Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 05:21 AM JST

PDB ID	:	6KYK
Title	:	Crystal structure of Shank3 NTD-ANK mutant in complex with Rap1
Authors	:	Cai, Q.; Zhang, M.
Deposited on	:	2019-09-19
Resolution	:	2.82 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:

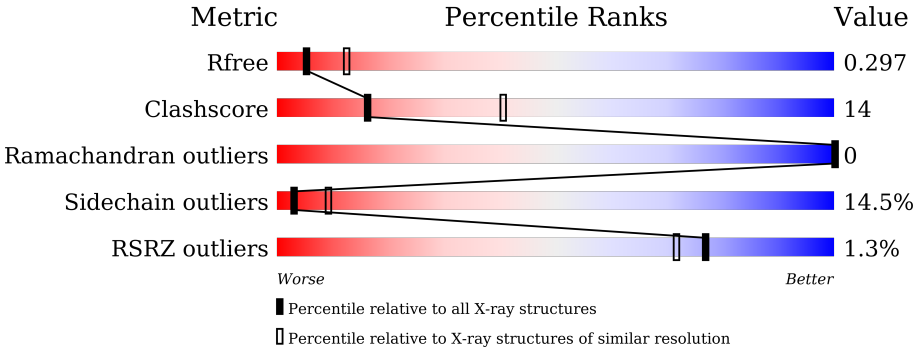
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	374	.% 69% 22% 5% •
1	B	374	.% 66% 25% 5% 5%
2	C	170	.% 70% 24% 6% •
2	D	170	2% 66% 28% 5% •
2	E	170	4% 67% 26% 6% •
2	F	170	.% 60% 33% 6% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11209 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 SH3 and multiple ankyrin repeat domains protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2817	1765	521	520	11	0	1	0
1	B	357	2809	1761	519	518	11	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q4ACU6
A	-4	PRO	-	expression tag	UNP Q4ACU6
A	-3	GLY	-	expression tag	UNP Q4ACU6
A	-2	SER	-	expression tag	UNP Q4ACU6
A	-1	GLU	-	expression tag	UNP Q4ACU6
A	0	PHE	-	expression tag	UNP Q4ACU6
A	231	ARG	LEU	engineered mutation	UNP Q4ACU6
A	304	TYR	PHE	engineered mutation	UNP Q4ACU6
B	-5	GLY	-	expression tag	UNP Q4ACU6
B	-4	PRO	-	expression tag	UNP Q4ACU6
B	-3	GLY	-	expression tag	UNP Q4ACU6
B	-2	SER	-	expression tag	UNP Q4ACU6
B	-1	GLU	-	expression tag	UNP Q4ACU6
B	0	PHE	-	expression tag	UNP Q4ACU6
B	231	ARG	LEU	engineered mutation	UNP Q4ACU6
B	304	TYR	PHE	engineered mutation	UNP Q4ACU6

- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	169	1348	844	232	264	8	0	0	0
2	D	168	1341	839	231	263	8	0	0	0

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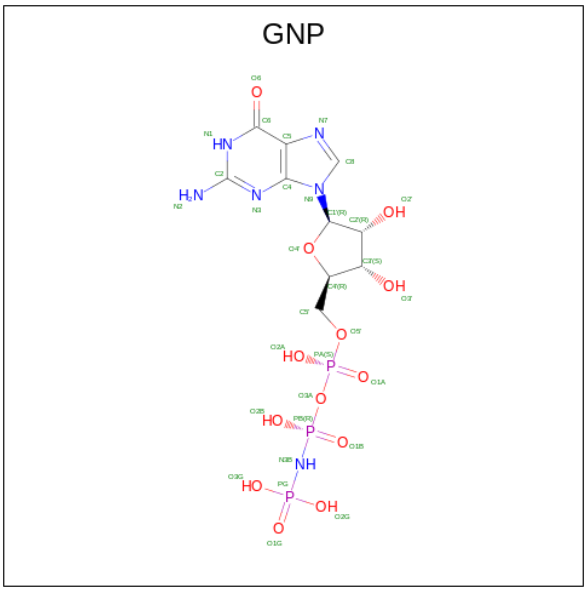
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	169	1348	844	232	264	8	0	0	0
			Total	C	N	O	S			
2	F	168	1341	839	231	263	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P61224
C	-1	PRO	-	expression tag	UNP P61224
C	0	HIS	-	expression tag	UNP P61224
D	-2	GLY	-	expression tag	UNP P61224
D	-1	PRO	-	expression tag	UNP P61224
D	0	HIS	-	expression tag	UNP P61224
E	-2	GLY	-	expression tag	UNP P61224
E	-1	PRO	-	expression tag	UNP P61224
E	0	HIS	-	expression tag	UNP P61224
F	-2	GLY	-	expression tag	UNP P61224
F	-1	PRO	-	expression tag	UNP P61224
F	0	HIS	-	expression tag	UNP P61224

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	C	1	32	10	6	13	3	0	0
3	D	1	32	10	6	13	3	0	0
3	E	1	32	10	6	13	3	0	0
3	F	1	32	10	6	13	3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	C	1	1	1	0	0
4	D	1	1	1	0	0
4	E	1	1	1	0	0
4	F	1	1	1	0	0

- Molecule 5 is water.

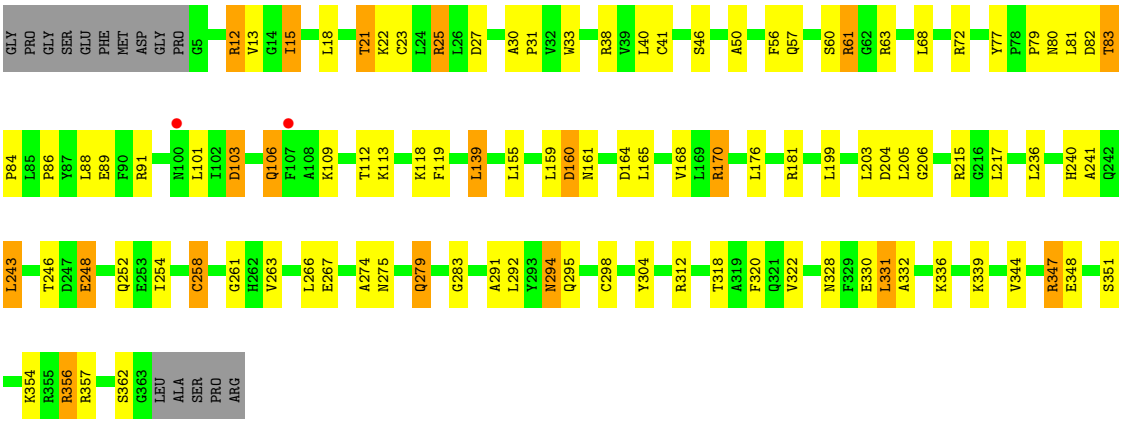
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	17	17	17	0	0
5	B	18	18	18	0	0
5	C	8	8	8	0	0
5	D	8	8	8	0	0
5	E	10	10	10	0	0
5	F	12	12	12	0	0

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.

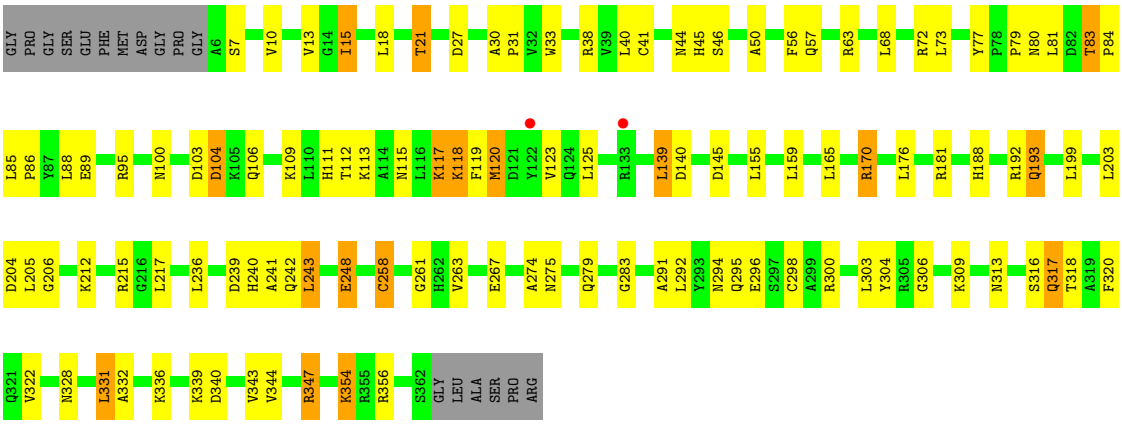
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 3

Chain A:



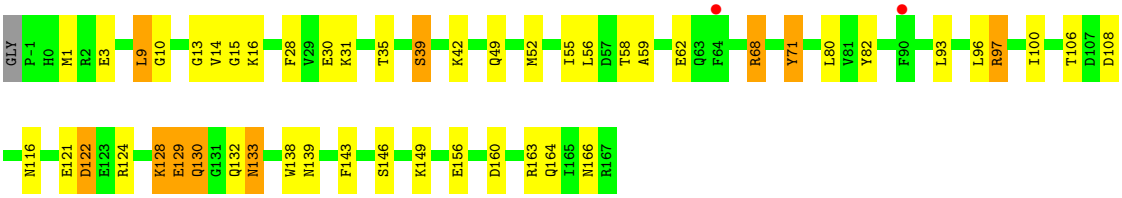
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 3

Chain B:



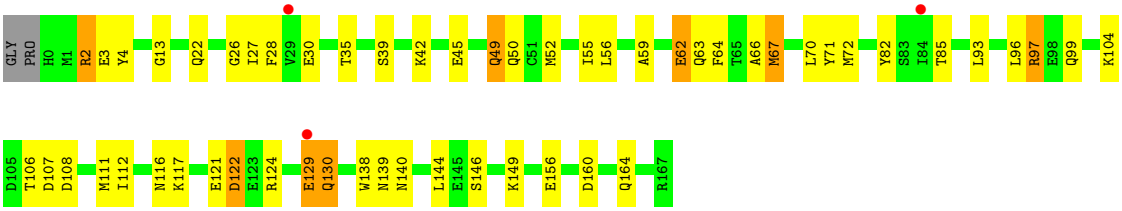
• Molecule 2: Ras-related protein Rap-1b

Chain C:



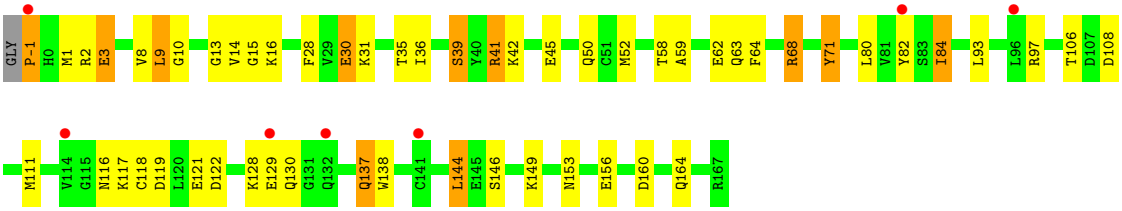
• Molecule 2: Ras-related protein Rap-1b

Chain D:



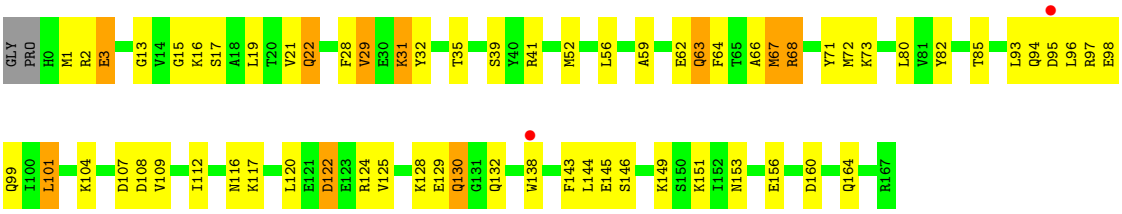
• Molecule 2: Ras-related protein Rap-1b

Chain E:



• Molecule 2: Ras-related protein Rap-1b

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	171.03Å 54.11Å 203.11Å 90.00° 109.51° 90.00°	Depositor
Resolution (Å)	49.00 – 2.82 48.95 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.00-2.82) 93.4 (48.95-2.82)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.240 , 0.300 0.241 , 0.297	Depositor DCC
R_{free} test set	1976 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11209	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.62% 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 (i)

5.1 Standard geometry (i)

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

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	0.69	0/2882	0.83	1/3909 (0.0%)
1	B	0.68	0/2874	0.82	0/3899
2	C	0.69	0/1366	0.83	0/1840
2	D	0.69	0/1358	0.84	0/1829
2	E	0.69	0/1366	0.85	1/1840 (0.1%)
2	F	0.69	0/1358	0.82	0/1829
All	All	0.68	0/11204	0.83	2/15146 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	-1	PRO	CA-N-CD	-6.96	101.76	111.50
1	A	25	ARG	NE-CZ-NH2	5.39	122.99	120.30

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	2817	0	2771	61	0
1	B	2809	0	2764	72	0
2	C	1348	0	1332	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1341	0	1327	46	0
2	E	1348	0	1334	47	0
2	F	1341	0	1326	69	0
3	C	32	0	13	4	0
3	D	32	0	13	2	0
3	E	32	0	13	4	0
3	F	32	0	13	5	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	17	0	0	1	0
5	B	18	0	0	4	0
5	C	8	0	0	4	0
5	D	8	0	0	2	0
5	E	10	0	0	1	0
5	F	12	0	0	3	0
All	All	11209	0	10906	318	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 14.

All (318) 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)
2:D:97:ARG:HB2	2:D:138:TRP:CH2	1.36	1.57
2:D:97:ARG:HB2	2:D:138:TRP:CZ2	1.56	1.38
2:D:97:ARG:CB	2:D:138:TRP:CH2	2.26	1.17
1:A:89:GLU:OE1	1:A:91:ARG:NH2	1.77	1.15
2:F:94:GLN:O	2:F:98:GLU:OE1	1.66	1.13
1:B:212:LYS:HE2	5:B:404:HOH:O	1.52	1.09
2:D:72:MET:O	2:D:104:LYS:NZ	1.86	1.07
2:F:94:GLN:O	2:F:98:GLU:CD	1.95	1.03
2:F:95:ASP:C	2:F:98:GLU:OE2	2.00	1.00
2:F:128:LYS:HD3	2:F:132:GLN:NE2	1.75	1.00
1:A:25:ARG:O	1:A:38:ARG:NH1	1.93	0.99
2:D:97:ARG:CB	2:D:138:TRP:CZ2	2.43	0.98
2:F:95:ASP:O	2:F:98:GLU:OE2	1.82	0.97
1:A:12:ARG:NH2	1:A:23:CYS:SG	2.42	0.92
1:A:275:ASN:HD21	1:B:275:ASN:HD21	1.18	0.90
1:B:33[A]:TRP:CD1	5:B:404:HOH:O	2.24	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:GLU:OE2	2:E:41:ARG:NH1	2.04	0.89
2:F:22:GLN:HA	2:F:22:GLN:HE21	1.35	0.89
2:E:97:ARG:NH2	2:E:138:TRP:HA	1.88	0.87
2:F:94:GLN:C	2:F:98:GLU:OE1	2.15	0.86
2:F:17:SER:O	2:F:21:VAL:HG23	1.76	0.85
2:F:63:GLN:O	2:F:63:GLN:NE2	2.12	0.83
2:F:95:ASP:CA	2:F:98:GLU:OE2	2.29	0.81
2:E:82:TYR:HB3	2:E:93:LEU:HD11	1.64	0.80
2:C:82:TYR:HB3	2:C:93:LEU:HD11	1.64	0.79
2:E:97:ARG:HH21	2:E:138:TRP:CB	1.95	0.79
2:F:97:ARG:HD2	2:F:138:TRP:CD2	2.17	0.79
2:F:82:TYR:HB3	2:F:93:LEU:HD11	1.65	0.79
2:F:56:LEU:HD21	2:F:71:TYR:CD1	2.18	0.79
2:D:82:TYR:HB3	2:D:93:LEU:HD11	1.63	0.78
2:D:97:ARG:HD2	2:D:138:TRP:CE2	2.19	0.78
2:E:9:LEU:HD12	2:E:9:LEU:H	1.49	0.77
2:D:111:MET:SD	2:D:138:TRP:HZ3	2.08	0.77
2:D:130:GLN:NE2	5:D:301:HOH:O	1.97	0.77
2:E:97:ARG:HH22	2:E:138:TRP:HA	1.46	0.77
2:F:112:ILE:HD11	2:F:144:LEU:HD12	1.67	0.76
2:C:9:LEU:HD12	2:C:9:LEU:H	1.50	0.76
1:A:89:GLU:CD	1:A:91:ARG:NH2	2.39	0.75
2:E:97:ARG:HH21	2:E:138:TRP:HB3	1.52	0.74
2:D:112:ILE:HD11	2:D:144:LEU:HD12	1.69	0.73
2:F:128:LYS:HD3	2:F:132:GLN:HE22	1.54	0.72
2:E:13:GLY:H	3:E:201:GNP:HNB3	1.35	0.72
2:E:97:ARG:HD3	2:E:138:TRP:CD2	2.24	0.71
2:E:97:ARG:NH2	2:E:138:TRP:CA	2.53	0.71
1:B:44:ASN:HA	5:B:410:HOH:O	1.91	0.71
2:C:1:MET:HE3	2:C:52:MET:HB2	1.73	0.71
1:A:21:THR:HB	2:C:39:SER:HB2	1.74	0.70
2:F:22:GLN:HA	2:F:22:GLN:NE2	2.06	0.70
2:C:163:ARG:HD2	5:C:304:HOH:O	1.91	0.70
2:F:97:ARG:HD2	2:F:138:TRP:CE2	2.27	0.70
1:B:313:ASN:OD1	1:B:317:GLN:O	2.10	0.70
1:B:294:ASN:CG	1:B:328:ASN:OD1	2.30	0.69
2:D:97:ARG:HD2	2:D:138:TRP:CD2	2.28	0.68
1:B:31:PRO:HB2	1:B:33[A]:TRP:CD1	2.29	0.68
2:C:97:ARG:HD3	2:C:138:TRP:CD2	2.28	0.68
2:D:97:ARG:CA	2:D:138:TRP:CH2	2.77	0.68
2:F:144:LEU:HD22	2:F:153:ASN:ND2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:GLU:CD	2:E:41:ARG:NH1	2.48	0.67
1:B:170:ARG:CZ	2:F:67:MET:CE	2.73	0.67
2:F:35:THR:O	2:F:59:ALA:HB2	1.95	0.66
2:F:97:ARG:NH1	2:F:101:LEU:HD21	2.11	0.66
2:F:95:ASP:HA	2:F:98:GLU:OE2	1.95	0.66
2:E:84:ILE:HG23	2:E:116:ASN:O	1.95	0.66
1:B:83:THR:HG22	1:B:84:PRO:HD2	1.77	0.66
1:A:294:ASN:CG	1:A:328:ASN:OD1	2.34	0.66
1:A:83:THR:HG22	1:A:84:PRO:HD2	1.77	0.65
2:F:19:LEU:HD21	2:F:116:ASN:HD21	1.61	0.65
1:B:193:GLN:HA	1:B:193:GLN:HE21	1.62	0.65
2:F:128:LYS:HD3	2:F:132:GLN:HE21	1.62	0.64
2:D:45:GLU:HB2	2:D:50:GLN:HE22	1.63	0.64
2:D:111:MET:SD	2:D:138:TRP:CZ3	2.91	0.63
2:E:30:GLU:O	3:E:201:GNP:O3'	2.11	0.63
1:A:176:LEU:H	1:A:176:LEU:HD22	1.63	0.62
1:A:72:ARG:NH2	2:D:62:GLU:OE2	2.31	0.62
1:A:294:ASN:HB2	1:A:328:ASN:OD1	1.99	0.62
1:B:279:GLN:NE2	1:B:283:GLY:O	2.32	0.62
1:A:31:PRO:HB2	1:A:33[A]:TRP:CD1	2.34	0.62
1:A:89:GLU:CD	1:A:91:ARG:HH22	1.99	0.62
2:C:13:GLY:H	3:C:201:GNP:HNB3	1.48	0.62
1:A:258:CYS:O	1:A:295:GLN:HG3	1.99	0.62
1:B:170:ARG:HD3	1:B:176:LEU:HD21	1.81	0.62
1:B:193:GLN:HA	1:B:193:GLN:NE2	2.15	0.61
1:A:279:GLN:NE2	1:A:283:GLY:O	2.32	0.61
2:D:56:LEU:HD21	2:D:71:TYR:CD1	2.36	0.61
2:E:97:ARG:NH2	2:E:138:TRP:CB	2.62	0.61
1:A:21:THR:HB	2:C:39:SER:CB	2.31	0.60
2:D:97:ARG:NE	2:D:138:TRP:CE3	2.69	0.60
2:F:94:GLN:O	2:F:98:GLU:OE2	2.19	0.60
1:B:356:ARG:HA	2:F:62:GLU:HG2	1.83	0.60
1:B:258:CYS:O	1:B:295:GLN:HG3	2.00	0.60
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.34	0.60
2:E:9:LEU:HD12	2:E:9:LEU:N	2.17	0.59
1:B:303:LEU:O	1:B:343:VAL:HG22	2.01	0.59
2:F:22:GLN:OE1	2:F:151:LYS:HG2	2.02	0.59
1:A:243:LEU:HD22	1:A:274:ALA:HA	1.85	0.58
1:B:104:ASP:OD1	1:B:104:ASP:N	2.36	0.58
2:E:144:LEU:CD2	2:E:153:ASN:ND2	2.66	0.57
1:A:248:GLU:CD	1:A:248:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLY:HA2	1:B:343:VAL:HG21	1.87	0.57
1:B:44:ASN:HB2	5:E:301:HOH:O	2.03	0.57
2:D:97:ARG:HB2	2:D:138:TRP:CZ3	2.25	0.57
2:C:97:ARG:HD3	2:C:138:TRP:CG	2.40	0.57
1:A:27:ASP:HB3	1:A:30:ALA:HB3	1.86	0.56
1:A:160:ASP:OD1	1:A:160:ASP:N	2.38	0.56
1:A:109:LYS:O	1:A:112:THR:HG23	2.05	0.56
2:D:67:MET:HE2	2:D:70:LEU:HD12	1.88	0.56
1:A:63:ARG:NH2	1:A:80:ASN:OD1	2.39	0.56
2:F:96:LEU:HD21	5:F:304:HOH:O	2.06	0.56
2:F:95:ASP:HA	2:F:98:GLU:CD	2.25	0.56
1:B:63:ARG:NH2	1:B:80:ASN:OD1	2.39	0.56
1:B:204:ASP:O	2:F:64:PHE:HB3	2.06	0.56
2:D:50:GLN:NE2	2:D:50:GLN:HA	2.21	0.56
2:F:122:ASP:OD1	2:F:122:ASP:N	2.39	0.56
1:A:294:ASN:CB	1:A:328:ASN:OD1	2.54	0.56
2:D:122:ASP:OD1	2:D:122:ASP:N	2.39	0.56
1:B:109:LYS:O	1:B:112:THR:HG23	2.05	0.55
2:E:28:PHE:CE2	2:E:149:LYS:HG3	2.42	0.55
2:E:45:GLU:HB2	2:E:50:GLN:HE22	1.71	0.55
1:A:304:TYR:CZ	1:A:344:VAL:HG21	2.41	0.55
1:B:206:GLY:HA2	2:F:64:PHE:CD1	2.42	0.55
1:B:304:TYR:CE1	1:B:344:VAL:CG2	2.89	0.55
2:E:36:ILE:HG23	2:E:64:PHE:CE1	2.42	0.55
2:C:122:ASP:OD1	2:C:122:ASP:N	2.40	0.54
2:D:121:GLU:OE2	2:D:124:ARG:NE	2.38	0.54
2:F:29:VAL:HB	2:F:31:LYS:NZ	2.22	0.54
1:A:356:ARG:HA	2:D:62:GLU:HG3	1.89	0.54
2:F:144:LEU:HD22	2:F:153:ASN:HD22	1.73	0.54
1:B:115:ASN:HA	1:B:118:LYS:HE2	1.90	0.54
1:B:236:LEU:O	1:B:241:ALA:HB2	2.07	0.54
2:F:29:VAL:HB	2:F:31:LYS:HZ2	1.72	0.54
1:B:318:THR:O	1:B:322:VAL:HG23	2.08	0.54
1:B:27:ASP:HB3	1:B:30:ALA:HB3	1.91	0.53
2:C:9:LEU:HD12	2:C:9:LEU:N	2.18	0.53
1:B:243:LEU:HD22	1:B:274:ALA:HA	1.89	0.53
1:B:188:HIS:O	1:B:192:ARG:HG3	2.09	0.53
2:F:156:GLU:OE1	2:F:156:GLU:N	2.42	0.53
2:E:97:ARG:HD3	2:E:138:TRP:CE2	2.44	0.53
2:F:19:LEU:HD11	2:F:116:ASN:ND2	2.23	0.53
1:A:236:LEU:O	1:A:241:ALA:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TYR:CE1	1:B:344:VAL:HG23	2.44	0.52
2:F:94:GLN:HE22	2:F:138:TRP:HE1	1.56	0.52
2:C:35:THR:O	2:C:59:ALA:HB2	2.10	0.52
1:B:294:ASN:HB2	1:B:328:ASN:OD1	2.09	0.52
2:C:58:THR:HG21	2:C:71:TYR:CZ	2.45	0.52
2:E:156:GLU:N	2:E:156:GLU:OE1	2.42	0.52
3:F:201:GNP:O2B	3:F:201:GNP:O3G	2.27	0.52
1:A:318:THR:O	1:A:322:VAL:HG23	2.10	0.52
2:D:156:GLU:OE1	2:D:156:GLU:N	2.42	0.52
1:B:294:ASN:CB	1:B:328:ASN:OD1	2.59	0.51
2:D:2:ARG:HD3	2:D:4:TYR:CZ	2.45	0.51
2:C:121:GLU:OE2	2:C:124:ARG:NE	2.37	0.51
1:A:72:ARG:HH22	2:D:62:GLU:CD	2.14	0.51
1:A:215:ARG:NH2	1:A:248:GLU:OE1	2.44	0.51
1:B:13:VAL:HA	1:B:88:LEU:O	2.11	0.51
2:C:133:ASN:C	2:C:133:ASN:HD22	2.14	0.51
1:A:13:VAL:HA	1:A:88:LEU:O	2.10	0.51
2:C:156:GLU:N	2:C:156:GLU:OE1	2.43	0.51
2:D:35:THR:O	2:D:59:ALA:HB2	2.10	0.51
2:F:68:ARG:O	2:F:72:MET:HG3	2.10	0.51
2:F:94:GLN:NE2	2:F:138:TRP:HE1	2.09	0.51
2:F:132:GLN:HG3	2:F:143:PHE:CD2	2.46	0.51
1:B:33[A]:TRP:CG	5:B:404:HOH:O	2.57	0.50
1:B:72:ARG:NH2	2:F:62:GLU:OE1	2.41	0.50
1:A:15:ILE:N	1:A:15:ILE:HD13	2.26	0.50
1:A:103:ASP:HB2	1:A:106:GLN:HB2	1.93	0.50
1:B:15:ILE:HD13	1:B:15:ILE:N	2.25	0.50
1:A:18:LEU:HD11	1:A:46:SER:HB2	1.93	0.50
2:D:22:GLN:HE21	2:D:26:GLY:HA2	1.75	0.50
2:F:94:GLN:HG3	2:F:98:GLU:OE1	2.10	0.50
2:F:144:LEU:CD2	2:F:153:ASN:ND2	2.74	0.50
1:B:119:PHE:CE2	1:B:139:LEU:HD22	2.46	0.50
1:A:119:PHE:CE2	1:A:139:LEU:HD22	2.46	0.50
1:B:291:ALA:HA	1:B:331:LEU:HD13	1.94	0.49
1:B:10:VAL:HG12	1:B:85:LEU:HD23	1.94	0.49
2:E:35:THR:O	2:E:59:ALA:HB2	2.13	0.49
2:F:19:LEU:HD21	2:F:116:ASN:ND2	2.26	0.49
1:B:117:LYS:HE2	1:B:145:ASP:OD2	2.11	0.49
1:B:215:ARG:HD2	1:B:248:GLU:OE1	2.13	0.49
2:D:62:GLU:HG2	2:D:64:PHE:CE2	2.48	0.49
2:E:15:GLY:HA2	3:E:201:GNP:O2A	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:N	1:B:347:ARG:HD3	2.27	0.49
2:C:122:ASP:HB2	5:C:308:HOH:O	2.13	0.49
2:F:97:ARG:CD	2:F:138:TRP:CG	2.96	0.49
2:E:3:GLU:CD	2:E:41:ARG:HH12	2.15	0.49
2:E:144:LEU:HD21	2:E:153:ASN:ND2	2.28	0.49
2:E:97:ARG:HH22	2:E:138:TRP:CA	2.22	0.49
2:F:97:ARG:CD	2:F:138:TRP:CD2	2.94	0.49
2:E:8:VAL:O	2:E:58:THR:OG1	2.22	0.48
2:E:58:THR:HG21	2:E:71:TYR:CZ	2.49	0.48
1:A:261:GLY:HA2	1:A:298:CYS:SG	2.53	0.48
2:C:132:GLN:HG3	2:C:143:PHE:CD2	2.48	0.48
1:A:25:ARG:HH21	1:A:25:ARG:HG3	1.79	0.48
1:B:68:LEU:HG	1:B:77:TYR:CD2	2.49	0.48
2:F:28:PHE:CE2	2:F:149:LYS:HG3	2.48	0.48
1:B:303:LEU:O	1:B:343:VAL:CG2	2.62	0.47
2:E:64:PHE:N	2:E:64:PHE:CD1	2.81	0.47
2:F:32:TYR:OH	3:F:201:GNP:O1G	2.24	0.47
2:C:28:PHE:CE2	2:C:149:LYS:HG3	2.50	0.47
3:C:201:GNP:O2B	5:C:301:HOH:O	2.20	0.47
1:A:205:LEU:CD2	2:D:66:ALA:HB1	2.44	0.47
1:A:246:THR:HG22	1:A:252:GLN:HG3	1.96	0.47
1:B:120:MET:HA	1:B:120:MET:CE	2.45	0.47
2:F:130:GLN:HG3	5:F:309:HOH:O	2.14	0.47
1:A:206:GLY:HA2	2:D:64:PHE:CD1	2.50	0.47
2:D:28:PHE:CE2	2:D:149:LYS:HG3	2.49	0.47
2:F:97:ARG:HH12	2:F:101:LEU:HD21	1.78	0.47
1:A:164:ASP:O	1:A:168:VAL:HG23	2.15	0.47
1:A:68:LEU:HG	1:A:77:TYR:CD2	2.49	0.47
2:F:116:ASN:HA	2:F:146:SER:O	2.15	0.47
2:F:97:ARG:HD2	2:F:138:TRP:CG	2.50	0.46
1:B:40:LEU:CD2	1:B:50:ALA:HB1	2.45	0.46
2:F:104:LYS:HG3	2:F:109:VAL:HG21	1.97	0.46
2:D:49:GLN:HE21	2:D:49:GLN:HB2	1.60	0.46
1:B:40:LEU:HD21	1:B:50:ALA:HB1	1.97	0.46
1:A:170:ARG:HD3	1:A:176:LEU:HD21	1.97	0.46
1:A:291:ALA:HA	1:A:331:LEU:HD13	1.97	0.46
1:B:313:ASN:HD21	1:B:317:GLN:HG3	1.81	0.46
1:B:320:PHE:CD1	1:B:332:ALA:HB1	2.51	0.46
2:C:128:LYS:HD3	2:C:132:GLN:NE2	2.30	0.46
1:A:79:PRO:HB2	1:A:86:PRO:HB3	1.98	0.46
2:D:13:GLY:O	2:D:117:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ASN:HA	2:D:146:SER:O	2.15	0.45
1:A:40:LEU:CD2	1:A:50:ALA:HB1	2.47	0.45
2:D:13:GLY:H	3:D:201:GNP:HNB3	1.64	0.45
1:A:56:PHE:N	1:A:89:GLU:O	2.46	0.45
2:E:9:LEU:CD1	2:E:80:LEU:HD12	2.46	0.45
1:B:18:LEU:HD11	1:B:46:SER:HB2	1.98	0.45
1:B:354:LYS:HD2	1:B:354:LYS:N	2.31	0.45
2:E:116:ASN:HA	2:E:146:SER:O	2.16	0.45
1:B:193:GLN:HE21	1:B:193:GLN:CA	2.26	0.45
2:C:68:ARG:HA	2:C:71:TYR:CE2	2.52	0.45
2:C:116:ASN:HA	2:C:146:SER:O	2.17	0.45
2:E:144:LEU:HD22	2:E:153:ASN:HB3	1.98	0.45
1:B:21:THR:OG1	2:E:39:SER:HB2	2.16	0.45
2:D:129:GLU:OE1	2:D:130:GLN:N	2.50	0.45
2:F:112:ILE:CD1	2:F:144:LEU:HD12	2.41	0.45
1:A:204:ASP:O	2:D:64:PHE:HB3	2.16	0.44
2:D:22:GLN:NE2	2:D:26:GLY:HA2	2.32	0.44
2:D:97:ARG:HA	2:D:138:TRP:CH2	2.51	0.44
2:D:117:LYS:HG3	3:D:201:GNP:C6	2.47	0.44
1:B:206:GLY:HA2	2:F:64:PHE:CE1	2.52	0.44
2:C:160:ASP:O	2:C:164:GLN:HG3	2.18	0.44
2:F:99:GLN:NE2	5:F:302:HOH:O	2.49	0.44
1:B:115:ASN:HA	1:B:118:LYS:CE	2.48	0.44
2:E:68:ARG:HA	2:E:71:TYR:CE2	2.52	0.44
1:A:25:ARG:HG3	1:A:25:ARG:NH2	2.33	0.44
1:B:56:PHE:N	1:B:89:GLU:O	2.46	0.44
2:C:82:TYR:HB3	2:C:93:LEU:CD1	2.42	0.44
2:C:166:ASN:HB2	5:C:302:HOH:O	2.17	0.44
1:A:347:ARG:HD3	1:A:348:GLU:H	1.82	0.44
2:E:137:GLN:HE21	2:E:137:GLN:HB3	1.63	0.44
1:B:111:HIS:CE1	1:B:139:LEU:HA	2.52	0.44
1:B:95:ARG:HB2	1:B:140:ASP:OD1	2.18	0.43
2:C:9:LEU:CD1	2:C:80:LEU:HD12	2.48	0.43
2:C:129:GLU:N	2:C:129:GLU:OE1	2.51	0.43
2:F:80:LEU:HB3	2:F:93:LEU:HD22	1.98	0.43
2:F:124:ARG:NH2	2:F:145:GLU:OE1	2.51	0.43
2:C:80:LEU:HB3	2:C:93:LEU:HD22	1.99	0.43
2:F:129:GLU:OE1	2:F:129:GLU:N	2.51	0.43
2:D:160:ASP:O	2:D:164:GLN:HG3	2.19	0.43
1:A:357:ARG:NH1	5:A:401:HOH:O	2.50	0.43
1:B:239:ASP:CG	1:B:356:ARG:HH22	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:GLU:N	2:E:30:GLU:OE1	2.52	0.43
1:A:320:PHE:CD1	1:A:332:ALA:HB1	2.54	0.43
1:B:313:ASN:HD21	1:B:317:GLN:CG	2.31	0.43
2:C:68:ARG:NH1	2:C:68:ARG:HG3	2.33	0.43
2:C:9:LEU:HD21	2:C:100:ILE:HD11	2.01	0.43
2:E:14:VAL:CG2	2:E:16:LYS:HG3	2.49	0.43
1:A:312:ARG:NH2	1:B:242:GLN:HG3	2.34	0.42
1:A:347:ARG:CD	1:A:347:ARG:N	2.82	0.42
2:C:129:GLU:OE1	2:C:130:GLN:N	2.48	0.42
2:E:97:ARG:HG3	2:E:111:MET:SD	2.58	0.42
2:E:10:GLY:N	2:E:16:LYS:HD3	2.34	0.42
2:E:84:ILE:HD13	2:E:117:LYS:O	2.20	0.42
1:B:203:LEU:HD13	1:B:239:ASP:OD2	2.20	0.42
2:D:45:GLU:CB	2:D:50:GLN:HE22	2.31	0.42
2:D:97:ARG:CD	2:D:138:TRP:CD2	3.00	0.42
2:F:13:GLY:H	3:F:201:GNP:HNB3	1.66	0.42
2:F:132:GLN:HG3	2:F:143:PHE:CE2	2.54	0.42
2:C:30:GLU:O	3:C:201:GNP:O3'	2.33	0.42
1:B:205:LEU:CD2	2:F:66:ALA:HB1	2.49	0.42
1:A:40:LEU:HD21	1:A:50:ALA:HB1	2.02	0.42
1:B:261:GLY:HA2	1:B:298:CYS:SG	2.60	0.42
2:E:14:VAL:HG23	2:E:16:LYS:HG3	2.02	0.42
1:B:296:GLU:OE2	1:B:300:ARG:NH2	2.52	0.42
2:C:97:ARG:HD3	2:C:138:TRP:CE2	2.54	0.42
2:E:80:LEU:HB3	2:E:93:LEU:HD22	2.02	0.42
2:E:160:ASP:O	2:E:164:GLN:HG3	2.19	0.42
2:F:117:LYS:HB3	2:F:120:LEU:HD12	2.01	0.42
1:A:176:LEU:HD22	1:A:176:LEU:N	2.34	0.42
1:B:31:PRO:HA	1:B:73:LEU:HA	2.02	0.42
2:D:112:ILE:CD1	2:D:144:LEU:HD12	2.43	0.42
2:E:82:TYR:HB3	2:E:93:LEU:CD1	2.42	0.42
2:D:130:GLN:CD	5:D:301:HOH:O	2.45	0.41
2:F:16:LYS:N	3:F:201:GNP:O1B	2.52	0.41
2:C:14:VAL:CG2	2:C:16:LYS:HG3	2.50	0.41
2:F:3:GLU:OE2	2:F:41:ARG:NH1	2.48	0.41
1:A:254:ILE:HG22	1:A:266:LEU:HD12	2.02	0.41
1:B:123:VAL:O	1:B:159:LEU:HD11	2.21	0.41
2:C:56:LEU:CD2	2:C:71:TYR:HB2	2.51	0.41
2:E:16:LYS:N	3:E:201:GNP:O1B	2.53	0.41
1:A:330:GLU:H	1:A:330:GLU:CD	2.21	0.41
1:B:79:PRO:HB2	1:B:86:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:GLN:HG3	2:C:143:PHE:CE2	2.55	0.41
1:A:27:ASP:HB3	1:A:30:ALA:CB	2.49	0.41
1:B:347:ARG:N	1:B:347:ARG:CD	2.84	0.41
2:C:15:GLY:HA2	3:C:201:GNP:O2A	2.20	0.41
1:B:199:LEU:O	1:B:203:LEU:HG	2.21	0.41
2:E:97:ARG:HD3	2:E:138:TRP:CG	2.55	0.41
2:F:160:ASP:O	2:F:164:GLN:HG3	2.20	0.41
1:A:199:LEU:O	1:A:203:LEU:HG	2.22	0.40
1:A:347:ARG:HD3	1:A:347:ARG:N	2.36	0.40
1:B:304:TYR:CE1	1:B:344:VAL:HG21	2.56	0.40
2:E:97:ARG:CD	2:E:138:TRP:CD2	3.01	0.40
2:F:82:TYR:HB3	2:F:93:LEU:CD1	2.43	0.40
2:C:10:GLY:N	2:C:16:LYS:HD3	2.36	0.40
2:C:35:THR:O	2:C:59:ALA:CB	2.69	0.40
2:F:15:GLY:HA2	3:F:201:GNP:O2A	2.21	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	358/374 (96%)	356 (99%)	2 (1%)	0	100	100
1	B	356/374 (95%)	353 (99%)	3 (1%)	0	100	100
2	C	167/170 (98%)	164 (98%)	3 (2%)	0	100	100
2	D	166/170 (98%)	164 (99%)	2 (1%)	0	100	100
2	E	167/170 (98%)	166 (99%)	1 (1%)	0	100	100
2	F	166/170 (98%)	164 (99%)	2 (1%)	0	100	100
All	All	1380/1428 (97%)	1367 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	296/306 (97%)	255 (86%)	41 (14%)	3 10
1	B	296/306 (97%)	255 (86%)	41 (14%)	3 10
2	C	149/149 (100%)	129 (87%)	20 (13%)	4 11
2	D	148/149 (99%)	124 (84%)	24 (16%)	2 7
2	E	149/149 (100%)	122 (82%)	27 (18%)	1 5
2	F	148/149 (99%)	129 (87%)	19 (13%)	4 13
All	All	1186/1208 (98%)	1014 (86%)	172 (14%)	3 9

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	15	ILE
1	A	21	THR
1	A	22	LYS
1	A	41	CYS
1	A	57	GLN
1	A	60	SER
1	A	61	ARG
1	A	81	LEU
1	A	83	THR
1	A	101	LEU
1	A	103	ASP
1	A	106	GLN
1	A	113	LYS
1	A	118	LYS
1	A	139	LEU
1	A	155	LEU
1	A	159	LEU
1	A	160	ASP
1	A	161	ASN
1	A	165	LEU
1	A	170	ARG

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Mol	Chain	Res	Type
1	A	181	ARG
1	A	217	LEU
1	A	240	HIS
1	A	243	LEU
1	A	248	GLU
1	A	258	CYS
1	A	263	VAL
1	A	267	GLU
1	A	279	GLN
1	A	292	LEU
1	A	294	ASN
1	A	331	LEU
1	A	336	LYS
1	A	339	LYS
1	A	347	ARG
1	A	351	SER
1	A	354	LYS
1	A	356	ARG
1	A	362	SER
1	B	7	SER
1	B	15	ILE
1	B	21	THR
1	B	38	ARG
1	B	41	CYS
1	B	45	HIS
1	B	57	GLN
1	B	81	LEU
1	B	83	THR
1	B	100	ASN
1	B	103	ASP
1	B	104	ASP
1	B	106	GLN
1	B	113	LYS
1	B	117	LYS
1	B	118	LYS
1	B	120	MET
1	B	125	LEU
1	B	139	LEU
1	B	155	LEU
1	B	165	LEU
1	B	170	ARG
1	B	181	ARG

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Mol	Chain	Res	Type
1	B	193	GLN
1	B	217	LEU
1	B	240	HIS
1	B	243	LEU
1	B	248	GLU
1	B	258	CYS
1	B	263	VAL
1	B	267	GLU
1	B	292	LEU
1	B	309	LYS
1	B	316	SER
1	B	317	GLN
1	B	331	LEU
1	B	336	LYS
1	B	339	LYS
1	B	340	ASP
1	B	347	ARG
1	B	354	LYS
2	C	3	GLU
2	C	9	LEU
2	C	31	LYS
2	C	39	SER
2	C	42	LYS
2	C	49	GLN
2	C	55	ILE
2	C	62	GLU
2	C	68	ARG
2	C	71	TYR
2	C	96	LEU
2	C	97	ARG
2	C	106	THR
2	C	108	ASP
2	C	122	ASP
2	C	128	LYS
2	C	129	GLU
2	C	130	GLN
2	C	133	ASN
2	C	139	ASN
2	D	2	ARG
2	D	3	GLU
2	D	27	ILE
2	D	30	GLU

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Mol	Chain	Res	Type
2	D	39	SER
2	D	42	LYS
2	D	49	GLN
2	D	52	MET
2	D	55	ILE
2	D	62	GLU
2	D	63	GLN
2	D	67	MET
2	D	85	THR
2	D	96	LEU
2	D	97	ARG
2	D	99	GLN
2	D	106	THR
2	D	107	ASP
2	D	108	ASP
2	D	122	ASP
2	D	129	GLU
2	D	130	GLN
2	D	139	ASN
2	D	140	ASN
2	E	-1	PRO
2	E	1	MET
2	E	2	ARG
2	E	3	GLU
2	E	9	LEU
2	E	30	GLU
2	E	31	LYS
2	E	39	SER
2	E	41	ARG
2	E	42	LYS
2	E	52	MET
2	E	62	GLU
2	E	63	GLN
2	E	68	ARG
2	E	71	TYR
2	E	84	ILE
2	E	106	THR
2	E	108	ASP
2	E	118	CYS
2	E	119	ASP
2	E	121	GLU
2	E	122	ASP

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Mol	Chain	Res	Type
2	E	128	LYS
2	E	129	GLU
2	E	130	GLN
2	E	137	GLN
2	E	144	LEU
2	F	1	MET
2	F	2	ARG
2	F	3	GLU
2	F	22	GLN
2	F	29	VAL
2	F	31	LYS
2	F	39	SER
2	F	52	MET
2	F	63	GLN
2	F	67	MET
2	F	68	ARG
2	F	73	LYS
2	F	85	THR
2	F	101	LEU
2	F	107	ASP
2	F	108	ASP
2	F	122	ASP
2	F	125	VAL
2	F	130	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	126	HIS
1	A	161	ASN
1	A	238	HIS
1	A	265	HIS
1	A	275	ASN
1	A	294	ASN
1	A	317	GLN
1	B	45	HIS
1	B	57	GLN
1	B	99	GLN
1	B	100	ASN
1	B	115	ASN
1	B	193	GLN

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Mol	Chain	Res	Type
1	B	238	HIS
1	B	265	HIS
1	B	317	GLN
2	C	74	ASN
2	C	99	GLN
2	C	133	ASN
2	C	137	GLN
2	C	139	ASN
2	D	22	GLN
2	D	43	GLN
2	D	49	GLN
2	D	50	GLN
2	D	74	ASN
2	D	130	GLN
2	D	137	GLN
2	D	139	ASN
2	D	140	ASN
2	E	43	GLN
2	E	50	GLN
2	E	74	ASN
2	E	130	GLN
2	E	137	GLN
2	F	49	GLN
2	F	74	ASN
2	F	94	GLN
2	F	116	ASN
2	F	132	GLN
2	F	137	GLN
2	F	153	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
3	GNP	F	201	4	29,34,34	1.37	3 (10%)	33,54,54	2.33	6 (18%)
3	GNP	E	201	4	29,34,34	1.37	6 (20%)	33,54,54	2.43	9 (27%)
3	GNP	D	201	4	29,34,34	1.57	4 (13%)	33,54,54	2.40	8 (24%)
3	GNP	C	201	4	29,34,34	1.54	4 (13%)	33,54,54	2.35	8 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	F	201	4	-	4/14/38/38	0/3/3/3
3	GNP	E	201	4	-	5/14/38/38	0/3/3/3
3	GNP	D	201	4	-	5/14/38/38	0/3/3/3
3	GNP	C	201	4	-	7/14/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	GNP	PG-O1G	4.77	1.53	1.46
3	C	201	GNP	PG-O1G	4.45	1.53	1.46
3	C	201	GNP	C6-N1	4.35	1.40	1.33
3	F	201	GNP	C6-N1	4.30	1.40	1.33
3	D	201	GNP	C6-N1	4.11	1.40	1.33
3	E	201	GNP	C6-N1	3.99	1.40	1.33
3	F	201	GNP	PG-O1G	3.52	1.51	1.46
3	E	201	GNP	PG-O1G	3.20	1.51	1.46
3	D	201	GNP	PB-O3A	2.68	1.62	1.59
3	C	201	GNP	PB-O1B	2.59	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	GNP	PB-O2B	-2.38	1.50	1.56
3	D	201	GNP	PB-O2B	-2.31	1.50	1.56
3	E	201	GNP	PB-O2B	-2.22	1.50	1.56
3	E	201	GNP	PB-O1B	2.21	1.49	1.46
3	F	201	GNP	PB-O2B	-2.14	1.51	1.56
3	E	201	GNP	PG-O3G	-2.12	1.51	1.56
3	E	201	GNP	PG-O2G	-2.07	1.51	1.56

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	201	GNP	C5-C6-N1	-8.86	111.31	123.43
3	E	201	GNP	C5-C6-N1	-8.81	111.38	123.43
3	F	201	GNP	C5-C6-N1	-8.74	111.48	123.43
3	D	201	GNP	C5-C6-N1	-8.73	111.49	123.43
3	F	201	GNP	C2-N1-C6	6.06	125.56	115.93
3	D	201	GNP	C2-N1-C6	5.97	125.41	115.93
3	E	201	GNP	C2-N1-C6	5.93	125.36	115.93
3	C	201	GNP	C2-N1-C6	5.92	125.34	115.93
3	F	201	GNP	O2B-PB-O1B	4.29	118.92	109.92
3	C	201	GNP	O2B-PB-O1B	4.03	118.38	109.92
3	E	201	GNP	O2B-PB-O1B	3.94	118.17	109.92
3	D	201	GNP	O2B-PB-O1B	3.80	117.90	109.92
3	E	201	GNP	O2G-PG-O1G	-3.66	104.25	113.45
3	D	201	GNP	O1B-PB-N3B	-3.54	106.56	111.77
3	F	201	GNP	N3-C2-N1	-3.48	122.58	127.22
3	D	201	GNP	O3G-PG-O1G	-3.43	104.83	113.45
3	E	201	GNP	PB-O3A-PA	-3.33	120.88	132.62
3	C	201	GNP	O2G-PG-O1G	-3.16	105.50	113.45
3	E	201	GNP	O3A-PB-N3B	3.15	115.32	106.59
3	E	201	GNP	N3-C2-N1	-2.99	123.23	127.22
3	D	201	GNP	N3-C2-N1	-2.99	123.23	127.22
3	C	201	GNP	N3-C2-N1	-2.93	123.32	127.22
3	F	201	GNP	PB-O3A-PA	-2.92	122.34	132.62
3	D	201	GNP	C2-N3-C4	-2.63	112.36	115.36
3	D	201	GNP	PB-O3A-PA	-2.60	123.47	132.62
3	C	201	GNP	C2-N3-C4	-2.42	112.59	115.36
3	E	201	GNP	C2-N3-C4	-2.30	112.73	115.36
3	F	201	GNP	C2-N3-C4	-2.25	112.79	115.36
3	C	201	GNP	PB-O3A-PA	-2.23	124.77	132.62
3	E	201	GNP	O3G-PG-O1G	-2.09	108.21	113.45
3	C	201	GNP	O3G-PG-O1G	-2.01	108.41	113.45

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	201	GNP	PB-N3B-PG-O1G
3	C	201	GNP	PG-N3B-PB-O1B
3	C	201	GNP	PA-O3A-PB-O1B
3	C	201	GNP	PA-O3A-PB-O2B
3	C	201	GNP	C5'-O5'-PA-O3A
3	C	201	GNP	C5'-O5'-PA-O1A
3	D	201	GNP	PB-N3B-PG-O1G
3	D	201	GNP	PG-N3B-PB-O1B
3	D	201	GNP	PA-O3A-PB-O1B
3	D	201	GNP	PA-O3A-PB-O2B
3	E	201	GNP	PB-N3B-PG-O1G
3	E	201	GNP	PG-N3B-PB-O1B
3	E	201	GNP	PA-O3A-PB-O2B
3	E	201	GNP	C5'-O5'-PA-O1A
3	F	201	GNP	PB-N3B-PG-O1G
3	F	201	GNP	PG-N3B-PB-O1B
3	F	201	GNP	O4'-C4'-C5'-O5'
3	E	201	GNP	C5'-O5'-PA-O3A
3	C	201	GNP	C5'-O5'-PA-O2A
3	F	201	GNP	C3'-C4'-C5'-O5'
3	D	201	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

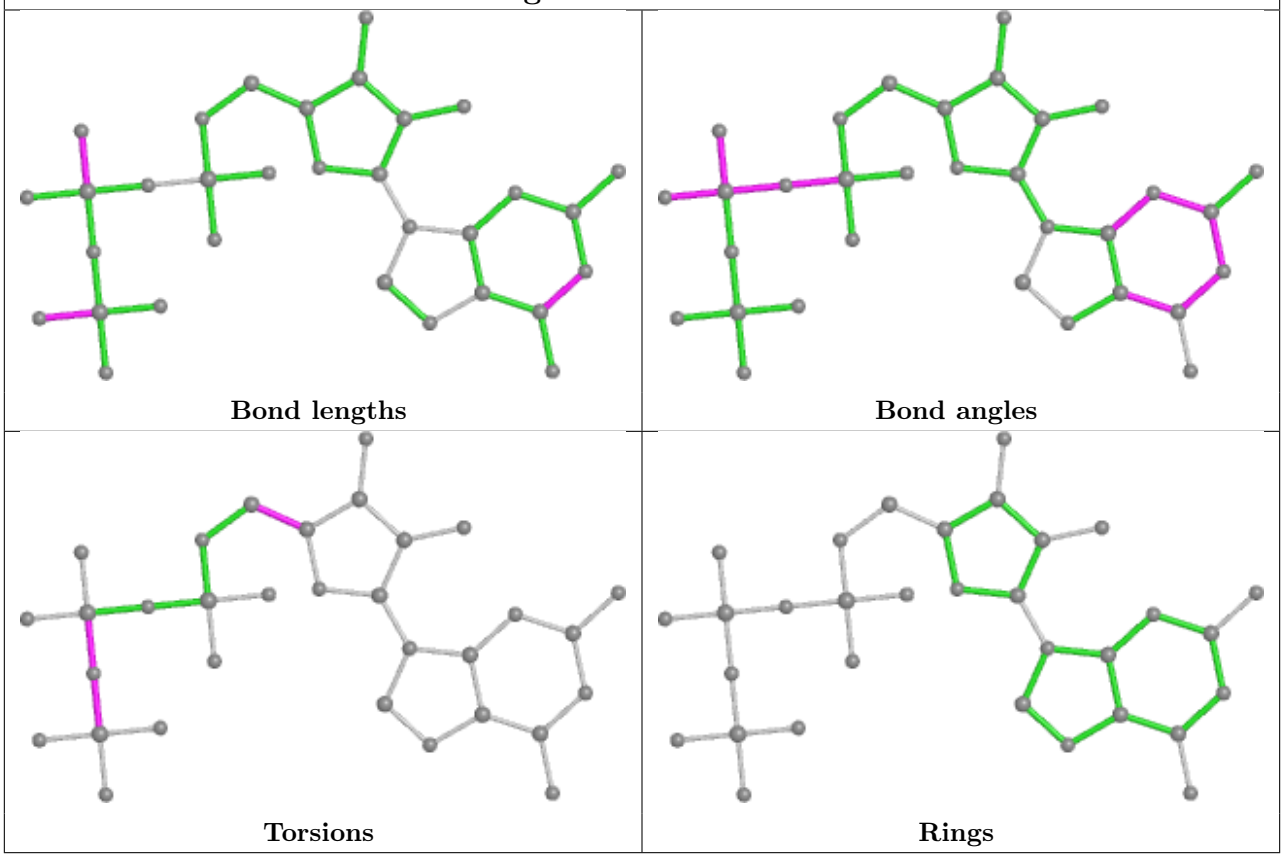
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	201	GNP	5	0
3	E	201	GNP	4	0
3	D	201	GNP	2	0
3	C	201	GNP	4	0

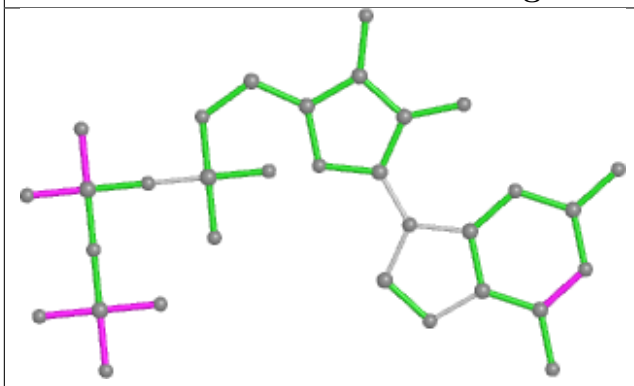
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

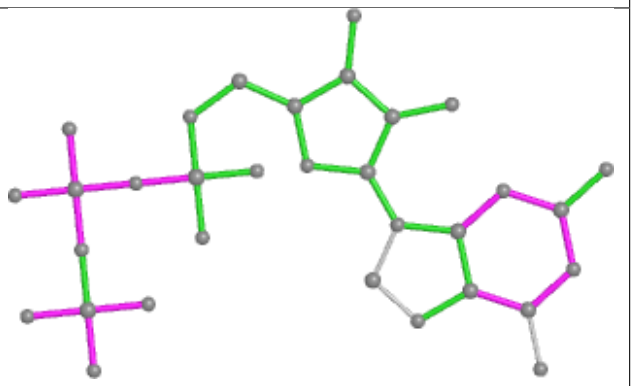
Ligand GNP F 201



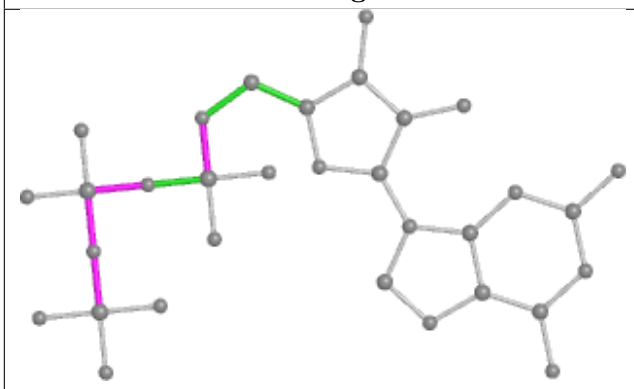
Ligand GNP E 201



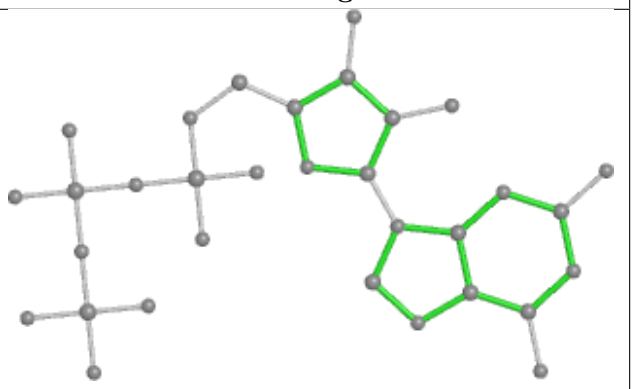
Bond lengths



Bond angles

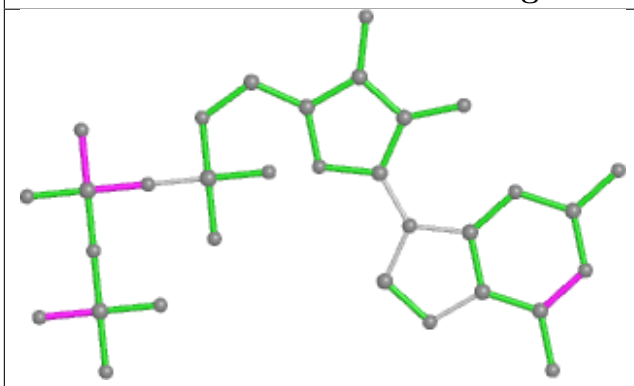


Torsions

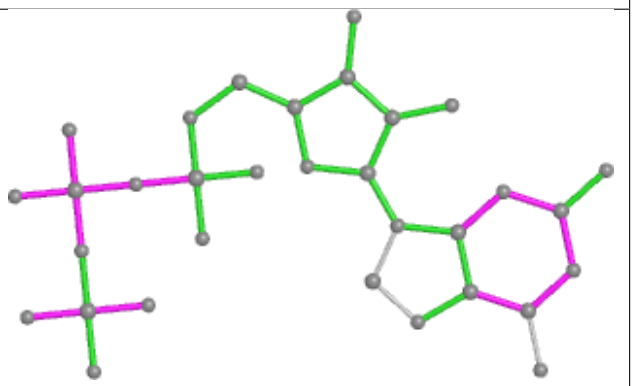


Rings

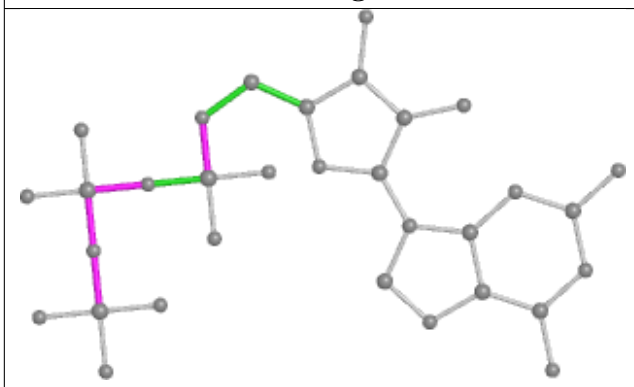
Ligand GNP D 201



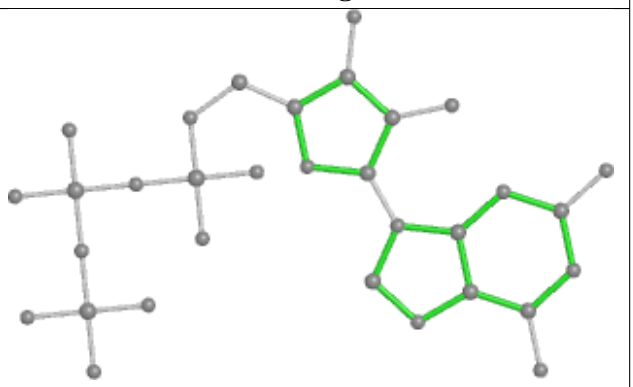
Bond lengths



Bond angles

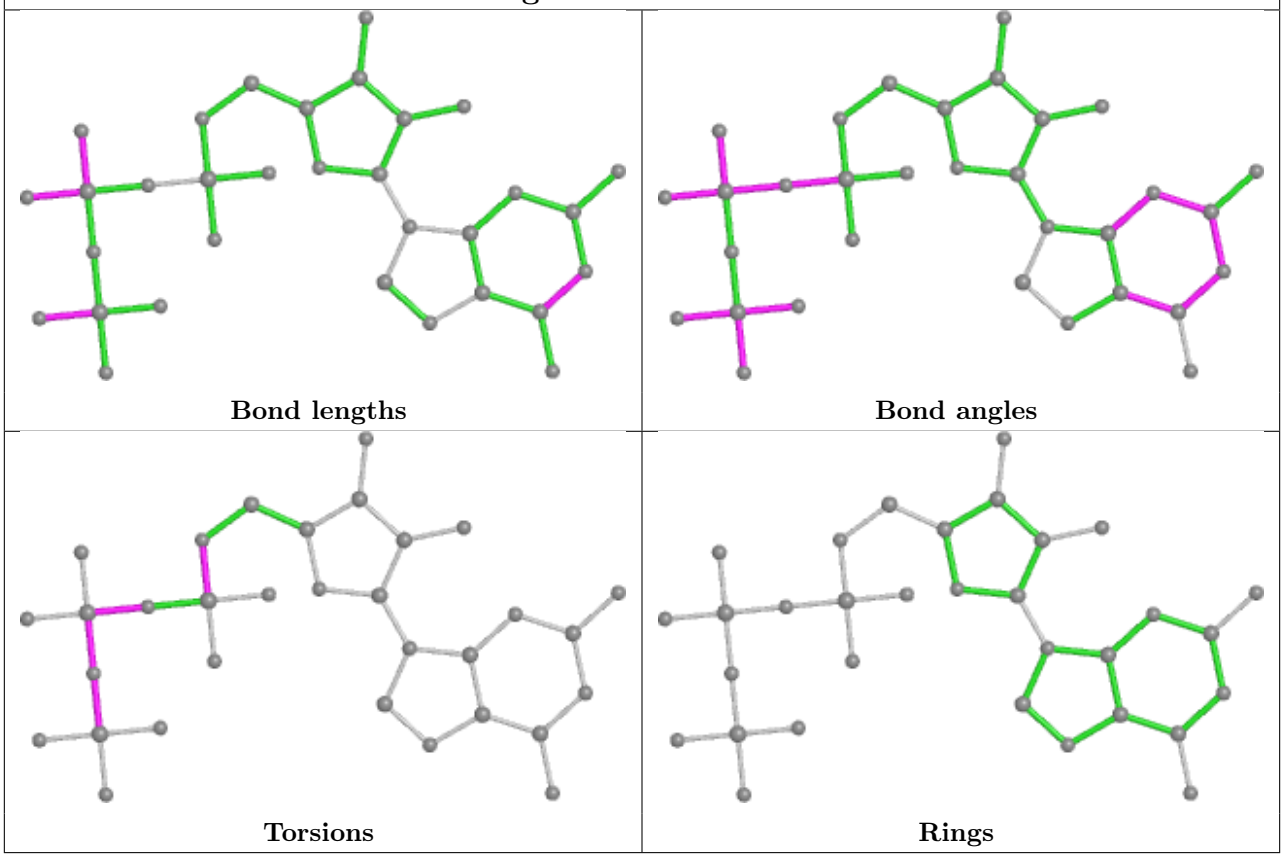


Torsions



Rings

Ligand GNP C 201



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	359/374 (95%)	-0.15	2 (0%)	89	86	35, 59, 95, 158	0
1	B	357/374 (95%)	-0.08	2 (0%)	89	86	35, 63, 99, 153	0
2	C	169/170 (99%)	-0.07	2 (1%)	79	73	48, 72, 104, 132	0
2	D	168/170 (98%)	0.21	3 (1%)	68	61	44, 75, 109, 128	0
2	E	169/170 (99%)	0.25	7 (4%)	37	27	56, 85, 114, 143	0
2	F	168/170 (98%)	0.08	2 (1%)	79	73	45, 72, 100, 112	0
All	All	1390/1428 (97%)	-0.00	18 (1%)	77	72	35, 69, 107, 158	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	132	GLN	3.1
2	E	141	CYS	2.9
2	E	129	GLU	2.8
2	D	129	GLU	2.7
2	C	64	PHE	2.6
2	E	82	TYR	2.5
1	A	107	PHE	2.4
1	B	122	TYR	2.3
2	D	29	VAL	2.3
1	A	100	ASN	2.3
2	F	138	TRP	2.2
2	D	84	ILE	2.2
2	C	90	PHE	2.2
2	E	96	LEU	2.1
1	B	133	ARG	2.1
2	E	114	VAL	2.1
2	F	95	ASP	2.0
2	E	-1	PRO	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)

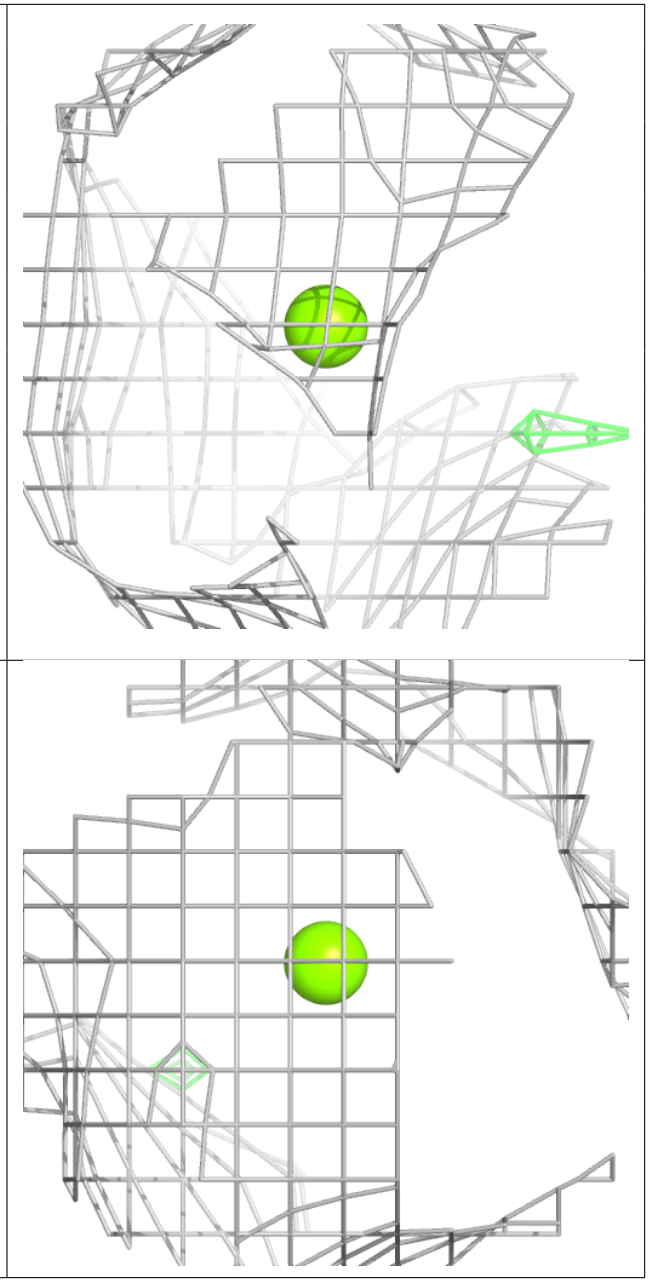
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	D	202	1/1	0.94	0.12	91,91,91,91	0
3	GNP	E	201	32/32	0.95	0.15	59,76,94,97	0
4	MG	E	202	1/1	0.95	0.05	64,64,64,64	0
3	GNP	D	201	32/32	0.96	0.15	44,62,71,72	0
3	GNP	F	201	32/32	0.96	0.14	49,62,71,73	0
3	GNP	C	201	32/32	0.97	0.13	51,62,80,89	0
4	MG	C	202	1/1	0.98	0.06	52,52,52,52	0
4	MG	F	202	1/1	0.98	0.12	85,85,85,85	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.

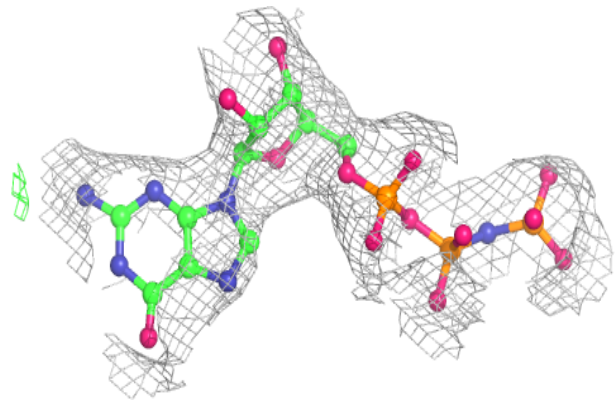
Electron density around MG D 202:

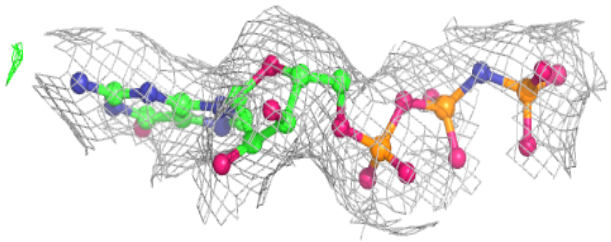
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

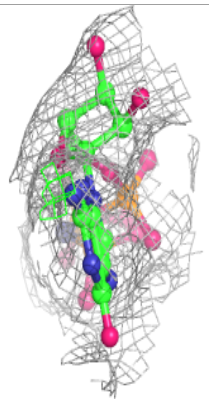


Electron density around GNP E 201:

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

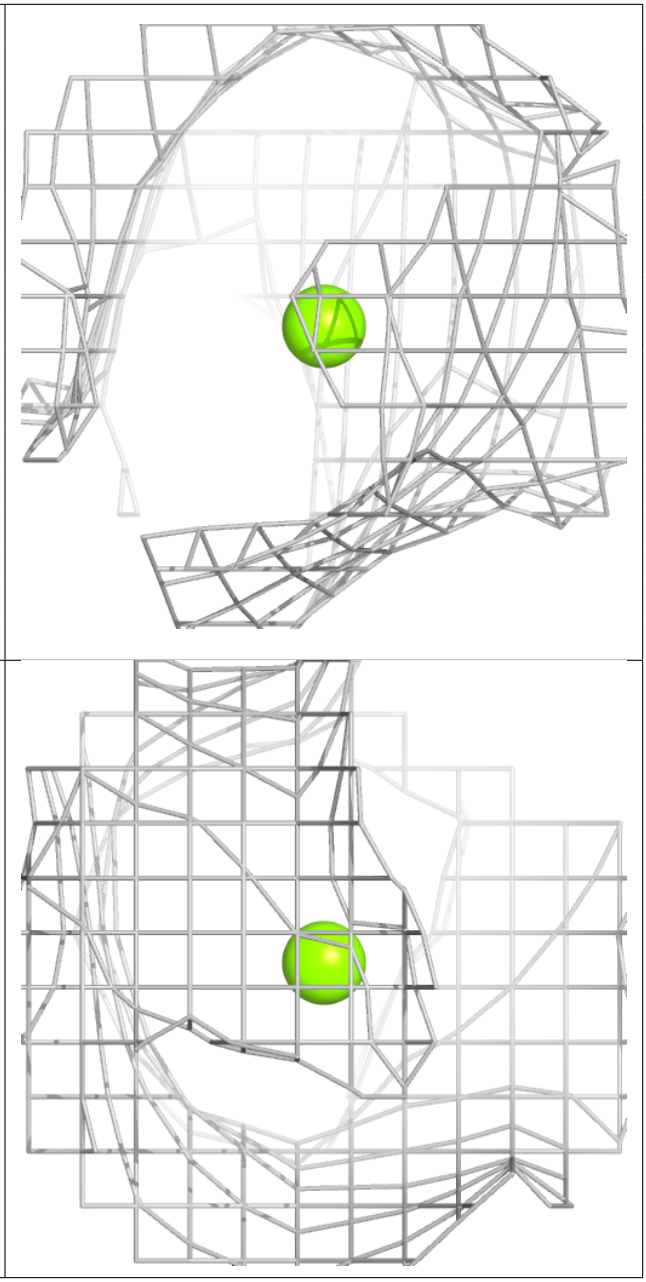






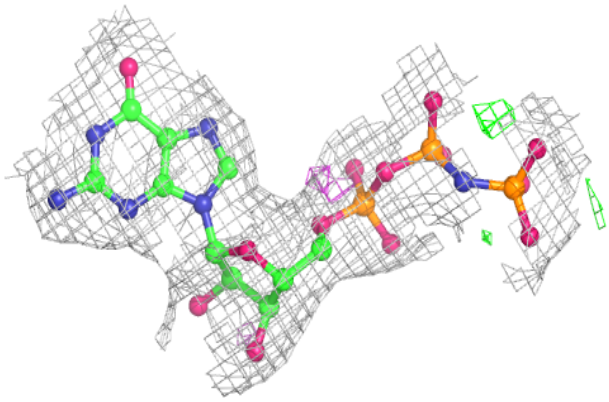
Electron density around MG E 202:

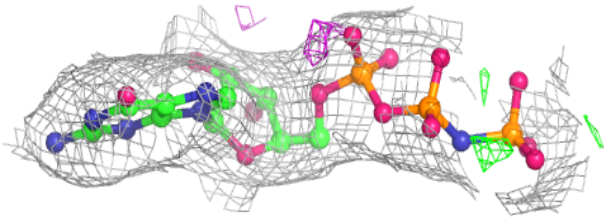
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

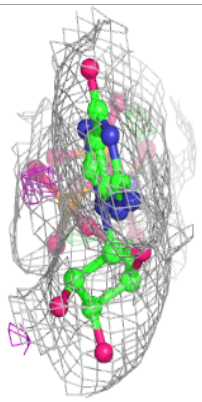


Electron density around GNP D 201:

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

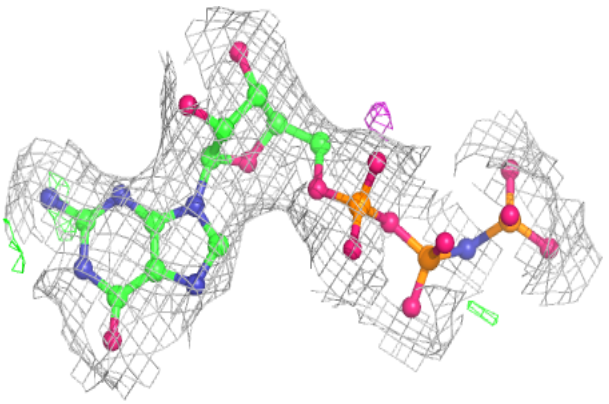


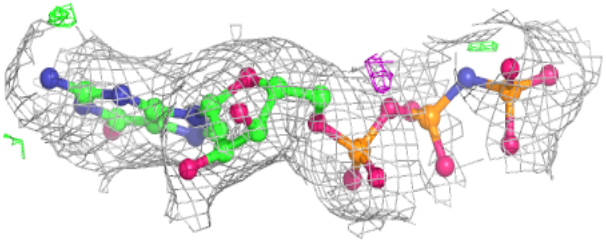


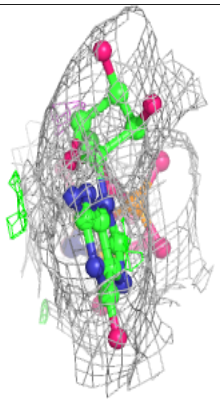


Electron density around GNP F 201:

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

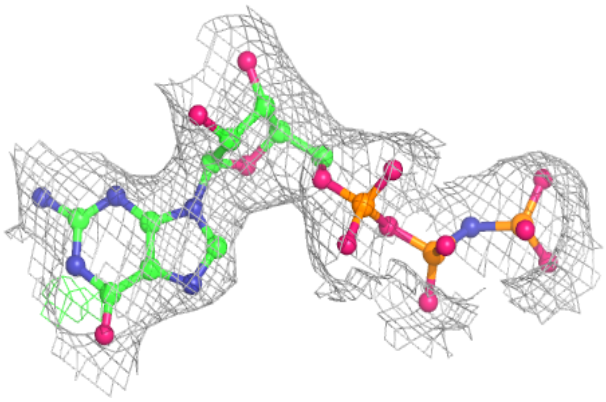


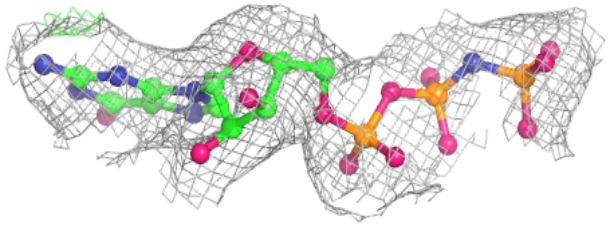


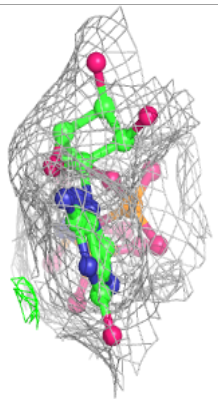


Electron density around GNP C 201:

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

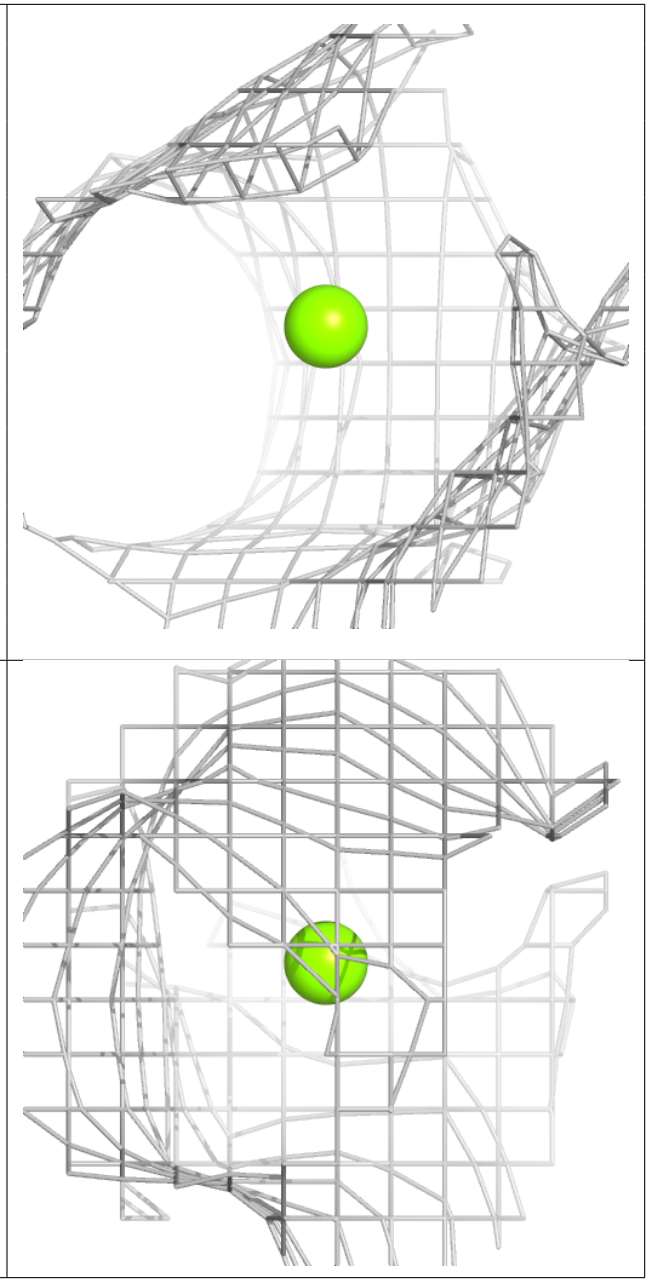






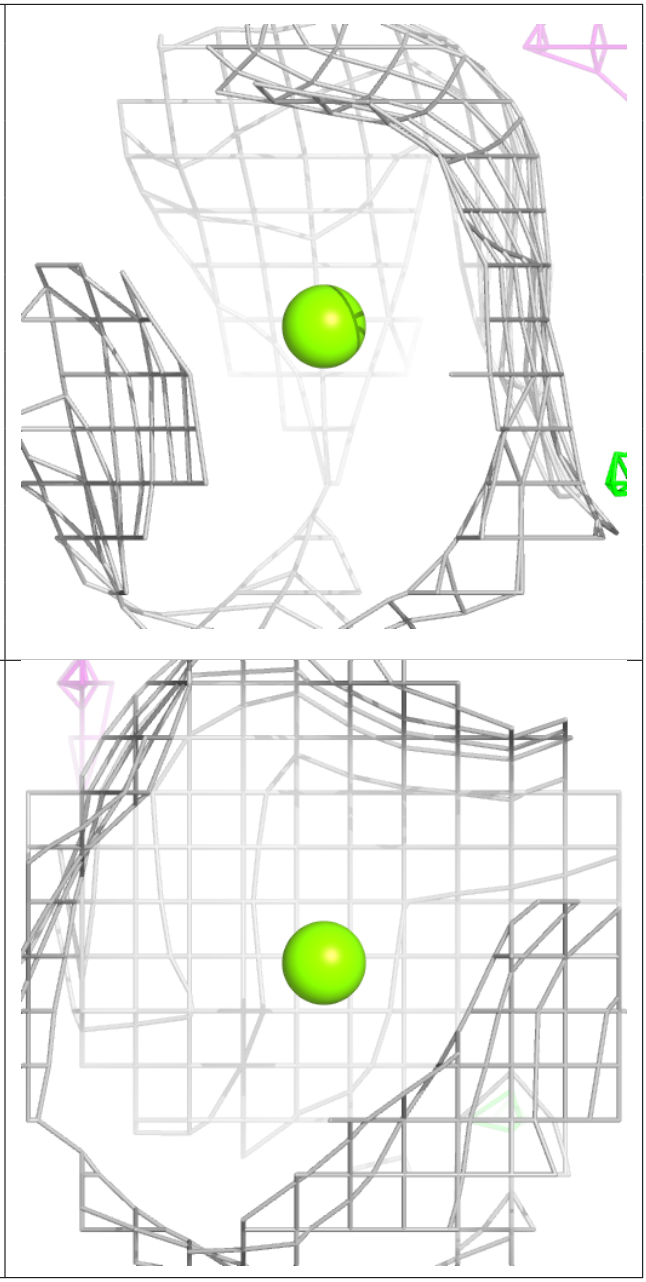
Electron density around MG C 202:

$2mF_o$-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 F 202:

$2mF_o$-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.