



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:07 PM UTC

PDB ID : 9HS1 / pdb_00009hs1
Title : Crystal structure of the Escherichia coli nucleosidase PpnN (partial alarmone form)
Authors : Baerentsen, R.L.; Brodersen, D.E.
Deposited on : 2024-12-18
Resolution : 2.36 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

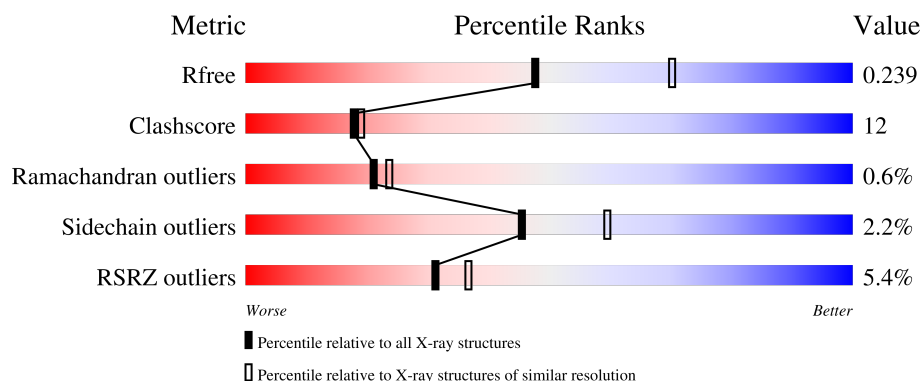
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


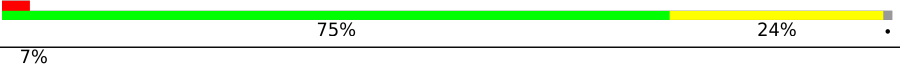
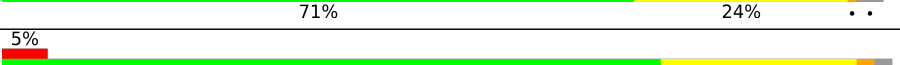

The reported resolution of this entry is 2.36 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	459	
1	B	459	
1	C	459	
1	D	459	

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
3	GUN	A	502	-	X	X	-
3	GUN	B	502	-	X	X	-
3	GUN	C	501	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14688 atoms, of which 48 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 Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3578	2265	638	652	23			
1	B	454	Total	C	N	O	S	0	0	0
			3570	2260	634	653	23			
1	C	444	Total	C	N	O	S	0	0	0
			3506	2221	624	639	22			
1	D	448	Total	C	N	O	S	0	0	0
			3521	2230	625	643	23			

There are 24 discrepancies between the modelled and reference sequences:

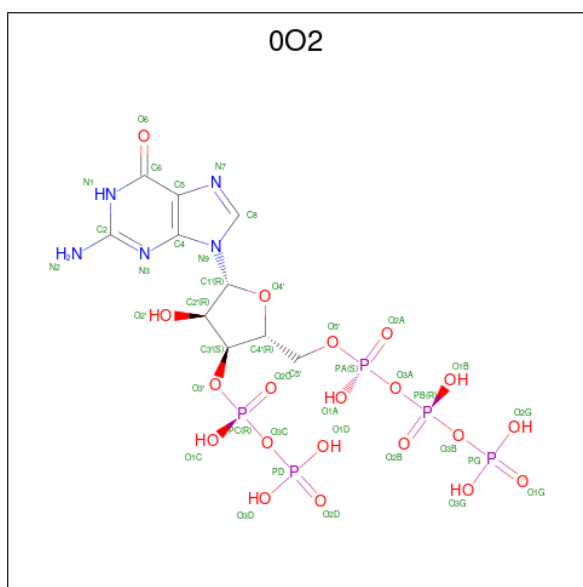
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP P0ADR8
A	-3	PRO	-	expression tag	UNP P0ADR8
A	-2	ALA	-	expression tag	UNP P0ADR8
A	-1	LEU	-	expression tag	UNP P0ADR8
A	0	ARG	-	expression tag	UNP P0ADR8
A	1	ALA	-	expression tag	UNP P0ADR8
B	-4	MET	-	initiating methionine	UNP P0ADR8
B	-3	PRO	-	expression tag	UNP P0ADR8
B	-2	ALA	-	expression tag	UNP P0ADR8
B	-1	LEU	-	expression tag	UNP P0ADR8
B	0	ARG	-	expression tag	UNP P0ADR8
B	1	ALA	-	expression tag	UNP P0ADR8
C	-4	MET	-	initiating methionine	UNP P0ADR8
C	-3	PRO	-	expression tag	UNP P0ADR8
C	-2	ALA	-	expression tag	UNP P0ADR8
C	-1	LEU	-	expression tag	UNP P0ADR8
C	0	ARG	-	expression tag	UNP P0ADR8
C	1	ALA	-	expression tag	UNP P0ADR8
D	-4	MET	-	initiating methionine	UNP P0ADR8
D	-3	PRO	-	expression tag	UNP P0ADR8
D	-2	ALA	-	expression tag	UNP P0ADR8

Continued on next page...

Continued from previous page...

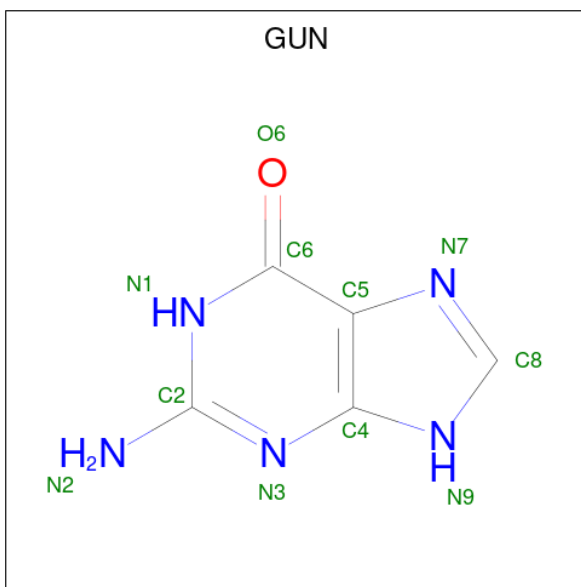
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	LEU	-	expression tag	UNP P0ADR8
D	0	ARG	-	expression tag	UNP P0ADR8
D	1	ALA	-	expression tag	UNP P0ADR8

- Molecule 2 is guanosine 5'-(tetrahydrogen triphosphate) 3'-(trihydrogen diphosphate) (CCD ID: 0O2) (formula: C₁₀H₁₈N₅O₂₀P₅) (labeled as "Ligand of Interest" by depositor).



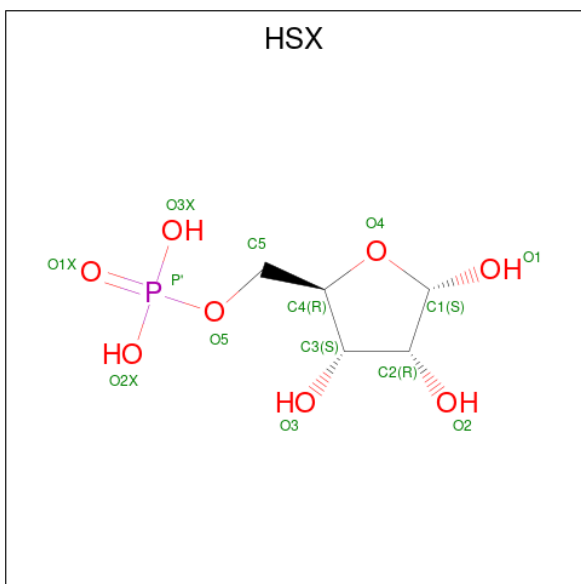
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	P	0	0
			51	10	11	5	20	5		
2	B	1	Total	C	H	N	O	P	0	0
			51	10	11	5	20	5		
2	C	1	Total	C	H	N	O	P	0	0
			51	10	11	5	20	5		

- Molecule 3 is GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			16	5	5	5	1		
3	B	1	Total	C	H	N	O	0	0
			16	5	5	5	1		
3	C	1	Total	C	H	N	O	0	0
			16	5	5	5	1		

- Molecule 4 is 5-O-phosphono-alpha-D-ribofuranose (CCD ID: HSX) (formula: $C_5H_{11}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O	P	0	0
			14	5	8	1		

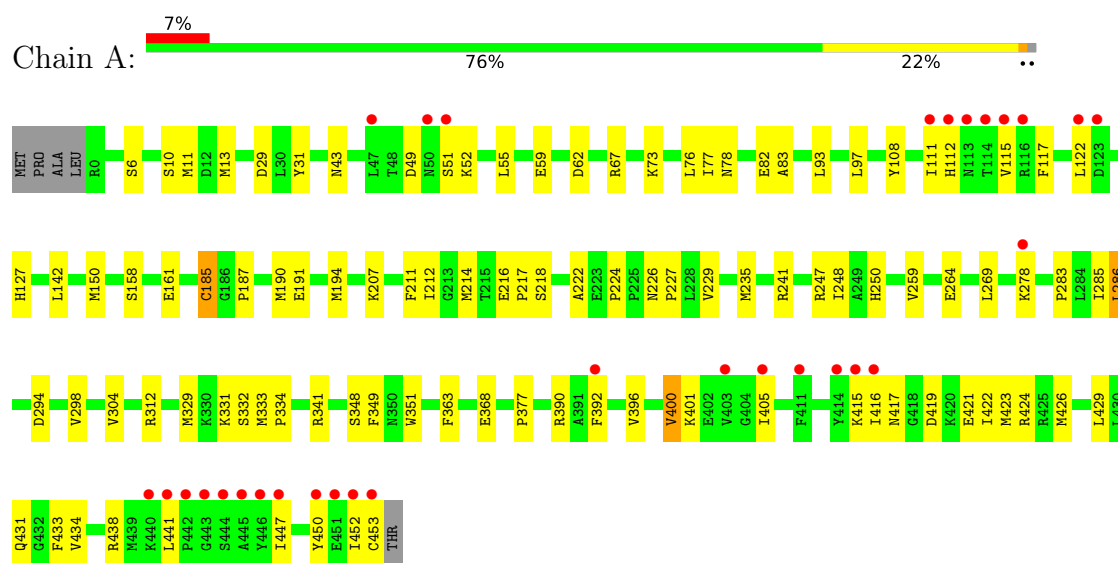
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	79	Total	O	0	0
			79	79		
5	C	71	Total	O	0	0
			71	71		
5	D	77	Total	O	0	0
			77	77		

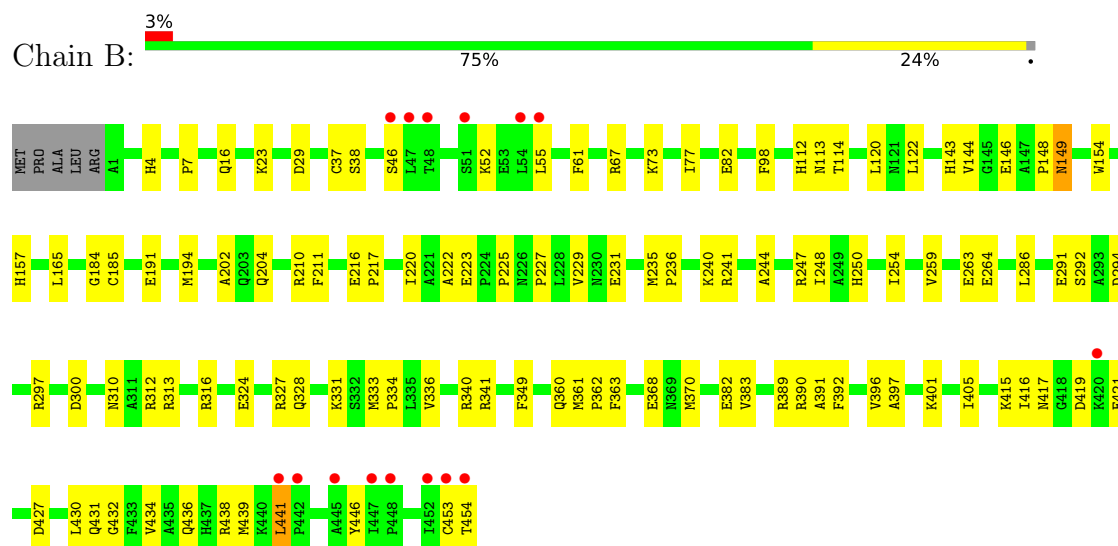
3 Residue-property plots

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: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase

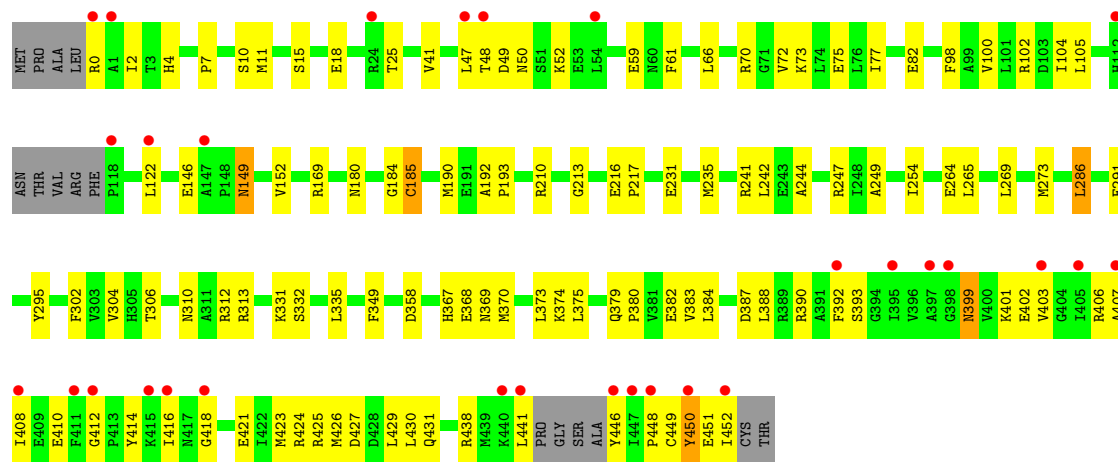


- Molecule 1: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase

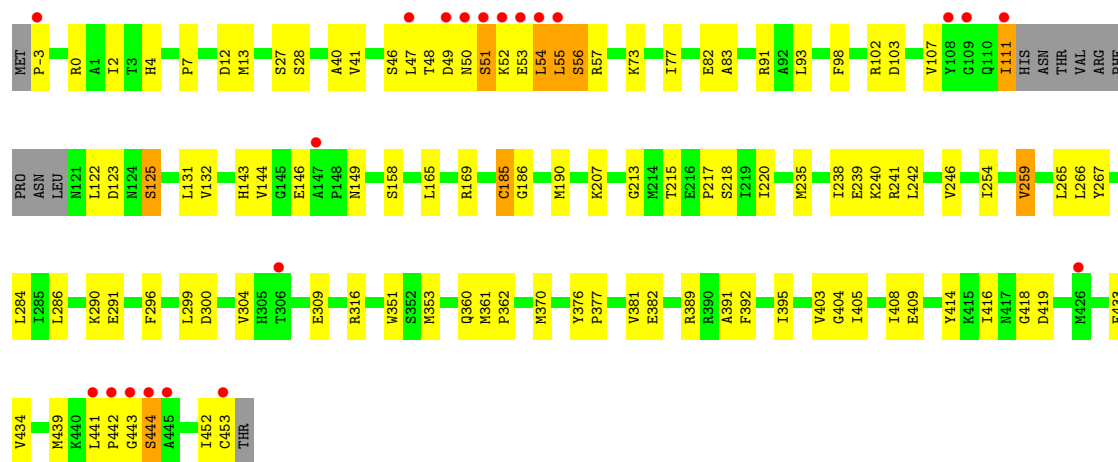
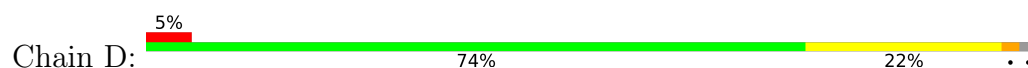


- Molecule 1: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase





● Molecule 1: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.66Å 152.66Å 224.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.36 49.63 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.63-2.36) 99.9 (49.63-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.241 0.195 , 0.239	Depositor DCC
R_{free} test set	5439 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14688	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HSX, OO2, GUN

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	0.39	1/3648 (0.0%)	0.55	0/4936
1	B	0.39	0/3640	0.52	2/4928 (0.0%)
1	C	0.34	0/3572	0.48	0/4828
1	D	0.40	0/3588	0.52	0/4852
All	All	0.38	1/14448 (0.0%)	0.52	2/19544 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	PRO	CA-C	5.57	1.54	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	GLN	CA-C-N	-5.00	111.99	123.15
1	B	360	GLN	C-N-CA	-5.00	111.99	123.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3578	0	3607	86	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3570	0	3590	87	0
1	C	3506	0	3537	99	0
1	D	3521	0	3554	85	1
2	A	40	11	11	3	0
2	B	40	11	13	2	0
2	C	40	11	12	0	1
3	A	11	5	5	7	0
3	B	11	5	5	4	0
3	C	11	5	5	5	0
4	D	14	0	0	0	0
5	A	71	0	0	4	0
5	B	79	0	0	5	0
5	C	71	0	0	6	0
5	D	77	0	0	6	0
All	All	14640	48	14339	353	2

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 12.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:NH1	1:B:328:GLN:OE1	1.87	1.06
1:C:427:ASP:OD1	1:C:450:TYR:OH	1.71	1.06
1:C:358:ASP:HB2	1:C:390:ARG:HH12	1.22	1.05
1:B:291:GLU:OE1	1:B:291:GLU:N	1.96	0.97
1:D:259:VAL:HG22	1:D:439:MET:HE1	1.47	0.95
1:A:82:GLU:OE2	1:A:82:GLU:N	1.99	0.94
1:C:291:GLU:N	1:C:291:GLU:OE2	2.01	0.93
1:B:361:MET:HG3	1:B:362:PRO:HD2	1.53	0.90
1:C:216:GLU:HG2	1:C:217:PRO:HD2	1.51	0.90
1:C:401:LYS:HE3	1:C:401:LYS:HA	1.55	0.89
1:D:353:MET:HG2	5:D:677:HOH:O	1.70	0.89
1:D:405:ILE:O	1:D:409:GLU:HG2	1.74	0.88
1:B:392:PHE:O	1:B:396:VAL:HG23	1.74	0.88
1:D:291:GLU:OE2	1:D:291:GLU:N	2.08	0.87
1:C:269:LEU:O	1:C:273:MET:HG3	1.73	0.86
1:B:316:ARG:NH1	1:B:328:GLN:CD	2.37	0.81
1:A:216:GLU:OE1	1:A:218:SER:HB2	1.81	0.81
1:C:451:GLU:C	1:C:452:ILE:HD12	2.05	0.80
1:D:439:MET:HE2	1:D:439:MET:HA	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:HD3	3:C:501:GUN:HN22	1.46	0.80
1:B:294:ASP:OD1	1:B:297:ARG:NH2	2.13	0.80
1:A:73:LYS:HE3	2:B:501:O02:O1G	1.83	0.79
1:B:370:MET:HE1	1:B:391:ALA:HA	1.64	0.79
1:B:316:ARG:HH12	1:B:328:GLN:CD	1.91	0.79
1:C:358:ASP:HB2	1:C:390:ARG:NH1	1.97	0.79
1:C:392:PHE:CD1	1:C:426:MET:HE3	2.18	0.78
1:C:216:GLU:HG2	1:C:217:PRO:CD	2.14	0.77
1:D:246:VAL:HG12	5:D:677:HOH:O	1.84	0.77
1:A:368:GLU:OE1	1:A:368:GLU:N	2.15	0.77
1:C:380:PRO:HB2	1:C:383:VAL:HG23	1.68	0.76
1:B:210:ARG:HD2	1:B:231:GLU:OE2	1.84	0.76
1:C:59:GLU:OE2	1:C:59:GLU:N	2.16	0.74
1:B:194:MET:HE2	1:B:211:PHE:HB3	1.70	0.74
1:A:392:PHE:CZ	1:A:429:LEU:HD23	2.22	0.74
1:C:146:GLU:OE2	1:C:146:GLU:HA	1.87	0.74
1:A:298:VAL:HG12	1:A:429:LEU:HD12	1.69	0.74
1:B:368:GLU:OE1	1:B:368:GLU:N	2.19	0.74
1:A:241:ARG:HD3	3:A:502:GUN:HN22	1.53	0.72
1:C:15:SER:OG	1:C:18:GLU:HG3	1.89	0.72
1:B:52:LYS:HE3	1:B:222:ALA:HB1	1.70	0.72
1:B:417:ASN:ND2	1:B:453:CYS:O	2.23	0.71
1:C:50:ASN:HD21	1:C:52:LYS:HG2	1.55	0.71
1:B:235:MET:HE3	1:B:236:PRO:HD2	1.73	0.71
1:C:302:PHE:O	1:C:306:THR:HG23	1.91	0.71
1:B:235:MET:HE3	1:B:236:PRO:CD	2.21	0.70
1:A:285:ILE:HD12	1:A:329:MET:HE2	1.74	0.70
1:B:220:ILE:HD11	1:B:225:PRO:HD3	1.74	0.69
1:C:392:PHE:HZ	1:C:429:LEU:HD23	1.56	0.69
1:B:397:ALA:CB	1:B:401:LYS:HE2	2.24	0.68
1:B:397:ALA:HB1	1:B:401:LYS:HE2	1.76	0.68
1:C:82:GLU:CD	1:C:82:GLU:H	2.02	0.68
1:A:392:PHE:HZ	1:A:429:LEU:HD23	1.58	0.67
1:B:120:LEU:HD21	1:B:122:LEU:HD21	1.76	0.67
1:C:392:PHE:CZ	1:C:429:LEU:HD23	2.30	0.67
1:D:125:SER:HB2	5:D:655:HOH:O	1.93	0.67
1:A:298:VAL:HG12	1:A:429:LEU:CD1	2.24	0.67
1:A:396:VAL:O	1:A:400:VAL:HG22	1.95	0.67
1:C:169:ARG:NH2	5:C:601:HOH:O	2.28	0.67
1:A:13:MET:HE2	1:B:144:VAL:HG22	1.77	0.67
1:A:401:LYS:O	1:A:405:ILE:HG13	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ASN:HD21	1:B:454:THR:HA	1.60	0.66
1:A:294:ASP:HB2	5:A:625:HOH:O	1.95	0.66
1:B:316:ARG:HH12	1:B:328:GLN:NE2	1.93	0.66
1:D:304:VAL:HG13	1:D:309:GLU:HA	1.77	0.66
1:B:310:ASN:HB2	5:B:628:HOH:O	1.96	0.65
1:C:70:ARG:HG3	1:D:351:TRP:CD1	2.31	0.65
1:C:310:ASN:O	1:C:313:ARG:HG3	1.96	0.65
1:D:102:ARG:O	1:D:107:VAL:HG23	1.96	0.65
1:A:298:VAL:CG1	1:A:429:LEU:HD12	2.26	0.65
1:C:217:PRO:HD3	1:C:235:MET:O	1.97	0.64
1:B:146:GLU:OE2	1:B:146:GLU:HA	1.97	0.64
1:A:341:ARG:HH22	2:A:501:OO2:PD	2.21	0.64
1:C:4:HIS:CD2	1:C:75:GLU:HG3	2.32	0.64
1:C:25:THR:HG22	1:C:105:LEU:HD22	1.80	0.64
2:A:501:OO2:O1A	1:B:73:LYS:NZ	2.31	0.64
1:A:421:GLU:OE2	1:A:424:ARG:NH2	2.31	0.64
1:D:4:HIS:HB3	1:D:73:LYS:HE2	1.80	0.64
1:C:185:CYS:HB2	1:C:213:GLY:HA3	1.79	0.63
1:C:423:MET:HE2	1:C:450:TYR:CD2	2.34	0.63
1:D:143:HIS:HB2	1:D:146:GLU:HG2	1.79	0.63
1:C:406:ARG:HB3	1:C:410:GLU:OE2	1.99	0.63
1:B:184:GLY:O	1:B:185:CYS:HB3	1.99	0.63
1:D:186:GLY:HA3	1:D:190:MET:HE3	1.81	0.62
1:C:331:LYS:NZ	5:C:602:HOH:O	2.32	0.62
1:D:82:GLU:CD	1:D:82:GLU:H	2.06	0.62
1:D:235:MET:CE	1:D:240:LYS:HB3	2.29	0.62
1:C:402:GLU:O	1:C:406:ARG:HG2	2.00	0.62
1:B:235:MET:HE2	1:B:240:LYS:HB3	1.80	0.61
1:A:115:VAL:HG22	1:A:117:PHE:H	1.65	0.61
1:D:304:VAL:CG1	1:D:309:GLU:HG3	2.31	0.61
1:D:13:MET:HE3	1:D:13:MET:HA	1.82	0.61
1:A:416:ILE:CD1	1:A:450:TYR:HB2	2.31	0.61
1:B:300:ASP:OD2	1:B:312:ARG:NH2	2.32	0.61
1:C:242:LEU:CD2	3:C:501:GUN:HN21	2.13	0.61
1:C:50:ASN:ND2	1:C:52:LYS:HG2	2.14	0.61
1:A:417:ASN:OD1	1:A:417:ASN:O	2.19	0.60
1:C:368:GLU:HG3	1:C:369:ASN:N	2.15	0.60
1:C:401:LYS:HE3	1:C:401:LYS:CA	2.31	0.60
1:C:235:MET:HE3	1:C:244:ALA:HB2	1.82	0.60
1:C:408:ILE:HD11	1:C:414:TYR:CD2	2.37	0.60
1:A:76:LEU:HD21	1:A:97:LEU:HD21	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:SER:HB3	5:B:645:HOH:O	2.02	0.59
1:D:416:ILE:HD12	1:D:452:ILE:CD1	2.33	0.59
1:C:399:ASN:ND2	1:C:449:CYS:SG	2.76	0.59
1:B:184:GLY:O	1:B:185:CYS:CB	2.49	0.59
1:C:0:ARG:O	1:C:2:ILE:HD12	2.03	0.59
1:D:217:PRO:HD3	1:D:235:MET:O	2.03	0.59
1:B:430:LEU:O	1:B:434:VAL:HG23	2.03	0.58
1:B:148:PRO:HB3	1:B:250:HIS:CD2	2.37	0.58
1:C:122:LEU:HG	5:C:610:HOH:O	2.03	0.58
1:D:300:ASP:O	1:D:304:VAL:HG23	2.03	0.58
1:C:304:VAL:HG21	1:C:312:ARG:CZ	2.34	0.58
1:A:111:ILE:HG22	1:A:112:HIS:CE1	2.38	0.58
1:A:431:GLN:O	1:A:434:VAL:HG22	2.04	0.58
1:B:324:GLU:HG3	1:B:328:GLN:NE2	2.19	0.57
1:D:286:LEU:HB3	1:D:296:PHE:CE1	2.39	0.57
1:A:217:PRO:HD3	1:A:235:MET:O	2.04	0.57
1:B:419:ASP:OD1	1:B:421:GLU:N	2.34	0.57
1:D:48:THR:HG22	1:D:49:ASP:N	2.20	0.57
1:D:416:ILE:HD12	1:D:452:ILE:HD13	1.87	0.57
1:A:392:PHE:O	1:A:396:VAL:HG23	2.05	0.56
1:B:324:GLU:OE1	1:B:327:ARG:NH1	2.37	0.56
1:C:375:LEU:HD23	1:C:375:LEU:N	2.19	0.56
1:D:215:THR:HA	1:D:241:ARG:HE	1.70	0.56
1:D:259:VAL:HG12	1:D:392:PHE:HD1	1.70	0.56
1:D:54:LEU:O	1:D:56:SER:N	2.38	0.56
1:C:264:GLU:CD	3:C:501:GUN:O6	2.49	0.56
1:C:414:TYR:N	1:C:449:CYS:O	2.37	0.56
1:D:377:PRO:HD3	1:D:419:ASP:HB2	1.87	0.56
1:C:401:LYS:HA	1:C:401:LYS:CE	2.23	0.56
1:D:254:ILE:HD12	1:D:284:LEU:HD11	1.88	0.55
1:B:241:ARG:NH1	3:B:502:GUN:HN22	2.04	0.55
1:D:246:VAL:CG1	5:D:677:HOH:O	2.49	0.55
1:B:436:GLN:HB2	1:B:438:ARG:HG2	1.89	0.55
1:A:115:VAL:HB	5:B:666:HOH:O	2.06	0.55
1:C:373:LEU:HD22	1:C:387:ASP:OD1	2.07	0.55
1:C:149:ASN:HD21	1:C:180:ASN:ND2	2.04	0.55
1:D:370:MET:HE1	1:D:391:ALA:HA	1.88	0.54
1:C:11:MET:HE3	1:C:102:ARG:HG3	1.90	0.54
1:D:111:ILE:O	1:D:111:ILE:HG23	2.07	0.54
1:A:51:SER:O	1:A:55:LEU:HG	2.08	0.54
1:A:419:ASP:O	1:A:423:MET:HG2	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:CD	3:A:502:GUN:O6	2.50	0.54
1:D:235:MET:HE2	1:D:240:LYS:HB3	1.90	0.54
1:C:295:TYR:CD1	1:C:438:ARG:HD2	2.43	0.54
1:B:4:HIS:HB3	1:B:73:LYS:HE2	1.89	0.53
1:D:185:CYS:HB2	1:D:213:GLY:HA3	1.91	0.53
1:C:379:GLN:OE1	1:C:379:GLN:HA	2.08	0.53
1:C:441:LEU:CD2	1:C:446:TYR:HA	2.38	0.53
1:C:10:SER:HB3	5:C:654:HOH:O	2.08	0.53
1:C:392:PHE:HD1	1:C:426:MET:HE3	1.70	0.53
1:A:241:ARG:CD	3:A:502:GUN:HN22	2.22	0.53
1:A:150:MET:HE3	1:A:212:ILE:HD12	1.90	0.53
1:C:254:ILE:HB	1:C:286:LEU:HD22	1.90	0.53
1:D:40:ALA:HA	1:D:54:LEU:HD21	1.91	0.53
1:A:304:VAL:HG21	1:A:312:ARG:NH1	2.24	0.53
1:A:416:ILE:HD11	1:A:450:TYR:HB2	1.90	0.53
1:B:427:ASP:O	1:B:431:GLN:HB2	2.08	0.53
1:B:220:ILE:O	1:B:220:ILE:HG13	2.09	0.53
1:D:50:ASN:O	1:D:52:LYS:N	2.40	0.53
1:B:194:MET:HE1	1:B:229:VAL:HG22	1.91	0.52
1:B:235:MET:HE3	1:B:236:PRO:HD3	1.92	0.52
1:C:190:MET:HG2	5:C:632:HOH:O	2.08	0.52
1:D:123:ASP:O	1:D:361:MET:HE1	2.10	0.52
1:B:264:GLU:CD	3:B:502:GUN:O6	2.52	0.52
1:D:48:THR:HB	1:D:53:GLU:HG3	1.92	0.52
1:B:23:LYS:HD3	1:B:67:ARG:NH1	2.24	0.51
1:A:190:MET:HG2	5:A:626:HOH:O	2.09	0.51
1:A:351:TRP:CE3	1:B:16:GLN:HG3	2.45	0.51
1:A:250:HIS:HB2	1:A:333:MET:HE1	1.92	0.51
1:A:416:ILE:HD11	1:A:450:TYR:CB	2.41	0.51
1:C:402:GLU:OE2	1:C:403:VAL:HG13	2.11	0.51
1:D:376:TYR:CZ	1:D:418:GLY:HA2	2.44	0.51
1:A:83:ALA:HB1	1:A:93:LEU:HD12	1.93	0.51
1:A:452:ILE:HG22	1:A:453:CYS:N	2.25	0.51
1:A:185:CYS:HB2	1:A:229:VAL:HG21	1.93	0.51
1:C:242:LEU:HD21	3:C:501:GUN:HN21	1.75	0.51
2:A:501:OO2:O2A	2:A:501:OO2:O1C	2.29	0.50
1:A:29:ASP:N	1:A:29:ASP:OD2	2.44	0.50
1:B:382:GLU:HG2	1:B:383:VAL:N	2.25	0.50
1:B:29:ASP:OD2	1:B:29:ASP:N	2.44	0.50
1:B:112:HIS:O	1:B:113:ASN:HB2	2.11	0.50
1:A:31:TYR:OH	1:A:62:ASP:OD1	2.14	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:HG22	1:A:112:HIS:CD2	2.47	0.50
1:C:247:ARG:HD2	1:C:349:PHE:CZ	2.46	0.50
1:A:241:ARG:HD3	3:A:502:GUN:N2	2.24	0.49
1:D:403:VAL:HG13	1:D:404:GLY:N	2.26	0.49
1:B:202:ALA:HB3	5:B:674:HOH:O	2.12	0.49
1:D:132:VAL:HG22	1:D:235:MET:HE1	1.94	0.49
1:B:55:LEU:N	1:B:55:LEU:HD23	2.27	0.49
1:A:247:ARG:HD2	1:A:349:PHE:CZ	2.48	0.49
1:D:404:GLY:O	1:D:408:ILE:HG12	2.12	0.49
1:B:313:ARG:NH1	1:B:313:ARG:HG2	2.28	0.49
1:C:406:ARG:O	1:C:410:GLU:HB2	2.13	0.49
1:C:427:ASP:O	1:C:431:GLN:HB2	2.13	0.48
1:D:51:SER:H	1:D:54:LEU:HD12	1.77	0.48
1:D:207:LYS:HA	5:D:649:HOH:O	2.13	0.48
1:B:154:TRP:CD2	3:B:502:GUN:O6	2.66	0.48
1:B:244:ALA:O	1:B:248:ILE:HG12	2.14	0.48
1:A:150:MET:HE3	1:A:212:ILE:CD1	2.44	0.48
1:B:82:GLU:CD	1:B:82:GLU:H	2.20	0.48
1:C:382:GLU:HG2	1:C:383:VAL:N	2.28	0.48
1:C:446:TYR:CE2	1:C:448:PRO:HG3	2.49	0.48
1:D:304:VAL:HG11	1:D:309:GLU:HG3	1.95	0.48
1:B:216:GLU:HB2	1:B:217:PRO:CD	2.44	0.48
1:B:316:ARG:NH1	1:B:328:GLN:NE2	2.59	0.48
1:A:351:TRP:CZ3	1:B:16:GLN:HG3	2.49	0.48
1:D:132:VAL:HG22	1:D:235:MET:CE	2.44	0.48
1:D:239:GLU:CD	1:D:362:PRO:HA	2.39	0.48
1:C:122:LEU:HG	1:C:122:LEU:O	2.14	0.48
1:A:241:ARG:NH1	3:A:502:GUN:HN22	2.11	0.47
1:B:419:ASP:OD1	1:B:421:GLU:HB3	2.14	0.47
1:B:401:LYS:O	1:B:405:ILE:HG13	2.14	0.47
1:C:184:GLY:O	1:C:185:CYS:HB3	2.14	0.47
1:B:157:HIS:HE1	1:B:223:GLU:OE1	1.97	0.47
1:A:363:PHE:CG	1:A:390:ARG:HD2	2.49	0.47
1:A:426:MET:HB2	1:A:426:MET:HE2	1.70	0.47
1:B:415:LYS:CB	5:B:678:HOH:O	2.63	0.47
1:A:10:SER:O	1:A:11:MET:HB2	2.14	0.47
1:A:83:ALA:CB	1:A:93:LEU:HD12	2.45	0.47
1:C:265:LEU:O	1:C:265:LEU:HD12	2.15	0.47
1:C:408:ILE:HD12	1:C:449:CYS:HB3	1.96	0.47
1:D:381:VAL:HG13	1:D:382:GLU:N	2.29	0.47
1:A:283:PRO:HG3	1:A:332:SER:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:O	1:A:334:PRO:HD2	2.15	0.47
1:B:254:ILE:HB	1:B:286:LEU:HD22	1.96	0.47
1:A:377:PRO:HG3	1:A:422:ILE:HD11	1.96	0.47
1:C:418:GLY:O	1:C:452:ILE:HG23	2.15	0.47
1:D:122:LEU:HD11	1:D:131:LEU:HD22	1.97	0.47
1:D:377:PRO:HD3	1:D:419:ASP:CB	2.45	0.47
1:A:52:LYS:HE2	1:A:222:ALA:HB1	1.96	0.46
1:C:421:GLU:OE1	1:C:424:ARG:NH2	2.48	0.46
1:B:441:LEU:HD13	1:B:446:TYR:HA	1.97	0.46
1:D:316:ARG:HE	1:D:316:ARG:HB2	1.58	0.46
1:D:443:GLY:O	1:D:444:SER:CB	2.62	0.46
1:C:185:CYS:HB2	1:C:213:GLY:CA	2.44	0.46
1:D:259:VAL:HG12	1:D:392:PHE:CD1	2.50	0.46
1:C:384:LEU:O	1:C:384:LEU:HD12	2.15	0.46
1:D:238:ILE:HD12	1:D:241:ARG:HD2	1.98	0.46
1:D:290:LYS:HG3	1:D:291:GLU:OE2	2.16	0.46
1:D:158:SER:OG	1:D:441:LEU:HD23	2.14	0.46
1:C:406:ARG:O	1:C:410:GLU:OE2	2.33	0.46
1:C:384:LEU:O	1:C:388:LEU:HB2	2.15	0.46
1:D:433:PHE:HB3	1:D:439:MET:HE3	1.98	0.46
1:A:161:GLU:HA	1:A:161:GLU:OE1	2.16	0.45
1:A:194:MET:HE2	1:A:211:PHE:HB3	1.98	0.45
1:A:415:LYS:NZ	1:A:453:CYS:HB2	2.31	0.45
1:C:0:ARG:C	1:C:2:ILE:HD12	2.41	0.45
1:C:450:TYR:N	1:C:450:TYR:CD1	2.84	0.45
1:D:291:GLU:N	1:D:291:GLU:CD	2.74	0.45
1:D:266:LEU:HD13	1:D:266:LEU:HA	1.80	0.45
1:C:370:MET:HG3	1:C:414:TYR:CD1	2.51	0.45
1:B:37:CYS:SG	1:B:220:ILE:HG23	2.56	0.45
1:B:361:MET:HE2	1:B:361:MET:HB2	1.85	0.45
1:C:425:ARG:HB3	5:C:624:HOH:O	2.17	0.45
1:C:302:PHE:CG	1:C:429:LEU:HD22	2.51	0.45
1:B:247:ARG:HD2	1:B:349:PHE:CZ	2.52	0.45
1:A:304:VAL:CG2	1:A:312:ARG:HD2	2.46	0.45
1:D:235:MET:HE3	1:D:240:LYS:HB3	1.99	0.45
1:C:210:ARG:HD2	1:C:231:GLU:OE2	2.17	0.44
1:B:143:HIS:HB3	1:B:146:GLU:HG2	1.99	0.44
1:C:265:LEU:HD22	1:C:286:LEU:HD11	1.99	0.44
1:D:122:LEU:N	1:D:122:LEU:HD22	2.31	0.44
1:D:391:ALA:O	1:D:395:ILE:HG13	2.17	0.44
1:A:278:LYS:HB3	1:A:278:LYS:HE2	1.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG11	1:B:439:MET:SD	2.58	0.44
1:B:341:ARG:NH2	2:B:501:OO2:O1B	2.50	0.44
1:A:207:LYS:HB2	1:A:207:LYS:HE3	1.72	0.44
1:B:363:PHE:HB2	1:B:390:ARG:CZ	2.48	0.44
1:A:283:PRO:HG3	1:A:332:SER:CB	2.47	0.44
1:B:120:LEU:CD2	1:B:122:LEU:HD21	2.44	0.44
1:D:54:LEU:O	1:D:55:LEU:C	2.60	0.44
1:A:122:LEU:HD23	1:A:127:HIS:NE2	2.33	0.44
1:D:93:LEU:N	1:D:93:LEU:HD23	2.32	0.44
1:D:408:ILE:HD11	1:D:414:TYR:CE2	2.53	0.44
1:D:441:LEU:HB3	1:D:442:PRO:HD2	1.98	0.44
1:A:264:GLU:OE2	3:A:502:GUN:O6	2.35	0.44
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.77	0.44
1:C:66:LEU:HD11	1:C:75:GLU:HB2	2.00	0.44
1:C:367:HIS:HE1	1:C:407:ALA:HB1	1.82	0.44
1:D:291:GLU:CD	1:D:291:GLU:H	2.17	0.44
1:D:242:LEU:HB3	1:D:267:TYR:CE2	2.53	0.43
1:D:0:ARG:HG3	1:D:2:ILE:HD11	2.01	0.43
1:D:48:THR:CG2	1:D:49:ASP:N	2.81	0.43
1:D:52:LYS:HG2	1:D:52:LYS:O	2.17	0.43
1:A:421:GLU:HG2	1:A:424:ARG:HH21	1.83	0.43
1:B:149:ASN:HA	1:B:333:MET:SD	2.58	0.43
1:B:432:GLY:O	1:B:436:GLN:HG3	2.18	0.43
1:A:214:MET:HE1	1:A:248:ILE:HD13	2.01	0.43
1:B:120:LEU:HG	1:B:122:LEU:HD23	2.01	0.43
1:B:241:ARG:CZ	3:B:502:GUN:HN22	2.31	0.43
1:A:77:ILE:O	1:A:78:ASN:HB2	2.19	0.43
1:A:286:LEU:N	1:A:286:LEU:HD23	2.33	0.43
1:A:452:ILE:CG2	1:A:453:CYS:N	2.82	0.43
1:C:48:THR:HG22	1:C:49:ASP:N	2.33	0.43
1:C:332:SER:HA	1:C:335:LEU:HD23	2.01	0.43
1:D:12:ASP:OD1	1:D:12:ASP:N	2.50	0.43
1:D:122:LEU:N	1:D:122:LEU:CD2	2.82	0.42
1:B:23:LYS:HE3	1:B:23:LYS:HB3	1.76	0.42
1:B:263:GLU:HG2	1:B:389:ARG:HG3	2.01	0.42
1:B:291:GLU:N	1:B:291:GLU:CD	2.76	0.42
1:C:70:ARG:HD3	1:C:70:ARG:HA	1.84	0.42
1:C:302:PHE:CE1	1:C:306:THR:HG21	2.54	0.42
1:D:7:PRO:HA	1:D:98:PHE:CZ	2.54	0.42
1:C:82:GLU:CD	1:C:82:GLU:N	2.76	0.42
1:C:192:ALA:N	1:C:193:PRO:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PRO:HA	1:B:98:PHE:CE2	2.54	0.42
1:A:438:ARG:HD2	5:A:620:HOH:O	2.20	0.42
1:D:53:GLU:HG2	1:D:57:ARG:HD2	2.02	0.42
1:B:415:LYS:C	1:B:416:ILE:HD13	2.44	0.42
1:C:264:GLU:OE1	3:C:501:GUN:O6	2.36	0.42
1:C:373:LEU:CD2	1:C:387:ASP:OD1	2.66	0.42
1:A:241:ARG:NH1	3:A:502:GUN:N2	2.68	0.42
1:C:61:PHE:HA	1:C:77:ILE:O	2.20	0.42
1:D:2:ILE:CD1	1:D:77:ILE:HG13	2.49	0.42
1:A:111:ILE:HG22	1:A:112:HIS:CG	2.55	0.42
1:C:100:VAL:HG13	1:C:104:ILE:HG13	2.01	0.42
1:D:389:ARG:NH2	5:D:606:HOH:O	2.53	0.41
1:D:265:LEU:HD23	1:D:299:LEU:HD11	2.02	0.41
1:A:108:TYR:CD1	1:A:108:TYR:C	2.98	0.41
1:D:304:VAL:HG13	1:D:309:GLU:CA	2.49	0.41
1:A:142:LEU:HB3	1:A:348:SER:OG	2.19	0.41
1:B:185:CYS:SG	1:B:225:PRO:HB3	2.60	0.41
1:C:235:MET:HE3	1:C:244:ALA:CB	2.50	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.71	0.41
1:B:61:PHE:HA	1:B:77:ILE:O	2.21	0.41
1:B:204:GLN:O	1:D:91:ARG:NH1	2.53	0.41
1:B:331:LYS:O	1:B:334:PRO:HD2	2.21	0.41
1:C:370:MET:HG3	1:C:414:TYR:CG	2.56	0.41
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.73	0.41
1:C:72:VAL:CG1	1:C:73:LYS:N	2.84	0.41
1:D:125:SER:HB2	1:D:360:GLN:OE1	2.20	0.41
1:D:165:LEU:O	1:D:169:ARG:HG3	2.21	0.41
1:D:434:VAL:HG22	1:D:439:MET:HG3	2.03	0.41
1:A:191:GLU:OE2	1:A:227:PRO:HD2	2.21	0.41
1:B:191:GLU:OE2	1:B:227:PRO:HD2	2.19	0.41
1:A:43:ASN:ND2	5:A:605:HOH:O	2.53	0.41
1:A:214:MET:HE1	1:A:248:ILE:CD1	2.51	0.41
1:A:226:ASN:HB2	1:A:227:PRO:HD2	2.03	0.41
1:C:7:PRO:HA	1:C:98:PHE:CE2	2.56	0.41
1:D:416:ILE:HD12	1:D:452:ILE:HD11	2.01	0.41
1:A:111:ILE:O	1:A:112:HIS:HB2	2.21	0.41
1:C:152:VAL:CG2	1:C:249:ALA:HB2	2.50	0.40
1:C:416:ILE:H	1:C:416:ILE:HG13	1.71	0.40
1:A:259:VAL:HG23	1:A:433:PHE:CE2	2.56	0.40
1:A:333:MET:HB2	1:A:334:PRO:HD3	2.02	0.40
1:C:408:ILE:HA	1:C:412:GLY:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ALA:HB1	1:D:93:LEU:HD12	2.04	0.40
1:A:111:ILE:HG22	1:A:112:HIS:NE2	2.36	0.40
1:C:374:LYS:C	1:C:375:LEU:HD23	2.46	0.40
1:D:103:ASP:O	1:D:107:VAL:HB	2.22	0.40
1:A:416:ILE:CD1	1:A:450:TYR:CB	3.00	0.40
1:B:336:VAL:O	1:B:340:ARG:HG2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-3:PRO:CD	2:C:502:O02:O1A[7_645]	1.37	0.83
1:A:67:ARG:NH1	1:A:278:LYS:CD[3_444]	1.97	0.23

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	452/459 (98%)	429 (95%)	20 (4%)	3 (1%)	18	20
1	B	452/459 (98%)	432 (96%)	19 (4%)	1 (0%)	43	52
1	C	438/459 (95%)	417 (95%)	20 (5%)	1 (0%)	43	52
1	D	444/459 (97%)	420 (95%)	19 (4%)	5 (1%)	11	11
All	All	1786/1836 (97%)	1698 (95%)	78 (4%)	10 (1%)	21	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	ASN
1	D	54	LEU
1	D	55	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	444	SER
1	D	28	SER
1	A	49	ASP
1	B	149	ASN
1	D	51	SER
1	A	187	PRO
1	A	400	VAL

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	386/390 (99%)	379 (98%)	7 (2%)	51	66
1	B	385/390 (99%)	381 (99%)	4 (1%)	68	81
1	C	378/390 (97%)	370 (98%)	8 (2%)	47	61
1	D	379/390 (97%)	365 (96%)	14 (4%)	30	40
All	All	1528/1560 (98%)	1495 (98%)	33 (2%)	45	59

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	59	GLU
1	A	158	SER
1	A	185	CYS
1	A	286	LEU
1	A	441	LEU
1	A	447	ILE
1	B	38	SER
1	B	46	SER
1	B	114	THR
1	B	441	LEU
1	C	41	VAL
1	C	47	LEU
1	C	185	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	286	LEU
1	C	393	SER
1	C	399	ASN
1	C	430	LEU
1	C	450	TYR
1	D	27	SER
1	D	41	VAL
1	D	46	SER
1	D	47	LEU
1	D	56	SER
1	D	111	ILE
1	D	125	SER
1	D	144	VAL
1	D	149	ASN
1	D	185	CYS
1	D	218	SER
1	D	220	ILE
1	D	259	VAL
1	D	453	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	110	GLN
1	A	113	ASN
1	A	124	ASN
1	A	138	ASN
1	A	162	ASN
1	A	339	ASN
1	A	417	ASN
1	A	431	GLN
1	B	64	ASN
1	B	112	HIS
1	B	157	HIS
1	B	203	GLN
1	B	314	HIS
1	B	339	ASN
1	B	417	ASN
1	C	138	ASN
1	C	149	ASN
1	C	399	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	431	GLN
1	D	314	HIS
1	D	372	ASN
1	D	379	GLN
1	D	417	ASN
1	D	431	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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	GUN	B	502	-	12,12,12	5.94	10 (83%)	15,17,17	4.13	11 (73%)
3	GUN	C	501	-	12,12,12	5.98	11 (91%)	15,17,17	4.11	12 (80%)
4	HSX	D	501	-	14,14,14	6.85	5 (35%)	19,21,21	1.32	1 (5%)
2	0O2	C	502	-	40,42,42	3.55	23 (57%)	61,68,68	2.47	21 (34%)
2	0O2	B	501	-	40,42,42	3.32	20 (50%)	61,68,68	2.28	17 (27%)
2	0O2	A	501	-	40,42,42	3.46	20 (50%)	61,68,68	2.44	22 (36%)
3	GUN	A	502	-	12,12,12	5.87	10 (83%)	15,17,17	4.17	11 (73%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GUN	B	502	-	-	-	0/2/2/2
3	GUN	C	501	-	-	-	0/2/2/2
4	HSX	D	501	-	-	4/6/22/22	0/1/1/1
2	0O2	C	502	-	-	8/33/49/49	0/3/3/3
2	0O2	B	501	-	-	3/33/49/49	0/3/3/3
2	0O2	A	501	-	-	11/33/49/49	0/3/3/3
3	GUN	A	502	-	-	-	0/2/2/2

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	HSX	C1-C2	-18.66	1.31	1.52
3	C	501	GUN	C2-N1	10.55	1.63	1.37
4	D	501	HSX	O4-C1	10.46	1.55	1.43
3	B	502	GUN	C2-N1	10.28	1.62	1.37
3	A	502	GUN	C2-N1	10.16	1.62	1.37
4	D	501	HSX	C3-C4	-10.12	1.27	1.53
2	C	502	0O2	O6-C6	8.73	1.40	1.23
2	A	501	0O2	O6-C6	8.63	1.39	1.23
2	B	501	0O2	O6-C6	8.41	1.39	1.23
3	B	502	GUN	O6-C6	8.28	1.39	1.23
3	C	501	GUN	O6-C6	7.96	1.38	1.23
3	A	502	GUN	O6-C6	7.88	1.38	1.23
2	C	502	0O2	C5-N7	7.58	1.54	1.39
3	C	501	GUN	C8-N7	-7.48	1.16	1.33
3	A	502	GUN	C8-N7	-7.41	1.16	1.33
3	B	502	GUN	C8-N7	-7.39	1.16	1.33
2	A	501	0O2	O4'-C1'	7.31	1.58	1.42
2	B	501	0O2	O4'-C1'	7.23	1.58	1.42
2	A	501	0O2	C5-N7	7.17	1.53	1.39
2	C	502	0O2	O4'-C1'	7.07	1.58	1.42
2	B	501	0O2	C5-N7	7.06	1.53	1.39
3	A	502	GUN	C8-N9	-7.02	1.23	1.35
3	B	502	GUN	C8-N9	-7.02	1.23	1.35
2	C	502	0O2	PA-O3A	6.67	1.66	1.59
3	C	501	GUN	C8-N9	-6.62	1.24	1.35
4	D	501	HSX	O4-C4	6.55	1.59	1.45
3	A	502	GUN	C4-N3	-6.38	1.26	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	GUN	C4-N3	-6.34	1.26	1.36
3	B	502	GUN	C4-N3	-6.30	1.26	1.36
4	D	501	HSX	C3-C2	6.26	1.70	1.53
3	C	501	GUN	C6-N1	6.05	1.50	1.38
2	C	502	0O2	PB-O3A	5.97	1.65	1.59
3	B	502	GUN	C6-N1	5.90	1.49	1.38
2	A	501	0O2	PA-O3A	5.84	1.65	1.59
2	A	501	0O2	PC-O3C	5.72	1.65	1.59
2	C	502	0O2	PB-O3B	5.41	1.65	1.59
3	C	501	GUN	C2-N2	5.40	1.46	1.34
3	A	502	GUN	C6-N1	5.27	1.48	1.38
3	A	502	GUN	C2-N2	5.18	1.46	1.34
2	B	501	0O2	PB-O3B	5.14	1.65	1.59
2	B	501	0O2	PC-O3C	5.10	1.65	1.59
2	A	501	0O2	PB-O3B	5.04	1.64	1.59
2	C	502	0O2	C2-N2	4.97	1.45	1.34
2	A	501	0O2	C2-N2	4.89	1.45	1.34
2	A	501	0O2	PB-O3A	4.83	1.64	1.59
2	C	502	0O2	PC-O3C	4.78	1.64	1.59
2	B	501	0O2	C2-N2	4.76	1.45	1.34
3	B	502	GUN	C2-N2	4.72	1.45	1.34
2	B	501	0O2	PA-O3A	4.68	1.64	1.59
3	C	501	GUN	C2-N3	4.61	1.44	1.33
3	A	502	GUN	C2-N3	4.59	1.44	1.33
2	B	501	0O2	C2-N1	4.57	1.48	1.37
3	B	502	GUN	C2-N3	4.47	1.44	1.33
2	C	502	0O2	C2-N1	4.42	1.48	1.37
2	A	501	0O2	O4'-C4'	4.35	1.54	1.45
3	B	502	GUN	C4-N9	4.35	1.44	1.36
3	A	502	GUN	C4-N9	4.31	1.44	1.36
3	C	501	GUN	C4-N9	4.29	1.44	1.36
2	B	501	0O2	O4'-C4'	4.24	1.54	1.45
2	C	502	0O2	C2-N3	4.14	1.43	1.33
2	A	501	0O2	C2-N1	4.02	1.47	1.37
2	C	502	0O2	O4'-C4'	3.98	1.53	1.45
2	A	501	0O2	C2-N3	3.96	1.42	1.33
2	B	501	0O2	C2-N3	3.68	1.42	1.33
2	A	501	0O2	PC-O3'	3.57	1.70	1.59
2	B	501	0O2	PB-O3A	3.57	1.63	1.59
2	A	501	0O2	C8-N9	-3.54	1.29	1.37
2	B	501	0O2	C2'-C3'	-3.51	1.45	1.53
2	C	502	0O2	C4-N9	-3.50	1.29	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	0O2	C8-N9	-3.49	1.29	1.37
2	B	501	0O2	C8-N9	-3.34	1.30	1.37
2	A	501	0O2	C4-N9	-3.28	1.29	1.38
2	C	502	0O2	C2'-C3'	-3.21	1.46	1.53
2	B	501	0O2	PC-O3'	3.19	1.69	1.59
2	B	501	0O2	C4-N9	-3.09	1.30	1.38
2	A	501	0O2	C2'-C3'	-3.06	1.46	1.53
2	C	502	0O2	PC-O3'	2.78	1.67	1.59
2	C	502	0O2	C8-N7	2.59	1.39	1.32
2	B	501	0O2	C8-N7	2.50	1.39	1.32
2	C	502	0O2	PG-O3G	-2.46	1.45	1.54
2	C	502	0O2	C2'-C1'	-2.44	1.45	1.53
2	A	501	0O2	C2'-C1'	-2.40	1.45	1.53
2	B	501	0O2	C2'-C1'	-2.38	1.46	1.53
2	C	502	0O2	C4-N3	2.36	1.39	1.34
2	C	502	0O2	PG-O2G	-2.35	1.46	1.54
2	B	501	0O2	PG-O3G	-2.33	1.46	1.54
2	C	502	0O2	PD-O3D	-2.33	1.46	1.54
3	A	502	GUN	C5-N7	2.32	1.43	1.39
3	B	502	GUN	C5-N7	2.31	1.43	1.39
2	A	501	0O2	C8-N7	2.31	1.39	1.32
2	A	501	0O2	PG-O2G	-2.28	1.46	1.54
2	B	501	0O2	C4-N3	2.17	1.39	1.34
2	C	502	0O2	C1'-N9	-2.16	1.41	1.47
2	B	501	0O2	PD-O3D	-2.13	1.46	1.54
2	A	501	0O2	PD-O3D	-2.12	1.46	1.54
2	C	502	0O2	PD-O1D	-2.07	1.47	1.54
3	C	501	GUN	C5-C6	-2.06	1.37	1.44
3	C	501	GUN	C5-N7	2.03	1.43	1.39
2	A	501	0O2	PD-O1D	-2.01	1.47	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	0O2	C8-N9-C4	8.73	122.39	106.03
3	C	501	GUN	N9-C4-N3	8.10	135.84	125.99
2	A	501	0O2	C8-N9-C4	8.08	121.17	106.03
2	B	501	0O2	C8-N9-C4	7.87	120.78	106.03
3	A	502	GUN	N9-C4-N3	7.83	135.51	125.99
3	B	502	GUN	N9-C4-N3	7.66	135.31	125.99
2	A	501	0O2	N9-C4-N3	5.94	137.83	125.95
2	B	501	0O2	N9-C4-N3	5.87	137.69	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	0O2	C4'-O4'-C1'	-5.85	96.56	109.47
3	C	501	GUN	C2-N3-C4	5.84	123.67	113.36
3	B	502	GUN	C2-N3-C4	5.80	123.60	113.36
3	A	502	GUN	C2-N3-C4	5.80	123.60	113.36
2	A	501	0O2	C5-C4-N3	-5.79	119.17	128.39
3	B	502	GUN	C8-N7-C5	5.78	112.20	104.38
3	A	502	GUN	C8-N7-C5	5.61	111.97	104.38
2	B	501	0O2	C5-C4-N3	-5.57	119.52	128.39
3	C	501	GUN	C2-N1-C6	-5.46	115.20	125.11
3	A	502	GUN	C2-N1-C6	-5.45	115.23	125.11
2	C	502	0O2	N9-C4-N3	5.44	136.84	125.95
3	B	502	GUN	C2-N1-C6	-5.31	115.48	125.11
2	A	501	0O2	C2-N3-C4	5.27	121.39	112.30
2	C	502	0O2	C5-C4-N3	-5.14	120.21	128.39
3	C	501	GUN	C8-N7-C5	4.84	110.93	104.38
2	C	502	0O2	C2-N3-C4	4.84	120.64	112.30
4	D	501	HSX	C1-C2-C3	4.80	108.19	102.29
3	A	502	GUN	C8-N9-C4	4.76	111.53	106.25
3	B	502	GUN	C4-C5-N7	-4.74	102.75	110.17
2	C	502	0O2	N9-C8-N7	-4.64	104.79	113.40
3	B	502	GUN	C8-N9-C4	4.63	111.39	106.25
3	A	502	GUN	C4-C5-N7	-4.55	103.06	110.17
2	A	501	0O2	C1'-N9-C8	-4.54	113.83	126.73
3	C	501	GUN	C5-C4-N9	-4.53	99.70	106.17
3	C	501	GUN	N1-C2-N3	-4.49	115.10	123.32
2	B	501	0O2	C2-N3-C4	4.39	119.86	112.30
3	C	501	GUN	C8-N9-C4	4.26	110.98	106.25
3	A	502	GUN	C5-C4-N9	-4.25	100.10	106.17
3	A	502	GUN	N1-C2-N3	-4.25	115.55	123.32
3	B	502	GUN	N1-C2-N3	-4.23	115.58	123.32
2	B	501	0O2	C1'-N9-C8	-4.14	114.96	126.73
3	B	502	GUN	C5-C4-N9	-4.14	100.27	106.17
2	A	501	0O2	N9-C8-N7	-4.06	105.88	113.40
3	C	501	GUN	C4-C5-N7	-3.89	104.07	110.17
2	C	502	0O2	C1'-N9-C8	-3.80	115.92	126.73
2	B	501	0O2	N9-C8-N7	-3.78	106.39	113.40
2	B	501	0O2	O2G-PG-O3B	3.71	117.08	104.64
2	B	501	0O2	C4'-O4'-C1'	-3.58	101.56	109.47
2	A	501	0O2	C4'-O4'-C1'	-3.58	101.57	109.47
2	C	502	0O2	O3G-PG-O3B	3.55	116.53	104.64
2	A	501	0O2	C2'-C1'-N9	3.36	122.60	113.25
3	B	502	GUN	N2-C2-N3	3.20	125.91	119.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	GUN	N2-C2-N3	3.16	125.85	119.67
2	A	501	0O2	O3D-PD-O3C	3.14	115.15	104.64
2	B	501	0O2	C2-N1-C6	-3.13	119.44	125.11
2	A	501	0O2	C2-N1-C6	-3.12	119.45	125.11
2	C	502	0O2	C2-N1-C6	-3.05	119.58	125.11
2	C	502	0O2	C4-C5-N7	-3.00	105.91	110.67
2	B	501	0O2	O6-C6-C5	-2.96	118.73	126.53
2	A	501	0O2	O1C-PC-O2C	-2.94	98.78	112.44
2	C	502	0O2	O1D-PD-O3C	2.92	114.42	104.64
2	B	501	0O2	O1D-PD-O3C	2.79	114.00	104.64
3	C	501	GUN	O6-C6-C5	-2.77	119.23	126.53
2	A	501	0O2	O2G-PG-O3B	2.73	113.78	104.64
2	A	501	0O2	O1D-PD-O3C	2.71	113.73	104.64
2	A	501	0O2	C4-C5-N7	-2.70	106.39	110.67
2	C	502	0O2	O2G-PG-O3B	2.70	113.70	104.64
2	B	501	0O2	O3D-PD-O3C	2.62	113.43	104.64
2	C	502	0O2	O3D-PD-O3C	2.62	113.41	104.64
2	A	501	0O2	O6-C6-C5	-2.55	119.79	126.53
2	A	501	0O2	O3G-PG-O3B	2.52	113.10	104.64
2	B	501	0O2	C6-C5-C4	2.52	122.62	118.83
3	A	502	GUN	C6-C5-N7	2.48	134.80	130.29
2	A	501	0O2	N1-C2-N3	-2.48	118.79	123.32
2	B	501	0O2	O1C-PC-O2C	-2.47	100.98	112.44
2	C	502	0O2	O6-C6-C5	-2.46	120.03	126.53
2	C	502	0O2	C5-C6-N1	2.45	119.49	113.25
2	C	502	0O2	N1-C2-N3	-2.43	118.87	123.32
3	B	502	GUN	C6-C5-N7	2.42	134.69	130.29
2	A	501	0O2	O1C-PC-O3C	2.41	113.79	107.27
2	A	501	0O2	C5-C6-N1	2.38	119.32	113.25
2	A	501	0O2	O1A-PA-O2A	-2.37	101.42	112.44
2	B	501	0O2	C4-C5-N7	-2.36	106.93	110.67
2	C	502	0O2	O1B-PB-O2B	-2.35	101.53	112.44
2	B	501	0O2	C2'-C3'-C4'	2.33	107.33	103.24
3	A	502	GUN	C5-C6-N1	2.29	119.08	113.25
2	C	502	0O2	O1C-PC-O2C	-2.24	102.01	112.44
2	C	502	0O2	O1B-PB-O3A	2.20	113.21	107.27
3	C	501	GUN	C5-C6-N1	2.18	118.79	113.25
3	C	501	GUN	N2-C2-N3	2.15	123.88	119.67
2	B	501	0O2	C5-C6-N1	2.12	118.66	113.25
2	C	502	0O2	C2'-C3'-C4'	2.12	106.96	103.24
2	A	501	0O2	O1B-PB-O2B	-2.11	102.65	112.44
2	A	501	0O2	C6-C5-C4	2.03	121.89	118.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	GUN	N2-C2-N1	2.01	121.01	116.76
2	C	502	0O2	O1A-PA-O3A	2.00	112.69	107.27
3	B	502	GUN	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	0O2	C5'-O5'-PA-O3A
2	A	501	0O2	C5'-O5'-PA-O2A
2	C	502	0O2	PC-O3C-PD-O3D
4	D	501	HSX	C5-O5-P'-O1X
4	D	501	HSX	C5-O5-P'-O2X
4	D	501	HSX	C5-O5-P'-O3X
2	A	501	0O2	O4'-C4'-C5'-O5'
2	C	502	0O2	O4'-C4'-C5'-O5'
2	C	502	0O2	C3'-C4'-C5'-O5'
2	A	501	0O2	C3'-C4'-C5'-O5'
2	A	501	0O2	C4'-C5'-O5'-PA
2	A	501	0O2	PB-O3A-PA-O5'
2	A	501	0O2	PD-O3C-PC-O3'
2	B	501	0O2	PB-O3A-PA-O5'
2	B	501	0O2	PD-O3C-PC-O3'
2	C	502	0O2	PA-O3A-PB-O1B
2	C	502	0O2	C5'-O5'-PA-O3A
2	C	502	0O2	C5'-O5'-PA-O2A
4	D	501	HSX	C3-C4-C5-O5
2	B	501	0O2	C4'-C5'-O5'-PA
2	A	501	0O2	PA-O3A-PB-O3B
2	A	501	0O2	PB-O3B-PG-O1G
2	A	501	0O2	PA-O3A-PB-O1B
2	C	502	0O2	PA-O3A-PB-O2B
2	C	502	0O2	PB-O3A-PA-O1A
2	A	501	0O2	PA-O3A-PB-O2B

There are no ring outliers.

6 monomers are involved in 22 short contacts:

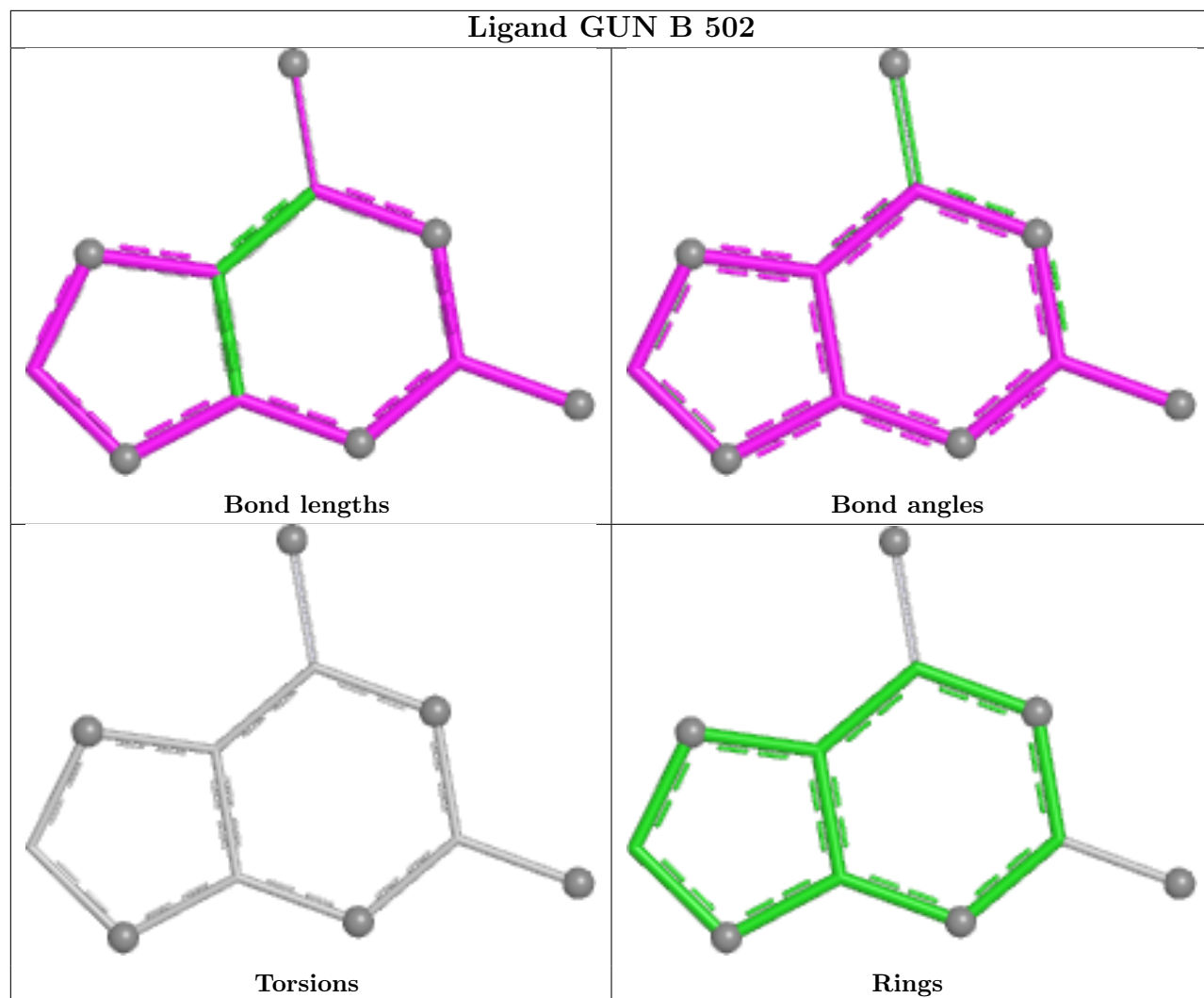
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	GUN	4	0
3	C	501	GUN	5	0

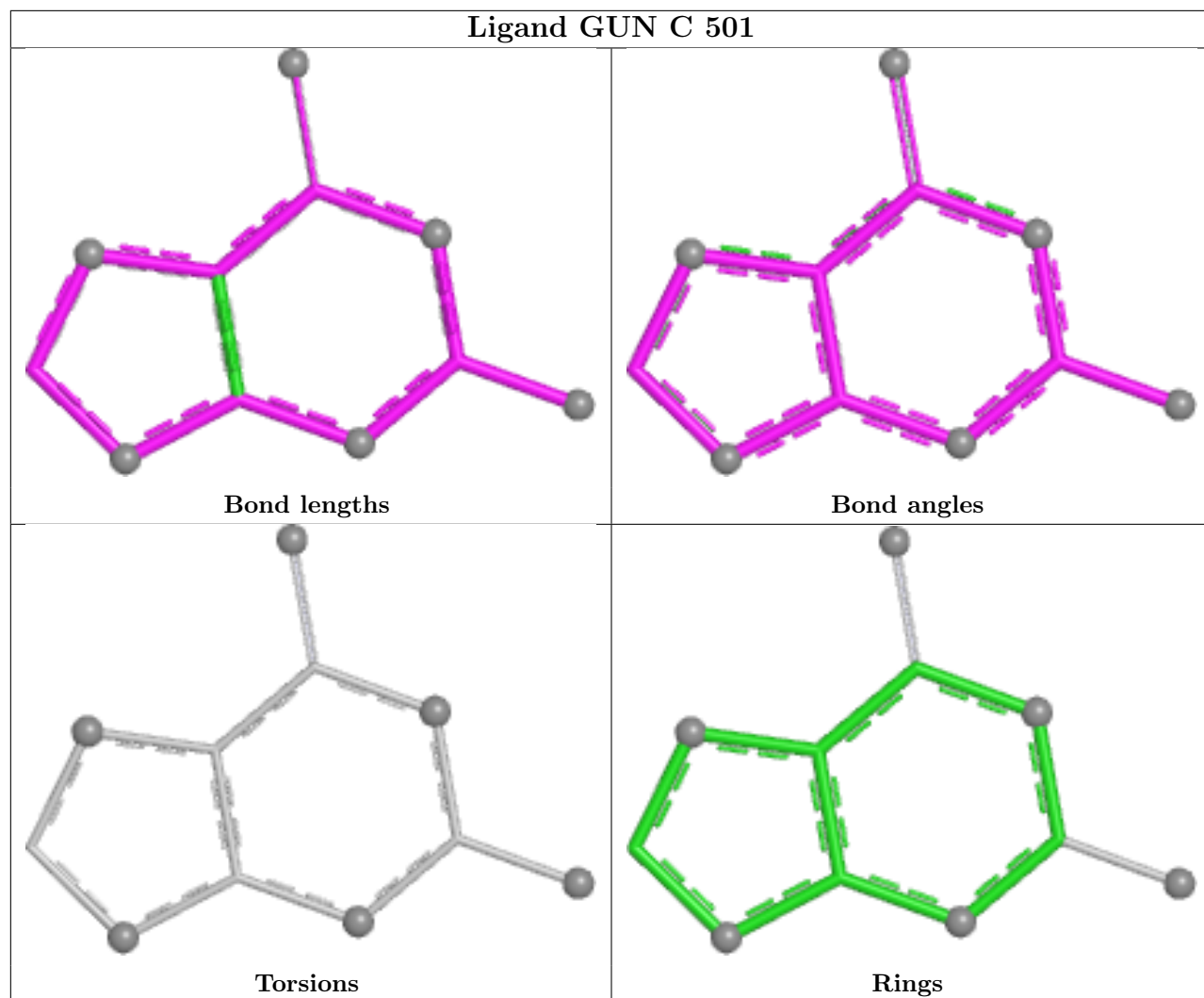
Continued on next page...

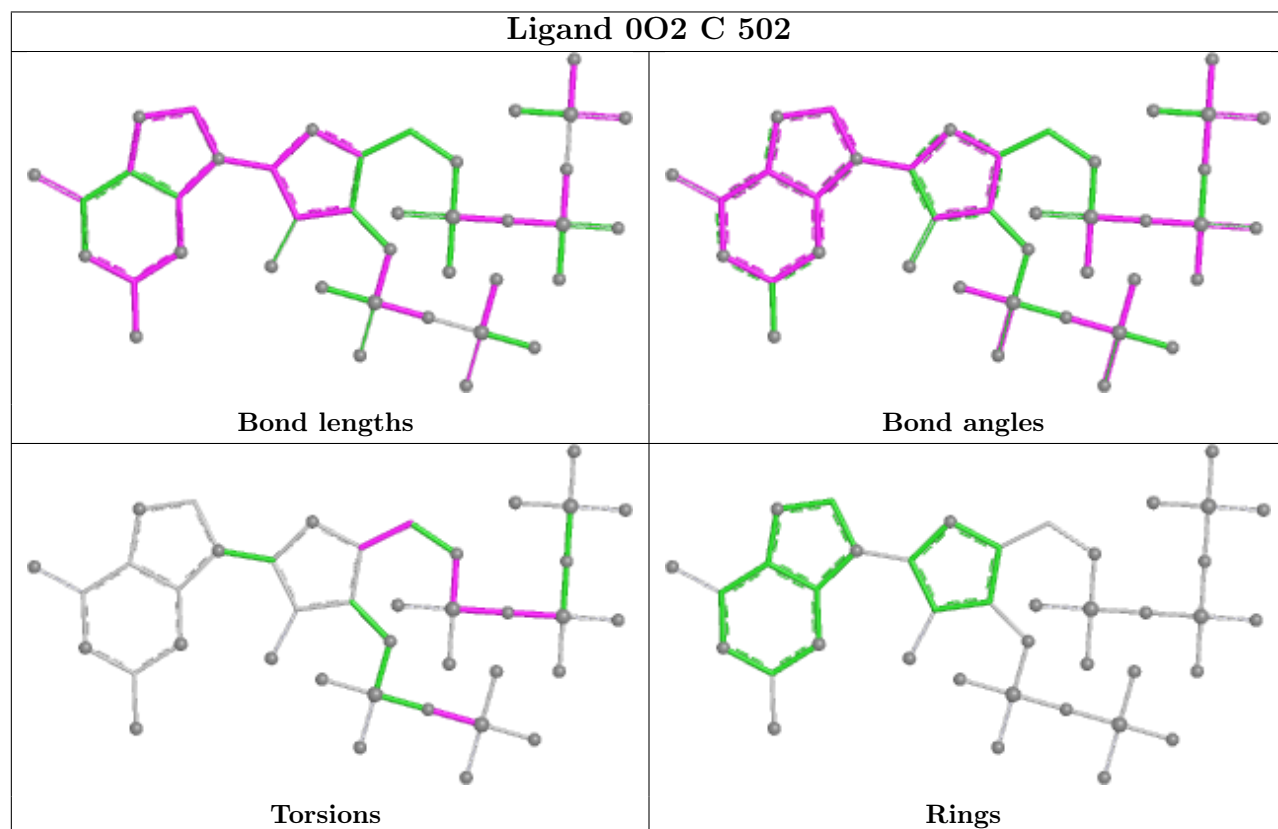
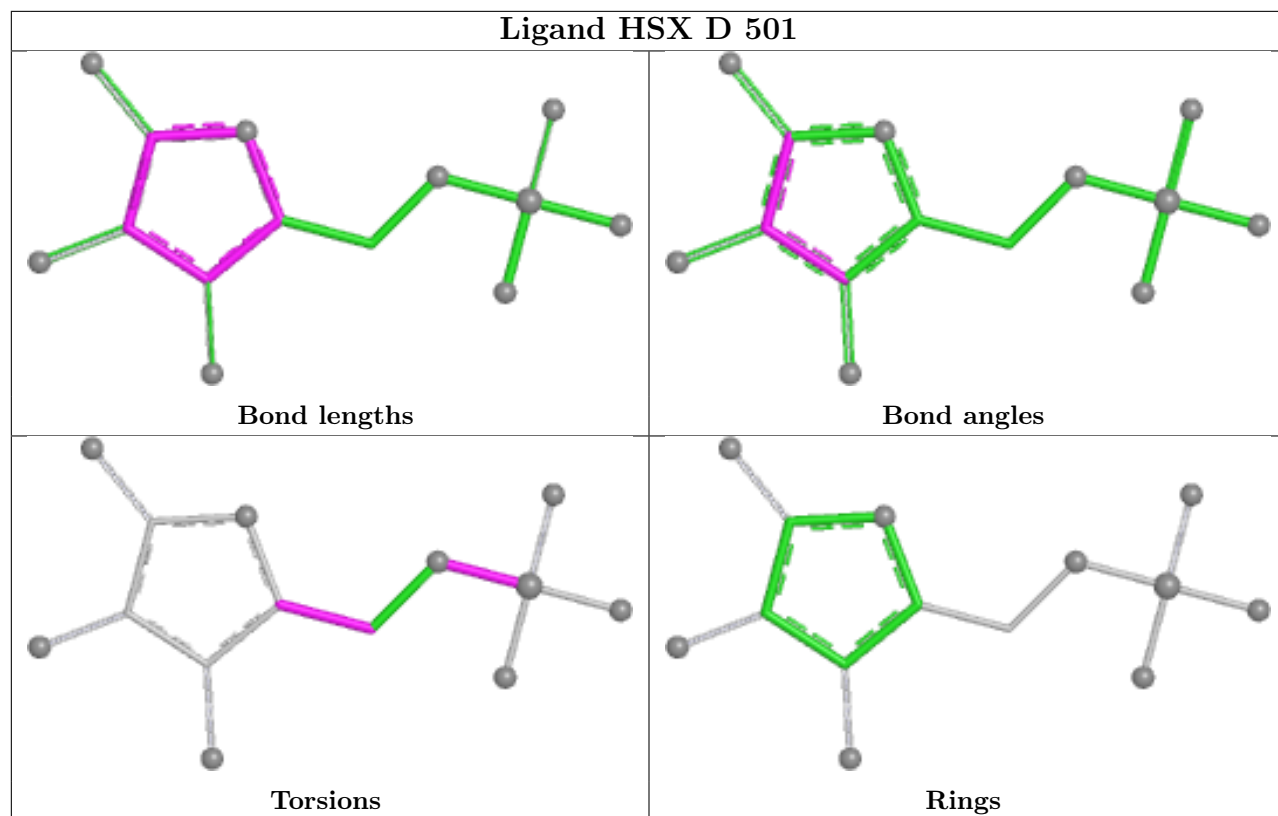
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	0O2	0	1
2	B	501	0O2	2	0
2	A	501	0O2	3	0
3	A	502	GUN	7	0

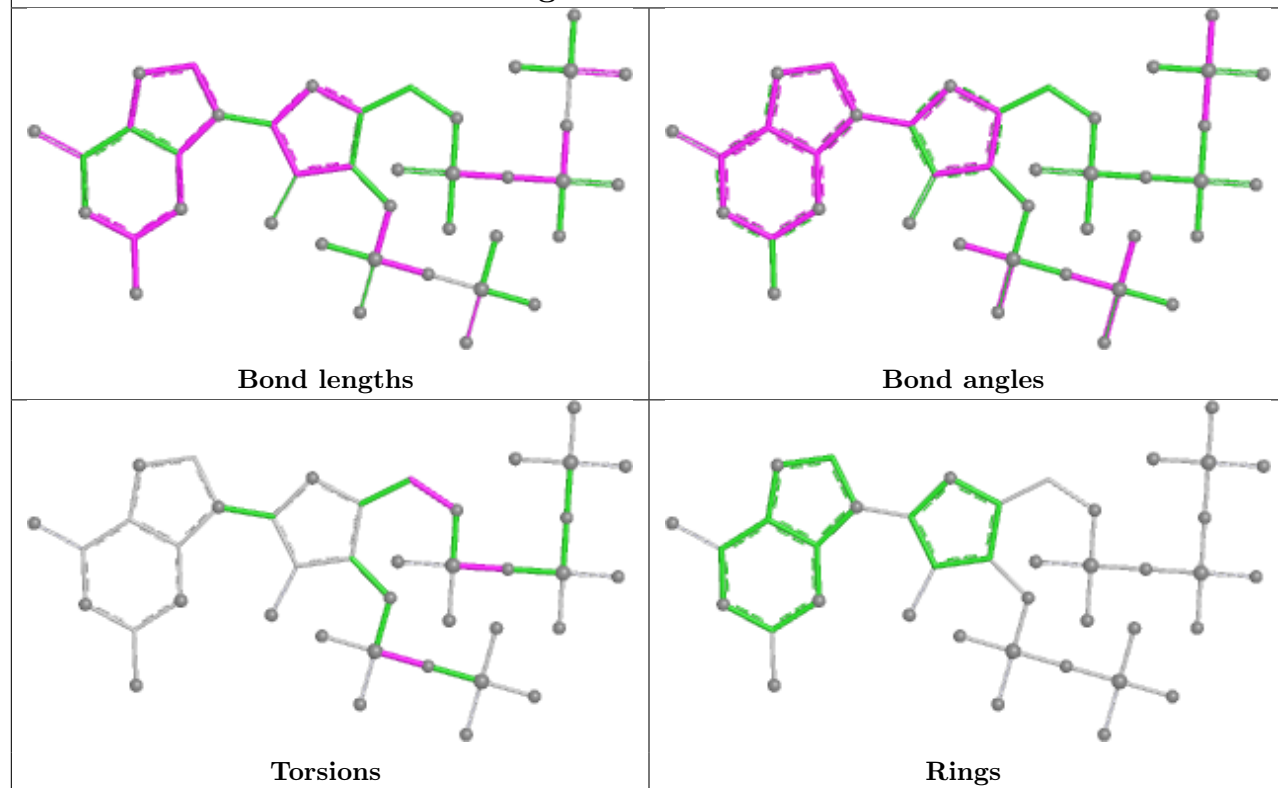
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



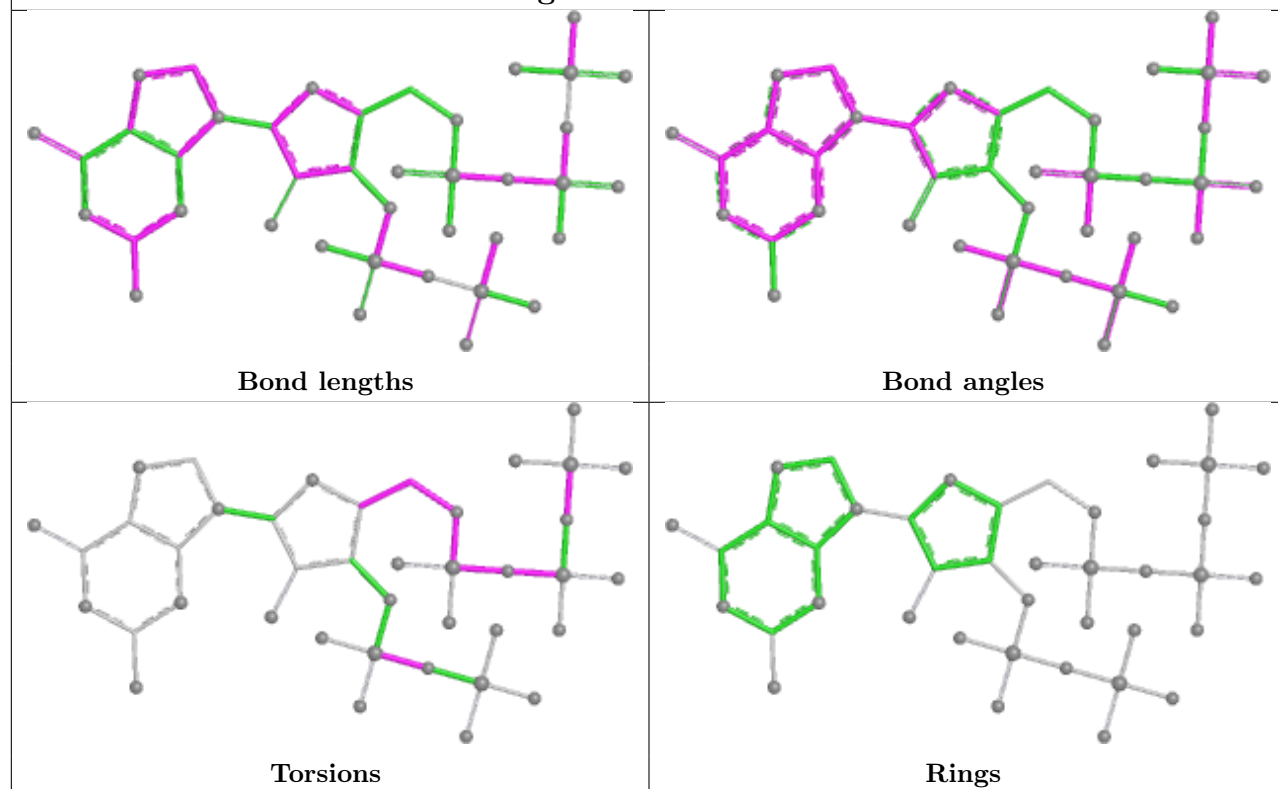


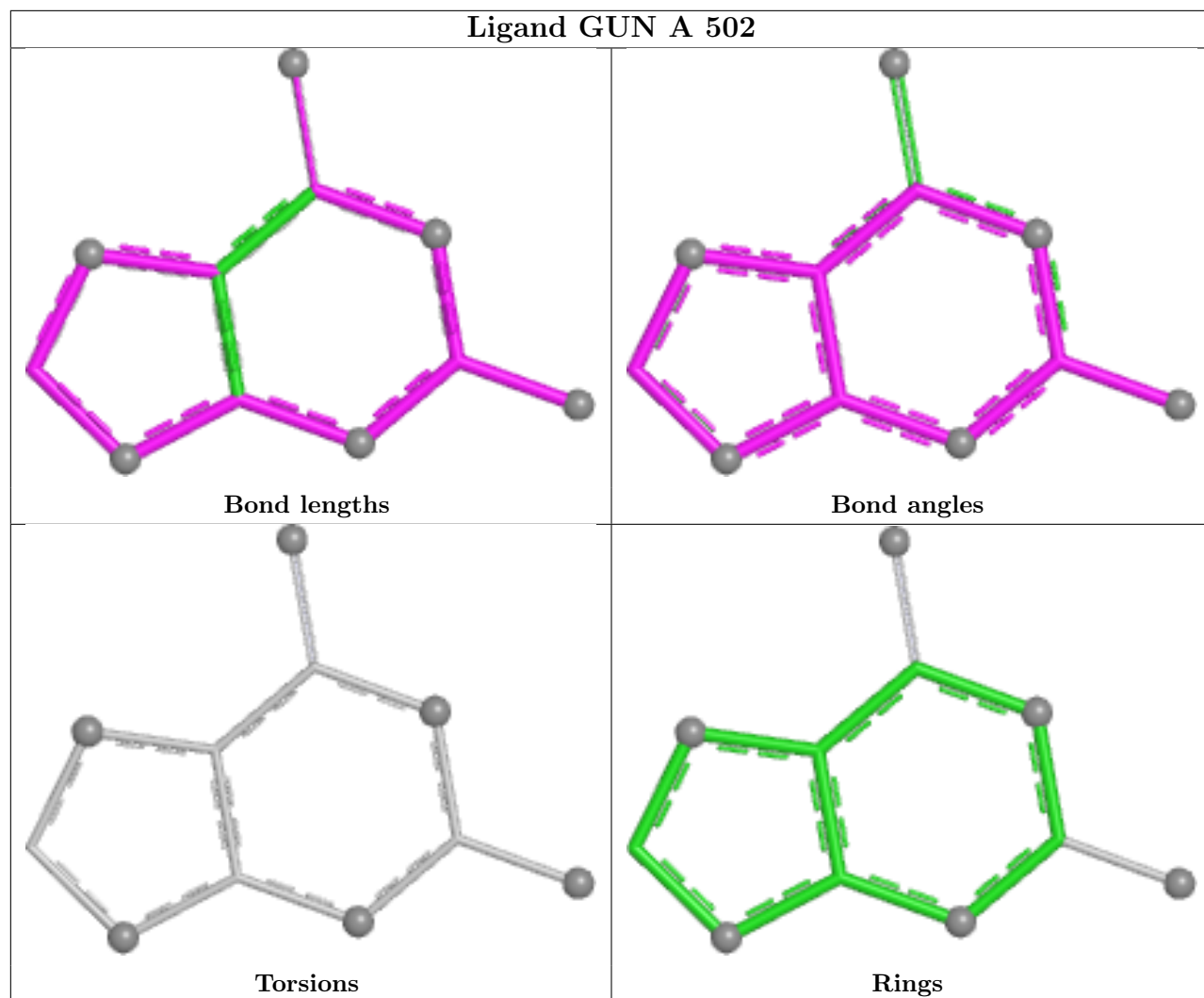


Ligand 0O2 B 501



Ligand 0O2 A 501





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	454/459 (98%)	0.23	31 (6%)	23 26	43, 56, 102, 120	10 (2%)
1	B	454/459 (98%)	0.10	15 (3%)	49 56	43, 56, 92, 123	8 (1%)
1	C	444/459 (96%)	0.33	30 (6%)	23 26	45, 60, 112, 130	8 (1%)
1	D	448/459 (97%)	0.16	21 (4%)	36 42	44, 57, 87, 115	6 (1%)
All	All	1800/1836 (98%)	0.21	97 (5%)	31 37	43, 57, 102, 130	32 (1%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	441	LEU	5.3
1	D	55	LEU	5.2
1	A	447	ILE	5.1
1	C	452	ILE	5.1
1	B	445	ALA	4.9
1	B	454	THR	4.8
1	C	47	LEU	4.6
1	C	118	PRO	4.6
1	D	445	ALA	4.5
1	C	441	LEU	4.4
1	D	453	CYS	4.3
1	D	47	LEU	4.3
1	A	445	ALA	4.2
1	B	47	LEU	4.2
1	C	447	ILE	4.2
1	A	452	ILE	4.1
1	D	111	ILE	4.1
1	C	450	TYR	4.1
1	B	441	LEU	4.0
1	C	411	PHE	4.0
1	A	403	VAL	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	108	TYR	3.7
1	B	442	PRO	3.6
1	C	405	ILE	3.5
1	A	442	PRO	3.5
1	C	416	ILE	3.5
1	A	115	VAL	3.4
1	B	447	ILE	3.4
1	C	403	VAL	3.3
1	C	448	PRO	3.3
1	D	442	PRO	3.3
1	B	448	PRO	3.3
1	A	111	ILE	3.3
1	A	47	LEU	3.2
1	C	112	HIS	3.1
1	A	441	LEU	3.1
1	C	122	LEU	3.1
1	B	452	ILE	3.0
1	C	398	GLY	3.0
1	A	114	THR	2.9
1	D	51	SER	2.8
1	A	444	SER	2.8
1	C	408	ILE	2.8
1	A	392	PHE	2.8
1	B	54	LEU	2.7
1	C	54	LEU	2.7
1	A	450	TYR	2.7
1	C	395	ILE	2.7
1	A	446	TYR	2.7
1	D	443	GLY	2.7
1	B	51	SER	2.7
1	A	122	LEU	2.6
1	C	407	ALA	2.6
1	A	116	ARG	2.6
1	C	1	ALA	2.6
1	C	440	LYS	2.6
1	C	415	LYS	2.5
1	B	453	CYS	2.5
1	C	397	ALA	2.5
1	C	392	PHE	2.4
1	C	446	TYR	2.4
1	D	53	GLU	2.4
1	A	443	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	453	CYS	2.4
1	A	411	PHE	2.4
1	C	0	ARG	2.4
1	D	49	ASP	2.4
1	D	109	GLY	2.4
1	A	278	LYS	2.4
1	D	-3	PRO	2.3
1	A	51	SER	2.3
1	D	444	SER	2.3
1	B	48	THR	2.3
1	A	113	ASN	2.2
1	A	451	GLU	2.2
1	A	50	ASN	2.2
1	A	123	ASP	2.2
1	C	412	GLY	2.2
1	A	414	TYR	2.2
1	A	416	ILE	2.1
1	A	112	HIS	2.1
1	C	418	GLY	2.1
1	B	420	LYS	2.1
1	B	46	SER	2.1
1	C	48	THR	2.1
1	D	147	ALA	2.1
1	D	54	LEU	2.1
1	C	24	ARG	2.1
1	A	415	LYS	2.1
1	A	440	LYS	2.0
1	D	426	MET	2.0
1	B	55	LEU	2.0
1	D	52	LYS	2.0
1	D	306	THR	2.0
1	C	147	ALA	2.0
1	D	50	ASN	2.0
1	A	405	ILE	2.0

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

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](#)

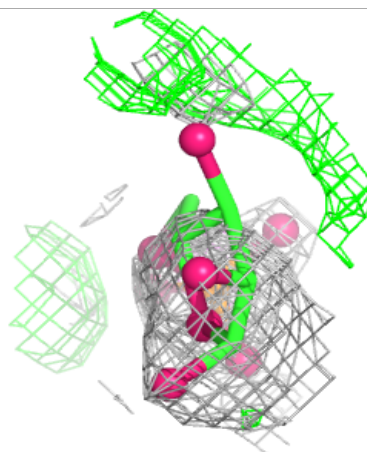
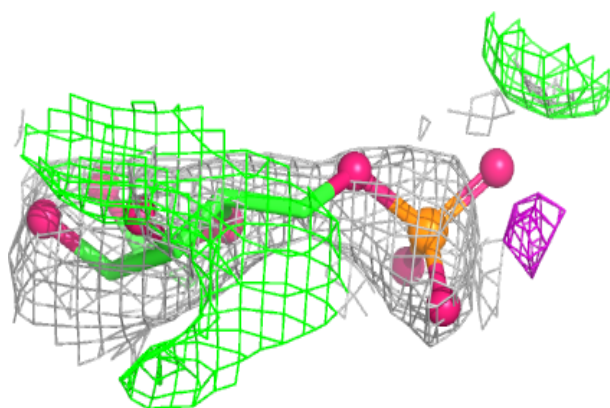
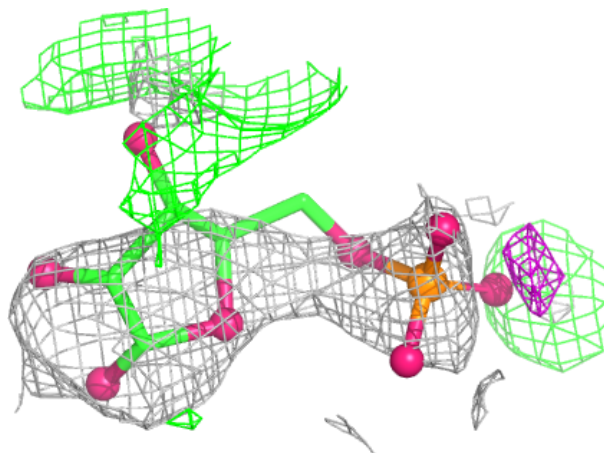
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HSX	D	501	14/14	0.68	0.21	60,73,80,167	14
3	GUN	C	501	11/11	0.76	0.28	57,64,77,79	16
3	GUN	A	502	11/11	0.77	0.35	58,60,77,77	16
2	0O2	C	502	40/40	0.81	0.13	66,85,103,106	24
2	0O2	B	501	40/40	0.88	0.09	53,77,111,128	0
3	GUN	B	502	11/11	0.88	0.16	58,65,80,82	7
2	0O2	A	501	40/40	0.89	0.10	46,82,110,118	51

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.

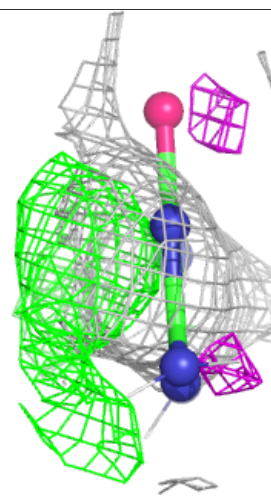
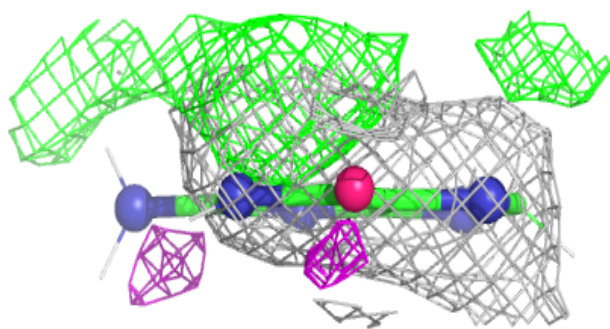
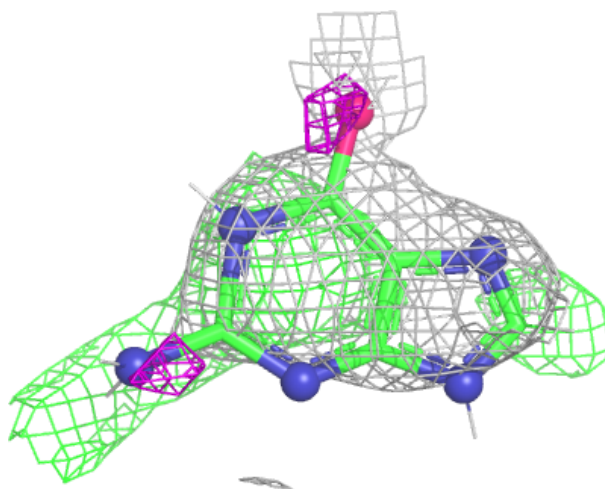
Electron density around HSX D 501:

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



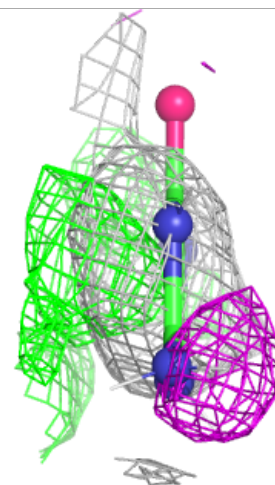
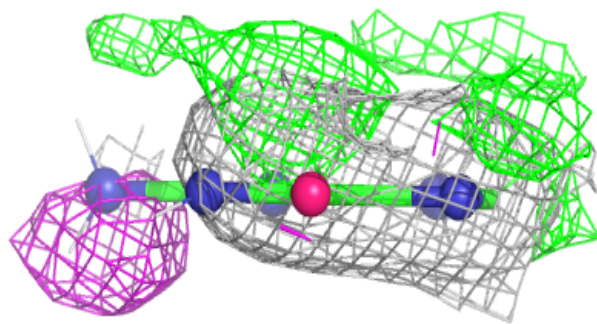
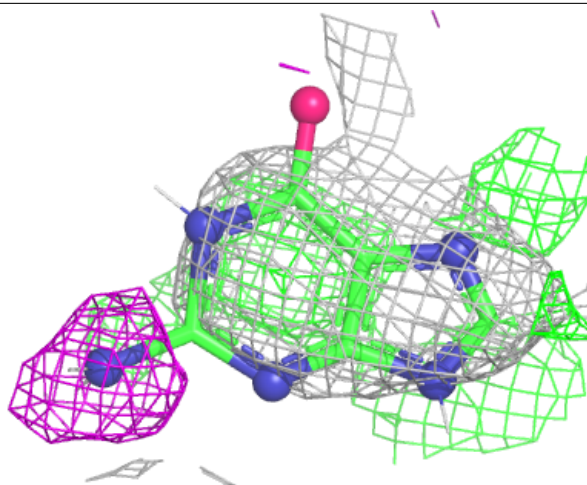
Electron density around GUN C 501:

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



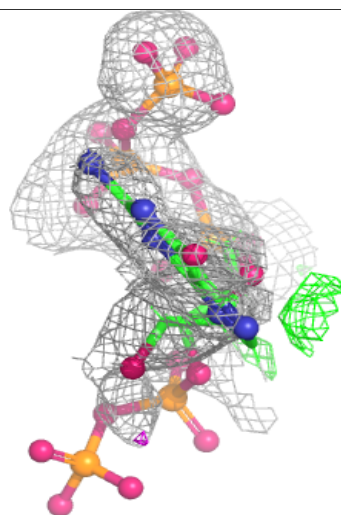
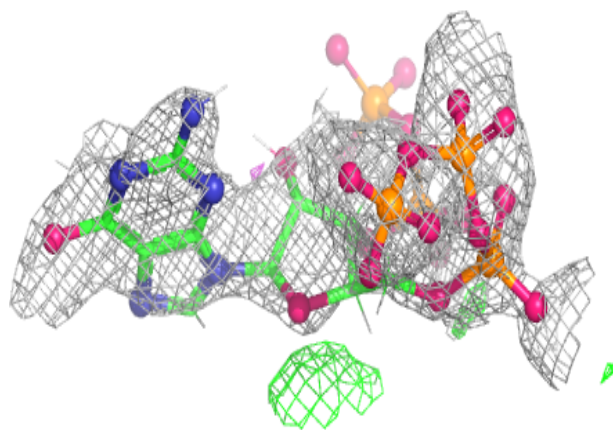
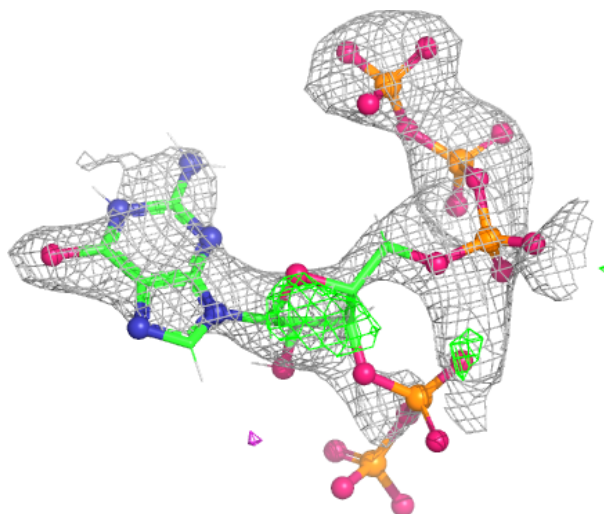
Electron density around GUN A 502:

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



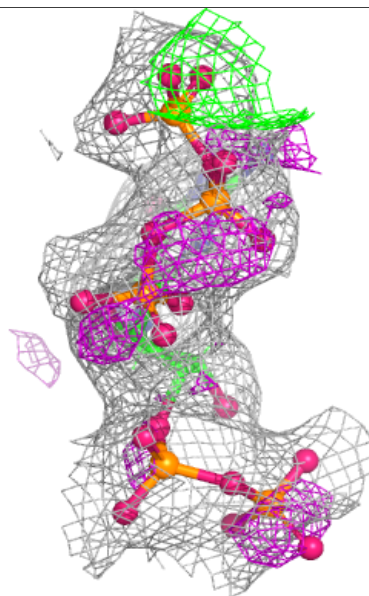
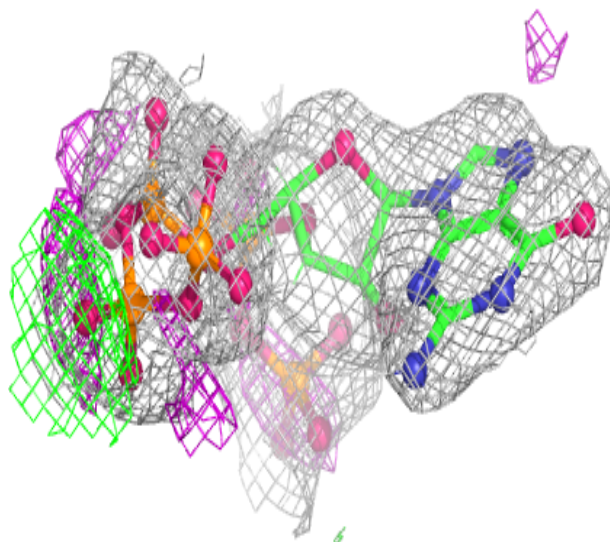
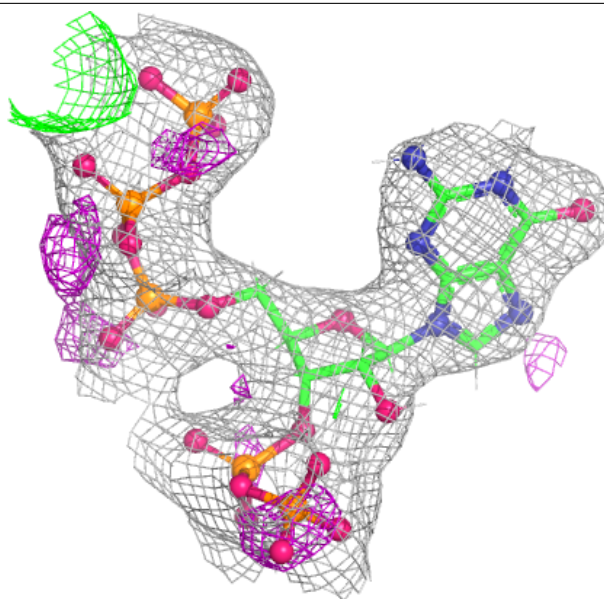
Electron density around 0O2 C 502:

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



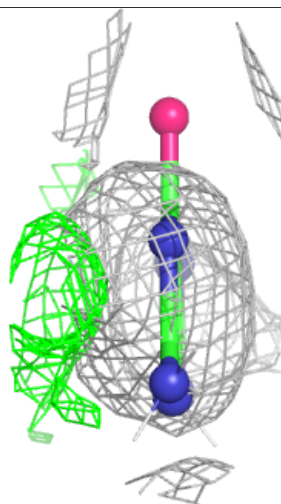
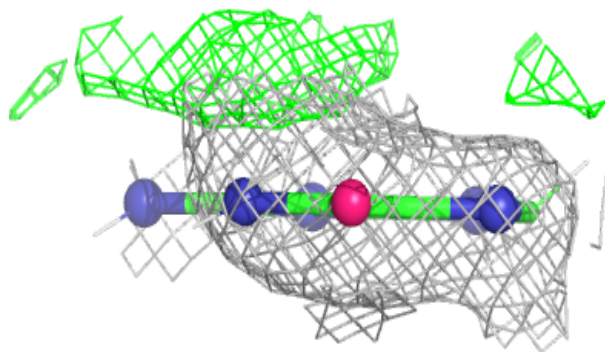
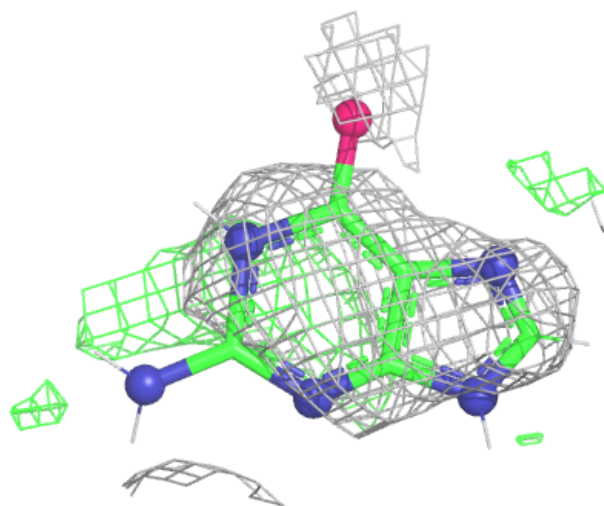
Electron density around 0O2 B 501:

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



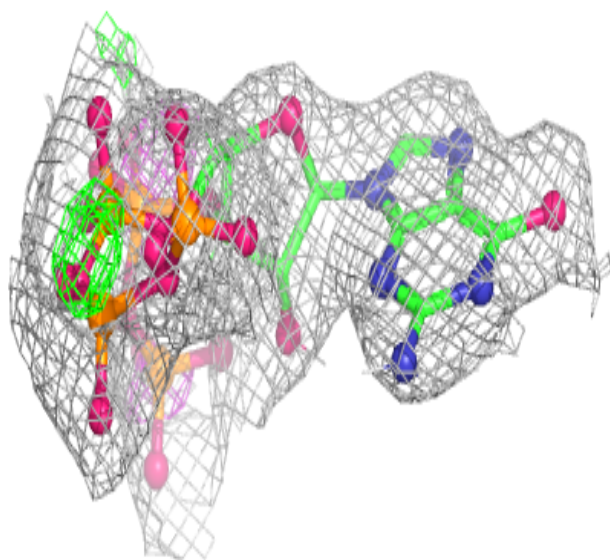
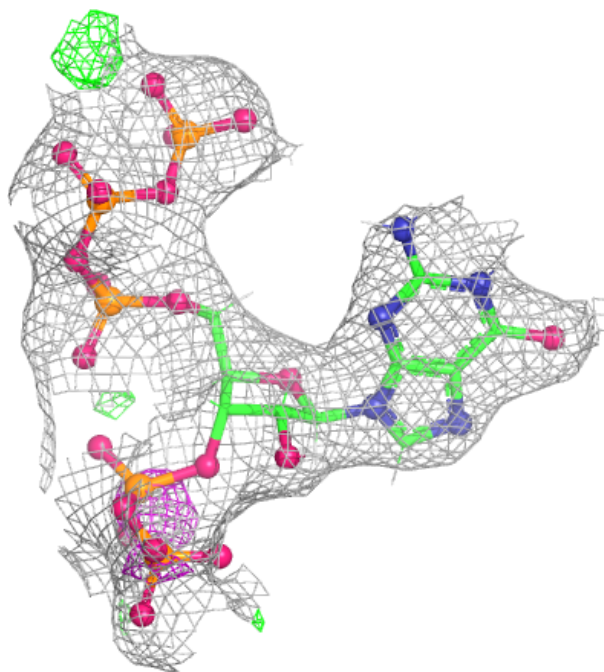
Electron density around GUN B 502:

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



Electron density around 0O2 A 501:

$2mF_o - DF_c$ (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.