Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 04:40 AM EDT

PDB ID	:	3BB1
Title	:	Crystal structure of Toc34 from Pisum sativum in complex with Mg2+ and GMPPNP
Authors	:	Koenig, P.; Sinning, I.; Schleiff, E.; Tews, I.
Deposited on	:	2007-11-09
Resolution	:	2.80 Å(reported)

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

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

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

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

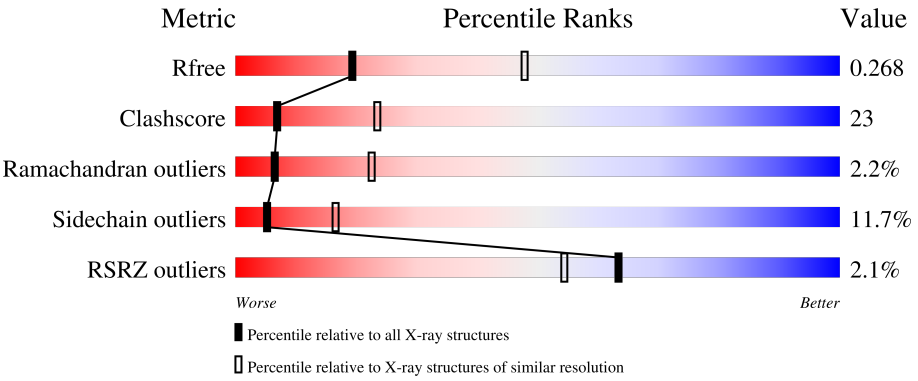
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	274	60% 25% 5% • 8%
1	B	274	2% 50% 30% 7% • 11%
1	C	274	% 58% 24% 6% • 10%
1	D	274	2% 51% 30% 7% • 10%
1	E	274	% 56% 30% • 9%

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Mol	Chain	Length	Quality of chain
1	F	274	3% 52% 28% 8% 11%
1	G	274	% 65% 22% 8%
1	H	274	4% 45% 37% 7% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	C	291	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15802 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 Translocase of chloroplast 34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1930	1226	328	372	4			
1	B	243	Total	C	N	O	S	0	0	0
			1853	1182	314	353	4			
1	C	246	Total	C	N	O	S	0	0	0
			1887	1202	320	361	4			
1	D	247	Total	C	N	O	S	0	0	0
			1882	1199	318	361	4			
1	E	248	Total	C	N	O	S	0	0	0
			1901	1211	323	363	4			
1	F	245	Total	C	N	O	S	0	0	0
			1882	1201	320	357	4			
1	G	251	Total	C	N	O	S	0	0	0
			1923	1221	327	371	4			
1	H	248	Total	C	N	O	S	0	0	0
			1897	1210	323	360	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	GLU	engineered mutation	UNP Q41009
A	267	LEU	-	expression tag	UNP Q41009
A	268	GLU	-	expression tag	UNP Q41009
A	269	HIS	-	expression tag	UNP Q41009
A	270	HIS	-	expression tag	UNP Q41009
A	271	HIS	-	expression tag	UNP Q41009
A	272	HIS	-	expression tag	UNP Q41009
A	273	HIS	-	expression tag	UNP Q41009
A	274	HIS	-	expression tag	UNP Q41009
B	10	GLY	GLU	engineered mutation	UNP Q41009
B	267	LEU	-	expression tag	UNP Q41009
B	268	GLU	-	expression tag	UNP Q41009
B	269	HIS	-	expression tag	UNP Q41009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	270	HIS	-	expression tag	UNP Q41009
B	271	HIS	-	expression tag	UNP Q41009
B	272	HIS	-	expression tag	UNP Q41009
B	273	HIS	-	expression tag	UNP Q41009
B	274	HIS	-	expression tag	UNP Q41009
C	10	GLY	GLU	engineered mutation	UNP Q41009
C	267	LEU	-	expression tag	UNP Q41009
C	268	GLU	-	expression tag	UNP Q41009
C	269	HIS	-	expression tag	UNP Q41009
C	270	HIS	-	expression tag	UNP Q41009
C	271	HIS	-	expression tag	UNP Q41009
C	272	HIS	-	expression tag	UNP Q41009
C	273	HIS	-	expression tag	UNP Q41009
C	274	HIS	-	expression tag	UNP Q41009
D	10	GLY	GLU	engineered mutation	UNP Q41009
D	267	LEU	-	expression tag	UNP Q41009
D	268	GLU	-	expression tag	UNP Q41009
D	269	HIS	-	expression tag	UNP Q41009
D	270	HIS	-	expression tag	UNP Q41009
D	271	HIS	-	expression tag	UNP Q41009
D	272	HIS	-	expression tag	UNP Q41009
D	273	HIS	-	expression tag	UNP Q41009
D	274	HIS	-	expression tag	UNP Q41009
E	10	GLY	GLU	engineered mutation	UNP Q41009
E	267	LEU	-	expression tag	UNP Q41009
E	268	GLU	-	expression tag	UNP Q41009
E	269	HIS	-	expression tag	UNP Q41009
E	270	HIS	-	expression tag	UNP Q41009
E	271	HIS	-	expression tag	UNP Q41009
E	272	HIS	-	expression tag	UNP Q41009
E	273	HIS	-	expression tag	UNP Q41009
E	274	HIS	-	expression tag	UNP Q41009
F	10	GLY	GLU	engineered mutation	UNP Q41009
F	267	LEU	-	expression tag	UNP Q41009
F	268	GLU	-	expression tag	UNP Q41009
F	269	HIS	-	expression tag	UNP Q41009
F	270	HIS	-	expression tag	UNP Q41009
F	271	HIS	-	expression tag	UNP Q41009
F	272	HIS	-	expression tag	UNP Q41009
F	273	HIS	-	expression tag	UNP Q41009
F	274	HIS	-	expression tag	UNP Q41009
G	10	GLY	GLU	engineered mutation	UNP Q41009

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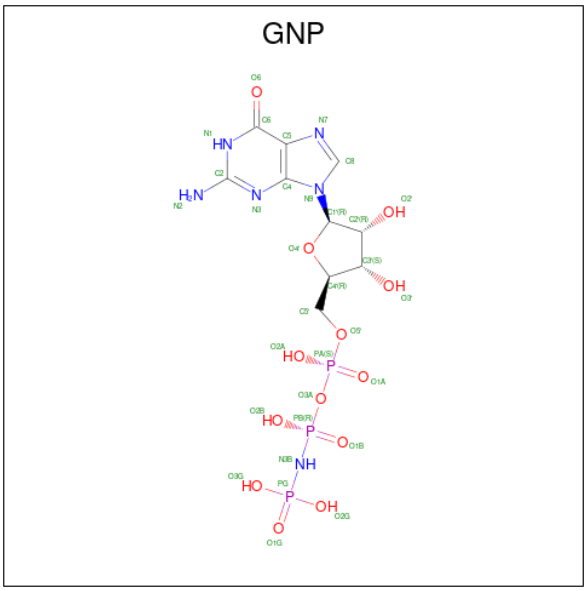
Chain	Residue	Modelled	Actual	Comment	Reference
G	267	LEU	-	expression tag	UNP Q41009
G	268	GLU	-	expression tag	UNP Q41009
G	269	HIS	-	expression tag	UNP Q41009
G	270	HIS	-	expression tag	UNP Q41009
G	271	HIS	-	expression tag	UNP Q41009
G	272	HIS	-	expression tag	UNP Q41009
G	273	HIS	-	expression tag	UNP Q41009
G	274	HIS	-	expression tag	UNP Q41009
H	10	GLY	GLU	engineered mutation	UNP Q41009
H	267	LEU	-	expression tag	UNP Q41009
H	268	GLU	-	expression tag	UNP Q41009
H	269	HIS	-	expression tag	UNP Q41009
H	270	HIS	-	expression tag	UNP Q41009
H	271	HIS	-	expression tag	UNP Q41009
H	272	HIS	-	expression tag	UNP Q41009
H	273	HIS	-	expression tag	UNP Q41009
H	274	HIS	-	expression tag	UNP Q41009

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

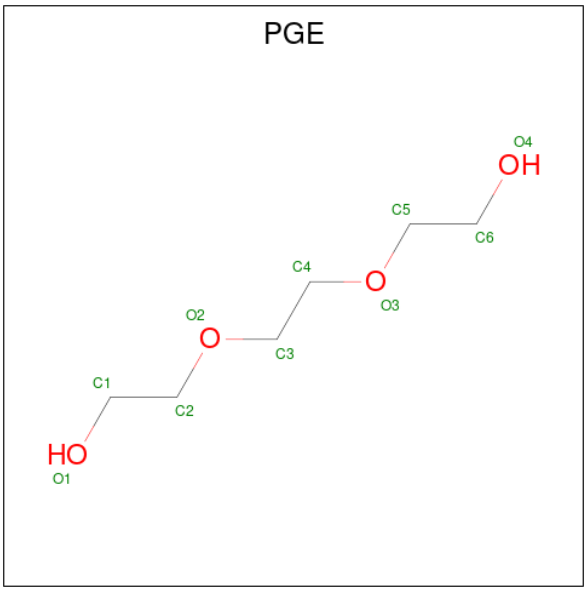
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



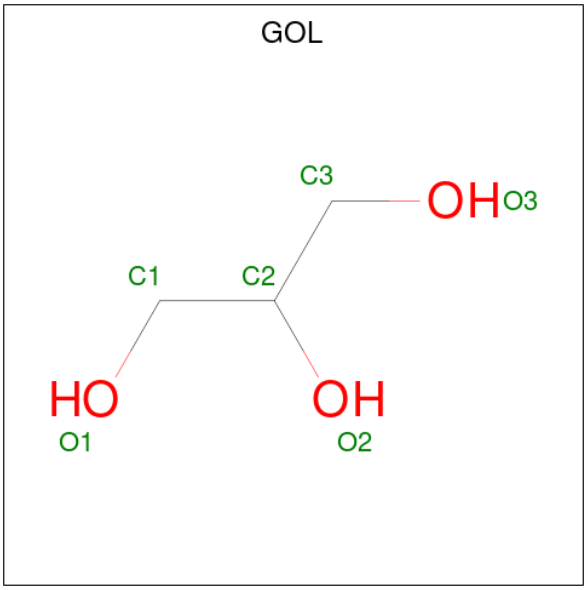
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	G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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	F	1	Total C O 10 6 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

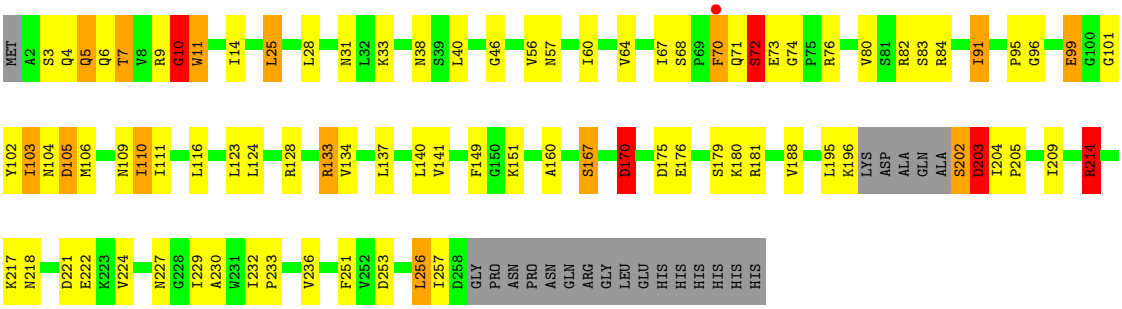
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	52	Total O 52 52	0	0
6	B	24	Total O 24 24	0	0
6	C	49	Total O 49 49	0	0
6	D	39	Total O 39 39	0	0
6	E	53	Total O 53 53	0	0
6	F	35	Total O 35 35	0	0
6	G	40	Total O 40 40	0	0
6	H	35	Total O 35 35	0	0

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.

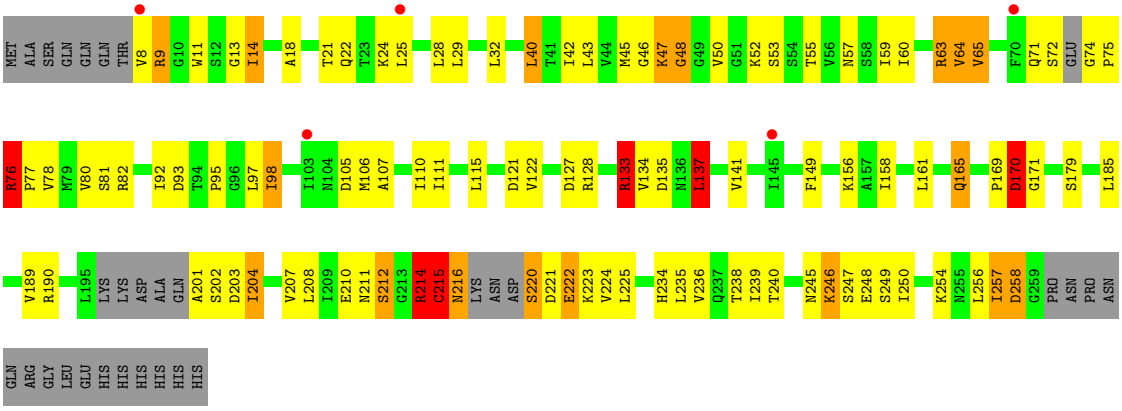
• Molecule 1: Translocase of chloroplast 34

Chain A:



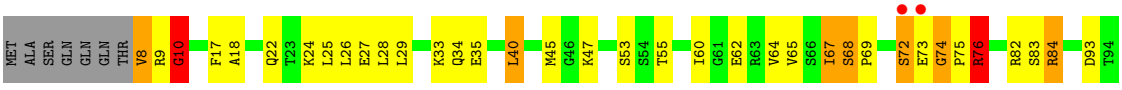
• Molecule 1: Translocase of chloroplast 34

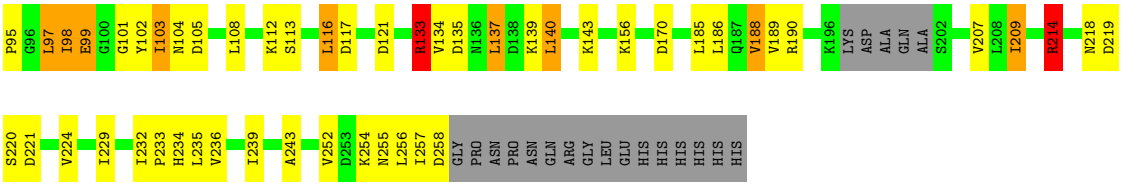
Chain B:



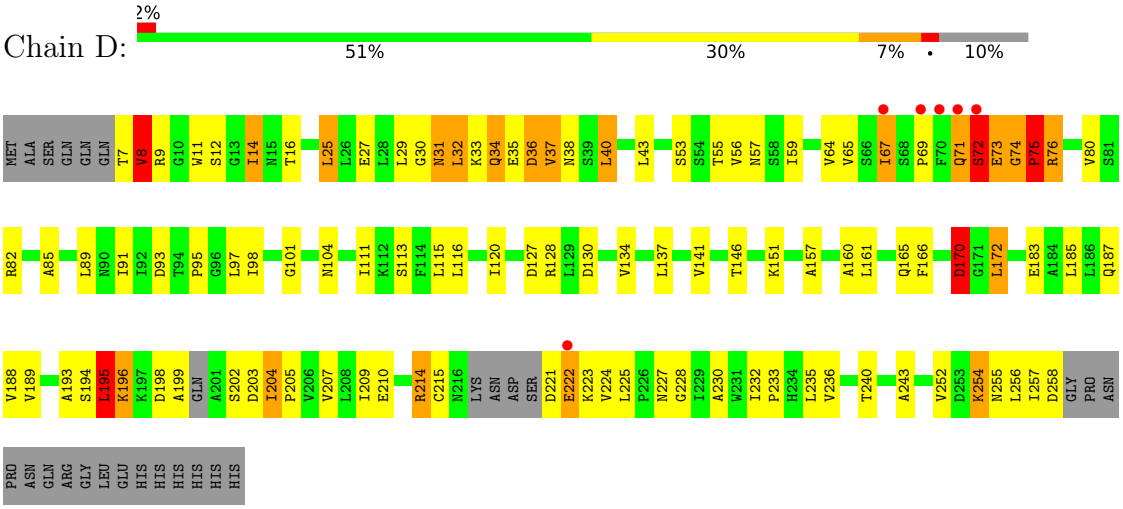
• Molecule 1: Translocase of chloroplast 34

Chain C:

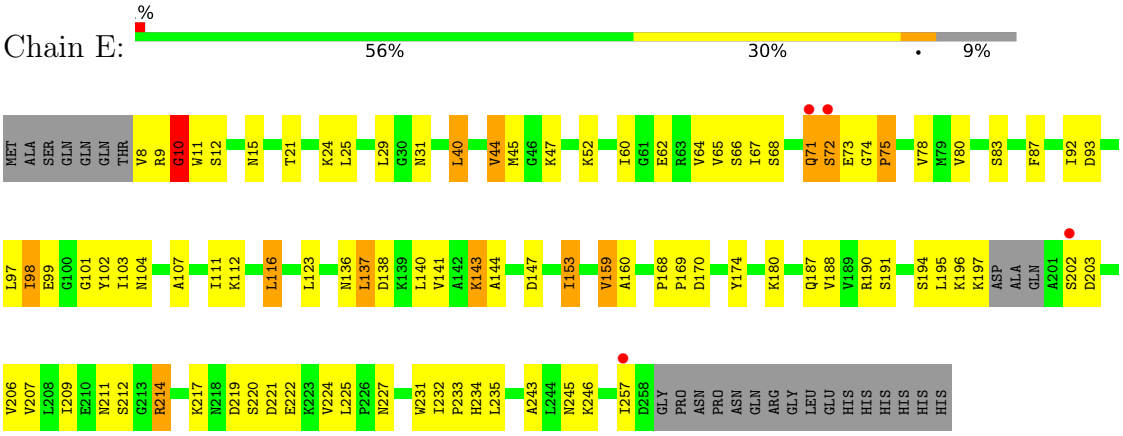




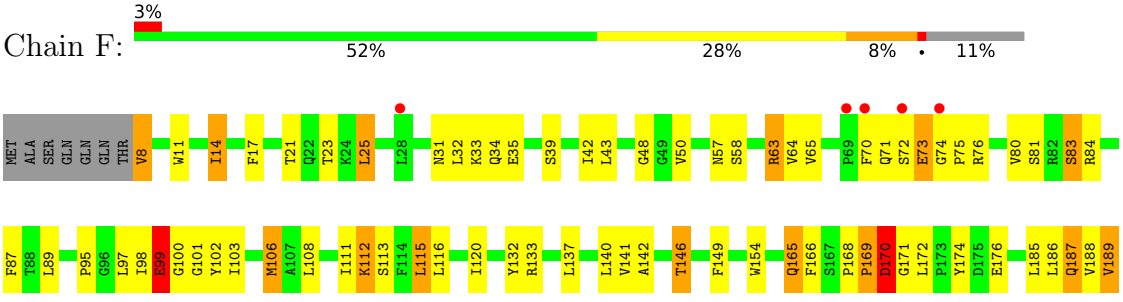
• Molecule 1: Translocase of chloroplast 34

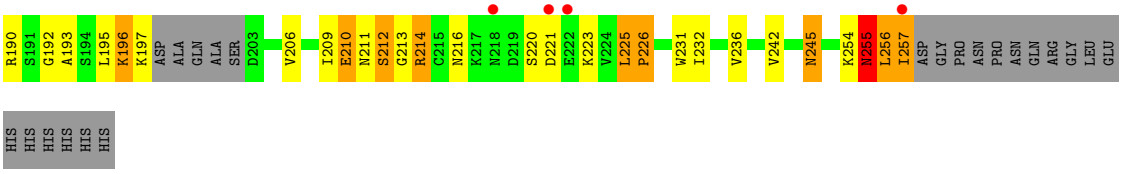


• Molecule 1: Translocase of chloroplast 34

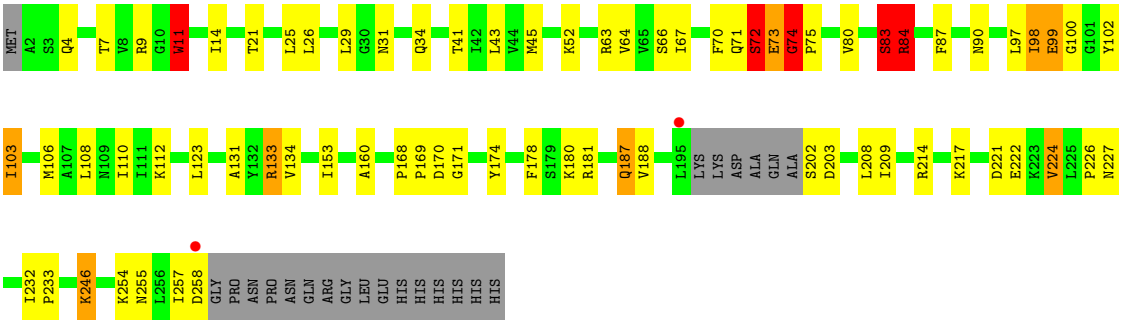


• Molecule 1: Translocase of chloroplast 34

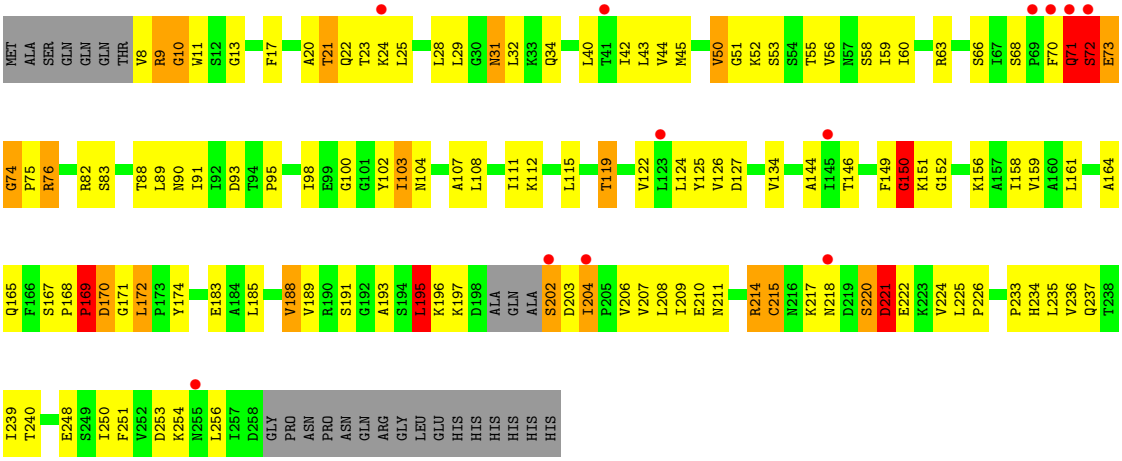




• Molecule 1: Translocase of chloroplast 34



• Molecule 1: Translocase of chloroplast 34



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	178.78Å 180.06Å 90.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.80 49.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.88-2.80) 97.5 (49.85-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.224 , 0.282 0.205 , 0.268	Depositor DCC
R_{free} test set	3668 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.207 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15802	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.85	1/1960 (0.1%)	0.95	4/2658 (0.2%)
1	B	0.77	0/1881	1.00	9/2549 (0.4%)
1	C	0.91	1/1917 (0.1%)	1.03	8/2599 (0.3%)
1	D	0.78	0/1911	1.04	6/2593 (0.2%)
1	E	0.88	1/1931 (0.1%)	0.93	4/2617 (0.2%)
1	F	0.78	0/1912	0.96	4/2591 (0.2%)
1	G	0.84	0/1953	0.93	5/2649 (0.2%)
1	H	0.72	0/1927	0.91	4/2612 (0.2%)
All	All	0.82	3/15392 (0.0%)	0.97	44/20868 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	5
1	B	6	8
1	C	2	7
1	D	3	8
1	E	2	3
1	F	2	5
1	G	3	2
1	H	2	9
All	All	21	47

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	GLU	CD-OE1	5.87	1.32	1.25
1	E	214	ARG	CG-CD	5.63	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	LYS	C-O	5.54	1.33	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	10	GLY	N-CA-C	9.71	137.37	113.10
1	F	99	GLU	N-CA-C	8.64	134.33	111.00
1	C	214	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	B	258	ASP	CB-CA-C	7.82	126.04	110.40
1	E	11	TRP	N-CA-C	-7.65	90.35	111.00
1	H	72	SER	N-CA-CB	7.63	121.94	110.50
1	B	76	ARG	C-N-CD	-6.86	105.52	120.60
1	C	84	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	H	195	LEU	CA-CB-CG	6.82	130.98	115.30
1	B	47	LYS	N-CA-C	6.80	129.35	111.00
1	D	37	VAL	CB-CA-C	6.70	124.14	111.40
1	A	10	GLY	N-CA-C	6.44	129.20	113.10
1	B	215	CYS	CB-CA-C	6.37	123.14	110.40
1	D	130	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	76	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	76	ARG	N-CA-C	6.00	127.21	111.00
1	H	150	GLY	N-CA-C	6.00	128.10	113.10
1	B	133	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	E	202	SER	N-CA-CB	5.92	119.38	110.50
1	E	93	ASP	CB-CG-OD1	5.92	123.63	118.30
1	D	25	LEU	CA-CB-CG	5.91	128.88	115.30
1	G	11	TRP	N-CA-C	5.79	126.64	111.00
1	G	224	VAL	CB-CA-C	-5.63	100.70	111.40
1	A	214	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	G	170	ASP	N-CA-CB	5.57	120.62	110.60
1	F	245	ASN	N-CA-C	5.52	125.89	111.00
1	A	170	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	H	221	ASP	CB-CA-C	5.46	121.32	110.40
1	C	135	ASP	CB-CG-OD1	5.44	123.20	118.30
1	D	195	LEU	CA-CB-CG	5.43	127.79	115.30
1	E	93	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	84	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	170	ASP	CB-CG-OD1	5.33	123.10	118.30
1	F	170	ASP	N-CA-C	5.24	125.14	111.00
1	B	215	CYS	CA-CB-SG	5.23	123.42	114.00
1	B	63	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	214	ARG	N-CA-C	5.18	124.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	83	SER	N-CA-C	5.17	124.96	111.00
1	C	133	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	F	83	SER	CB-CA-C	-5.11	100.40	110.10
1	A	99	GLU	N-CA-C	5.09	124.74	111.00
1	G	170	ASP	CB-CA-C	5.05	120.49	110.40
1	B	137	LEU	CB-CA-C	5.03	119.76	110.20
1	B	170	ASP	CB-CG-OD2	-5.01	113.79	118.30

All (21) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	99	GLU	CA
1	B	47	LYS	CA
1	B	137	LEU	CA
1	B	203	ASP	CA
1	B	215	CYS	CA
1	B	256	LEU	CA
1	B	258	ASP	CA
1	C	34	GLN	CA
1	C	72	SER	CA
1	D	37	VAL	CA
1	D	214	ARG	CA
1	D	246	LYS	CA
1	E	136	ASN	CA
1	E	202	SER	CA
1	F	76	ARG	CA
1	F	99	GLU	CA
1	G	83	SER	CA
1	G	99	GLU	CA
1	G	170	ASP	CA
1	H	72	SER	CA
1	H	221	ASP	CA

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLY	Peptide
1	A	203	ASP	Peptide
1	A	70	PHE	Peptide
1	A	72	SER	Peptide
1	A	9	ARG	Peptide
1	B	211	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	214	ARG	Peptide
1	B	222	GLU	Peptide
1	B	46	GLY	Peptide
1	B	47	LYS	Peptide
1	B	48	GLY	Peptide
1	B	74	GLY	Peptide
1	B	76	ARG	Peptide
1	C	10	GLY	Peptide
1	C	74	GLY	Peptide
1	C	75	PRO	Peptide
1	C	76	ARG	Peptide
1	C	8	VAL	Peptide
1	C	9	ARG	Peptide
1	C	97	LEU	Peptide
1	D	195	LEU	Peptide
1	D	196	LYS	Peptide
1	D	221	ASP	Peptide
1	D	34	GLN	Peptide
1	D	71	GLN	Peptide
1	D	72	SER	Peptide
1	D	75	PRO	Peptide
1	D	8	VAL	Peptide
1	E	10	GLY	Peptide
1	E	71	GLN	Peptide
1	E	75	PRO	Peptide
1	F	169	PRO	Peptide
1	F	192	GLY	Peptide
1	F	212	SER	Peptide
1	F	256	LEU	Peptide
1	F	76	ARG	Peptide
1	G	74	GLY	Peptide
1	G	98	ILE	Peptide
1	H	149	PHE	Peptide
1	H	169	PRO	Peptide
1	H	171	GLY	Peptide
1	H	195	LEU	Peptide
1	H	202	SER	Peptide
1	H	71	GLN	Peptide
1	H	72	SER	Peptide
1	H	73	GLU	Peptide
1	H	9	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1930	0	1969	86	0
1	B	1853	0	1899	111	0
1	C	1887	0	1935	94	0
1	D	1882	0	1918	113	0
1	E	1901	0	1953	70	0
1	F	1882	0	1939	99	0
1	G	1923	0	1963	67	0
1	H	1897	0	1945	115	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	32	0	13	0	0
3	B	32	0	13	1	0
3	C	32	0	13	1	0
3	D	32	0	13	5	0
3	E	32	0	13	0	0
3	F	32	0	13	0	0
3	G	32	0	13	1	0
3	H	32	0	13	2	0
4	A	10	0	14	0	0
4	F	10	0	14	4	0
5	A	6	0	8	1	0
5	C	6	0	8	4	0
5	E	6	0	8	0	0
5	F	6	0	8	0	0
5	G	12	0	16	3	0
6	A	52	0	0	9	0
6	B	24	0	0	8	0
6	C	49	0	0	10	0
6	D	39	0	0	8	0
6	E	53	0	0	2	0
6	F	35	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	40	0	0	12	0
6	H	35	0	0	16	0
All	All	15802	0	15701	721	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 23.

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:VAL:HG21	6:H:315:HOH:O	1.31	1.26
1:G:67:ILE:O	1:G:67:ILE:HD12	1.38	1.20
1:F:189:VAL:O	1:F:193:ALA:HB2	1.43	1.19
1:A:116:LEU:HD21	1:A:257:ILE:CD1	1.73	1.18
1:B:246:LYS:CB	1:B:247:SER:HA	1.63	1.14
1:B:214:ARG:HH11	1:D:214:ARG:HG2	1.08	1.09
1:B:246:LYS:HB2	1:B:247:SER:HA	1.07	1.05
1:G:110:ILE:HG23	6:G:330:HOH:O	1.57	1.04
1:H:71:GLN:HB3	1:H:72:SER:CB	1.89	1.01
1:D:75:PRO:HB2	1:D:76:ARG:HA	1.40	1.00
1:D:198:ASP:CB	1:D:199:ALA:HB3	1.92	1.00
1:A:116:LEU:CD2	1:A:257:ILE:HD11	1.92	1.00
1:A:253:ASP:HB2	6:A:339:HOH:O	1.60	1.00
1:A:203:ASP:HB2	1:A:204:ILE:HA	1.44	0.98
1:B:214:ARG:HH11	1:D:214:ARG:CG	1.75	0.98
1:A:116:LEU:HD21	1:A:257:ILE:HD11	0.98	0.97
1:B:246:LYS:HB2	1:B:247:SER:CA	1.93	0.97
1:D:116:LEU:HD11	1:D:257:ILE:HD12	1.47	0.95
1:D:198:ASP:HB3	1:D:199:ALA:HB3	1.50	0.94
1:D:8:VAL:HA	6:D:310:HOH:O	1.65	0.94
1:C:98:ILE:HD11	1:C:137:LEU:HD11	1.47	0.94
1:A:203:ASP:HB2	1:A:205:PRO:HD3	1.47	0.94
1:B:214:ARG:NH1	1:D:214:ARG:HG2	1.84	0.92
1:B:257:ILE:HD12	1:B:258:ASP:N	1.84	0.92
1:E:112:LYS:HB3	1:E:257:ILE:HD12	1.51	0.92
1:H:256:LEU:HB3	6:H:317:HOH:O	1.68	0.90
1:H:250:ILE:HG23	1:H:256:LEU:HD11	1.54	0.89
1:D:207:VAL:HG21	1:D:235:LEU:CD1	2.03	0.89
1:F:142:ALA:O	1:F:146:THR:HG22	1.72	0.88
1:F:101:GLY:HA3	1:F:137:LEU:HD21	1.56	0.87
1:C:10:GLY:HA2	1:C:82:ARG:HD2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ASN:OD1	1:B:247:SER:HB2	1.75	0.86
1:C:98:ILE:CD1	1:C:137:LEU:HD11	2.06	0.86
1:F:225:LEU:HD21	1:F:231:TRP:HB3	1.59	0.85
1:D:38:ASN:HA	6:D:295:HOH:O	1.76	0.84
1:F:8:VAL:HA	6:F:311:HOH:O	1.76	0.84
1:H:71:GLN:HB3	1:H:72:SER:OG	1.77	0.83
1:D:160:ALA:HB1	1:D:209:ILE:CD1	2.08	0.83
1:G:52:LYS:NZ	3:G:281:GNP:O1B	2.12	0.83
1:D:160:ALA:HB1	1:D:209:ILE:HD13	1.61	0.83
1:A:203:ASP:CB	1:A:205:PRO:HD3	2.09	0.82
1:B:207:VAL:HG21	1:B:235:LEU:HD13	1.59	0.82
1:D:257:ILE:HG22	6:D:321:HOH:O	1.79	0.82
1:C:98:ILE:O	1:C:98:ILE:HG23	1.78	0.82
1:C:143:LYS:HD2	1:E:102:TYR:CZ	2.14	0.81
1:H:71:GLN:HB3	1:H:72:SER:HB2	1.59	0.81
1:C:98:ILE:O	1:C:98:ILE:HD13	1.79	0.81
1:A:116:LEU:CD2	1:A:257:ILE:CD1	2.55	0.81
1:F:58:SER:OG	1:F:211:ASN:ND2	2.12	0.81
1:B:97:LEU:HD12	1:B:141:VAL:HG13	1.63	0.81
1:E:159:VAL:HG22	1:E:206:VAL:HG13	1.62	0.81
1:E:98:ILE:HD13	1:E:141:VAL:HG22	1.63	0.80
1:A:203:ASP:HB2	1:A:204:ILE:CA	2.11	0.80
1:H:28:LEU:HD13	1:H:236:VAL:HG12	1.62	0.80
1:E:160:ALA:HB1	1:E:209:ILE:HD12	1.65	0.78
1:E:112:LYS:HB3	1:E:257:ILE:CD1	2.12	0.78
1:D:207:VAL:HG21	1:D:235:LEU:HD12	1.64	0.78
1:G:67:ILE:O	1:G:67:ILE:CD1	2.27	0.78
1:H:53:SER:OG	1:H:93:ASP:OD2	2.00	0.78
1:A:11:TRP:HZ3	1:A:60:ILE:O	1.67	0.78
1:B:236:VAL:O	1:B:240:THR:HG23	1.84	0.78
1:D:198:ASP:HB2	1:D:199:ALA:HB3	1.64	0.77
1:G:160:ALA:HB1	1:G:209:ILE:CD1	2.15	0.77
1:D:32:LEU:HD23	1:D:37:VAL:HB	1.67	0.77
1:B:257:ILE:HD12	1:B:257:ILE:C	2.04	0.77
1:C:99:GLU:N	1:C:99:GLU:OE1	2.18	0.76
1:D:89:LEU:HD21	1:D:91:ILE:HD11	1.66	0.76
1:F:112:LYS:NZ	1:F:257:ILE:HD13	2.01	0.76
1:D:116:LEU:HD11	1:D:257:ILE:CD1	2.16	0.76
1:F:100:GLY:HA2	1:F:102:TYR:H	1.50	0.76
1:D:204:ILE:HG22	1:D:205:PRO:HD2	1.67	0.76
1:H:172:LEU:HD12	1:H:172:LEU:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:VAL:HG23	1:D:228:GLY:O	1.86	0.75
1:C:258:ASP:C	6:C:338:HOH:O	2.25	0.75
1:G:134:VAL:HG21	1:G:188:VAL:HG21	1.68	0.75
1:E:64:VAL:HG13	1:E:65:VAL:HG13	1.67	0.75
1:D:53:SER:HB2	1:D:67:ILE:HG22	1.67	0.75
1:H:253:ASP:HB2	6:H:305:HOH:O	1.86	0.74
1:D:74:GLY:HA3	1:D:75:PRO:C	2.08	0.74
1:B:156:LYS:HE2	1:B:245:ASN:OD1	1.87	0.74
1:H:119:THR:O	1:H:119:THR:HG22	1.85	0.74
1:A:167:SER:OG	1:D:16:THR:HG22	1.88	0.73
1:B:214:ARG:HH11	1:D:214:ARG:CD	2.01	0.73
1:D:116:LEU:CD1	1:D:257:ILE:CD1	2.67	0.73
1:H:58:SER:OG	1:H:211:ASN:ND2	2.20	0.73
1:F:25:LEU:CD2	1:F:236:VAL:HG21	2.19	0.73
1:C:76:ARG:HA	6:C:332:HOH:O	1.89	0.73
1:A:110:ILE:HG13	6:A:343:HOH:O	1.89	0.73
1:F:25:LEU:HD21	1:F:236:VAL:HG21	1.71	0.72
1:A:56:VAL:HG22	1:A:91:ILE:HD11	1.70	0.72
1:B:165:GLN:OE1	1:B:215:CYS:HB2	1.90	0.72
1:D:116:LEU:HD13	1:D:257:ILE:HD11	1.72	0.72
1:B:223:LYS:HA	6:B:305:HOH:O	1.89	0.72
1:H:103:ILE:HD12	1:H:144:ALA:HB2	1.70	0.72
1:B:214:ARG:NH1	1:D:214:ARG:CD	2.53	0.71
1:G:188:VAL:HG23	6:G:329:HOH:O	1.88	0.71
1:H:250:ILE:CG2	1:H:256:LEU:HD11	2.20	0.71
1:C:103:ILE:HD13	1:C:140:LEU:HD13	1.72	0.71
1:H:134:VAL:CG1	1:H:188:VAL:HG11	2.20	0.71
1:F:257:ILE:N	6:F:313:HOH:O	2.24	0.71
1:B:42:ILE:HD11	1:B:239:ILE:HG21	1.72	0.70
1:C:28:LEU:HD13	1:C:236:VAL:HG12	1.73	0.70
1:D:257:ILE:CG2	6:D:321:HOH:O	2.37	0.70
1:H:75:PRO:O	1:H:76:ARG:C	2.29	0.70
1:B:223:LYS:CD	6:B:306:HOH:O	2.39	0.70
1:F:185:LEU:O	1:F:189:VAL:HG13	1.93	0.69
1:G:67:ILE:HD12	1:G:67:ILE:C	2.12	0.69
1:H:55:THR:HG23	1:H:209:ILE:HD13	1.74	0.69
1:G:98:ILE:HG22	6:G:326:HOH:O	1.92	0.69
1:A:202:SER:OG	1:A:203:ASP:O	2.10	0.69
1:B:185:LEU:O	1:B:189:VAL:HG13	1.91	0.69
1:D:69:PRO:HB3	3:D:281:GNP:O3'	1.91	0.69
1:F:31:ASN:HA	1:F:34:GLN:HE21	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:GLN:CB	1:H:72:SER:HB2	2.22	0.69
1:B:32:LEU:HD11	1:B:240:THR:HB	1.75	0.69
1:C:112:LYS:HD2	1:C:257:ILE:HG23	1.75	0.69
1:E:10:GLY:CA	1:E:83:SER:H	2.06	0.69
1:E:45:MET:CE	1:E:97:LEU:HD11	2.23	0.68
1:F:195:LEU:HD13	1:F:197:LYS:HG2	1.76	0.68
1:G:112:LYS:NZ	1:G:257:ILE:HG23	2.08	0.68
1:B:257:ILE:HD11	6:B:304:HOH:O	1.93	0.67
1:C:133:ARG:NH1	3:D:281:GNP:HNB3	1.92	0.67
1:G:160:ALA:HB1	1:G:209:ILE:HD11	1.76	0.67
1:G:187:GLN:NE2	6:G:329:HOH:O	2.28	0.67
1:B:64:VAL:CG1	1:B:80:VAL:HG11	2.25	0.67
1:F:112:LYS:HZ1	1:F:257:ILE:HD13	1.58	0.67
1:F:189:VAL:O	1:F:193:ALA:CB	2.32	0.67
1:G:134:VAL:CG2	1:G:188:VAL:HG21	2.23	0.67
1:D:32:LEU:HD12	1:D:240:THR:HG22	1.77	0.67
1:B:214:ARG:NH1	1:D:214:ARG:CG	2.49	0.66
1:H:183:GLU:HB3	6:H:309:HOH:O	1.96	0.66
1:D:11:TRP:CD1	1:D:14:ILE:HG22	2.30	0.66
1:H:204:ILE:HD13	1:H:204:ILE:C	2.16	0.66
1:C:47:LYS:HG2	1:C:98:ILE:HG21	1.78	0.66
1:G:202:SER:N	1:G:203:ASP:HA	2.11	0.66
1:F:42:ILE:HD12	1:F:89:LEU:HD11	1.78	0.66
1:A:101:GLY:CA	1:B:137:LEU:HD21	2.25	0.66
1:B:215:CYS:SG	1:B:223:LYS:HB2	2.36	0.66
1:D:32:LEU:CD2	1:D:37:VAL:HB	2.26	0.66
1:F:14:ILE:HG23	1:F:84:ARG:NH1	2.11	0.66
1:F:196:LYS:HE2	6:F:296:HOH:O	1.96	0.66
1:C:257:ILE:HG22	1:C:258:ASP:OD1	1.96	0.65
1:B:8:VAL:HG22	1:B:81:SER:HB2	1.78	0.65
1:B:18:ALA:N	1:B:222:GLU:OE1	2.30	0.65
1:F:169:PRO:HG3	6:F:317:HOH:O	1.97	0.65
1:G:102:TYR:CD1	6:H:306:HOH:O	2.48	0.65
1:B:28:LEU:HD13	1:B:236:VAL:HG12	1.79	0.65
1:C:255:ASN:C	6:C:340:HOH:O	2.35	0.65
1:F:146:THR:HB	1:F:193:ALA:O	1.97	0.65
1:A:11:TRP:HB2	1:A:83:SER:O	1.96	0.64
1:H:119:THR:O	1:H:119:THR:CG2	2.44	0.64
1:D:254:LYS:HA	1:D:257:ILE:HB	1.79	0.64
1:H:8:VAL:O	1:H:8:VAL:HG13	1.98	0.64
1:A:25:LEU:HD11	1:A:236:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:SER:N	1:H:203:ASP:HA	2.12	0.64
1:F:21:THR:O	1:F:25:LEU:HB2	1.98	0.64
1:A:106:MET:O	1:A:110:ILE:HG22	1.98	0.64
1:C:116:LEU:HD23	1:C:257:ILE:HD11	1.79	0.64
1:F:213:GLY:HA3	6:F:320:HOH:O	1.98	0.64
1:G:64:VAL:HG21	1:G:80:VAL:HG11	1.78	0.64
1:B:207:VAL:HG21	1:B:235:LEU:CD1	2.28	0.64
1:C:99:GLU:HG2	1:C:104:ASN:HB2	1.79	0.64
1:H:239:ILE:HG23	6:H:315:HOH:O	1.98	0.63
1:C:116:LEU:HD21	1:C:257:ILE:HD12	1.80	0.63
1:E:45:MET:HE1	1:E:97:LEU:HD11	1.80	0.63
1:F:254:LYS:O	1:F:255:ASN:CB	2.46	0.63
1:E:40:LEU:HD21	1:E:243:ALA:HB2	1.80	0.63
1:F:100:GLY:CA	1:F:102:TYR:H	2.10	0.63
1:G:160:ALA:HB1	1:G:209:ILE:HD12	1.79	0.63
1:H:70:PHE:O	1:H:71:GLN:CG	2.46	0.63
1:A:11:TRP:CH2	1:A:60:ILE:HA	2.34	0.63
1:C:98:ILE:C	1:C:99:GLU:OE1	2.37	0.63
1:B:201:ALA:N	1:B:202:SER:HA	2.14	0.63
1:C:10:GLY:HA2	1:C:82:ARG:CD	2.27	0.63
1:A:10:GLY:HA3	1:A:83:SER:H	1.64	0.62
1:G:72:SER:O	1:G:73:GLU:C	2.38	0.62
1:F:101:GLY:CA	1:F:137:LEU:HD21	2.28	0.62
1:D:40:LEU:HD11	1:D:243:ALA:HB1	1.81	0.62
1:D:53:SER:CB	1:D:67:ILE:HG22	2.30	0.62
1:B:158:ILE:CD1	1:B:238:THR:HG22	2.29	0.62
1:D:116:LEU:CD1	1:D:257:ILE:HD11	2.29	0.62
1:A:134:VAL:CG1	1:A:188:VAL:HG21	2.29	0.62
1:E:143:LYS:HE3	1:E:147:ASP:OD2	2.00	0.62
1:A:101:GLY:HA2	1:B:137:LEU:HD21	1.82	0.62
1:B:64:VAL:HG11	1:B:80:VAL:HG11	1.82	0.62
1:B:216:ASN:C	1:B:224:VAL:HG12	2.21	0.62
1:H:43:LEU:HD21	1:H:45:MET:SD	2.40	0.62
1:B:8:VAL:HG22	1:B:81:SER:CB	2.29	0.61
1:G:169:PRO:HA	1:H:214:ARG:NH2	2.15	0.61
1:G:21:THR:HG22	1:G:25:LEU:HD13	1.81	0.61
1:H:10:GLY:HA3	1:H:82:ARG:HD2	1.81	0.61
1:B:8:VAL:HG23	1:B:9:ARG:H	1.65	0.61
1:C:10:GLY:CA	1:C:82:ARG:HD2	2.28	0.61
1:C:143:LYS:HD2	1:E:102:TYR:CE2	2.35	0.61
1:E:101:GLY:HA3	1:F:101:GLY:HA3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:PRO:HB2	1:D:76:ARG:CA	2.23	0.61
1:E:64:VAL:HG11	1:E:80:VAL:HG21	1.82	0.61
1:D:98:ILE:HD12	1:D:137:LEU:HD22	1.83	0.61
1:F:172:LEU:HD22	1:F:176:GLU:HG2	1.83	0.61
1:H:250:ILE:HG23	1:H:256:LEU:CD1	2.30	0.60
1:F:165:GLN:HE21	1:F:165:GLN:HA	1.64	0.60
1:H:207:VAL:HG13	1:H:234:HIS:CD2	2.36	0.60
1:C:185:LEU:O	1:C:189:VAL:HG23	1.99	0.60
1:C:139:LYS:HG3	1:C:188:VAL:HG22	1.84	0.60
1:H:70:PHE:O	1:H:71:GLN:HG2	2.02	0.60
1:A:203:ASP:HB2	1:A:205:PRO:CD	2.26	0.60
1:C:103:ILE:CD1	1:C:140:LEU:HD22	2.30	0.60
1:D:29:LEU:O	1:D:33:LYS:HB2	2.02	0.60
1:G:9:ARG:HD2	6:G:295:HOH:O	2.01	0.60
1:C:65:VAL:HB	1:C:76:ARG:NH2	2.17	0.60
1:F:146:THR:HG21	1:F:193:ALA:O	2.00	0.60
1:D:36:ASP:OD1	1:D:36:ASP:O	2.19	0.59
1:E:67:ILE:HD11	1:F:170:ASP:OD1	2.02	0.59
1:E:232:ILE:HB	1:E:233:PRO:HD3	1.85	0.59
1:H:218:ASN:HD21	1:H:222:GLU:HB2	1.67	0.59
1:E:98:ILE:CD1	1:E:141:VAL:HG22	2.32	0.59
1:B:247:SER:N	1:B:248:GLU:HA	2.17	0.59
1:H:103:ILE:CD1	1:H:144:ALA:HB2	2.32	0.59
1:D:75:PRO:CB	1:D:76:ARG:HA	2.24	0.59
1:H:250:ILE:CG2	1:H:256:LEU:CD1	2.81	0.59
1:G:72:SER:O	1:G:74:GLY:N	2.35	0.59
1:A:203:ASP:CB	1:A:204:ILE:HA	2.27	0.59
1:E:10:GLY:HA3	1:E:83:SER:H	1.67	0.58
1:G:246:LYS:O	1:G:246:LYS:HG3	2.03	0.58
1:F:146:THR:CB	1:F:193:ALA:O	2.52	0.58
1:C:99:GLU:OE1	1:C:99:GLU:CA	2.51	0.58
1:B:57:ASN:OD1	1:B:65:VAL:HG22	2.04	0.58
1:D:202:SER:N	1:D:203:ASP:HA	2.18	0.58
1:H:75:PRO:HB3	1:H:95:PRO:HG3	1.86	0.58
1:H:74:GLY:HA3	6:H:293:HOH:O	2.02	0.58
1:H:88:THR:HG22	1:H:90:ASN:ND2	2.19	0.58
1:D:97:LEU:HD12	1:D:141:VAL:HG13	1.85	0.58
1:A:137:LEU:O	1:A:141:VAL:HG23	2.03	0.58
1:F:146:THR:CG2	1:F:193:ALA:O	2.52	0.57
1:C:76:ARG:HD2	6:C:292:HOH:O	2.04	0.57
1:C:10:GLY:HA3	1:C:83:SER:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:THR:HG23	1:G:233:PRO:HG3	1.85	0.57
1:G:133:ARG:NH1	3:H:281:GNP:O1G	2.36	0.57
1:D:27:GLU:O	1:D:30:GLY:N	2.37	0.57
1:D:203:ASP:N	1:D:204:ILE:HA	2.20	0.57
1:G:180:LYS:HB2	1:H:70:PHE:CZ	2.40	0.57
1:H:193:ALA:HB3	1:H:195:LEU:CD1	2.35	0.57
1:A:11:TRP:HH2	1:A:60:ILE:HA	1.70	0.57
1:A:110:ILE:CD1	6:A:343:HOH:O	2.51	0.57
1:H:90:ASN:N	1:H:90:ASN:HD22	2.02	0.57
1:D:67:ILE:HD12	1:D:67:ILE:O	2.04	0.57
1:D:75:PRO:HB3	1:D:95:PRO:CG	2.35	0.57
1:C:22:GLN:O	1:C:26:LEU:HG	2.03	0.56
1:E:40:LEU:HB2	1:E:87:PHE:HZ	1.70	0.56
1:E:196:LYS:O	1:E:196:LYS:HG2	2.05	0.56
1:F:63:ARG:HG3	1:G:171:GLY:HA3	1.86	0.56
1:A:110:ILE:CG1	6:A:343:HOH:O	2.51	0.56
1:E:24:LYS:HE3	1:E:222:GLU:OE2	2.06	0.56
1:F:98:ILE:HG21	1:F:137:LEU:HD13	1.86	0.56
1:G:112:LYS:HZ2	1:G:257:ILE:HG23	1.69	0.56
1:G:133:ARG:NH2	1:H:68:SER:O	2.38	0.56
1:H:71:GLN:CB	1:H:72:SER:CB	2.73	0.56
1:B:18:ALA:HB3	1:B:222:GLU:HB2	1.87	0.56
1:B:257:ILE:CD1	6:B:304:HOH:O	2.51	0.56
1:D:203:ASP:H	1:D:204:ILE:HA	1.70	0.56
1:G:169:PRO:HA	1:H:214:ARG:HH21	1.70	0.56
1:E:116:LEU:CD1	1:E:257:ILE:HG13	2.35	0.56
1:E:40:LEU:HD11	1:E:243:ALA:HB1	1.86	0.56
1:E:207:VAL:HG21	1:E:235:LEU:HD13	1.88	0.56
6:G:324:HOH:O	1:H:70:PHE:HD1	1.89	0.56
1:B:111:ILE:O	1:B:115:LEU:HD12	2.06	0.56
1:B:257:ILE:HD12	1:B:258:ASP:CB	2.36	0.56
1:C:103:ILE:CD1	1:C:140:LEU:HD13	2.36	0.56
1:D:71:GLN:HG2	6:D:301:HOH:O	2.05	0.56
1:D:89:LEU:CD2	1:D:91:ILE:HD11	2.33	0.56
1:C:76:ARG:C	6:C:332:HOH:O	2.43	0.56
1:B:220:SER:N	1:B:221:ASP:HA	2.21	0.55
1:B:32:LEU:HD23	1:B:40:LEU:HD12	1.88	0.55
1:A:214:ARG:HG3	1:A:214:ARG:HH11	1.71	0.55
1:C:98:ILE:O	1:C:98:ILE:CG2	2.52	0.55
1:D:113:SER:O	1:D:116:LEU:HB2	2.06	0.55
1:D:202:SER:HB3	1:D:203:ASP:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:SER:HB3	1:H:71:GLN:O	2.06	0.55
1:D:116:LEU:CD1	1:D:257:ILE:HD12	2.23	0.55
1:E:190:ARG:HG2	1:E:195:LEU:HB2	1.89	0.55
1:H:134:VAL:CG1	1:H:188:VAL:CG1	2.84	0.55
1:B:40:LEU:HD23	1:B:121:ASP:CB	2.37	0.55
1:C:60:ILE:HG22	1:C:60:ILE:O	2.07	0.55
1:C:116:LEU:CD2	1:C:257:ILE:HD11	2.35	0.55
1:G:83:SER:O	1:G:87:PHE:O	2.24	0.55
1:A:160:ALA:HB1	1:A:209:ILE:HD12	1.88	0.55
1:C:103:ILE:HD13	1:C:140:LEU:HD22	1.87	0.55
1:G:99:GLU:HG2	1:G:100:GLY:H	1.70	0.55
1:A:11:TRP:CE3	1:A:11:TRP:HA	2.41	0.55
1:H:40:LEU:HD23	1:H:42:ILE:HG13	1.88	0.55
1:B:48:GLY:HA3	1:B:52:LYS:NZ	2.22	0.55
1:H:59:ILE:HD11	1:H:235:LEU:HD21	1.88	0.55
1:B:257:ILE:CD1	1:B:258:ASP:N	2.65	0.54
1:D:127:ASP:OD1	1:D:128:ARG:N	2.40	0.54
1:F:14:ILE:HD12	1:F:25:LEU:HD12	1.90	0.54
1:C:102:TYR:CE1	1:E:143:LYS:HD2	2.42	0.54
1:D:11:TRP:HA	1:D:82:ARG:HD2	1.88	0.54
1:A:11:TRP:CZ3	1:A:60:ILE:O	2.53	0.54
1:A:202:SER:CB	1:A:203:ASP:C	2.76	0.54
1:B:111:ILE:HG22	1:B:115:LEU:CD1	2.37	0.54
1:C:116:LEU:CD2	1:C:257:ILE:CD1	2.84	0.54
1:H:185:LEU:O	1:H:189:VAL:HG23	2.07	0.54
1:B:257:ILE:C	1:B:257:ILE:CD1	2.76	0.54
1:D:223:LYS:NZ	6:D:306:HOH:O	2.30	0.54
1:G:123:LEU:HD22	1:G:153:ILE:HD13	1.90	0.54
1:H:10:GLY:H	1:H:82:ARG:HD3	1.73	0.54
1:D:14:ILE:HD12	1:D:25:LEU:HD12	1.88	0.54
1:C:232:ILE:HB	1:C:233:PRO:HD3	1.90	0.54
1:H:156:LYS:NZ	1:H:248:GLU:C	2.61	0.54
1:F:64:VAL:HG11	1:F:80:VAL:HG11	1.90	0.53
1:C:67:ILE:HG13	1:C:67:ILE:O	2.08	0.53
1:A:175:ASP:HB3	6:D:302:HOH:O	2.08	0.53
1:B:257:ILE:HD12	1:B:258:ASP:HB2	1.90	0.53
1:D:33:LYS:CD	1:D:85:ALA:O	2.56	0.53
1:D:72:SER:HB3	1:D:73:GLU:HA	1.91	0.53
1:B:257:ILE:HD12	1:B:258:ASP:CA	2.38	0.53
1:H:88:THR:HG22	1:H:90:ASN:HD21	1.73	0.53
1:D:193:ALA:HB3	1:D:195:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ASN:OD1	1:F:65:VAL:HG22	2.09	0.53
1:C:116:LEU:HD21	1:C:257:ILE:CD1	2.38	0.53
1:E:24:LYS:HD2	1:E:233:PRO:HB3	1.90	0.53
1:F:187:GLN:HA	1:F:187:GLN:OE1	2.09	0.53
1:F:223:LYS:CE	4:F:290:PGE:H5	2.39	0.53
1:F:223:LYS:HE3	4:F:290:PGE:H5	1.90	0.53
1:B:185:LEU:O	1:B:189:VAL:CG1	2.57	0.53
1:D:11:TRP:CG	1:D:14:ILE:HG22	2.44	0.53
1:F:42:ILE:CD1	1:F:89:LEU:HD11	2.38	0.53
1:D:37:VAL:CA	6:D:295:HOH:O	2.57	0.53
1:E:45:MET:HE2	1:E:97:LEU:HD11	1.91	0.53
1:G:70:PHE:HD1	6:H:299:HOH:O	1.91	0.53
1:E:102:TYR:HE1	1:F:102:TYR:HH	1.56	0.53
1:C:97:LEU:CD2	1:C:108:LEU:HD13	2.39	0.52
1:G:67:ILE:CD1	1:G:67:ILE:C	2.73	0.52
5:G:290:GOL:H11	6:G:331:HOH:O	2.09	0.52
1:F:108:LEU:HA	1:F:111:ILE:HD12	1.91	0.52
1:B:165:GLN:HB2	1:B:210:GLU:HG2	1.91	0.52
1:B:21:THR:HG22	1:B:25:LEU:HD12	1.92	0.52
1:C:55:THR:HG23	1:C:209:ILE:HD12	1.91	0.52
1:D:75:PRO:HB3	1:D:95:PRO:HG2	1.91	0.52
1:F:210:GLU:OE1	1:F:212:SER:HB3	2.09	0.52
1:H:203:ASP:CB	1:H:204:ILE:HA	2.39	0.52
1:B:55:THR:O	1:B:59:ILE:HG13	2.09	0.52
1:C:101:GLY:HA3	1:D:101:GLY:HA3	1.90	0.52
1:E:10:GLY:HA2	1:E:83:SER:H	1.75	0.52
1:H:165:GLN:HB2	1:H:210:GLU:HG2	1.92	0.52
1:C:133:ARG:NH2	1:D:71:GLN:O	2.43	0.52
1:F:232:ILE:HD12	6:F:326:HOH:O	2.08	0.52
1:H:169:PRO:O	1:H:170:ASP:O	2.28	0.52
1:B:223:LYS:HD3	6:B:306:HOH:O	2.07	0.52
1:C:28:LEU:CD1	1:C:236:VAL:HG12	2.38	0.51
1:F:242:VAL:HA	1:F:245:ASN:HB3	1.92	0.51
1:G:232:ILE:HB	1:G:233:PRO:HD3	1.92	0.51
1:F:149:PHE:HA	1:F:256:LEU:HD23	1.93	0.51
1:G:99:GLU:HG2	1:G:100:GLY:N	2.26	0.51
1:B:190:ARG:HH21	1:B:204:ILE:CG2	2.23	0.51
1:C:218:ASN:HB3	1:C:224:VAL:HG11	1.92	0.51
1:E:141:VAL:O	1:E:144:ALA:HB3	2.11	0.51
1:F:8:VAL:CG2	1:F:83:SER:OG	2.59	0.51
1:C:207:VAL:HA	5:C:291:GOL:H31	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:SER:N	1:G:203:ASP:CA	2.74	0.51
1:A:7:THR:HB	6:A:332:HOH:O	2.09	0.51
1:D:160:ALA:HB1	1:D:209:ILE:HD11	1.90	0.51
1:B:134:VAL:O	1:B:135:ASP:HB3	2.11	0.50
1:C:103:ILE:HD13	1:C:140:LEU:CD1	2.40	0.50
1:F:112:LYS:HZ3	1:F:257:ILE:HD13	1.74	0.50
1:A:3:SER:HB2	6:A:335:HOH:O	2.11	0.50
1:A:11:TRP:CD2	1:A:14:ILE:HG13	2.47	0.50
1:C:55:THR:CG2	1:C:209:ILE:HD12	2.41	0.50
1:F:97:LEU:HD12	1:F:141:VAL:HG13	1.94	0.50
1:F:165:GLN:HB2	1:F:210:GLU:HG3	1.93	0.50
1:A:103:ILE:CG2	1:A:104:ASN:N	2.74	0.50
1:A:105:ASP:O	1:A:109:ASN:ND2	2.44	0.50
1:F:170:ASP:N	1:F:171:GLY:HA2	2.26	0.50
1:F:256:LEU:O	1:F:257:ILE:CG2	2.60	0.50
1:H:146:THR:HA	1:H:150:GLY:HA2	1.93	0.50
1:B:13:GLY:HA3	1:B:60:ILE:O	2.12	0.50
1:D:64:VAL:HG21	1:D:80:VAL:HG11	1.93	0.50
1:G:98:ILE:HD13	1:G:103:ILE:HD12	1.93	0.50
1:H:156:LYS:NZ	1:H:248:GLU:O	2.43	0.50
1:B:223:LYS:NZ	6:B:306:HOH:O	2.43	0.50
1:F:146:THR:HG21	1:F:193:ALA:C	2.32	0.50
1:E:107:ALA:O	1:E:111:ILE:HG13	2.11	0.50
1:F:213:GLY:CA	6:F:320:HOH:O	2.58	0.50
1:H:9:ARG:C	6:H:316:HOH:O	2.50	0.50
1:G:98:ILE:CD1	1:G:103:ILE:HD12	2.42	0.49
1:D:202:SER:CB	1:D:203:ASP:HA	2.41	0.49
1:E:98:ILE:HD13	1:E:141:VAL:CG2	2.39	0.49
1:A:217:LYS:HA	1:A:222:GLU:O	2.12	0.49
1:B:222:GLU:HG3	1:B:223:LYS:H	1.78	0.49
1:D:120:ILE:HD12	1:D:252:VAL:CG2	2.43	0.49
1:B:246:LYS:HB3	1:B:247:SER:HA	1.79	0.49
1:H:146:THR:O	1:H:150:GLY:CA	2.61	0.49
1:B:57:ASN:ND2	1:B:65:VAL:HG23	2.27	0.49
1:E:12:SER:O	1:E:15:ASN:HB2	2.13	0.49
1:E:21:THR:HG23	1:E:233:PRO:HG3	1.94	0.49
1:E:78:VAL:O	1:E:92:ILE:HA	2.12	0.49
1:E:225:LEU:HD21	1:E:231:TRP:HB3	1.93	0.49
1:A:64:VAL:HG21	1:A:80:VAL:HG11	1.95	0.49
1:B:14:ILE:CD1	1:B:22:GLN:HG2	2.43	0.49
1:F:11:TRP:O	1:F:14:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:GLU:HB3	1:F:74:GLY:HA2	1.94	0.49
1:A:11:TRP:HA	1:A:11:TRP:HE3	1.78	0.49
1:D:33:LYS:HD2	1:D:85:ALA:O	2.14	0.48
1:D:72:SER:CB	1:D:73:GLU:HA	2.42	0.48
1:A:56:VAL:HG22	1:A:91:ILE:CD1	2.41	0.48
1:B:9:ARG:O	1:B:82:ARG:HA	2.13	0.48
1:C:45:MET:HA	6:C:337:HOH:O	2.14	0.48
1:F:48:GLY:O	1:F:50:VAL:HG13	2.13	0.48
1:E:47:LYS:O	1:E:52:LYS:NZ	2.46	0.48
1:F:225:LEU:CD2	1:F:231:TRP:HB3	2.39	0.48
1:G:67:ILE:CD1	6:G:327:HOH:O	2.61	0.48
1:G:84:ARG:HA	1:G:84:ARG:HD3	1.51	0.48
1:G:174:TYR:CE2	1:G:226:PRO:HG2	2.49	0.48
1:H:28:LEU:CD1	1:H:236:VAL:HG12	2.39	0.48
1:E:160:ALA:HB1	1:E:209:ILE:CD1	2.40	0.48
1:A:133:ARG:HD2	1:B:71:GLN:HA	1.95	0.48
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.26	0.48
1:D:157:ALA:O	1:D:204:ILE:HG22	2.13	0.48
1:G:168:PRO:O	1:H:214:ARG:NH2	2.47	0.48
1:F:214:ARG:NH1	6:F:318:HOH:O	2.46	0.48
1:H:51:GLY:O	1:H:55:THR:OG1	2.30	0.48
1:H:108:LEU:HA	1:H:111:ILE:HD12	1.95	0.48
1:B:190:ARG:HH21	1:B:204:ILE:HG22	1.78	0.47
1:D:111:ILE:O	1:D:115:LEU:CD2	2.62	0.47
1:E:168:PRO:HG2	1:E:174:TYR:HA	1.96	0.47
1:A:110:ILE:HD12	6:A:343:HOH:O	2.14	0.47
1:B:216:ASN:N	1:B:216:ASN:ND2	2.63	0.47
1:C:121:ASP:O	1:C:156:LYS:HD2	2.14	0.47
1:D:36:ASP:OD1	1:D:36:ASP:C	2.52	0.47
1:D:215:CYS:SG	1:D:223:LYS:HB3	2.54	0.47
1:B:98:ILE:HD12	1:B:137:LEU:HB2	1.95	0.47
1:F:99:GLU:O	1:F:99:GLU:HG3	2.14	0.47
1:A:251:PHE:O	1:A:256:LEU:HD13	2.14	0.47
1:C:53:SER:OG	1:C:93:ASP:OD2	2.33	0.47
1:E:60:ILE:HG22	1:E:62:GLU:HG3	1.97	0.47
1:E:196:LYS:O	1:E:196:LYS:CG	2.63	0.47
1:C:229:ILE:HD12	5:C:291:GOL:O1	2.14	0.47
1:D:232:ILE:N	1:D:233:PRO:HD2	2.29	0.47
1:A:10:GLY:CA	1:A:83:SER:H	2.28	0.47
1:A:25:LEU:HD11	1:A:236:VAL:CG2	2.45	0.47
1:A:67:ILE:HG22	6:A:340:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLY:HA3	1:C:82:ARG:HA	1.97	0.47
1:B:40:LEU:HD23	1:B:121:ASP:HB3	1.97	0.47
1:D:31:ASN:H	1:D:31:ASN:ND2	2.13	0.47
1:F:132:TYR:O	1:F:133:ARG:HD3	2.15	0.47
1:A:71:GLN:O	1:A:72:SER:HB2	2.15	0.47
1:A:149:PHE:HA	1:A:256:LEU:HD23	1.96	0.47
1:F:64:VAL:HG13	1:F:80:VAL:HG21	1.96	0.47
1:F:209:ILE:HG23	1:F:231:TRP:CZ3	2.49	0.47
1:B:48:GLY:HA3	1:B:52:LYS:HZ2	1.80	0.47
1:E:98:ILE:HG12	1:E:137:LEU:HD21	1.96	0.47
1:D:34:GLN:O	1:D:36:ASP:HA	2.15	0.47
1:F:165:GLN:HB2	1:F:210:GLU:CG	2.45	0.47
1:D:120:ILE:HD12	1:D:252:VAL:HG23	1.97	0.46
1:H:251:PHE:CE2	1:H:253:ASP:OD1	2.67	0.46
1:B:25:LEU:HD23	1:B:236:VAL:HG11	1.97	0.46
1:F:165:GLN:O	1:F:165:GLN:HG3	2.16	0.46
1:C:76:ARG:CA	6:C:332:HOH:O	2.55	0.46
1:D:75:PRO:HB3	1:D:95:PRO:HG3	1.97	0.46
1:G:134:VAL:HG21	1:G:188:VAL:CG2	2.40	0.46
1:A:202:SER:N	1:A:203:ASP:CA	2.78	0.46
1:B:75:PRO:HA	1:B:95:PRO:HG3	1.97	0.46
1:C:102:TYR:CZ	1:E:143:LYS:HD2	2.50	0.46
1:D:198:ASP:HB2	1:D:199:ALA:CB	2.39	0.46
1:B:42:ILE:HD11	1:B:239:ILE:CG2	2.42	0.46
1:B:43:LEU:HG	1:B:45:MET:HG3	1.97	0.46
1:D:11:TRP:O	1:D:14:ILE:CG2	2.63	0.46
1:D:111:ILE:HG23	1:D:115:LEU:HD21	1.98	0.46
1:A:10:GLY:HA3	1:A:83:SER:O	2.16	0.46
1:B:165:GLN:OE1	1:B:215:CYS:CB	2.62	0.46
1:C:28:LEU:HD23	6:C:336:HOH:O	2.16	0.46
1:D:224:VAL:HG22	1:D:225:LEU:O	2.15	0.46
1:F:17:PHE:CD1	4:F:290:PGE:H4	2.51	0.46
1:H:98:ILE:HG22	1:H:100:GLY:O	2.15	0.46
1:E:40:LEU:HD21	1:E:243:ALA:CB	2.46	0.46
1:A:11:TRP:HD1	1:A:84:ARG:HB2	1.81	0.46
1:D:56:VAL:HG21	1:D:93:ASP:HB2	1.98	0.46
1:E:123:LEU:HD22	1:E:153:ILE:HD13	1.98	0.46
1:H:197:LYS:HA	6:H:298:HOH:O	2.16	0.46
1:A:170:ASP:OD1	1:B:63:ARG:NH2	2.49	0.46
1:C:235:LEU:HG	1:C:239:ILE:HD12	1.98	0.46
1:D:55:THR:O	1:D:59:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:GLU:HG2	1:D:74:GLY:N	2.28	0.46
1:A:214:ARG:HH11	1:A:214:ARG:CG	2.28	0.45
1:B:122:VAL:HG21	1:B:239:ILE:HG23	1.97	0.45
1:B:210:GLU:HG3	1:B:212:SER:HB3	1.97	0.45
1:D:134:VAL:HG13	1:D:188:VAL:HG11	1.98	0.45
1:E:25:LEU:C	1:E:25:LEU:HD23	2.36	0.45
1:F:254:LYS:O	1:F:255:ASN:HB2	2.15	0.45
1:G:217:LYS:HA	1:G:222:GLU:O	2.16	0.45
1:E:44:VAL:HG13	1:E:92:ILE:O	2.15	0.45
1:E:102:TYR:HH	1:F:102:TYR:HE2	1.59	0.45
1:H:44:VAL:HG22	1:H:44:VAL:O	2.15	0.45
1:H:250:ILE:N	1:H:250:ILE:HD12	2.31	0.45
1:A:217:LYS:HD3	1:A:221:ASP:OD1	2.17	0.45
1:B:60:ILE:HG21	1:B:64:VAL:HG21	1.98	0.45
1:B:165:GLN:CD	1:B:216:ASN:HD21	2.20	0.45
1:B:214:ARG:NH1	1:D:214:ARG:HD2	2.31	0.45
1:C:10:GLY:HA3	1:C:82:ARG:CA	2.47	0.45
1:D:43:LEU:HD13	1:D:115:LEU:HD11	1.99	0.45
1:D:57:ASN:OD1	1:D:65:VAL:HG22	2.17	0.45
1:H:188:VAL:O	1:H:188:VAL:CG2	2.64	0.45
1:H:207:VAL:CG1	1:H:234:HIS:HD2	2.29	0.45
1:A:60:ILE:HD12	1:A:82:ARG:HG3	1.99	0.45
1:H:169:PRO:O	1:H:170:ASP:C	2.53	0.45
1:A:64:VAL:CG2	1:A:80:VAL:HG21	2.47	0.45
1:B:107:ALA:O	1:B:111:ILE:HG13	2.16	0.45
1:F:17:PHE:HD1	4:F:290:PGE:H4	1.81	0.45
1:F:223:LYS:CD	6:F:324:HOH:O	2.64	0.45
1:H:53:SER:HA	1:H:56:VAL:HG13	1.98	0.45
1:F:186:LEU:O	1:F:190:ARG:HG3	2.16	0.45
1:H:10:GLY:HA3	1:H:11:TRP:HA	1.70	0.45
1:B:169:PRO:O	1:B:171:GLY:N	2.49	0.45
1:D:189:VAL:O	1:D:193:ALA:HB2	2.16	0.45
1:F:25:LEU:HD22	1:F:236:VAL:HG21	1.98	0.45
1:H:20:ALA:HB2	1:H:220:SER:HB3	1.99	0.45
1:A:103:ILE:HD13	1:A:140:LEU:HB3	1.98	0.45
1:C:98:ILE:HD11	1:C:137:LEU:CD1	2.34	0.45
1:E:197:LYS:HB2	6:E:330:HOH:O	2.16	0.45
1:H:50:VAL:HG11	1:H:126:VAL:O	2.16	0.45
1:H:146:THR:O	1:H:150:GLY:HA2	2.17	0.45
1:A:230:ALA:O	1:A:233:PRO:HD2	2.17	0.45
1:F:43:LEU:HD22	1:F:120:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:TRP:CH2	1:G:14:ILE:HD11	2.52	0.45
1:H:17:PHE:O	1:H:22:GLN:NE2	2.47	0.45
1:H:83:SER:N	6:H:316:HOH:O	2.50	0.45
1:A:202:SER:N	1:A:203:ASP:HA	2.32	0.44
1:C:185:LEU:O	1:C:188:VAL:HG12	2.17	0.44
1:D:165:GLN:OE1	1:D:215:CYS:HA	2.17	0.44
1:F:101:GLY:CA	1:F:137:LEU:CD2	2.94	0.44
1:B:106:MET:O	1:B:110:ILE:HG13	2.17	0.44
1:C:76:ARG:HG2	1:C:95:PRO:HD3	1.99	0.44
1:F:75:PRO:HA	1:F:95:PRO:HG3	1.99	0.44
1:B:208:LEU:HB3	1:B:225:LEU:HD13	2.00	0.44
1:C:234:HIS:CD2	5:C:291:GOL:H32	2.52	0.44
1:D:25:LEU:HD22	1:D:236:VAL:HG21	1.99	0.44
1:F:101:GLY:HA3	1:F:137:LEU:CD2	2.39	0.44
1:G:227:ASN:HD21	5:G:291:GOL:H31	1.81	0.44
1:H:28:LEU:HA	1:H:31:ASN:HD21	1.82	0.44
1:A:103:ILE:HG23	1:A:104:ASN:N	2.31	0.44
1:B:111:ILE:HG22	1:B:115:LEU:HD11	1.99	0.44
1:B:53:SER:OG	1:B:93:ASP:OD2	2.34	0.44
1:B:115:LEU:HD13	1:B:149:PHE:CZ	2.52	0.44
1:D:146:THR:HG21	1:D:193:ALA:O	2.18	0.44
1:F:103:ILE:HD11	1:F:140:LEU:O	2.17	0.44
1:F:168:PRO:HG2	1:F:174:TYR:HA	1.99	0.44
1:G:102:TYR:CE1	6:H:306:HOH:O	2.71	0.44
1:G:131:ALA:HB3	1:G:181:ARG:NH2	2.31	0.44
1:H:50:VAL:CG1	1:H:126:VAL:HG12	2.47	0.44
1:A:72:SER:CB	1:A:73:GLU:HA	2.48	0.44
1:C:97:LEU:HD22	1:C:108:LEU:HD13	1.99	0.44
1:C:133:ARG:NH1	3:D:281:GNP:N3B	2.63	0.44
1:H:52:LYS:NZ	3:H:281:GNP:O3G	2.41	0.44
1:H:134:VAL:HG12	1:H:188:VAL:HG11	1.98	0.44
1:A:227:ASN:HD21	5:A:291:GOL:H32	1.83	0.44
1:B:32:LEU:CD2	1:B:40:LEU:HD12	2.47	0.44
1:E:217:LYS:HA	1:E:222:GLU:O	2.18	0.44
1:F:32:LEU:HD13	1:F:87:PHE:CE2	2.53	0.44
1:F:112:LYS:CE	1:F:257:ILE:HG21	2.48	0.44
1:G:112:LYS:HZ1	1:G:257:ILE:HG23	1.80	0.44
1:H:150:GLY:O	1:H:152:GLY:N	2.51	0.44
1:B:8:VAL:HG22	1:B:81:SER:HB3	1.99	0.43
1:C:60:ILE:O	1:C:60:ILE:CG2	2.65	0.43
1:H:59:ILE:HD11	1:H:235:LEU:CD2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:CG	1:A:74:GLY:N	2.81	0.43
1:A:218:ASN:HB3	1:A:224:VAL:HG11	2.00	0.43
1:B:127:ASP:OD1	1:B:128:ARG:N	2.50	0.43
1:H:203:ASP:CB	1:H:204:ILE:CA	2.96	0.43
1:G:11:TRP:CZ3	1:G:14:ILE:HD11	2.53	0.43
1:A:95:PRO:HD2	1:A:111:ILE:HD11	2.01	0.43
1:B:216:ASN:C	6:B:305:HOH:O	2.56	0.43
1:C:17:PHE:O	1:C:18:ALA:C	2.54	0.43
1:C:99:GLU:OE1	1:C:99:GLU:HA	2.18	0.43
1:D:91:ILE:HD12	1:D:91:ILE:HG23	1.73	0.43
1:H:193:ALA:HB3	1:H:195:LEU:HD11	2.00	0.43
1:H:196:LYS:N	6:H:313:HOH:O	2.51	0.43
1:A:28:LEU:O	1:A:31:ASN:HB2	2.18	0.43
1:D:116:LEU:HD13	1:D:257:ILE:CD1	2.38	0.43
1:E:180:LYS:HB2	1:F:70:PHE:CE1	2.53	0.43
1:G:31:ASN:O	1:G:34:GLN:HB3	2.17	0.43
1:A:57:ASN:HD22	1:A:67:ILE:HD11	1.84	0.43
1:E:217:LYS:HD3	1:E:221:ASP:OD1	2.19	0.43
1:E:234:HIS:HE1	6:E:319:HOH:O	2.01	0.43
1:F:43:LEU:HD22	1:F:120:ILE:CD1	2.49	0.43
1:F:112:LYS:HE2	1:F:257:ILE:HG21	2.00	0.43
1:F:169:PRO:C	1:F:171:GLY:HA2	2.39	0.43
1:G:26:LEU:HD23	1:G:29:LEU:HD12	2.00	0.43
1:H:55:THR:O	1:H:59:ILE:HG12	2.18	0.43
1:H:165:GLN:HE21	1:H:226:PRO:HG3	1.84	0.43
1:A:33:LYS:NZ	1:A:38:ASN:OD1	2.37	0.43
1:A:202:SER:CB	1:A:203:ASP:O	2.67	0.43
1:C:40:LEU:HD12	1:C:121:ASP:CB	2.48	0.43
1:D:170:ASP:HB2	1:D:172:LEU:HG	2.00	0.43
1:F:100:GLY:HA3	1:F:101:GLY:HA2	1.85	0.43
1:E:170:ASP:N	6:F:318:HOH:O	2.52	0.43
1:H:13:GLY:HA3	1:H:60:ILE:O	2.18	0.43
1:B:48:GLY:HA2	1:B:50:VAL:HG13	2.01	0.43
1:C:68:SER:HA	1:C:69:PRO:HD3	1.91	0.43
1:D:161:LEU:HD21	1:D:185:LEU:CD2	2.49	0.43
1:A:116:LEU:CD2	1:A:257:ILE:HD13	2.45	0.43
1:B:207:VAL:HG12	1:B:234:HIS:CD2	2.54	0.43
1:E:116:LEU:HD11	1:E:257:ILE:HG13	2.00	0.43
1:F:112:LYS:HZ3	1:F:257:ILE:CD1	2.32	0.43
1:H:82:ARG:HA	6:H:316:HOH:O	2.19	0.43
1:H:164:ALA:CB	1:H:225:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG2	1:A:180:LYS:HZ3	1.84	0.42
1:B:249:SER:C	1:B:250:ILE:HD12	2.39	0.42
1:C:17:PHE:O	1:C:22:GLN:NE2	2.48	0.42
1:A:128:ARG:O	1:A:181:ARG:NH2	2.47	0.42
1:A:134:VAL:HG11	1:A:188:VAL:HG21	2.02	0.42
1:B:223:LYS:HD2	6:B:306:HOH:O	2.13	0.42
1:D:198:ASP:CB	1:D:199:ALA:CB	2.80	0.42
1:F:169:PRO:O	1:F:171:GLY:HA2	2.19	0.42
1:G:255:ASN:HA	1:G:258:ASP:HB2	2.02	0.42
1:H:103:ILE:CD1	1:H:144:ALA:CB	2.97	0.42
1:C:24:LYS:O	1:C:28:LEU:HG	2.19	0.42
1:E:245:ASN:OD1	1:E:245:ASN:C	2.58	0.42
1:F:146:THR:HB	1:F:154:TRP:HE1	1.84	0.42
1:G:41:THR:HA	1:G:90:ASN:O	2.19	0.42
1:C:62:GLU:HB2	1:C:64:VAL:HG13	2.01	0.42
1:D:14:ILE:HG21	1:D:14:ILE:HD13	1.81	0.42
1:F:31:ASN:HA	1:F:34:GLN:HB2	2.00	0.42
1:F:111:ILE:HG22	1:F:115:LEU:CD2	2.49	0.42
1:H:102:TYR:HE1	6:H:306:HOH:O	2.01	0.42
1:C:99:GLU:CG	1:C:104:ASN:HD22	2.33	0.42
1:C:256:LEU:N	6:C:340:HOH:O	2.52	0.42
1:H:183:GLU:OE1	1:H:183:GLU:HA	2.19	0.42
1:B:222:GLU:HG3	1:B:223:LYS:HG2	2.01	0.42
1:C:25:LEU:O	1:C:29:LEU:HG	2.20	0.42
1:C:117:ASP:N	1:C:252:VAL:O	2.52	0.42
1:D:111:ILE:O	1:D:115:LEU:HD22	2.20	0.42
1:D:111:ILE:HG22	1:D:115:LEU:HD23	2.02	0.42
1:E:8:VAL:O	1:E:8:VAL:HG13	2.20	0.42
1:E:99:GLU:HB2	1:E:104:ASN:HB2	2.01	0.42
1:H:89:LEU:HD21	1:H:91:ILE:HD11	2.02	0.42
1:B:257:ILE:CD1	1:B:258:ASP:HB2	2.49	0.42
1:C:186:LEU:O	1:C:190:ARG:HG3	2.20	0.42
1:E:64:VAL:CG1	1:E:80:VAL:HG21	2.47	0.42
1:E:103:ILE:HD11	1:E:144:ALA:HB2	2.00	0.42
1:G:73:GLU:HG3	6:G:312:HOH:O	2.19	0.42
1:A:72:SER:HA	1:B:133:ARG:NH2	2.35	0.42
1:C:133:ARG:HH12	3:D:281:GNP:HNB3	1.65	0.42
1:H:104:ASN:HB3	1:H:107:ALA:HB3	2.00	0.42
1:A:133:ARG:HH21	3:B:281:GNP:HNB3	1.67	0.42
1:H:208:LEU:HB2	1:H:225:LEU:HD13	2.02	0.42
1:B:111:ILE:HG22	1:B:115:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:HD12	1:B:250:ILE:N	2.35	0.42
1:C:67:ILE:HD12	3:C:281:GNP:C2'	2.50	0.42
1:C:72:SER:HA	1:C:73:GLU:HA	1.96	0.42
1:C:73:GLU:HB2	1:C:74:GLY:O	2.20	0.42
1:F:31:ASN:CA	1:F:34:GLN:HE21	2.29	0.42
1:F:81:SER:HA	1:F:89:LEU:O	2.20	0.42
1:H:70:PHE:O	1:H:71:GLN:HG3	2.20	0.42
1:H:88:THR:CG2	1:H:90:ASN:HD21	2.32	0.42
1:A:170:ASP:CG	1:B:63:ARG:HH22	2.23	0.41
1:B:43:LEU:HD12	1:B:92:ILE:HB	2.02	0.41
1:C:98:ILE:HD12	1:C:137:LEU:HD11	1.94	0.41
1:D:32:LEU:HD12	1:D:240:THR:CG2	2.48	0.41
1:D:53:SER:HB3	1:D:65:VAL:CG2	2.50	0.41
1:H:204:ILE:C	1:H:204:ILE:CD1	2.88	0.41
1:D:74:GLY:HA3	1:D:75:PRO:O	2.20	0.41
1:F:8:VAL:HG21	1:F:83:SER:OG	2.20	0.41
5:G:290:GOL:C1	6:G:331:HOH:O	2.68	0.41
1:A:46:GLY:O	1:A:96:GLY:HA2	2.20	0.41
1:B:158:ILE:HD11	1:B:238:THR:HG22	1.99	0.41
1:B:220:SER:HB2	1:B:221:ASP:C	2.41	0.41
1:G:66:SER:HB2	1:G:73:GLU:HG2	2.02	0.41
1:C:18:ALA:HB2	1:C:221:ASP:O	2.20	0.41
1:G:43:LEU:O	1:G:123:LEU:HD12	2.20	0.41
1:E:102:TYR:OH	1:F:102:TYR:CE2	2.66	0.41
1:E:170:ASP:O	1:H:63:ARG:HD2	2.20	0.41
1:H:40:LEU:CD2	1:H:42:ILE:HG13	2.50	0.41
1:A:123:LEU:HD12	1:A:124:LEU:N	2.36	0.41
1:B:78:VAL:O	1:B:92:ILE:HA	2.21	0.41
1:D:32:LEU:CD1	1:D:240:THR:HG22	2.46	0.41
1:D:32:LEU:HD11	1:D:40:LEU:HD21	2.02	0.41
1:H:125:TYR:O	1:H:159:VAL:HA	2.21	0.41
1:A:64:VAL:HG21	1:A:80:VAL:HG21	2.03	0.41
1:C:257:ILE:CG2	1:C:258:ASP:OD1	2.68	0.41
1:E:168:PRO:HA	1:E:169:PRO:HD3	1.80	0.41
1:G:83:SER:O	1:G:84:ARG:C	2.59	0.41
1:G:178:PHE:CD1	1:G:208:LEU:HD21	2.55	0.41
1:H:124:LEU:HD12	1:H:158:ILE:HB	2.03	0.41
1:E:138:ASP:HB2	1:E:188:VAL:HG11	2.02	0.41
1:F:99:GLU:O	1:F:99:GLU:CG	2.68	0.41
1:G:108:LEU:O	1:G:112:LYS:HG3	2.21	0.41
1:H:32:LEU:HD11	1:H:240:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:SER:N	1:H:203:ASP:CA	2.83	0.41
1:B:63:ARG:HD2	1:C:170:ASP:O	2.21	0.41
1:C:45:MET:CE	1:C:97:LEU:HD11	2.51	0.41
1:D:72:SER:HB2	1:F:106:MET:HE1	2.03	0.41
1:E:211:ASN:O	1:E:212:SER:C	2.59	0.41
1:G:21:THR:HG23	1:G:233:PRO:HD3	2.02	0.41
1:G:45:MET:CE	1:G:97:LEU:HD11	2.51	0.41
1:G:67:ILE:HG12	1:H:170:ASP:OD2	2.21	0.41
1:H:28:LEU:HD11	1:H:237:GLN:HB2	2.03	0.41
1:H:217:LYS:HD3	1:H:221:ASP:HB2	2.03	0.41
1:A:70:PHE:HD1	6:A:324:HOH:O	2.04	0.41
1:B:161:LEU:HB2	1:B:208:LEU:HD23	2.03	0.41
1:C:8:VAL:CA	6:C:300:HOH:O	2.69	0.41
1:E:60:ILE:HG13	1:E:80:VAL:HG11	2.03	0.41
1:A:5:GLN:O	1:A:5:GLN:HG3	2.21	0.40
1:C:73:GLU:HB2	1:C:74:GLY:C	2.41	0.40
1:H:21:THR:CG2	1:H:233:PRO:HD3	2.50	0.40
1:D:116:LEU:HD12	1:D:116:LEU:HA	1.89	0.40
1:D:223:LYS:O	1:D:230:ALA:HA	2.21	0.40
1:F:254:LYS:O	1:F:255:ASN:HB3	2.21	0.40
1:G:67:ILE:HD11	6:G:327:HOH:O	2.19	0.40
1:H:168:PRO:HG2	1:H:174:TYR:HA	2.03	0.40
1:A:151:LYS:HD2	1:A:195:LEU:HD23	2.03	0.40
1:D:157:ALA:O	1:D:204:ILE:CG2	2.70	0.40
1:E:225:LEU:HB2	1:E:227:ASN:OD1	2.21	0.40
1:G:106:MET:HE2	6:G:328:HOH:O	2.21	0.40
1:H:127:ASP:O	1:H:161:LEU:HA	2.21	0.40
1:B:222:GLU:HG3	1:B:223:LYS:N	2.36	0.40
1:C:133:ARG:NH1	3:D:281:GNP:O1G	2.54	0.40
1:H:195:LEU:HD22	6:H:313:HOH:O	2.20	0.40
1:A:232:ILE:O	1:A:236:VAL:HG23	2.22	0.40
1:C:229:ILE:HD12	5:C:291:GOL:C1	2.51	0.40
1:E:29:LEU:HD22	1:E:87:PHE:CD2	2.57	0.40
1:H:115:LEU:HA	1:H:115:LEU:HD22	1.82	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	248/274 (90%)	234 (94%)	13 (5%)	1 (0%)	34 66
1	B	235/274 (86%)	204 (87%)	25 (11%)	6 (3%)	5 18
1	C	242/274 (88%)	222 (92%)	17 (7%)	3 (1%)	13 39
1	D	241/274 (88%)	216 (90%)	17 (7%)	8 (3%)	4 13
1	E	244/274 (89%)	220 (90%)	20 (8%)	4 (2%)	9 31
1	F	241/274 (88%)	218 (90%)	20 (8%)	3 (1%)	13 39
1	G	247/274 (90%)	222 (90%)	18 (7%)	7 (3%)	5 17
1	H	244/274 (89%)	213 (87%)	20 (8%)	11 (4%)	2 8
All	All	1942/2192 (89%)	1749 (90%)	150 (8%)	43 (2%)	6 22

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	B	77	PRO
1	B	170	ASP
1	B	215	CYS
1	D	9	ARG
1	D	75	PRO
1	D	196	LYS
1	D	222	GLU
1	E	72	SER
1	E	74	GLY
1	G	73	GLU
1	H	10	GLY
1	H	73	GLU
1	H	74	GLY
1	H	150	GLY
1	H	170	ASP
1	H	214	ARG

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Mol	Chain	Res	Type
1	C	10	GLY
1	D	8	VAL
1	D	74	GLY
1	E	10	GLY
1	F	221	ASP
1	F	255	ASN
1	G	11	TRP
1	G	246	LYS
1	H	169	PRO
1	H	191	SER
1	B	11	TRP
1	G	72	SER
1	H	34	GLN
1	H	71	GLN
1	H	215	CYS
1	B	203	ASP
1	B	246	LYS
1	G	74	GLY
1	C	243	ALA
1	D	151	LYS
1	G	75	PRO
1	G	84	ARG
1	D	67	ILE
1	C	76	ARG
1	F	226	PRO
1	E	75	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	217/236 (92%)	193 (89%)	24 (11%)	6 19
1	B	208/236 (88%)	183 (88%)	25 (12%)	5 15
1	C	213/236 (90%)	189 (89%)	24 (11%)	6 18
1	D	210/236 (89%)	183 (87%)	27 (13%)	4 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	214/236 (91%)	188 (88%)	26 (12%)	5 15
1	F	212/236 (90%)	178 (84%)	34 (16%)	2 7
1	G	217/236 (92%)	202 (93%)	15 (7%)	15 41
1	H	212/236 (90%)	187 (88%)	25 (12%)	5 16
All	All	1703/1888 (90%)	1503 (88%)	200 (12%)	5 16

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	6	GLN
1	A	7	THR
1	A	11	TRP
1	A	25	LEU
1	A	40	LEU
1	A	68	SER
1	A	76	ARG
1	A	91	ILE
1	A	99	GLU
1	A	102	TYR
1	A	103	ILE
1	A	105	ASP
1	A	110	ILE
1	A	133	ARG
1	A	167	SER
1	A	170	ASP
1	A	179	SER
1	A	202	SER
1	A	203	ASP
1	A	214	ARG
1	A	229	ILE
1	A	256	LEU
1	B	9	ARG
1	B	14	ILE
1	B	24	LYS
1	B	29	LEU
1	B	40	LEU
1	B	64	VAL
1	B	65	VAL
1	B	72	SER

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Mol	Chain	Res	Type
1	B	76	ARG
1	B	98	ILE
1	B	105	ASP
1	B	133	ARG
1	B	137	LEU
1	B	165	GLN
1	B	170	ASP
1	B	179	SER
1	B	204	ILE
1	B	212	SER
1	B	214	ARG
1	B	215	CYS
1	B	216	ASN
1	B	220	SER
1	B	254	LYS
1	B	256	LEU
1	B	257	ILE
1	C	27	GLU
1	C	33	LYS
1	C	34	GLN
1	C	40	LEU
1	C	67	ILE
1	C	68	SER
1	C	72	SER
1	C	84	ARG
1	C	98	ILE
1	C	99	GLU
1	C	103	ILE
1	C	105	ASP
1	C	113	SER
1	C	116	LEU
1	C	133	ARG
1	C	134	VAL
1	C	137	LEU
1	C	140	LEU
1	C	188	VAL
1	C	209	ILE
1	C	214	ARG
1	C	219	ASP
1	C	220	SER
1	C	254	LYS
1	D	7	THR

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Mol	Chain	Res	Type
1	D	12	SER
1	D	14	ILE
1	D	31	ASN
1	D	32	LEU
1	D	35	GLU
1	D	36	ASP
1	D	40	LEU
1	D	72	SER
1	D	73	GLU
1	D	76	ARG
1	D	104	ASN
1	D	166	PHE
1	D	170	ASP
1	D	172	LEU
1	D	183	GLU
1	D	187	GLN
1	D	194	SER
1	D	195	LEU
1	D	204	ILE
1	D	210	GLU
1	D	222	GLU
1	D	227	ASN
1	D	254	LYS
1	D	255	ASN
1	D	256	LEU
1	D	258	ASP
1	E	9	ARG
1	E	31	ASN
1	E	40	LEU
1	E	44	VAL
1	E	66	SER
1	E	68	SER
1	E	71	GLN
1	E	72	SER
1	E	73	GLU
1	E	98	ILE
1	E	116	LEU
1	E	136	ASN
1	E	137	LEU
1	E	140	LEU
1	E	143	LYS
1	E	153	ILE

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Mol	Chain	Res	Type
1	E	159	VAL
1	E	187	GLN
1	E	191	SER
1	E	194	SER
1	E	203	ASP
1	E	214	ARG
1	E	219	ASP
1	E	220	SER
1	E	224	VAL
1	E	246	LYS
1	F	8	VAL
1	F	14	ILE
1	F	23	THR
1	F	25	LEU
1	F	33	LYS
1	F	35	GLU
1	F	39	SER
1	F	63	ARG
1	F	71	GLN
1	F	72	SER
1	F	73	GLU
1	F	99	GLU
1	F	106	MET
1	F	112	LYS
1	F	113	SER
1	F	115	LEU
1	F	116	LEU
1	F	146	THR
1	F	165	GLN
1	F	166	PHE
1	F	170	ASP
1	F	187	GLN
1	F	188	VAL
1	F	189	VAL
1	F	196	LYS
1	F	206	VAL
1	F	210	GLU
1	F	214	ARG
1	F	216	ASN
1	F	220	SER
1	F	225	LEU
1	F	226	PRO

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Mol	Chain	Res	Type
1	F	255	ASN
1	F	257	ILE
1	G	4	GLN
1	G	7	THR
1	G	63	ARG
1	G	71	GLN
1	G	72	SER
1	G	83	SER
1	G	84	ARG
1	G	99	GLU
1	G	103	ILE
1	G	133	ARG
1	G	187	GLN
1	G	214	ARG
1	G	221	ASP
1	G	224	VAL
1	G	254	LYS
1	H	21	THR
1	H	23	THR
1	H	24	LYS
1	H	25	LEU
1	H	29	LEU
1	H	31	ASN
1	H	50	VAL
1	H	66	SER
1	H	72	SER
1	H	76	ARG
1	H	103	ILE
1	H	112	LYS
1	H	119	THR
1	H	151	LYS
1	H	167	SER
1	H	172	LEU
1	H	188	VAL
1	H	195	LEU
1	H	204	ILE
1	H	206	VAL
1	H	215	CYS
1	H	220	SER
1	H	221	ASP
1	H	224	VAL
1	H	254	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	109	ASN
1	B	22	GLN
1	B	136	ASN
1	B	216	ASN
1	B	234	HIS
1	C	31	ASN
1	C	109	ASN
1	C	255	ASN
1	D	31	ASN
1	D	104	ASN
1	D	155	ASN
1	D	187	GLN
1	D	227	ASN
1	E	31	ASN
1	E	136	ASN
1	E	237	GLN
1	F	34	GLN
1	F	71	GLN
1	F	165	GLN
1	F	211	ASN
1	F	216	ASN
1	F	234	HIS
1	F	255	ASN
1	G	31	ASN
1	G	109	ASN
1	G	187	GLN
1	G	234	HIS
1	H	31	ASN
1	H	71	GLN
1	H	90	ASN
1	H	165	GLN
1	H	211	ASN
1	H	216	ASN
1	H	234	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
5	GOL	F	291	-	5,5,5	0.35	0	5,5,5	0.51	0
3	GNP	E	281	2	29,34,34	1.70	8 (27%)	33,54,54	2.96	14 (42%)
5	GOL	G	291	-	5,5,5	0.46	0	5,5,5	0.74	0
3	GNP	G	281	2	29,34,34	1.59	7 (24%)	33,54,54	3.17	14 (42%)
3	GNP	H	281	2	29,34,34	1.49	7 (24%)	33,54,54	2.57	10 (30%)
4	PGE	A	290	-	9,9,9	0.82	0	8,8,8	0.71	0
3	GNP	C	281	2	29,34,34	1.85	9 (31%)	33,54,54	2.73	9 (27%)
4	PGE	F	290	-	9,9,9	0.69	0	8,8,8	0.85	0
5	GOL	A	291	-	5,5,5	0.33	0	5,5,5	0.82	0
3	GNP	B	281	2	29,34,34	1.52	5 (17%)	33,54,54	2.30	6 (18%)
5	GOL	G	290	-	5,5,5	0.38	0	5,5,5	0.56	0
3	GNP	A	281	2	29,34,34	1.57	6 (20%)	33,54,54	3.11	11 (33%)
3	GNP	D	281	2	29,34,34	1.51	8 (27%)	33,54,54	2.33	12 (36%)
3	GNP	F	281	2	29,34,34	1.97	8 (27%)	33,54,54	2.04	5 (15%)
5	GOL	C	291	-	5,5,5	0.43	0	5,5,5	0.96	0
5	GOL	E	290	-	5,5,5	0.55	0	5,5,5	1.11	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
5	GOL	F	291	-	-	0/4/4/4	-
3	GNP	E	281	2	-	4/14/38/38	0/3/3/3
5	GOL	G	291	-	-	2/4/4/4	-
3	GNP	G	281	2	-	2/14/38/38	0/3/3/3
3	GNP	H	281	2	-	4/14/38/38	0/3/3/3
4	PGE	A	290	-	-	3/7/7/7	-
3	GNP	C	281	2	-	2/14/38/38	0/3/3/3
4	PGE	F	290	-	-	5/7/7/7	-
5	GOL	A	291	-	-	2/4/4/4	-
3	GNP	B	281	2	-	2/14/38/38	0/3/3/3
5	GOL	G	290	-	-	2/4/4/4	-
3	GNP	A	281	2	-	2/14/38/38	0/3/3/3
3	GNP	D	281	2	-	2/14/38/38	0/3/3/3
3	GNP	F	281	2	-	2/14/38/38	0/3/3/3
5	GOL	C	291	-	-	2/4/4/4	-
5	GOL	E	290	-	-	4/4/4/4	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	281	GNP	PB-O3A	5.19	1.65	1.59
3	A	281	GNP	C6-N1	4.48	1.40	1.33
3	F	281	GNP	PG-O1G	4.30	1.53	1.46
3	C	281	GNP	PB-O3A	4.29	1.64	1.59
3	F	281	GNP	C6-N1	4.13	1.40	1.33
3	G	281	GNP	C6-N1	4.04	1.40	1.33
3	E	281	GNP	PG-O3G	-3.52	1.47	1.56
3	B	281	GNP	C6-N1	3.50	1.39	1.33
3	E	281	GNP	PB-O2B	-3.44	1.47	1.56
3	C	281	GNP	C6-N1	3.39	1.38	1.33
3	C	281	GNP	PG-O3G	-3.38	1.47	1.56
3	E	281	GNP	C6-N1	3.35	1.38	1.33
3	E	281	GNP	PB-O3A	3.25	1.63	1.59
3	B	281	GNP	PG-O3G	-3.25	1.48	1.56
3	H	281	GNP	PB-O3A	3.21	1.63	1.59
3	G	281	GNP	PB-O2B	-3.16	1.48	1.56
3	C	281	GNP	C5-C4	-3.08	1.32	1.40
3	D	281	GNP	PB-O2B	-2.98	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	281	GNP	PG-O1G	2.93	1.50	1.46
3	D	281	GNP	C5-C4	-2.91	1.33	1.40
3	D	281	GNP	C6-N1	2.90	1.38	1.33
3	G	281	GNP	PB-O3A	2.88	1.62	1.59
3	A	281	GNP	PG-O3G	-2.85	1.49	1.56
3	C	281	GNP	PG-N3B	2.84	1.70	1.63
3	F	281	GNP	PG-O2G	-2.80	1.49	1.56
3	B	281	GNP	PB-O3A	2.79	1.62	1.59
3	D	281	GNP	PG-O3G	-2.77	1.49	1.56
3	G	281	GNP	PG-O3G	-2.77	1.49	1.56
3	A	281	GNP	PG-N3B	2.76	1.70	1.63
3	F	281	GNP	PG-O3G	-2.73	1.49	1.56
3	E	281	GNP	C8-N7	-2.72	1.29	1.34
3	E	281	GNP	PB-O1B	2.71	1.50	1.46
3	H	281	GNP	PG-O1G	2.68	1.50	1.46
3	G	281	GNP	PG-O1G	2.67	1.50	1.46
3	C	281	GNP	C8-N7	-2.65	1.30	1.34
3	H	281	GNP	PB-O2B	-2.60	1.49	1.56
3	F	281	GNP	C5-C4	-2.60	1.34	1.40
3	B	281	GNP	PG-O1G	2.59	1.50	1.46
3	C	281	GNP	PG-O1G	2.57	1.50	1.46
3	H	281	GNP	C5-C4	-2.54	1.34	1.40
3	E	281	GNP	C5-C4	-2.43	1.34	1.40
3	C	281	GNP	PB-O1B	2.39	1.49	1.46
3	F	281	GNP	PB-O2B	-2.36	1.50	1.56
3	E	281	GNP	PG-O1G	2.32	1.49	1.46
3	D	281	GNP	PB-O3A	2.32	1.62	1.59
3	H	281	GNP	PG-O3G	-2.27	1.50	1.56
3	D	281	GNP	PG-O2G	-2.24	1.50	1.56
3	H	281	GNP	PG-N3B	2.23	1.69	1.63
3	G	281	GNP	PB-O1B	2.22	1.49	1.46
3	D	281	GNP	C8-N7	-2.17	1.30	1.34
3	D	281	GNP	PG-N3B	2.17	1.69	1.63
3	F	281	GNP	PG-N3B	2.16	1.69	1.63
3	A	281	GNP	PB-O2B	-2.11	1.51	1.56
3	B	281	GNP	C5-C4	-2.06	1.35	1.40
3	H	281	GNP	PG-O2G	-2.05	1.51	1.56
3	C	281	GNP	PB-O2B	-2.04	1.51	1.56
3	G	281	GNP	C5-C4	-2.02	1.35	1.40
3	A	281	GNP	C8-N7	-2.01	1.31	1.34

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	281	GNP	C5-C6-N1	-10.58	108.96	123.43
3	G	281	GNP	C5-C6-N1	-9.90	109.89	123.43
3	G	281	GNP	O1G-PG-N3B	-9.87	97.24	111.77
3	B	281	GNP	C5-C6-N1	-8.86	111.31	123.43
3	F	281	GNP	C5-C6-N1	-8.52	111.78	123.43
3	E	281	GNP	C5-C6-N1	-8.16	112.27	123.43
3	H	281	GNP	C5-C6-N1	-7.74	112.85	123.43
3	A	281	GNP	C2-N1-C6	7.64	128.07	115.93
3	C	281	GNP	O1G-PG-N3B	-7.44	100.81	111.77
3	D	281	GNP	C5-C6-N1	-6.81	114.12	123.43
3	C	281	GNP	C5-C6-N1	-6.47	114.58	123.43
3	E	281	GNP	O1B-PB-N3B	6.15	120.83	111.77
3	C	281	GNP	C2-N1-C6	5.69	124.96	115.93
3	A	281	GNP	O1G-PG-N3B	-5.59	103.54	111.77
3	E	281	GNP	C2-N1-C6	5.56	124.77	115.93
3	G	281	GNP	C2-N1-C6	5.40	124.50	115.93
3	C	281	GNP	C4-C5-N7	5.19	114.81	109.40
3	E	281	GNP	N2-C2-N3	5.15	126.18	117.79
3	B	281	GNP	C2-N1-C6	5.08	124.00	115.93
3	D	281	GNP	O1G-PG-N3B	-5.06	104.32	111.77
3	H	281	GNP	C2-N1-C6	4.89	123.69	115.93
3	E	281	GNP	N2-C2-N1	-4.85	109.71	117.25
3	H	281	GNP	O2B-PB-O1B	4.52	119.41	109.92
3	F	281	GNP	C2-N1-C6	4.51	123.10	115.93
3	C	281	GNP	N3-C2-N1	-4.47	121.26	127.22
3	H	281	GNP	O2G-PG-O3G	4.39	119.32	107.64
3	G	281	GNP	C2-N3-C4	-4.23	110.52	115.36
3	E	281	GNP	C4-C5-N7	4.20	113.77	109.40
3	D	281	GNP	C2-N1-C6	4.10	122.44	115.93
3	H	281	GNP	O3A-PB-N3B	-4.04	95.39	106.59
3	C	281	GNP	N2-C2-N3	3.97	124.25	117.79
3	B	281	GNP	C2-N3-C4	-3.93	110.86	115.36
3	H	281	GNP	O2G-PG-O1G	-3.90	103.65	113.45
3	A	281	GNP	C2-N3-C4	-3.77	111.05	115.36
3	A	281	GNP	N3-C2-N1	-3.70	122.28	127.22
3	C	281	GNP	C4-C5-C6	-3.67	117.30	120.80
3	E	281	GNP	C2-N3-C4	-3.63	111.21	115.36
3	B	281	GNP	O2B-PB-O1B	3.61	117.50	109.92
3	D	281	GNP	N2-C2-N3	3.60	123.66	117.79
3	G	281	GNP	O4'-C1'-C2'	-3.50	101.80	106.93
3	A	281	GNP	C4-C5-N7	3.44	112.98	109.40
3	A	281	GNP	PB-O3A-PA	-3.41	120.61	132.62
3	D	281	GNP	O3A-PB-N3B	-3.39	97.19	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	281	GNP	O3G-PG-O1G	-3.31	105.14	113.45
3	E	281	GNP	O3A-PB-N3B	-3.25	97.58	106.59
3	A	281	GNP	O1B-PB-N3B	3.21	116.50	111.77
3	G	281	GNP	O2G-PG-O3G	3.20	116.16	107.64
3	D	281	GNP	O2G-PG-O1G	-3.16	105.51	113.45
3	A	281	GNP	O2G-PG-O3G	3.14	115.99	107.64
3	A	281	GNP	O2G-PG-O1G	-3.09	105.68	113.45
3	F	281	GNP	O2B-PB-O1B	3.07	116.37	109.92
3	H	281	GNP	C2-N3-C4	-3.06	111.86	115.36
3	D	281	GNP	N2-C2-N1	-2.94	112.67	117.25
3	H	281	GNP	O1B-PB-N3B	2.90	116.04	111.77
3	F	281	GNP	O3A-PB-N3B	-2.83	98.74	106.59
3	D	281	GNP	C4-C5-N7	2.82	112.34	109.40
3	G	281	GNP	N2-C2-N1	-2.80	112.90	117.25
3	D	281	GNP	N3-C2-N1	-2.67	123.67	127.22
3	G	281	GNP	O4'-C4'-C5'	-2.63	100.72	109.37
3	B	281	GNP	PB-O3A-PA	-2.55	123.63	132.62
3	D	281	GNP	O3'-C3'-C4'	-2.49	103.85	111.05
3	A	281	GNP	O3'-C3'-C2'	-2.46	103.87	111.82
3	G	281	GNP	C4-C5-N7	2.45	111.95	109.40
3	E	281	GNP	O1G-PG-N3B	-2.43	108.19	111.77
3	E	281	GNP	O4'-C1'-C2'	-2.43	103.38	106.93
3	F	281	GNP	C2-N3-C4	-2.39	112.63	115.36
3	G	281	GNP	O2A-PA-O1A	2.38	124.00	112.24
3	E	281	GNP	N3-C2-N1	-2.34	124.10	127.22
3	E	281	GNP	O4'-C4'-C5'	-2.28	101.87	109.37
3	H	281	GNP	N3-C2-N1	-2.28	124.19	127.22
3	G	281	GNP	O3A-PB-N3B	-2.26	100.33	106.59
3	E	281	GNP	PB-O3A-PA	-2.24	124.71	132.62
3	G	281	GNP	O5'-PA-O1A	-2.22	100.39	109.07
3	B	281	GNP	O4'-C1'-C2'	-2.15	103.79	106.93
3	C	281	GNP	C2-N3-C4	-2.14	112.91	115.36
3	H	281	GNP	C3'-C2'-C1'	2.11	104.15	100.98
3	G	281	GNP	C3'-C2'-C1'	-2.10	97.81	100.98
3	D	281	GNP	O4'-C1'-C2'	-2.10	103.86	106.93
3	G	281	GNP	N2-C2-N3	2.09	121.20	117.79
3	D	281	GNP	O2B-PB-O3A	2.05	111.50	104.64
3	C	281	GNP	O2'-C2'-C1'	-2.01	103.43	110.85

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	281	GNP	PG-N3B-PB-O1B
3	A	281	GNP	PA-O3A-PB-O1B
3	B	281	GNP	PG-N3B-PB-O1B
3	B	281	GNP	PG-N3B-PB-O3A
3	C	281	GNP	PB-N3B-PG-O1G
3	C	281	GNP	PG-N3B-PB-O1B
3	D	281	GNP	PG-N3B-PB-O1B
3	D	281	GNP	PG-N3B-PB-O3A
3	E	281	GNP	PG-N3B-PB-O1B
3	E	281	GNP	PG-N3B-PB-O3A
3	E	281	GNP	PA-O3A-PB-O1B
3	F	281	GNP	PG-N3B-PB-O1B
3	F	281	GNP	PG-N3B-PB-O3A
3	G	281	GNP	PG-N3B-PB-O1B
3	H	281	GNP	PG-N3B-PB-O1B
3	H	281	GNP	PG-N3B-PB-O3A
3	H	281	GNP	PA-O3A-PB-O1B
3	H	281	GNP	PA-O3A-PB-O2B
5	A	291	GOL	O1-C1-C2-O2
5	A	291	GOL	O1-C1-C2-C3
5	C	291	GOL	C1-C2-C3-O3
5	E	290	GOL	O1-C1-C2-C3
5	G	290	GOL	C1-C2-C3-O3
5	C	291	GOL	O2-C2-C3-O3
5	E	290	GOL	O1-C1-C2-O2
5	E	290	GOL	C1-C2-C3-O3
5	G	291	GOL	C1-C2-C3-O3
4	A	290	PGE	O3-C5-C6-O4
5	G	290	GOL	O2-C2-C3-O3
4	F	290	PGE	O3-C5-C6-O4
5	E	290	GOL	O2-C2-C3-O3
4	A	290	PGE	C1-C2-O2-C3
4	F	290	PGE	C3-C4-O3-C5
4	F	290	PGE	C6-C5-O3-C4
5	G	291	GOL	O2-C2-C3-O3
3	G	281	GNP	PG-N3B-PB-O3A
4	F	290	PGE	O1-C1-C2-O2
4	A	290	PGE	O2-C3-C4-O3
3	E	281	GNP	PA-O3A-PB-O2B
4	F	290	PGE	C1-C2-O2-C3

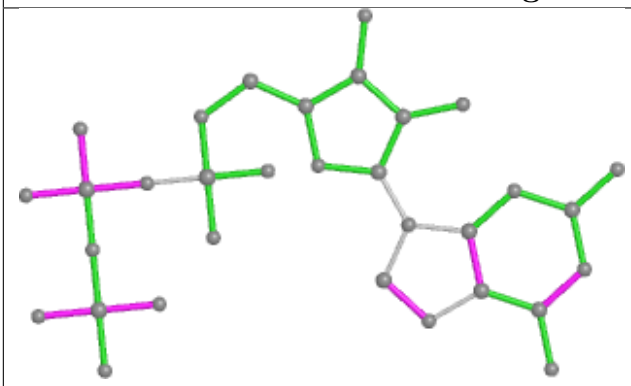
There are no ring outliers.

10 monomers are involved in 22 short contacts:

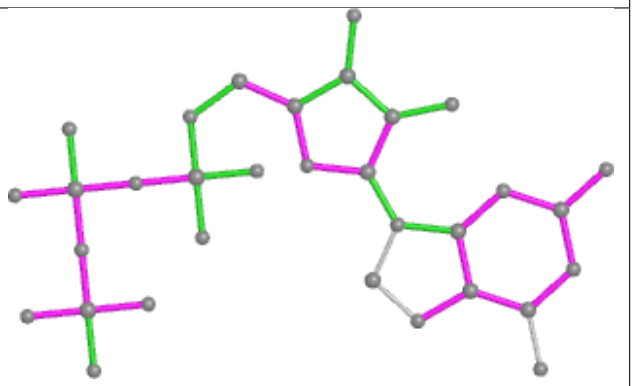
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	291	GOL	1	0
3	G	281	GNP	1	0
3	H	281	GNP	2	0
3	C	281	GNP	1	0
4	F	290	PGE	4	0
5	A	291	GOL	1	0
3	B	281	GNP	1	0
5	G	290	GOL	2	0
3	D	281	GNP	5	0
5	C	291	GOL	4	0

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.

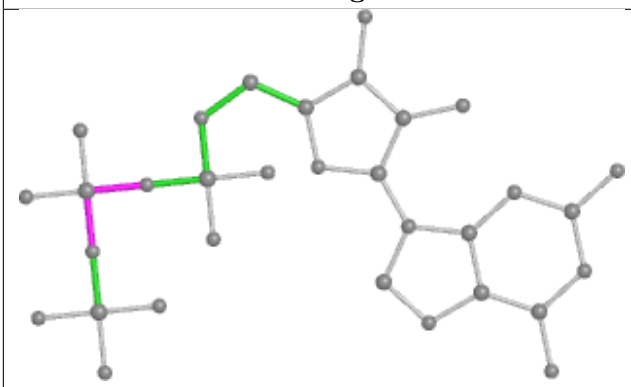
Ligand GNP E 281



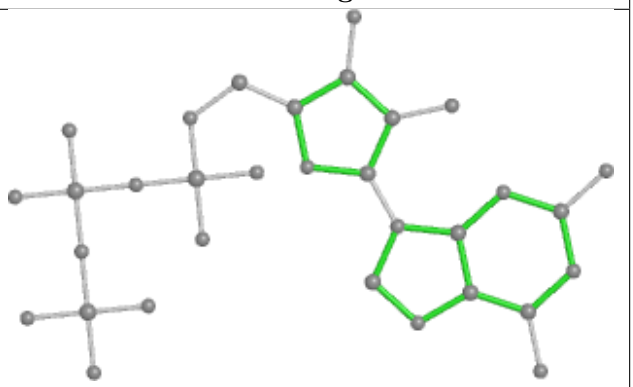
Bond lengths



Bond angles

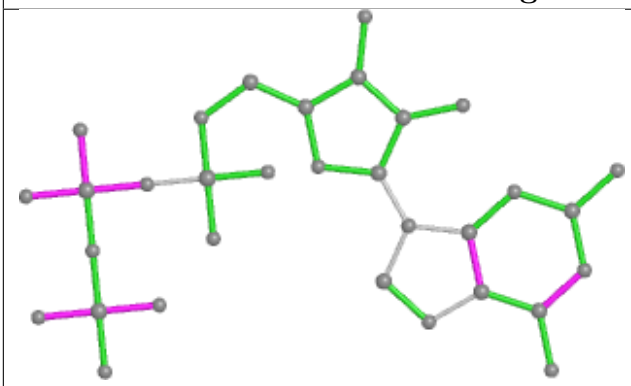


Torsions



Rings

Ligand GNP G 281



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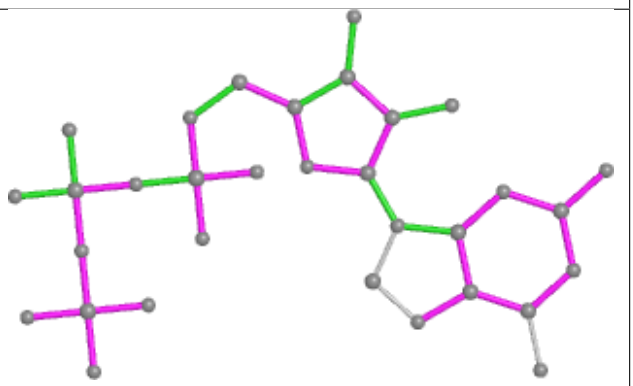
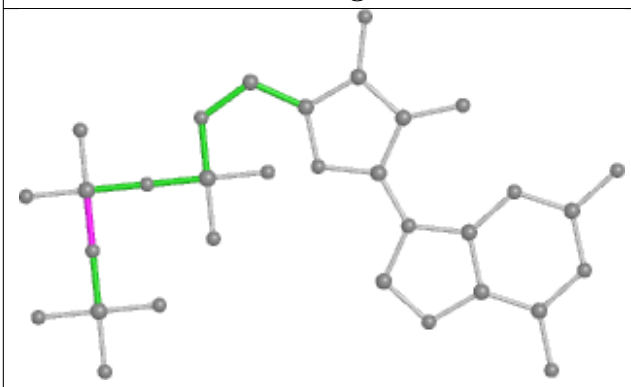


Bond angles



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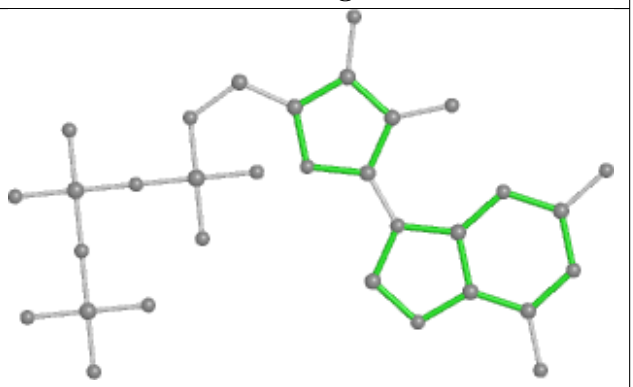
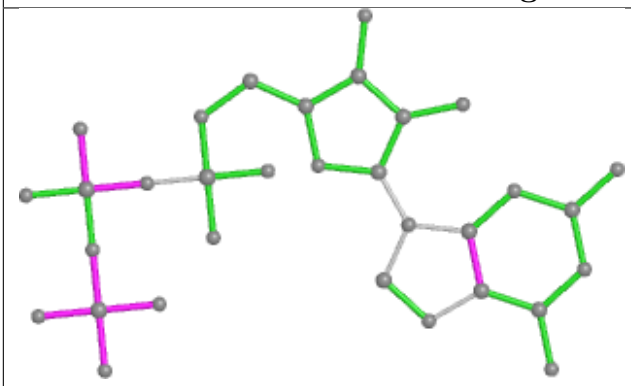
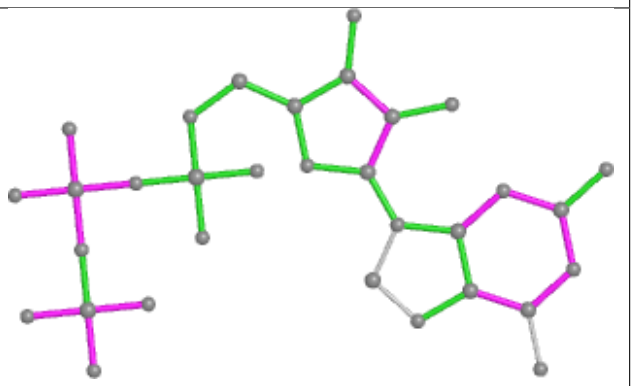


Rings

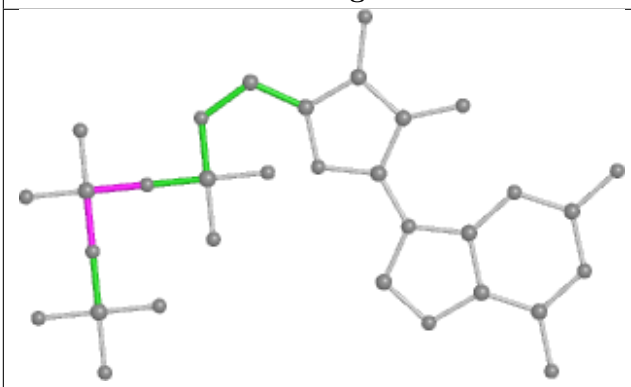
Ligand GNP H 281



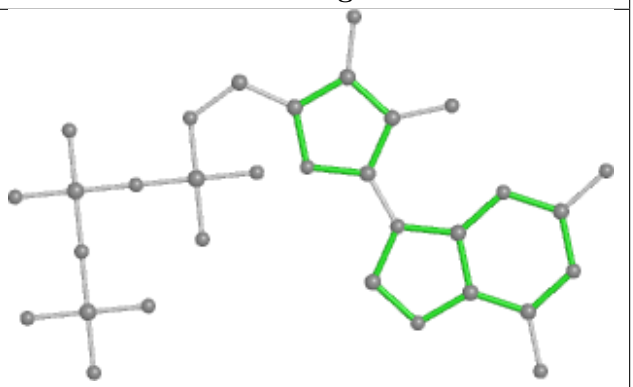
Bond lengths



Bond angles

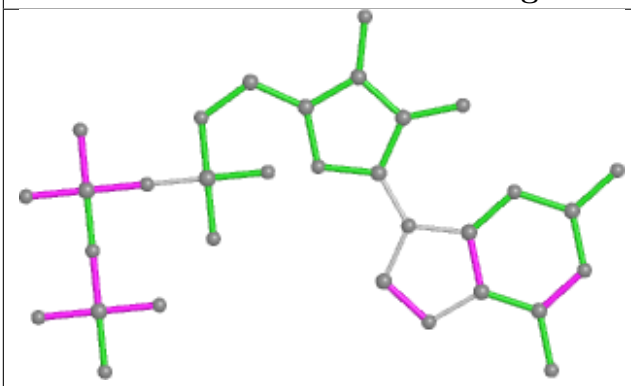


Torsions



Rings

Ligand GNP C 281



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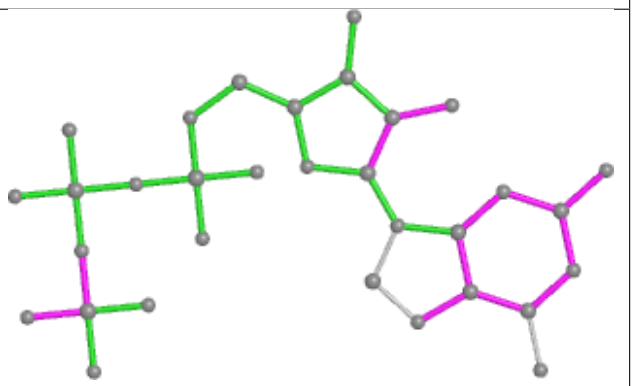
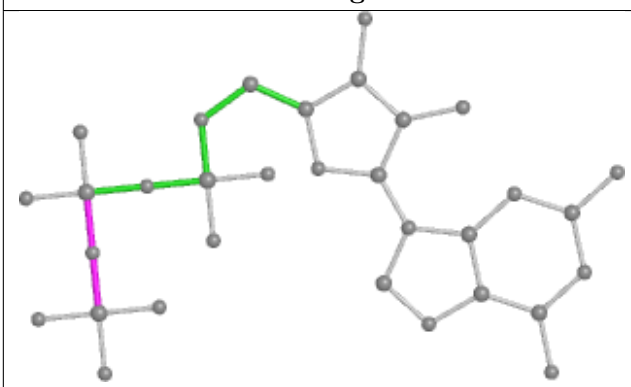
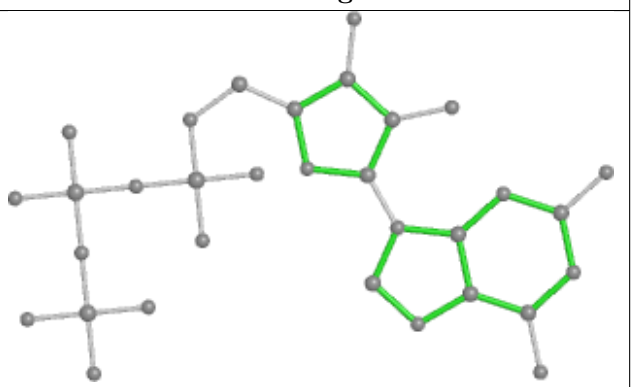


Bond angles

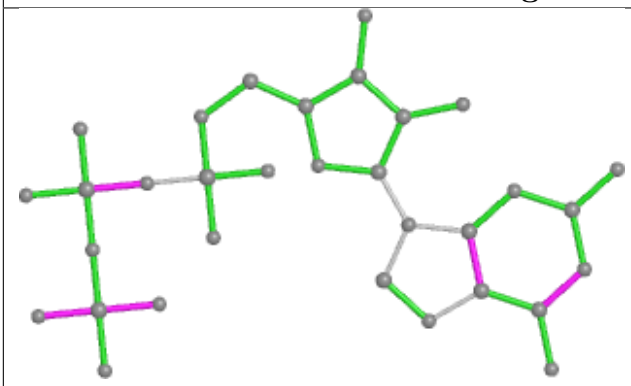


Torsions

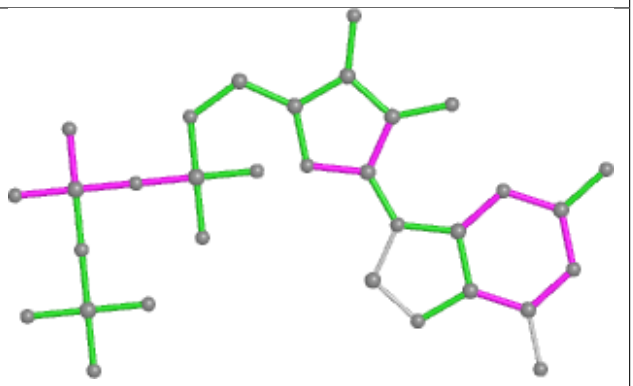


Rings

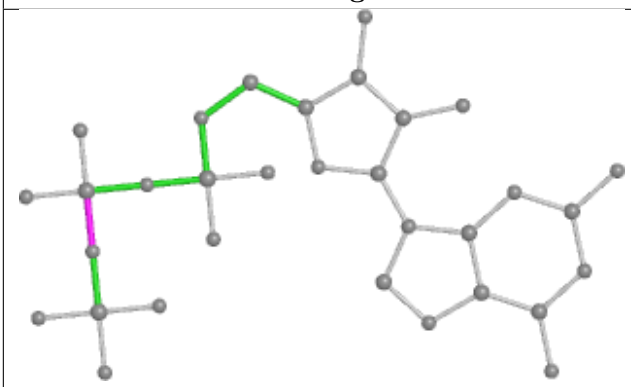
Ligand GNP B 281



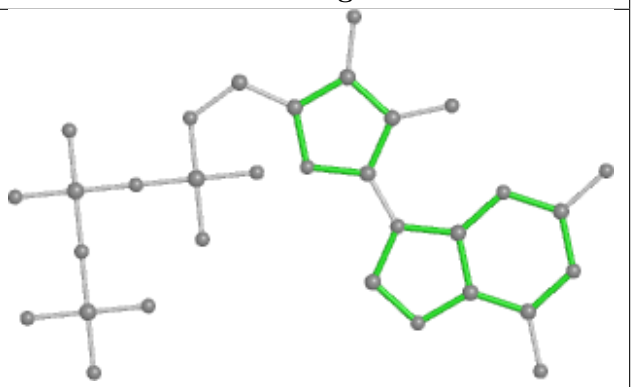
Bond lengths



Bond angles

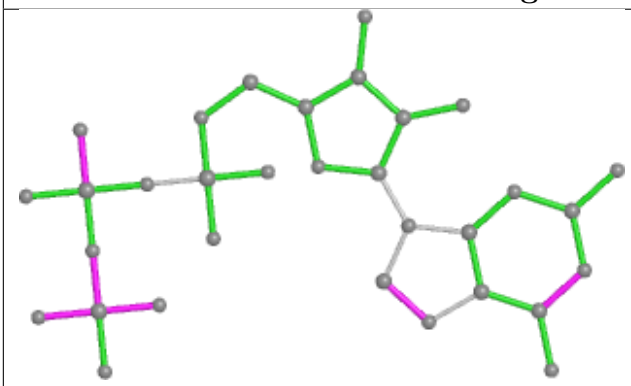


Torsions

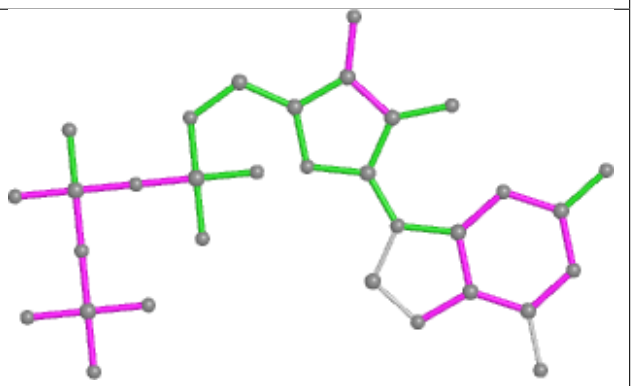


Rings

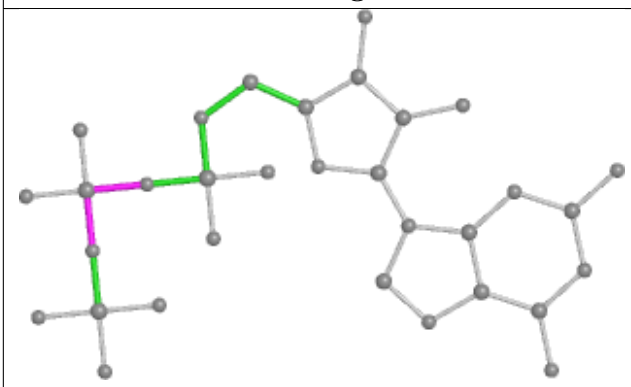
Ligand GNP A 281



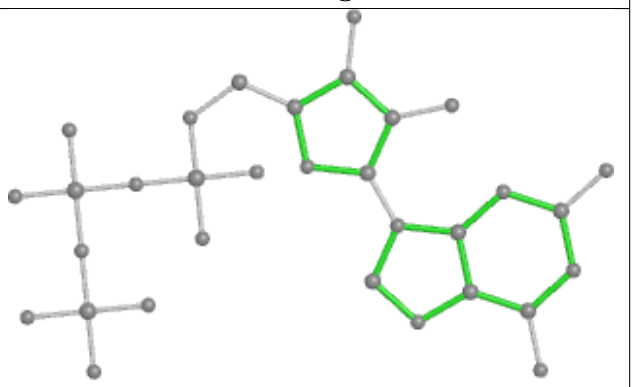
Bond lengths



Bond angles

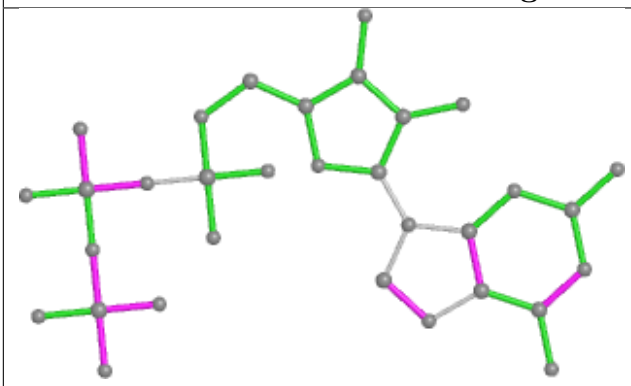


Torsions

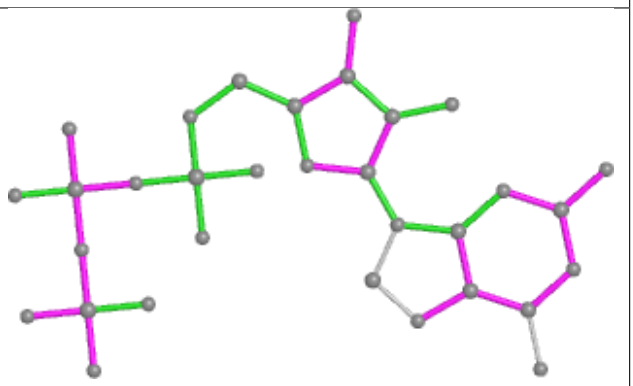


Rings

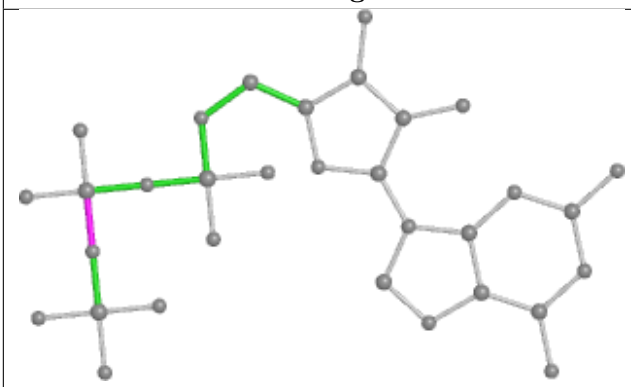
Ligand GNP D 281



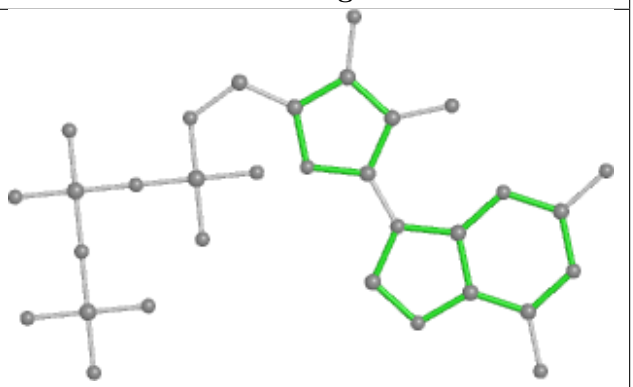
Bond lengths



Bond angles

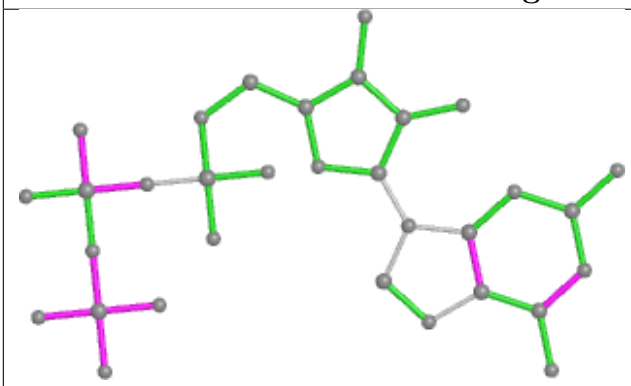


Torsions

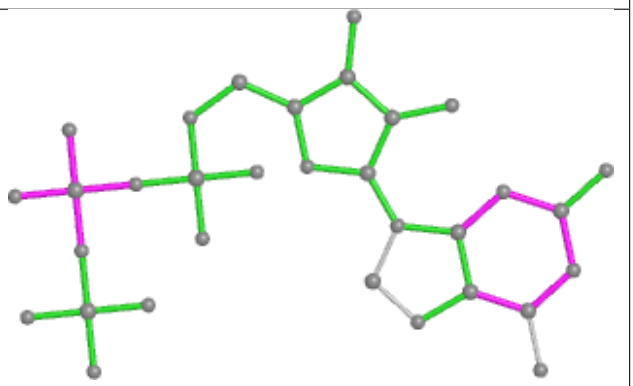


Rings

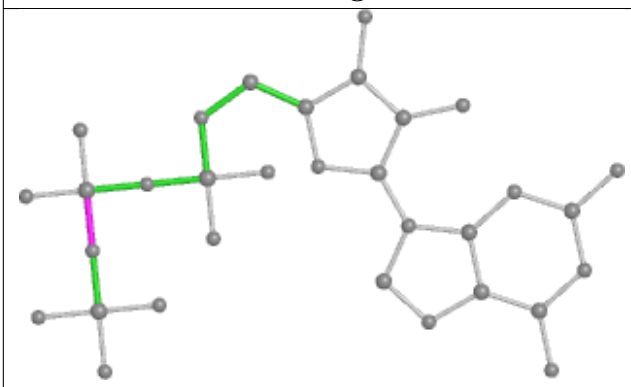
Ligand GNP F 281



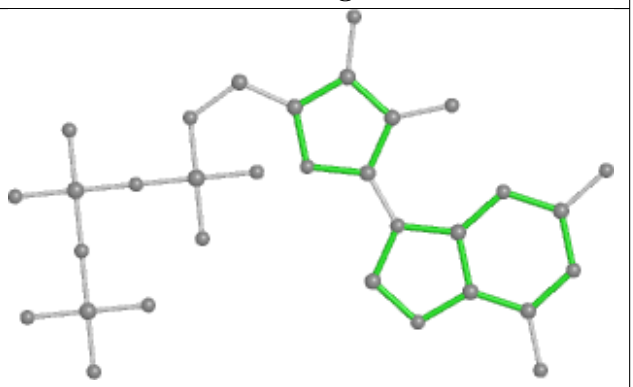
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	252/274 (91%)	0.03	1 (0%)	92	91	58, 66, 84, 99	0
1	B	243/274 (88%)	0.28	5 (2%)	63	54	66, 82, 104, 116	0
1	C	246/274 (89%)	0.11	2 (0%)	86	81	55, 64, 84, 100	0
1	D	247/274 (90%)	0.23	6 (2%)	59	49	62, 76, 99, 114	0
1	E	248/274 (90%)	0.06	4 (1%)	72	66	54, 63, 88, 94	0
1	F	245/274 (89%)	0.21	9 (3%)	41	31	62, 74, 97, 109	0
1	G	251/274 (91%)	0.01	2 (0%)	86	81	56, 67, 86, 100	0
1	H	248/274 (90%)	0.33	12 (4%)	30	21	70, 85, 102, 111	0
All	All	1980/2192 (90%)	0.16	41 (2%)	63	54	54, 72, 98, 116	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	SER	4.8
1	C	73	GLU	4.3
1	H	202	SER	4.2
1	D	69	PRO	3.9
1	F	70	PHE	3.6
1	E	72	SER	3.5
1	D	70	PHE	3.4
1	F	69	PRO	3.3
1	H	69	PRO	3.1
1	B	103	ILE	2.9
1	G	258	ASP	2.8
1	H	218	ASN	2.8
1	E	202	SER	2.8
1	E	71	GLN	2.7
1	H	41	THR	2.7
1	F	74	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	70	PHE	2.6
1	H	204	ILE	2.6
1	F	28	LEU	2.6
1	D	72	SER	2.5
1	D	71	GLN	2.5
1	F	221	ASP	2.5
1	G	195	LEU	2.5
1	H	70	PHE	2.5
1	H	255	ASN	2.4
1	B	8	VAL	2.4
1	H	72	SER	2.4
1	D	222	GLU	2.3
1	B	25	LEU	2.3
1	D	67	ILE	2.2
1	A	70	PHE	2.2
1	E	257	ILE	2.1
1	H	145	ILE	2.1
1	F	218	ASN	2.1
1	H	71	GLN	2.1
1	F	257	ILE	2.1
1	F	222	GLU	2.1
1	H	24	LYS	2.1
1	H	123	LEU	2.0
1	B	145	ILE	2.0
1	F	72	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

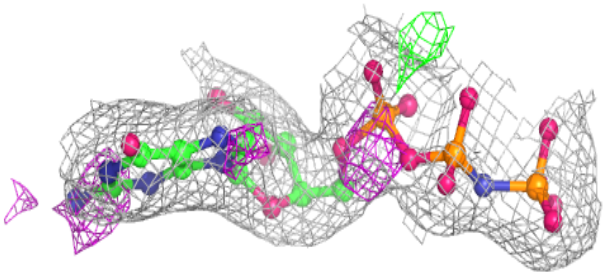
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

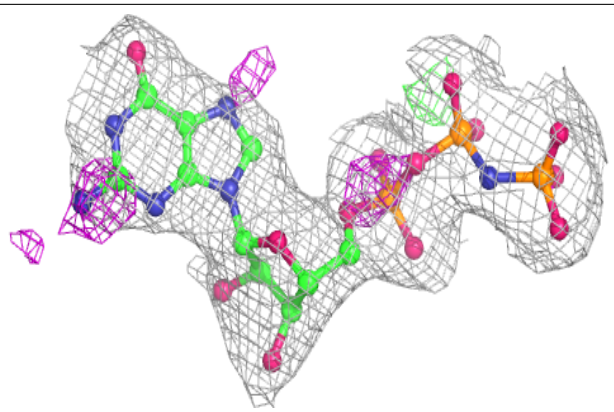
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	G	290	6/6	0.78	0.27	110,110,111,111	0
4	PGE	F	290	10/10	0.82	0.22	99,103,104,104	0
5	GOL	G	291	6/6	0.86	0.42	87,90,91,93	0
5	GOL	A	291	6/6	0.88	0.23	96,98,99,99	0
4	PGE	A	290	10/10	0.89	0.50	75,81,82,82	0
5	GOL	F	291	6/6	0.89	0.17	88,89,89,90	0
5	GOL	C	291	6/6	0.90	0.29	89,91,91,91	0
5	GOL	E	290	6/6	0.95	0.20	55,59,61,62	0
2	MG	H	282	1/1	0.95	0.10	71,71,71,71	0
3	GNP	H	281	32/32	0.97	0.15	67,71,75,76	0
2	MG	B	282	1/1	0.97	0.08	66,66,66,66	0
3	GNP	G	281	32/32	0.97	0.15	59,62,65,66	0
3	GNP	F	281	32/32	0.98	0.17	56,64,65,66	0
2	MG	C	282	1/1	0.98	0.07	63,63,63,63	0
2	MG	D	282	1/1	0.98	0.07	58,58,58,58	0
2	MG	E	282	1/1	0.98	0.04	64,64,64,64	0
2	MG	F	282	1/1	0.98	0.06	63,63,63,63	0
2	MG	A	282	1/1	0.98	0.10	65,65,65,65	0
3	GNP	A	281	32/32	0.98	0.17	58,63,65,66	0
3	GNP	B	281	32/32	0.98	0.15	67,70,73,77	0
3	GNP	C	281	32/32	0.98	0.13	60,64,66,67	0
3	GNP	D	281	32/32	0.98	0.15	60,65,68,69	0
3	GNP	E	281	32/32	0.98	0.13	59,62,67,72	0
2	MG	G	282	1/1	0.99	0.12	63,63,63,63	0

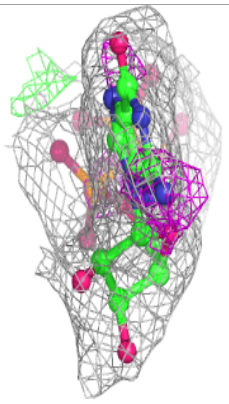
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP H 281:

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

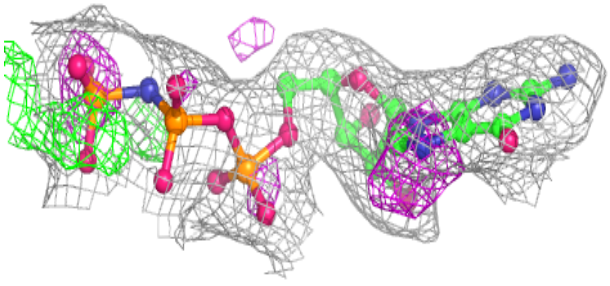


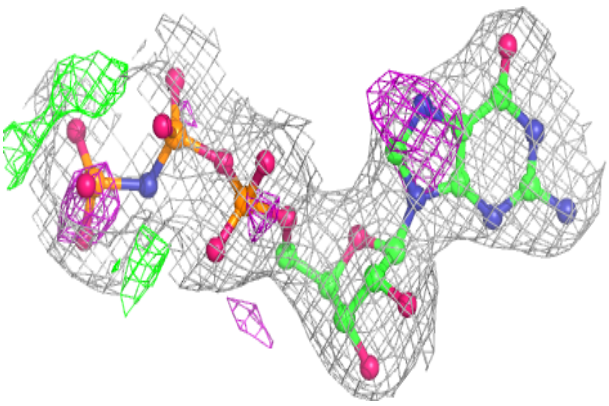


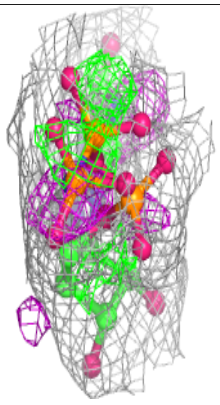


Electron density around GNP G 281:

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

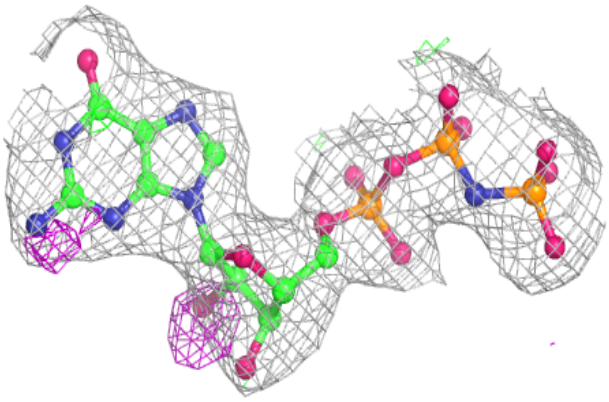


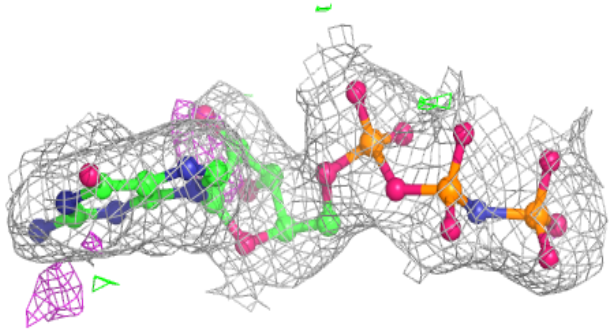


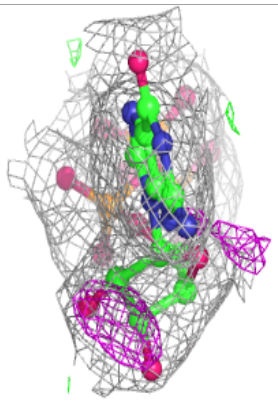


Electron density around GNP F 281:

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

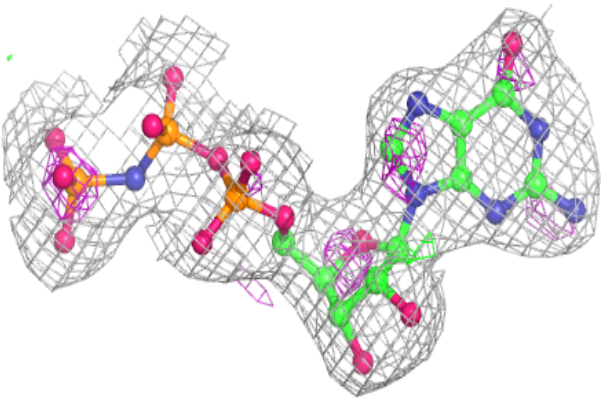


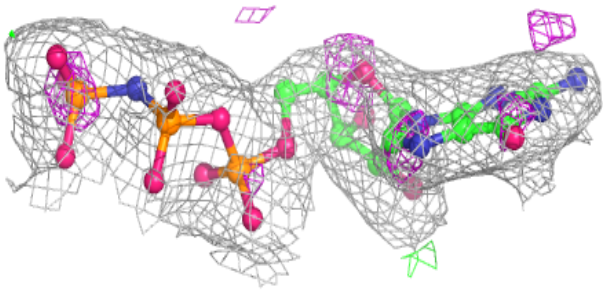


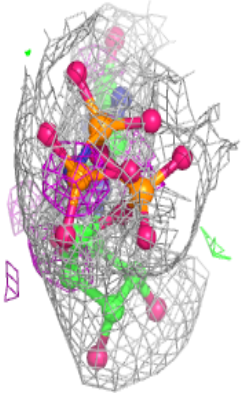


Electron density around GNP A 281:

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

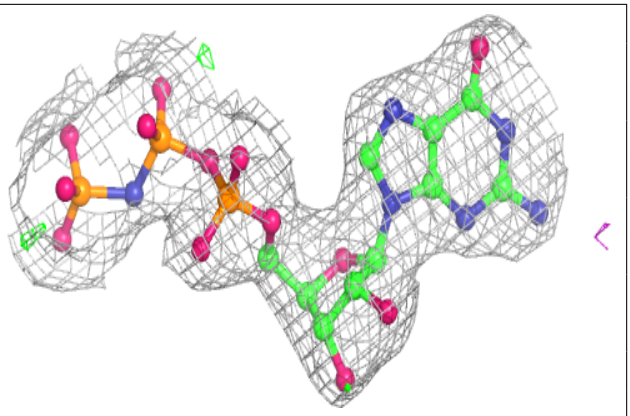


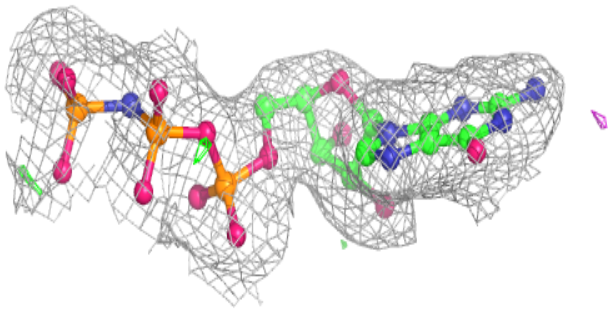


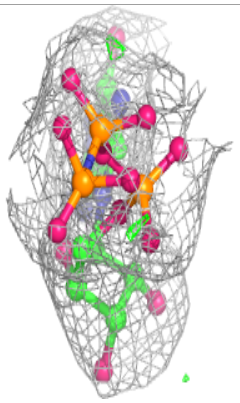


Electron density around GNP B 281:

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

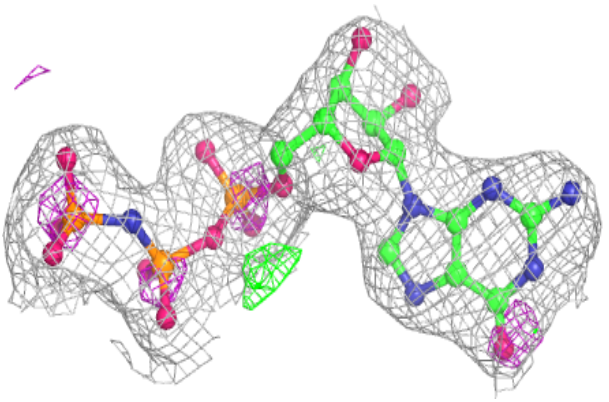


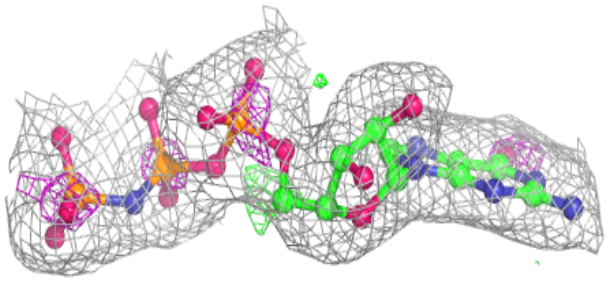


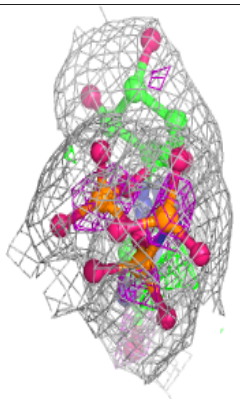


Electron density around GNP C 281:

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

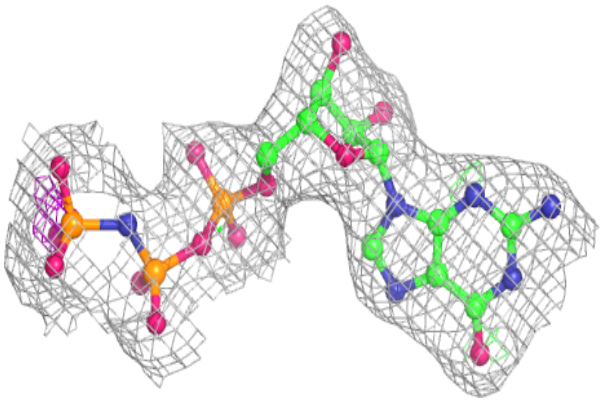


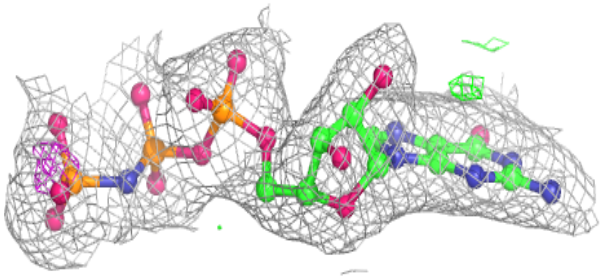


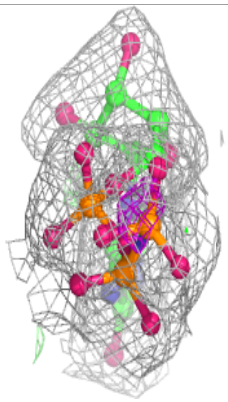


Electron density around GNP D 281:

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

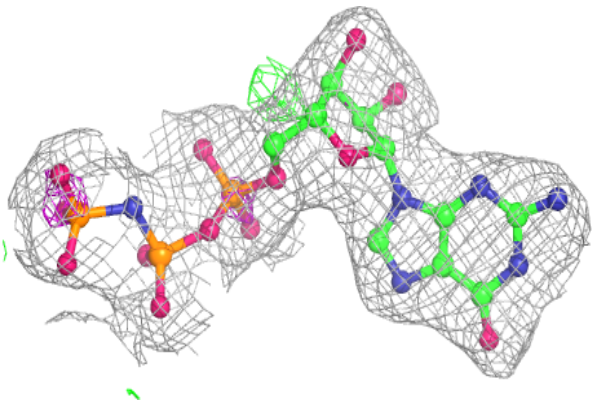


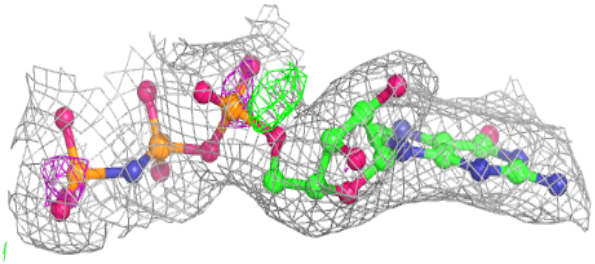


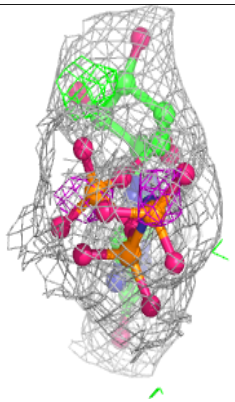


Electron density around GNP E 281:

$2mF_o$-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.