



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 10:27 AM JST

PDB ID : 6IUY
Title : Structure of DsGPDH of *Dunaliella salina*
Authors : He, Q.; Toh, J.D.; Ero, R.; Qiao, Z.; Kumar, V.; Gao, Y.G.
Deposited on : 2018-12-01
Resolution : 2.20 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

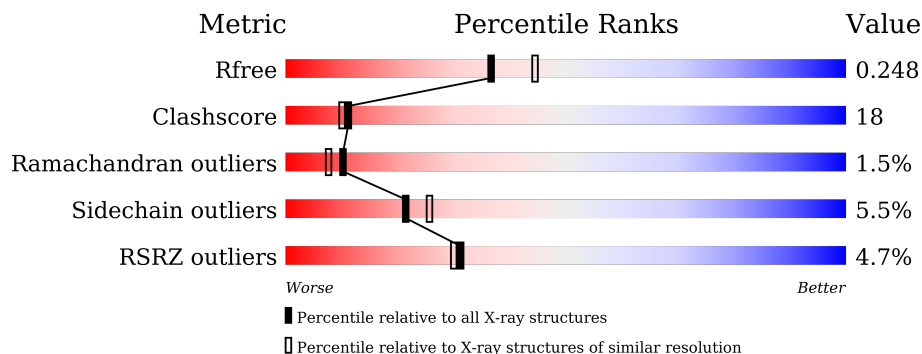
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	624	 5% (Poor fit), 65% (0-1 outliers), 26% (1-2 outliers), 6% (3+ outliers or not modelled)
1	B	624	 3% (Poor fit), 61% (0-1 outliers), 20% (1-2 outliers), 15% (3+ outliers or not modelled)

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	13P	A	702	-	-	X	-
3	13P	B	702	-	-	X	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 9078 atoms, of which 62 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 Glycerol-3-phosphate dehydrogenase [NAD(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	585	Total	C	N	O	S	0	0	0
			4468	2815	787	836	30			
1	B	531	Total	C	N	O	S	0	0	0
			4067	2564	721	752	30			

There are 44 discrepancies between the modelled and reference sequences:

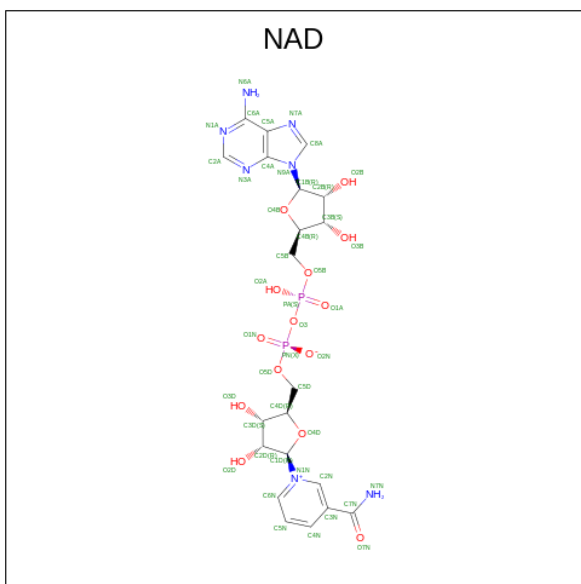
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	expression tag	UNP Q52ZA0
A	77	HIS	-	expression tag	UNP Q52ZA0
A	78	HIS	-	expression tag	UNP Q52ZA0
A	79	HIS	-	expression tag	UNP Q52ZA0
A	80	HIS	-	expression tag	UNP Q52ZA0
A	81	HIS	-	expression tag	UNP Q52ZA0
A	82	HIS	-	expression tag	UNP Q52ZA0
A	83	SER	-	expression tag	UNP Q52ZA0
A	84	SER	-	expression tag	UNP Q52ZA0
A	85	GLY	-	expression tag	UNP Q52ZA0
A	86	VAL	-	expression tag	UNP Q52ZA0
A	87	ASP	-	expression tag	UNP Q52ZA0
A	88	LEU	-	expression tag	UNP Q52ZA0
A	89	GLY	-	expression tag	UNP Q52ZA0
A	90	THR	-	expression tag	UNP Q52ZA0
A	91	GLU	-	expression tag	UNP Q52ZA0
A	92	ASN	-	expression tag	UNP Q52ZA0
A	93	LEU	-	expression tag	UNP Q52ZA0
A	94	TYR	-	expression tag	UNP Q52ZA0
A	95	PHE	-	expression tag	UNP Q52ZA0
A	96	GLN	-	expression tag	UNP Q52ZA0
A	97	SER	-	expression tag	UNP Q52ZA0
B	76	MET	-	expression tag	UNP Q52ZA0
B	77	HIS	-	expression tag	UNP Q52ZA0
B	78	HIS	-	expression tag	UNP Q52ZA0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	79	HIS	-	expression tag	UNP Q52ZA0
B	80	HIS	-	expression tag	UNP Q52ZA0
B	81	HIS	-	expression tag	UNP Q52ZA0
B	82	HIS	-	expression tag	UNP Q52ZA0
B	83	SER	-	expression tag	UNP Q52ZA0
B	84	SER	-	expression tag	UNP Q52ZA0
B	85	GLY	-	expression tag	UNP Q52ZA0
B	86	VAL	-	expression tag	UNP Q52ZA0
B	87	ASP	-	expression tag	UNP Q52ZA0
B	88	LEU	-	expression tag	UNP Q52ZA0
B	89	GLY	-	expression tag	UNP Q52ZA0
B	90	THR	-	expression tag	UNP Q52ZA0
B	91	GLU	-	expression tag	UNP Q52ZA0
B	92	ASN	-	expression tag	UNP Q52ZA0
B	93	LEU	-	expression tag	UNP Q52ZA0
B	94	TYR	-	expression tag	UNP Q52ZA0
B	95	PHE	-	expression tag	UNP Q52ZA0
B	96	GLN	-	expression tag	UNP Q52ZA0
B	97	SER	-	expression tag	UNP Q52ZA0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



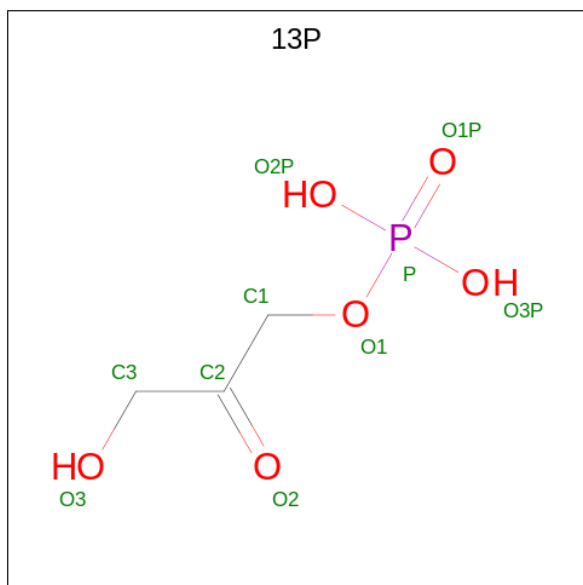
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	70	21	26	7	14	2	0	0

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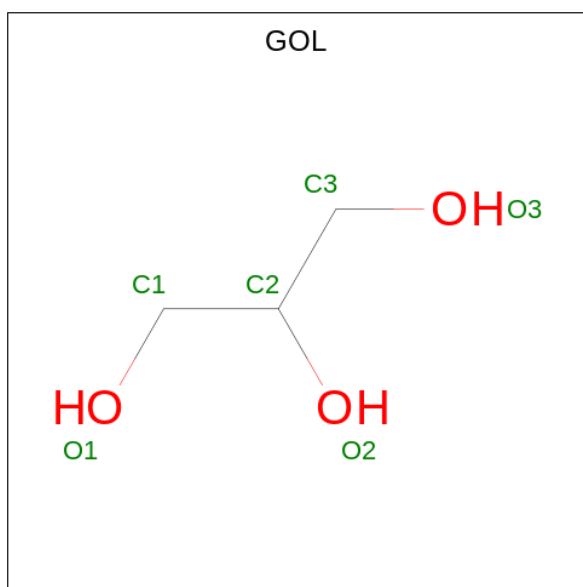
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	B	1	70	21	26	7	14	2	0	0

- Molecule 3 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
3	A	1	15	3	5	6	1	0	0
3	B	1	15	3	5	6	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

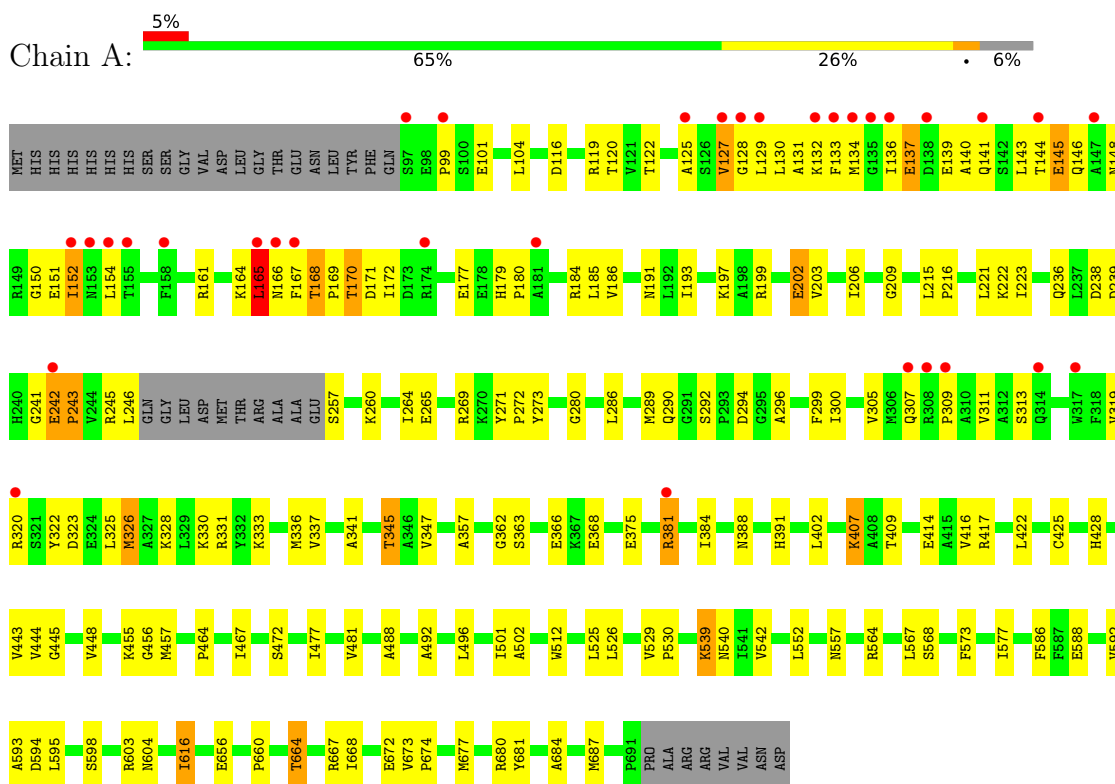
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	194	Total O 194 194	0	0
6	B	171	Total O 171 171	0	0

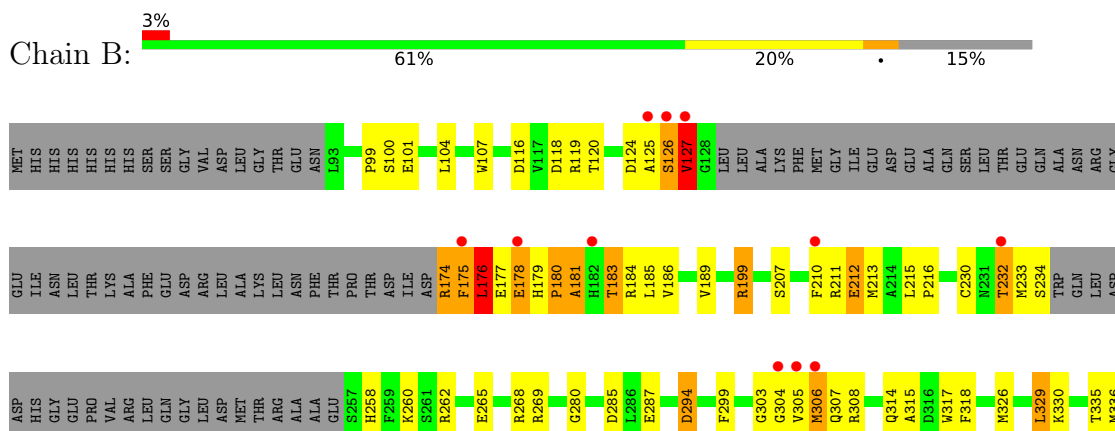
3 Residue-property plots

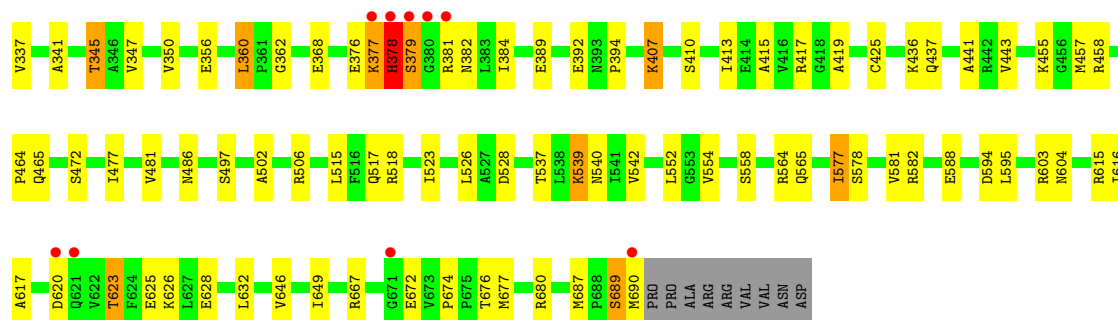
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycerol-3-phosphate dehydrogenase [NAD(+)]



- Molecule 1: Glycerol-3-phosphate dehydrogenase [NAD(+)]





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.33Å 91.33Å 348.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 2.20 48.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.36-2.20) 100.0 (48.99-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.248 0.203 , 0.248	Depositor DCC
R_{free} test set	3808 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9078	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: MG, GOL, NAD, 13P

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	0.41	0/4552	0.55	0/6158
1	B	0.43	0/4142	0.57	1/5595 (0.0%)
All	All	0.42	0/8694	0.56	1/11753 (0.0%)

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	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	176	LEU	CA-CB-CG	6.58	130.44	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LEU	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	4468	0	4410	179	0
1	B	4067	0	4050	128	0
2	A	44	26	24	0	0
2	B	44	26	25	2	0
3	A	10	5	5	7	0
3	B	10	5	5	5	0
4	A	6	0	8	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	194	0	0	24	1
6	B	171	0	0	13	0
All	All	9016	62	8527	308	1

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 18.

All (308) 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:199:ARG:NH1	1:B:330:LYS:O	1.81	1.13
1:B:336:MET:SD	6:B:953:HOH:O	2.07	1.12
1:A:336:MET:SD	6:A:979:HOH:O	2.08	1.11
1:A:464:PRO:HG3	1:A:577:ILE:HD13	1.32	1.07
1:B:336:MET:HE1	1:B:425:CYS:HB3	1.38	1.01
1:A:289:MET:SD	6:A:813:HOH:O	2.25	0.95
1:A:457:MET:SD	6:A:994:HOH:O	2.25	0.93
1:A:168:THR:HG23	1:A:170:THR:HG23	1.51	0.92
1:A:141:GLN:HA	1:A:144:THR:HG22	1.50	0.92
1:A:333:LYS:HG2	1:A:366:GLU:HG3	1.53	0.88
1:A:684:ALA:HA	1:A:687:MET:HG2	1.56	0.86
1:A:120:THR:HG21	1:A:280:GLY:HA2	1.57	0.86
1:A:444:VAL:HG13	1:A:448:VAL:HG11	1.59	0.85
1:A:375:GLU:OE2	6:A:802:HOH:O	1.95	0.84
1:B:174:ARG:HG3	1:B:175:PHE:H	1.43	0.83
1:B:336:MET:CE	1:B:425:CYS:HB3	2.08	0.82
1:B:603:ARG:NE	3:B:702:13P:O3P	2.12	0.82
1:A:368:GLU:OE1	6:A:801:HOH:O	1.95	0.82
1:A:136:ILE:HG13	1:A:139:GLU:HB3	1.60	0.82
1:B:180:PRO:HB2	1:B:183:THR:HG22	1.63	0.81
1:B:603:ARG:HG3	3:B:702:13P:O2P	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HD11	1:A:139:GLU:HG2	1.63	0.79
1:B:179:HIS:CG	1:B:180:PRO:HD3	2.17	0.79
1:B:603:ARG:N	3:B:702:13P:O2P	2.16	0.79
1:A:122:THR:HG21	1:A:184:ARG:HH21	1.47	0.78
1:A:122:THR:HB	6:A:803:HOH:O	1.83	0.78
1:A:336:MET:HE3	1:A:337:VAL:N	1.99	0.78
1:A:168:THR:CG2	1:A:170:THR:HG23	2.14	0.77
1:A:238:ASP:OD1	1:A:239:ASP:N	2.17	0.77
1:A:197:LYS:NZ	1:A:222:LYS:O	2.18	0.77
1:B:326:MET:HA	1:B:329:LEU:HD22	1.67	0.76
1:B:181:ALA:HA	1:B:184:ARG:HG3	1.67	0.75
1:A:660:PRO:O	1:A:664:THR:HG23	1.87	0.75
1:B:308:ARG:NH1	6:B:806:HOH:O	2.22	0.72
1:B:417:ARG:HA	1:B:443:VAL:CG2	2.18	0.72
1:B:360:LEU:O	6:B:802:HOH:O	2.08	0.72
1:B:623:THR:HG22	1:B:626:LYS:H	1.53	0.71
1:A:381:ARG:NH1	6:A:802:HOH:O	2.24	0.71
1:B:335:THR:HG21	1:B:415:ALA:O	1.90	0.71
1:A:141:GLN:HA	1:A:144:THR:CG2	2.20	0.70
1:A:168:THR:HG22	1:A:171:ASP:OD2	1.92	0.70
1:A:236:GLN:O	1:A:243:PRO:HD2	1.91	0.70
1:B:265:GLU:HG2	1:B:294:ASP:HB3	1.73	0.70
1:B:554:VAL:HG13	1:B:558:SER:HB2	1.72	0.69
1:A:122:THR:HG23	1:A:184:ARG:HB3	1.75	0.69
1:A:168:THR:OG1	1:A:169:PRO:HD2	1.93	0.68
1:A:664:THR:HG21	1:A:681:TYR:HA	1.76	0.68
1:B:537:THR:OG1	6:B:801:HOH:O	2.06	0.68
1:B:564:ARG:NH2	1:B:565:GLN:OE1	2.27	0.68
1:A:129:LEU:HD11	1:A:179:HIS:NE2	2.09	0.68
1:A:132:LYS:O	1:A:133:PHE:HB3	1.94	0.67
1:A:299:PHE:N	6:A:813:HOH:O	2.27	0.67
1:B:180:PRO:HB2	1:B:183:THR:CG2	2.24	0.66
1:B:539:LYS:HG2	1:B:540:ASN:N	2.11	0.66
1:A:286:LEU:HD11	1:A:290:GLN:NE2	2.10	0.66
1:A:414:GLU:OE1	6:A:805:HOH:O	2.13	0.66
1:A:417:ARG:O	6:A:804:HOH:O	2.12	0.66
1:B:120:THR:HG21	1:B:280:GLY:HA2	1.78	0.65
1:A:444:VAL:CG1	1:A:448:VAL:HG11	2.26	0.65
1:A:169:PRO:O	1:A:172:ILE:HG22	1.97	0.65
1:A:445:GLY:O	1:A:448:VAL:HG12	1.97	0.65
1:B:119:ARG:HD3	1:B:306:MET:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:SER:O	1:B:127:VAL:HG22	1.98	0.64
1:A:129:LEU:HD11	1:A:179:HIS:CD2	2.32	0.64
1:A:186:VAL:HG21	1:A:322:TYR:HE2	1.63	0.64
1:A:539:LYS:NZ	3:A:702:13P:O3	2.31	0.64
1:A:526:LEU:HD21	1:A:588:GLU:HG3	1.80	0.63
1:A:122:THR:HG21	1:A:184:ARG:NH2	2.13	0.63
1:A:202:GLU:HG3	1:A:273:TYR:OH	1.98	0.63
1:A:448:VAL:CG1	1:A:477:ILE:HG21	2.29	0.63
1:A:203:VAL:HG12	1:A:223:ILE:HD13	1.80	0.63
1:A:236:GLN:HB2	1:A:246:LEU:HD23	1.80	0.62
1:A:333:LYS:HG2	1:A:366:GLU:CG	2.29	0.62
1:A:165:LEU:HD13	1:A:166:ASN:H	1.65	0.62
1:B:124:ASP:OD2	1:B:184:ARG:NH2	2.33	0.62
1:B:667:ARG:NH2	1:B:687:MET:O	2.23	0.62
1:B:341:ALA:O	1:B:345:THR:HG23	2.00	0.61
1:A:193:ILE:HD13	1:A:221:LEU:HD13	1.80	0.61
1:B:326:MET:HA	1:B:329:LEU:CD2	2.30	0.61
1:A:127:VAL:HG23	1:A:161:ARG:HH11	1.65	0.61
1:A:417:ARG:HA	1:A:443:VAL:HG22	1.82	0.61
1:B:212:GLU:OE2	1:B:233:MET:HB2	2.01	0.60
1:A:309:PRO:O	1:A:313:SER:OG	2.19	0.60
1:B:175:PHE:HB3	1:B:177:GLU:OE2	2.00	0.60
1:A:165:LEU:HD13	1:A:166:ASN:N	2.17	0.59
1:B:232:THR:OG1	1:B:233:MET:N	2.35	0.59
1:A:455:LYS:HD2	3:A:702:13P:H31	1.83	0.59
1:A:464:PRO:CG	1:A:577:ILE:HD13	2.20	0.59
1:A:177:GLU:O	1:A:180:PRO:HD3	2.02	0.59
1:A:140:ALA:O	1:A:143:LEU:N	2.34	0.58
1:A:193:ILE:CD1	1:A:221:LEU:HD13	2.33	0.58
1:A:191:ASN:HB3	1:A:326:MET:CE	2.32	0.58
1:B:314:GLN:O	1:B:315:ALA:HB3	2.03	0.58
1:A:336:MET:HE2	1:A:425:CYS:HB3	1.85	0.58
1:A:540:ASN:HD21	3:A:702:13P:H32	1.69	0.57
1:A:542:VAL:HG11	1:A:595:LEU:HD11	1.85	0.57
1:A:586:PHE:O	1:A:592:VAL:HG23	2.03	0.57
1:A:136:ILE:HG13	1:A:136:ILE:O	2.04	0.57
1:A:168:THR:O	1:A:171:ASP:HB2	2.05	0.57
1:B:417:ARG:HA	1:B:443:VAL:HG22	1.86	0.57
1:B:436:LYS:NZ	6:B:819:HOH:O	2.38	0.57
1:A:116:ASP:OD1	1:A:260:LYS:NZ	2.38	0.57
1:A:185:LEU:N	1:A:185:LEU:HD12	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:PRO:HG3	1:A:577:ILE:CD1	2.22	0.57
1:B:502:ALA:HA	1:B:526:LEU:O	2.04	0.57
1:B:305:VAL:HG12	1:B:306:MET:HG2	1.87	0.56
1:B:603:ARG:H	3:B:702:13P:P	2.29	0.56
1:A:428:HIS:CG	1:A:456:GLY:HA3	2.40	0.56
1:B:384:ILE:HD11	1:B:410:SER:HB3	1.89	0.55
1:B:623:THR:CG2	1:B:625:GLU:H	2.19	0.55
1:A:238:ASP:OD1	6:A:807:HOH:O	2.18	0.55
1:B:233:MET:O	1:B:234:SER:OG	2.17	0.54
1:B:299:PHE:CE2	1:B:315:ALA:HB2	2.42	0.54
1:B:506:ARG:NH2	6:B:821:HOH:O	2.40	0.54
1:B:674:PRO:HG2	1:B:677:MET:HG2	1.90	0.54
1:A:341:ALA:O	1:A:345:THR:HG23	2.07	0.54
2:B:701:NAD:H2N	2:B:701:NAD:H51N	1.90	0.54
1:A:119:ARG:CZ	1:A:125:ALA:HB2	2.38	0.53
1:A:209:GLY:O	6:A:809:HOH:O	2.19	0.53
1:B:179:HIS:CD2	1:B:180:PRO:HG3	2.44	0.53
1:B:207:SER:HB3	1:B:230:CYS:SG	2.47	0.53
1:A:116:ASP:O	1:A:120:THR:OG1	2.25	0.53
1:B:458:ARG:HH11	1:B:465:GLN:HE22	1.55	0.53
1:A:604:ASN:HB2	6:A:832:HOH:O	2.08	0.53
1:B:350:VAL:HG22	1:B:515:LEU:HG	1.90	0.53
1:B:667:ARG:HD2	1:B:672:GLU:OE2	2.08	0.53
1:A:564:ARG:NH1	6:A:806:HOH:O	2.16	0.53
1:A:417:ARG:HA	1:A:443:VAL:CG2	2.39	0.52
1:B:180:PRO:CB	1:B:183:THR:CG2	2.87	0.52
1:A:206:ILE:HG22	1:A:260:LYS:HG2	1.91	0.52
1:B:497:SER:OG	6:B:804:HOH:O	2.18	0.52
1:B:517:GLN:HA	1:B:523:ILE:HD12	1.92	0.52
1:B:199:ARG:NH2	1:B:362:GLY:O	2.42	0.52
1:A:320:ARG:NH2	6:A:808:HOH:O	2.43	0.52
1:B:119:ARG:CD	1:B:306:MET:HG3	2.39	0.52
1:A:300:ILE:HD13	1:A:325:LEU:HD21	1.92	0.52
1:B:623:THR:HG23	1:B:625:GLU:H	1.75	0.52
1:A:573:PHE:CE2	1:A:577:ILE:HD12	2.46	0.51
1:A:684:ALA:CA	1:A:687:MET:HG2	2.36	0.51
1:B:526:LEU:HD11	1:B:588:GLU:HG3	1.92	0.51
1:A:186:VAL:HG21	1:A:322:TYR:CE2	2.46	0.51
1:B:215:LEU:HB2	1:B:216:PRO:HD3	1.92	0.51
1:B:539:LYS:HD2	1:B:594:ASP:CG	2.30	0.51
1:A:345:THR:HG21	1:A:488:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:SER:O	1:B:101:GLU:HB3	2.10	0.51
1:A:307:GLN:OE1	6:A:808:HOH:O	2.18	0.51
1:B:552:LEU:HD11	1:B:676:THR:HA	1.92	0.51
1:B:384:ILE:CD1	1:B:410:SER:HB3	2.41	0.51
1:A:381:ARG:NH2	1:A:384:ILE:HG21	2.26	0.51
1:A:132:LYS:HG2	1:A:137:GLU:OE1	2.12	0.50
1:B:526:LEU:CD1	1:B:588:GLU:HG3	2.42	0.50
1:A:667:ARG:HD2	1:A:672:GLU:OE1	2.12	0.50
1:A:336:MET:CE	1:A:425:CYS:HB3	2.41	0.50
1:B:107:TRP:NE1	1:B:329:LEU:HD13	2.27	0.50
1:B:178:GLU:OE2	1:B:181:ALA:HB2	2.12	0.50
1:A:388:ASN:OD1	1:A:407:LYS:HD2	2.12	0.50
1:A:257:SER:CB	6:A:812:HOH:O	2.60	0.50
1:B:308:ARG:N	6:B:810:HOH:O	2.28	0.50
1:B:265:GLU:O	1:B:269:ARG:HG3	2.12	0.49
1:A:119:ARG:HG2	1:A:305:VAL:HG11	1.94	0.49
1:A:241:GLY:O	1:A:242:GLU:HB3	2.12	0.49
1:B:179:HIS:CD2	1:B:180:PRO:HD3	2.47	0.49
1:B:458:ARG:HH11	1:B:465:GLN:NE2	2.10	0.49
1:A:128:GLY:HA2	1:A:131:ALA:HB3	1.93	0.49
1:B:676:THR:O	6:B:803:HOH:O	2.18	0.49
1:A:603:ARG:HH21	3:A:702:13P:C1	2.25	0.49
1:B:376:GLU:HB2	1:B:378:HIS:CE1	2.46	0.49
1:A:130:LEU:C	1:A:161:ARG:HH22	2.16	0.49
1:A:130:LEU:HB3	1:A:161:ARG:HH12	1.78	0.49
1:A:557:ASN:HB2	6:A:862:HOH:O	2.12	0.49
1:A:131:ALA:HA	1:A:161:ARG:NH2	2.28	0.49
1:A:345:THR:HB	1:A:492:ALA:HB2	1.95	0.49
1:A:199:ARG:NH2	1:A:362:GLY:O	2.45	0.49
1:A:257:SER:HB2	6:A:812:HOH:O	2.13	0.49
1:B:689:SER:O	1:B:690:MET:HB2	2.12	0.49
1:B:526:LEU:HD21	1:B:528:ASP:HB3	1.95	0.49
1:B:577:ILE:HG22	1:B:578:SER:OG	2.13	0.49
1:A:448:VAL:HG12	1:A:477:ILE:HG21	1.93	0.48
1:A:455:LYS:HD2	3:A:702:13P:C3	2.43	0.48
1:A:552:LEU:HD21	1:A:616:ILE:HD11	1.94	0.48
1:A:357:ALA:O	1:A:363:SER:HB2	2.12	0.48
1:A:673:VAL:HG13	1:A:674:PRO:HD2	1.94	0.48
1:A:265:GLU:O	1:A:269:ARG:HG3	2.12	0.48
1:B:628:GLU:O	1:B:632:LEU:HB2	2.12	0.48
1:A:525:LEU:O	1:A:526:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:MET:HE3	1:A:680:ARG:HB2	1.96	0.48
1:B:176:LEU:O	1:B:176:LEU:HD23	2.14	0.48
1:B:299:PHE:CD2	1:B:315:ALA:HB2	2.48	0.48
1:B:455:LYS:HD3	1:B:539:LYS:HE2	1.95	0.48
1:B:604:ASN:HD22	3:B:702:13P:H12	1.78	0.48
1:A:146:GLN:HA	1:A:150:GLY:CA	2.43	0.48
1:A:539:LYS:HE3	1:A:594:ASP:OD1	2.13	0.48
1:B:186:VAL:O	1:B:189:VAL:HG12	2.14	0.48
1:B:623:THR:HG22	1:B:625:GLU:N	2.28	0.48
1:B:210:PHE:O	1:B:213:MET:HB2	2.14	0.48
1:B:356:GLU:OE2	1:B:518:ARG:NH2	2.42	0.48
1:B:368:GLU:OE2	6:B:805:HOH:O	2.20	0.48
1:A:128:GLY:HA2	1:A:131:ALA:CB	2.43	0.47
1:A:148:ASN:O	1:A:152:ILE:HA	2.14	0.47
1:A:542:VAL:CG1	1:A:595:LEU:HD11	2.43	0.47
1:B:377:LYS:O	1:B:378:HIS:HB3	2.14	0.47
1:B:552:LEU:CD1	1:B:676:THR:HA	2.43	0.47
3:A:702:13P:C1	6:A:819:HOH:O	2.62	0.47
1:A:130:LEU:O	1:A:134:MET:HB2	2.14	0.47
1:A:539:LYS:HE2	1:A:598:SER:OG	2.14	0.47
1:B:118:ASP:OD2	1:B:125:ALA:HA	2.14	0.47
1:A:286:LEU:HD21	1:A:290:GLN:HE22	1.79	0.47
1:B:677:MET:HE3	1:B:680:ARG:HB2	1.95	0.47
1:B:258:HIS:O	1:B:262:ARG:HB2	2.14	0.47
1:B:542:VAL:HB	1:B:595:LEU:HD11	1.97	0.47
1:B:116:ASP:O	1:B:120:THR:OG1	2.32	0.47
1:A:238:ASP:CG	1:A:239:ASP:H	2.17	0.47
1:A:539:LYS:HE3	1:A:594:ASP:CG	2.36	0.46
1:B:554:VAL:HG13	1:B:558:SER:CB	2.41	0.46
1:A:165:LEU:HD12	1:A:165:LEU:N	2.31	0.46
1:B:100:SER:O	1:B:101:GLU:CB	2.62	0.46
1:B:307:GLN:CD	6:B:834:HOH:O	2.52	0.46
1:A:539:LYS:HD3	1:A:540:ASN:N	2.30	0.46
1:A:203:VAL:HG12	1:A:223:ILE:CD1	2.45	0.46
1:A:141:GLN:CA	1:A:144:THR:HG22	2.33	0.46
1:A:119:ARG:NH2	1:A:125:ALA:HB2	2.31	0.46
1:A:186:VAL:CG2	1:A:322:TYR:HE2	2.27	0.46
1:A:146:GLN:O	1:A:150:GLY:HA3	2.15	0.46
1:A:199:ARG:NH1	1:A:330:LYS:O	2.37	0.46
1:A:132:LYS:C	1:A:134:MET:H	2.19	0.46
1:A:529:VAL:N	1:A:530:PRO:HD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:MET:CE	1:B:680:ARG:HB2	2.46	0.46
1:A:136:ILE:CD1	1:A:139:GLU:HG2	2.40	0.45
1:A:137:GLU:O	1:A:141:GLN:NE2	2.49	0.45
1:A:127:VAL:O	1:A:127:VAL:HG22	2.15	0.45
1:A:136:ILE:CG1	1:A:139:GLU:HB3	2.40	0.45
1:A:331:ARG:HD2	1:A:366:GLU:OE2	2.17	0.45
1:A:593:ALA:HB2	1:B:564:ARG:HB2	1.99	0.45
1:A:336:MET:HE3	1:A:337:VAL:H	1.80	0.45
1:A:603:ARG:HH21	3:A:702:13P:H11	1.81	0.45
1:B:260:LYS:NZ	1:B:285:ASP:OD1	2.38	0.45
1:A:127:VAL:HG23	1:A:161:ARG:HD3	1.99	0.45
1:A:145:GLU:HB2	1:A:146:GLN:H	1.53	0.45
1:A:168:THR:HG23	1:A:170:THR:CG2	2.36	0.45
1:A:264:ILE:CD1	1:A:296:ALA:HB2	2.47	0.45
1:A:120:THR:CG2	1:A:280:GLY:HA2	2.39	0.44
1:A:271:TYR:HB3	1:A:272:PRO:HD2	1.99	0.44
1:B:180:PRO:O	1:B:181:ALA:CB	2.65	0.44
1:B:368:GLU:OE1	1:B:407:LYS:NZ	2.46	0.44
1:A:381:ARG:O	1:A:381:ARG:HG3	2.17	0.44
1:B:304:GLY:O	1:B:305:VAL:HB	2.18	0.44
1:B:437:GLN:NE2	6:B:837:HOH:O	2.49	0.44
1:B:101:GLU:HA	1:B:104:LEU:HB2	2.00	0.44
1:B:623:THR:CG2	1:B:625:GLU:N	2.81	0.44
1:A:146:GLN:HA	1:A:150:GLY:N	2.33	0.43
1:B:616:ILE:HD12	1:B:617:ALA:N	2.33	0.43
1:A:664:THR:O	1:A:668:ILE:HG13	2.18	0.43
1:A:684:ALA:HA	1:A:687:MET:CG	2.37	0.43
1:B:378:HIS:CE1	1:B:379:SER:HB3	2.53	0.43
1:B:126:SER:C	1:B:127:VAL:HG13	2.38	0.43
1:B:564:ARG:NE	6:B:807:HOH:O	2.22	0.43
1:A:481:VAL:HG22	1:A:502:ALA:HB3	2.01	0.43
1:A:539:LYS:HE2	1:A:598:SER:CB	2.48	0.43
1:B:481:VAL:HG22	1:B:502:ALA:HB3	2.01	0.43
1:A:345:THR:CG2	1:A:488:ALA:HB1	2.48	0.43
1:A:122:THR:HG23	1:A:184:ARG:O	2.19	0.43
1:A:680:ARG:NE	6:A:817:HOH:O	2.30	0.43
1:A:167:PHE:CE1	1:A:171:ASP:HB3	2.53	0.42
1:B:174:ARG:HG3	1:B:175:PHE:N	2.23	0.42
1:B:472:SER:HA	1:B:477:ILE:O	2.19	0.42
1:A:119:ARG:NE	6:A:810:HOH:O	2.19	0.42
1:B:268:ARG:HD2	1:B:294:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:CD2	1:B:616:ILE:HG21	2.49	0.42
1:B:578:SER:O	1:B:581:VAL:HG23	2.20	0.42
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.89	0.42
1:B:517:GLN:CA	1:B:523:ILE:HD12	2.49	0.42
1:A:165:LEU:CD1	1:A:166:ASN:H	2.31	0.42
1:A:501:ILE:HD13	1:A:512:TRP:HB3	2.01	0.42
1:B:335:THR:HG23	1:B:419:ALA:HB2	2.01	0.42
1:B:464:PRO:HG3	1:B:577:ILE:HG13	2.00	0.42
1:A:165:LEU:HD23	1:A:245:ARG:CB	2.49	0.42
1:A:341:ALA:O	1:A:345:THR:CG2	2.68	0.42
1:A:265:GLU:HG2	1:A:294:ASP:HB2	2.02	0.42
1:B:99:PRO:HG3	1:B:317:TRP:CE2	2.55	0.42
1:B:392:GLU:O	1:B:394:PRO:HD3	2.20	0.42
1:B:526:LEU:CD2	1:B:528:ASP:HB3	2.49	0.42
1:A:140:ALA:O	1:A:143:LEU:HB2	2.20	0.41
1:A:323:ASP:HA	1:A:326:MET:HB2	2.01	0.41
1:B:119:ARG:HD3	1:B:306:MET:CG	2.48	0.41
1:B:615:ARG:NE	1:B:620:ASP:HA	2.36	0.41
1:A:104:LEU:HD11	1:A:328:LYS:HB3	2.01	0.41
1:A:391:HIS:HB3	1:A:402:LEU:O	2.21	0.41
1:A:552:LEU:HA	1:A:552:LEU:HD23	1.87	0.41
1:B:413:ILE:CD1	1:B:441:ALA:HB2	2.51	0.41
1:A:448:VAL:HG13	1:A:477:ILE:HD13	2.03	0.41
1:A:472:SER:HA	1:A:477:ILE:O	2.21	0.41
1:A:567:LEU:HD21	1:A:592:VAL:HG22	2.02	0.41
1:A:132:LYS:HB3	1:A:132:LYS:HE3	1.80	0.41
1:A:136:ILE:HG13	1:A:139:GLU:CB	2.42	0.41
1:A:448:VAL:HG13	1:A:477:ILE:HG21	2.00	0.41
1:A:573:PHE:CZ	1:A:577:ILE:HD12	2.56	0.41
1:B:457:MET:CE	1:B:649:ILE:HD12	2.51	0.41
1:B:486:ASN:O	2:B:701:NAD:H4N	2.21	0.41
1:A:322:TYR:N	6:A:814:HOH:O	2.28	0.40
1:B:215:LEU:N	1:B:216:PRO:CD	2.85	0.40
1:B:303:GLY:HA3	1:B:318:PHE:CZ	2.56	0.40
1:B:336:MET:HE2	1:B:337:VAL:C	2.41	0.40
1:B:457:MET:HE1	1:B:646:VAL:HA	2.03	0.40
1:A:416:VAL:HG13	1:A:422:LEU:HD21	2.02	0.40
1:A:552:LEU:CD2	1:A:616:ILE:HD11	2.51	0.40
1:A:215:LEU:N	1:A:216:PRO:CD	2.84	0.40
1:A:467:ILE:HG12	6:A:844:HOH:O	2.22	0.40
1:A:184:ARG:HB3	1:A:184:ARG:HE	1.72	0.40

All (1) 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)
6:A:902:HOH:O	6:A:919:HOH:O[5_455]	2.01	0.19

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	581/624 (93%)	539 (93%)	34 (6%)	8 (1%)	11	8
1	B	525/624 (84%)	489 (93%)	27 (5%)	9 (2%)	9	6
All	All	1106/1248 (89%)	1028 (93%)	61 (6%)	17 (2%)	10	8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLU
1	A	242	GLU
1	B	127	VAL
1	B	180	PRO
1	B	181	ALA
1	B	378	HIS
1	B	379	SER
1	A	152	ILE
1	A	165	LEU
1	B	689	SER
1	A	243	PRO
1	B	126	SER
1	B	175	PHE
1	A	151	GLU
1	B	232	THR
1	A	154	LEU
1	A	99	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	465/511 (91%)	442 (95%)	23 (5%)	25	31
1	B	426/511 (83%)	400 (94%)	26 (6%)	18	21
All	All	891/1022 (87%)	842 (94%)	49 (6%)	21	26

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	137	GLU
1	A	145	GLU
1	A	164	LYS
1	A	165	LEU
1	A	168	THR
1	A	170	THR
1	A	202	GLU
1	A	292	SER
1	A	311	VAL
1	A	319	VAL
1	A	326	MET
1	A	345	THR
1	A	347	VAL
1	A	381	ARG
1	A	407	LYS
1	A	409	THR
1	A	496	LEU
1	A	539	LYS
1	A	568	SER
1	A	616	ILE
1	A	656	GLU
1	A	664	THR
1	B	127	VAL
1	B	174	ARG
1	B	176	LEU
1	B	178	GLU

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Mol	Chain	Res	Type
1	B	183	THR
1	B	185	LEU
1	B	199	ARG
1	B	211	ARG
1	B	212	GLU
1	B	287	GLU
1	B	294	ASP
1	B	306	MET
1	B	329	LEU
1	B	345	THR
1	B	347	VAL
1	B	360	LEU
1	B	377	LYS
1	B	378	HIS
1	B	381	ARG
1	B	382	ASN
1	B	389	GLU
1	B	407	LYS
1	B	539	LYS
1	B	577	ILE
1	B	582	ARG
1	B	623	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	B	465	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	701	-	42,48,48	5.16	16 (38%)	50,73,73	1.52	7 (14%)
3	13P	A	702	-	9,9,9	1.00	1 (11%)	10,12,12	1.40	1 (10%)
4	GOL	A	703	-	5,5,5	0.34	0	5,5,5	0.30	0
2	NAD	B	701	-	42,48,48	5.09	15 (35%)	50,73,73	1.61	9 (18%)
3	13P	B	702	-	9,9,9	1.11	1 (11%)	10,12,12	1.40	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	701	-	-	8/26/62/62	0/5/5/5
3	13P	A	702	-	-	7/7/8/8	-
4	GOL	A	703	-	-	4/4/4/4	-
2	NAD	B	701	-	-	11/26/62/62	0/5/5/5
3	13P	B	702	-	-	5/7/8/8	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAD	C2B-C1B	-16.07	1.29	1.53
2	A	701	NAD	O4D-C1D	15.50	1.62	1.41
2	B	701	NAD	C2B-C1B	-15.28	1.30	1.53
2	B	701	NAD	O4D-C1D	15.24	1.62	1.41
2	A	701	NAD	C2D-C1D	-15.15	1.30	1.53
2	B	701	NAD	O4B-C1B	14.04	1.60	1.41
2	A	701	NAD	O4B-C1B	14.02	1.60	1.41
2	B	701	NAD	C2D-C1D	-13.90	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	NAD	O4D-C4D	-6.54	1.30	1.45
2	B	701	NAD	O4B-C4B	-6.42	1.30	1.45
2	A	701	NAD	O4B-C4B	-6.28	1.31	1.45
2	B	701	NAD	C7N-N7N	6.23	1.44	1.33
2	A	701	NAD	C7N-N7N	6.10	1.44	1.33
2	A	701	NAD	O4D-C4D	-5.61	1.32	1.45
2	B	701	NAD	C2N-N1N	4.16	1.40	1.35
2	B	701	NAD	O3D-C3D	-3.72	1.34	1.43
2	B	701	NAD	C3N-C7N	3.47	1.55	1.50
2	A	701	NAD	O3D-C3D	-3.45	1.34	1.43
2	B	701	NAD	O2B-C2B	3.31	1.50	1.43
2	A	701	NAD	O3B-C3B	-3.09	1.35	1.43
2	A	701	NAD	O2B-C2B	2.97	1.50	1.43
2	A	701	NAD	C3N-C7N	2.86	1.54	1.50
2	B	701	NAD	O2D-C2D	2.84	1.49	1.43
2	A	701	NAD	C2N-N1N	2.80	1.38	1.35
3	B	702	13P	O1-C1	-2.65	1.41	1.43
2	A	701	NAD	O2D-C2D	2.60	1.49	1.43
2	B	701	NAD	C2A-N3A	2.59	1.36	1.32
3	A	702	13P	O1-C1	-2.54	1.41	1.43
2	B	701	NAD	O3B-C3B	-2.53	1.37	1.43
2	A	701	NAD	C6A-N6A	2.38	1.42	1.34
2	B	701	NAD	C6A-N6A	2.31	1.42	1.34
2	A	701	NAD	C5A-C4A	-2.23	1.35	1.40
2	A	701	NAD	C2A-N3A	2.23	1.35	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	NAD	N3A-C2A-N1A	-5.20	120.56	128.68
2	A	701	NAD	N3A-C2A-N1A	-5.11	120.70	128.68
2	B	701	NAD	O4B-C1B-C2B	-4.73	100.02	106.93
2	A	701	NAD	C5A-C6A-N6A	4.14	126.64	120.35
2	B	701	NAD	C6N-N1N-C2N	-4.06	118.27	121.97
2	A	701	NAD	C6N-N1N-C2N	-3.82	118.49	121.97
3	A	702	13P	O1-P-O1P	3.42	116.07	106.47
2	B	701	NAD	C5A-C6A-N6A	3.31	125.39	120.35
2	A	701	NAD	N6A-C6A-N1A	-2.55	113.28	118.57
2	B	701	NAD	C2N-N1N-C1D	2.48	124.65	119.14
2	A	701	NAD	C2N-C3N-C4N	2.40	120.98	118.26
2	B	701	NAD	O4D-C4D-C5D	-2.37	101.58	109.37
3	B	702	13P	O1-P-O1P	2.26	112.82	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	NAD	PN-O5D-C5D	-2.20	108.76	121.68
2	B	701	NAD	C3D-C2D-C1D	2.17	104.24	100.98
2	A	701	NAD	C1B-N9A-C4A	-2.11	122.94	126.64
2	B	701	NAD	N6A-C6A-N1A	-2.10	114.22	118.57
2	A	701	NAD	O4D-C1D-C2D	-2.06	103.91	106.93

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NAD	O4D-C1D-N1N-C2N
2	A	701	NAD	O4D-C1D-N1N-C6N
2	A	701	NAD	C2D-C1D-N1N-C2N
2	A	701	NAD	C2D-C1D-N1N-C6N
2	B	701	NAD	C5D-O5D-PN-O1N
2	B	701	NAD	O4D-C1D-N1N-C2N
2	B	701	NAD	O4D-C1D-N1N-C6N
2	B	701	NAD	C2D-C1D-N1N-C2N
2	B	701	NAD	C2D-C1D-N1N-C6N
3	A	702	13P	C1-O1-P-O1P
3	A	702	13P	C1-O1-P-O2P
3	A	702	13P	C1-O1-P-O3P
3	A	702	13P	C2-C1-O1-P
3	A	702	13P	O2-C2-C3-O3
3	B	702	13P	C1-O1-P-O1P
3	B	702	13P	C1-O1-P-O2P
3	B	702	13P	C1-O1-P-O3P
4	A	703	GOL	O1-C1-C2-C3
4	A	703	GOL	C1-C2-C3-O3
2	B	701	NAD	C3D-C4D-C5D-O5D
4	A	703	GOL	O2-C2-C3-O3
3	A	702	13P	O1-C1-C2-C3
4	A	703	GOL	O1-C1-C2-O2
2	A	701	NAD	C5B-O5B-PA-O3
2	B	701	NAD	PA-O3-PN-O2N
2	A	701	NAD	O4D-C4D-C5D-O5D
2	B	701	NAD	O4D-C4D-C5D-O5D
3	B	702	13P	O2-C2-C3-O3
2	A	701	NAD	C4B-C5B-O5B-PA
3	A	702	13P	O1-C1-C2-O2
2	B	701	NAD	C5D-O5D-PN-O3
2	B	701	NAD	PA-O3-PN-O1N

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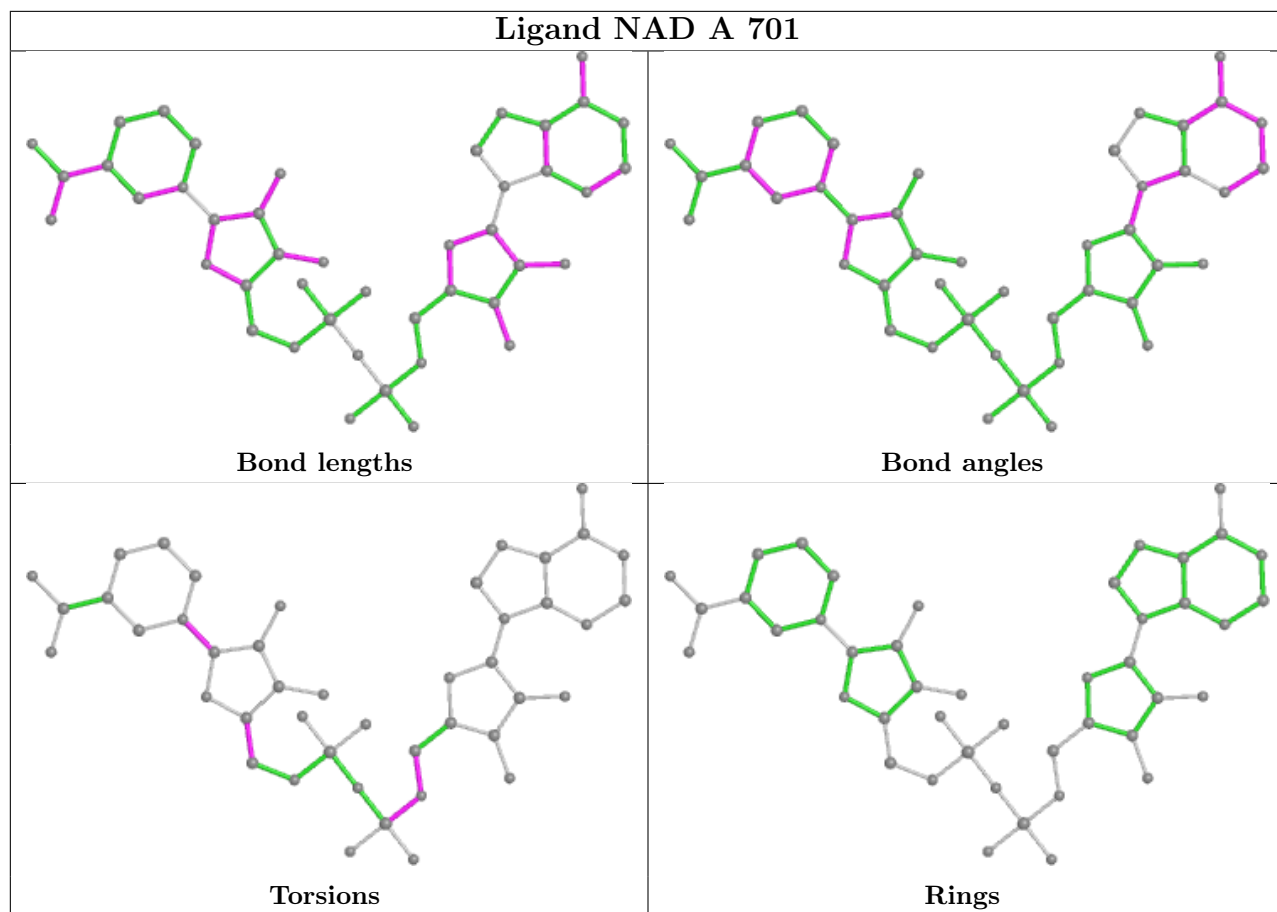
Mol	Chain	Res	Type	Atoms
2	A	701	NAD	C5B-O5B-PA-O2A
2	B	701	NAD	O4B-C4B-C5B-O5B
3	B	702	13P	O1-C1-C2-O2

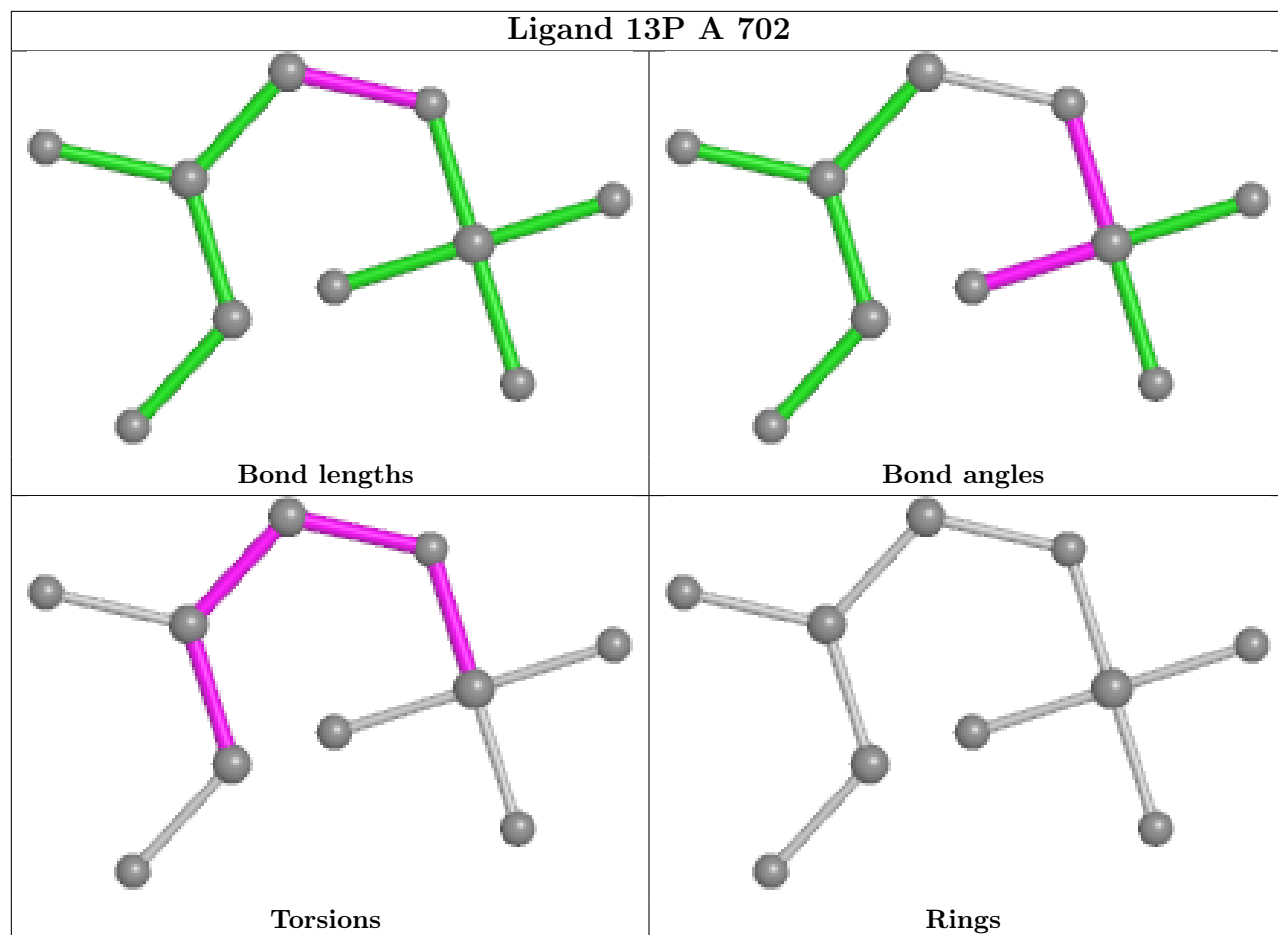
There are no ring outliers.

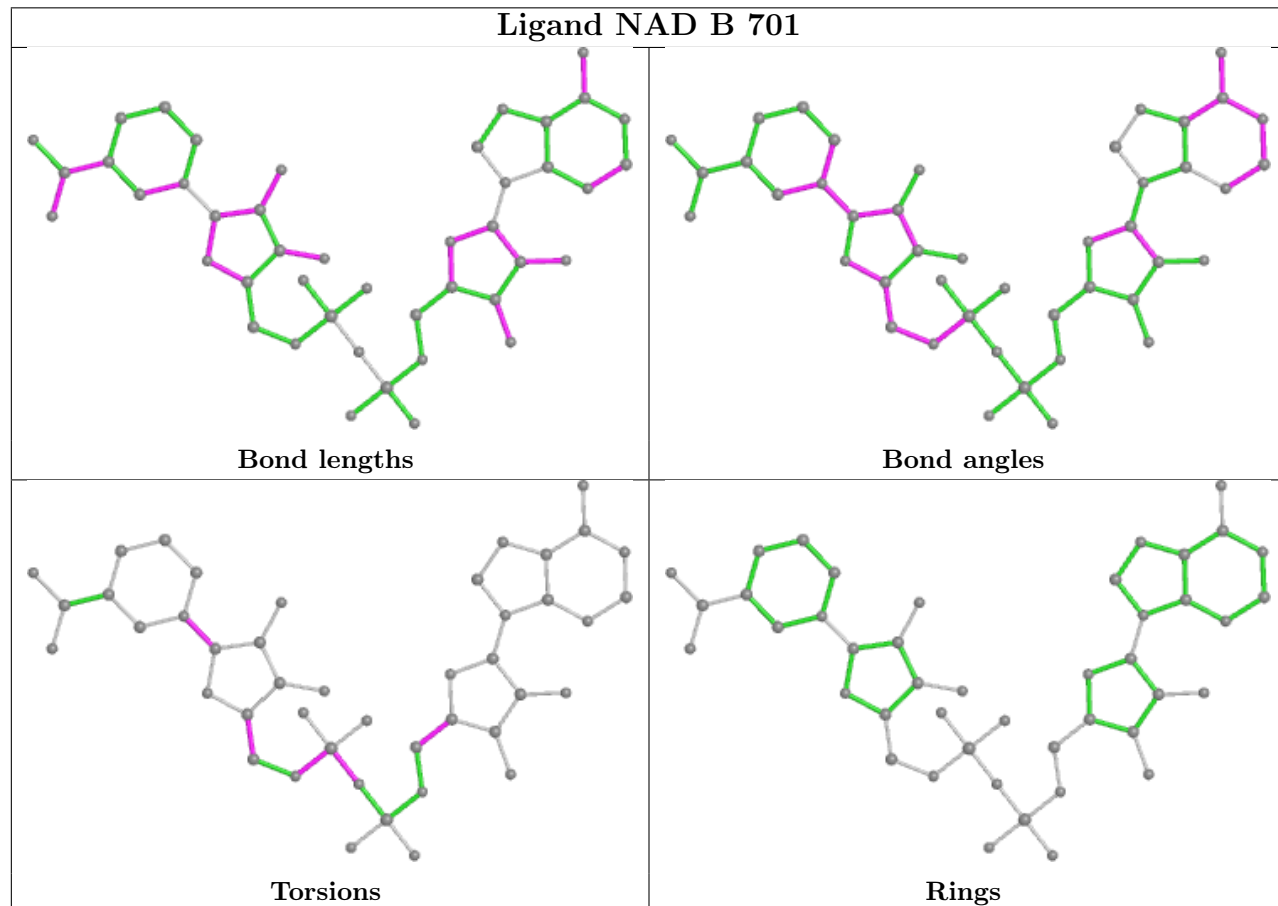
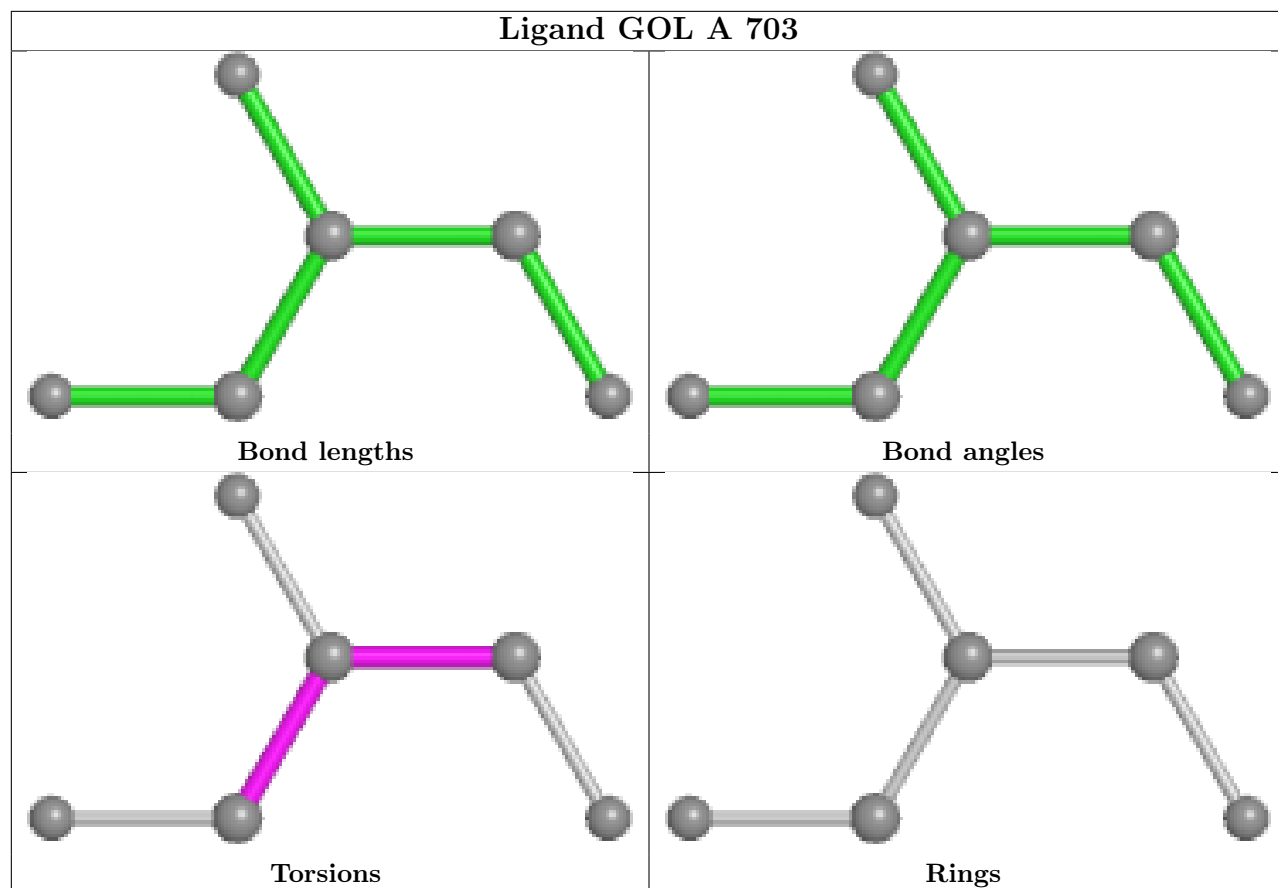
3 monomers are involved in 14 short contacts:

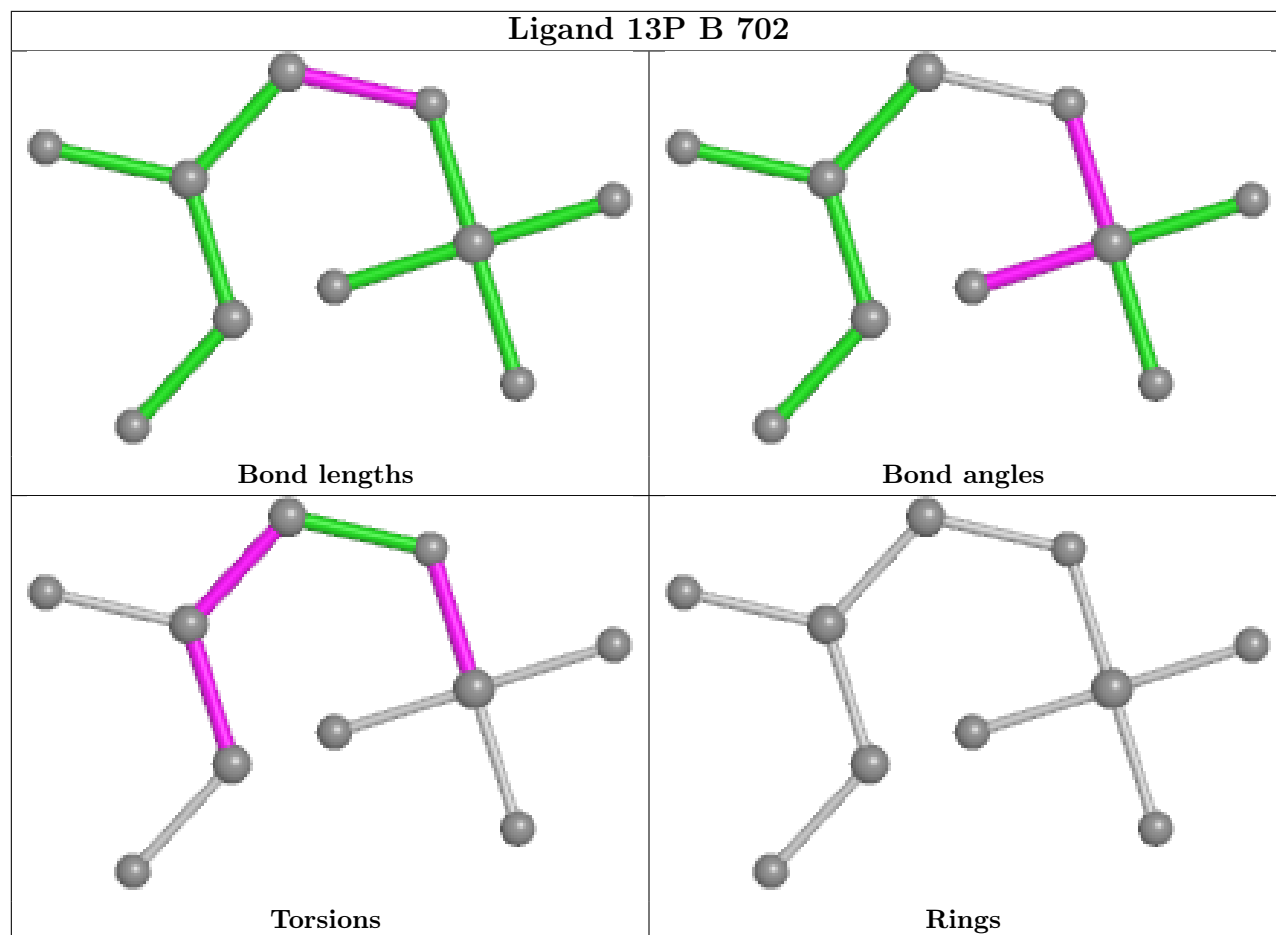
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	13P	7	0
2	B	701	NAD	2	0
3	B	702	13P	5	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/624 (93%)	0.15	33 (5%) 24 23	34, 51, 89, 119	0
1	B	531/624 (85%)	0.05	20 (3%) 40 38	35, 49, 79, 103	0
All	All	1116/1248 (89%)	0.10	53 (4%) 31 30	34, 50, 87, 119	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	SER	10.1
1	A	153	ASN	9.6
1	B	379	SER	8.1
1	A	154	LEU	8.0
1	B	378	HIS	7.1
1	A	147	ALA	6.9
1	A	152	ILE	5.3
1	A	155	THR	5.1
1	B	305	VAL	4.8
1	B	377	LYS	4.6
1	A	167	PHE	4.5
1	B	232	THR	4.3
1	A	135	GLY	4.2
1	A	309	PRO	4.0
1	B	127	VAL	3.4
1	B	210	PHE	3.4
1	B	380	GLY	3.4
1	A	138	ASP	3.3
1	A	307	GLN	3.2
1	A	174	ARG	3.2
1	B	306	MET	3.1
1	B	178	GLU	3.0
1	A	133	PHE	2.9
1	A	128	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	165	LEU	2.9
1	B	304	GLY	2.8
1	B	381	ARG	2.7
1	A	129	LEU	2.7
1	A	308	ARG	2.7
1	A	320	ARG	2.6
1	A	132	LYS	2.6
1	B	621	GLN	2.5
1	A	127	VAL	2.5
1	A	134	MET	2.5
1	A	144	THR	2.5
1	A	314	GLN	2.4
1	B	690	MET	2.4
1	A	317	TRP	2.4
1	A	99	PRO	2.4
1	A	381	ARG	2.3
1	B	175	PHE	2.3
1	B	671	GLY	2.3
1	B	620	ASP	2.3
1	B	182	HIS	2.3
1	B	126	SER	2.3
1	A	166	ASN	2.2
1	A	242	GLU	2.2
1	A	136	ILE	2.2
1	A	125	ALA	2.1
1	A	158	PHE	2.1
1	A	181	ALA	2.1
1	A	141	GLN	2.1
1	B	125	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

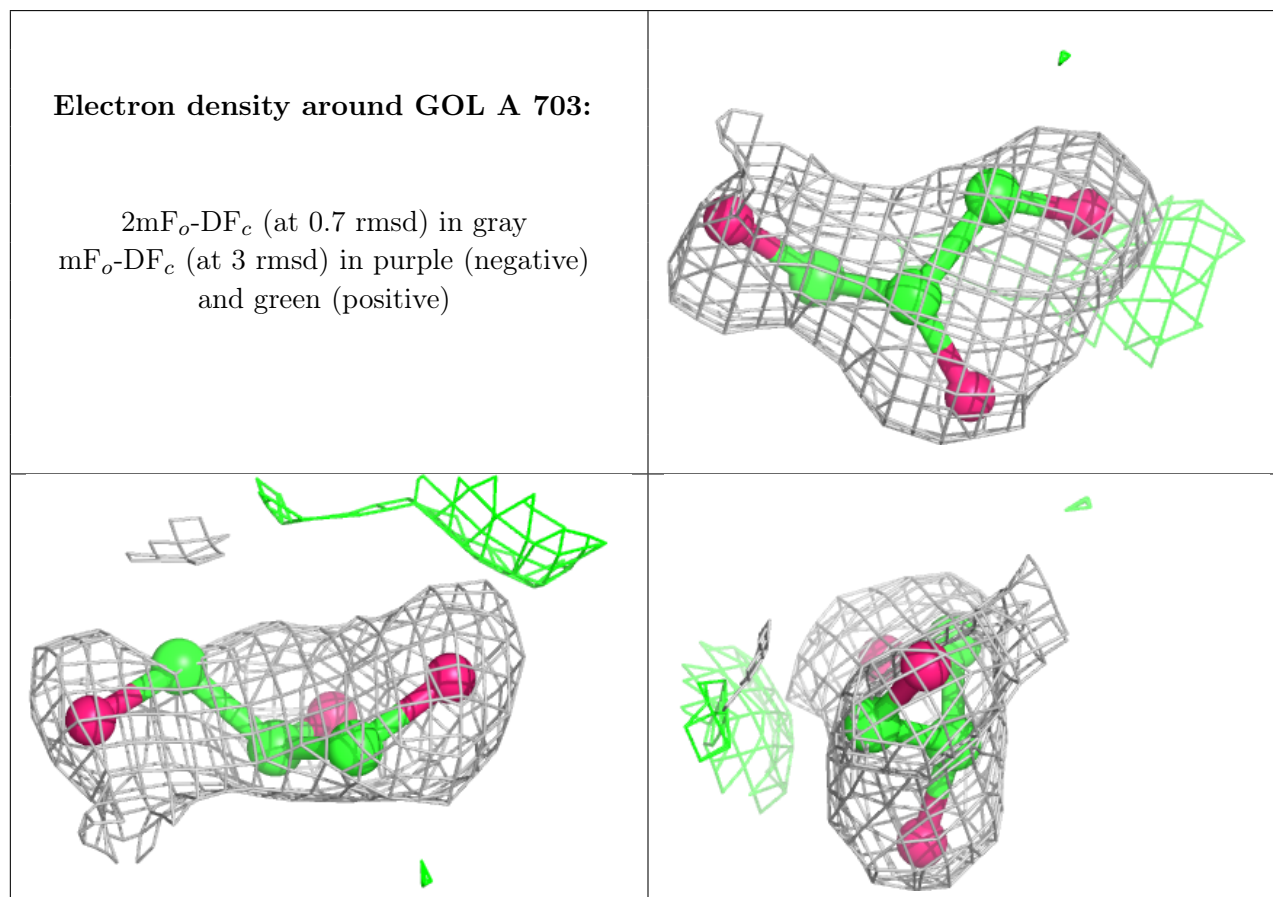
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

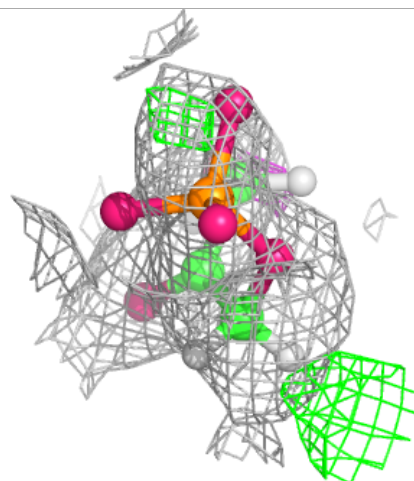
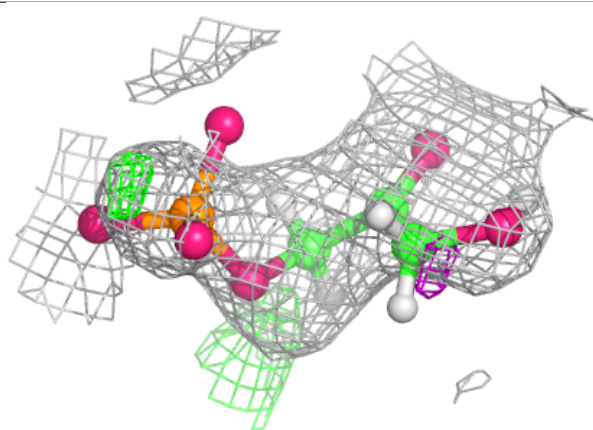
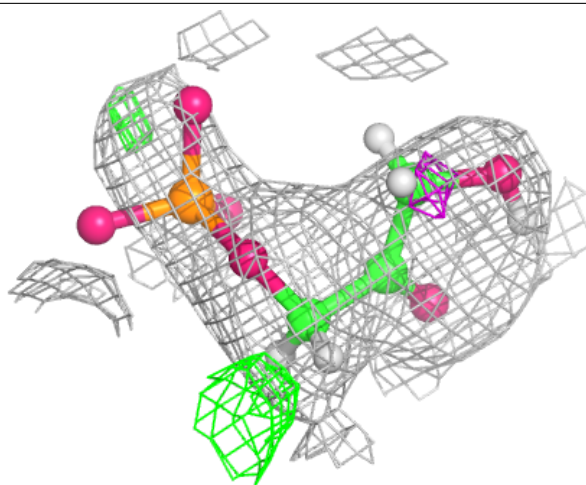
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	703	6/6	0.78	0.30	67,69,72,74	0
3	13P	B	702	10/10	0.89	0.18	48,54,66,66	5
5	MG	A	704	1/1	0.92	0.10	59,59,59,59	0
3	13P	A	702	10/10	0.93	0.24	38,42,54,54	7
2	NAD	B	701	44/44	0.93	0.11	38,52,63,72	0
5	MG	B	703	1/1	0.97	0.07	73,73,73,73	0
2	NAD	A	701	44/44	0.98	0.12	30,40,50,52	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.



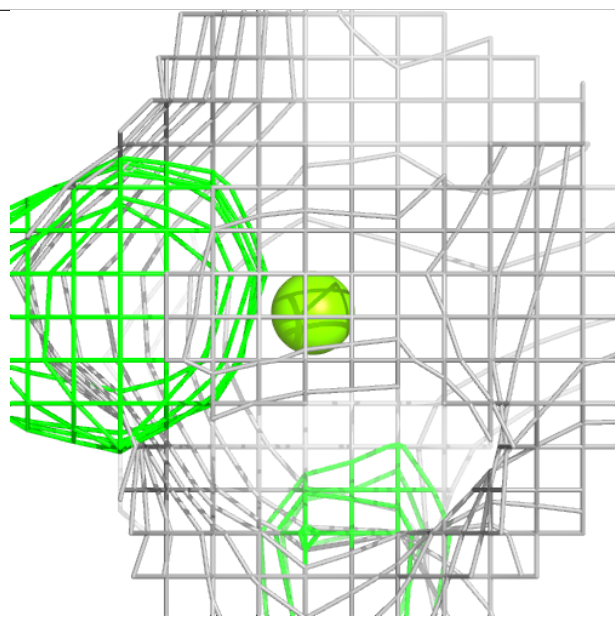
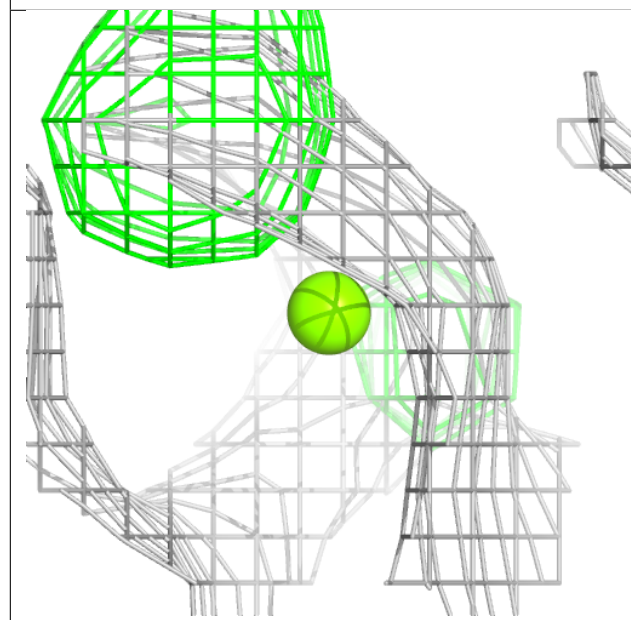
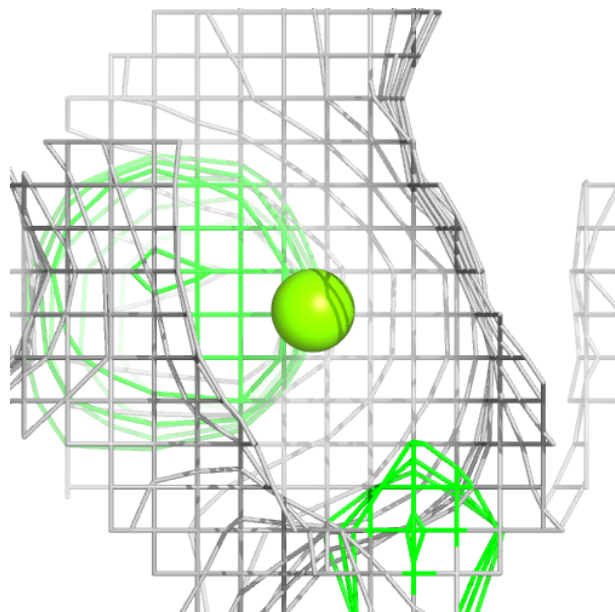
Electron density around 13P B 702:

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



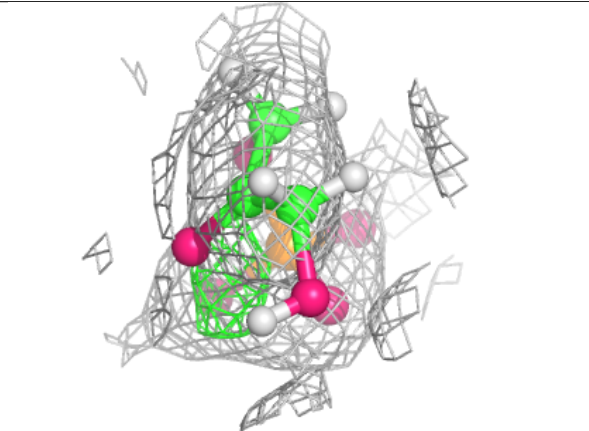
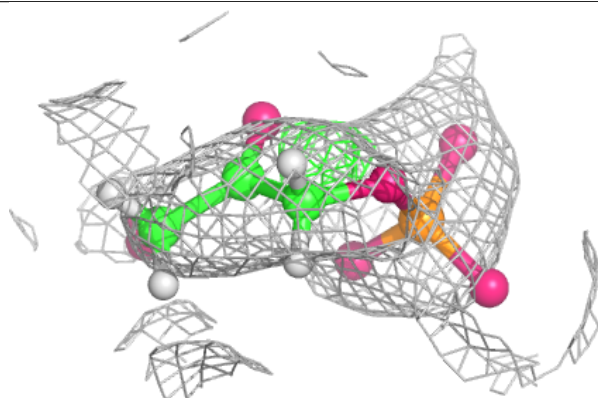
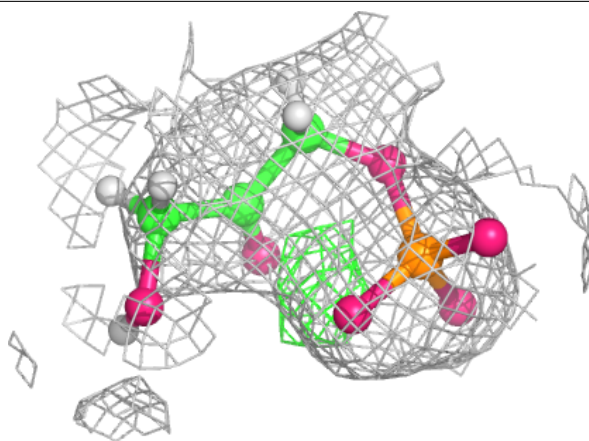
Electron density around MG A 704:

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

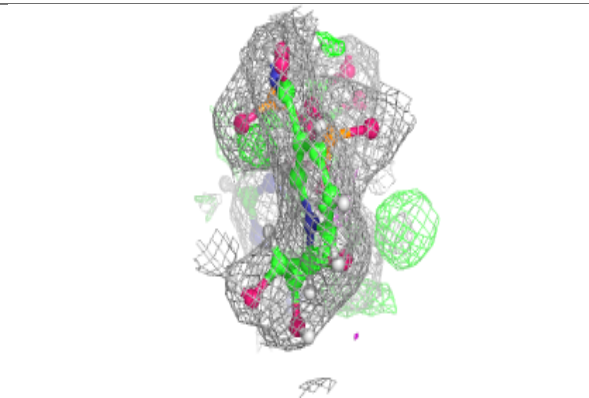
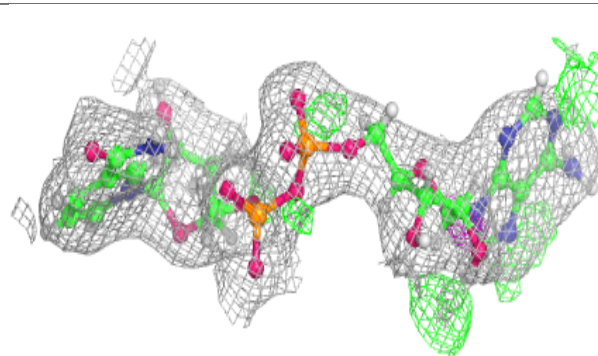
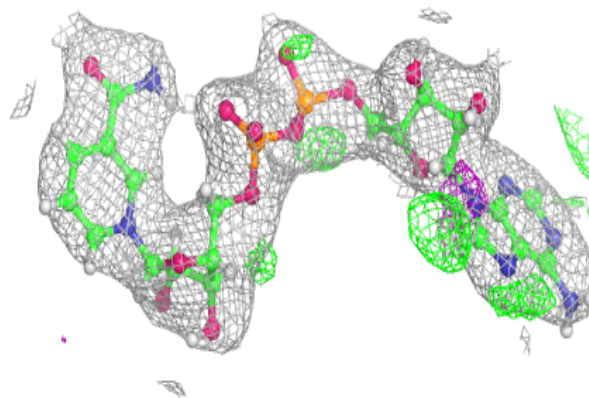


Electron density around 13P A 702:

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

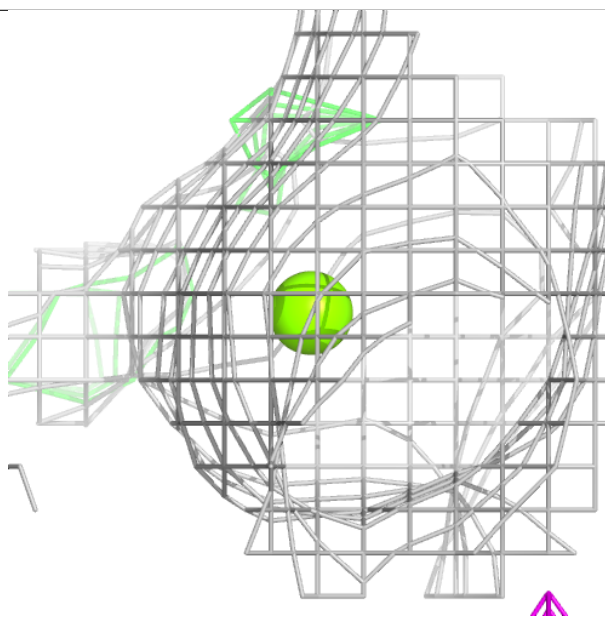
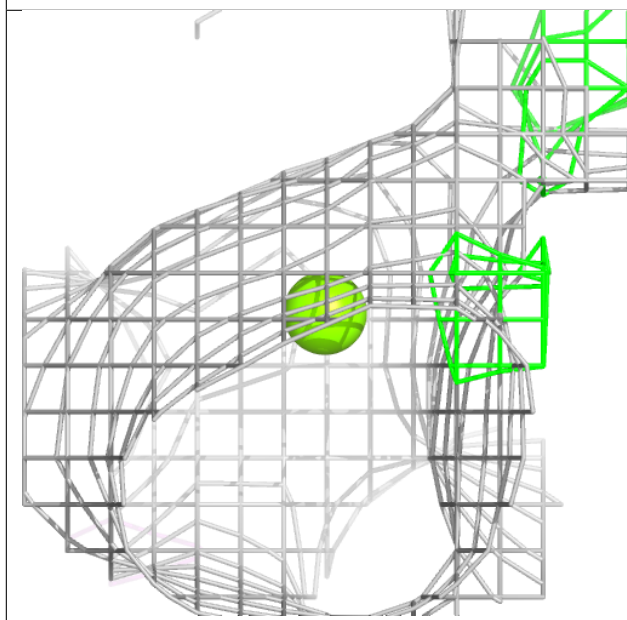
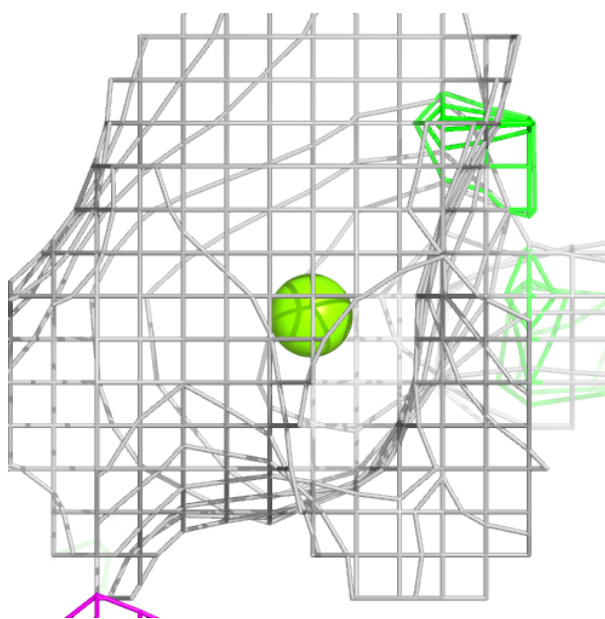
**Electron density around NAD B 701:**

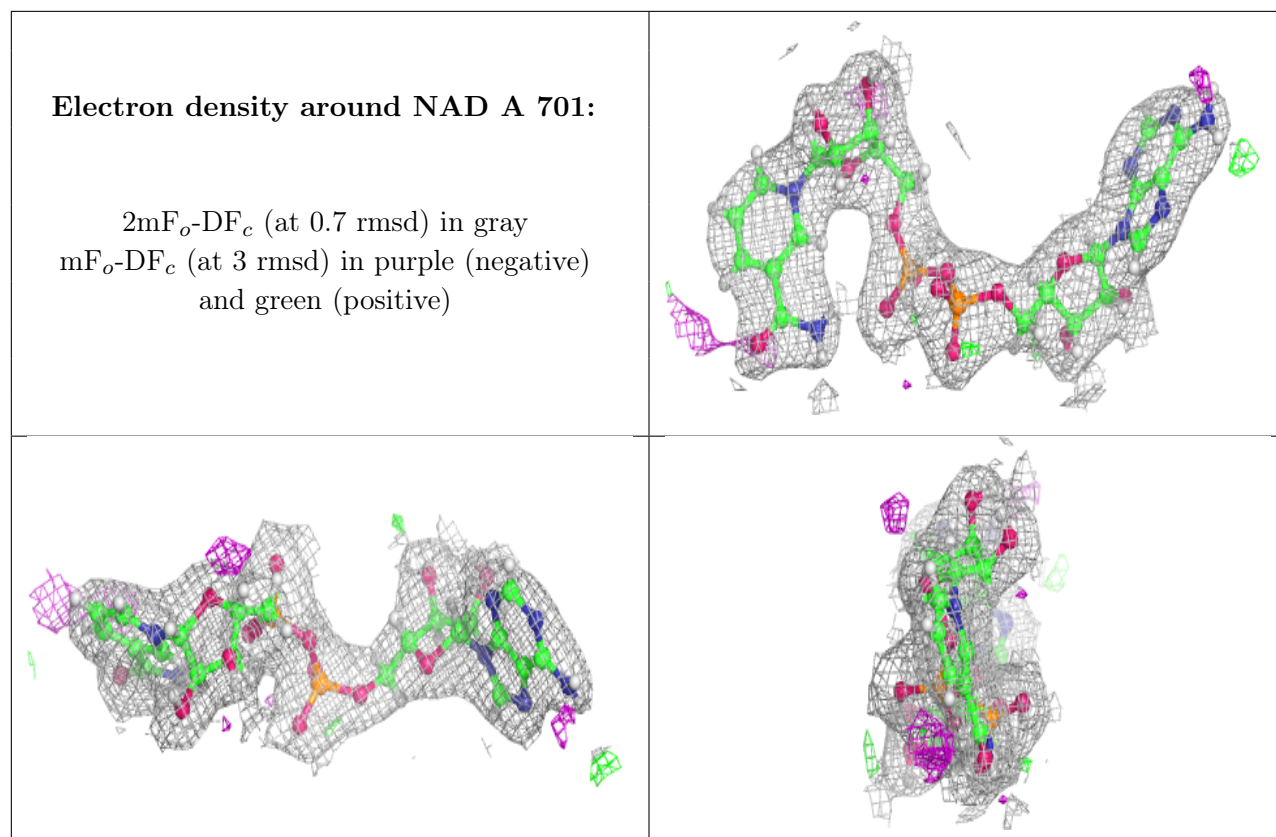
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 703:

$2mF_o-DF_c$ (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.