



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:36 PM UTC

PDB ID : 3A58 / pdb_00003a58
Title : Crystal structure of Sec3p - Rho1p complex from *Saccharomyces cerevisiae*
Authors : Yamashita, M.; Sato, Y.; Yamagata, A.; Mimura, H.; Yoshikawa, A.; Fukai, S.
Deposited on : 2009-08-03
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

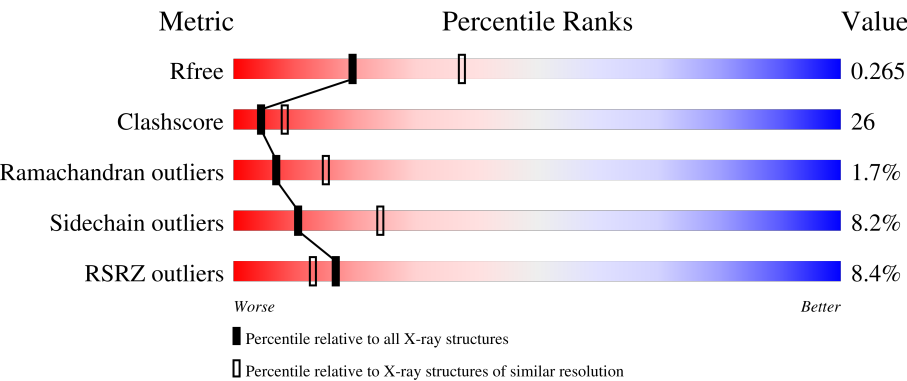
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	320	0% 35%19%42%
1	C	320	2% 31%21%44%
1	E	320	16% 19%31%48%
2	B	188	6% 49%41%5%
2	D	188	2% 63%24%6%5%

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Mol	Chain	Length	Quality of chain
2	F	188	6% 55% 35% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8792 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 Exocyst complex component SEC3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	Se	0	0	0
			1522	969	268	282	2	1			
1	C	180	Total	C	N	O	S	Se	0	0	0
			1485	944	262	276	2	1			
1	E	166	Total	C	N	O	S	Se	0	0	0
			1377	882	238	254	2	1			

- Molecule 2 is a protein called GTP-binding protein RHO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1385	871	235	272	7			
2	D	178	Total	C	N	O	S	0	0	0
			1385	871	235	272	7			
2	F	181	Total	C	N	O	S	0	0	0
			1406	883	240	276	7			

There are 3 discrepancies between the modelled and reference sequences:

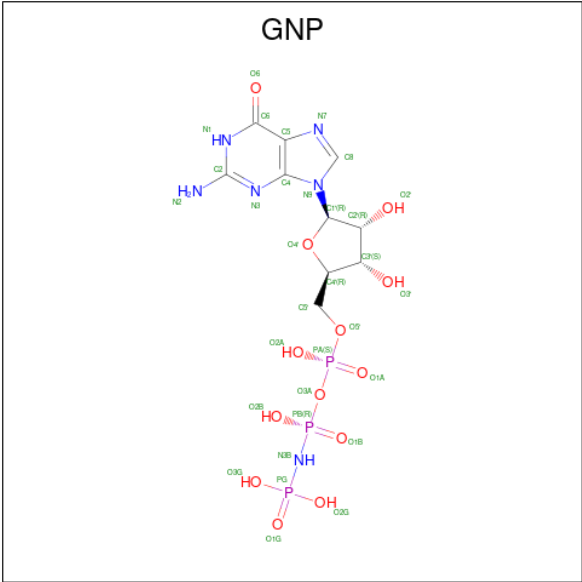
Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ASN	PHE	engineered mutation	UNP P06780
D	30	ASN	PHE	engineered mutation	UNP P06780
F	30	ASN	PHE	engineered mutation	UNP P06780

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

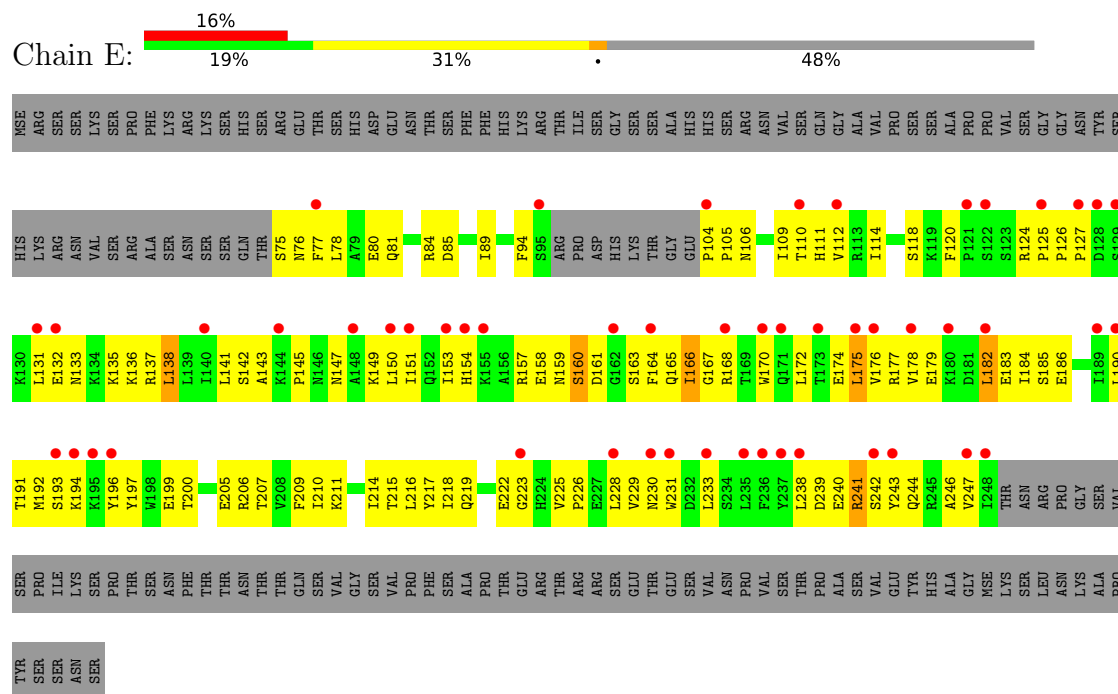
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	7	Total	O	0	0
			7	7		
6	C	24	Total	O	0	0
			24	24		

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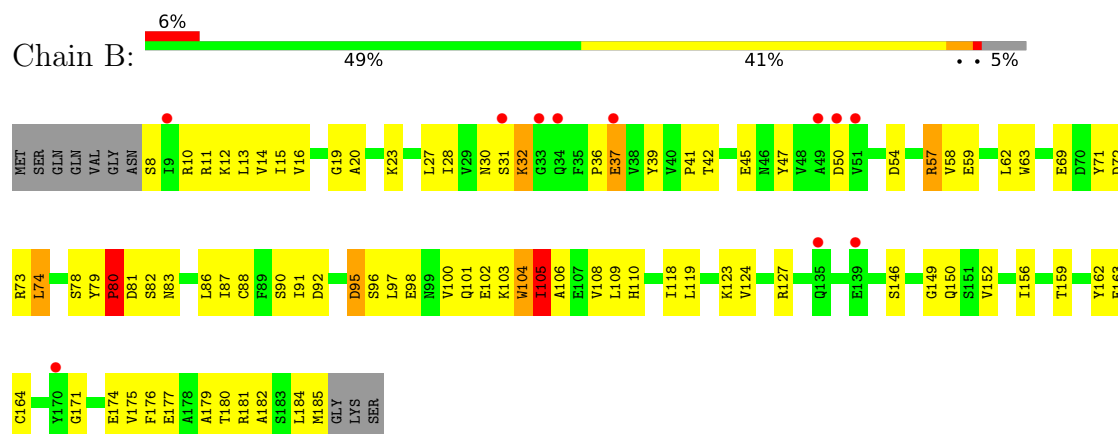
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	25	Total 25	O 25	0	0
6	E	6	Total 6	O 6	0	0
6	F	7	Total 7	O 7	0	0

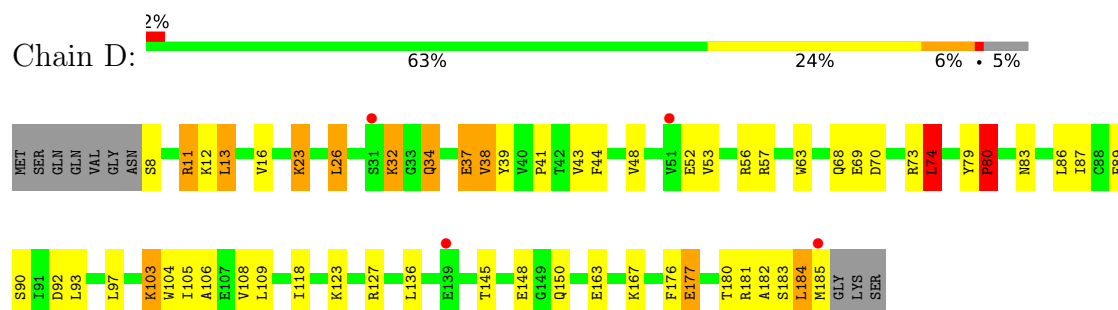
- Molecule 1: Exocyst complex component SEC3



- Molecule 2: GTP-binding protein RHO1

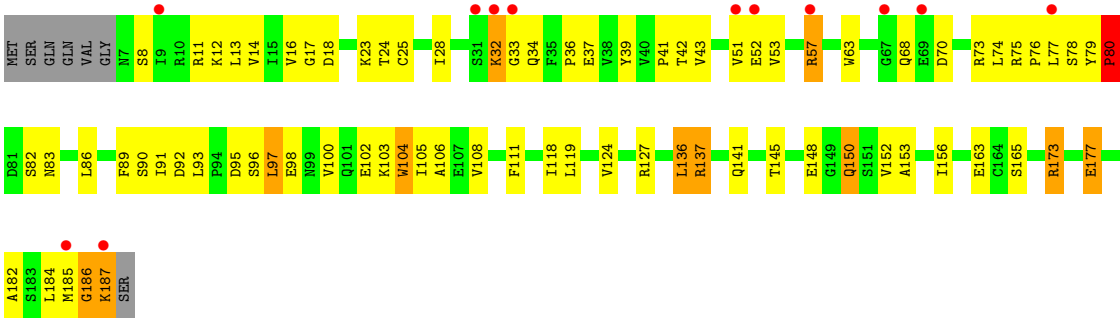


- Molecule 2: GTP-binding protein RHO1



- Molecule 2: GTP-binding protein RHO1





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.00Å 116.05Å 247.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.85 – 2.60 47.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.85-2.60) 99.7 (47.85-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.265 0.234 , 0.265	Depositor DCC
R_{free} test set	2663 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, GNP

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	0.52	0/1556	1.00	6/2101 (0.3%)
1	C	0.48	0/1518	0.93	4/2049 (0.2%)
1	E	0.37	0/1406	0.87	2/1895 (0.1%)
2	B	0.42	0/1409	0.96	4/1915 (0.2%)
2	D	0.54	0/1409	0.97	7/1915 (0.4%)
2	F	0.42	0/1430	0.93	3/1942 (0.2%)
All	All	0.46	0/8728	0.94	26/11817 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	43	VAL	N-CA-C	-9.96	102.21	111.67
1	A	193	SER	N-CA-C	-7.75	102.91	111.36
1	A	254	SER	N-CA-C	7.45	120.46	111.82
2	B	105	ILE	CB-CA-C	-6.96	103.07	111.97
2	B	104	TRP	N-CA-C	6.45	117.97	111.07
1	C	96	ARG	CA-C-N	6.34	127.77	119.84
1	C	96	ARG	C-N-CA	6.34	127.77	119.84
2	F	104	TRP	N-CA-C	5.97	117.46	111.07
1	E	246	ALA	N-CA-C	5.85	117.73	111.36
2	D	79	TYR	N-CA-C	5.63	121.15	113.16
2	D	177	GLU	N-CA-C	-5.55	105.15	111.14
2	F	177	GLU	N-CA-C	-5.54	105.32	111.36
1	C	91	ASN	N-CA-C	5.53	118.06	111.71
1	C	232	ASP	N-CA-C	-5.48	100.18	108.67
2	B	74	LEU	N-CA-C	5.37	119.54	112.89
2	D	80	PRO	N-CA-C	5.34	123.47	112.47
2	D	104	TRP	N-CA-C	5.32	116.77	111.07
1	A	246	ALA	N-CA-C	5.32	119.48	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	SER	N-CA-C	-5.31	105.58	111.36
2	D	74	LEU	N-CA-C	5.22	119.36	112.89
1	A	120	PHE	CA-C-N	5.19	124.81	119.56
1	A	120	PHE	C-N-CA	5.19	124.81	119.56
1	A	109	ILE	N-CA-C	-5.10	107.59	111.62
2	D	89	PHE	N-CA-C	-5.09	101.33	109.07
2	B	177	GLU	N-CA-C	-5.08	105.82	111.36
2	D	23	LYS	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1522	0	1533	58	0
1	C	1485	0	1488	71	0
1	E	1377	0	1387	117	0
2	B	1385	0	1361	83	0
2	D	1385	0	1360	52	0
2	F	1406	0	1383	89	0
3	A	15	0	0	1	0
3	C	15	0	0	1	0
3	E	5	0	0	0	0
4	B	32	0	13	2	0
4	D	32	0	13	1	0
4	F	32	0	13	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	29	0	0	0	0
6	B	7	0	0	0	0
6	C	24	0	0	0	0
6	D	25	0	0	4	0
6	E	6	0	0	0	0
6	F	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8792	0	8551	451	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 26.

All (451) 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:34:GLN:HE21	2:D:34:GLN:HA	1.16	1.10
1:C:102:GLY:HA3	2:F:11:ARG:HH22	1.15	1.06
1:E:147:ASN:HD22	1:E:150:LEU:HG	1.16	1.03
1:E:112:VAL:HG11	1:E:209:PHE:HB2	1.41	1.02
2:B:97:LEU:HD11	2:B:152:VAL:HG21	1.40	1.00
1:E:75:SER:HB2	1:E:78:LEU:HD13	1.45	0.97
2:F:12:LYS:H	2:F:83:ASN:HD22	0.99	0.97
1:E:190:LEU:HB3	1:E:192:MSE:HE1	1.48	0.94
2:D:182:ALA:HA	2:D:185:MET:HE3	1.50	0.94
1:A:159:ASN:HD21	1:A:163:SER:HB3	1.31	0.94
1:A:146:ASN:H	1:A:146:ASN:HD22	0.96	0.94
1:E:120:PHE:HB2	1:E:125:PRO:HG3	1.47	0.94
1:A:151:ILE:HD11	1:A:172:LEU:HG	1.49	0.93
2:D:12:LYS:H	2:D:83:ASN:HD22	1.18	0.91
1:C:98:ASP:HB2	1:C:103:GLU:H	1.34	0.91
2:F:12:LYS:H	2:F:83:ASN:ND2	1.68	0.91
2:B:12:LYS:H	2:B:83:ASN:HD22	1.18	0.90
1:E:240:GLU:O	1:E:244:GLN:HG2	1.72	0.89
2:D:37:GLU:CD	2:D:37:GLU:H	1.82	0.88
1:C:98:ASP:HB3	1:C:102:GLY:H	1.40	0.87
1:E:135:LYS:HB3	1:E:137:ARG:HH12	1.41	0.86
2:F:137:ARG:HH11	2:F:137:ARG:HB3	1.42	0.85
2:B:124:VAL:HG23	2:B:164:CYS:O	1.76	0.85
1:E:135:LYS:HB3	1:E:137:ARG:NH1	1.92	0.83
2:D:34:GLN:HA	2:D:34:GLN:NE2	1.93	0.82
1:A:146:ASN:H	1:A:146:ASN:ND2	1.67	0.82
1:C:98:ASP:HB3	1:C:102:GLY:N	1.94	0.82
1:A:147:ASN:HD22	1:A:150:LEU:HG	1.45	0.82
2:F:12:LYS:N	2:F:83:ASN:HD22	1.78	0.81
1:E:147:ASN:ND2	1:E:150:LEU:HG	1.95	0.81
1:E:182:LEU:H	1:E:182:LEU:HD23	1.44	0.80
1:C:118:SER:HB3	1:C:135:LYS:HE3	1.63	0.80
1:C:216:LEU:O	1:C:220:THR:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:HA3	2:F:11:ARG:NH2	1.96	0.79
1:E:151:ILE:HG22	1:E:172:LEU:HB2	1.63	0.79
1:C:186:GLU:HG2	2:D:73:ARG:NH2	1.97	0.79
1:C:241:ARG:O	1:C:245:ARG:HG3	1.81	0.79
2:F:57:ARG:HH11	2:F:57:ARG:HB3	1.45	0.78
2:F:32:LYS:HG3	2:F:33:GLY:H	1.48	0.78
2:B:101:GLN:O	2:B:105:ILE:HD11	1.83	0.77
1:E:151:ILE:HG12	1:E:216:LEU:HD11	1.65	0.76
2:D:12:LYS:H	2:D:83:ASN:ND2	1.82	0.76
1:C:100:LYS:HD3	2:F:187:LYS:HZ2	1.49	0.76
1:C:214:ILE:HD11	1:C:236:PHE:HB3	1.66	0.75
1:E:154:HIS:HB3	1:E:166:ILE:HD13	1.66	0.74
1:A:240:GLU:O	1:A:244:GLN:HG2	1.86	0.74
1:E:240:GLU:HB2	1:E:241:ARG:HE	1.52	0.74
2:F:37:GLU:CD	2:F:37:GLU:H	1.96	0.74
2:F:97:LEU:HD21	2:F:152:VAL:HG21	1.70	0.72
1:E:184:ILE:HD12	1:E:197:TYR:OH	1.89	0.72
2:D:127:ARG:HH22	2:D:163:GLU:CD	1.99	0.71
2:B:127:ARG:HH22	2:B:163:GLU:CD	1.98	0.71
1:E:124:ARG:NH1	1:E:183:GLU:HB3	2.06	0.71
1:E:118:SER:HB2	1:E:135:LYS:HE3	1.74	0.70
2:B:12:LYS:H	2:B:83:ASN:ND2	1.91	0.69
2:B:91:ILE:CD1	2:B:124:VAL:HA	2.23	0.69
1:A:105:PRO:O	1:A:145:PRO:HG3	1.93	0.68
1:E:178:VAL:HG12	1:E:231:TRP:HE1	1.57	0.68
1:A:151:ILE:HG13	1:A:172:LEU:HB2	1.74	0.68
2:D:145:THR:OG1	2:D:148:GLU:HG3	1.93	0.68
1:E:75:SER:HB2	1:E:78:LEU:CD1	2.21	0.68
1:E:217:TYR:CD2	1:E:226:PRO:HD3	2.29	0.68
1:E:110:THR:HG22	1:E:111:HIS:N	2.08	0.68
1:E:168:ARG:HH12	1:E:194:LYS:NZ	1.91	0.68
2:F:78:SER:C	2:F:80:PRO:HD2	2.20	0.67
2:D:12:LYS:N	2:D:83:ASN:HD22	1.90	0.67
1:C:194:LYS:HB2	1:C:194:LYS:NZ	2.09	0.67
2:B:101:GLN:C	2:B:105:ILE:HD11	2.20	0.67
2:B:180:THR:O	2:B:184:LEU:HD13	1.95	0.67
1:C:168:ARG:HD2	1:C:169:THR:H	1.59	0.67
1:E:77:PHE:HE2	2:F:41:PRO:HG2	1.59	0.67
2:B:91:ILE:HD13	2:B:124:VAL:HA	1.76	0.66
2:B:105:ILE:HD12	2:B:106:ALA:H	1.59	0.66
1:A:86:ARG:O	1:A:90:ILE:HG22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLU:CD	2:B:37:GLU:H	2.02	0.66
2:F:76:PRO:HB3	2:F:111:PHE:HE1	1.60	0.66
1:A:184:ILE:HG22	1:A:186:GLU:H	1.61	0.65
2:D:182:ALA:O	2:D:185:MET:HG2	1.95	0.65
1:E:179:GLU:HG3	1:E:229:VAL:HB	1.78	0.65
1:E:109:ILE:HG12	1:E:142:SER:HA	1.77	0.65
2:F:137:ARG:HB3	2:F:137:ARG:NH1	2.12	0.65
1:A:184:ILE:N	1:A:184:ILE:HD12	2.10	0.65
2:B:10:ARG:HG2	2:B:59:GLU:HB3	1.76	0.65
2:F:12:LYS:HE3	2:F:63:TRP:CE2	2.32	0.65
1:E:182:LEU:HD23	1:E:182:LEU:N	2.12	0.65
2:F:76:PRO:HB3	2:F:111:PHE:CE1	2.32	0.65
1:A:247:VAL:HB	1:A:249:THR:HG22	1.79	0.64
1:E:243:TYR:O	1:E:247:VAL:HG13	1.97	0.64
2:B:87:ILE:HD11	2:B:108:VAL:HG21	1.80	0.64
1:C:101:THR:HG22	1:C:103:GLU:OE2	1.97	0.64
1:A:101:THR:HB	1:A:103:GLU:OE2	1.98	0.63
1:A:147:ASN:ND2	1:A:150:LEU:HG	2.10	0.63
1:A:146:ASN:ND2	1:A:146:ASN:N	2.43	0.63
1:A:241:ARG:HD2	1:A:245:ARG:CZ	2.28	0.63
2:B:100:VAL:O	2:B:105:ILE:HG13	1.98	0.63
1:C:225:VAL:HG11	1:C:228:LEU:HD21	1.81	0.63
2:F:124:VAL:HG12	2:F:165:SER:HB2	1.80	0.63
2:D:8:SER:HB2	2:D:57:ARG:O	1.99	0.63
1:E:217:TYR:CE2	1:E:226:PRO:HD3	2.33	0.63
1:A:146:ASN:HD22	1:A:146:ASN:N	1.81	0.63
1:E:78:LEU:HD12	1:E:78:LEU:H	1.64	0.63
2:B:105:ILE:CG2	2:B:156:ILE:HB	2.29	0.62
2:B:12:LYS:N	2:B:83:ASN:HD22	1.94	0.62
1:C:175:LEU:HD13	1:C:226:PRO:HG2	1.81	0.62
1:C:214:ILE:C	1:C:214:ILE:HD12	2.25	0.62
1:E:137:ARG:HG2	1:E:137:ARG:HH11	1.65	0.62
1:E:106:ASN:ND2	1:E:145:PRO:HD3	2.14	0.62
1:C:105:PRO:O	1:C:145:PRO:HG3	1.99	0.62
2:F:73:ARG:HH11	2:F:74:LEU:HD11	1.64	0.62
2:F:86:LEU:HD22	2:F:118:ILE:HB	1.82	0.62
2:F:182:ALA:HA	2:F:185:MET:SD	2.40	0.62
1:E:76:ASN:O	1:E:80:GLU:HG2	1.99	0.61
1:E:200:THR:HG21	1:E:206:ARG:HB2	1.82	0.61
2:B:13:LEU:C	2:B:13:LEU:HD23	2.25	0.61
2:B:90:SER:OG	2:B:92:ASP:OD1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:ILE:HD13	2:F:156:ILE:HB	1.82	0.61
1:A:118:SER:HB3	1:A:135:LYS:HE2	1.83	0.61
1:C:214:ILE:HG12	1:C:236:PHE:CD1	2.35	0.61
1:E:175:LEU:HD21	1:E:178:VAL:HG23	1.82	0.61
1:E:177:ARG:HE	1:E:229:VAL:HG21	1.66	0.60
1:C:200:THR:CG2	1:C:202:SER:O	2.50	0.60
1:E:233:LEU:HB3	1:E:238:LEU:HD12	1.84	0.60
1:C:202:SER:HB2	2:D:70:ASP:HB3	1.83	0.59
2:F:127:ARG:HH22	2:F:163:GLU:CD	2.10	0.59
1:A:200:THR:HG23	1:A:205:GLU:HB2	1.85	0.59
1:E:174:GLU:O	1:E:176:VAL:HG23	2.01	0.59
1:C:211:LYS:HD2	1:C:235:LEU:HD22	1.84	0.59
2:F:18:ASP:OD1	2:F:96:SER:HA	2.02	0.59
1:E:241:ARG:CD	1:E:241:ARG:H	2.15	0.59
2:F:73:ARG:HG3	2:F:74:LEU:HD22	1.83	0.59
1:C:100:LYS:HD3	2:F:187:LYS:NZ	2.18	0.58
1:C:98:ASP:CB	1:C:103:GLU:H	2.12	0.58
2:B:182:ALA:O	2:B:185:MET:HG2	2.04	0.58
2:D:68:GLN:HG3	6:D:195:HOH:O	2.04	0.58
1:E:110:THR:HG22	1:E:111:HIS:H	1.68	0.58
2:B:152:VAL:O	2:B:156:ILE:HG23	2.04	0.58
2:B:127:ARG:NH2	2:B:163:GLU:OE2	2.38	0.57
2:B:12:LYS:HE3	2:B:63:TRP:CE2	2.40	0.57
1:E:191:THR:C	1:E:192:MSE:HE3	2.30	0.57
1:A:120:PHE:HB2	1:A:125:PRO:HB3	1.86	0.56
1:C:201:ASN:O	2:D:73:ARG:NH2	2.38	0.56
2:D:34:GLN:HE21	2:D:34:GLN:CA	1.98	0.56
2:F:97:LEU:CD1	2:F:152:VAL:HG11	2.35	0.56
2:B:16:VAL:C	2:B:23:LYS:HD3	2.30	0.56
2:B:58:VAL:HG21	2:B:180:THR:HG23	1.87	0.56
1:E:154:HIS:HB3	1:E:166:ILE:CD1	2.36	0.56
1:E:78:LEU:HD12	1:E:78:LEU:N	2.21	0.56
2:B:57:ARG:HG3	2:B:57:ARG:HH11	1.70	0.56
2:F:145:THR:HG23	2:F:148:GLU:H	1.71	0.56
2:B:30:ASN:ND2	2:B:176:PHE:CD1	2.74	0.56
2:B:31:SER:O	2:B:32:LYS:HG2	2.06	0.56
1:E:120:PHE:CE1	1:E:126:PRO:HD2	2.41	0.56
2:F:91:ILE:HD12	2:F:124:VAL:HA	1.88	0.55
2:F:39:TYR:CZ	2:F:41:PRO:HG3	2.41	0.55
2:F:102:GLU:OE1	2:F:102:GLU:HA	2.06	0.55
1:A:151:ILE:CD1	1:A:172:LEU:HG	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TYR:O	1:A:247:VAL:HG22	2.06	0.55
1:E:147:ASN:HD22	1:E:150:LEU:CG	2.06	0.55
2:F:57:ARG:HB3	2:F:57:ARG:NH1	2.17	0.55
1:A:200:THR:CG2	1:A:202:SER:O	2.55	0.55
2:B:78:SER:C	2:B:80:PRO:HD2	2.31	0.55
1:E:118:SER:CB	1:E:135:LYS:HE3	2.36	0.55
2:D:11:ARG:HA	2:D:83:ASN:ND2	2.21	0.54
1:E:124:ARG:NH1	1:E:183:GLU:CB	2.69	0.54
1:C:147:ASN:HB3	1:C:150:LEU:HG	1.88	0.54
1:E:78:LEU:HD21	2:F:70:ASP:OD2	2.08	0.54
1:A:200:THR:CG2	1:A:205:GLU:HB2	2.37	0.54
2:B:58:VAL:HG21	2:B:180:THR:CG2	2.37	0.54
2:F:13:LEU:C	2:F:13:LEU:HD23	2.32	0.54
2:F:86:LEU:CD2	2:F:118:ILE:HB	2.37	0.54
2:B:105:ILE:O	2:B:109:LEU:HG	2.07	0.54
1:E:131:LEU:HG	2:F:77:LEU:HB3	1.89	0.54
1:E:160:SER:O	1:E:161:ASP:CG	2.51	0.54
2:F:186:GLY:O	2:F:187:LYS:HB3	2.09	0.54
2:B:98:GLU:HB3	2:B:102:GLU:OE1	2.09	0.53
1:C:77:PHE:CZ	2:D:68:GLN:HG2	2.43	0.53
2:D:52:GLU:HA	2:D:52:GLU:OE1	2.07	0.53
2:F:79:TYR:N	2:F:80:PRO:HD2	2.24	0.53
1:E:166:ILE:HD12	1:E:167:GLY:N	2.23	0.53
1:A:77:PHE:CD2	2:B:41:PRO:HG2	2.44	0.53
1:A:76:ASN:O	1:A:80:GLU:HG2	2.09	0.53
2:B:73:ARG:HG2	2:B:74:LEU:HD22	1.91	0.53
1:A:171:GLN:O	1:A:174:GLU:HG3	2.09	0.53
1:E:120:PHE:CZ	1:E:126:PRO:HD2	2.44	0.53
1:A:151:ILE:C	1:A:151:ILE:HD12	2.33	0.53
2:B:171:GLY:O	2:B:175:VAL:HG23	2.08	0.53
2:F:73:ARG:NH1	2:F:74:LEU:HD11	2.24	0.53
2:B:8:SER:HB2	2:B:57:ARG:O	2.08	0.53
1:C:194:LYS:HB2	1:C:194:LYS:HZ2	1.74	0.53
2:F:14:VAL:CG2	2:F:82:SER:HB3	2.39	0.52
2:D:13:LEU:C	2:D:13:LEU:HD23	2.34	0.52
2:D:37:GLU:CD	2:D:37:GLU:N	2.61	0.52
1:C:159:ASN:C	1:C:160:SER:O	2.52	0.52
2:F:16:VAL:HG22	2:F:17:GLY:H	1.75	0.52
2:B:45:GLU:HG2	2:B:47:TYR:CZ	2.44	0.52
1:E:207:THR:O	1:E:211:LYS:HG3	2.09	0.52
2:B:118:ILE:CD1	2:B:179:ALA:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:LEU:N	1:E:138:LEU:HD12	2.25	0.52
1:A:258:ILE:C	1:A:258:ILE:HD12	2.35	0.52
2:D:11:ARG:HG2	2:D:183:SER:OG	2.09	0.52
2:D:16:VAL:C	2:D:23:LYS:HD3	2.35	0.52
1:E:136:LYS:O	1:E:137:ARG:HD3	2.10	0.52
2:F:32:LYS:CG	2:F:33:GLY:H	2.21	0.52
1:A:151:ILE:HD12	1:A:152:GLN:N	2.26	0.51
1:E:110:THR:CG2	1:E:111:HIS:N	2.73	0.51
1:E:75:SER:CB	1:E:78:LEU:HD13	2.30	0.51
1:E:244:GLN:O	1:E:247:VAL:HG22	2.11	0.51
2:B:105:ILE:CD1	2:B:106:ALA:H	2.23	0.51
1:E:105:PRO:O	1:E:145:PRO:HG3	2.10	0.51
1:E:217:TYR:CD2	1:E:225:VAL:HA	2.45	0.51
1:A:101:THR:O	1:A:103:GLU:HG2	2.11	0.51
2:F:97:LEU:HD11	2:F:152:VAL:HG11	1.92	0.51
1:C:186:GLU:HG2	2:D:73:ARG:CZ	2.39	0.51
1:E:141:LEU:CD2	1:E:153:ILE:HG12	2.40	0.51
1:E:114:ILE:HD11	1:E:137:ARG:HB2	1.93	0.51
1:E:137:ARG:NH2	1:E:157:ARG:HH11	2.09	0.51
2:F:8:SER:HB2	2:F:57:ARG:O	2.12	0.50
2:D:11:ARG:HD3	2:D:184:LEU:HD13	1.93	0.50
1:E:225:VAL:HG22	1:E:228:LEU:HD11	1.94	0.50
2:F:145:THR:HG22	2:F:148:GLU:CD	2.36	0.50
1:C:99:HIS:O	1:C:100:LYS:HG3	2.11	0.50
2:F:24:THR:O	2:F:28:ILE:HG12	2.11	0.50
2:B:104:TRP:O	2:B:108:VAL:HG23	2.11	0.50
2:B:105:ILE:HG21	2:B:156:ILE:HB	1.92	0.50
1:C:158:GLU:HB2	1:C:164:PHE:CE2	2.47	0.50
2:F:79:TYR:N	2:F:80:PRO:CD	2.74	0.50
2:B:97:LEU:HD12	2:B:100:VAL:HG21	1.93	0.49
1:C:174:GLU:O	1:C:176:VAL:HG23	2.13	0.49
1:E:210:ILE:O	1:E:214:ILE:HG12	2.13	0.49
2:B:124:VAL:HG23	2:B:164:CYS:C	2.37	0.49
1:E:136:LYS:HB2	1:E:136:LYS:NZ	2.27	0.49
1:E:178:VAL:HG12	1:E:231:TRP:NE1	2.25	0.49
1:C:168:ARG:HD2	1:C:169:THR:N	2.27	0.49
2:D:37:GLU:HG2	2:D:38:VAL:HG12	1.93	0.49
2:D:167:LYS:HE2	6:D:202:HOH:O	2.13	0.49
2:F:68:GLN:HA	2:F:68:GLN:NE2	2.28	0.49
1:A:166:ILE:HG13	1:A:166:ILE:O	2.11	0.49
1:E:217:TYR:CE2	1:E:225:VAL:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ILE:HG12	2:B:23:LYS:HD2	1.95	0.48
1:E:185:SER:HB2	1:E:186:GLU:OE2	2.13	0.48
2:F:150:GLN:HE21	2:F:150:GLN:CA	2.26	0.48
2:B:101:GLN:HA	2:B:105:ILE:CG1	2.43	0.48
2:D:105:ILE:HG23	2:D:106:ALA:N	2.28	0.48
2:F:90:SER:OG	2:F:92:ASP:OD1	2.30	0.48
1:C:228:LEU:HD22	1:C:243:TYR:CE1	2.47	0.48
2:D:43:VAL:HG12	2:D:44:PHE:HD1	1.78	0.48
1:E:77:PHE:HE2	2:F:41:PRO:CG	2.26	0.48
1:E:133:ASN:HD22	1:E:133:ASN:N	2.11	0.48
1:A:159:ASN:HD21	1:A:163:SER:CB	2.16	0.48
1:E:112:VAL:HG11	1:E:209:PHE:CB	2.28	0.48
2:F:16:VAL:HG22	2:F:17:GLY:N	2.28	0.48
1:A:200:THR:HG21	1:A:206:ARG:N	2.29	0.48
2:F:11:ARG:HD2	2:F:184:LEU:HD23	1.94	0.48
1:A:180:LYS:HB2	1:A:231:TRP:CE2	2.49	0.48
2:D:39:TYR:CZ	2:D:41:PRO:HG3	2.49	0.48
1:C:160:SER:C	1:C:162:GLY:H	2.21	0.47
1:E:184:ILE:HD13	1:E:199:GLU:OE1	2.14	0.47
2:F:89:PHE:CG	2:F:97:LEU:HD23	2.49	0.47
1:A:209:PHE:O	1:A:212:SER:HB2	2.15	0.47
1:E:110:THR:CG2	1:E:111:HIS:H	2.26	0.47
1:E:200:THR:CG2	1:E:206:ARG:HB2	2.44	0.47
2:F:96:SER:O	2:F:100:VAL:HG23	2.14	0.47
1:C:151:ILE:N	1:C:151:ILE:HD12	2.30	0.47
1:C:247:VAL:C	1:C:249:THR:H	2.23	0.47
2:D:69:GLU:N	6:D:195:HOH:O	2.48	0.47
1:E:137:ARG:NH2	1:E:157:ARG:NH1	2.62	0.47
1:A:158:GLU:HB2	1:A:164:PHE:CE2	2.50	0.47
1:E:114:ILE:HD12	1:E:114:ILE:O	2.15	0.47
2:F:13:LEU:HD23	2:F:14:VAL:N	2.30	0.47
2:B:118:ILE:HD11	2:B:179:ALA:HA	1.97	0.47
1:C:194:LYS:HB2	1:C:194:LYS:HZ3	1.80	0.47
2:D:145:THR:HG23	2:D:148:GLU:OE2	2.15	0.47
2:D:180:THR:O	2:D:184:LEU:HD22	2.15	0.47
2:F:14:VAL:HG23	2:F:82:SER:HB3	1.96	0.47
2:B:95:ASP:OD2	2:B:95:ASP:N	2.48	0.46
1:E:120:PHE:CD1	1:E:125:PRO:HB3	2.50	0.46
1:C:86:ARG:HG3	1:C:108:TYR:CE2	2.50	0.46
1:C:200:THR:HG21	1:C:206:ARG:N	2.31	0.46
2:B:105:ILE:HG23	2:B:156:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:LYS:NZ	1:C:194:LYS:CB	2.77	0.46
2:F:105:ILE:HG23	2:F:106:ALA:N	2.31	0.46
1:A:241:ARG:HD2	1:A:245:ARG:NH2	2.31	0.46
2:B:79:TYR:N	2:B:80:PRO:HD2	2.31	0.46
1:E:85:ASP:O	1:E:89:ILE:HG13	2.15	0.46
1:E:147:ASN:HD21	1:E:149:LYS:HB2	1.80	0.46
2:B:91:ILE:HD11	2:B:124:VAL:HA	1.96	0.46
2:F:95:ASP:O	2:F:98:GLU:HB2	2.16	0.46
2:B:12:LYS:HE3	2:B:63:TRP:CD2	2.51	0.46
1:C:200:THR:HG21	1:C:202:SER:O	2.15	0.46
1:E:175:LEU:HG	1:E:192:MSE:HE2	1.98	0.46
1:E:178:VAL:HG22	1:E:190:LEU:CD2	2.46	0.46
1:E:182:LEU:H	1:E:182:LEU:CD2	2.21	0.46
1:A:142:SER:OG	1:A:154:HIS:NE2	2.45	0.45
2:B:12:LYS:HD3	2:B:81:ASP:O	2.16	0.45
1:C:110:THR:HG22	1:C:141:LEU:HD12	1.97	0.45
1:C:146:ASN:H	1:C:146:ASN:ND2	2.12	0.45
2:D:127:ARG:NH2	2:D:163:GLU:OE2	2.48	0.45
1:A:81:GLN:OE1	1:A:84:ARG:NH1	2.50	0.45
2:B:14:VAL:HG21	2:B:82:SER:OG	2.17	0.45
2:B:19:GLY:O	2:B:20:ALA:HB3	2.16	0.45
2:D:74:LEU:HD22	2:D:74:LEU:H	1.82	0.45
2:D:177:GLU:O	2:D:181:ARG:HG3	2.17	0.45
1:E:81:GLN:HE22	1:E:84:ARG:HD3	1.81	0.45
1:A:183:GLU:HB2	1:A:184:ILE:HD12	1.98	0.45
1:C:86:ARG:HG3	1:C:108:TYR:CZ	2.52	0.45
1:E:218:ILE:HG23	1:E:223:GLY:HA2	1.99	0.45
2:F:186:GLY:O	2:F:187:LYS:CB	2.64	0.45
1:E:137:ARG:NH1	1:E:137:ARG:HG2	2.31	0.45
1:E:225:VAL:CG2	1:E:228:LEU:HD11	2.47	0.45
1:E:239:ASP:OD2	1:E:241:ARG:HG2	2.16	0.45
2:F:152:VAL:O	2:F:156:ILE:HG12	2.17	0.45
1:A:106:ASN:ND2	1:A:145:PRO:HD3	2.32	0.45
2:D:53:VAL:HG21	2:D:180:THR:HG22	1.99	0.45
2:F:119:LEU:HD23	2:F:153:ALA:HB2	1.99	0.45
1:A:98:ASP:OD2	1:A:100:LYS:HB2	2.17	0.45
1:E:229:VAL:HG12	1:E:230:ASN:ND2	2.32	0.45
2:B:87:ILE:HG21	2:B:100:VAL:HG13	1.99	0.44
2:F:12:LYS:HE3	2:F:63:TRP:CD2	2.52	0.44
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.82	0.44
1:C:224:HIS:CE1	1:C:251:ARG:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:GLN:HB2	6:D:194:HOH:O	2.16	0.44
1:A:239:ASP:C	1:A:239:ASP:OD1	2.61	0.44
2:F:11:ARG:HH11	2:F:11:ARG:HG2	1.83	0.44
2:B:96:SER:O	2:B:100:VAL:HG23	2.18	0.44
1:E:120:PHE:CZ	1:E:126:PRO:CD	3.00	0.44
1:E:190:LEU:CB	1:E:192:MSE:HE1	2.34	0.44
2:F:39:TYR:CE2	2:F:41:PRO:HG3	2.52	0.44
2:B:79:TYR:N	2:B:80:PRO:CD	2.80	0.44
2:B:39:TYR:CZ	2:B:41:PRO:HG3	2.53	0.44
2:D:11:ARG:HA	2:D:83:ASN:HD22	1.83	0.44
1:E:111:HIS:O	1:E:112:VAL:HG13	2.17	0.44
1:E:168:ARG:HH12	1:E:194:LYS:CE	2.30	0.44
2:F:104:TRP:O	2:F:108:VAL:HG23	2.17	0.44
1:C:192:MSE:HG2	1:C:196:TYR:HE1	1.82	0.44
1:C:202:SER:OG	1:C:205:GLU:HG3	2.18	0.44
1:A:124:ARG:HE	1:A:184:ILE:CD1	2.29	0.44
2:B:42:THR:HB	4:B:301:GNP:O2G	2.18	0.44
2:B:174:GLU:CD	2:B:174:GLU:H	2.25	0.44
1:C:75:SER:C	1:C:77:PHE:H	2.25	0.44
1:C:77:PHE:CD2	2:D:41:PRO:HG2	2.53	0.44
2:F:111:PHE:N	2:F:111:PHE:CD2	2.86	0.44
1:A:101:THR:C	1:A:103:GLU:H	2.26	0.43
2:B:91:ILE:CD1	2:B:127:ARG:HB2	2.48	0.43
1:C:224:HIS:ND1	1:C:251:ARG:HD3	2.33	0.43
1:E:238:LEU:HB2	1:E:242:SER:HB2	1.99	0.43
1:A:101:THR:O	1:A:103:GLU:N	2.51	0.43
2:B:13:LEU:HD23	2:B:14:VAL:N	2.33	0.43
2:B:123:LYS:HG2	4:B:301:GNP:C6	2.47	0.43
2:B:86:LEU:HD22	2:B:118:ILE:HB	2.00	0.43
2:B:91:ILE:HD12	2:B:127:ARG:HB2	1.99	0.43
2:D:90:SER:OG	2:D:92:ASP:OD1	2.35	0.43
1:E:151:ILE:HG21	1:E:172:LEU:HD22	2.00	0.43
1:A:157:ARG:HH21	3:A:323:PO4:P	2.42	0.43
1:A:159:ASN:ND2	1:A:163:SER:HB3	2.15	0.43
1:E:178:VAL:HG22	1:E:190:LEU:HD22	2.01	0.43
1:C:100:LYS:HE2	2:F:187:LYS:HB2	2.01	0.43
1:C:174:GLU:O	1:C:192:MSE:HA	2.18	0.43
1:E:157:ARG:O	1:E:165:GLN:HG2	2.18	0.43
1:E:157:ARG:HD3	1:E:165:GLN:CD	2.43	0.43
2:F:136:LEU:HD12	2:F:136:LEU:HA	1.86	0.43
1:A:200:THR:HG21	1:A:202:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HA	2:B:100:VAL:HG23	2.00	0.43
1:C:98:ASP:C	1:C:100:LYS:H	2.27	0.43
1:E:114:ILE:CD1	1:E:137:ARG:HB2	2.47	0.43
2:F:73:ARG:HE	2:F:74:LEU:HD21	1.83	0.43
2:F:136:LEU:HB3	2:F:141:GLN:O	2.19	0.43
1:C:228:LEU:HD22	1:C:243:TYR:HE1	1.84	0.43
2:F:25:CYS:SG	2:F:36:PRO:HD2	2.59	0.43
2:B:28:ILE:CD1	2:B:36:PRO:HG2	2.49	0.42
2:F:74:LEU:HD22	2:F:74:LEU:H	1.84	0.42
2:F:150:GLN:CA	2:F:150:GLN:NE2	2.81	0.42
1:A:141:LEU:CD2	1:A:153:ILE:HG12	2.49	0.42
2:B:50:ASP:OD1	2:B:59:GLU:HA	2.20	0.42
1:E:78:LEU:CD1	1:E:78:LEU:H	2.30	0.42
1:C:202:SER:CB	2:D:70:ASP:HB3	2.49	0.42
2:D:48:VAL:HG23	2:D:48:VAL:O	2.19	0.42
2:F:16:VAL:HG22	2:F:104:TRP:CZ3	2.54	0.42
1:C:184:ILE:HG22	1:C:186:GLU:OE1	2.20	0.42
2:D:43:VAL:HG12	2:D:44:PHE:CD1	2.55	0.42
1:E:78:LEU:HD11	2:F:70:ASP:OD2	2.19	0.42
2:F:75:ARG:HB3	2:F:76:PRO:HD3	2.01	0.42
2:F:119:LEU:CD2	2:F:152:VAL:HG23	2.50	0.42
1:A:202:SER:OG	1:A:205:GLU:HG3	2.19	0.42
2:D:74:LEU:HD13	2:D:74:LEU:N	2.34	0.42
2:B:119:LEU:CD2	2:B:152:VAL:HG23	2.50	0.42
1:C:123:SER:O	1:C:124:ARG:C	2.63	0.42
1:E:106:ASN:HB3	1:E:143:ALA:O	2.20	0.42
2:F:16:VAL:CG2	2:F:104:TRP:CZ3	3.03	0.42
1:E:158:GLU:HB2	1:E:164:PHE:CE2	2.55	0.42
2:B:174:GLU:CD	2:B:174:GLU:N	2.78	0.42
1:C:159:ASN:O	1:C:160:SER:O	2.38	0.42
2:D:87:ILE:HD11	2:D:108:VAL:HG21	2.02	0.42
1:E:114:ILE:HD12	1:E:114:ILE:C	2.45	0.42
1:A:244:GLN:OE1	1:A:244:GLN:HA	2.20	0.41
2:B:10:ARG:HD3	2:B:59:GLU:OE1	2.20	0.41
1:C:97:PRO:HA	1:C:103:GLU:O	2.19	0.41
1:C:131:LEU:O	1:C:134:LYS:HG2	2.20	0.41
1:E:215:THR:O	1:E:219:GLN:HG2	2.20	0.41
1:E:243:TYR:CE1	1:E:247:VAL:HG12	2.54	0.41
1:A:201:ASN:HB3	2:B:71:TYR:CE1	2.55	0.41
1:C:160:SER:O	1:C:162:GLY:N	2.52	0.41
1:E:194:LYS:HE3	1:E:196:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:GLY:C	2:F:34:GLN:HG3	2.44	0.41
2:F:127:ARG:NH2	2:F:163:GLU:OE2	2.53	0.41
1:C:160:SER:C	1:C:162:GLY:N	2.78	0.41
1:E:126:PRO:HA	1:E:127:PRO:HD3	1.93	0.41
2:F:53:VAL:O	2:F:53:VAL:HG23	2.21	0.41
2:B:11:ARG:HA	2:B:83:ASN:ND2	2.36	0.41
2:B:110:HIS:ND1	2:B:110:HIS:C	2.79	0.41
1:E:133:ASN:N	1:E:133:ASN:ND2	2.67	0.41
1:E:229:VAL:O	1:E:230:ASN:HB2	2.21	0.41
2:F:51:VAL:HG12	2:F:52:GLU:N	2.35	0.41
1:C:99:HIS:O	1:C:100:LYS:CG	2.68	0.41
2:D:26:LEU:HD22	2:D:176:PHE:HE1	1.86	0.41
1:E:161:ASP:OD1	1:E:163:SER:HB2	2.21	0.41
1:E:168:ARG:HH12	1:E:194:LYS:HZ3	1.68	0.41
2:B:54:ASP:OD1	2:B:181:ARG:NH1	2.54	0.41
2:B:69:GLU:O	2:B:72:ASP:OD2	2.39	0.41
2:D:26:LEU:HD22	2:D:176:PHE:CE1	2.56	0.41
1:E:170:TRP:CD1	1:E:192:MSE:HG2	2.55	0.41
1:A:108:TYR:CZ	1:A:110:THR:HA	2.56	0.41
2:B:13:LEU:C	2:B:13:LEU:CD2	2.94	0.41
1:C:168:ARG:HH12	3:C:321:PO4:P	2.44	0.41
2:F:16:VAL:C	2:F:23:LYS:HD3	2.46	0.41
2:B:149:GLY:O	2:B:152:VAL:HG22	2.21	0.41
1:C:87:LYS:O	1:C:91:ASN:HB2	2.21	0.41
1:C:237:TYR:O	1:C:238:LEU:HD12	2.20	0.41
2:D:123:LYS:HG2	4:D:301:GNP:C6	2.51	0.41
1:E:177:ARG:NH2	1:E:179:GLU:OE2	2.54	0.41
2:F:73:ARG:HE	2:F:74:LEU:CD2	2.33	0.41
2:B:15:ILE:HD11	2:B:88:CYS:SG	2.61	0.41
2:B:95:ASP:O	2:B:98:GLU:HB2	2.21	0.41
1:C:200:THR:HG23	1:C:205:GLU:HB2	2.03	0.41
2:D:86:LEU:HD22	2:D:118:ILE:HB	2.03	0.41
1:E:200:THR:OG1	1:E:205:GLU:HB3	2.21	0.41
2:F:16:VAL:CG2	2:F:75:ARG:HD2	2.51	0.41
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.89	0.40
2:B:28:ILE:HD12	2:B:36:PRO:HG2	2.02	0.40
1:E:159:ASN:C	1:E:160:SER:O	2.63	0.40
2:B:162:TYR:CD1	2:B:162:TYR:N	2.89	0.40
2:F:97:LEU:HD13	2:F:152:VAL:HG11	2.04	0.40
2:B:27:LEU:HD22	2:B:62:LEU:HD13	2.04	0.40
2:D:109:LEU:HD23	2:D:109:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:ARG:O	2:F:177:GLU:HG3	2.20	0.40
1:E:94:PHE:HA	1:E:105:PRO:HB2	2.04	0.40
2:F:187:LYS:NZ	2:F:187:LYS:HB3	2.36	0.40
1:A:239:ASP:H	1:A:242:SER:HG	1.68	0.40
1:C:146:ASN:H	1:C:146:ASN:HD22	1.69	0.40
1:C:229:VAL:O	1:C:230:ASN:HB2	2.21	0.40
2:D:12:LYS:HE3	2:D:63:TRP:CD2	2.57	0.40
1:E:238:LEU:HD12	1:E:238:LEU:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	183/320 (57%)	172 (94%)	9 (5%)	2 (1%)	11	25
1	C	178/320 (56%)	161 (90%)	12 (7%)	5 (3%)	4	6
1	E	162/320 (51%)	144 (89%)	17 (10%)	1 (1%)	21	42
2	B	176/188 (94%)	166 (94%)	7 (4%)	3 (2%)	7	15
2	D	176/188 (94%)	167 (95%)	6 (3%)	3 (2%)	7	15
2	F	179/188 (95%)	166 (93%)	9 (5%)	4 (2%)	5	10
All	All	1054/1524 (69%)	976 (93%)	60 (6%)	18 (2%)	7	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	80	PRO
1	C	97	PRO
2	D	80	PRO
2	F	80	PRO

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Mol	Chain	Res	Type
1	C	160	SER
1	C	161	ASP
2	D	32	LYS
2	F	186	GLY
2	B	32	LYS
2	B	103	LYS
1	C	252	PRO
2	D	103	LYS
1	E	160	SER
2	F	32	LYS
2	F	103	LYS
1	A	160	SER
1	C	253	GLY
1	A	102	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/290 (59%)	158 (92%)	14 (8%)	11	24
1	C	167/290 (58%)	145 (87%)	22 (13%)	4	8
1	E	155/290 (53%)	147 (95%)	8 (5%)	21	44
2	B	153/161 (95%)	145 (95%)	8 (5%)	21	44
2	D	153/161 (95%)	137 (90%)	16 (10%)	6	14
2	F	155/161 (96%)	145 (94%)	10 (6%)	15	35
All	All	955/1353 (71%)	877 (92%)	78 (8%)	10	24

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ILE
1	A	140	ILE
1	A	146	ASN
1	A	151	ILE

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Mol	Chain	Res	Type
1	A	159	ASN
1	A	161	ASP
1	A	172	LEU
1	A	175	LEU
1	A	184	ILE
1	A	193	SER
1	A	200	THR
1	A	228	LEU
1	A	247	VAL
1	A	258	ILE
2	B	37	GLU
2	B	57	ARG
2	B	80	PRO
2	B	95	ASP
2	B	105	ILE
2	B	146	SER
2	B	150	GLN
2	B	159	THR
1	C	91	ASN
1	C	96	ARG
1	C	97	PRO
1	C	171	GLN
1	C	172	LEU
1	C	175	LEU
1	C	182	LEU
1	C	183	GLU
1	C	185	SER
1	C	192	MSE
1	C	194	LYS
1	C	195	LYS
1	C	200	THR
1	C	207	THR
1	C	212	SER
1	C	214	ILE
1	C	216	LEU
1	C	220	THR
1	C	222	GLU
1	C	228	LEU
1	C	238	LEU
1	C	247	VAL
2	D	11	ARG
2	D	13	LEU

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Mol	Chain	Res	Type
2	D	26	LEU
2	D	32	LYS
2	D	34	GLN
2	D	37	GLU
2	D	38	VAL
2	D	56	ARG
2	D	74	LEU
2	D	80	PRO
2	D	93	LEU
2	D	97	LEU
2	D	103	LYS
2	D	136	LEU
2	D	150	GLN
2	D	184	LEU
1	E	104	PRO
1	E	132	GLU
1	E	138	LEU
1	E	166	ILE
1	E	175	LEU
1	E	182	LEU
1	E	222	GLU
1	E	241	ARG
2	F	42	THR
2	F	57	ARG
2	F	80	PRO
2	F	93	LEU
2	F	97	LEU
2	F	136	LEU
2	F	137	ARG
2	F	150	GLN
2	F	173	ARG
2	F	187	LYS

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

Mol	Chain	Res	Type
1	A	106	ASN
1	A	107	ASN
1	A	133	ASN
1	A	146	ASN
1	A	147	ASN
1	A	152	GLN

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Mol	Chain	Res	Type
1	A	159	ASN
1	A	171	GLN
2	B	68	GLN
2	B	83	ASN
2	B	101	GLN
2	B	141	GLN
2	B	150	GLN
2	B	155	GLN
1	C	106	ASN
1	C	133	ASN
1	C	146	ASN
1	C	152	GLN
1	C	165	GLN
1	C	171	GLN
2	D	34	GLN
2	D	83	ASN
2	D	101	GLN
2	D	141	GLN
2	D	142	GLN
2	D	147	GLN
2	D	150	GLN
1	E	106	ASN
1	E	107	ASN
1	E	147	ASN
1	E	152	GLN
1	E	201	ASN
1	E	230	ASN
2	F	46	ASN
2	F	68	GLN
2	F	83	ASN
2	F	101	GLN
2	F	141	GLN
2	F	142	GLN
2	F	150	GLN
2	F	155	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	PO4	C	322	-	4,4,4	1.72	0	6,6,6	0.49	0
3	PO4	A	322	-	4,4,4	1.70	0	6,6,6	0.45	0
4	GNP	B	301	5	34,34,34	1.43	5 (14%)	47,54,54	1.09	3 (6%)
3	PO4	A	321	-	4,4,4	1.68	0	6,6,6	0.46	0
3	PO4	C	323	-	4,4,4	1.73	0	6,6,6	0.47	0
3	PO4	A	323	-	4,4,4	1.67	1 (25%)	6,6,6	0.45	0
3	PO4	E	321	-	4,4,4	1.65	0	6,6,6	0.46	0
4	GNP	D	301	5	34,34,34	1.44	5 (14%)	47,54,54	1.07	4 (8%)
4	GNP	F	301	5	34,34,34	1.93	6 (17%)	47,54,54	1.09	4 (8%)
3	PO4	C	321	-	4,4,4	1.67	0	6,6,6	0.49	0

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
4	GNP	F	301	5	-	3/18/38/38	0/3/3/3
4	GNP	B	301	5	-	3/18/38/38	0/3/3/3
4	GNP	D	301	5	-	3/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	GNP	PA-O3A	-6.94	1.52	1.59
4	F	301	GNP	PB-O3A	-5.58	1.52	1.59
4	B	301	GNP	PA-O3A	-3.84	1.55	1.59
4	D	301	GNP	PA-O3A	-3.81	1.55	1.59
4	F	301	GNP	PG-O1G	3.56	1.51	1.46
4	B	301	GNP	PB-O3A	-3.49	1.54	1.59
4	D	301	GNP	PB-O2B	-3.29	1.48	1.56
4	B	301	GNP	PB-O2B	-3.15	1.48	1.56
4	B	301	GNP	PG-O1G	3.15	1.50	1.46
4	D	301	GNP	PG-O1G	3.00	1.50	1.46
4	D	301	GNP	PB-O3A	-3.00	1.55	1.59
4	F	301	GNP	PB-O2B	-2.83	1.49	1.56
4	D	301	GNP	PG-O3G	-2.50	1.50	1.56
4	B	301	GNP	PG-O3G	-2.49	1.50	1.56
4	F	301	GNP	PG-O3G	-2.23	1.50	1.56
4	F	301	GNP	C4-N3	2.22	1.39	1.34
3	A	323	PO4	P-O4	-2.03	1.48	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	GNP	O3G-PG-O1G	-4.21	102.89	113.45
4	F	301	GNP	O3G-PG-O1G	-3.91	103.65	113.45
4	D	301	GNP	O3G-PG-O1G	-3.76	104.01	113.45
4	F	301	GNP	O2B-PB-O1B	3.47	117.32	109.87
4	B	301	GNP	O2B-PB-O1B	2.91	116.11	109.87
4	B	301	GNP	O2G-PG-O3G	2.54	114.42	107.59
4	D	301	GNP	O2B-PB-O1B	2.51	115.26	109.87
4	D	301	GNP	O4'-C1'-N9	2.33	113.64	108.36
4	D	301	GNP	O1B-PB-N3B	-2.30	108.38	111.77
4	F	301	GNP	O4'-C1'-N9	2.22	113.40	108.36
4	F	301	GNP	O1B-PB-N3B	-2.17	108.57	111.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GNP	PB-N3B-PG-O1G
4	B	301	GNP	PG-N3B-PB-O1B
4	B	301	GNP	PG-N3B-PB-O3A
4	D	301	GNP	PB-N3B-PG-O1G

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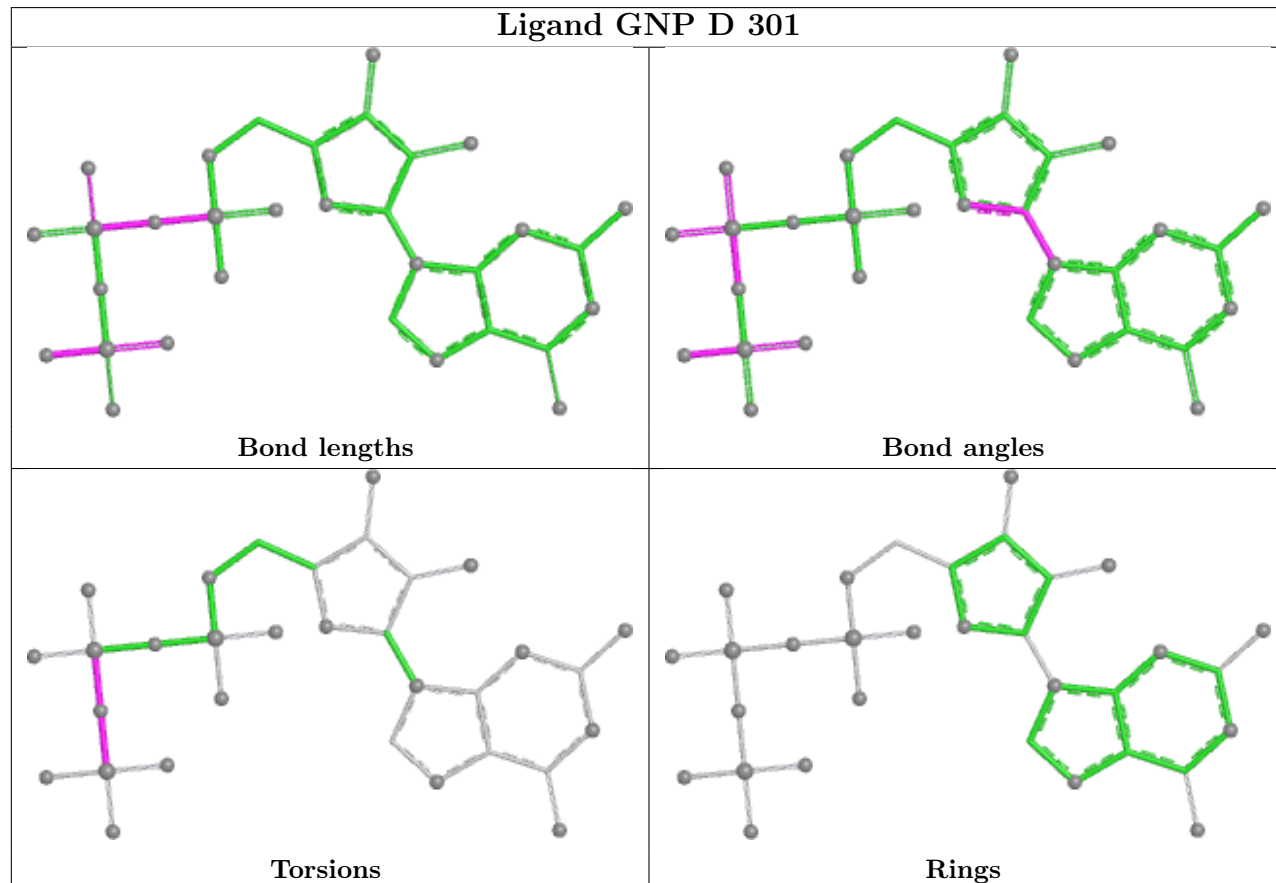
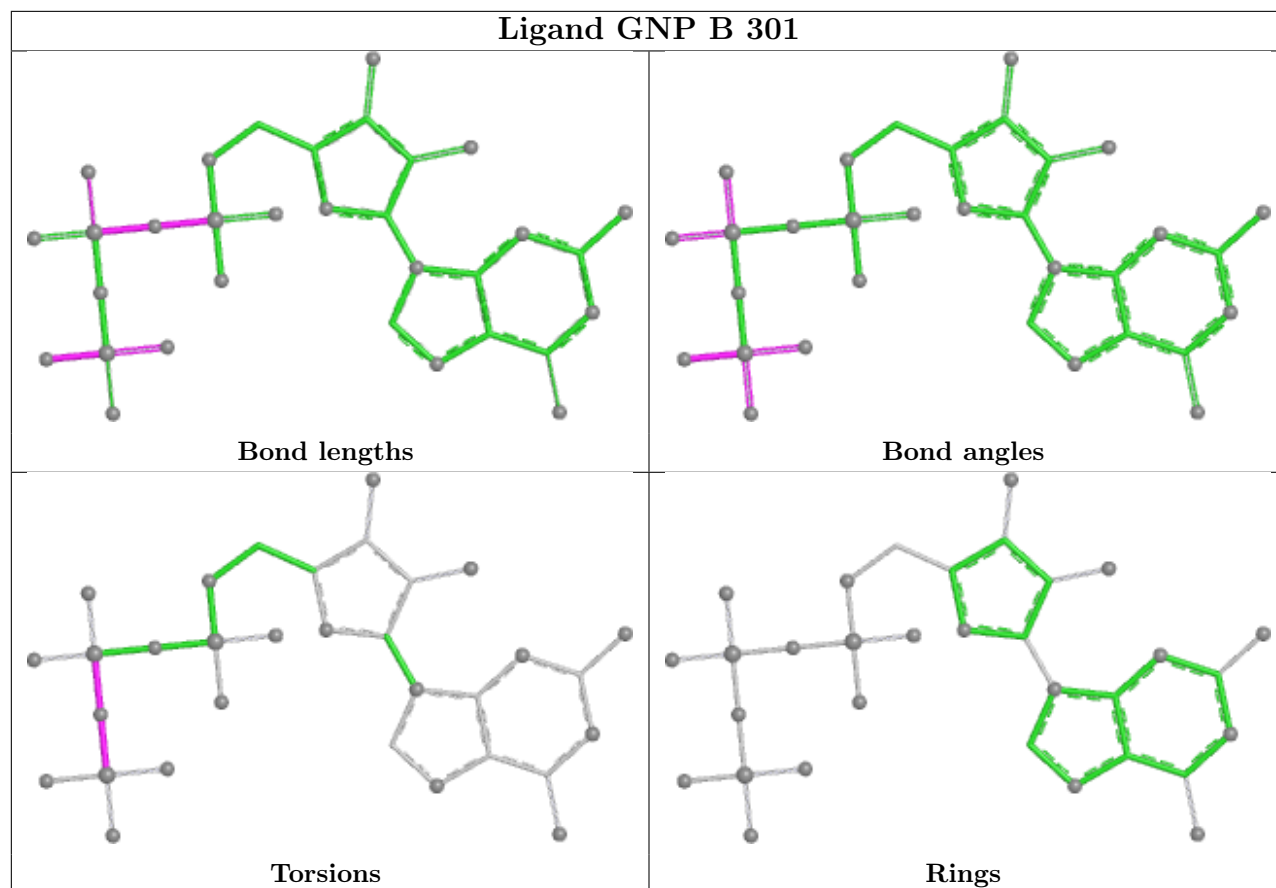
Mol	Chain	Res	Type	Atoms
4	D	301	GNP	PG-N3B-PB-O1B
4	D	301	GNP	PG-N3B-PB-O3A
4	F	301	GNP	PB-N3B-PG-O1G
4	F	301	GNP	PG-N3B-PB-O1B
4	F	301	GNP	PG-N3B-PB-O3A

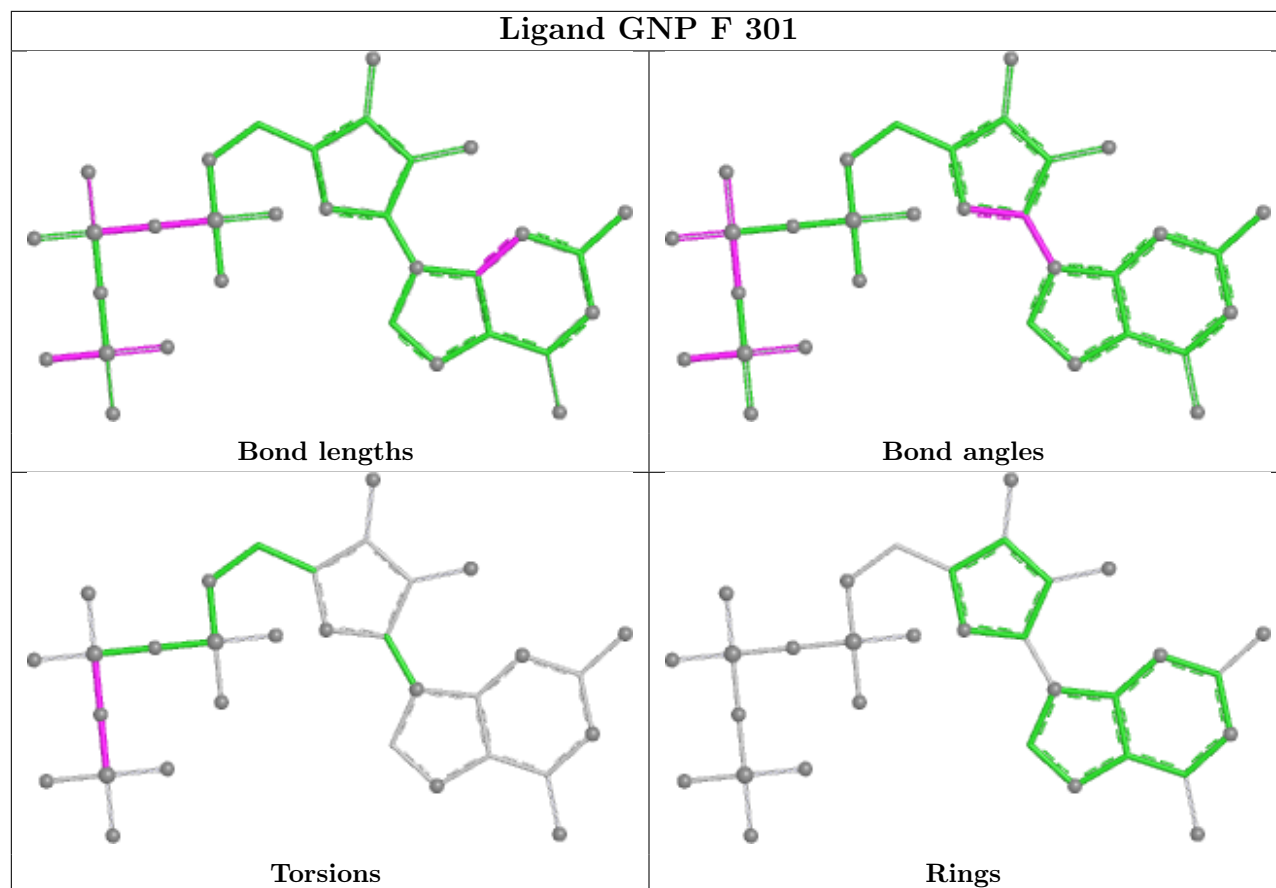
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	GNP	2	0
3	A	323	PO4	1	0
4	D	301	GNP	1	0
3	C	321	PO4	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	184/320 (57%)	0.06	4 (2%) 62 57	31, 53, 84, 119	0
1	C	179/320 (55%)	0.01	7 (3%) 43 38	36, 57, 97, 123	0
1	E	165/320 (51%)	1.61	51 (30%) 1 1	72, 108, 129, 133	0
2	B	178/188 (94%)	0.67	11 (6%) 26 21	52, 74, 97, 108	0
2	D	178/188 (94%)	-0.04	4 (2%) 62 57	34, 47, 78, 99	0
2	F	181/188 (96%)	0.60	12 (6%) 24 19	51, 76, 95, 108	0
All	All	1065/1524 (69%)	0.47	89 (8%) 17 13	31, 67, 116, 133	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	128	ASP	5.2
1	E	248	ILE	4.3
1	E	223	GLY	4.0
1	A	161	ASP	3.9
1	E	104	PRO	3.5
1	E	178	VAL	3.5
2	B	31	SER	3.4
1	E	164	PHE	3.4
2	B	33	GLY	3.4
1	E	193	SER	3.3
1	E	170	TRP	3.3
1	E	162	GLY	3.2
1	A	101	THR	3.2
1	E	148	ALA	3.2
1	E	182	LEU	3.1
2	B	139	GLU	3.1
2	F	31	SER	3.1
1	E	154	HIS	3.1
1	E	127	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	185	MET	3.1
1	E	77	PHE	3.0
1	E	230	ASN	3.0
1	A	99	HIS	3.0
2	D	31	SER	3.0
1	E	121	PRO	2.9
2	B	9	ILE	2.9
1	E	150	LEU	2.9
2	D	139	GLU	2.9
1	E	195	LYS	2.9
2	F	32	LYS	2.8
1	E	235	LEU	2.8
2	D	51	VAL	2.8
1	E	228	LEU	2.7
1	E	112	VAL	2.7
1	E	151	ILE	2.7
2	F	51	VAL	2.7
2	B	37	GLU	2.7
1	E	129	SER	2.6
2	B	49	ALA	2.6
1	A	260	SER	2.6
1	C	101	THR	2.6
1	E	190	LEU	2.6
1	E	238	LEU	2.6
2	B	51	VAL	2.5
2	F	57	ARG	2.5
1	E	243	TYR	2.5
2	F	67	GLY	2.5
2	D	185	MET	2.5
1	E	95	SER	2.5
2	F	9	ILE	2.5
1	E	196	TYR	2.5
1	E	237	TYR	2.5
1	E	236	PHE	2.4
1	E	171	GLN	2.4
1	E	131	LEU	2.4
2	B	135	GLN	2.4
1	E	110	THR	2.4
1	E	176	VAL	2.4
1	E	233	LEU	2.3
1	E	189	ILE	2.3
2	B	50	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	140	ILE	2.3
1	C	104	PRO	2.3
1	E	153	ILE	2.3
1	E	194	LYS	2.2
1	E	144	LYS	2.2
1	E	180	LYS	2.2
2	F	69	GLU	2.2
2	B	170	TYR	2.2
2	F	33	GLY	2.2
1	C	99	HIS	2.2
1	E	132	GLU	2.2
2	F	52	GLU	2.2
2	B	34	GLN	2.2
1	E	125	PRO	2.1
2	F	187	LYS	2.1
1	E	175	LEU	2.1
2	F	77	LEU	2.1
1	C	103	GLU	2.1
1	C	102	GLY	2.1
1	C	254	SER	2.1
1	E	231	TRP	2.1
1	E	173	THR	2.1
1	E	247	VAL	2.1
1	E	122	SER	2.0
1	C	119	LYS	2.0
1	E	155	LYS	2.0
1	E	242	SER	2.0
1	E	168	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

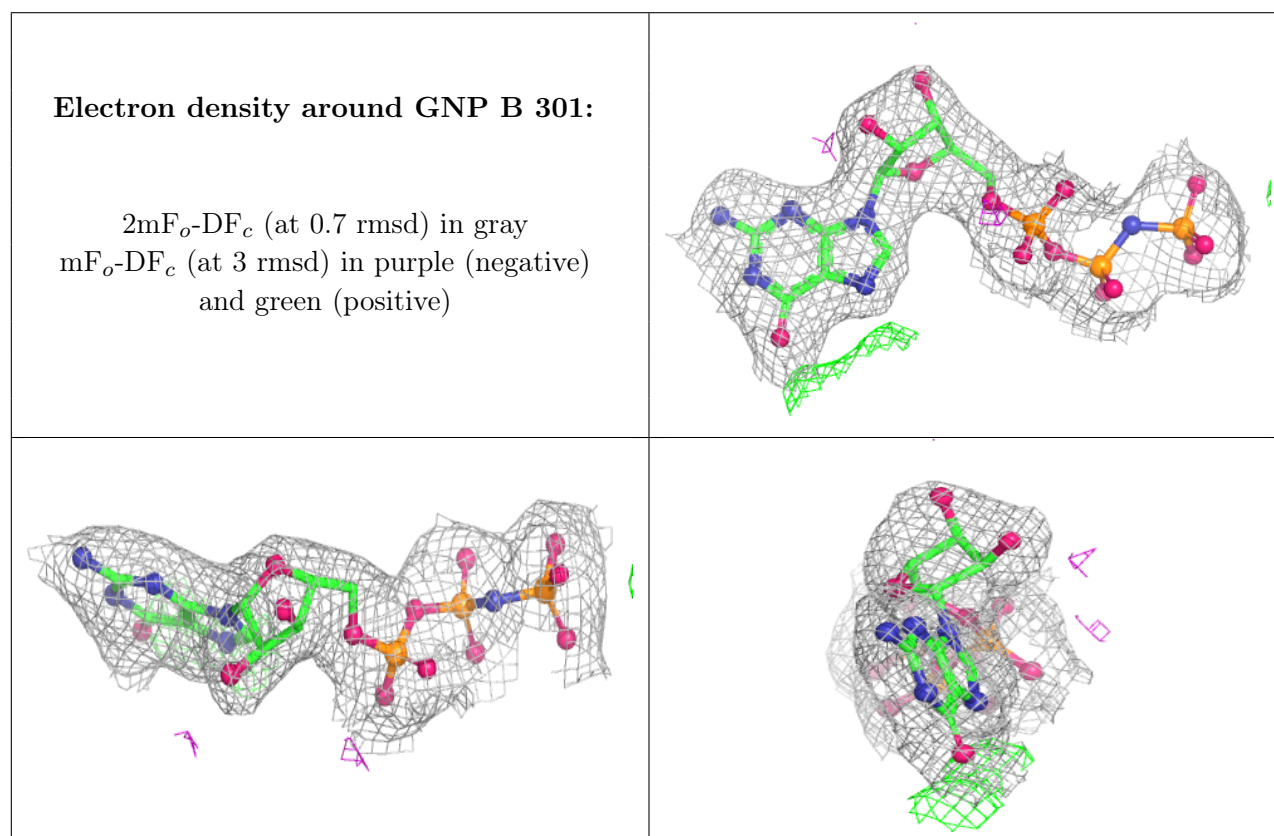
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

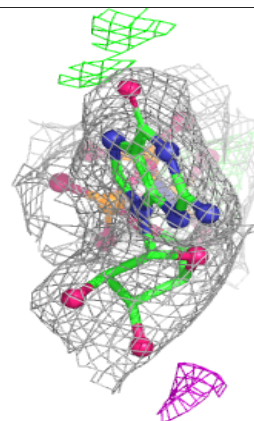
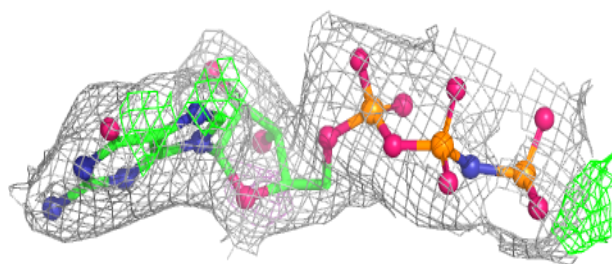
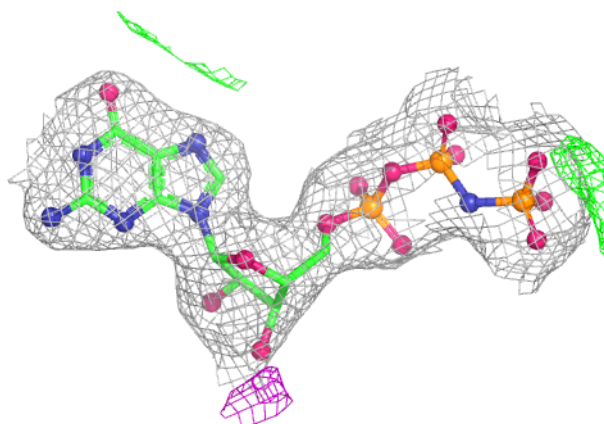
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	E	321	5/5	0.41	0.14	146,147,147,147	0
3	PO4	A	323	5/5	0.78	0.13	110,110,111,111	0
3	PO4	A	321	5/5	0.82	0.10	109,110,110,110	0
3	PO4	C	323	5/5	0.88	0.15	93,94,95,95	0
3	PO4	C	321	5/5	0.93	0.11	71,72,72,73	0
3	PO4	A	322	5/5	0.95	0.06	82,83,83,84	0
3	PO4	C	322	5/5	0.96	0.08	67,67,68,70	0
4	GNP	B	301	32/32	0.96	0.07	49,57,60,61	0
4	GNP	F	301	32/32	0.96	0.07	58,62,65,68	0
4	GNP	D	301	32/32	0.98	0.06	27,34,39,42	0
5	MG	F	401	1/1	0.98	0.06	57,57,57,57	0
5	MG	D	401	1/1	0.99	0.02	38,38,38,38	0
5	MG	B	401	1/1	0.99	0.03	46,46,46,46	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.



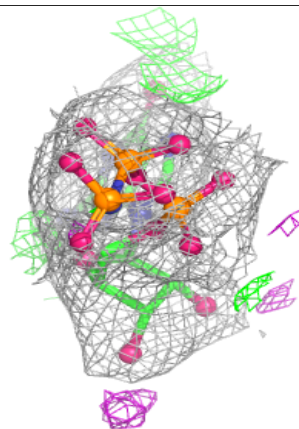
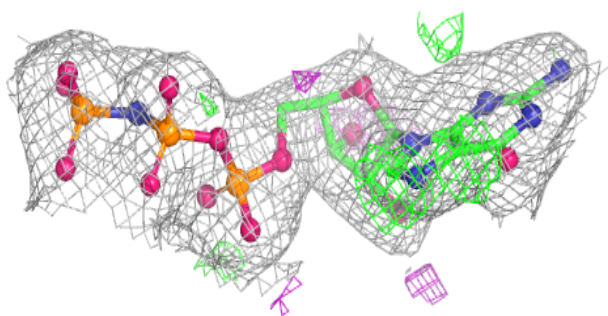
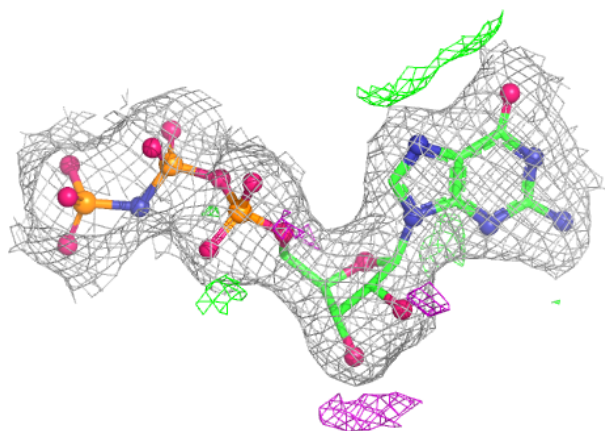
Electron density around GNP F 301:

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



Electron density around GNP D 301:

$2mF_o-DF_c$ (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.