



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:55 AM EDT

PDB ID : 8VGB / pdb_00008vgb
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

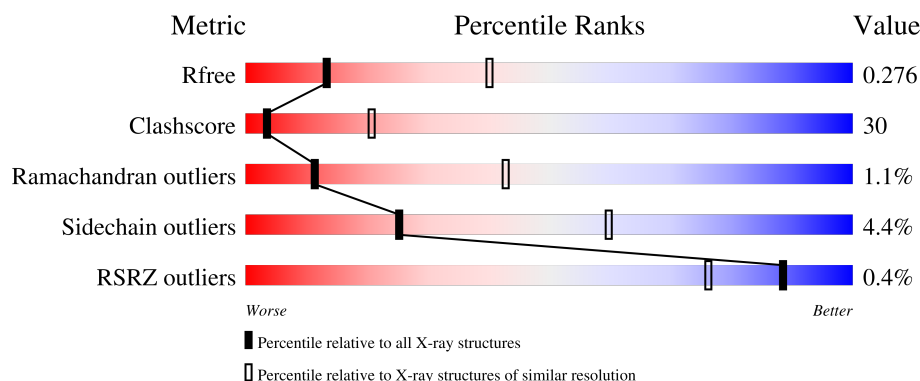
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	383	% 35% 38% • 25%
1	B	383	37% 37% • 23%
1	C	383	% 35% 38% • 23%
1	D	383	38% 36% • 22%

2 Entry composition

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.

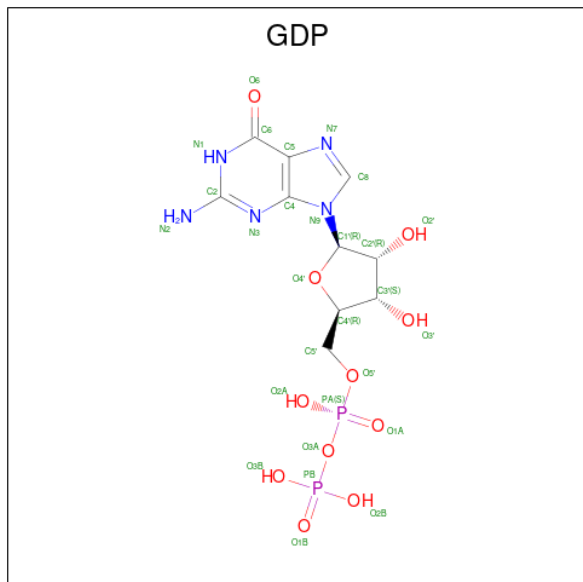
- Molecule 1 is a protein called Guanine nucleotide-binding protein alpha-1 subunit.

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

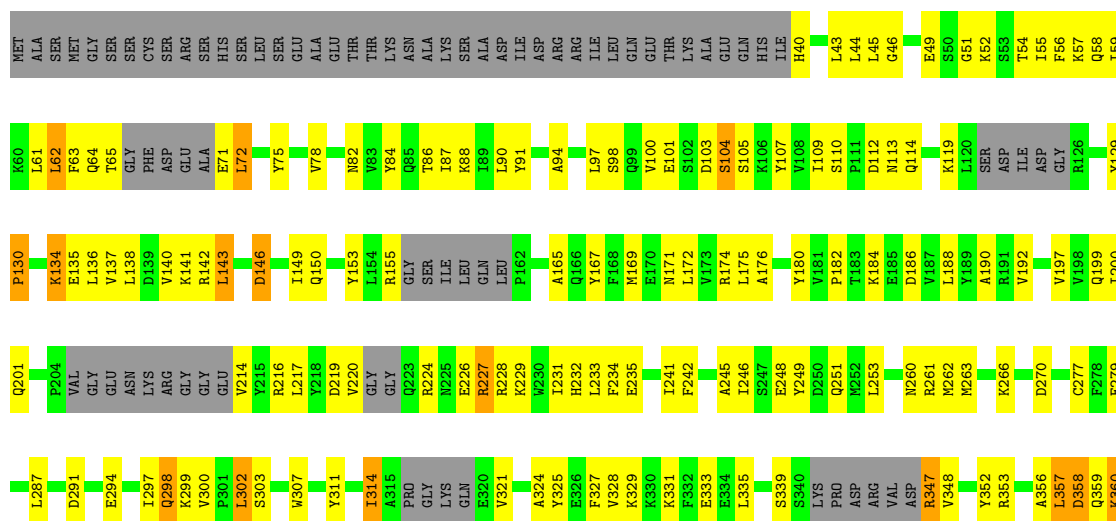
- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: 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		



L361	V362	K363	K364	T365	F366	K367	L368	I369	D370	E371	S372	M373	R374	R375	SER	ARG	GLU	GLY	THR
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4 Data and refinement statistics

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) 95.0 (48.37-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ 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	1932 reflections (6.10%)	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 , 111.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: 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	0.23	0/2441	0.66	6/3276 (0.2%)
1	B	0.19	0/2513	0.54	4/3371 (0.1%)
1	C	0.25	0/2473	0.71	7/3325 (0.2%)
1	D	0.19	0/2553	0.61	7/3426 (0.2%)
All	All	0.22	0/9980	0.63	24/13398 (0.2%)

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 (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	GLU	CA-C-N	12.14	143.55	121.70
1	A	69	GLU	C-N-CA	12.14	143.55	121.70
1	C	69	GLU	CA-C-N	11.98	143.26	121.70
1	C	69	GLU	C-N-CA	11.98	143.26	121.70
1	C	362	VAL	N-CA-C	-10.52	102.84	113.47
1	C	360	LYS	CA-C-N	9.74	139.24	121.70
1	C	360	LYS	C-N-CA	9.74	139.24	121.70
1	D	360	LYS	CA-C-N	9.21	138.28	121.70
1	D	360	LYS	C-N-CA	9.21	138.28	121.70
1	C	64	GLN	CA-C-N	8.40	136.83	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	GLN	C-N-CA	8.40	136.83	121.70
1	B	227	ARG	CA-C-N	8.08	136.25	121.70
1	B	227	ARG	C-N-CA	8.08	136.25	121.70
1	B	104	SER	CA-C-N	7.90	135.92	121.70
1	B	104	SER	C-N-CA	7.90	135.92	121.70
1	D	104	SER	CA-C-N	7.57	135.33	121.70
1	D	104	SER	C-N-CA	7.57	135.33	121.70
1	A	64	GLN	CA-C-N	7.42	135.06	121.70
1	A	64	GLN	C-N-CA	7.42	135.06	121.70
1	A	67	PHE	CA-C-N	6.96	134.22	121.70
1	A	67	PHE	C-N-CA	6.96	134.22	121.70
1	D	62	LEU	CA-CB-CG	6.78	140.01	116.30
1	D	227	ARG	CA-C-N	6.00	132.50	121.70
1	D	227	ARG	C-N-CA	6.00	132.50	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

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	157	0
1	B	2468	0	2490	149	0
1	C	2428	0	2460	157	0
1	D	2507	0	2530	132	0
2	A	28	0	12	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
All	All	9917	0	9932	587	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 30.

All (587) 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:138:LEU:HD12	1:C:141:LYS:HZ3	1.42	0.84
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	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:160:GLN:HG3	1:C:162:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:42:LEU:HD21	1:B:373:MET:HE1	1.78	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:B:87:ILE:HG23	1:B:169:MET:HE3	1.80	0.63
1:D:150:GLN:HA	1:D:153:TYR:HB3	1.80	0.63
1:C:114:GLN:C	1:C:116:ILE:H	2.07	0.63
1:C:116:ILE:HD12	1:C:119:LYS:HD3	1.81	0.63
1:B:167:TYR:OH	1:B:186:ASP:OD1	2.14	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:B:110:SER:OG	1:B:112:ASP:OD1	2.17	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: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:116:ILE:HD11	1:C:139:ASP:CG	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:227:ARG:C	1:D:227:ARG:HD2	2.26	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:103:ASP:C	1:D:105:SER:HA	2.27	0.59
1:A:67:PHE:HA	1:A:68:ASP:C	2.28	0.59
1:D:169:MET:HA	1:D:172:LEU:HG	1.83	0.59
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:B:112:ASP:OD1	1:B:113:ASN:ND2	2.36	0.58
1:C:174:ARG:HH22	1:C:186:ASP:CG	2.10	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:B:263:MET:HE3	1:B:306:GLU:HB3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:69:GLU:HB3	1:A:70:ALA:C	2.29	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:A:144:TRP:HZ2	1:A:150:GLN:CD	2.13	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:369:ILE:O	1:D:373:MET:HG2	2.05	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
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: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:C:336:TYR:O	1:C:344:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:288:ASN:HD21	1:A:356:ALA:HB2	1.73	0.53
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:B:133:ASN:CG	1:B:137:VAL:HG23	2.34	0.52
1:C:215:TYR:CZ	1:C:366:PHE:HZ	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:PHE:CZ	1:D:200:ILE:HG13	2.45	0.51
1:D:227:ARG:HD2	1:D:227:ARG:O	2.08	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: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:A:174:ARG:HH22	1:A:186:ASP:CG	2.18	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: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:B:365:THR:C	1:B:369:ILE:HD12	2.36	0.50
1:C:134:LYS:HA	1:C:137:VAL:HG22	1.92	0.50
1:C:167:TYR:OH	1:C:186:ASP:OD1	2.26	0.50
1:C:138:LEU:HA	1:C:141:LYS:HZ3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:365:THR:C	1:D:369:ILE:HD12	2.39	0.47
1:B:333:GLU:O	1:B:337:PHE:HD1	1.97	0.47
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:D:359:GLN:C	1:D:361:LEU:HB2	2.40	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:54:THR:HA	1:C:57:LYS:HE2	1.98	0.45
1:C:114:GLN:C	1:C:116:ILE:N	2.69	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
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:41:LYS:C	1:B:42:LEU:HD23	2.42	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:A:64:GLN:HA	1:A:65:THR:C	2.42	0.45
1:A:255:GLU:H	1:A:255:GLU:CD	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:246:ILE:HA	1:C:262:MET:HE1	1.99	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:101:GLU:CD	1:B:155:ARG:HH22	2.26	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:64:GLN:HA	1:D:65:THR:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:295:LYS:HD3	1:C:295:LYS:C	2.44	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:C:183:THR:HG22	1:C:186:ASP:CG	2.44	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
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:199:GLN:OE1	1:C:216:ARG:NE	2.34	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:297:ILE:O	1:D:298:GLN:C	2.63	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:327:PHE:C	1:A:327:PHE:CD2	2.98	0.41
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:71:GLU:N	1:B:71:GLU:CD	2.79	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: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:A:47:ALA:O	1:A:50:SER:OG	2.39	0.41
1:B:40:HIS:HB3	1:B:214:VAL:O	2.21	0.41
1:B:87:ILE:HG23	1:B:169:MET:CE	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:88:LYS:HZ1	1:D:119:LYS:HB3	1.86	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:D:75:TYR:O	1:D:78:VAL:HG22	2.21	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:53:SER:OG	2:A:500:GDP:O2A	2.34	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:C:346:ASP:OD2	1:C:346:ASP:N	2.52	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 65
1	B	280/383 (73%)	272 (97%)	6 (2%)	2 (1%)	18 53
1	C	281/383 (73%)	258 (92%)	20 (7%)	3 (1%)	11 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	283/383 (74%)	264 (93%)	13 (5%)	6 (2%)	5	27
All	All	1116/1532 (73%)	1052 (94%)	52 (5%)	12 (1%)	11	43

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 ⓘ

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%)	255 (96%)	10 (4%)	29	63
1	B	272/344 (79%)	254 (93%)	18 (7%)	15	46
1	C	269/344 (78%)	259 (96%)	10 (4%)	30	64
1	D	277/344 (80%)	267 (96%)	10 (4%)	31	65
All	All	1083/1376 (79%)	1035 (96%)	48 (4%)	25	60

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	PHE
1	A	77	SER

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Mol	Chain	Res	Type
1	A	82	ASN
1	A	127	LEU
1	A	155	ARG
1	A	166	GLN
1	A	310	ASP
1	A	348	VAL
1	A	350	LYS
1	A	362	VAL
1	B	39	ILE
1	B	40	HIS
1	B	49	GLU
1	B	52	LYS
1	B	58	GLN
1	B	78	VAL
1	B	104	SER
1	B	116	ILE
1	B	151	GLU
1	B	164	CYS
1	B	198	VAL
1	B	214	VAL
1	B	232	HIS
1	B	280	LYS
1	B	350	LYS
1	B	358	ASP
1	B	360	LYS
1	B	371	GLU
1	C	72	LEU
1	C	142	ARG
1	C	154	LEU
1	C	161	LEU
1	C	173	VAL
1	C	274	LYS
1	C	310	ASP
1	C	330	LYS
1	C	353	ARG
1	C	365	THR
1	D	143	LEU
1	D	146	ASP
1	D	220	VAL
1	D	224	ARG
1	D	302	LEU
1	D	303	SER

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Mol	Chain	Res	Type
1	D	314	ILE
1	D	347	ARG
1	D	357	LEU
1	D	358	ASP

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

Mol	Chain	Res	Type
1	A	64	GLN
1	A	99	GLN
1	A	114	GLN
1	B	40	HIS
1	B	58	GLN
1	B	145	GLN
1	B	199	GLN
1	B	298	GLN
1	B	359	GLN
1	C	99	GLN
1	D	80	HIS
1	D	82	ASN
1	D	113	ASN
1	D	298	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 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	C	401	3	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
2	GDP	A	500	3	29,30,30	1.15	2 (6%)	45,47,47	1.75	5 (11%)
2	GDP	D	401	3	29,30,30	1.15	2 (6%)	45,47,47	1.81	7 (15%)
2	GDP	B	401	3	29,30,30	1.17	3 (10%)	45,47,47	1.86	9 (20%)

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	C	401	3	-	3/16/32/32	0/3/3/3
2	GDP	A	500	3	-	4/16/32/32	0/3/3/3
2	GDP	D	401	3	-	5/16/32/32	0/3/3/3
2	GDP	B	401	3	-	6/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	GDP	C5-C4	3.14	1.47	1.38
2	D	401	GDP	C5-C4	3.13	1.47	1.38
2	C	401	GDP	C5-C4	3.11	1.47	1.38
2	B	401	GDP	C5-C4	3.07	1.47	1.38
2	A	500	GDP	C6-N1	-2.55	1.34	1.38
2	C	401	GDP	C6-N1	-2.53	1.34	1.38
2	D	401	GDP	C6-N1	-2.51	1.34	1.38
2	B	401	GDP	C6-N1	-2.40	1.34	1.38
2	B	401	GDP	C5-N7	-2.15	1.34	1.39
2	C	401	GDP	C5-N7	-2.07	1.34	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GDP	C5-C4-N3	-6.31	118.34	128.39
2	D	401	GDP	C5-C4-N3	-6.23	118.47	128.39
2	C	401	GDP	C5-C4-N3	-6.16	118.59	128.39
2	A	500	GDP	C5-C4-N3	-6.03	118.80	128.39
2	B	401	GDP	C2-N3-C4	5.12	121.11	112.30
2	D	401	GDP	C2-N3-C4	5.11	121.10	112.30
2	C	401	GDP	C2-N3-C4	5.04	120.98	112.30
2	A	500	GDP	C2-N3-C4	5.03	120.96	112.30
2	B	401	GDP	N9-C4-N3	4.69	135.33	125.95
2	C	401	GDP	N9-C4-N3	4.55	135.05	125.95
2	D	401	GDP	N9-C4-N3	4.49	134.94	125.95
2	A	500	GDP	N9-C4-N3	4.36	134.67	125.95
2	D	401	GDP	C6-C5-N7	3.66	136.94	130.29
2	A	500	GDP	C6-C5-N7	3.54	136.72	130.29
2	C	401	GDP	C6-C5-N7	3.48	136.63	130.29
2	B	401	GDP	C6-C5-N7	3.37	136.41	130.29
2	D	401	GDP	C4-C5-N7	-3.05	105.84	110.67
2	B	401	GDP	C4-C5-N7	-2.94	106.00	110.67
2	C	401	GDP	C4-C5-N7	-2.81	106.22	110.67
2	A	500	GDP	C4-C5-N7	-2.67	106.44	110.67
2	D	401	GDP	C3'-C2'-C1'	2.39	105.99	101.46
2	B	401	GDP	C3'-C2'-C1'	2.31	105.83	101.46
2	B	401	GDP	C8-N7-C5	2.31	108.38	104.26
2	D	401	GDP	C8-N7-C5	2.28	108.32	104.26
2	B	401	GDP	O2A-PA-O3A	2.17	113.13	107.27
2	C	401	GDP	C3'-C2'-C1'	2.12	105.48	101.46
2	C	401	GDP	C8-N7-C5	2.11	108.01	104.26
2	B	401	GDP	O6-C6-C5	-2.08	121.04	126.53

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'
2	A	500	GDP	C3'-C4'-C5'-O5'

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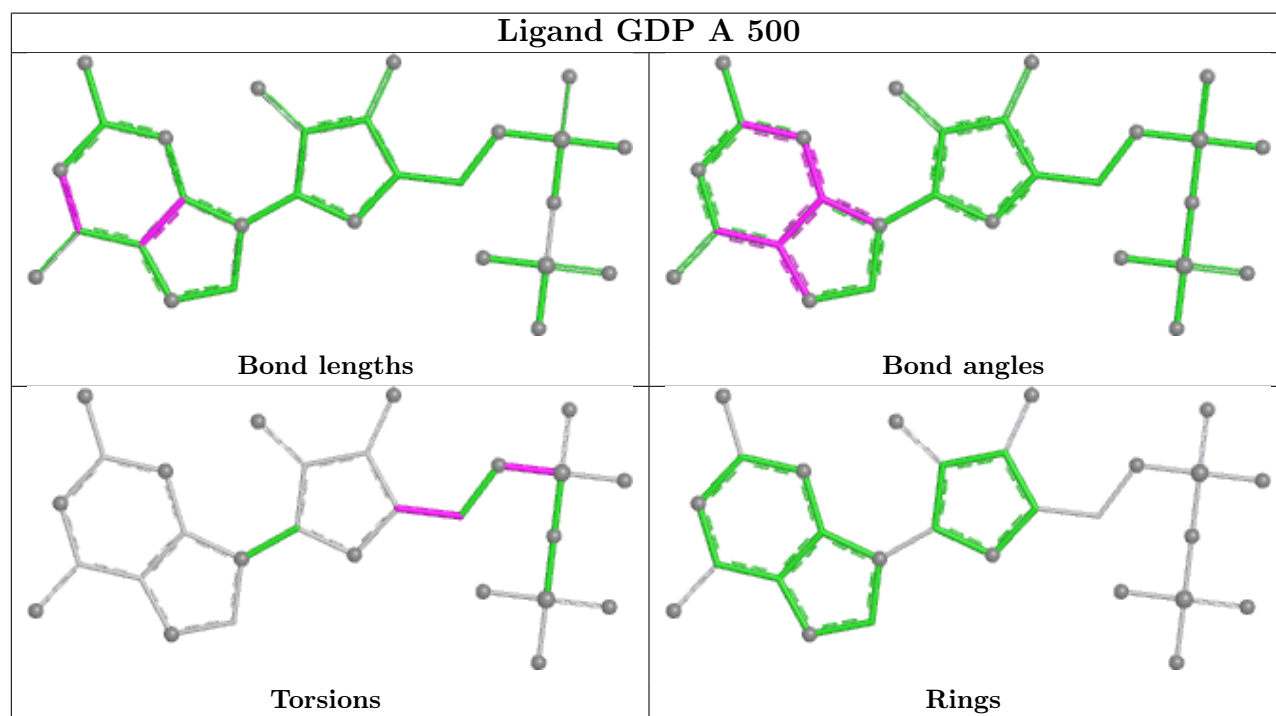
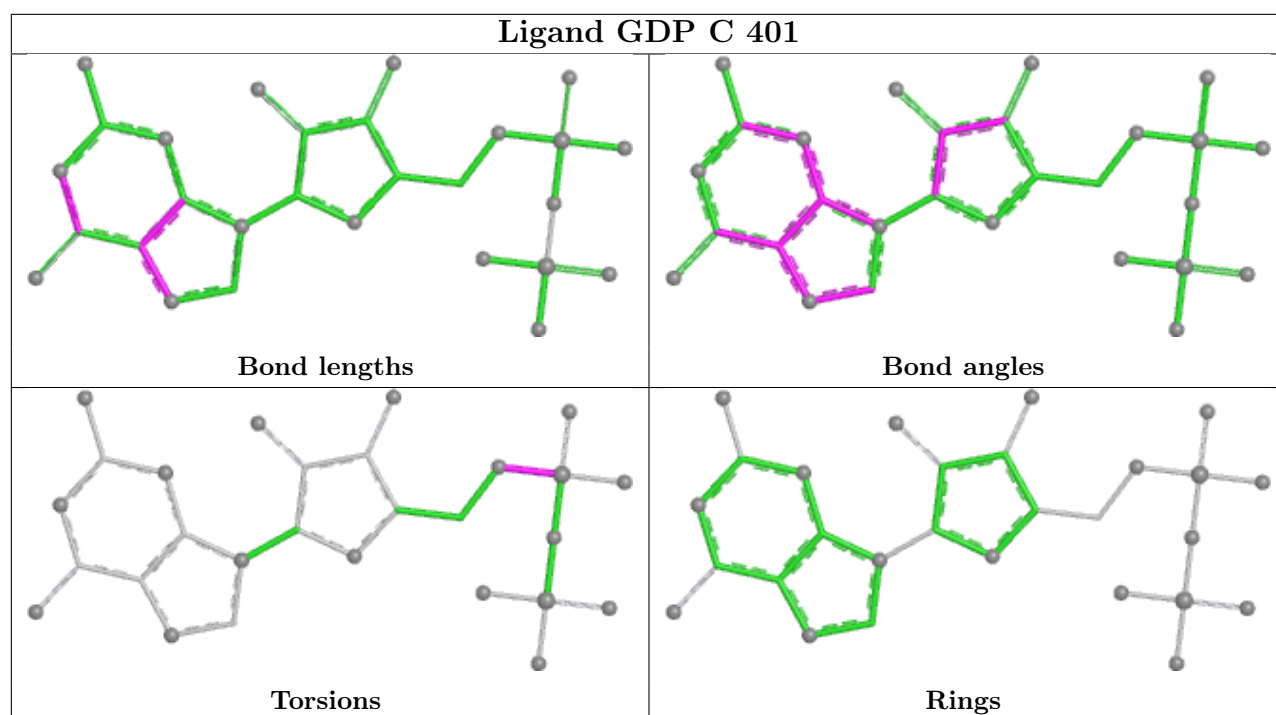
Mol	Chain	Res	Type	Atoms
2	D	401	GDP	PA-O3A-PB-O1B
2	B	401	GDP	PB-O3A-PA-O2A
2	A	500	GDP	C5'-O5'-PA-O2A
2	B	401	GDP	C5'-O5'-PA-O1A
2	C	401	GDP	C5'-O5'-PA-O1A
2	D	401	GDP	C5'-O5'-PA-O2A
2	B	401	GDP	O4'-C4'-C5'-O5'
2	B	401	GDP	C3'-C4'-C5'-O5'

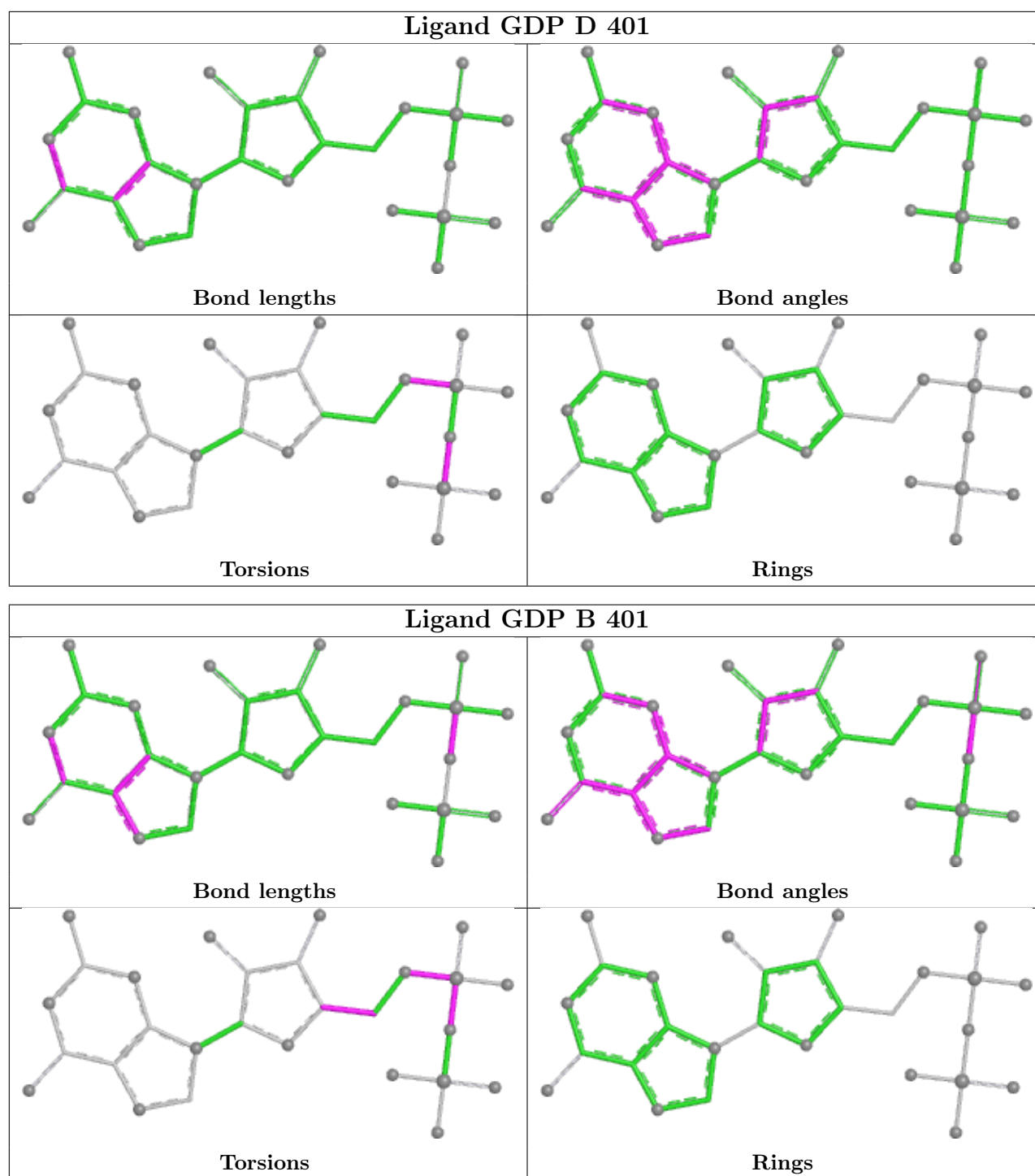
There are no ring outliers.

4 monomers are involved in 19 short contacts:

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/383 (75%)	-0.52	2 (0%) 84 66	56, 90, 129, 186	0
1	B	296/383 (77%)	-0.56	1 (0%) 90 79	62, 91, 138, 213	0
1	C	293/383 (76%)	-0.53	2 (0%) 84 66	62, 95, 145, 209	0
1	D	299/383 (78%)	-0.58	0 100 100	60, 90, 137, 233	0
All	All	1176/1532 (76%)	-0.55	5 (0%) 88 76	56, 92, 139, 233	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	358	ASP	2.7
1	B	360	LYS	2.6
1	A	85	GLN	2.5
1	C	249	TYR	2.3
1	A	189	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

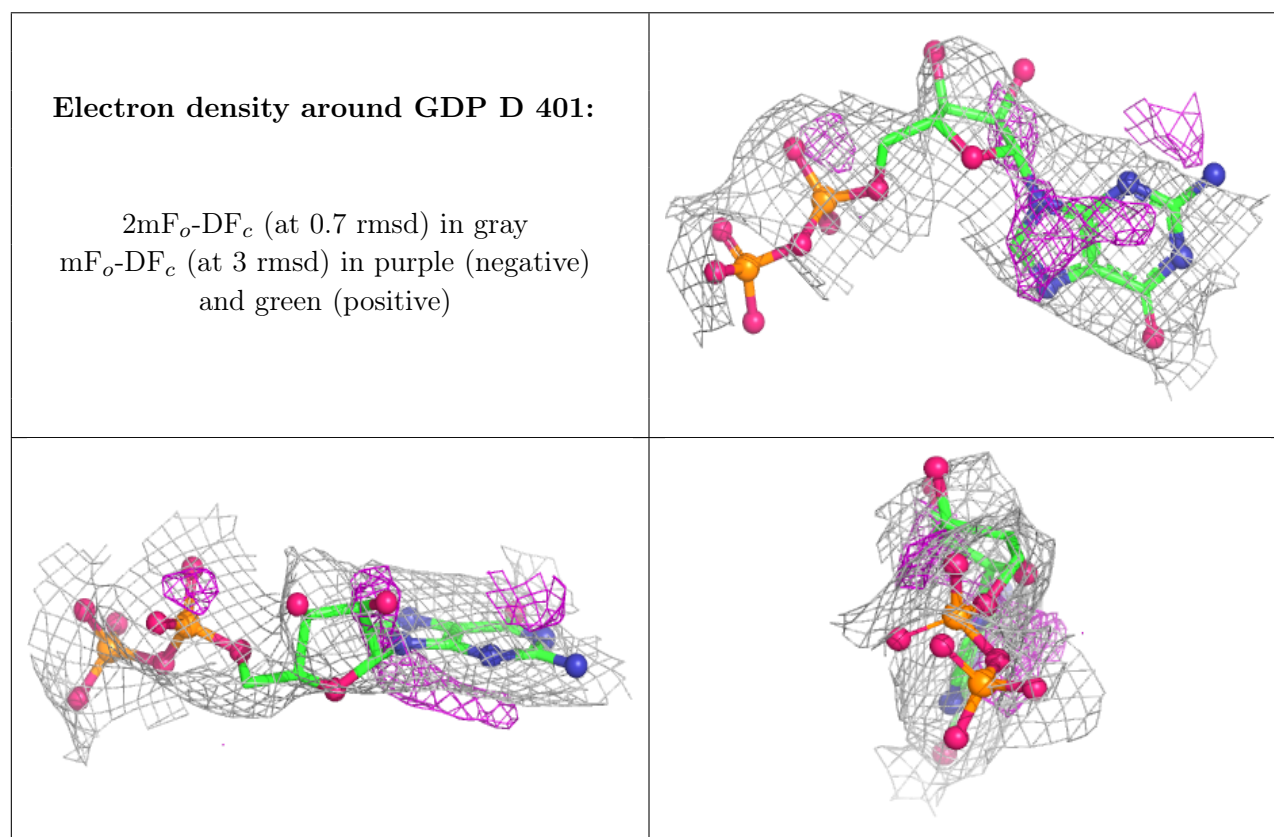
6.4 Ligands [i](#)

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.

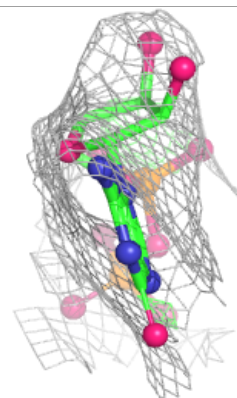
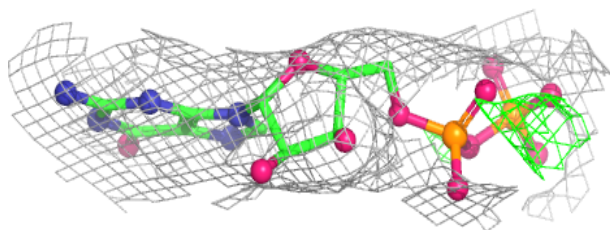
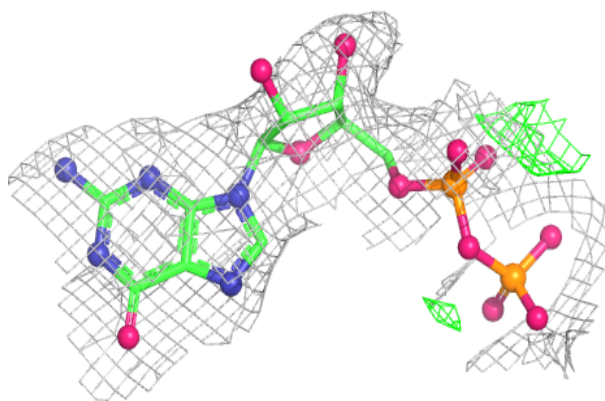
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	402	1/1	0.96	0.05	85,85,85,85	0
2	GDP	D	401	28/28	0.98	0.07	70,78,88,92	0
3	MG	A	501	1/1	0.98	0.07	98,98,98,98	0
3	MG	B	402	1/1	0.98	0.05	80,80,80,80	0
2	GDP	B	401	28/28	0.98	0.05	73,81,90,99	0
2	GDP	A	500	28/28	0.99	0.06	77,83,92,96	0
3	MG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

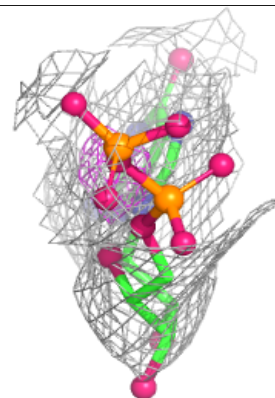
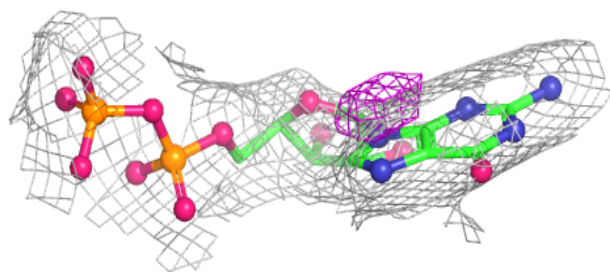
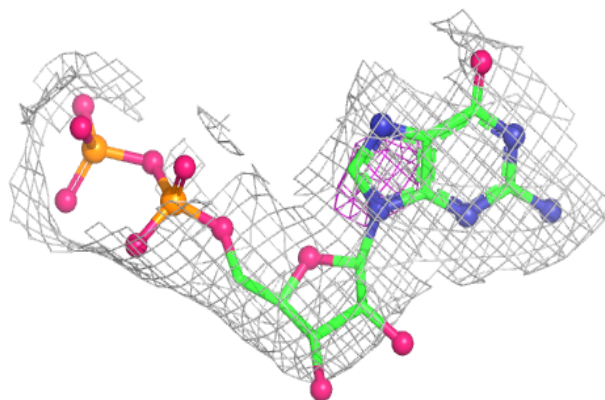


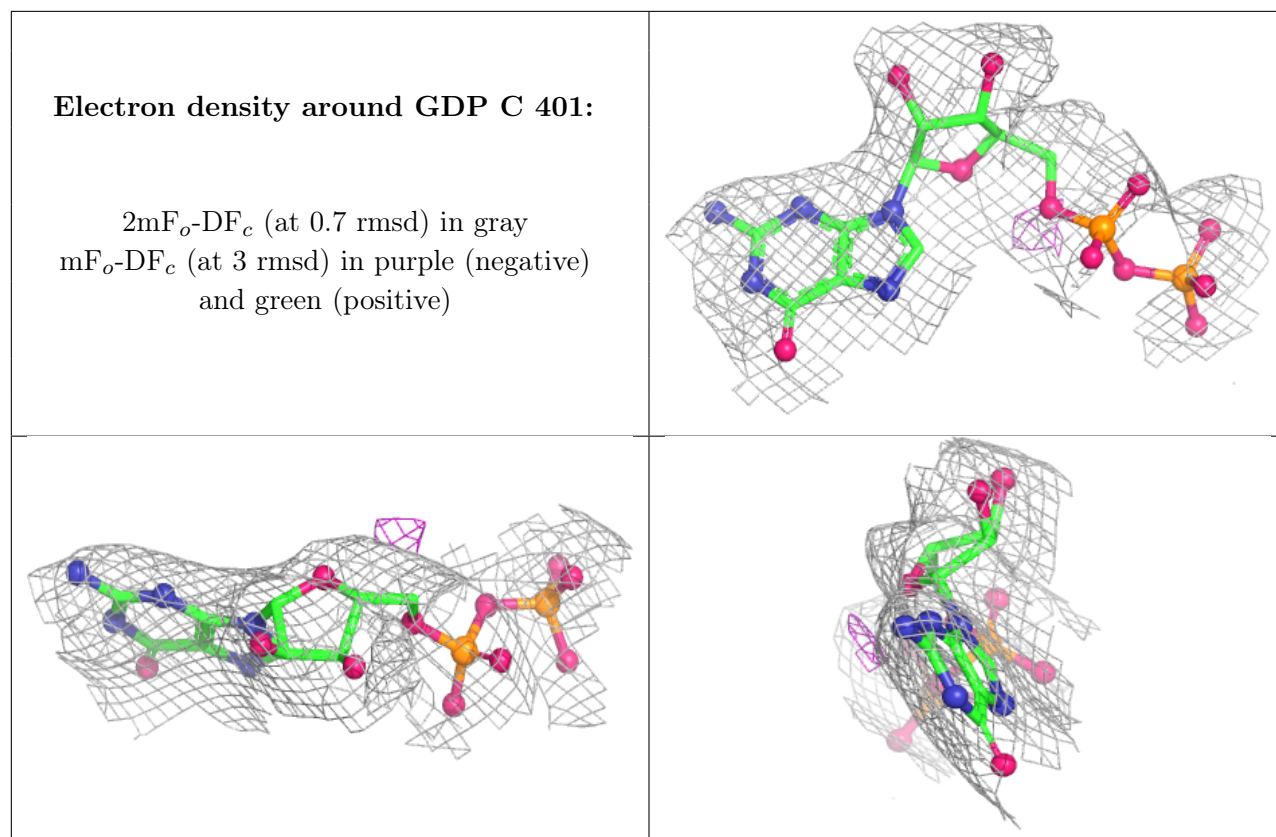
Electron density around GDP B 401:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.