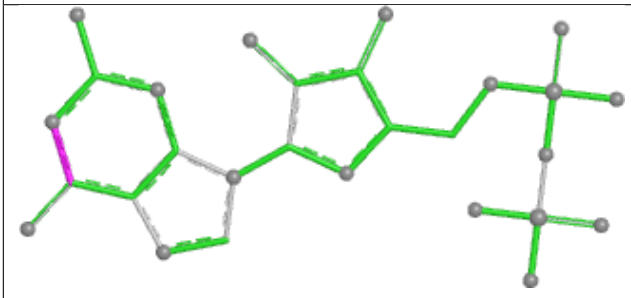
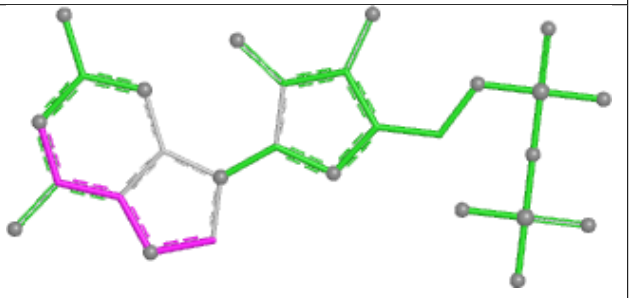
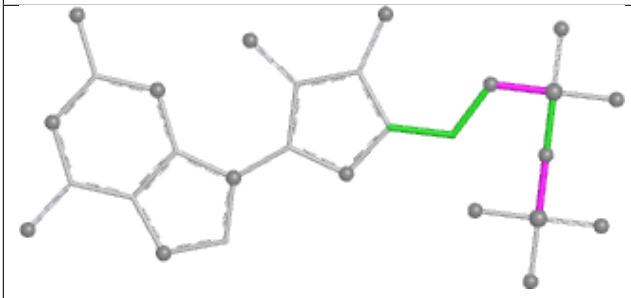
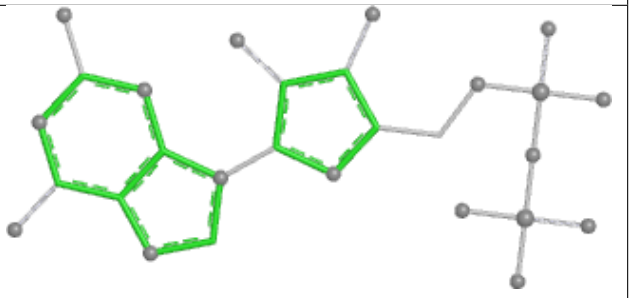
There are no ring outliers.

4 monomers are involved in 18 short contacts:

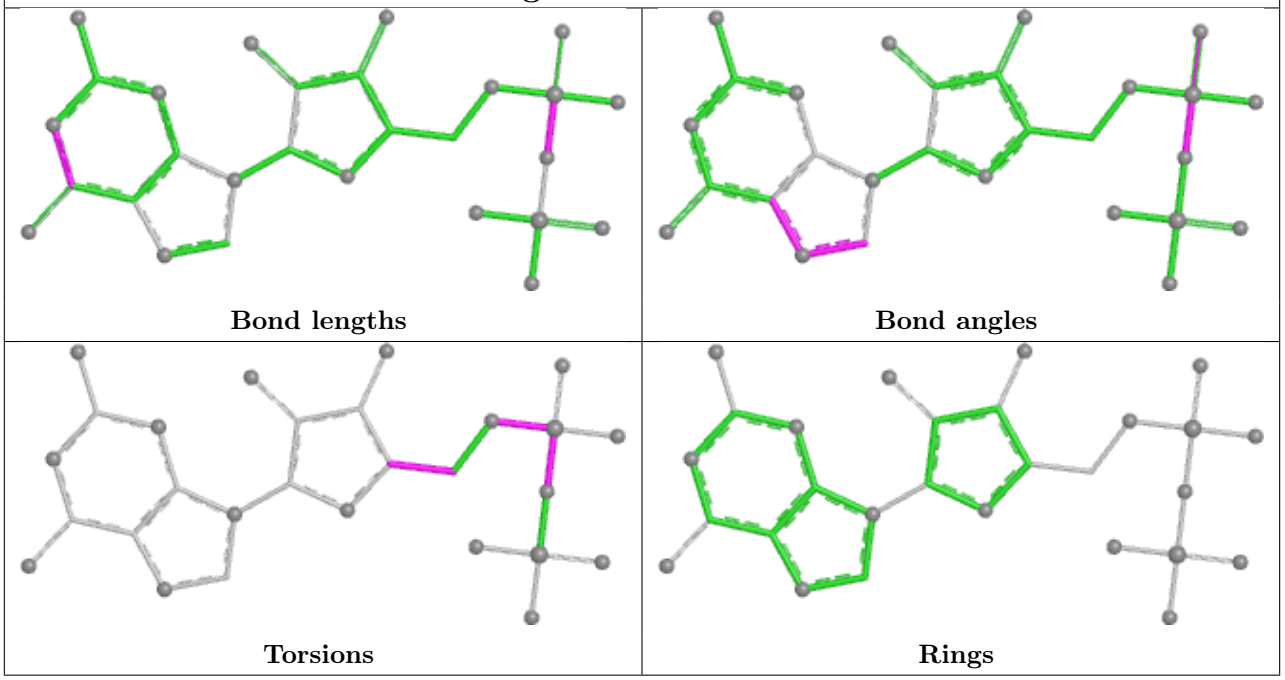
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	GDP	4	0
2	D	401	GDP	6	0
2	B	401	GDP	5	0
2	C	401	GDP	3	0

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

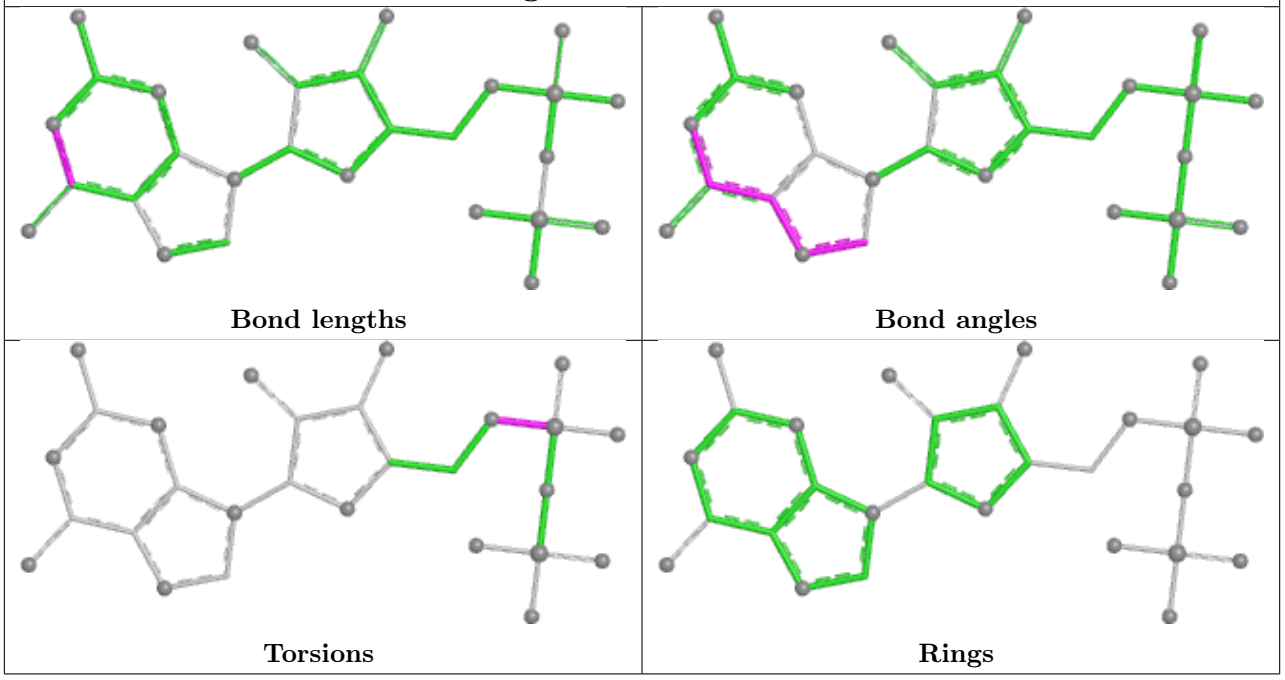
Ligand GDP A 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B 401



Ligand GDP C 401



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	288/383 (75%)	-0.67	1 (0%)	90	81	56, 90, 129, 186	0
1	B	296/383 (77%)	-0.71	1 (0%)	90	81	62, 91, 138, 213	0
1	C	293/383 (76%)	-0.68	2 (0%)	84	68	62, 95, 145, 209	0
1	D	299/383 (78%)	-0.73	0	100	100	60, 90, 137, 233	0
All	All	1176/1532 (76%)	-0.70	4 (0%)	90	81	56, 92, 139, 233	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	LYS	2.6
1	C	358	ASP	2.5
1	A	85	GLN	2.4
1	C	249	TYR	2.2

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 monosaccharides in this entry.

6.4 Ligands

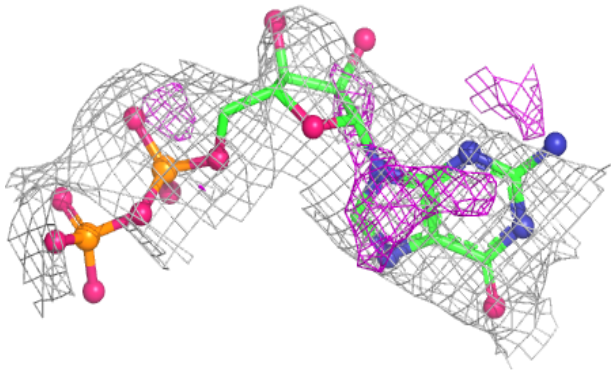
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

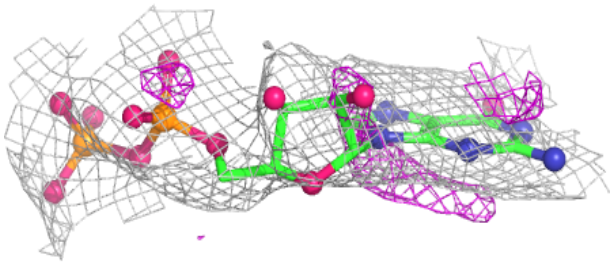
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	402	1/1	0.96	0.05	85,85,85,85	0
2	GDP	D	401	28/28	0.98	0.07	70,78,88,92	0
3	MG	A	501	1/1	0.98	0.07	98,98,98,98	0
3	MG	B	402	1/1	0.98	0.05	80,80,80,80	0
2	GDP	B	401	28/28	0.98	0.05	73,81,90,99	0
2	GDP	A	500	28/28	0.99	0.06	77,83,92,96	0
3	MG	C	402	1/1	0.99	0.08	83,83,83,83	0
2	GDP	C	401	28/28	0.99	0.05	70,82,97,111	0

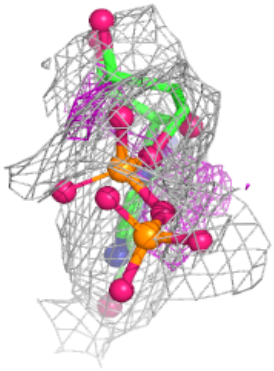
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP D 401:

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

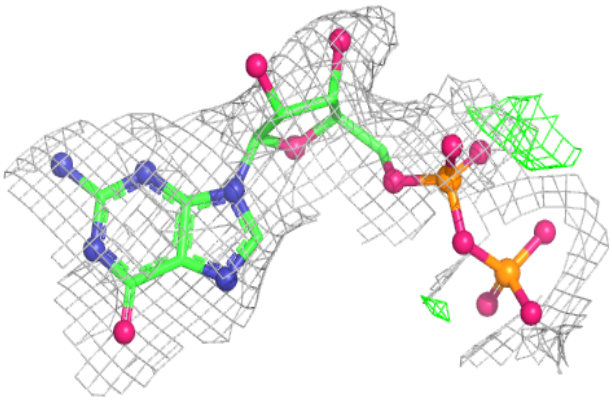


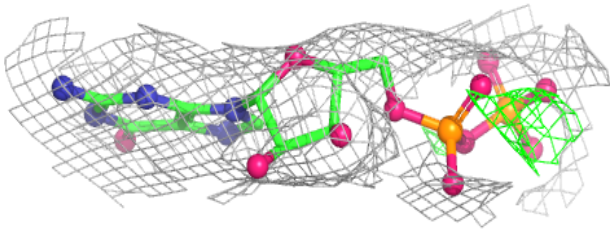


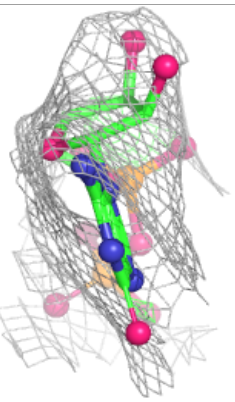


Electron density around GDP B 401:

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

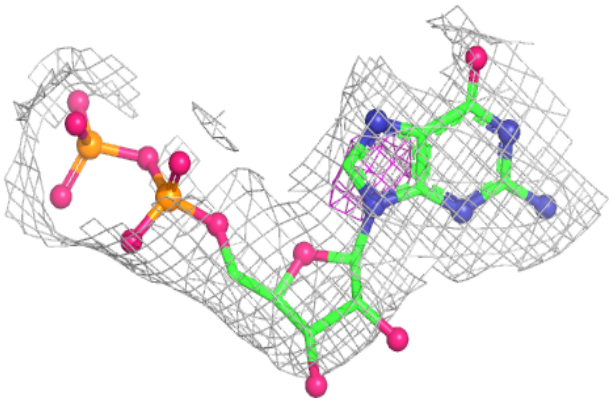


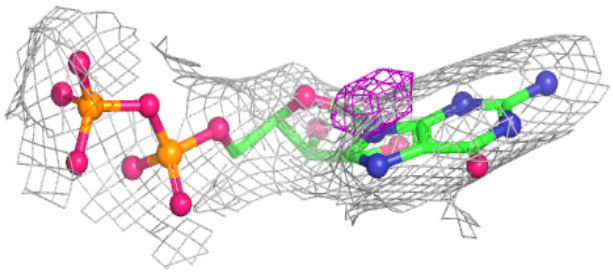


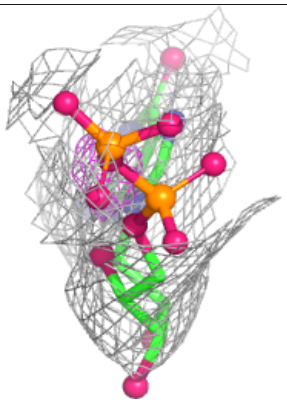


Electron density around GDP A 500:

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

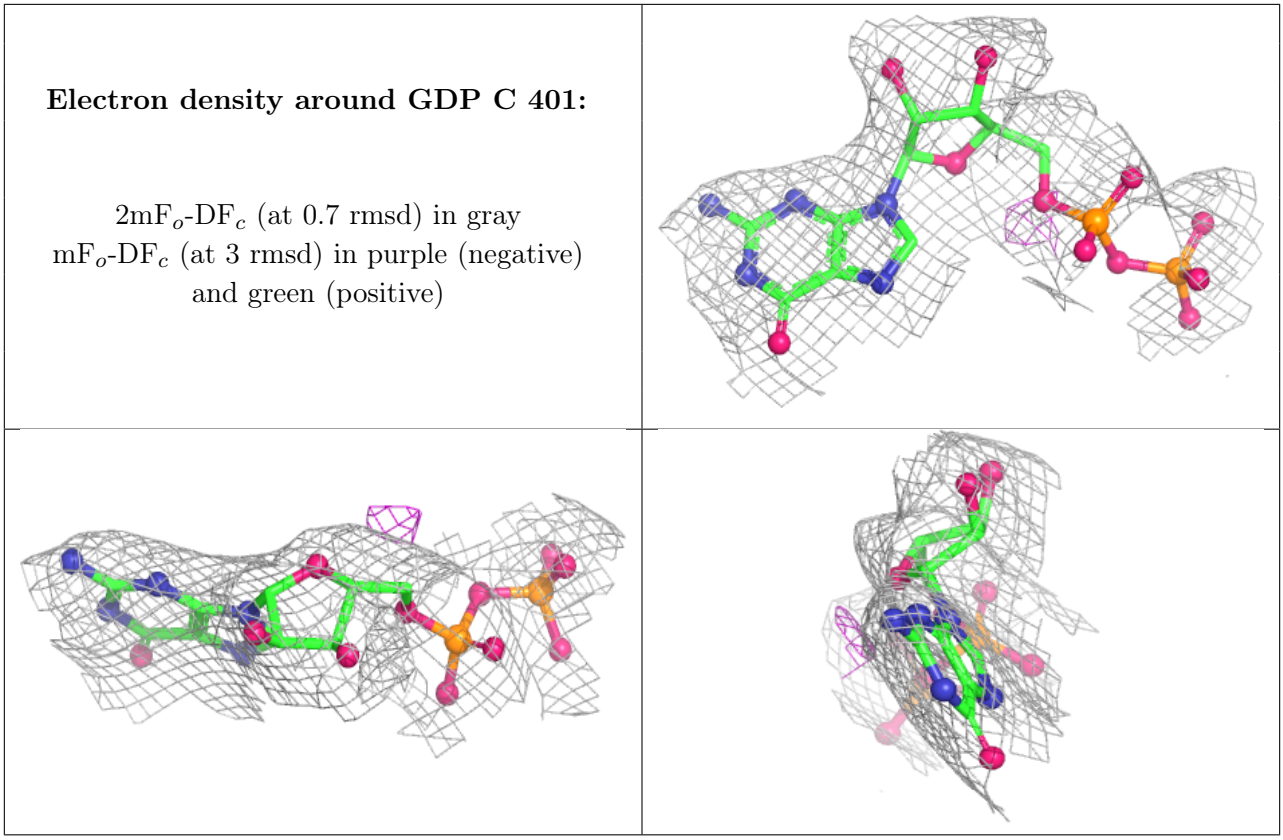






Electron density around GDP C 401:

$2mF_o$-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.