



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:42 PM EDT

PDB ID : 6IUYY / pdb_00006iuy
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	:	4-5-2 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

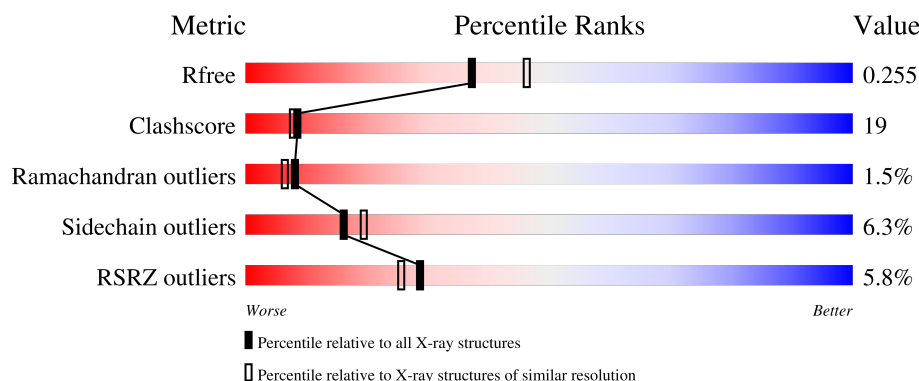
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	6% 63% 27% • 6%
1	B	624	5% 60% 20% • 15%

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

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
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:

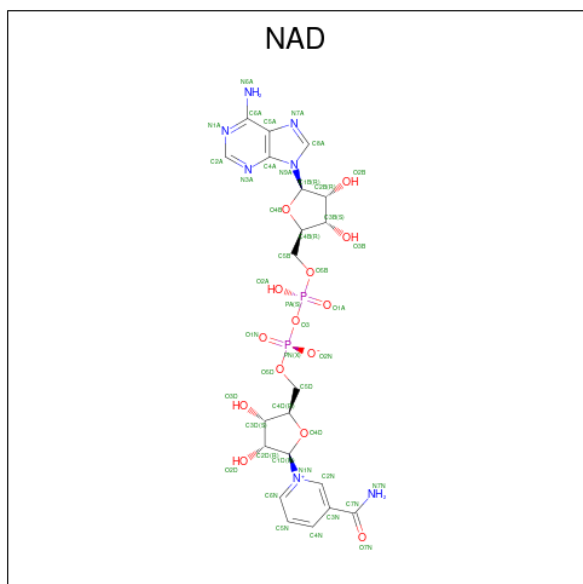
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	expression tag	UNP Q52ZA0
A	77	HIS	-	expression tag	UNP Q52ZA0
A	78	HIS	-	expression tag	UNP Q52ZA0
A	79	HIS	-	expression tag	UNP Q52ZA0
A	80	HIS	-	expression tag	UNP Q52ZA0
A	81	HIS	-	expression tag	UNP Q52ZA0
A	82	HIS	-	expression tag	UNP Q52ZA0
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

Continued on next page...

Continued from previous page...

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 (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



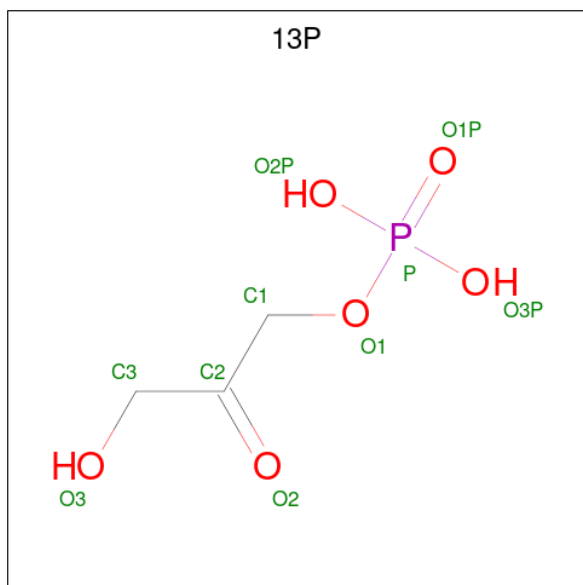
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			70	21	26	7	14	2	

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 4 is GLYCEROL (CCD ID: 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	0	0
			6	3	3		

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

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

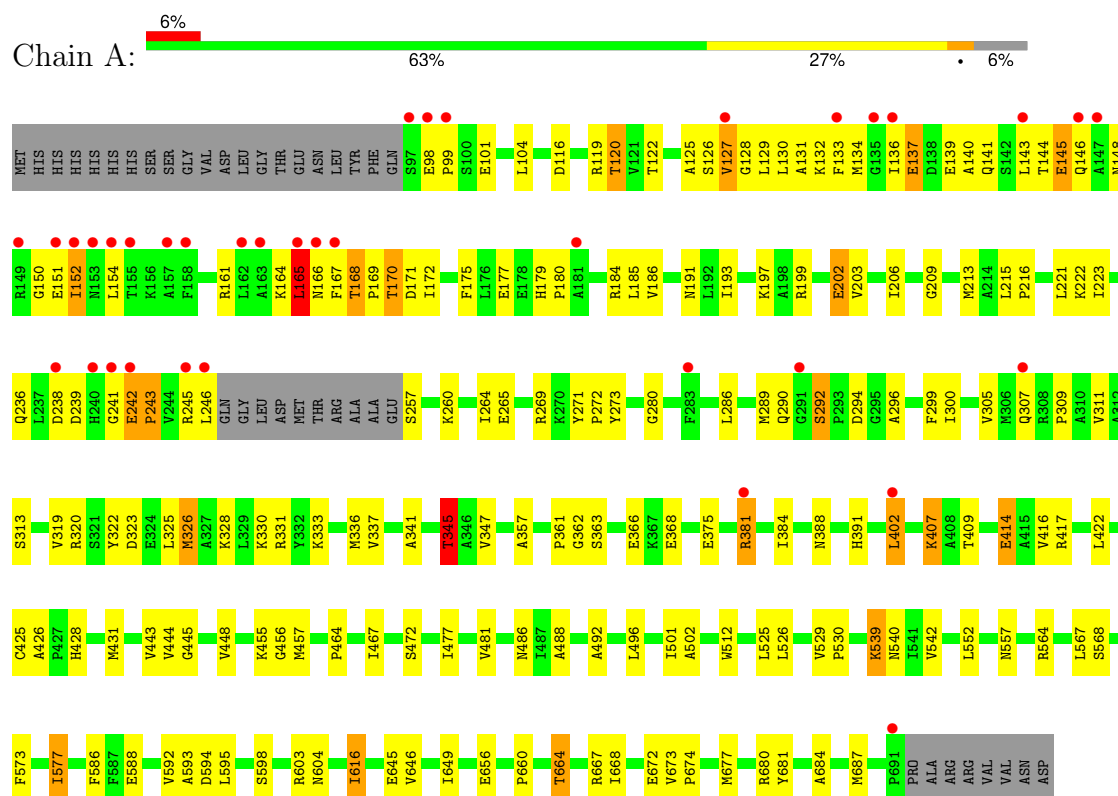
- Molecule 6 is water.

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

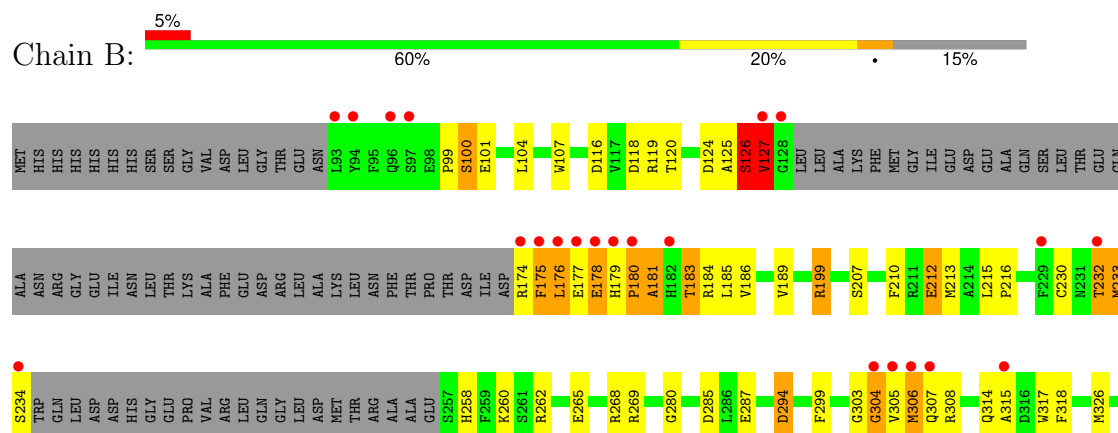
3 Residue-property plots

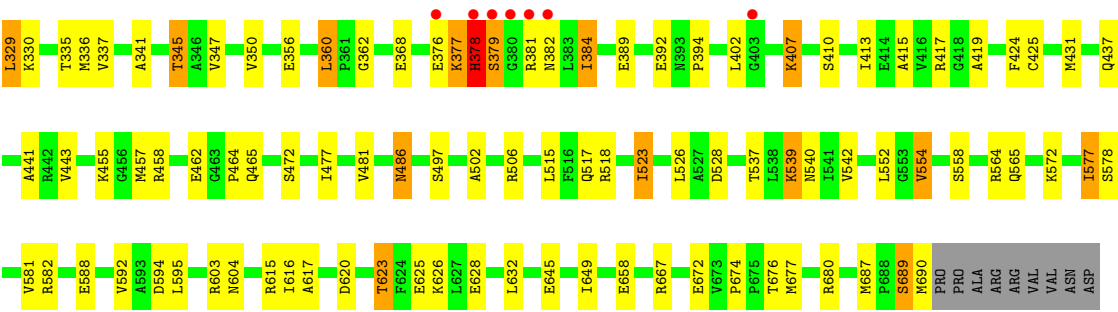
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 47.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.36-2.20) 100.0 (47.36-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.248 0.210 , 0.255	Depositor DCC
R_{free} test set	3808 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAD, 13P, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/4552	0.87	7/6158 (0.1%)
1	B	0.55	0/4142	0.86	5/5595 (0.1%)
All	All	0.53	0/8694	0.87	12/11753 (0.1%)

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 (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	402	LEU	N-CA-C	-7.38	100.79	110.53
1	A	402	LEU	N-CA-C	-7.03	99.87	110.28
1	A	292	SER	CA-C-N	6.36	126.06	119.64
1	A	292	SER	C-N-CA	6.36	126.06	119.64
1	A	486	ASN	N-CA-C	6.12	117.78	110.44
1	A	98	GLU	CA-C-N	5.91	127.22	119.84
1	A	98	GLU	C-N-CA	5.91	127.22	119.84
1	A	345	THR	N-CA-C	-5.67	105.09	112.23
1	B	100	SER	N-CA-C	5.56	119.70	113.02
1	B	304	GLY	N-CA-C	-5.18	105.45	112.14
1	B	486	ASN	N-CA-C	5.12	116.59	110.44
1	B	592	VAL	N-CA-C	5.08	115.69	110.36

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

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	194	0
1	B	4067	0	4050	132	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	12	0
All	All	9016	62	8527	327	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 19.

All (327) 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	1.37	1.05
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:336:MET:HE1	1:B:425:CYS:CB	2.10	0.82
1:A:136:ILE:HG13	1:A:139:GLU:HB3	1.60	0.82
1:A:175:PHE:CE2	1:A:213:MET:HE1	2.15	0.81
1:A:426:ALA:HB3	1:A:431:MET:HE2	1.62	0.81
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
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: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:A:175:PHE:HE2	1:A:213:MET:HE1	1.54	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:336:MET:HE3	1:A:337:VAL:N	2.06	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:457:MET:HE3	1:A:645:GLU:HB3	1.75	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:132:LYS:O	1:A:133:PHE:HB3	1.94	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
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:B:677:MET:HE3	1:B:680:ARG:HB2	1.80	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:B:210:PHE:CG	1:B:233:MET:HE3	2.35	0.62
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:539:LYS:HD2	1:B:594:ASP:CG	2.30	0.56
1:A:336:MET:HE3	1:A:337:VAL:H	1.70	0.56
1:A:326:MET:HE1	1:A:361:PRO:HB2	1.88	0.56
1:A:677:MET:HE3	1:A:680:ARG:HB2	1.88	0.55
1:B:384:ILE:HD11	1:B:410:SER:HB3	1.89	0.55
1:B:537:THR:OG1	6:B:801:HOH:O	2.06	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:457:MET:HE1	1:B:649:ILE:HD12	1.90	0.54
1:A:130:LEU:C	1:A:161:ARG:HH22	2.16	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:457:MET:HE1	1:A:649:ILE:HD12	1.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:336:MET:HE3	1:B:337:VAL:C	2.33	0.53
1:A:191:ASN:C	1:A:326:MET:HE2	2.34	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:336:MET:HE1	1:A:425:CYS:CB	2.40	0.51
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:307:GLN:CD	6:B:834:HOH:O	2.52	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:A:345:THR:HG21	1:A:488:ALA:HB1	1.93	0.51
1:A:539:LYS:HE3	1:A:594:ASP:CG	2.36	0.51
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:336:MET:CE	1:A:425:CYS: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:233:MET:O	1:B:234:SER:OG	2.17	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: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:132:LYS:C	1:A:134:MET:H	2.19	0.50
1:A:388:ASN:OD1	1:A:407:LYS:HD2	2.12	0.50
1:A:238:ASP:CG	1:A:239:ASP:H	2.17	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:126:SER:C	1:B:127:VAL:HG13	2.38	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:B:689:SER:O	1:B:690:MET:HB2	2.12	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:134:MET:HE2	1:A:167:PHE:HD1	1.77	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: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:126:SER:HB3	1:A:213:MET:HE2	1.96	0.47
1:A:457:MET:HE3	1:A:645:GLU:CB	2.44	0.47
1:B:424:PHE:CD1	1:B:431:MET:HE1	2.50	0.46
1:B:554:VAL:HG13	1:B:558:SER:CB	2.41	0.46
1:B:377:LYS:O	1:B:378:HIS:HB3	2.14	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: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:457:MET:HE2	1:A:646:VAL:HG23	1.96	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:B:457:MET:HE3	1:B:645:GLU:HB3	1.97	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:529:VAL:N	1:A:530:PRO:HD2	2.29	0.46
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:B:572:LYS:NZ	1:B:658:GLU:O	2.40	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:381:ARG:O	1:A:381:ARG:HG3	2.17	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:336:MET:HE1	1:A:425:CYS:N	2.34	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:677:MET:HE3	1:A:680:ARG:CB	2.51	0.41
1:B:486:ASN:O	2:B:701:NAD:H4N	2.21	0.41
1:A:238:ASP:CG	1:A:239:ASP:N	2.74	0.40
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: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:336:MET:HE1	1:A:425:CYS:HB3	2.03	0.40
1:A:467:ILE:HG12	6:A:844:HOH:O	2.22	0.40
1:B:210:PHE:CD2	1:B:233:MET:HE3	2.57	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%)	9	7
1	B	525/624 (84%)	489 (93%)	27 (5%)	9 (2%)	7	5
All	All	1106/1248 (89%)	1028 (93%)	61 (6%)	17 (2%)	8	6

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%)	439 (94%)	26 (6%)	19	24
1	B	426/511 (83%)	396 (93%)	30 (7%)	14	16
All	All	891/1022 (87%)	835 (94%)	56 (6%)	16	19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	THR
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	414	GLU
1	A	496	LEU
1	A	539	LYS
1	A	568	SER
1	A	577	ILE
1	A	616	ILE
1	A	656	GLU
1	A	664	THR
1	B	126	SER
1	B	127	VAL
1	B	176	LEU
1	B	178	GLU
1	B	183	THR
1	B	185	LEU
1	B	199	ARG
1	B	212	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	233	MET
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	384	ILE
1	B	389	GLU
1	B	407	LYS
1	B	462	GLU
1	B	523	ILE
1	B	539	LYS
1	B	554	VAL
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	290	GLN
1	A	390	ASN
1	A	486	ASN
1	A	505	ASN
1	A	514	GLN
1	B	390	ASN
1	B	437	GLN
1	B	465	GLN
1	B	486	ASN
1	B	513	GLN
1	B	604	ASN

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 ⓘ

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$
4	GOL	A	703	-	5,5,5	0.34	0	5,5,5	0.30	0
3	13P	A	702	-	9,9,9	0.87	1 (11%)	10,12,12	1.44	1 (10%)
2	NAD	A	701	-	46,48,48	3.64	16 (34%)	64,73,73	1.79	14 (21%)
3	13P	B	702	-	9,9,9	0.97	1 (11%)	10,12,12	1.42	1 (10%)
2	NAD	B	701	-	46,48,48	3.70	14 (30%)	64,73,73	1.79	13 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	703	-	-	4/4/4/4	-
3	13P	A	702	-	-	8/8/8/8	-
2	NAD	A	701	-	-	6/30/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	13P	B	702	-	-	6/8/8/8	-
2	NAD	B	701	-	-	9/30/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAD	O4D-C1D	16.62	1.62	1.40
2	B	701	NAD	O4D-C1D	16.35	1.62	1.40
2	B	701	NAD	O4B-C1B	8.08	1.60	1.42
2	A	701	NAD	O4B-C1B	8.07	1.60	1.42
2	A	701	NAD	C2B-C1B	-7.67	1.29	1.53
2	B	701	NAD	C2B-C1B	-7.29	1.30	1.53
2	B	701	NAD	O4D-C4D	-6.57	1.30	1.45
2	B	701	NAD	C7N-N7N	6.46	1.44	1.33
2	B	701	NAD	O4B-C4B	-6.46	1.30	1.45
2	A	701	NAD	C7N-N7N	6.33	1.44	1.33
2	A	701	NAD	O4B-C4B	-6.31	1.31	1.45
2	A	701	NAD	O4D-C4D	-5.64	1.32	1.45
2	B	701	NAD	C2N-N1N	4.59	1.40	1.35
2	B	701	NAD	O3D-C3D	-3.53	1.34	1.43
2	B	701	NAD	C3N-C7N	3.49	1.55	1.50
2	A	701	NAD	C6A-N6A	3.33	1.42	1.34
2	A	701	NAD	O3D-C3D	-3.27	1.34	1.43
2	B	701	NAD	C6A-N6A	3.22	1.42	1.34
2	B	701	NAD	O2B-C2B	3.16	1.50	1.43
2	A	701	NAD	C2N-N1N	3.08	1.38	1.35
2	A	701	NAD	O3B-C3B	-2.93	1.35	1.43
2	A	701	NAD	C3N-C7N	2.87	1.54	1.50
2	A	701	NAD	O2B-C2B	2.84	1.50	1.43
2	B	701	NAD	C8A-N7A	2.74	1.36	1.31
2	B	701	NAD	O2D-C2D	2.71	1.49	1.43
2	A	701	NAD	O2D-C2D	2.48	1.49	1.43
2	B	701	NAD	O3B-C3B	-2.40	1.37	1.43
2	A	701	NAD	C5A-C4A	-2.28	1.35	1.39
3	B	702	13P	O1-C1	-2.09	1.41	1.43
2	A	701	NAD	C1B-N9A	-2.08	1.40	1.46
2	A	701	NAD	C8A-N7A	2.04	1.35	1.31
3	A	702	13P	O1-C1	-2.01	1.41	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	NAD	N3A-C2A-N1A	-5.30	120.56	128.58
2	A	701	NAD	N3A-C2A-N1A	-5.21	120.70	128.58
2	A	701	NAD	N9A-C8A-N7A	-4.64	107.36	113.94
2	B	701	NAD	C4D-O4D-C1D	-4.62	105.69	109.92
2	A	701	NAD	C5A-C4A-N3A	-4.61	120.38	126.72
2	B	701	NAD	C6N-N1N-C2N	-4.24	118.27	121.88
2	B	701	NAD	C4B-O4B-C1B	-3.99	100.66	109.47
2	A	701	NAD	C6N-N1N-C2N	-3.98	118.49	121.88
2	B	701	NAD	C5A-C4A-N3A	-3.71	121.61	126.72
3	A	702	13P	O1-P-O1P	3.56	116.07	106.44
2	A	701	NAD	C4B-O4B-C1B	-3.50	101.75	109.47
2	A	701	NAD	C5A-N7A-C8A	3.38	108.75	103.45
2	B	701	NAD	N9A-C8A-N7A	-3.30	109.26	113.94
2	A	701	NAD	C2A-N3A-C4A	3.25	119.76	111.83
2	B	701	NAD	O4B-C1B-C2B	-3.08	100.02	106.62
2	B	701	NAD	C2A-N3A-C4A	2.79	118.65	111.83
2	A	701	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
2	A	701	NAD	C4A-C5A-N7A	-2.64	107.57	110.58
2	A	701	NAD	N3A-C4A-N9A	2.57	131.54	127.17
2	B	701	NAD	C2N-N1N-C1D	2.50	124.65	119.13
2	B	701	NAD	O4D-C4D-C5D	-2.42	101.58	109.33
2	A	701	NAD	C4A-N9A-C8A	2.37	108.22	105.74
3	B	702	13P	O1-P-O1P	2.36	112.82	106.44
2	A	701	NAD	C2N-C3N-C4N	2.34	120.98	118.26
2	B	701	NAD	O4B-C1B-N9A	2.32	112.55	108.09
2	B	701	NAD	O2N-PN-O3	2.32	113.53	107.27
2	A	701	NAD	N6A-C6A-N1A	-2.29	113.28	118.38
2	B	701	NAD	PN-O5D-C5D	-2.20	108.76	121.35
2	A	701	NAD	C5A-C4A-N9A	2.09	108.09	105.81

There are no chirality outliers.

All (33) 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

Continued on next page...

Continued from previous page...

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

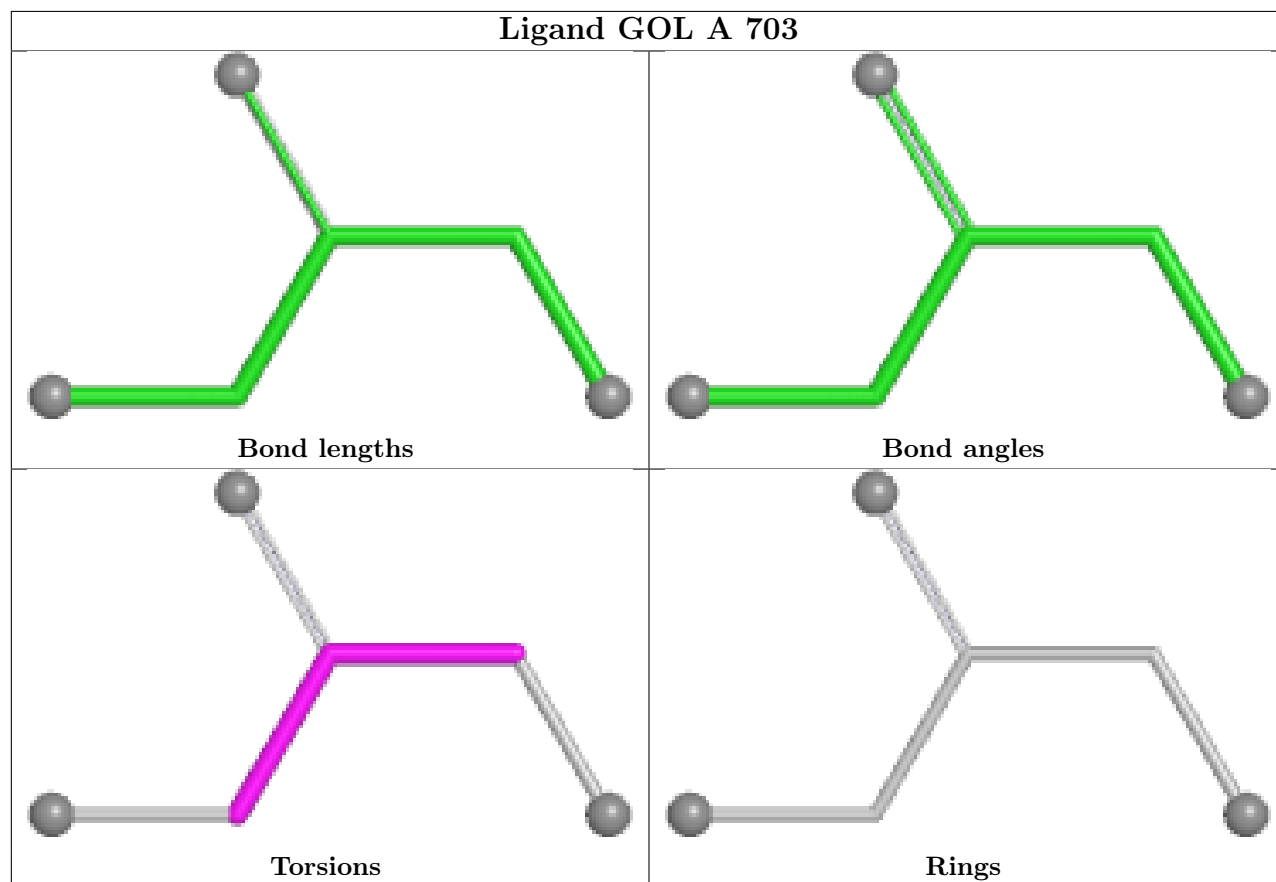
There are no ring outliers.

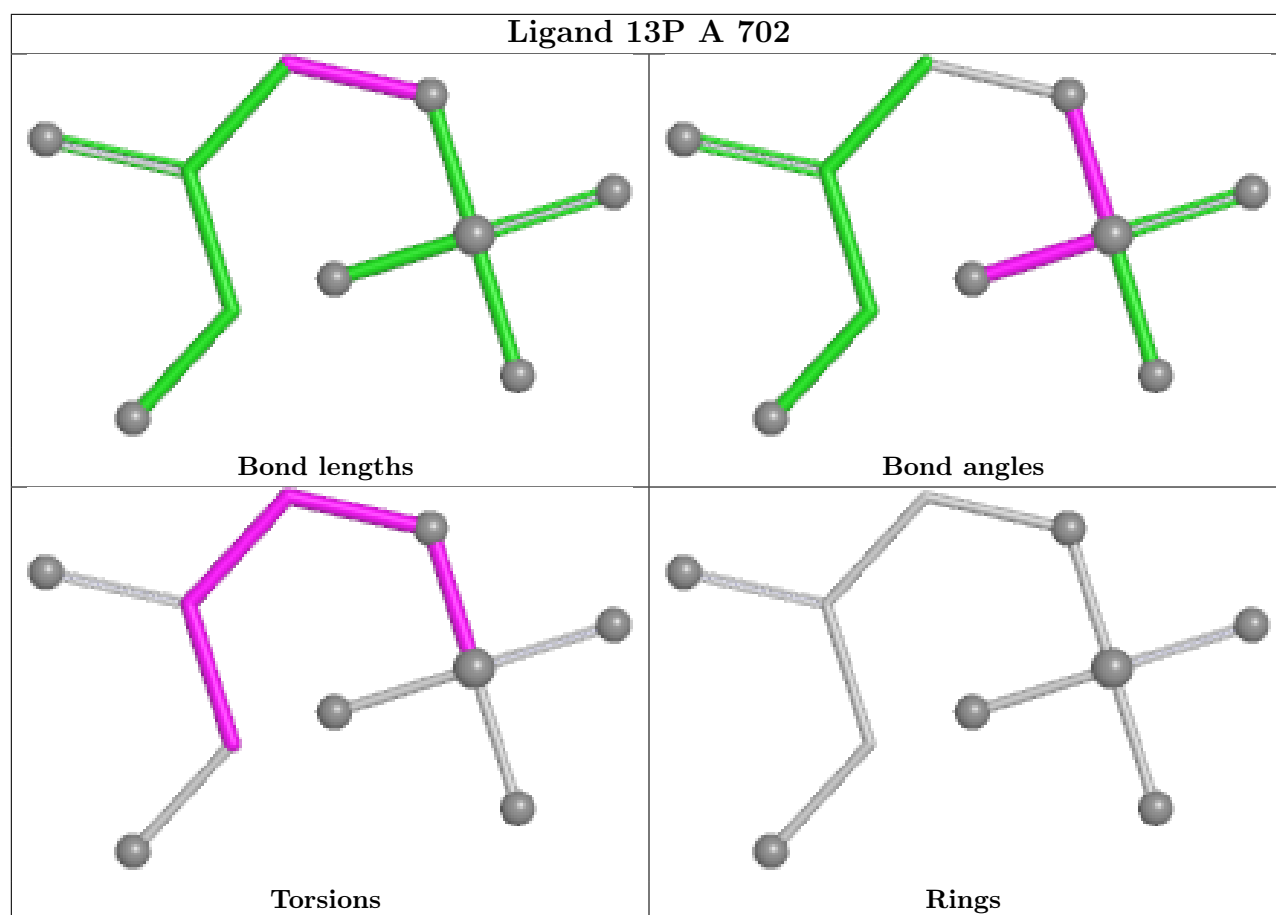
3 monomers are involved in 14 short contacts:

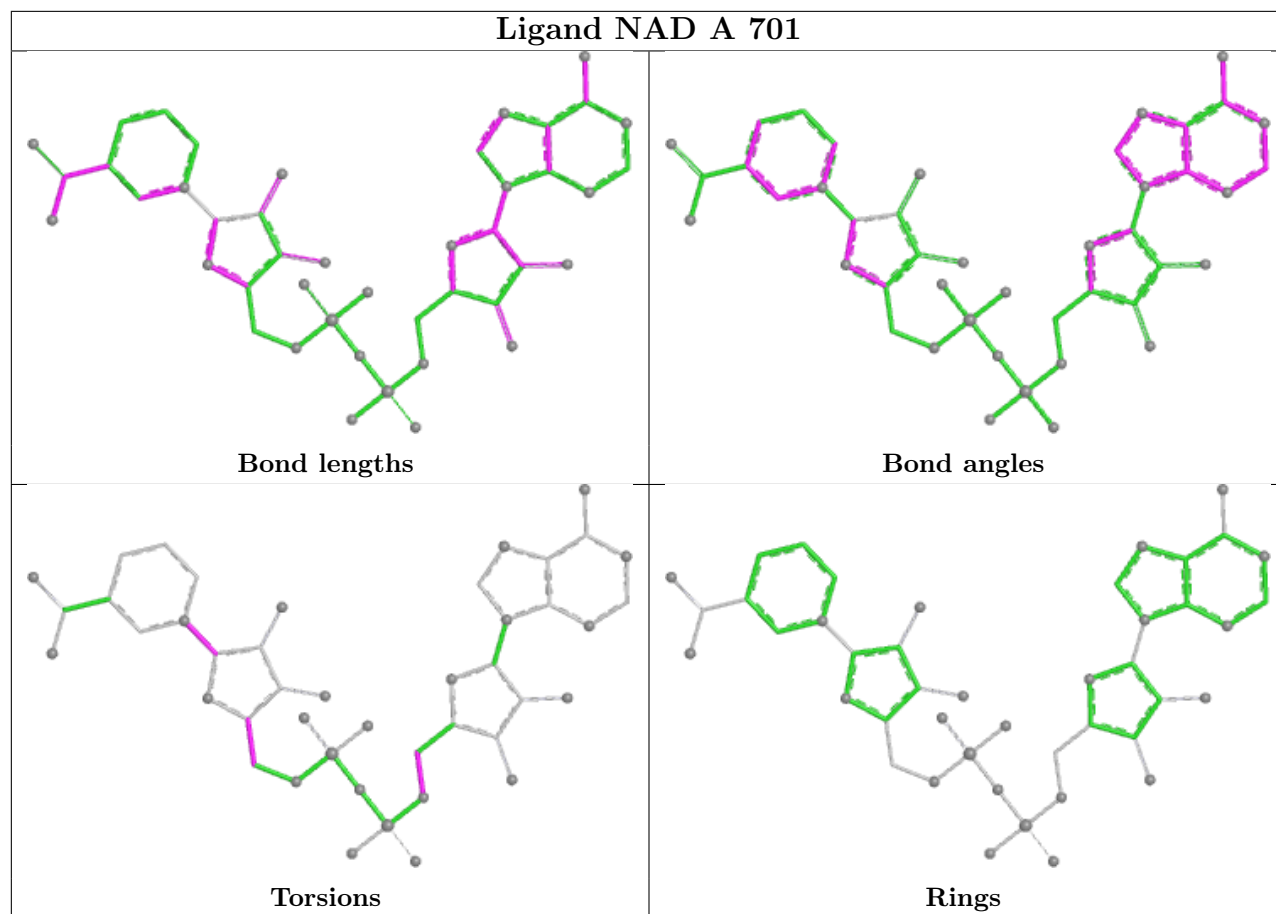
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	13P	7	0
3	B	702	13P	5	0
2	B	701	NAD	2	0

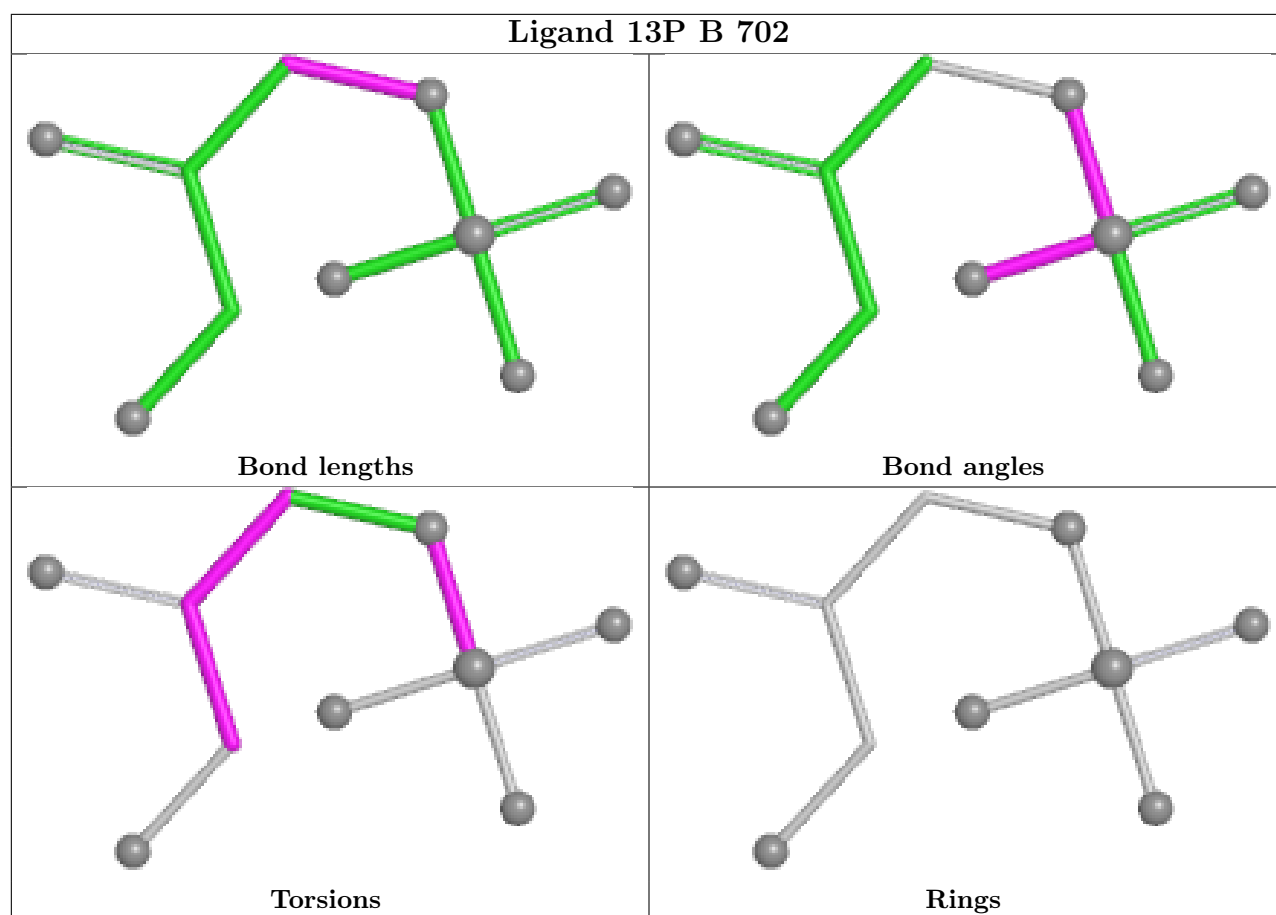
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

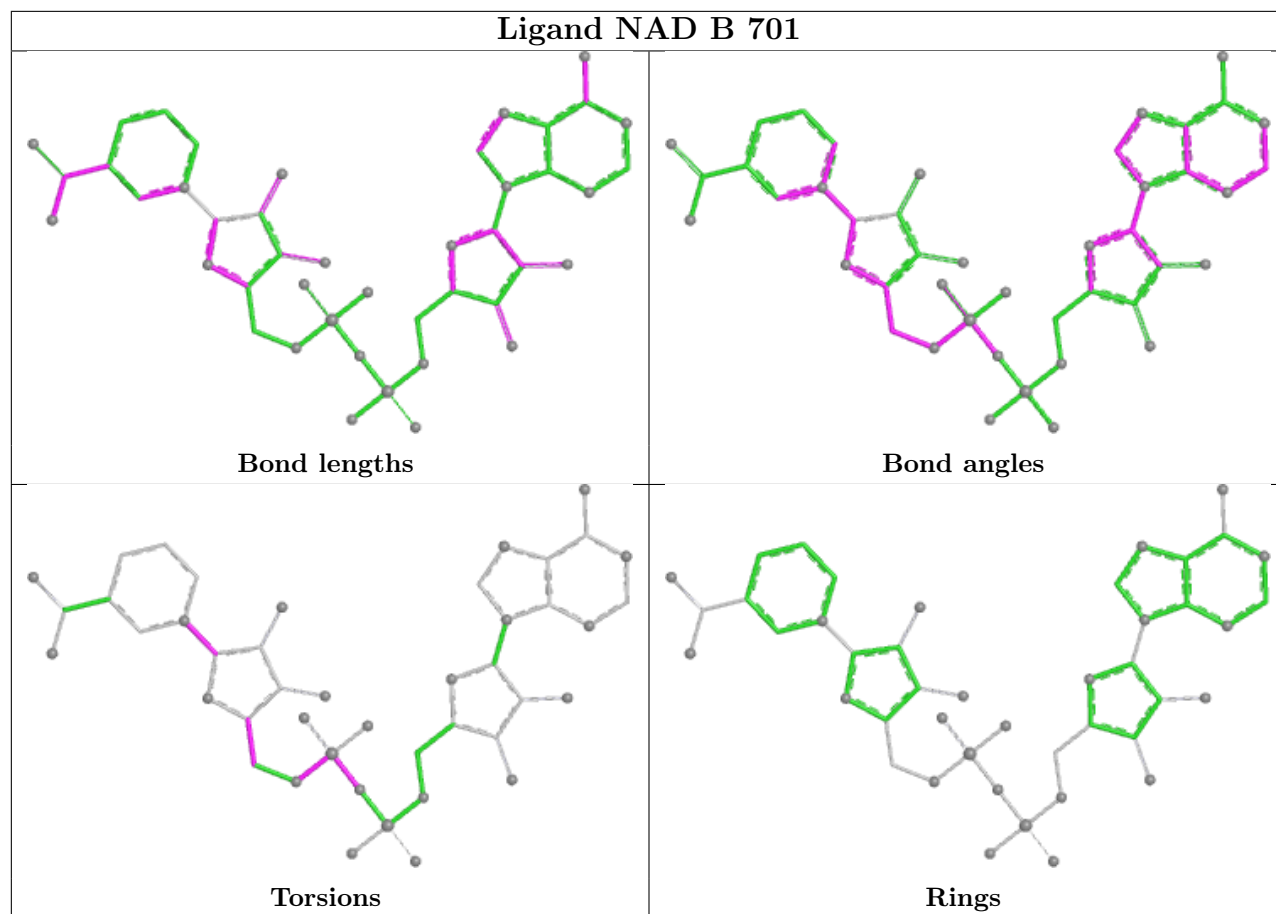
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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%)	0.34	36 (6%) 26 23	34, 51, 89, 119	0
1	B	531/624 (85%)	0.26	29 (5%) 30 27	35, 49, 79, 103	0
All	All	1116/1248 (89%)	0.30	65 (5%) 29 25	34, 50, 87, 119	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	ALA	6.8
1	A	153	ASN	6.7
1	B	128	GLY	5.9
1	A	154	LEU	5.8
1	B	379	SER	5.6
1	A	97	SER	5.4
1	A	155	THR	5.2
1	A	165	LEU	4.8
1	B	304	GLY	4.7
1	B	127	VAL	4.6
1	B	176	LEU	4.3
1	B	305	VAL	4.2
1	B	380	GLY	4.1
1	A	152	ILE	4.1
1	B	378	HIS	4.1
1	B	179	HIS	3.8
1	B	175	PHE	3.8
1	A	163	ALA	3.7
1	A	99	PRO	3.6
1	A	238	ASP	3.5
1	B	93	LEU	3.5
1	A	167	PHE	3.3
1	A	127	VAL	3.2
1	B	174	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	291	GLY	3.1
1	A	146	GLN	3.1
1	A	381	ARG	3.1
1	A	181	ALA	3.1
1	B	178	GLU	3.0
1	A	246	LEU	3.0
1	B	234	SER	3.0
1	A	162	LEU	3.0
1	B	97	SER	3.0
1	B	180	PRO	3.0
1	A	158	PHE	2.9
1	B	232	THR	2.9
1	A	143	LEU	2.8
1	A	157	ALA	2.7
1	A	166	ASN	2.6
1	B	306	MET	2.6
1	A	151	GLU	2.6
1	B	96	GLN	2.6
1	A	242	GLU	2.6
1	B	177	GLU	2.6
1	B	229	PHE	2.5
1	A	241	GLY	2.5
1	B	94	TYR	2.4
1	B	381	ARG	2.4
1	B	376	GLU	2.4
1	A	240	HIS	2.3
1	A	135	GLY	2.3
1	A	133	PHE	2.3
1	B	307	GLN	2.3
1	A	691	PRO	2.2
1	B	403	GLY	2.2
1	A	149	ARG	2.2
1	B	382	ASN	2.2
1	B	182	HIS	2.2
1	A	98	GLU	2.2
1	A	283	PHE	2.1
1	A	307	GLN	2.0
1	A	136	ILE	2.0
1	A	245	ARG	2.0
1	B	315	ALA	2.0
1	A	402	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

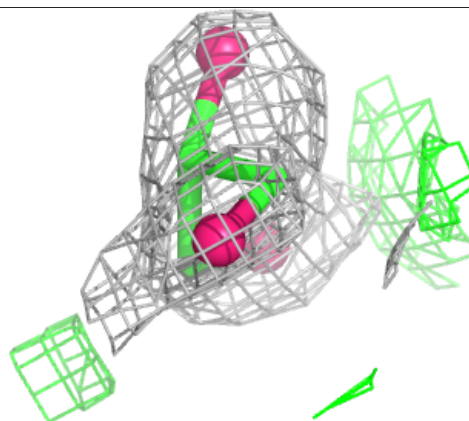
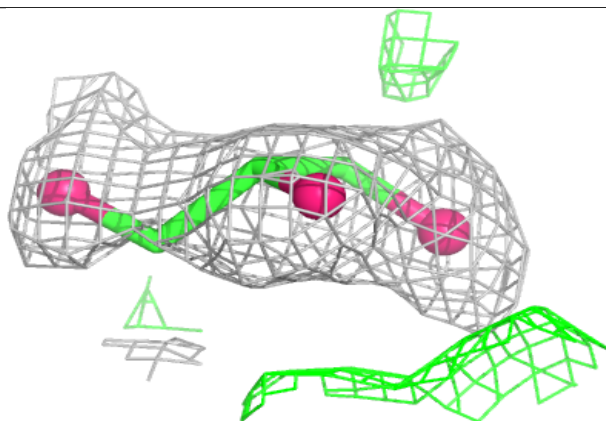
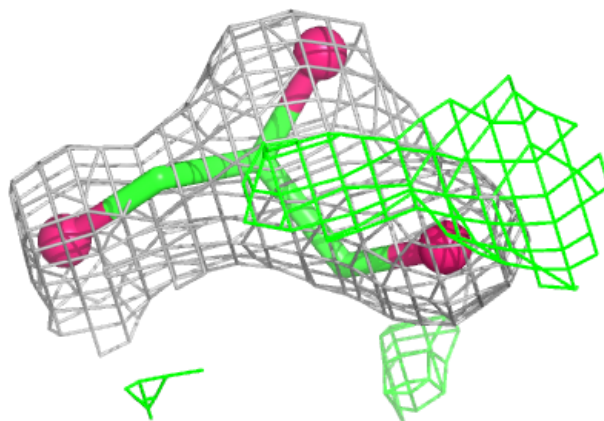
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	703	6/6	0.71	0.19	67,69,72,74	0
3	13P	B	702	10/10	0.85	0.16	48,54,66,66	5
5	MG	A	704	1/1	0.85	0.13	59,59,59,59	0
5	MG	B	703	1/1	0.88	0.14	73,73,73,73	0
2	NAD	B	701	44/44	0.92	0.09	38,52,63,72	0
3	13P	A	702	10/10	0.92	0.14	38,42,54,54	7
2	NAD	A	701	44/44	0.97	0.06	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.

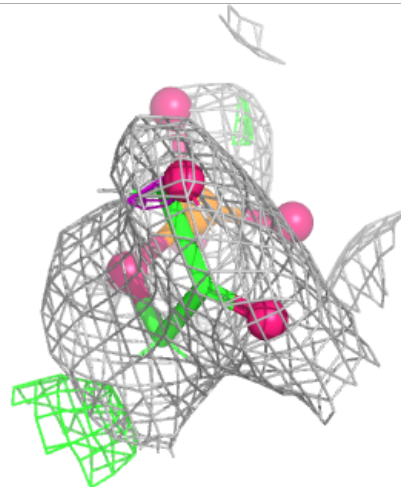
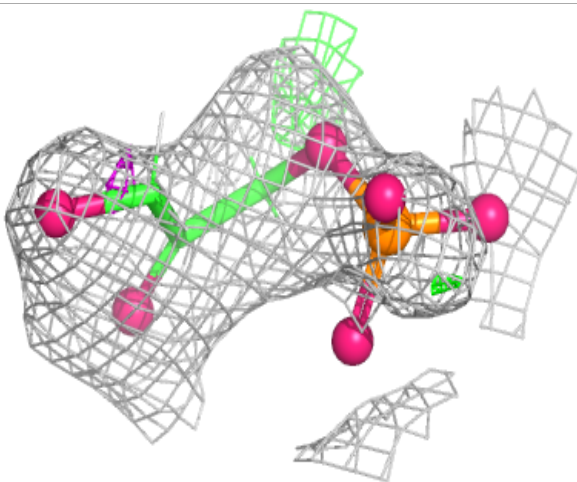
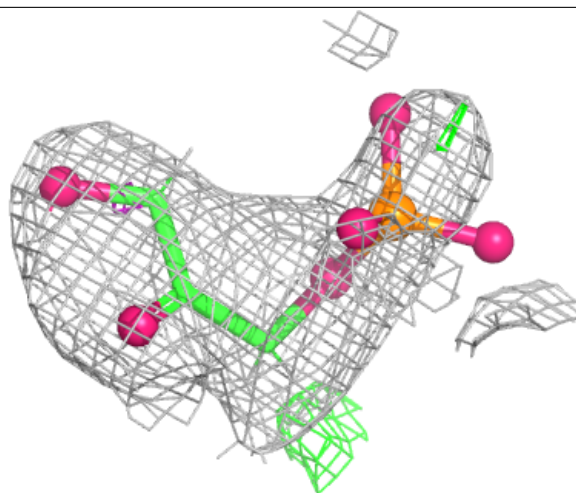
Electron density around GOL A 703:

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



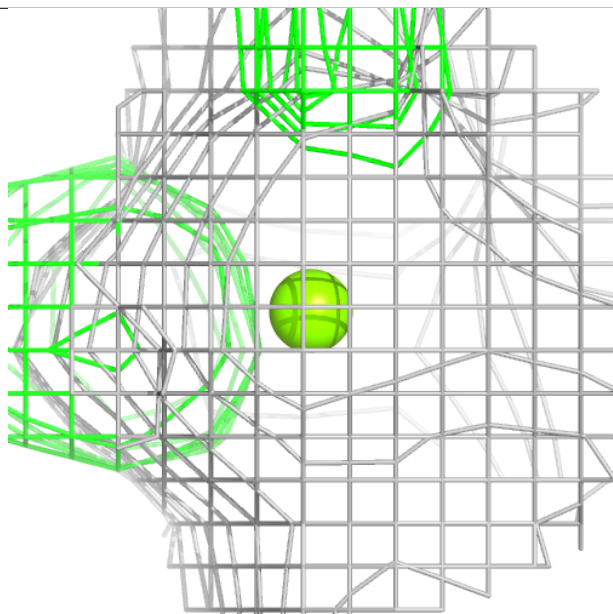
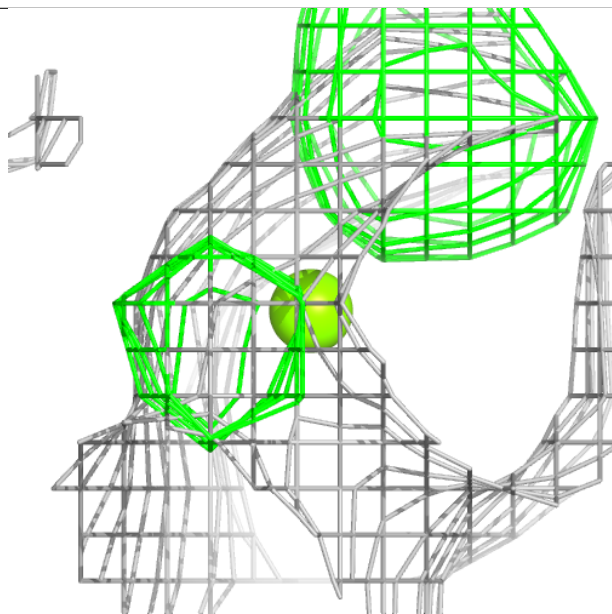
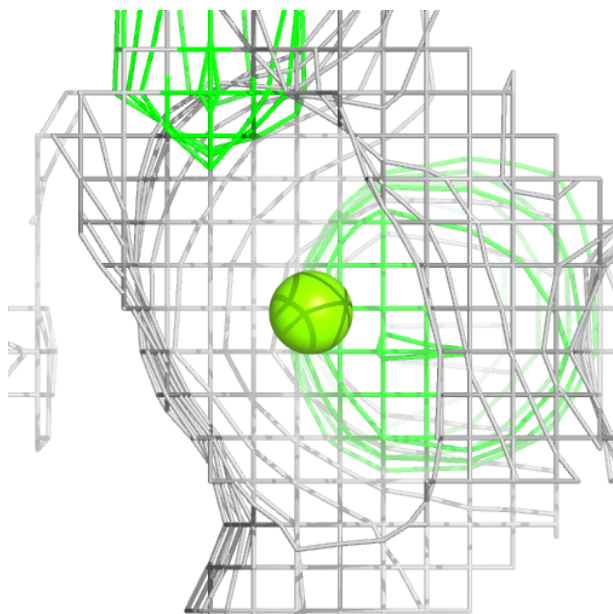
Electron density around 13P B 702:

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



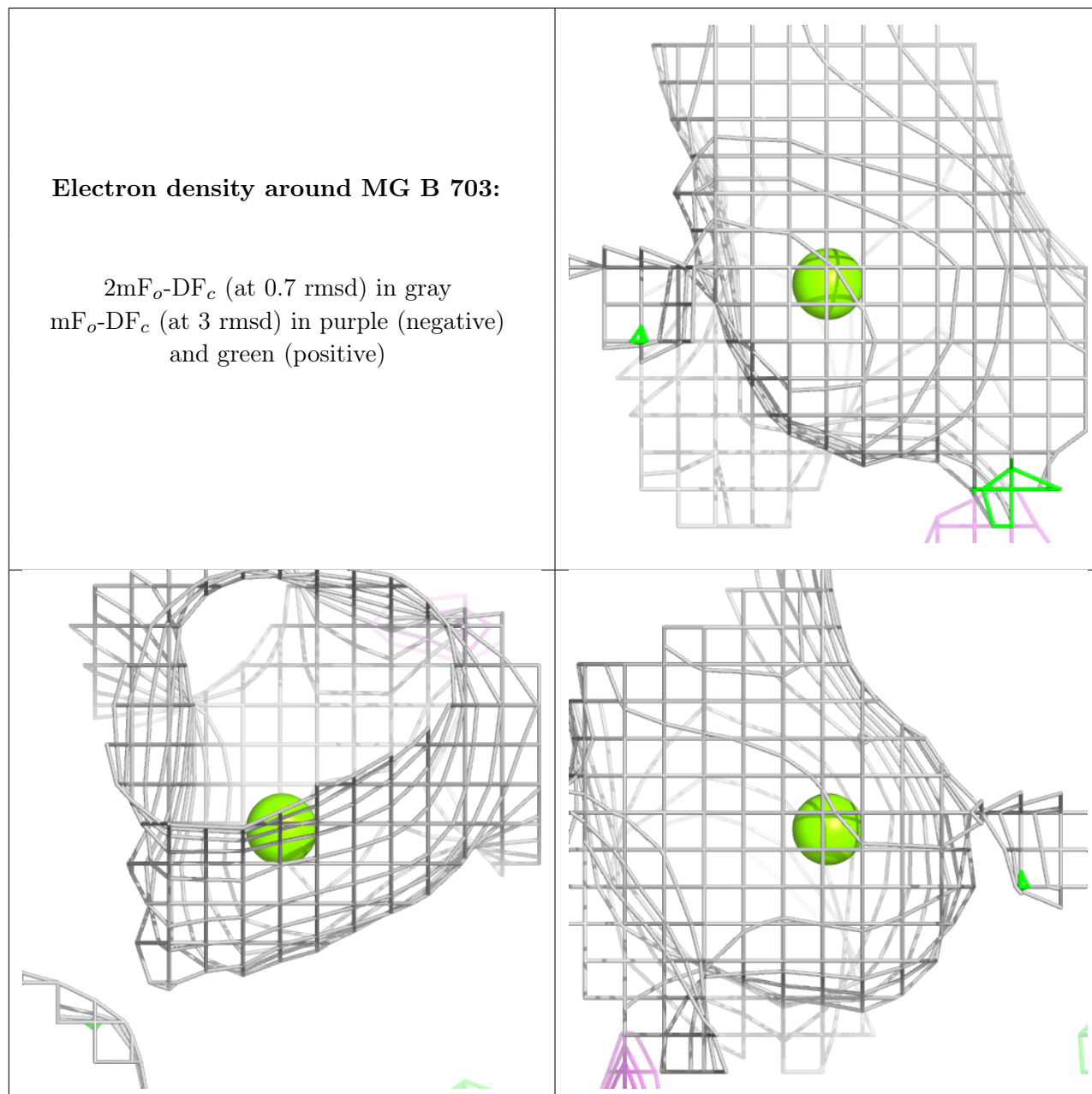
Electron density around MG A 704:

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



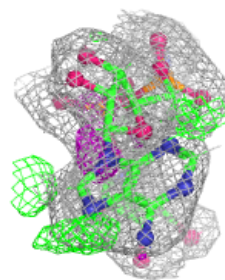
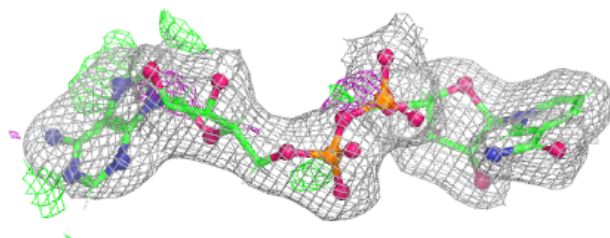
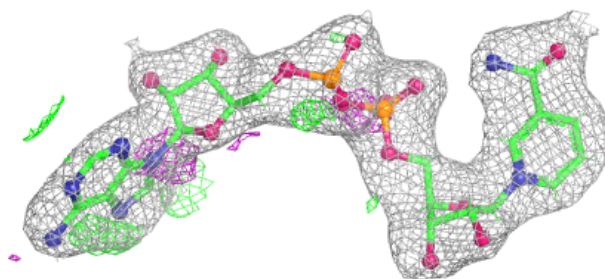
Electron density around MG B 703:

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

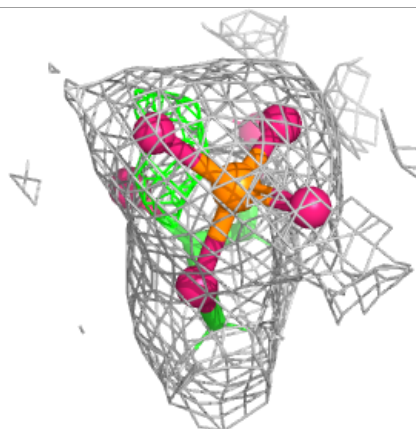
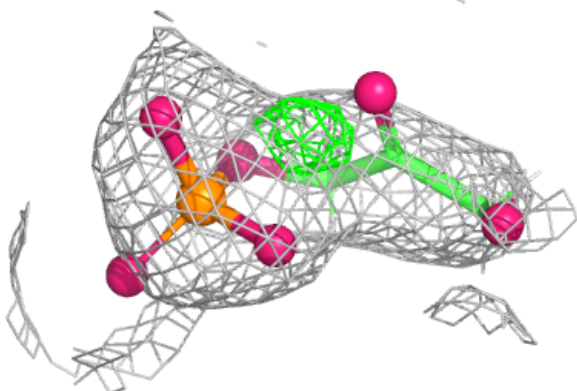
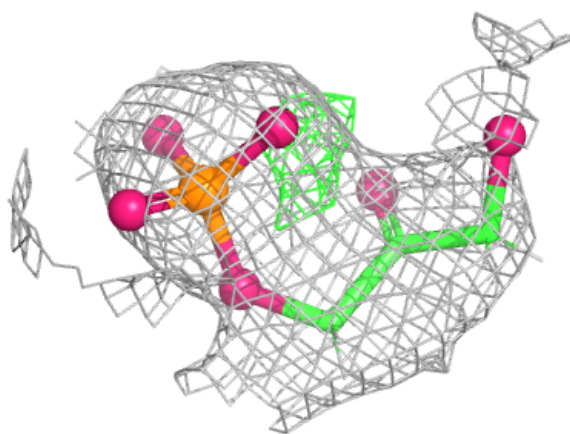


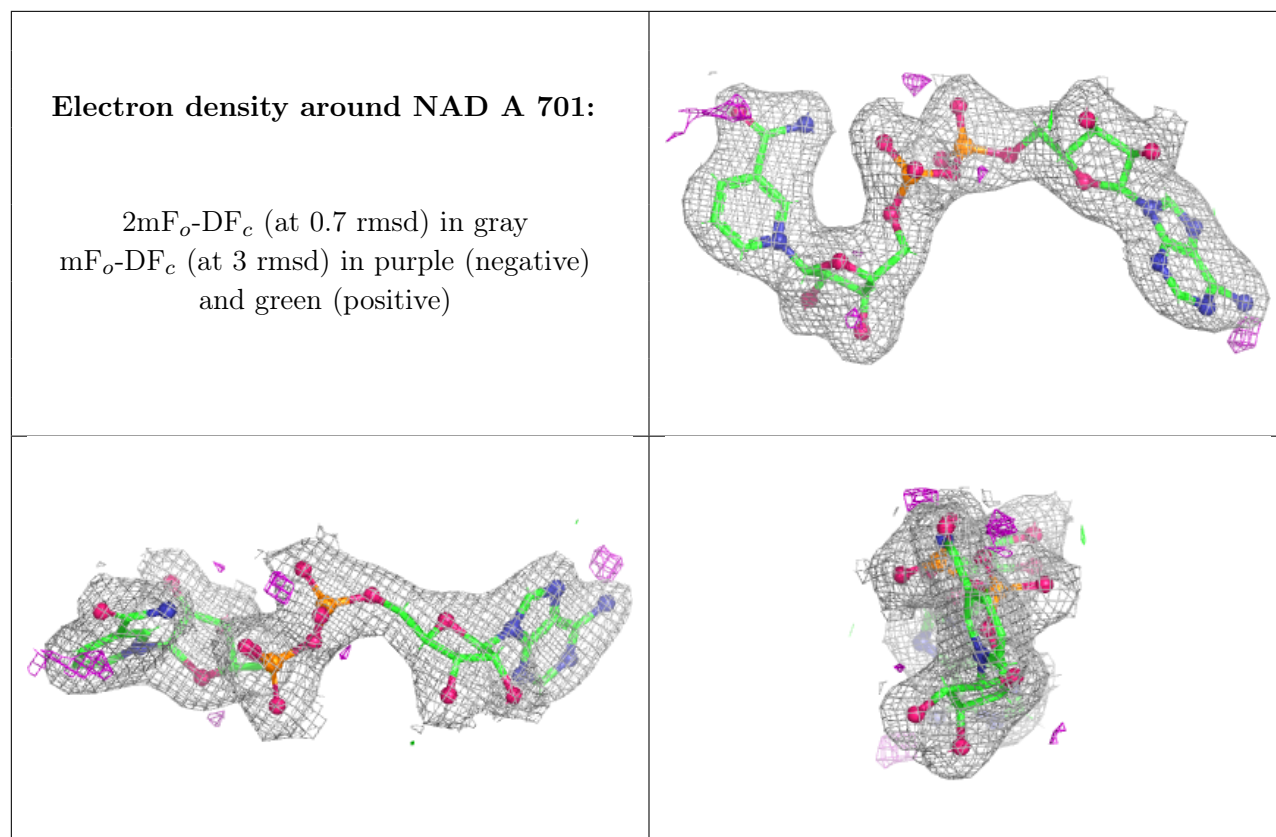
Electron density around NAD B 701:

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

**Electron density around 13P A 702:**

$2mF_o-DF_c$ (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.