Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 11:45 AM JST

PDB ID	:	7VOK
Title	:	The Crystal structure of EF-Tu and GDP from Mycobacterium tuberculosis
Authors	:	Zhan, B.W.; Li, J.X.
Deposited on	:	2021-10-14
Resolution	:	3.40 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 (i) 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 (i)) were used in the production of this report:

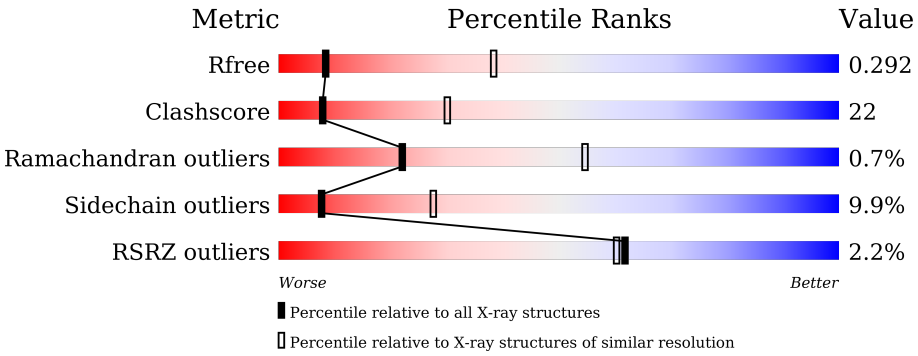
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	396	66% 28%
1	B	396	59% 32% 5%
1	C	396	68% 23% 5%
1	D	396	6% 61% 30% 5% 5%

2 Entry composition

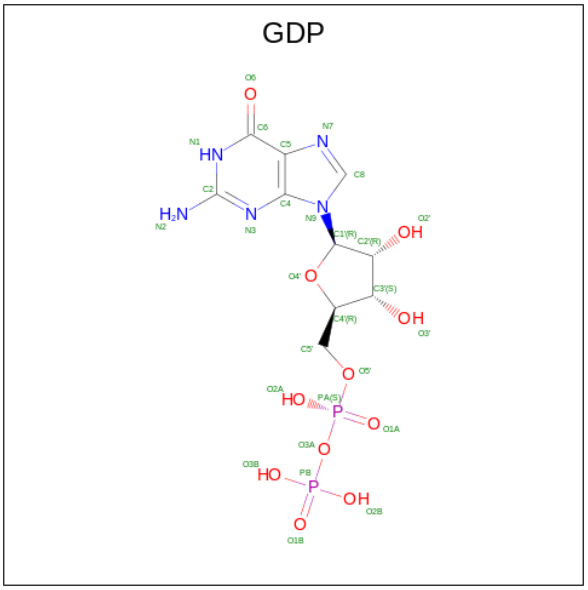
There are 3 unique types of molecules in this entry. The entry contains 11912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Elongation factor Tu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2981	1868	524	579	10			
1	B	382	Total	C	N	O	S	0	0	0
			2948	1845	519	574	10			
1	C	384	Total	C	N	O	S	0	0	0
			2966	1859	521	576	10			
1	D	376	Total	C	N	O	S	0	0	0
			2901	1816	510	565	10			

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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) (labeled as "Ligand of Interest" by depositor).

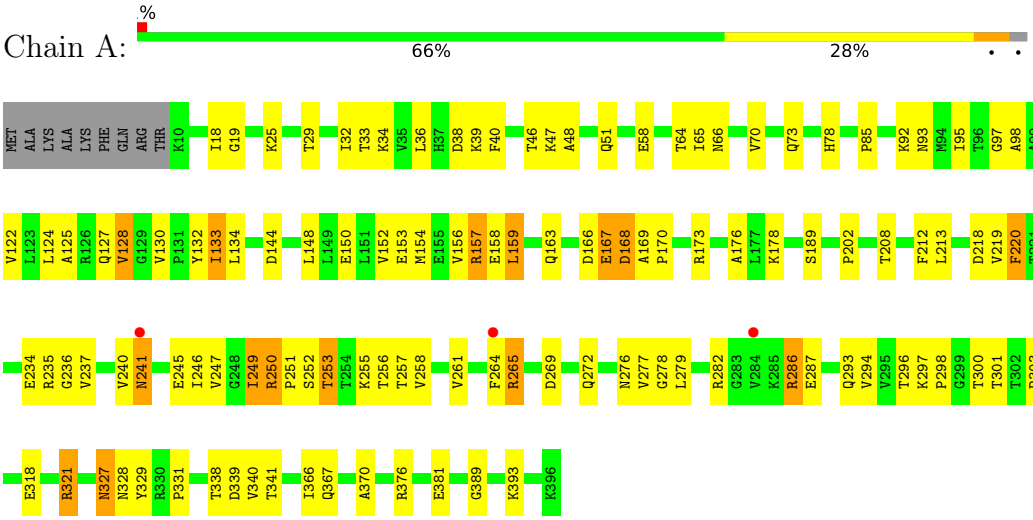
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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.

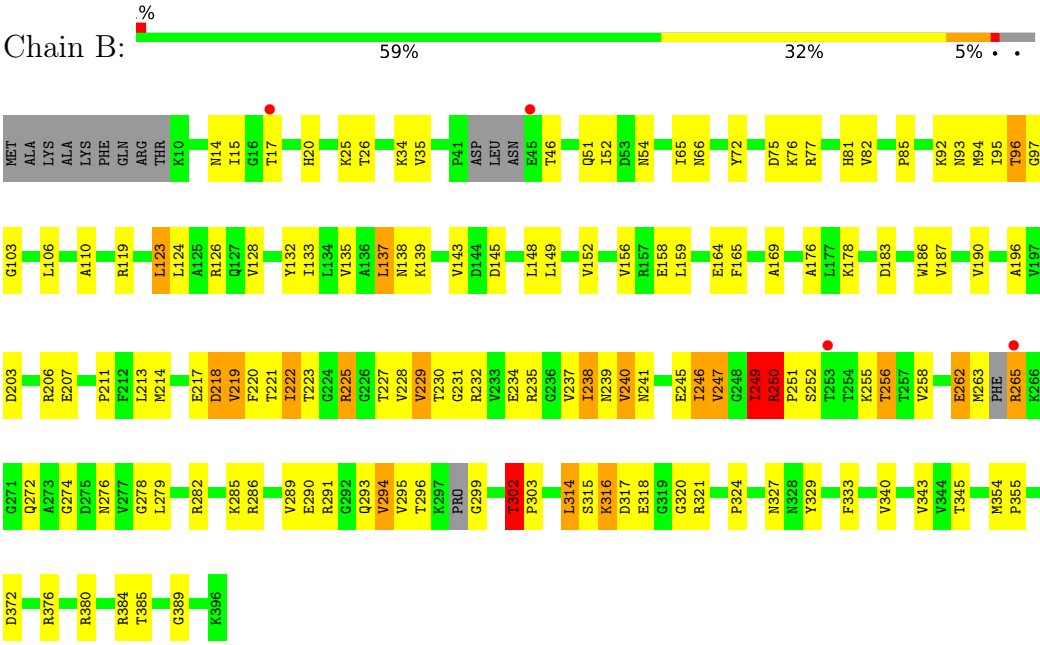
• Molecule 1: Elongation factor Tu

Chain A:



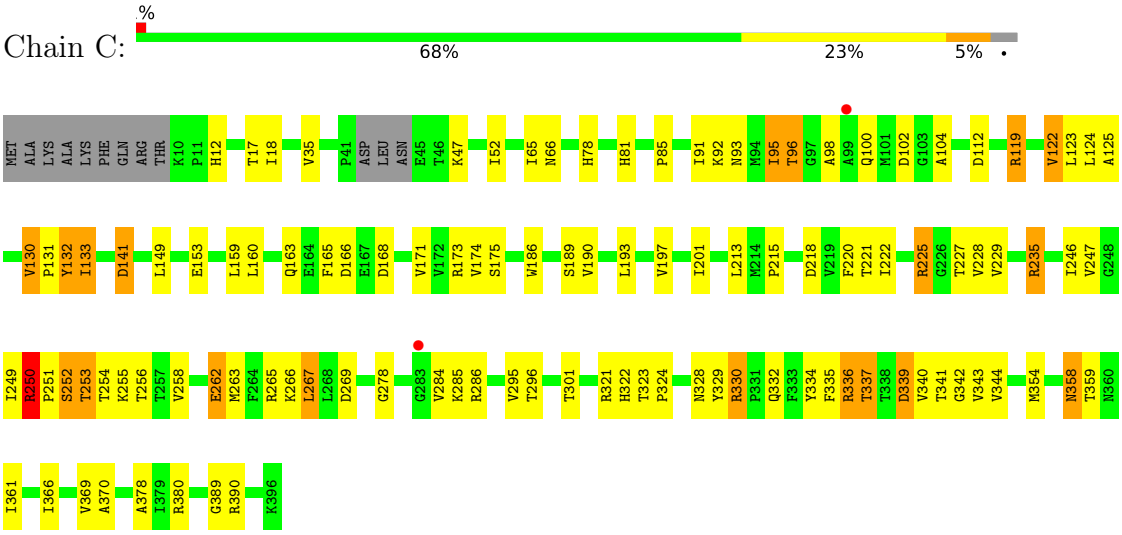
• Molecule 1: Elongation factor Tu

Chain B:



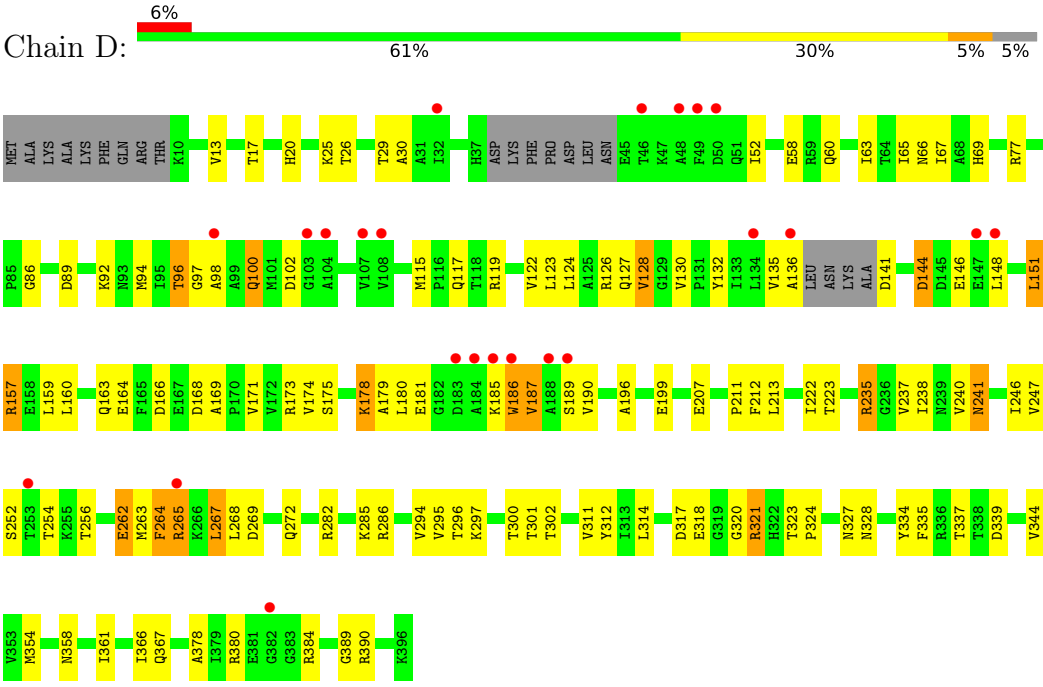
• Molecule 1: Elongation factor Tu

Chain C:



• Molecule 1: Elongation factor Tu

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.06Å 75.18Å 127.18Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	29.95 – 3.40 29.95 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.1 (29.95-3.40) 68.9 (29.95-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.97 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.244 , 0.302 0.243 , 0.292	Depositor DCC
R_{free} test set	1017 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , -28.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	11912	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% 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	0.49	1/3032 (0.0%)	0.78	2/4119 (0.0%)
1	B	0.45	1/2994 (0.0%)	0.75	1/4061 (0.0%)
1	C	0.42	1/3016 (0.0%)	0.72	1/4095 (0.0%)
1	D	0.45	2/2948 (0.1%)	0.72	2/4002 (0.0%)
All	All	0.45	5/11990 (0.0%)	0.74	6/16277 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	VAL	C-N	8.53	1.50	1.34
1	A	169	ALA	C-N	8.49	1.50	1.34
1	C	330	ARG	C-N	8.46	1.50	1.34
1	D	302	THR	C-N	8.30	1.50	1.34
1	B	302	THR	C-N	8.19	1.49	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	302	THR	CB-CA-C	-5.97	95.47	111.60
1	C	322	HIS	C-N-CA	5.75	136.08	121.70
1	A	220	PHE	CB-CA-C	-5.68	99.03	110.40
1	B	302	THR	CB-CA-C	-5.42	96.97	111.60
1	D	241	ASN	N-CA-CB	5.29	120.12	110.60
1	A	253	THR	CB-CA-C	-5.23	97.49	111.60

There are no chirality outliers.

There are no planarity outliers.

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	2981	0	2972	133	0
1	B	2948	0	2947	147	0
1	C	2966	0	2965	109	0
1	D	2901	0	2896	142	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
2	C	28	0	12	0	0
2	D	28	0	12	1	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	11912	0	11828	513	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 22.

All (513) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:CG1	1:A:370:ALA:HB2	1.55	1.37
1:B:250:ARG:HB2	1:B:251:PRO:CD	1.52	1.37
1:B:247:VAL:CG2	1:B:370:ALA:HB2	1.69	1.22
1:B:94:MET:SD	1:B:124:LEU:HD23	1.82	1.19
1:B:250:ARG:CB	1:B:251:PRO:HD2	1.73	1.19
1:B:94:MET:SD	1:B:124:LEU:CD2	2.31	1.18
1:A:247:VAL:HG11	1:A:370:ALA:HB2	1.26	1.17
1:C:225:ARG:NH1	1:C:267:LEU:HD11	1.58	1.16
1:C:250:ARG:CB	1:C:251:PRO:HD2	1.74	1.16
1:C:92:LYS:O	1:C:96:THR:HG23	1.47	1.15
1:A:250:ARG:HD3	1:A:251:PRO:HD2	1.27	1.14
1:D:178:LYS:HG3	1:D:186:TRP:CD1	1.83	1.12
1:D:250:ARG:HB2	1:D:251:PRO:HD2	1.25	1.12
1:D:124:LEU:O	1:D:128:VAL:HG23	1.52	1.09
1:C:250:ARG:HB2	1:C:251:PRO:HD2	1.14	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:HG21	1:B:370:ALA:CB	1.83	1.08
1:B:247:VAL:HG21	1:B:370:ALA:HB2	1.26	1.07
1:C:250:ARG:CB	1:C:251:PRO:CD	2.28	1.07
1:B:240:VAL:HG12	1:B:269:ASP:OD1	1.51	1.07
1:A:247:VAL:HG12	1:A:370:ALA:HB2	1.27	1.05
1:A:240:VAL:CG2	1:A:269:ASP:HA	1.87	1.03
1:D:178:LYS:CG	1:D:186:TRP:HD1	1.70	1.03
1:D:250:ARG:HB2	1:D:251:PRO:CD	1.89	1.03
1:D:250:ARG:CB	1:D:251:PRO:CD	2.39	1.00
1:C:250:ARG:HB2	1:C:251:PRO:CD	1.93	0.98
1:A:277:VAL:C	1:D:264:PHE:HZ	1.67	0.97
1:B:302:THR:HG22	1:B:303:PRO:HD2	1.46	0.96
1:C:249:ILE:HD12	1:C:249:ILE:H	1.33	0.94
1:B:247:VAL:CG2	1:B:370:ALA:CB	2.42	0.93
1:B:94:MET:CE	1:B:124:LEU:HD23	1.98	0.93
1:B:247:VAL:HG23	1:B:370:ALA:HB2	1.50	0.92
1:D:178:LYS:HG3	1:D:186:TRP:HD1	1.24	0.92
1:C:250:ARG:HB3	1:C:251:PRO:CD	1.96	0.92
1:A:247:VAL:HG11	1:A:370:ALA:CB	2.00	0.92
1:C:330:ARG:HB2	1:C:343:VAL:HG12	1.50	0.91
1:C:247:VAL:HG12	1:C:370:ALA:HB2	1.49	0.91
1:B:240:VAL:O	1:B:258:VAL:HG13	1.71	0.90
1:C:225:ARG:HH12	1:C:267:LEU:HD11	1.36	0.89
1:D:60:GLN:OE1	1:D:98:ALA:HB2	1.73	0.89
1:A:327:ASN:HD22	1:A:327:ASN:H	1.21	0.89
1:A:277:VAL:C	1:D:264:PHE:CZ	2.47	0.88
1:A:240:VAL:HG23	1:A:269:ASP:HA	1.53	0.88
1:C:247:VAL:CG1	1:C:370:ALA:HB2	2.03	0.87
1:D:240:VAL:HG11	1:D:269:ASP:HA	1.55	0.87
1:B:94:MET:SD	1:B:124:LEU:HD21	2.12	0.87
1:A:240:VAL:HG21	1:A:269:ASP:HA	1.53	0.87
1:C:91:ILE:HD13	1:C:124:LEU:HD11	1.53	0.87
1:D:97:GLY:CA	1:D:390:ARG:HH22	1.88	0.87
1:A:247:VAL:CG1	1:A:370:ALA:CB	2.50	0.86
1:D:235:ARG:HH11	1:D:235:ARG:HG2	1.40	0.86
1:C:102:ASP:O	1:C:131:PRO:HG2	1.76	0.85
1:C:225:ARG:NH1	1:C:267:LEU:CD1	2.39	0.84
1:D:213:LEU:HB3	1:D:235:ARG:HG3	1.58	0.84
1:A:250:ARG:CD	1:A:251:PRO:HD2	2.07	0.83
1:B:229:VAL:HG22	1:B:279:LEU:O	1.79	0.83
1:B:225:ARG:HA	1:B:225:ARG:NE	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:CG1	1:B:269:ASP:OD1	2.27	0.81
1:D:240:VAL:HG13	1:D:269:ASP:O	1.80	0.81
1:D:250:ARG:HB3	1:D:251:PRO:HD3	1.63	0.81
1:B:229:VAL:HG23	1:B:279:LEU:HB2	1.63	0.81
1:C:250:ARG:HB3	1:C:251:PRO:HD3	1.63	0.80
1:D:212:PHE:CE2	1:D:295:VAL:HG23	2.17	0.79
1:B:100:GLN:H	1:B:100:GLN:HE21	1.31	0.79
1:B:250:ARG:HB2	1:B:251:PRO:HD2	0.81	0.79
1:D:211:PRO:O	1:D:235:ARG:HD2	1.82	0.79
1:C:339:ASP:OD2	1:C:380:ARG:CZ	2.31	0.78
1:B:138:ASN:HD21	1:B:176:ALA:CB	1.96	0.78
1:A:245:GLU:HG3	1:A:298:PRO:HA	1.66	0.77
1:A:340:VAL:HG13	1:A:367:GLN:HG3	1.66	0.77
1:B:135:VAL:HG21	1:B:156:VAL:HG11	1.64	0.77
1:B:247:VAL:HG22	1:B:294:VAL:CG2	2.15	0.77
1:D:240:VAL:CG1	1:D:269:ASP:HA	2.14	0.77
1:B:249:ILE:HD13	1:B:249:ILE:N	2.00	0.76
1:C:358:ASN:ND2	1:C:358:ASN:O	2.17	0.76
1:A:246:ILE:N	1:A:246:ILE:HD12	2.01	0.76
1:B:138:ASN:HD21	1:B:176:ALA:HB3	1.51	0.75
1:D:235:ARG:HG2	1:D:235:ARG:NH1	2.00	0.75
1:A:246:ILE:HG21	1:A:293:GLN:OE1	1.87	0.75
1:D:339:ASP:OD2	1:D:380:ARG:NH2	2.20	0.74
1:D:178:LYS:CG	1:D:186:TRP:CD1	2.54	0.74
1:A:340:VAL:CG1	1:A:367:GLN:HB2	2.17	0.74
1:A:327:ASN:H	1:A:327:ASN:ND2	1.85	0.74
1:D:92:LYS:O	1:D:96:THR:HG23	1.87	0.74
1:B:256:THR:HG22	1:B:282:ARG:O	1.88	0.73
1:C:92:LYS:O	1:C:96:THR:CG2	2.31	0.73
1:C:91:ILE:O	1:C:95:ILE:HG12	1.88	0.73
1:A:36:LEU:O	1:A:40:PHE:HB2	1.88	0.72
1:A:240:VAL:HG23	1:A:269:ASP:CA	2.19	0.72
1:D:250:ARG:CB	1:D:251:PRO:HD3	2.18	0.72
1:D:249:ILE:HD13	1:D:249:ILE:N	2.05	0.71
1:C:249:ILE:HD12	1:C:249:ILE:N	2.04	0.71
1:C:91:ILE:O	1:C:95:ILE:CG1	2.38	0.70
1:C:339:ASP:OD2	1:C:380:ARG:NE	2.24	0.70
1:A:321:ARG:NH2	1:A:381:GLU:OE2	2.23	0.70
1:B:314:LEU:HD23	1:B:318:GLU:HB3	1.72	0.70
1:A:237:VAL:HG12	1:A:272:GLN:HA	1.73	0.70
1:B:106:LEU:HD23	1:B:135:VAL:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ILE:HG23	1:B:223:THR:HG23	1.72	0.70
1:C:91:ILE:HD13	1:C:124:LEU:CD1	2.22	0.70
1:B:133:ILE:HD11	1:B:165:PHE:CZ	2.26	0.70
1:C:249:ILE:H	1:C:249:ILE:CD1	2.02	0.70
1:D:175:SER:HB3	1:D:178:LYS:HB2	1.73	0.69
1:B:100:GLN:H	1:B:100:GLN:NE2	1.89	0.69
1:D:212:PHE:HE2	1:D:295:VAL:HG23	1.56	0.69
1:A:278:GLY:N	1:D:264:PHE:HZ	1.91	0.69
1:C:100:GLN:OE1	1:C:100:GLN:N	2.26	0.69
1:D:213:LEU:HD23	1:D:235:ARG:CZ	2.23	0.69
1:A:340:VAL:HG11	1:A:367:GLN:HB2	1.74	0.69
1:B:14:ASN:HB2	1:B:102:ASP:OD1	1.93	0.68
1:B:92:LYS:O	1:B:96:THR:HG23	1.94	0.68
1:D:265:ARG:O	1:D:265:ARG:HG2	1.92	0.68
1:B:240:VAL:O	1:B:258:VAL:CG1	2.40	0.68
1:B:265:ARG:HH11	1:B:265:ARG:CG	2.06	0.68
1:C:125:ALA:HB1	1:C:130:VAL:HG21	1.76	0.67
1:C:296:THR:HG21	1:C:301:THR:HB	1.77	0.67
1:A:148:LEU:O	1:A:152:VAL:HG23	1.94	0.67
1:A:157:ARG:NH1	1:A:157:ARG:HG2	2.10	0.67
1:A:277:VAL:N	1:D:264:PHE:HE2	1.93	0.67
1:D:148:LEU:C	1:D:148:LEU:HD23	2.15	0.67
1:C:324:PRO:HB3	1:C:354:MET:HA	1.76	0.66
1:A:39:LYS:O	1:A:39:LYS:HG2	1.96	0.66
1:B:229:VAL:CG2	1:B:279:LEU:HB2	2.26	0.65
1:B:94:MET:CE	1:B:124:LEU:CD2	2.71	0.65
1:C:225:ARG:HG2	1:C:225:ARG:NH2	2.12	0.65
1:C:122:VAL:HG21	1:C:159:LEU:HG	1.79	0.65
1:A:277:VAL:N	1:D:264:PHE:CE2	2.65	0.65
1:A:97:GLY:C	1:A:100:GLN:HE22	2.00	0.65
1:B:135:VAL:HG21	1:B:156:VAL:CG1	2.27	0.65
1:D:144:ASP:OD1	1:D:144:ASP:N	2.30	0.65
1:A:154:MET:O	1:A:158:GLU:HG2	1.97	0.64
1:A:166:ASP:OD1	1:A:166:ASP:N	2.25	0.64
1:B:250:ARG:CB	1:B:251:PRO:CD	2.39	0.64
1:A:34:LYS:HE2	1:C:253:THR:HB	1.79	0.64
1:B:252:SER:OG	1:B:252:SER:O	2.13	0.64
1:C:123:LEU:HA	1:C:163:GLN:HG2	1.79	0.64
1:D:222:ILE:HG12	1:D:223:THR:HG23	1.80	0.64
1:D:60:GLN:HE22	1:D:98:ALA:HB1	1.62	0.64
1:B:237:VAL:HG12	1:B:272:GLN:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:VAL:HG13	1:D:361:ILE:HG13	1.80	0.63
1:D:97:GLY:HA3	1:D:390:ARG:HH22	1.61	0.63
1:D:157:ARG:NH1	1:D:169:ALA:O	2.31	0.63
1:D:185:LYS:HG3	1:D:185:LYS:O	1.98	0.63
1:A:163:GLN:OE1	1:A:163:GLN:HA	1.99	0.63
1:B:232:ARG:NH2	1:B:276:ASN:OD1	2.31	0.63
1:D:247:VAL:HG21	1:D:301:THR:O	1.98	0.63
1:B:316:LYS:H	1:B:316:LYS:HD3	1.63	0.63
1:B:265:ARG:HH11	1:B:265:ARG:HG2	1.63	0.63
1:D:249:ILE:HG23	1:D:367:GLN:HE21	1.64	0.62
1:C:119:ARG:CG	1:C:119:ARG:HH11	2.12	0.62
1:A:219:VAL:HG22	1:A:286:ARG:HG2	1.82	0.62
1:A:100:GLN:OE1	1:A:376:ARG:CZ	2.48	0.62
1:B:106:LEU:HB3	1:B:135:VAL:HG22	1.81	0.62
1:B:133:ILE:CD1	1:B:165:PHE:CE2	2.83	0.62
1:D:327:ASN:OD1	1:D:346:LEU:HD12	2.00	0.61
1:C:225:ARG:CG	1:C:225:ARG:HH21	2.13	0.61
1:B:249:ILE:HG21	1:B:290:GLU:HG3	1.80	0.61
1:B:106:LEU:HD23	1:B:135:VAL:CG2	2.31	0.61
1:D:321:ARG:NH1	1:D:323:THR:O	2.34	0.61
1:D:60:GLN:OE1	1:D:98:ALA:CB	2.46	0.61
1:D:166:ASP:OD2	1:D:168:ASP:HB2	2.01	0.60
1:B:133:ILE:CD1	1:B:165:PHE:CZ	2.84	0.60
1:B:247:VAL:HG22	1:B:294:VAL:HG23	1.82	0.60
1:C:225:ARG:HG2	1:C:225:ARG:HH21	1.66	0.60
1:D:246:ILE:O	1:D:246:ILE:HG22	2.00	0.60
1:B:302:THR:CG2	1:B:303:PRO:HD2	2.28	0.60
1:D:86:GLY:O	1:D:89:ASP:N	2.35	0.60
1:A:277:VAL:O	1:D:264:PHE:CZ	2.54	0.60
1:C:102:ASP:O	1:C:131:PRO:CG	2.49	0.60
1:D:126:ARG:HD2	1:D:164:GLU:OE2	2.03	0.59
1:B:93:ASN:O	1:B:97:GLY:N	2.35	0.59
1:A:246:ILE:CG2	1:A:293:GLN:OE1	2.50	0.59
1:B:225:ARG:HA	1:B:225:ARG:HE	1.66	0.59
1:C:321:ARG:HD3	1:C:323:THR:O	2.02	0.59
1:A:173:ARG:O	1:A:189:SER:OG	2.21	0.59
1:C:18:ILE:HD11	1:C:133:ILE:HD11	1.85	0.59
1:D:187:VAL:O	1:D:190:VAL:HG22	2.02	0.59
1:A:100:GLN:OE1	1:A:376:ARG:NH2	2.36	0.59
1:A:329:TYR:CE2	1:A:331:PRO:HG3	2.37	0.59
1:B:123:LEU:HD23	1:B:123:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLU:N	1:D:207:GLU:OE1	2.36	0.59
1:C:330:ARG:O	1:C:330:ARG:HG2	2.02	0.58
1:A:246:ILE:HD12	1:A:246:ILE:H	1.65	0.58
1:D:249:ILE:CG2	1:D:367:GLN:HE21	2.16	0.58
1:D:296:THR:HG21	1:D:301:THR:HB	1.85	0.58
1:D:136:ALA:HB1	1:D:174:VAL:HG21	1.85	0.58
1:D:211:PRO:HB3	1:D:300:THR:HG21	1.85	0.58
1:D:60:GLN:CD	1:D:98:ALA:HB2	2.23	0.58
1:A:247:VAL:HG12	1:A:370:ALA:CB	2.19	0.58
1:B:217:GLU:HG3	1:B:231:GLY:HA2	1.86	0.58
1:B:246:ILE:HG22	1:B:293:GLN:OE1	2.04	0.58
1:C:332:GLN:HB3	1:C:339:ASP:HB3	1.86	0.58
1:D:265:ARG:HG2	1:D:265:ARG:NH1	2.19	0.58
1:C:122:VAL:HG12	1:C:133:ILE:HD12	1.86	0.57
1:B:238:ILE:HG23	1:B:238:ILE:O	2.04	0.57
1:C:221:THR:HG23	1:C:286:ARG:HB2	1.85	0.57
1:D:123:LEU:O	1:D:127:GLN:HG3	2.04	0.57
1:A:303:PRO:HA	1:A:370:ALA:HA	1.86	0.57
1:B:94:MET:HE1	1:B:124:LEU:HD23	1.85	0.57
1:C:246:ILE:HD12	1:C:254:THR:HG21	1.87	0.57
1:D:237:VAL:HG12	1:D:272:GLN:HA	1.85	0.57
1:A:93:ASN:ND2	1:A:98:ALA:HB3	2.19	0.57
1:A:227:THR:OG1	1:A:227:THR:O	2.16	0.57
1:B:143:VAL:HG11	1:B:148:LEU:HD22	1.86	0.57
1:D:17:THR:HG23	1:D:81:HIS:CE1	2.40	0.57
1:A:97:GLY:O	1:A:376:ARG:NH1	2.38	0.57
1:D:178:LYS:CD	1:D:186:TRP:HD1	2.16	0.57
1:C:119:ARG:NH1	1:C:119:ARG:HG3	2.19	0.56
1:A:48:ALA:H	1:A:51:GLN:NE2	2.03	0.56
1:C:334:TYR:HB3	1:C:378:ALA:HB3	1.86	0.56
1:A:46:THR:HG23	1:A:46:THR:O	2.03	0.56
1:B:137:LEU:HD12	1:B:137:LEU:O	2.05	0.56
1:C:123:LEU:HB2	1:C:163:GLN:HE21	1.71	0.56
1:C:215:PRO:HB3	1:C:336:ARG:HD3	1.88	0.56
1:D:178:LYS:CB	1:D:186:TRP:HD1	2.17	0.56
1:B:246:ILE:CG2	1:B:293:GLN:OE1	2.53	0.56
1:C:247:VAL:HG11	1:C:370:ALA:HB2	1.86	0.56
1:D:256:THR:OG1	1:D:282:ARG:O	2.23	0.56
1:A:34:LYS:NZ	1:C:253:THR:O	2.39	0.56
1:A:222:ILE:HD12	1:D:222:ILE:HD12	1.87	0.56
1:D:65:ILE:HG22	1:D:66:ASN:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ILE:HG22	1:C:389:GLY:HA2	1.86	0.56
1:C:213:LEU:HB3	1:C:235:ARG:HB2	1.87	0.56
1:A:124:LEU:HD23	1:A:124:LEU:O	2.06	0.56
1:B:139:LYS:HG2	2:B:401:GDP:C6	2.42	0.56
1:D:97:GLY:HA2	1:D:390:ARG:HH22	1.66	0.56
1:B:229:VAL:O	1:B:278:GLY:HA2	2.07	0.55
1:B:249:ILE:HG22	1:B:249:ILE:O	2.07	0.55
1:B:265:ARG:HG2	1:B:265:ARG:NH1	2.20	0.55
1:C:249:ILE:HG22	1:C:250:ARG:HD3	1.88	0.55
1:D:157:ARG:HH11	1:D:157:ARG:CG	2.19	0.55
1:A:220:PHE:CG	1:D:222:ILE:HD11	2.41	0.55
1:C:247:VAL:HA	1:C:252:SER:HB2	1.88	0.55
1:D:25:LYS:NZ	2:D:401:GDP:O3B	2.29	0.55
1:B:232:ARG:NH1	1:B:274:GLY:O	2.40	0.55
1:B:119:ARG:O	1:B:123:LEU:HB2	2.06	0.55
1:C:339:ASP:OD2	1:C:380:ARG:NH2	2.39	0.55
1:C:359:THR:HG23	1:C:359:THR:O	2.06	0.55
1:C:222:ILE:HG23	1:C:222:ILE:O	2.07	0.55
1:C:225:ARG:HH11	1:C:267:LEU:CD1	2.16	0.54
1:B:320:GLY:O	1:B:384:ARG:NH2	2.40	0.54
1:C:91:ILE:O	1:C:95:ILE:HG13	2.06	0.54
1:B:138:ASN:HD21	1:B:176:ALA:HB2	1.72	0.54
1:C:334:TYR:HB2	1:C:380:ARG:HD3	1.89	0.54
1:A:246:ILE:CG2	1:A:293:GLN:CD	2.76	0.54
1:D:97:GLY:CA	1:D:390:ARG:NH2	2.67	0.54
1:D:212:PHE:CE2	1:D:295:VAL:CG2	2.90	0.54
1:D:100:GLN:H	1:D:100:GLN:HE21	1.53	0.54
1:D:235:ARG:HH11	1:D:235:ARG:CG	2.15	0.54
1:A:212:PHE:CB	1:A:297:LYS:HE3	2.37	0.54
1:A:213:LEU:HD23	1:A:296:THR:HG22	1.88	0.54
1:C:132:TYR:OH	1:C:168:ASP:HB3	2.07	0.54
1:D:262:GLU:HB3	1:D:267:LEU:HA	1.90	0.53
1:A:247:VAL:HG13	1:A:303:PRO:HB3	1.91	0.53
1:A:250:ARG:HD3	1:A:251:PRO:CD	2.19	0.53
1:B:247:VAL:HG21	1:B:370:ALA:HB1	1.86	0.53
1:A:156:VAL:O	1:A:159:LEU:N	2.33	0.53
1:D:265:ARG:HG2	1:D:265:ARG:HH11	1.74	0.53
1:A:18:ILE:HD11	1:A:133:ILE:HD13	1.91	0.53
1:C:17:THR:HG23	1:C:81:HIS:CE1	2.44	0.53
1:A:247:VAL:HG12	1:A:247:VAL:O	2.08	0.53
1:B:20:HIS:O	1:B:25:LYS:NZ	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:HA	1:C:342:GLY:O	2.09	0.52
1:D:17:THR:HG23	1:D:81:HIS:NE2	2.24	0.52
1:B:35:VAL:HG21	1:B:190:VAL:HG21	1.91	0.52
1:B:119:ARG:HA	1:B:159:LEU:HD21	1.91	0.52
1:D:262:GLU:O	1:D:262:GLU:HG3	2.10	0.52
1:B:219:VAL:HG23	1:B:229:VAL:HG12	1.92	0.52
1:D:312:TYR:CE2	1:D:314:LEU:HD23	2.45	0.52
1:A:246:ILE:N	1:A:246:ILE:CD1	2.73	0.52
1:B:93:ASN:O	1:B:97:GLY:HA2	2.09	0.52
1:C:330:ARG:HB2	1:C:343:VAL:CG1	2.33	0.52
1:B:225:ARG:NE	1:B:225:ARG:CA	2.72	0.51
1:C:174:VAL:HA	1:C:189:SER:OG	2.10	0.51
1:D:67:ILE:HD13	1:D:84:ALA:HB2	1.91	0.51
1:D:265:ARG:HH11	1:D:265:ARG:CG	2.22	0.51
1:C:197:VAL:HG13	1:C:201:ILE:HD12	1.92	0.51
1:A:276:ASN:HB3	1:D:264:PHE:CD2	2.45	0.51
1:C:119:ARG:CG	1:C:119:ARG:NH1	2.73	0.51
1:D:157:ARG:NH1	1:D:157:ARG:CG	2.73	0.51
1:A:276:ASN:HB3	1:D:264:PHE:HD2	1.76	0.51
1:C:123:LEU:C	1:C:123:LEU:HD23	2.31	0.50
1:D:178:LYS:CB	1:D:186:TRP:CD1	2.93	0.50
1:D:246:ILE:HA	1:D:294:VAL:O	2.11	0.50
1:C:65:ILE:HG22	1:C:66:ASN:H	1.76	0.50
1:C:123:LEU:HD23	1:C:123:LEU:O	2.11	0.50
1:C:227:THR:O	1:C:227:THR:OG1	2.28	0.50
1:D:66:ASN:O	1:D:84:ALA:HB1	2.12	0.50
1:B:94:MET:CB	1:B:124:LEU:HD21	2.42	0.50
1:B:158:GLU:HG3	1:C:269:ASP:HB3	1.93	0.50
1:D:366:ILE:HG13	1:D:367:GLN:HG2	1.93	0.50
1:D:123:LEU:HA	1:D:163:GLN:HG2	1.94	0.50
1:B:100:GLN:NE2	1:B:100:GLN:N	2.59	0.50
1:C:166:ASP:CG	1:C:168:ASP:HB2	2.33	0.50
1:A:246:ILE:HA	1:A:294:VAL:O	2.11	0.49
1:C:344:VAL:HG13	1:C:361:ILE:HG13	1.93	0.49
1:C:337:THR:O	1:C:337:THR:HG22	2.11	0.49
1:D:141:ASP:HB3	1:D:186:TRP:HE1	1.77	0.49
1:D:286:ARG:O	1:D:286:ARG:HG2	2.10	0.49
1:A:241:ASN:HA	1:A:258:VAL:O	2.13	0.49
1:D:20:HIS:ND1	1:D:117:GLN:HB2	2.27	0.49
1:B:133:ILE:HD11	1:B:165:PHE:CE2	2.47	0.49
1:C:119:ARG:HH11	1:C:119:ARG:HG3	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:MET:HB3	1:D:128:VAL:HG21	1.94	0.49
1:B:135:VAL:HG12	1:B:135:VAL:O	2.12	0.49
1:B:138:ASN:OD1	1:B:176:ALA:N	2.41	0.49
1:B:148:LEU:O	1:B:152:VAL:HG23	2.12	0.49
1:B:15:ILE:O	1:B:82:VAL:HG12	2.13	0.48
1:A:247:VAL:HB	1:A:294:VAL:HG23	1.96	0.48
1:B:219:VAL:HG21	1:B:289:VAL:CG1	2.43	0.48
1:C:251:PRO:HG2	1:C:251:PRO:O	2.13	0.48
1:A:157:ARG:HH11	1:A:157:ARG:CG	2.26	0.48
1:B:14:ASN:HB3	1:B:101:MET:HA	1.95	0.48
1:B:77:ARG:NH2	1:B:203:ASP:OD1	2.47	0.48
1:A:32:ILE:O	1:A:36:LEU:HD13	2.12	0.48
1:A:47:LYS:HD2	1:A:70:VAL:HG22	1.96	0.48
1:B:219:VAL:HG21	1:B:289:VAL:HG11	1.96	0.48
1:B:329:TYR:O	1:B:343:VAL:HA	2.13	0.48
1:B:380:ARG:HA	1:B:385:THR:HA	1.96	0.48
1:A:212:PHE:HB2	1:A:297:LYS:HE3	1.94	0.48
1:D:249:ILE:HD13	1:D:249:ILE:H	1.78	0.48
1:A:240:VAL:HG23	1:A:269:ASP:C	2.33	0.48
1:C:341:THR:HB	1:C:366:ILE:HD13	1.96	0.48
1:D:60:GLN:NE2	1:D:98:ALA:HB1	2.29	0.48
1:A:297:LYS:HB3	1:A:300:THR:CG2	2.43	0.48
1:B:93:ASN:O	1:B:97:GLY:CA	2.62	0.48
1:B:262:GLU:HB3	1:B:267:LEU:HG	1.95	0.48
1:A:176:ALA:N	2:A:401:GDP:O6	2.46	0.48
1:A:18:ILE:HD11	1:A:133:ILE:CD1	2.44	0.48
1:C:141:ASP:OD2	1:C:175:SER:OG	2.28	0.48
1:A:256:THR:HG23	1:A:282:ARG:O	2.14	0.47
1:B:217:GLU:O	1:B:291:ARG:CG	2.62	0.47
1:A:150:GLU:O	1:A:153:GLU:HB2	2.14	0.47
1:C:104:ALA:HB3	1:C:133:ILE:HG12	1.96	0.47
1:B:17:THR:HG23	1:B:81:HIS:CE1	2.49	0.47
1:D:327:ASN:OD1	1:D:346:LEU:HB2	2.14	0.47
1:A:327:ASN:ND2	1:A:327:ASN:N	2.58	0.47
1:C:153:GLU:HG2	1:C:171:VAL:HG11	1.96	0.47
1:B:196:ALA:HA	1:B:199:GLU:HG3	1.96	0.47
1:D:321:ARG:HA	1:D:384:ARG:HH12	1.80	0.47
1:A:29:THR:O	1:A:33:THR:HG23	2.15	0.47
1:B:76:LYS:HB2	1:B:198:ASP:OD2	2.14	0.47
1:B:220:PHE:HB2	1:B:228:VAL:CG1	2.45	0.47
1:D:179:ALA:HA	1:D:187:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD23	1:A:159:LEU:O	2.15	0.47
1:B:183:ASP:O	1:B:187:VAL:HG23	2.15	0.47
1:B:217:GLU:O	1:B:291:ARG:HG3	2.15	0.47
1:A:34:LYS:CE	1:C:253:THR:O	2.62	0.47
1:A:64:THR:O	1:A:92:LYS:NZ	2.36	0.47
1:A:95:ILE:CG2	1:A:389:GLY:HA2	2.45	0.47
1:A:222:ILE:HG23	1:A:223:THR:HG23	1.97	0.47
1:C:35:VAL:HG21	1:C:190:VAL:CG2	2.44	0.47
1:C:321:ARG:NH2	1:C:329:TYR:CE1	2.83	0.47
1:D:240:VAL:HG13	1:D:269:ASP:C	2.35	0.47
1:B:65:ILE:HG22	1:B:66:ASN:H	1.80	0.47
1:C:125:ALA:HB1	1:C:130:VAL:CG2	2.44	0.46
1:D:136:ALA:HB1	1:D:174:VAL:CG2	2.45	0.46
1:B:265:ARG:CG	1:B:265:ARG:NH1	2.73	0.46
1:D:196:ALA:HA	1:D:199:GLU:HG2	1.96	0.46
1:A:308:GLU:N	1:A:393:LYS:O	2.35	0.46
1:D:141:ASP:OD2	1:D:178:LYS:NZ	2.45	0.46
1:D:264:PHE:HD1	1:D:264:PHE:HA	1.59	0.46
1:A:264:PHE:HB3	1:A:265:ARG:H	1.48	0.46
1:B:75:ASP:OD1	1:B:75:ASP:C	2.54	0.46
1:C:262:GLU:O	1:C:262:GLU:HG2	2.16	0.46
1:A:100:GLN:HE21	1:A:100:GLN:N	2.14	0.46
1:A:234:GLU:OE1	1:A:235:ARG:NH1	2.49	0.46
1:D:20:HIS:CG	1:D:115:MET:HB2	2.49	0.46
1:B:249:ILE:HG21	1:B:290:GLU:CG	2.45	0.46
1:D:67:ILE:HG23	1:D:82:VAL:HG23	1.96	0.46
1:D:186:TRP:HA	1:D:186:TRP:CE3	2.51	0.46
1:B:15:ILE:HA	1:B:103:GLY:O	2.16	0.46
1:B:137:LEU:HD12	1:B:137:LEU:C	2.37	0.46
1:B:247:VAL:HA	1:B:252:SER:HB2	1.97	0.46
1:C:123:LEU:C	1:C:123:LEU:CD2	2.84	0.46
1:D:179:ALA:HA	1:D:187:VAL:HG22	1.99	0.45
1:B:240:VAL:HG22	1:B:241:ASN:ND2	2.31	0.45
1:B:345:THR:HB	1:B:362:SER:HB2	1.98	0.45
1:C:246:ILE:HD12	1:C:254:THR:CG2	2.46	0.45
1:D:323:THR:HG22	1:D:324:PRO:O	2.16	0.45
1:A:38:ASP:OD1	1:A:38:ASP:N	2.48	0.45
1:B:132:TYR:OH	1:B:169:ALA:HA	2.16	0.45
1:D:157:ARG:HH11	1:D:157:ARG:HG3	1.82	0.45
1:D:240:VAL:HG23	1:D:240:VAL:O	2.15	0.45
1:A:261:VAL:HG22	1:A:279:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:C	1:D:264:PHE:CE2	2.90	0.45
1:D:312:TYR:HE2	1:D:314:LEU:HD23	1.79	0.45
1:C:256:THR:HG21	1:C:284:VAL:HG13	1.98	0.45
1:A:166:ASP:HB2	1:A:168:ASP:H	1.81	0.45
1:B:333:PHE:N	1:B:340:VAL:O	2.50	0.45
1:D:100:GLN:HE21	1:D:100:GLN:N	2.14	0.45
1:A:19:GLY:N	1:A:25:LYS:HD3	2.32	0.45
1:B:247:VAL:HG23	1:B:370:ALA:CB	2.31	0.45
1:C:295:VAL:HG23	1:C:295:VAL:O	2.16	0.45
1:D:324:PRO:HB2	1:D:352:MET:HG3	1.98	0.45
1:B:123:LEU:C	1:B:123:LEU:CD2	2.85	0.45
1:B:221:THR:OG1	1:B:286:ARG:HB2	2.16	0.45
1:C:149:LEU:HD13	1:C:173:ARG:HE	1.82	0.45
1:C:12:HIS:ND1	1:C:78:HIS:HB3	2.32	0.44
1:B:247:VAL:HG22	1:B:294:VAL:HG22	1.94	0.44
1:A:246:ILE:H	1:A:246:ILE:CD1	2.30	0.44
1:B:77:ARG:HH21	1:B:203:ASP:HA	1.82	0.44
1:A:34:LYS:HE2	1:C:253:THR:O	2.18	0.44
1:D:148:LEU:HD23	1:D:148:LEU:O	2.17	0.44
1:A:159:LEU:C	1:A:159:LEU:CD2	2.85	0.44
1:B:110:ALA:HB2	1:B:137:LEU:CD1	2.48	0.44
1:D:240:VAL:CG1	1:D:269:ASP:CA	2.90	0.44
1:A:34:LYS:HD2	1:A:46:THR:OG1	2.18	0.44
1:B:14:ASN:N	1:B:102:ASP:OD1	2.49	0.44
1:C:160:LEU:HB3	1:C:165:PHE:HB2	1.99	0.44
1:A:297:LYS:HB3	1:A:300:THR:HG23	2.00	0.44
1:B:26:THR:HG23	1:B:52:ILE:HG22	2.00	0.44
1:B:196:ALA:O	1:B:200:SER:HB2	2.18	0.44
1:B:211:PRO:O	1:B:235:ARG:HB3	2.17	0.44
1:A:341:THR:O	1:A:366:ILE:HG12	2.16	0.43
1:C:340:VAL:HG21	1:C:369:VAL:HG21	2.00	0.43
1:C:358:ASN:ND2	1:C:358:ASN:C	2.72	0.43
1:C:174:VAL:HG11	1:C:193:LEU:HD22	1.98	0.43
1:D:26:THR:HG23	1:D:52:ILE:HG22	2.00	0.43
1:D:60:GLN:NE2	1:D:98:ALA:CB	2.82	0.43
1:A:393:LYS:HB2	1:A:393:LYS:HE3	1.84	0.43
1:B:302:THR:HG22	1:B:303:PRO:CD	2.34	0.43
1:C:141:ASP:HB3	1:C:186:TRP:NE1	2.34	0.43
1:D:135:VAL:HB	1:D:171:VAL:HG22	2.00	0.43
1:D:335:PHE:O	1:D:337:THR:N	2.47	0.43
1:A:249:ILE:HB	1:A:293:GLN:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ARG:CG	1:B:251:PRO:HD2	2.43	0.43
1:B:267:LEU:C	1:B:267:LEU:HD23	2.38	0.43
1:D:13:VAL:HG21	1:D:77:ARG:HD3	1.99	0.43
1:A:93:ASN:HD22	1:A:98:ALA:HB3	1.84	0.43
1:A:130:VAL:O	1:A:130:VAL:HG12	2.18	0.43
1:A:341:THR:HB	1:A:366:ILE:HD11	2.01	0.43
1:B:229:VAL:CG2	1:B:279:LEU:O	2.58	0.43
1:D:151:LEU:HD22	1:D:154:MET:SD	2.58	0.43
1:C:221:THR:O	1:C:221:THR:OG1	2.35	0.43
1:A:124:LEU:O	1:A:128:VAL:HG13	2.19	0.42
1:B:138:ASN:ND2	1:B:176:ALA:HB2	2.34	0.42
1:A:327:ASN:HD22	1:A:327:ASN:N	2.01	0.42
1:A:48:ALA:H	1:A:51:GLN:HE22	1.67	0.42
1:A:122:VAL:HG22	1:A:133:ILE:HD12	2.00	0.42
1:B:77:ARG:NH2	1:B:203:ASP:HA	2.34	0.42
1:D:262:GLU:CB	1:D:267:LEU:HA	2.49	0.42
1:A:125:ALA:O	1:A:128:VAL:O	2.37	0.42
1:A:212:PHE:HB3	1:A:297:LYS:HE3	2.01	0.42
1:D:63:ILE:HG12	1:D:314:LEU:HD21	2.00	0.42
1:A:73:GLN:HB3	1:A:78:HIS:ND1	2.34	0.42
1:A:154:MET:HE3	1:A:154:MET:HB3	1.77	0.42
1:B:213:LEU:HD12	1:B:234:GLU:OE2	2.19	0.42
1:D:334:TYR:HB3	1:D:378:ALA:HB3	2.01	0.42
1:A:106:LEU:N	1:A:134:LEU:O	2.41	0.42
1:A:241:ASN:O	1:A:257:THR:HG23	2.20	0.42
1:B:178:LYS:HB2	1:B:186:TRP:HD1	1.85	0.42
1:D:122:VAL:HG11	1:D:159:LEU:HD22	2.02	0.42
1:A:65:ILE:HG22	1:A:66:ASN:H	1.85	0.42
1:B:34:LYS:HA	1:B:46:THR:HG22	2.02	0.42
1:B:295:VAL:O	1:B:295:VAL:HG22	2.19	0.42
1:D:119:ARG:HA	1:D:159:LEU:HD11	2.01	0.42
1:D:249:ILE:CG2	1:D:367:GLN:NE2	2.81	0.42
1:D:324:PRO:HB3	1:D:354:MET:HA	2.02	0.42
1:A:240:VAL:HG23	1:A:269:ASP:O	2.20	0.41
1:B:246:ILE:HG21	1:B:293:GLN:OE1	2.20	0.41
1:C:95:ILE:HG12	1:C:95:ILE:H	1.48	0.41
1:D:156:VAL:O	1:D:160:LEU:HG	2.20	0.41
1:D:320:GLY:O	1:D:384:ARG:NH2	2.52	0.41
1:A:167:GLU:H	1:A:167:GLU:HG3	1.43	0.41
1:D:30:ALA:HB3	1:D:180:LEU:HD11	2.01	0.41
1:C:93:ASN:OD1	1:C:98:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:THR:HG23	1:D:81:HIS:CD2	2.56	0.41
1:D:311:VAL:HG12	1:D:389:GLY:HA3	2.01	0.41
1:A:156:VAL:C	1:A:158:GLU:N	2.73	0.41
1:B:245:GLU:OE2	1:B:299:GLY:N	2.54	0.41
1:D:212:PHE:CE2	1:D:238:ILE:HD13	2.54	0.41
1:A:253:THR:O	1:A:253:THR:OG1	2.33	0.41
1:B:138:ASN:ND2	1:B:176:ALA:CB	2.75	0.41
1:B:145:ASP:O	1:B:149:LEU:HG	2.20	0.41
1:B:256:THR:CG2	1:B:282:ARG:O	2.64	0.41
1:C:47:LYS:HB2	1:C:52:ILE:HD11	2.02	0.41
1:D:173:ARG:O	1:D:189:SER:OG	2.32	0.41
1:B:128:VAL:O	1:B:128:VAL:CG1	2.68	0.41
1:D:58:GLU:OE2	1:D:69:HIS:ND1	2.38	0.41
1:A:127:GLN:H	1:A:127:GLN:HG2	1.71	0.41
1:A:178:LYS:HA	1:A:178:LYS:HD3	1.90	0.41
1:A:208:THR:O	1:A:236:GLY:HA2	2.20	0.41
1:A:340:VAL:HG13	1:A:367:GLN:CG	2.43	0.41
1:B:218:ASP:H	1:B:230:THR:HG1	1.68	0.41
1:B:315:SER:HA	1:B:355:PRO:HB3	2.02	0.41
1:C:47:LYS:CB	1:C:52:ILE:HD11	2.50	0.41
1:A:58:GLU:O	1:A:65:ILE:N	2.50	0.41
1:B:100:GLN:HE21	1:B:100:GLN:N	2.08	0.41
1:B:214:MET:SD	1:B:231:GLY:HA3	2.60	0.41
1:C:35:VAL:HG21	1:C:190:VAL:HG21	2.02	0.41
1:D:213:LEU:CD2	1:D:235:ARG:CZ	2.96	0.41
1:A:95:ILE:HG22	1:A:389:GLY:HA2	2.02	0.40
1:A:156:VAL:O	1:A:158:GLU:N	2.54	0.40
1:A:159:LEU:O	1:A:159:LEU:CD2	2.70	0.40
1:A:303:PRO:O	1:A:303:PRO:HG2	2.21	0.40
1:B:15:ILE:HD11	1:B:72:TYR:OH	2.21	0.40
1:B:102:ASP:OD1	1:B:102:ASP:N	2.54	0.40
1:B:324:PRO:HB3	1:B:354:MET:HA	2.03	0.40
1:C:246:ILE:HD12	1:C:254:THR:HB	2.03	0.40
1:A:246:ILE:HG22	1:A:293:GLN:CD	2.41	0.40
1:B:249:ILE:O	1:B:249:ILE:CG2	2.69	0.40
1:C:229:VAL:O	1:C:278:GLY:HA2	2.21	0.40
1:B:227:THR:HG21	1:B:285:LYS:HA	2.02	0.40
1:A:321:ARG:NH2	1:A:329:TYR:OH	2.55	0.40
1:B:219:VAL:HG23	1:B:229:VAL:CG1	2.52	0.40
1:C:337:THR:O	1:C:337:THR:CG2	2.69	0.40
1:A:220:PHE:CD2	1:D:222:ILE:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HZ	1:D:263:MET:CE	2.34	0.40
1:B:95:ILE:CG2	1:B:389:GLY:HA2	2.52	0.40
1:C:262:GLU:O	1:C:262:GLU:CG	2.68	0.40
1:C:266:LYS:H	1:C:266:LYS:HG2	1.36	0.40
1:D:178:LYS:HG3	1:D:186:TRP:NE1	2.28	0.40
1:D:240:VAL:O	1:D:240:VAL:CG2	2.70	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	385/396 (97%)	363 (94%)	20 (5%)	2 (0%)	29	61
1	B	374/396 (94%)	352 (94%)	19 (5%)	3 (1%)	19	51
1	C	380/396 (96%)	364 (96%)	13 (3%)	3 (1%)	19	51
1	D	370/396 (93%)	349 (94%)	19 (5%)	2 (0%)	29	61
All	All	1509/1584 (95%)	1428 (95%)	71 (5%)	10 (1%)	22	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	249	ILE
1	B	250	ARG
1	C	250	ARG
1	D	250	ARG
1	A	157	ARG
1	C	337	THR
1	C	85	PRO
1	D	241	ASN
1	A	85	PRO

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Mol	Chain	Res	Type
1	B	85	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	322/332 (97%)	294 (91%)	28 (9%)	10 34
1	B	320/332 (96%)	281 (88%)	39 (12%)	5 18
1	C	322/332 (97%)	292 (91%)	30 (9%)	9 31
1	D	315/332 (95%)	286 (91%)	29 (9%)	9 31
All	All	1279/1328 (96%)	1153 (90%)	126 (10%)	8 27

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	128	VAL
1	A	132	TYR
1	A	133	ILE
1	A	144	ASP
1	A	159	LEU
1	A	167	GLU
1	A	168	ASP
1	A	170	PRO
1	A	202	PRO
1	A	218	ASP
1	A	222	ILE
1	A	241	ASN
1	A	249	ILE
1	A	250	ARG
1	A	252	SER
1	A	255	LYS
1	A	265	ARG
1	A	286	ARG
1	A	287	GLU

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Mol	Chain	Res	Type
1	A	301	THR
1	A	315	SER
1	A	318	GLU
1	A	321	ARG
1	A	327	ASN
1	A	328	ASN
1	A	338	THR
1	A	339	ASP
1	B	51	GLN
1	B	54	ASN
1	B	96	THR
1	B	100	GLN
1	B	102	ASP
1	B	123	LEU
1	B	126	ARG
1	B	137	LEU
1	B	164	GLU
1	B	200	SER
1	B	206	ARG
1	B	207	GLU
1	B	218	ASP
1	B	219	VAL
1	B	222	ILE
1	B	225	ARG
1	B	229	VAL
1	B	238	ILE
1	B	239	ASN
1	B	240	VAL
1	B	246	ILE
1	B	247	VAL
1	B	249	ILE
1	B	250	ARG
1	B	255	LYS
1	B	256	THR
1	B	262	GLU
1	B	263	MET
1	B	265	ARG
1	B	294	VAL
1	B	296	THR
1	B	302	THR
1	B	314	LEU
1	B	316	LYS

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Mol	Chain	Res	Type
1	B	317	ASP
1	B	321	ARG
1	B	327	ASN
1	B	372	ASP
1	B	376	ARG
1	C	95	ILE
1	C	96	THR
1	C	112	ASP
1	C	119	ARG
1	C	122	VAL
1	C	130	VAL
1	C	132	TYR
1	C	133	ILE
1	C	141	ASP
1	C	218	ASP
1	C	220	PHE
1	C	225	ARG
1	C	228	VAL
1	C	235	ARG
1	C	250	ARG
1	C	252	SER
1	C	253	THR
1	C	255	LYS
1	C	258	VAL
1	C	262	GLU
1	C	263	MET
1	C	265	ARG
1	C	267	LEU
1	C	285	LYS
1	C	328	ASN
1	C	335	PHE
1	C	336	ARG
1	C	339	ASP
1	C	358	ASN
1	C	390	ARG
1	D	96	THR
1	D	100	GLN
1	D	102	ASP
1	D	128	VAL
1	D	132	TYR
1	D	144	ASP
1	D	146	GLU

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Mol	Chain	Res	Type
1	D	151	LEU
1	D	157	ARG
1	D	178	LYS
1	D	181	GLU
1	D	186	TRP
1	D	187	VAL
1	D	235	ARG
1	D	249	ILE
1	D	252	SER
1	D	254	THR
1	D	262	GLU
1	D	264	PHE
1	D	265	ARG
1	D	267	LEU
1	D	268	LEU
1	D	285	LYS
1	D	297	LYS
1	D	317	ASP
1	D	318	GLU
1	D	321	ARG
1	D	328	ASN
1	D	358	ASN

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	12	HIS
1	A	14	ASN
1	A	37	HIS
1	A	93	ASN
1	A	327	ASN
1	B	69	HIS
1	B	100	GLN
1	B	241	ASN
1	C	358	ASN
1	D	100	GLN
1	D	367	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	401	-	24,30,30	0.95	1 (4%)	30,47,47	1.24	4 (13%)
2	GDP	C	401	3	24,30,30	0.93	1 (4%)	30,47,47	1.28	4 (13%)
2	GDP	A	401	3	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
2	GDP	B	401	3	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GDP	C6-N1	-2.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDP	C6-N1	-2.38	1.34	1.37
2	D	401	GDP	C6-N1	-2.33	1.34	1.37
2	C	401	GDP	C6-N1	-2.29	1.34	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GDP	PA-O3A-PB	-4.05	118.94	132.83
2	A	401	GDP	PA-O3A-PB	-3.64	120.33	132.83
2	D	401	GDP	PA-O3A-PB	-3.44	121.01	132.83
2	C	401	GDP	PA-O3A-PB	-3.41	121.11	132.83
2	B	401	GDP	C3'-C2'-C1'	3.23	105.84	100.98
2	C	401	GDP	C3'-C2'-C1'	2.96	105.44	100.98
2	A	401	GDP	C3'-C2'-C1'	2.82	105.23	100.98
2	D	401	GDP	C3'-C2'-C1'	2.74	105.10	100.98
2	D	401	GDP	C8-N7-C5	2.44	107.64	102.99
2	A	401	GDP	C8-N7-C5	2.37	107.51	102.99
2	C	401	GDP	C8-N7-C5	2.34	107.45	102.99
2	B	401	GDP	C5-C6-N1	2.32	118.05	113.95
2	B	401	GDP	C8-N7-C5	2.31	107.38	102.99
2	A	401	GDP	C5-C6-N1	2.28	117.98	113.95
2	D	401	GDP	C5-C6-N1	2.27	117.96	113.95
2	C	401	GDP	C5-C6-N1	2.24	117.91	113.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

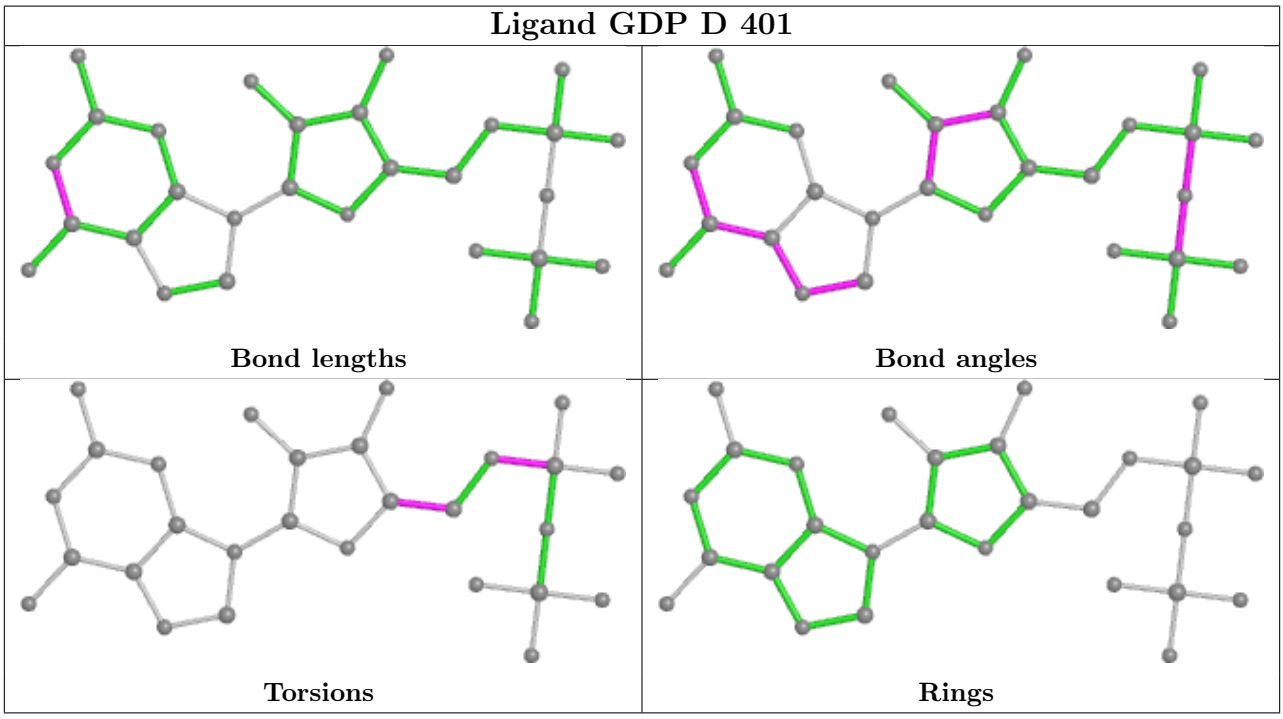
Mol	Chain	Res	Type	Atoms
2	A	401	GDP	PA-O3A-PB-O2B
2	A	401	GDP	PA-O3A-PB-O3B
2	B	401	GDP	C5'-O5'-PA-O1A
2	D	401	GDP	C5'-O5'-PA-O1A
2	D	401	GDP	C5'-O5'-PA-O2A
2	D	401	GDP	O4'-C4'-C5'-O5'
2	D	401	GDP	C3'-C4'-C5'-O5'
2	B	401	GDP	PA-O3A-PB-O1B
2	B	401	GDP	PA-O3A-PB-O2B
2	D	401	GDP	C5'-O5'-PA-O3A
2	B	401	GDP	C5'-O5'-PA-O2A
2	B	401	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

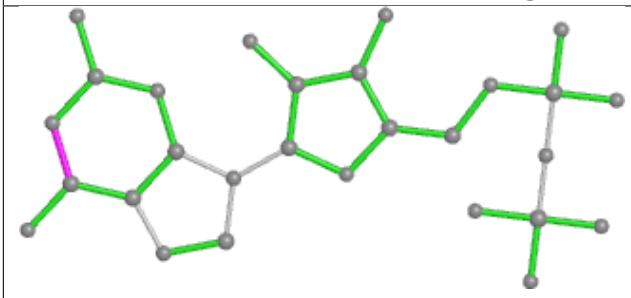
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	GDP	1	0
2	A	401	GDP	1	0
2	B	401	GDP	1	0

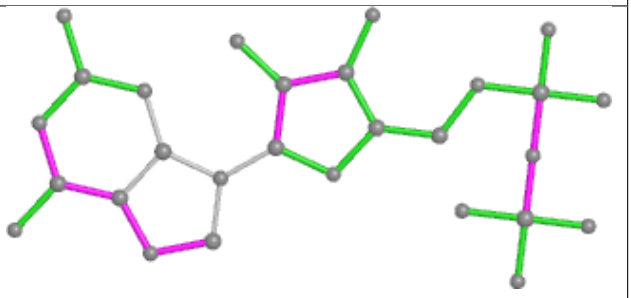
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



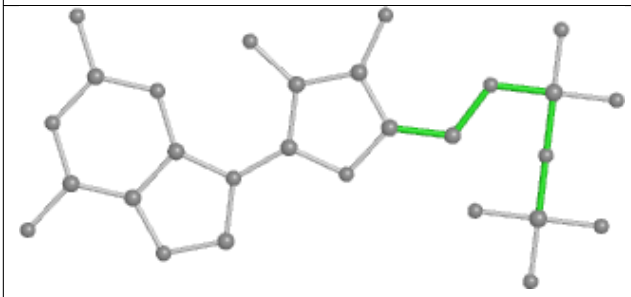
Ligand GDP C 401



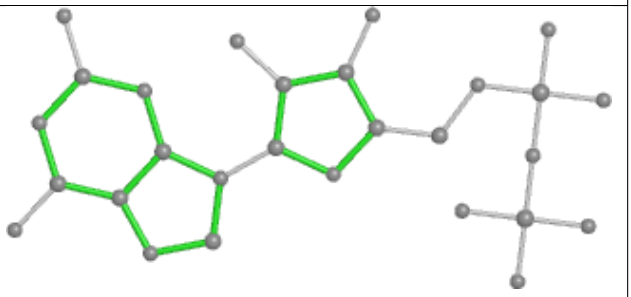
Bond lengths



Bond angles

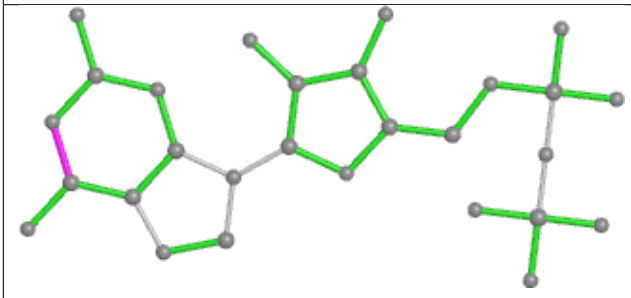


Torsions

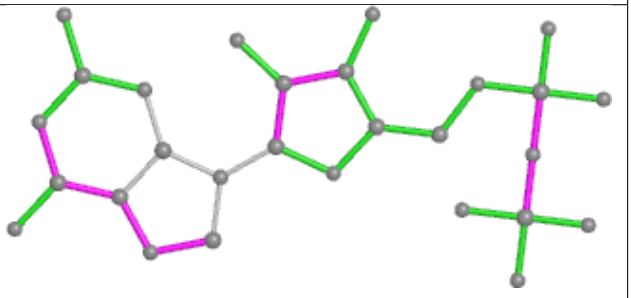


Rings

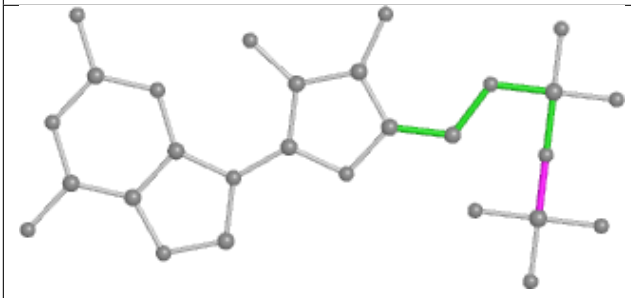
Ligand GDP A 401



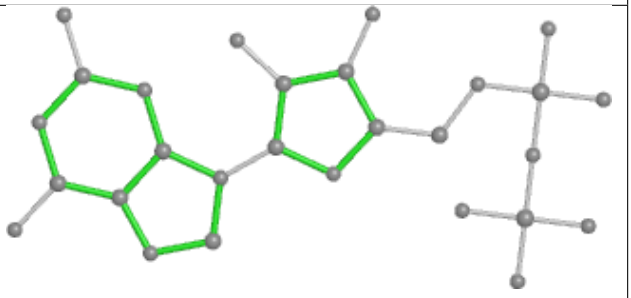
Bond lengths



Bond angles

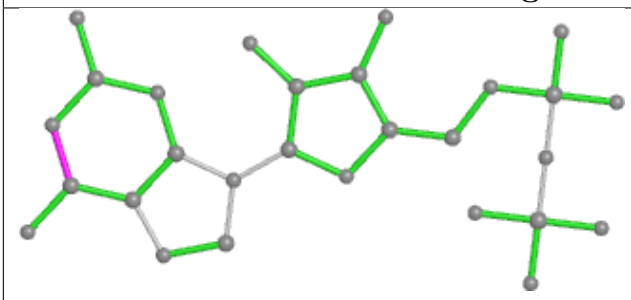


Torsions

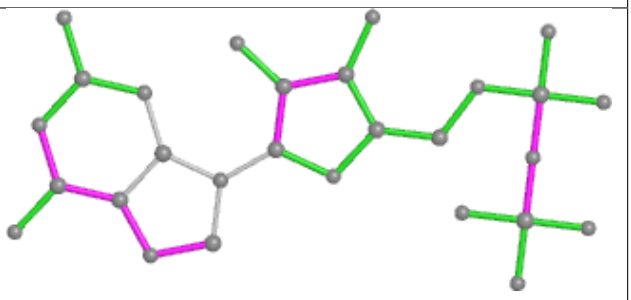


Rings

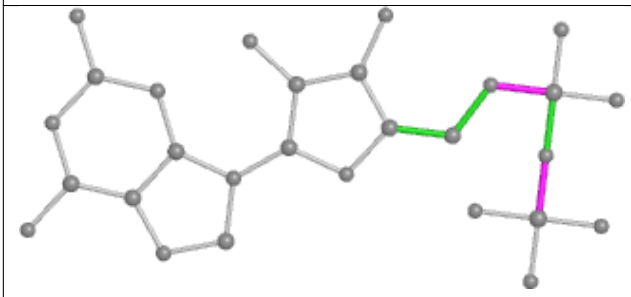
Ligand GDP B 401



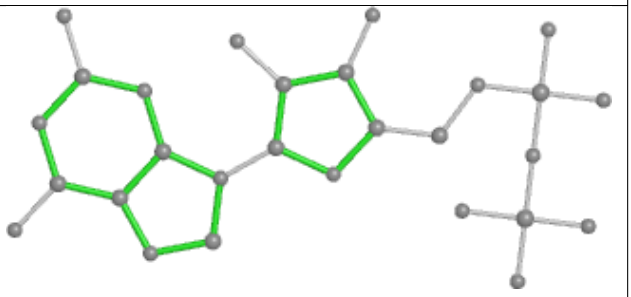
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	387/396 (97%)	-0.18	3 (0%)	86	85	12, 35, 71, 96	0
1	B	382/396 (96%)	0.03	5 (1%)	77	76	23, 59, 90, 127	0
1	C	384/396 (96%)	-0.13	2 (0%)	91	90	24, 41, 71, 109	0
1	D	376/396 (94%)	0.29	23 (6%)	21	22	21, 66, 122, 138	0
All	All	1529/1584 (96%)	0.00	33 (2%)	62	60	12, 47, 100, 138	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	108	VAL	5.2
1	D	186	TRP	4.2
1	D	148	LEU	4.2
1	D	185	LYS	3.9
1	D	189	SER	3.8
1	D	147	GLU	3.7
1	D	183	ASP	3.2
1	D	265	ARG	3.0
1	A	264	PHE	3.0
1	D	134	LEU	2.9
1	D	48	ALA	2.9
1	D	188	ALA	2.8
1	D	46	THR	2.8
1	D	382	GLY	2.8
1	C	99	ALA	2.7
1	C	283	GLY	2.6
1	D	98	ALA	2.6
1	D	104	ALA	2.6
1	B	17	THR	2.6
1	D	136	ALA	2.5
1	D	253	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	184	ALA	2.4
1	A	241	ASN	2.3
1	A	284	VAL	2.2
1	B	270	GLN	2.1
1	D	32	ILE	2.1
1	B	265	ARG	2.1
1	B	253	THR	2.1
1	D	50	ASP	2.0
1	B	45	GLU	2.0
1	D	49	PHE	2.0
1	D	107	VAL	2.0
1	D	103	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

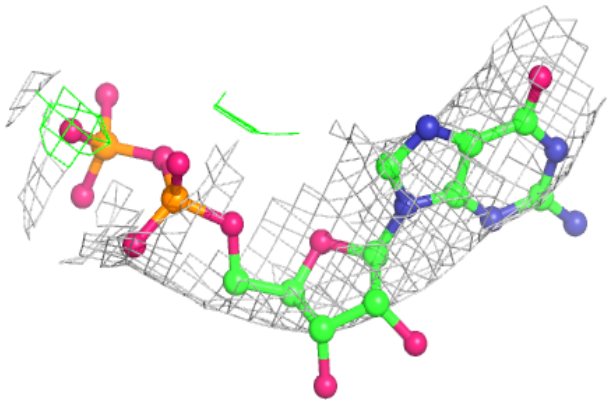
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GDP	D	401	28/28	0.86	0.24	104,121,127,132	0
3	MG	D	402	1/1	0.87	0.23	86,86,86,86	0
2	GDP	B	401	28/28	0.89	0.19	55,77,84,93	0
2	GDP	C	401	28/28	0.94	0.17	30,45,60,62	0
2	GDP	A	401	28/28	0.96	0.15	16,19,30,31	0
3	MG	B	402	1/1	0.98	0.18	46,46,46,46	0
3	MG	A	402	1/1	0.98	0.32	7,7,7,7	0
3	MG	C	402	1/1	0.99	0.33	19,19,19,19	0

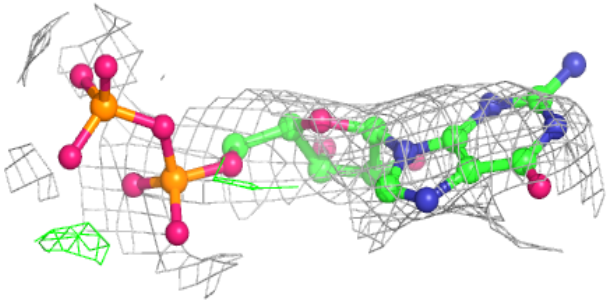
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

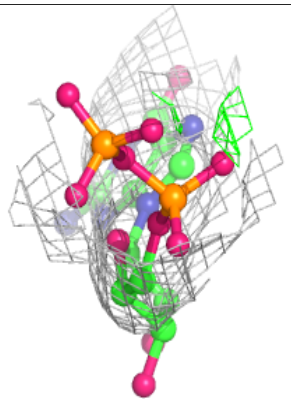
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

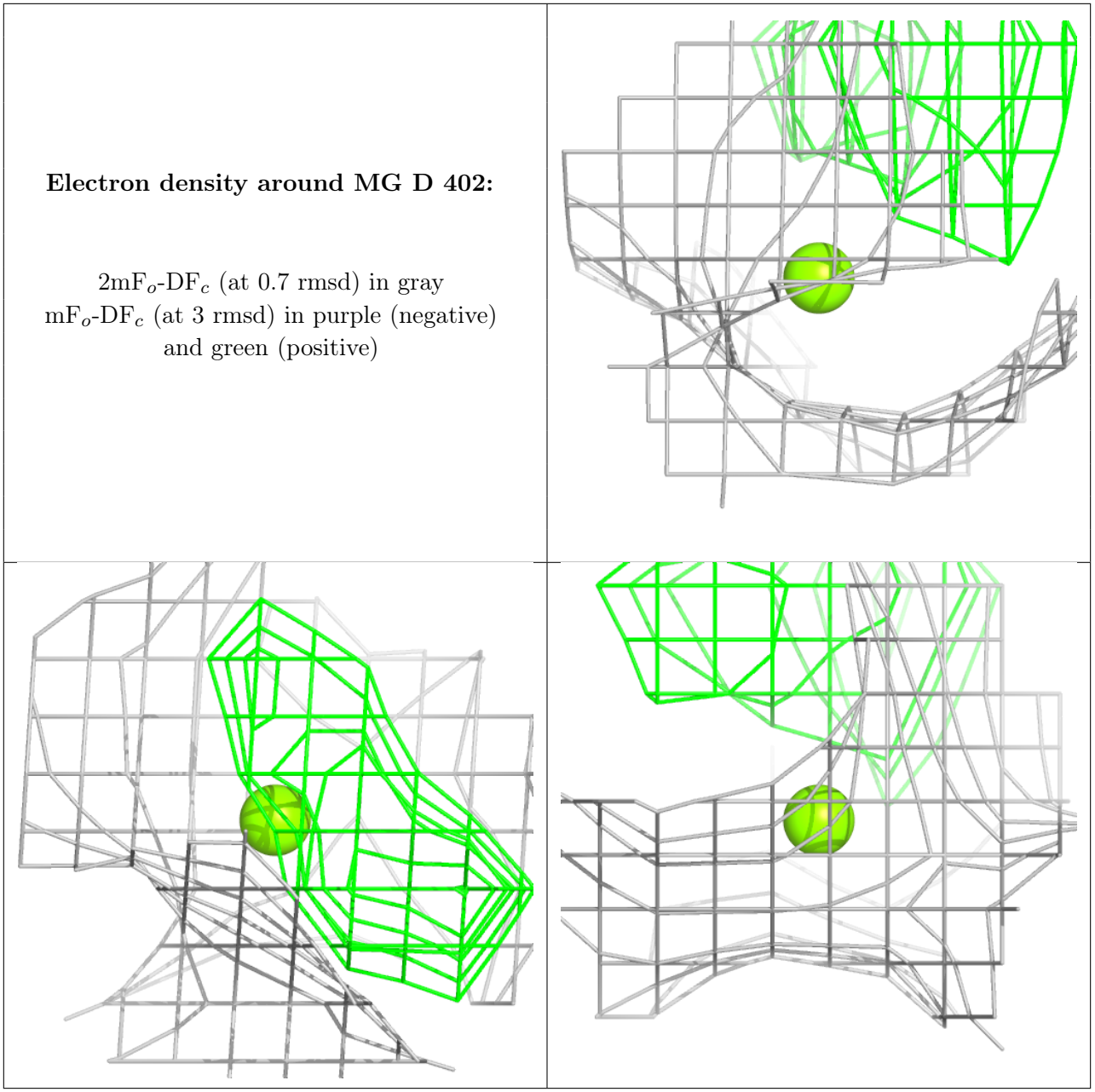






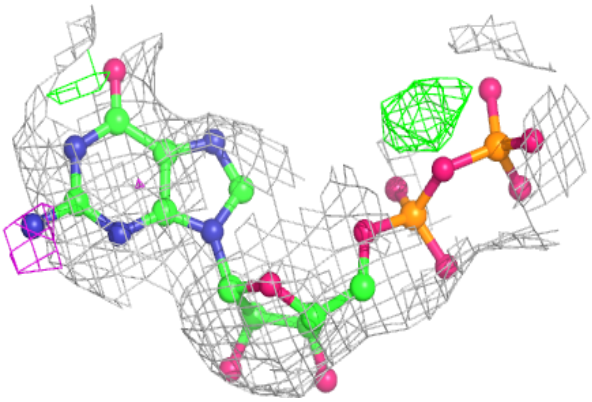
Electron density around MG D 402:

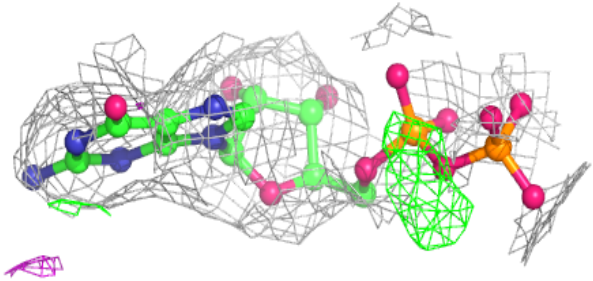
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

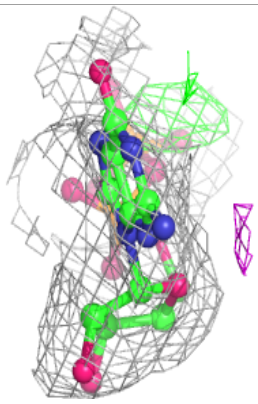


Electron density around GDP B 401:

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

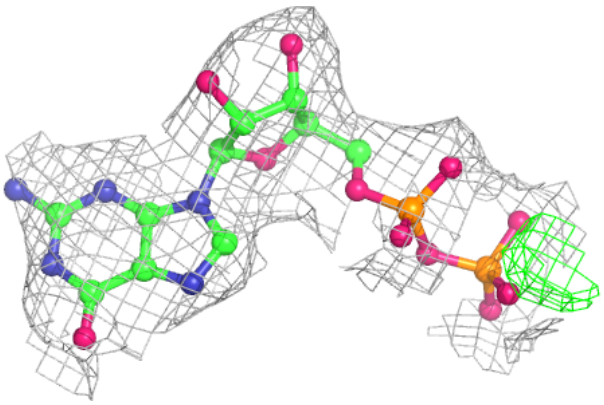


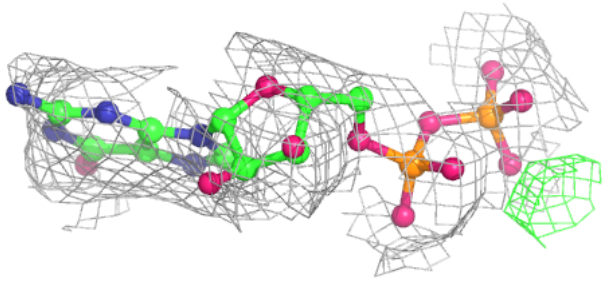


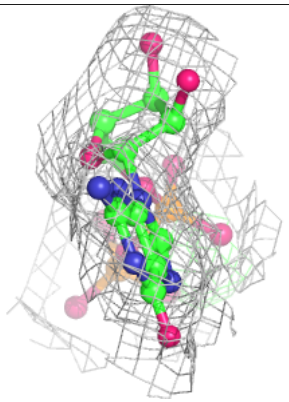


Electron density around GDP C 401:

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

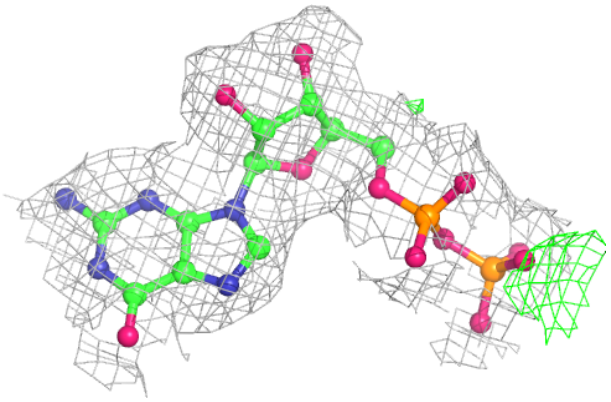


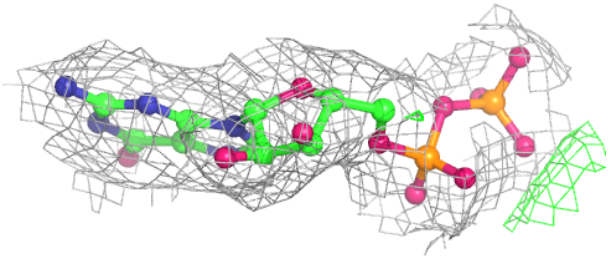


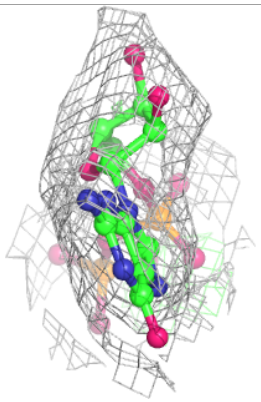


Electron density around GDP A 401:

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

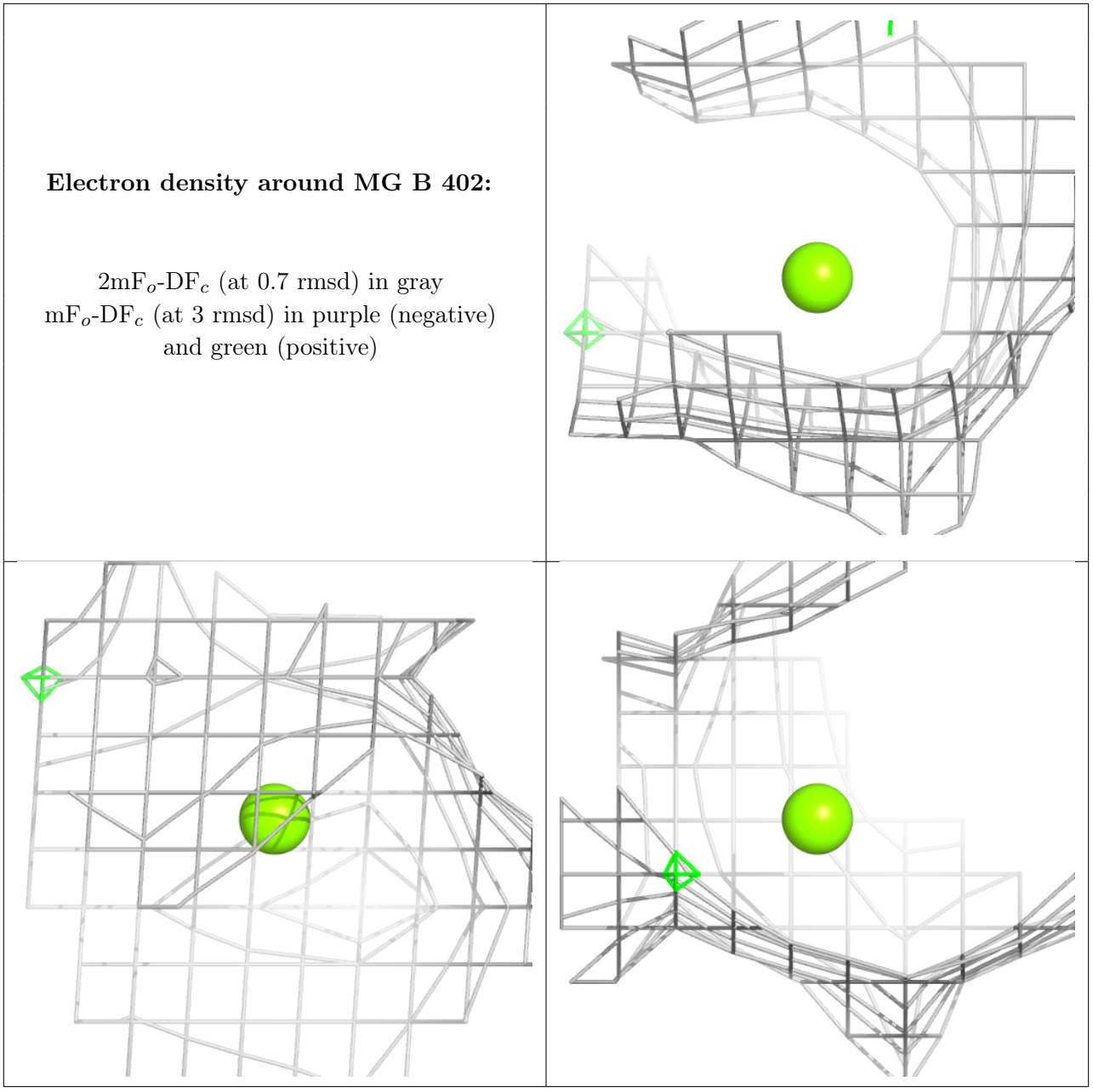






Electron density around MG B 402:

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



Electron density around MG A 402:

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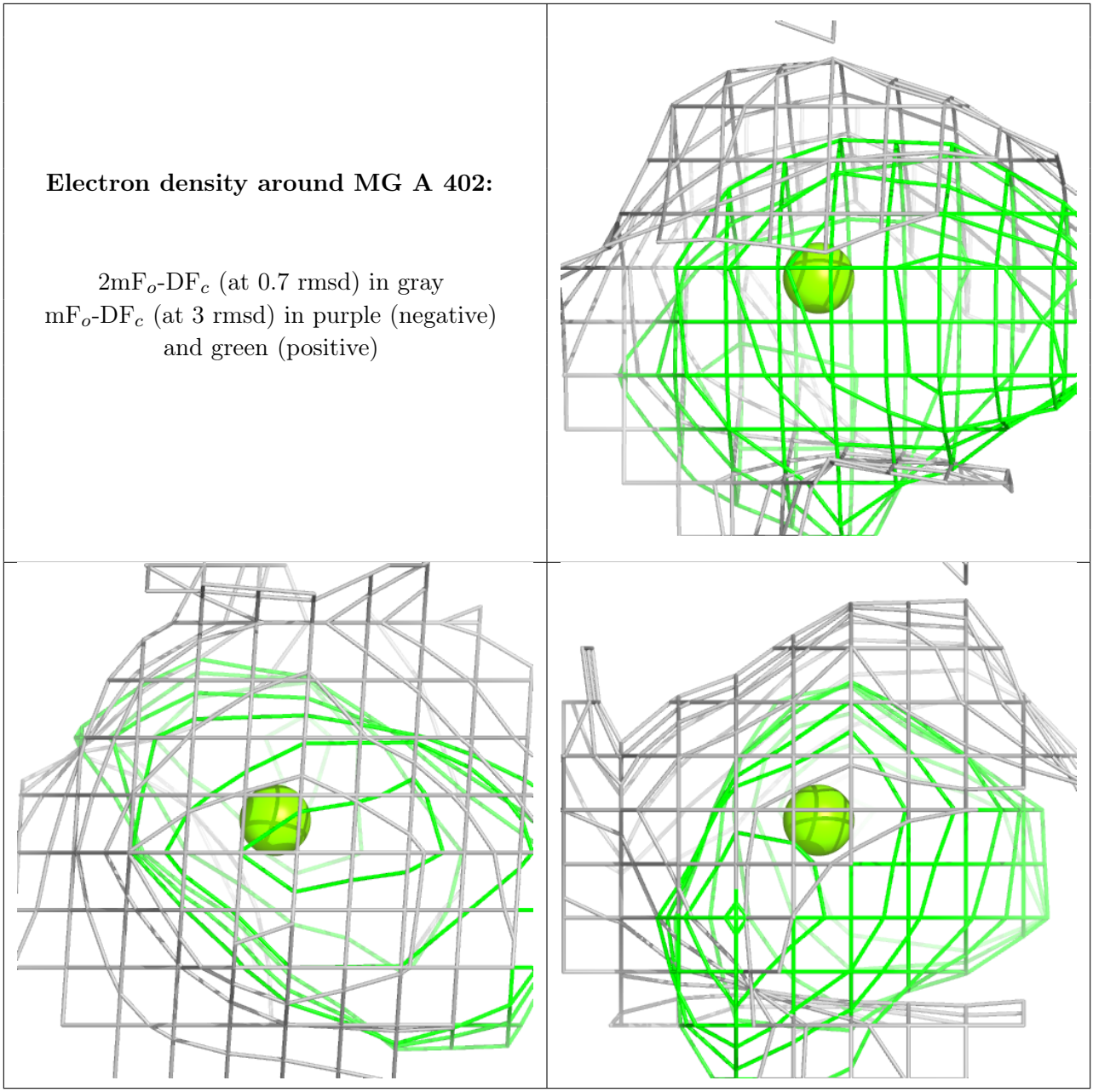
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MG C 402:

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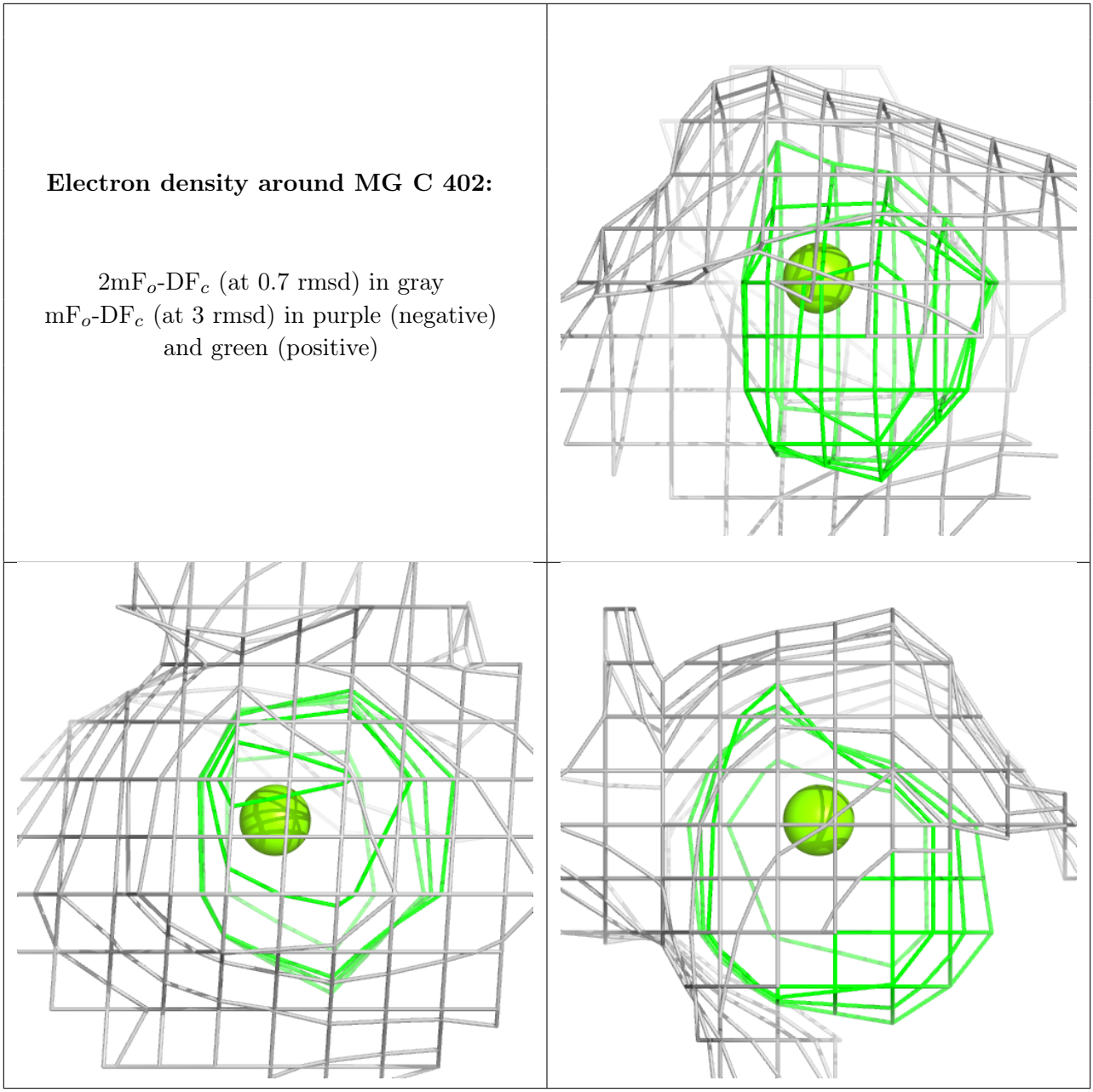
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.