



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:09 pm BST

PDB ID : 1O0S  
Title : Crystal Structure of Ascaris suum Malic Enzyme Complexed with NADH  
Authors : Rao, G.S.; Coleman, D.E.; Karsten, W.E.; Cook, P.F.; Harris, B.G.  
Deposited on : 2003-02-24  
Resolution : 2.00 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](mailto: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.

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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 : 2.11  
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) : 2.11

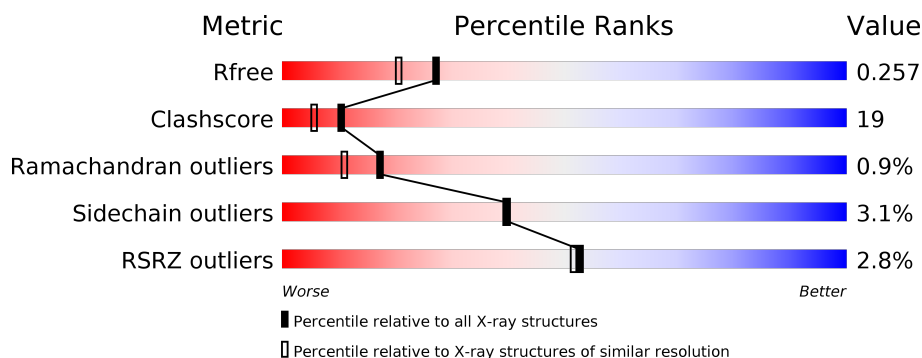
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	605	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>.</div> </div> </div>
1	B	605	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

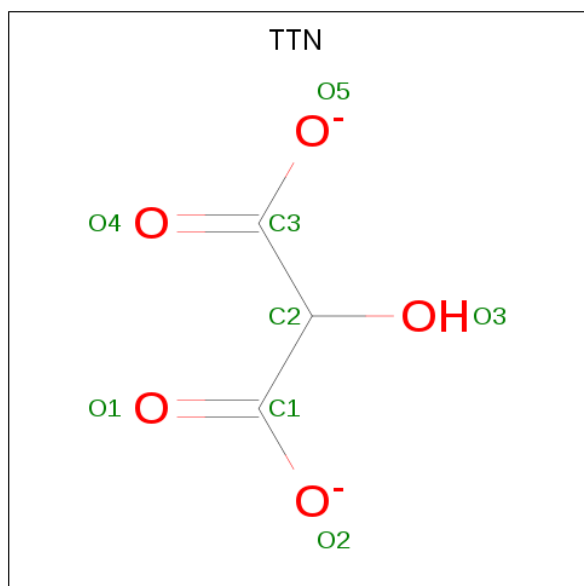
There are 4 unique types of molecules in this entry. The entry contains 10335 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NAD-dependent malic enzyme.

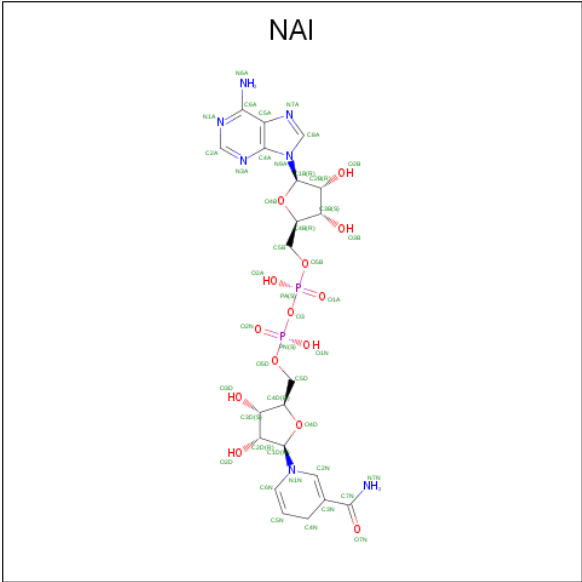
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	48	0	0
			4797	3060	822	889	26			
1	B	592	Total	C	N	O	S	41	0	0
			4719	3011	807	876	25			

- Molecule 2 is TARTRONATE (three-letter code: TTN) (formula:  $C_3H_2O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	3	5		
2	B	1	Total	C	O	0	0
			8	3	5		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

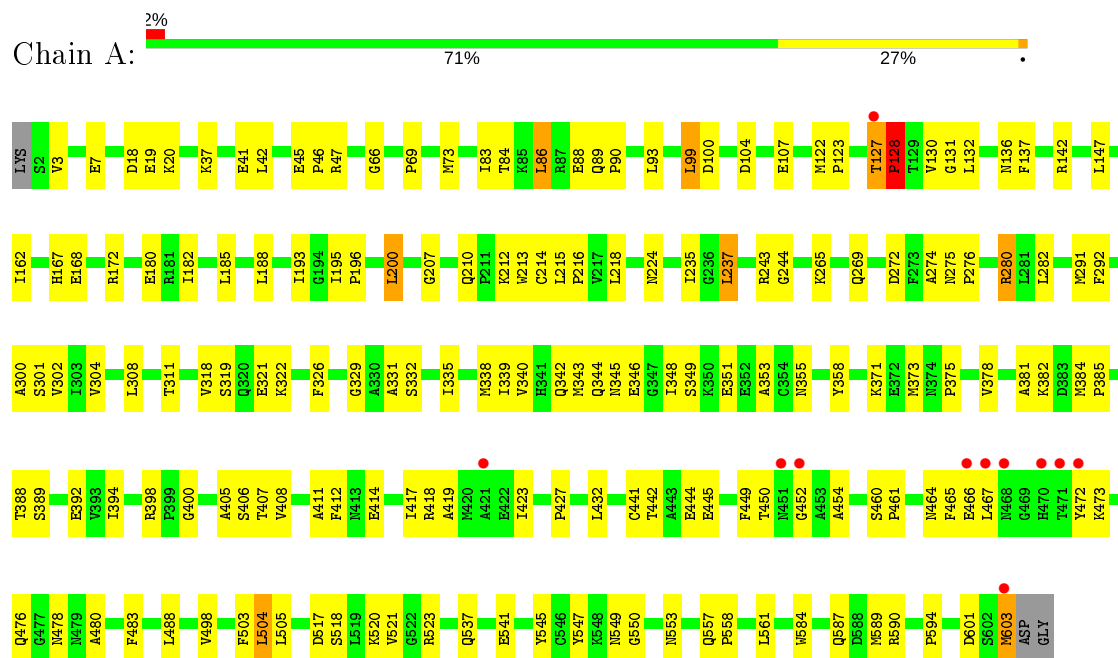
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total	O	0	0
			335	335		
4	B	380	Total	O	0	0
			380	380		

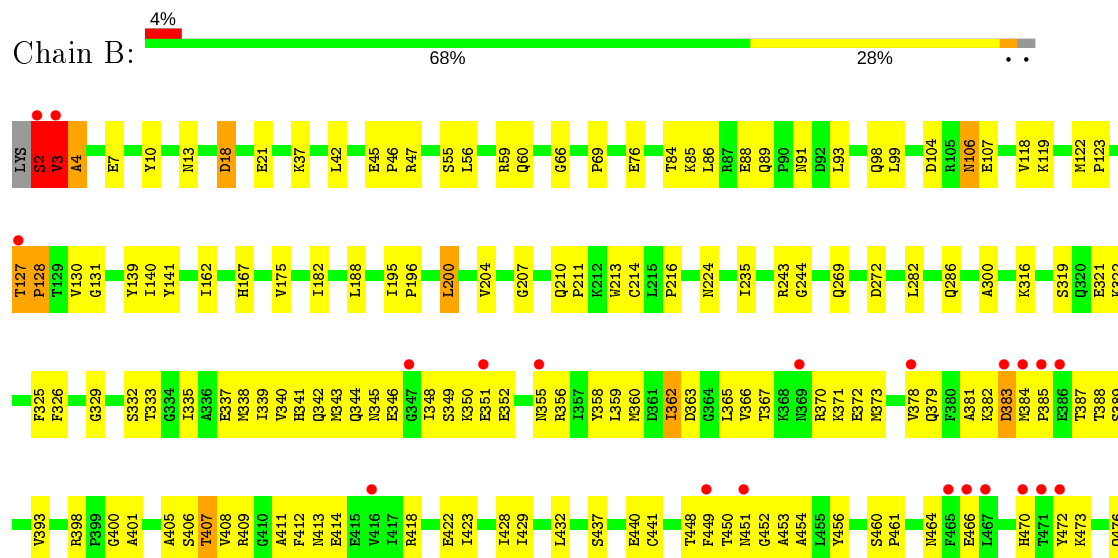
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: NAD-dependent malic enzyme



#### • Molecule 1: NAD-dependent malic enzyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.95Å 130.95Å 149.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 49.71 – 1.97	Depositor EDS
% Data completeness (in resolution range)	82.2 (50.00-2.00) 81.0 (49.71-1.97)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.97Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.264 0.214 , 0.257	Depositor DCC
$R_{free}$ test set	4104 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAI, TTN

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	1/4902 (0.0%)	0.59	1/6639 (0.0%)
1	B	0.87	11/4821 (0.2%)	0.83	11/6527 (0.2%)
All	All	0.68	12/9723 (0.1%)	0.72	12/13166 (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	B	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	VAL	N-CA	33.84	2.14	1.46
1	B	3	VAL	CA-C	28.94	2.28	1.52
1	B	3	VAL	CA-CB	17.96	1.92	1.54
1	B	2	SER	N-CA	16.88	1.80	1.46
1	A	603	MET	C-O	16.25	1.54	1.23
1	B	2	SER	CA-C	11.07	1.81	1.52
1	B	3	VAL	CB-CG1	10.74	1.75	1.52
1	B	2	SER	CB-OG	-8.49	1.31	1.42
1	B	3	VAL	C-N	7.58	1.51	1.34
1	B	3	VAL	CB-CG2	-7.21	1.37	1.52
1	B	2	SER	C-N	6.54	1.49	1.34
1	B	4	ALA	N-CA	5.27	1.56	1.46

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	SER	N-CA-CB	-18.65	82.52	110.50
1	B	2	SER	O-C-N	-18.46	93.17	122.70
1	B	3	VAL	CB-CA-C	-18.16	76.90	111.40
1	B	3	VAL	N-CA-C	17.53	158.33	111.00
1	B	2	SER	N-CA-C	14.51	150.18	111.00
1	B	3	VAL	CA-CB-CG1	13.19	130.69	110.90
1	B	3	VAL	O-C-N	-11.64	104.07	122.70
1	B	2	SER	CA-CB-OG	-11.51	80.11	111.20
1	B	3	VAL	CA-C-N	9.62	138.37	117.20
1	A	603	MET	N-CA-C	8.89	135.00	111.00
1	B	2	SER	C-N-CA	7.74	141.06	121.70
1	B	2	SER	CA-C-N	5.37	129.02	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	SER	Mainchain
1	B	3	VAL	Mainchain

## 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	4797	0	4789	158	0
1	B	4719	0	4710	198	4
2	A	8	0	2	0	0
2	B	8	0	2	0	0
3	A	44	0	27	2	0
3	B	44	0	27	3	0
4	A	335	0	0	13	4
4	B	380	0	0	19	0
All	All	10335	0	9557	352	4

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 (352) 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:3:VAL:CG1	1:B:3:VAL:CB	1.75	1.54
1:B:2:SER:C	1:B:2:SER:CA	1.81	1.47
1:B:3:VAL:CA	1:B:3:VAL:CB	1.92	1.44
1:B:2:SER:N	1:B:2:SER:CA	1.80	1.43
1:B:2:SER:CB	1:B:581:THR:OG1	1.72	1.36
1:B:2:SER:OG	1:B:581:THR:OG1	1.58	1.16
1:B:3:VAL:CA	1:B:3:VAL:N	2.14	1.10
1:B:2:SER:HB2	1:B:581:THR:OG1	1.47	1.09
1:B:2:SER:HB2	1:B:581:THR:CB	1.85	1.04
1:B:2:SER:N	1:B:2:SER:CB	2.19	1.04
1:B:3:VAL:C	1:B:3:VAL:CA	2.28	1.02
1:B:2:SER:C	1:B:2:SER:HA	1.77	1.01
1:B:2:SER:CB	1:B:581:THR:HG1	1.64	0.98
1:B:571:ASN:HD21	1:B:573:GLU:HG2	1.27	0.97
1:B:2:SER:HB2	1:B:581:THR:CG2	1.96	0.94
1:B:383:ASP:N	1:B:383:ASP:OD1	1.98	0.94
1:B:573:GLU:OE2	4:B:1226:HOH:O	1.86	0.93
1:B:3:VAL:HA	1:B:3:VAL:N	1.84	0.92
1:A:200:LEU:HG	1:A:214:CYS:HB3	1.50	0.92
1:B:3:VAL:HB	1:B:3:VAL:CA	1.98	0.91
1:B:571:ASN:ND2	1:B:573:GLU:HG2	1.86	0.90
1:A:343:MET:HE3	1:A:353:ALA:HB1	1.54	0.90
1:B:200:LEU:HG	1:B:214:CYS:HB3	1.54	0.90
1:A:127:THR:HB	1:A:128:PRO:HD3	1.56	0.88
1:B:3:VAL:N	1:B:581:THR:O	2.08	0.86
1:B:571:ASN:HD21	1:B:573:GLU:CG	1.89	0.85
1:B:3:VAL:CG1	1:B:3:VAL:CG2	2.54	0.85
1:B:2:SER:HB2	1:B:581:THR:HG23	1.57	0.84
1:B:2:SER:C	1:B:2:SER:OG	2.14	0.84
1:B:3:VAL:HB	1:B:3:VAL:CG1	2.06	0.84
1:B:517:ASP:O	1:B:520:LYS:HG2	1.77	0.84
1:A:587:GLN:NE2	1:A:590:ARG:HD3	1.95	0.81
1:B:384:MET:HB2	1:B:385:PRO:HD2	1.60	0.81
1:A:384:MET:HB2	1:A:385:PRO:HD2	1.64	0.80
1:B:127:THR:HB	1:B:128:PRO:CD	2.12	0.80
1:B:2:SER:HB3	1:B:2:SER:N	1.97	0.80
1:B:408:VAL:HG23	1:B:411:ALA:HB2	1.64	0.78
1:A:182:ILE:HD12	1:A:188:LEU:HD12	1.64	0.78
1:B:3:VAL:N	4:B:943:HOH:O	2.18	0.77
1:A:127:THR:HB	1:A:128:PRO:CD	2.14	0.77
1:B:319:SER:HB2	1:B:348:ILE:HD12	1.66	0.77
1:A:195:ILE:HB	1:A:196:PRO:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:CB	1:A:128:PRO:HD3	2.16	0.75
1:A:398:ARG:HB3	1:A:423:ILE:HG21	1.67	0.75
1:B:282:LEU:O	1:B:286:GLN:HB2	1.89	0.72
1:A:342:GLN:O	1:A:346:GLU:HG3	1.89	0.72
1:A:47:ARG:HG2	1:A:107:GLU:OE2	1.90	0.72
1:A:518:SER:HB2	1:A:523:ARG:HD2	1.71	0.71
1:A:326:PHE:HE2	1:A:408:VAL:HG21	1.55	0.71
1:A:182:ILE:HD12	1:A:188:LEU:HB2	1.73	0.70
1:B:450:THR:O	1:B:451:ASN:HB2	1.90	0.70
1:A:3:VAL:CG1	1:A:7:GLU:HB2	2.21	0.69
1:B:2:SER:C	4:B:943:HOH:O	2.29	0.69
1:B:340:VAL:HA	1:B:343:MET:HE2	1.75	0.69
1:A:319:SER:HB2	1:A:348:ILE:HD12	1.75	0.68
1:B:398:ARG:HH21	1:B:423:ILE:HG12	1.59	0.68
1:B:333:THR:O	1:B:337:GLU:HG3	1.94	0.67
1:B:3:VAL:C	1:B:3:VAL:CB	2.63	0.67
1:A:442:THR:OG1	1:A:445:GLU:HG3	1.93	0.67
1:B:407:THR:N	4:B:942:HOH:O	2.28	0.67
1:B:3:VAL:HG13	1:B:4:ALA:N	2.09	0.67
1:B:505:LEU:HD21	1:B:541:GLU:HB3	1.76	0.67
1:B:326:PHE:HE2	1:B:408:VAL:HG21	1.60	0.66
1:B:363:ASP:HB2	1:B:370:ARG:HH12	1.60	0.66
1:B:332:SER:OG	1:B:405:ALA:HB3	1.96	0.66
1:B:182:ILE:HD12	1:B:188:LEU:HB2	1.76	0.66
1:B:573:GLU:CD	4:B:1226:HOH:O	2.30	0.66
1:B:365:LEU:HB3	4:B:1053:HOH:O	1.96	0.66
1:A:182:ILE:CD1	1:A:188:LEU:HD12	2.26	0.66
1:B:2:SER:CB	1:B:581:THR:CG2	2.73	0.65
1:A:275:ASN:HB2	1:A:276:PRO:HD3	1.77	0.65
1:A:46:PRO:HG3	1:A:104:ASP:O	1.96	0.65
1:B:373:MET:HE1	1:B:381:ALA:HB2	1.78	0.65
1:A:300:ALA:HB1	1:A:338:MET:HG3	1.78	0.65
1:A:123:PRO:O	1:A:128:PRO:HD2	1.97	0.65
1:B:406:SER:OG	1:B:408:VAL:HG22	1.97	0.64
1:A:3:VAL:HG13	1:A:7:GLU:HB2	1.79	0.64
1:B:407:THR:O	1:B:407:THR:HG22	1.98	0.64
1:B:571:ASN:CG	1:B:573:GLU:HG2	2.19	0.63
1:A:321:GLU:OE2	1:A:400:GLY:HA3	1.98	0.63
1:B:348:ILE:CG2	1:B:352:GLU:HB2	2.28	0.63
1:B:47:ARG:HG3	1:B:107:GLU:OE2	1.99	0.62
1:B:127:THR:HB	1:B:128:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:VAL:O	1:B:521:VAL:HG12	2.00	0.62
1:B:56:LEU:O	1:B:60:GLN:HG3	2.00	0.62
1:A:319:SER:HB2	1:A:348:ILE:CD1	2.30	0.61
1:A:127:THR:CG2	1:A:128:PRO:HD3	2.30	0.61
1:A:450:THR:HG21	1:A:454:ALA:HB2	1.83	0.61
1:A:280:ARG:NH1	1:A:280:ARG:HB3	2.16	0.61
1:A:406:SER:OG	1:A:408:VAL:HG22	2.01	0.61
1:B:450:THR:HG21	1:B:454:ALA:N	2.16	0.60
1:B:571:ASN:OD1	1:B:573:GLU:HG2	2.01	0.60
1:A:412:PHE:HB2	1:A:441:CYS:HB3	1.83	0.60
1:B:319:SER:HB2	1:B:348:ILE:CD1	2.31	0.60
1:A:406:SER:O	1:A:408:VAL:N	2.34	0.60
1:A:558:PRO:HG2	1:A:561:LEU:HD23	1.84	0.60
1:A:93:LEU:HD13	4:A:950:HOH:O	2.00	0.60
1:B:505:LEU:HD23	1:B:505:LEU:C	2.21	0.60
1:B:321:GLU:OE2	1:B:400:GLY:HA3	2.01	0.59
1:B:127:THR:CG2	1:B:128:PRO:HD3	2.32	0.59
1:B:46:PRO:HG3	1:B:104:ASP:O	2.02	0.59
1:A:41:GLU:HG3	4:A:958:HOH:O	2.03	0.59
1:B:195:ILE:HB	1:B:196:PRO:HD3	1.83	0.58
1:A:408:VAL:HG23	1:A:408:VAL:O	2.03	0.58
1:B:413:ASN:HB2	4:B:1103:HOH:O	2.03	0.58
1:A:318:VAL:HG23	4:A:1229:HOH:O	2.03	0.58
1:B:127:THR:CB	1:B:128:PRO:CD	2.80	0.58
1:A:537:GLN:HG3	4:A:1144:HOH:O	2.03	0.58
1:B:348:ILE:HG22	1:B:349:SER:N	2.19	0.58
1:A:331:ALA:O	1:A:335:ILE:HG13	2.03	0.58
1:A:461:PRO:HG3	1:A:476:GLN:CD	2.24	0.58
1:A:147:LEU:HD12	1:A:215:LEU:HD11	1.85	0.58
1:B:106:ASN:HD22	1:B:106:ASN:C	2.06	0.57
1:B:84:THR:O	1:B:88:GLU:HG3	2.04	0.57
1:A:123:PRO:HA	1:A:127:THR:HB	1.86	0.57
1:B:558:PRO:HG2	1:B:561:LEU:HD23	1.86	0.57
1:A:465:PHE:CE2	1:A:467:LEU:HB2	2.40	0.57
1:A:210:GLN:HB2	1:A:213:TRP:CD2	2.40	0.57
1:A:417:ILE:HD12	1:A:449:PHE:HD1	1.70	0.57
1:A:419:ALA:O	1:A:423:ILE:HD12	2.05	0.57
1:B:348:ILE:CG2	1:B:349:SER:N	2.68	0.57
1:B:464:ASN:OD1	1:B:473:LYS:HG2	2.05	0.56
1:B:2:SER:CB	1:B:581:THR:HG23	2.33	0.56
1:A:127:THR:CB	1:A:128:PRO:CD	2.80	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:ND2	1:A:243:ARG:HH21	2.03	0.56
1:B:182:ILE:HD12	1:B:188:LEU:HD12	1.87	0.56
1:B:360:MET:SD	1:B:393:VAL:HG21	2.45	0.56
1:B:406:SER:O	1:B:408:VAL:N	2.31	0.56
1:B:3:VAL:CG1	1:B:7:GLU:HB2	2.35	0.56
1:B:371:LYS:O	1:B:372:GLU:HB2	2.06	0.56
1:B:450:THR:HG22	1:B:453:ALA:H	1.71	0.56
1:A:351:GLU:H	1:A:351:GLU:CD	2.09	0.56
1:A:308:LEU:O	1:A:311:THR:HB	2.06	0.56
1:B:127:THR:CB	1:B:128:PRO:HD3	2.36	0.56
1:B:412:PHE:HB2	1:B:441:CYS:HB3	1.87	0.56
1:A:332:SER:OG	1:A:405:ALA:HB3	2.06	0.55
1:A:300:ALA:O	1:A:304:VAL:HG23	2.06	0.55
1:A:587:GLN:HE21	1:A:590:ARG:HD3	1.71	0.55
1:B:408:VAL:HG23	1:B:408:VAL:O	2.06	0.55
1:A:182:ILE:HD12	1:A:188:LEU:CD1	2.36	0.55
1:B:204:VAL:HG11	1:B:211:PRO:HG3	1.88	0.55
1:B:122:MET:N	1:B:123:PRO:HD2	2.21	0.55
1:A:300:ALA:CB	1:A:338:MET:HG3	2.37	0.55
1:B:300:ALA:HB1	1:B:338:MET:HG3	1.89	0.55
1:B:348:ILE:HG23	1:B:352:GLU:HB2	1.89	0.55
1:B:366:VAL:HA	1:B:370:ARG:HE	1.71	0.55
1:A:523:ARG:HG3	1:A:523:ARG:HH21	1.71	0.54
1:B:340:VAL:HG12	1:B:344:GLN:HE21	1.73	0.54
1:A:193:ILE:O	1:A:196:PRO:HD2	2.06	0.54
1:B:18:ASP:HB3	1:B:21:GLU:OE2	2.07	0.54
1:A:182:ILE:CD1	1:A:188:LEU:HB2	2.36	0.54
1:A:42:LEU:HD23	1:A:42:LEU:C	2.28	0.54
1:B:127:THR:HG22	1:B:128:PRO:HD3	1.90	0.54
1:A:329:GLY:HA3	3:A:920:NAI:O5B	2.08	0.54
1:B:418:ARG:O	1:B:422:GLU:HG3	2.08	0.53
1:A:224:ASN:HD21	1:A:243:ARG:HH21	1.56	0.53
1:B:339:ILE:HG22	1:B:343:MET:CE	2.37	0.53
1:A:348:ILE:HG22	1:A:349:SER:N	2.23	0.53
1:A:182:ILE:HA	1:A:272:ASP:OD2	2.07	0.53
1:A:408:VAL:HG23	1:A:411:ALA:HB2	1.90	0.53
1:A:301:SER:HA	1:A:338:MET:HE2	1.90	0.53
1:B:342:GLN:O	1:B:346:GLU:HG3	2.08	0.53
1:B:461:PRO:HB3	1:B:476:GLN:NE2	2.24	0.53
1:A:521:VAL:HG12	1:A:521:VAL:O	2.09	0.53
1:A:587:GLN:HE22	1:A:590:ARG:HD3	1.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ASN:C	1:B:549:ASN:HD22	2.11	0.53
1:A:340:VAL:O	1:A:344:GLN:HG3	2.09	0.52
1:B:123:PRO:HA	1:B:127:THR:HB	1.90	0.52
1:A:444:GLU:HG3	1:A:465:PHE:CE1	2.45	0.52
1:A:584:TRP:HB2	1:A:589:MET:HG2	1.91	0.52
1:B:224:ASN:HD21	1:B:243:ARG:HH21	1.58	0.52
1:A:20:LYS:HD2	4:A:1054:HOH:O	2.08	0.52
1:A:408:VAL:HG11	3:A:920:NAI:N6A	2.25	0.52
1:B:182:ILE:CD1	1:B:188:LEU:HD12	2.38	0.52
1:B:362:ILE:HG12	3:B:930:NAI:O2B	2.09	0.52
1:B:3:VAL:C	1:B:3:VAL:CG1	2.77	0.52
1:B:406:SER:C	1:B:408:VAL:H	2.13	0.52
1:A:398:ARG:HB3	1:A:423:ILE:CG2	2.38	0.52
1:B:321:GLU:HG3	1:B:322:LYS:N	2.24	0.52
1:B:350:LYS:HE2	1:B:379:GLN:OE1	2.10	0.52
1:A:280:ARG:HD3	4:A:1172:HOH:O	2.09	0.52
1:B:452:GLY:HA3	1:B:472:TYR:OH	2.10	0.52
1:A:66:GLY:HA3	1:B:162:ILE:HG23	1.93	0.51
1:B:243:ARG:HG2	4:B:1132:HOH:O	2.10	0.51
1:B:300:ALA:CB	1:B:338:MET:HG3	2.40	0.51
1:A:505:LEU:C	1:A:505:LEU:HD23	2.31	0.51
1:B:91:ASN:HB2	4:B:1203:HOH:O	2.11	0.51
1:B:564:TYR:O	1:B:568:GLN:HG2	2.10	0.51
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.75	0.51
1:B:530:GLU:O	1:B:534:ILE:HG13	2.11	0.51
1:A:282:LEU:HA	1:A:291:MET:CE	2.41	0.51
1:B:450:THR:HG21	1:B:454:ALA:HB2	1.92	0.51
1:A:18:ASP:OD1	1:A:19:GLU:N	2.44	0.50
1:B:2:SER:HB2	1:B:581:THR:N	2.26	0.50
1:B:3:VAL:CA	1:B:3:VAL:CG2	2.80	0.50
1:B:3:VAL:HG13	1:B:7:GLU:HB2	1.92	0.50
1:A:339:ILE:O	1:A:343:MET:HG3	2.11	0.50
1:B:139:TYR:HB2	1:B:235:ILE:HG12	1.94	0.50
1:A:505:LEU:HD21	1:A:541:GLU:HB3	1.93	0.50
1:B:561:LEU:O	1:B:565:VAL:HG23	2.11	0.49
1:A:388:THR:O	1:A:388:THR:HG22	2.11	0.49
1:A:200:LEU:HD23	1:A:216:PRO:HG3	1.95	0.49
1:A:461:PRO:HG3	1:A:476:GLN:OE1	2.12	0.49
1:B:352:GLU:O	1:B:356:ARG:HG3	2.13	0.49
1:A:480:ALA:HA	1:A:483:PHE:CE2	2.48	0.49
1:B:76:GLU:HG2	4:B:1302:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:CG1	1:B:3:VAL:HG21	2.42	0.48
1:A:291:MET:HG2	1:A:292:PHE:N	2.27	0.48
1:B:401:ALA:CB	1:B:428:ILE:HB	2.42	0.48
1:A:473:LYS:HG3	1:A:521:VAL:HG11	1.95	0.48
1:A:100:ASP:OD2	1:A:142:ARG:HD3	2.13	0.48
1:A:343:MET:HE3	1:A:353:ALA:CB	2.37	0.48
1:B:210:GLN:HB2	1:B:213:TRP:CD2	2.48	0.48
1:A:348:ILE:CG2	1:A:349:SER:N	2.77	0.48
1:A:408:VAL:CG2	1:A:411:ALA:HB2	2.44	0.48
1:B:340:VAL:HA	1:B:343:MET:CE	2.42	0.48
1:B:360:MET:HG2	1:B:365:LEU:HA	1.96	0.48
1:A:523:ARG:NH2	1:A:523:ARG:HG3	2.29	0.47
1:B:42:LEU:C	1:B:42:LEU:HD23	2.34	0.47
1:B:86:LEU:HD13	1:B:98:GLN:NE2	2.28	0.47
1:A:182:ILE:HD12	1:A:188:LEU:CB	2.43	0.47
1:A:406:SER:C	1:A:408:VAL:H	2.17	0.47
1:B:326:PHE:HE2	1:B:408:VAL:CG2	2.27	0.47
1:B:549:ASN:C	1:B:549:ASN:ND2	2.68	0.47
1:B:483:PHE:CG	1:B:484:PRO:HD3	2.49	0.47
1:B:37:LYS:NZ	1:B:45:GLU:OE2	2.48	0.47
1:B:466:GLU:HA	1:B:470:HIS:O	2.15	0.47
1:A:348:ILE:HG22	1:A:349:SER:O	2.14	0.47
1:A:73:MET:HE2	4:A:1182:HOH:O	2.14	0.47
1:B:326:PHE:CE2	1:B:408:VAL:HG21	2.47	0.47
1:A:93:LEU:HB3	1:A:137:PHE:HZ	1.78	0.47
1:A:127:THR:HG22	1:A:128:PRO:HD3	1.95	0.47
1:A:280:ARG:CB	1:A:280:ARG:HH11	2.28	0.47
1:A:389:SER:HB3	1:A:392:GLU:HG3	1.95	0.47
1:A:417:ILE:HG21	1:A:449:PHE:HB2	1.97	0.47
1:B:224:ASN:ND2	1:B:243:ARG:HH21	2.12	0.47
1:A:389:SER:CB	1:A:392:GLU:HG3	2.44	0.47
1:A:394:ILE:O	1:A:398:ARG:N	2.43	0.47
1:B:300:ALA:HA	1:B:335:ILE:HG12	1.97	0.47
1:A:590:ARG:NH2	1:A:594:PRO:HA	2.30	0.47
1:B:473:LYS:HD2	1:B:521:VAL:HG11	1.97	0.47
1:A:136:ASN:N	1:A:136:ASN:HD22	2.14	0.46
1:B:348:ILE:HG22	1:B:349:SER:O	2.14	0.46
1:A:122:MET:N	1:A:123:PRO:HD2	2.29	0.46
1:B:141:TYR:HA	4:B:1108:HOH:O	2.15	0.46
1:B:341:HIS:CD2	1:B:345:ASN:HD21	2.33	0.46
1:A:131:GLY:C	1:A:185:LEU:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PHE:HZ	1:B:339:ILE:HD12	1.80	0.46
1:A:452:GLY:HA3	1:A:472:TYR:OH	2.15	0.46
1:B:370:ARG:HB3	1:B:373:MET:HB3	1.97	0.46
1:B:367:THR:HA	1:B:382:LYS:O	2.16	0.46
1:A:584:TRP:HB2	1:A:589:MET:CG	2.45	0.46
1:B:118:VAL:HG13	1:B:119:LYS:N	2.30	0.46
1:B:85:LYS:O	1:B:89:GLN:HG2	2.15	0.46
1:A:42:LEU:O	1:A:42:LEU:HD23	2.16	0.45
1:B:408:VAL:CG2	1:B:411:ALA:HB2	2.40	0.45
1:A:545:TYR:HB2	4:A:1179:HOH:O	2.15	0.45
1:B:359:LEU:O	1:B:365:LEU:HD12	2.16	0.45
1:B:358:TYR:CD1	1:B:358:TYR:N	2.85	0.45
1:A:517:ASP:HA	1:A:520:LYS:HE2	1.98	0.45
1:A:547:TYR:CE1	1:A:557:GLN:HG3	2.52	0.45
1:A:473:LYS:HD3	1:A:523:ARG:HH11	1.81	0.45
1:B:329:GLY:HA3	3:B:930:NAI:O5B	2.17	0.45
1:B:546:CYS:HA	1:B:549:ASN:ND2	2.32	0.45
1:A:460:SER:HA	1:A:461:PRO:HD3	1.82	0.45
1:A:342:GLN:OE1	1:A:504:LEU:HG	2.17	0.45
1:A:587:GLN:O	1:A:590:ARG:HG2	2.17	0.45
1:B:339:ILE:HG22	1:B:343:MET:HE1	1.99	0.45
1:A:280:ARG:CB	1:A:280:ARG:NH1	2.80	0.44
1:B:437:SER:HB3	4:B:1305:HOH:O	2.17	0.44
1:A:373:MET:HE1	1:A:381:ALA:HB2	2.00	0.44
1:A:414:GLU:O	1:A:418:ARG:HG2	2.17	0.44
1:A:466:GLU:HA	4:A:1027:HOH:O	2.16	0.44
1:B:384:MET:HB2	1:B:385:PRO:CD	2.40	0.44
1:B:182:ILE:HA	1:B:272:ASP:OD2	2.17	0.44
1:B:409:ARG:HD2	1:B:437:SER:O	2.18	0.44
1:B:224:ASN:ND2	1:B:243:ARG:NH2	2.65	0.44
1:A:461:PRO:HG3	1:A:476:GLN:HG2	1.98	0.44
1:A:302:VAL:HG21	1:A:478:ASN:O	2.17	0.44
1:B:207:GLY:O	1:B:488:LEU:HD22	2.17	0.44
1:A:182:ILE:HD12	1:A:188:LEU:CG	2.48	0.43
1:A:218:LEU:HD23	1:A:218:LEU:C	2.39	0.43
1:A:461:PRO:HG3	1:A:476:GLN:CG	2.47	0.43
1:A:358:TYR:CD2	1:A:382:LYS:HG3	2.54	0.43
1:B:118:VAL:HG13	1:B:119:LYS:H	1.84	0.43
1:B:2:SER:HA	4:B:943:HOH:O	2.17	0.43
1:B:2:SER:HB2	1:B:581:THR:CA	2.46	0.43
1:A:93:LEU:HD11	1:A:132:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:HG2	1:A:274:ALA:HB2	2.00	0.43
1:B:473:LYS:H	1:B:521:VAL:HG12	1.82	0.43
1:A:345:ASN:HD22	1:A:504:LEU:HD23	1.83	0.43
1:B:557:GLN:NE2	4:B:1008:HOH:O	2.52	0.43
1:A:498:VAL:HG12	1:A:503:PHE:CE1	2.54	0.43
1:B:122:MET:N	1:B:123:PRO:CD	2.82	0.43
1:A:93:LEU:HB3	1:A:137:PHE:CZ	2.53	0.42
1:B:408:VAL:HG11	3:B:930:NAI:N6A	2.33	0.42
1:B:584:TRP:HB2	1:B:589:MET:HG2	2.00	0.42
1:A:321:GLU:HG3	1:A:322:LYS:N	2.34	0.42
1:A:326:PHE:HE2	1:A:408:VAL:CG2	2.28	0.42
1:B:505:LEU:HD23	1:B:505:LEU:O	2.18	0.42
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.85	0.42
1:A:373:MET:CE	1:A:381:ALA:HB2	2.49	0.42
1:B:55:SER:O	1:B:59:ARG:HG3	2.20	0.42
1:B:460:SER:HB3	1:B:461:PRO:HD2	2.01	0.42
1:B:286:GLN:HG3	4:B:948:HOH:O	2.19	0.42
1:B:366:VAL:O	1:B:381:ALA:HA	2.19	0.42
1:B:389:SER:O	1:B:393:VAL:HG23	2.19	0.42
1:B:429:ILE:O	1:B:456:TYR:HA	2.19	0.42
1:A:131:GLY:C	1:A:185:LEU:HD11	2.40	0.42
1:B:495:ILE:HD13	1:B:546:CYS:SG	2.59	0.42
1:A:162:ILE:HG23	1:B:66:GLY:HA3	2.01	0.42
1:A:207:GLY:O	1:A:488:LEU:HD22	2.19	0.42
1:A:243:ARG:HG2	4:A:1021:HOH:O	2.19	0.42
1:A:587:GLN:CB	4:A:1200:HOH:O	2.67	0.42
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.90	0.42
1:A:172:ARG:HB2	1:A:213:TRP:HB3	2.02	0.42
1:A:464:ASN:OD1	1:A:473:LYS:HG2	2.19	0.42
1:B:473:LYS:CG	1:B:521:VAL:HG11	2.50	0.42
1:A:168:GLU:HG2	1:A:212:LYS:O	2.20	0.42
1:B:406:SER:C	4:B:942:HOH:O	2.57	0.42
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.94	0.41
1:A:69:PRO:HB3	1:B:235:ILE:HD13	2.01	0.41
1:A:550:GLY:HA2	4:A:1051:HOH:O	2.20	0.41
1:B:224:ASN:HD21	1:B:243:ARG:NH2	2.17	0.41
1:A:37:LYS:NZ	1:A:45:GLU:OE2	2.53	0.41
1:A:427:PRO:HG2	1:A:454:ALA:HA	2.01	0.41
1:B:182:ILE:CD1	1:B:188:LEU:HB2	2.48	0.41
1:A:244:GLY:HA3	4:A:983:HOH:O	2.19	0.41
1:B:130:VAL:HG13	1:B:131:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:SER:OG	1:B:351:GLU:HB2	2.21	0.41
1:B:182:ILE:HD12	1:B:188:LEU:CB	2.48	0.41
1:B:387:THR:OG1	1:B:388:THR:N	2.53	0.41
1:A:89:GLN:HA	1:A:90:PRO:HD3	1.84	0.41
1:A:473:LYS:HB3	1:A:523:ARG:NH1	2.35	0.41
1:B:338:MET:HE1	1:B:504:LEU:HD12	2.03	0.41
1:B:379:GLN:HB3	4:B:1295:HOH:O	2.20	0.41
1:B:3:VAL:HG11	1:B:7:GLU:HB2	2.01	0.41
1:A:375:PRO:O	1:A:378:VAL:HG23	2.21	0.41
1:B:440:GLU:N	1:B:440:GLU:OE1	2.50	0.41
1:B:448:THR:C	1:B:450:THR:H	2.24	0.41
1:B:450:THR:O	1:B:451:ASN:CB	2.62	0.41
1:A:84:THR:O	1:A:88:GLU:HG3	2.22	0.40
1:A:343:MET:HE1	1:A:353:ALA:O	2.21	0.40
1:B:316:LYS:NZ	4:B:1088:HOH:O	2.54	0.40
1:A:590:ARG:HG3	1:A:590:ARG:O	2.21	0.40
1:B:175:VAL:CG2	1:B:200:LEU:HD13	2.51	0.40
1:B:407:THR:HG23	4:B:1065:HOH:O	2.20	0.40
1:B:200:LEU:HD23	1:B:216:PRO:HG3	2.03	0.40
1:A:235:ILE:HD13	1:B:69:PRO:HB3	2.04	0.40
1:A:130:VAL:HG13	1:A:131:GLY:N	2.35	0.40
1:B:414:GLU:O	1:B:418:ARG:HG2	2.22	0.40
1:B:549:ASN:HD22	1:B:550:GLY:N	2.20	0.40

All (4) 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:B:2:SER:N	4:A:1058:HOH:O[4_556]	1.39	0.81
1:B:2:SER:CB	4:A:1058:HOH:O[4_556]	1.44	0.76
1:B:2:SER:CA	4:A:1058:HOH:O[4_556]	1.72	0.48
1:B:2:SER:OG	4:A:1058:HOH:O[4_556]	1.88	0.32

## 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	600/605 (99%)	568 (95%)	28 (5%)	4 (1%)	22	16
1	B	590/605 (98%)	560 (95%)	23 (4%)	7 (1%)	13	7
All	All	1190/1210 (98%)	1128 (95%)	51 (4%)	11 (1%)	17	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	THR
1	A	128	PRO
1	A	407	THR
1	B	127	THR
1	B	407	THR
1	A	371	LYS
1	B	244	GLY
1	B	449	PHE
1	B	10	TYR
1	B	128	PRO
1	B	378	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	515/517 (100%)	498 (97%)	17 (3%)	38	37
1	B	505/517 (98%)	490 (97%)	15 (3%)	41	41
All	All	1020/1034 (99%)	988 (97%)	32 (3%)	40	40

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ILE
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	128	PRO
1	A	167	HIS
1	A	200	LEU
1	A	237	LEU
1	A	265	LYS
1	A	269	GLN
1	A	280	ARG
1	A	355	ASN
1	A	432	LEU
1	A	504	LEU
1	A	549	ASN
1	A	553	ASN
1	A	601	ASP
1	A	603	MET
1	B	2	SER
1	B	13	ASN
1	B	18	ASP
1	B	93	LEU
1	B	99	LEU
1	B	106	ASN
1	B	140	ILE
1	B	167	HIS
1	B	200	LEU
1	B	269	GLN
1	B	355	ASN
1	B	362	ILE
1	B	383	ASP
1	B	432	LEU
1	B	549	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	136	ASN
1	A	320	GLN
1	A	341	HIS
1	A	345	ASN
1	A	355	ASN
1	A	468	ASN
1	A	549	ASN

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Mol	Chain	Res	Type
1	A	587	GLN
1	B	106	ASN
1	B	286	GLN
1	B	344	GLN
1	B	345	ASN
1	B	355	ASN
1	B	468	ASN
1	B	549	ASN
1	B	557	GLN
1	B	571	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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
2	TTN	A	810	-	1,7,7	0.49	0	0,9,9	0.00	-
2	TTN	B	815	-	1,7,7	0.31	0	0,9,9	0.00	-
3	NAI	A	920	-	42,48,48	3.41	12 (28%)	47,73,73	1.35	6 (12%)
3	NAI	B	930	-	42,48,48	2.86	12 (28%)	47,73,73	1.31	6 (12%)

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	TTN	A	810	-	-	0/0/8/8	-
2	TTN	B	815	-	-	0/0/8/8	-
3	NAI	A	920	-	-	5/25/72/72	0/5/5/5
3	NAI	B	930	-	-	6/25/72/72	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	920	NAI	C4A-N3A	17.77	1.60	1.35
3	B	930	NAI	C4A-N3A	14.66	1.55	1.35
3	A	920	NAI	C2A-N1A	5.85	1.44	1.33
3	B	930	NAI	C6N-C5N	5.11	1.42	1.33
3	A	920	NAI	C6N-C5N	5.02	1.42	1.33
3	A	920	NAI	C5A-C4A	4.98	1.54	1.40
3	A	920	NAI	C2A-N3A	4.16	1.38	1.32
3	B	930	NAI	C5A-C4A	4.02	1.51	1.40
3	B	930	NAI	C2A-N3A	3.30	1.37	1.32
3	A	920	NAI	C4N-C3N	-3.24	1.43	1.49
3	B	930	NAI	C2A-N1A	3.17	1.39	1.33
3	B	930	NAI	C4N-C3N	-3.03	1.44	1.49
3	A	920	NAI	PN-O2N	2.85	1.61	1.50
3	B	930	NAI	C2N-C3N	2.75	1.42	1.34
3	A	920	NAI	PA-O1A	2.73	1.60	1.50
3	B	930	NAI	C4N-C5N	-2.70	1.41	1.48
3	A	920	NAI	C2N-C3N	2.66	1.42	1.34
3	B	930	NAI	O4B-C1B	2.58	1.44	1.41
3	B	930	NAI	PA-O1A	2.54	1.59	1.50
3	B	930	NAI	C1D-N1N	2.52	1.53	1.46
3	B	930	NAI	PN-O2N	2.44	1.59	1.50
3	A	920	NAI	C4N-C5N	-2.44	1.42	1.48
3	A	920	NAI	O4B-C1B	2.20	1.44	1.41
3	A	920	NAI	C1D-N1N	2.18	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	930	NAI	PN-O3-PA	-4.90	116.00	132.83
3	A	920	NAI	PN-O3-PA	-4.76	116.48	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	920	NAI	C5A-C6A-N6A	3.73	126.02	120.35
3	A	920	NAI	O7N-C7N-N7N	-3.58	114.50	122.88
3	B	930	NAI	O7N-C7N-N7N	-3.47	114.76	122.88
3	B	930	NAI	C5A-C6A-N6A	3.16	125.16	120.35
3	B	930	NAI	C3N-C7N-N7N	2.46	122.04	117.67
3	A	920	NAI	C3N-C7N-N7N	2.42	121.96	117.67
3	A	920	NAI	C2A-N1A-C6A	2.40	122.86	118.75
3	A	920	NAI	N6A-C6A-N1A	-2.36	113.67	118.57
3	B	930	NAI	N6A-C6A-N1A	-2.29	113.82	118.57
3	B	930	NAI	C2A-N1A-C6A	2.04	122.24	118.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	930	NAI	C2D-C1D-N1N-C6N
3	A	920	NAI	C2D-C1D-N1N-C2N
3	A	920	NAI	C2D-C1D-N1N-C6N
3	B	930	NAI	C2D-C1D-N1N-C2N
3	B	930	NAI	O4B-C4B-C5B-O5B
3	A	920	NAI	O4D-C1D-N1N-C6N
3	B	930	NAI	O4D-C1D-N1N-C6N
3	A	920	NAI	O4D-C1D-N1N-C2N
3	B	930	NAI	O4D-C1D-N1N-C2N
3	B	930	NAI	C3B-C4B-C5B-O5B
3	A	920	NAI	O4B-C4B-C5B-O5B

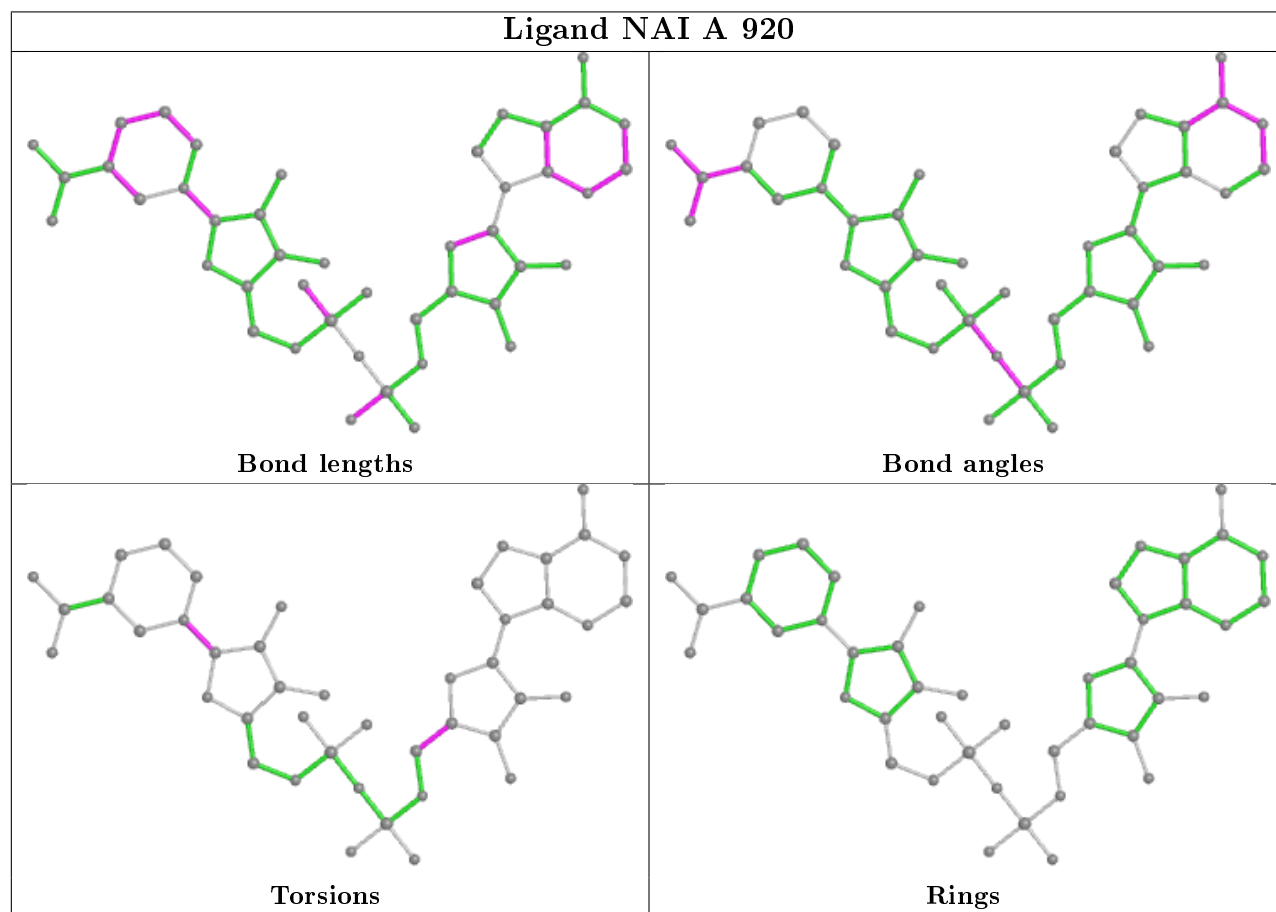
There are no ring outliers.

2 monomers are involved in 5 short contacts:

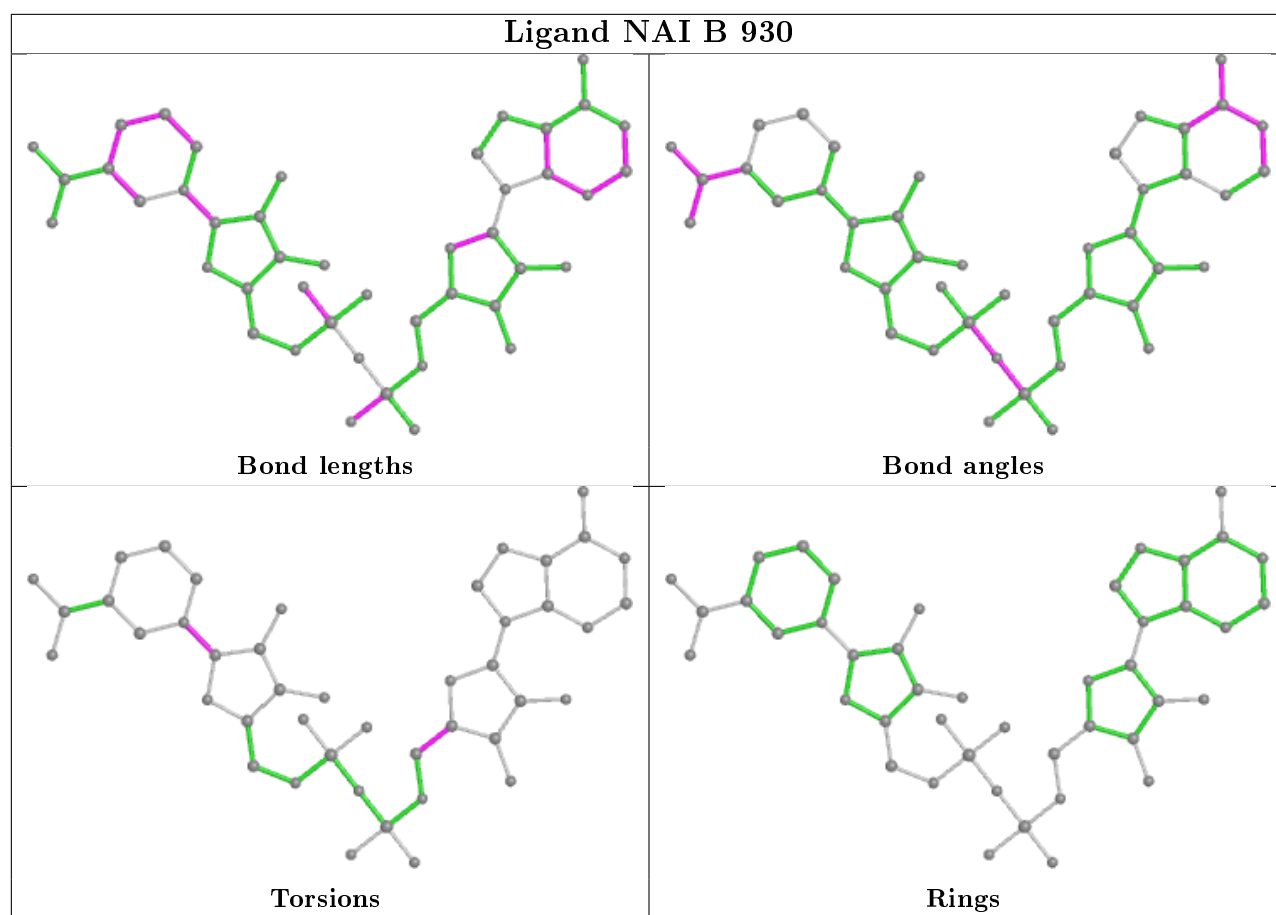
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	920	NAI	2	0
3	B	930	NAI	3	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	602/605 (99%)	-0.24	11 (1%) 68 66	19, 37, 65, 90	13 (2%)
1	B	592/605 (97%)	-0.17	23 (3%) 39 38	19, 34, 66, 88	11 (1%)
All	All	1194/1210 (98%)	-0.21	34 (2%) 53 51	19, 36, 66, 90	24 (2%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	8.9
1	B	383	ASP	4.8
1	B	369	ASN	3.7
1	B	385	PRO	3.7
1	B	470	HIS	3.7
1	A	468	ASN	3.6
1	B	467	LEU	3.3
1	B	3	VAL	3.3
1	A	603	MET	3.3
1	A	467	LEU	3.3
1	B	593	PHE	3.0
1	A	451	ASN	3.0
1	B	127	THR	2.9
1	B	416	VAL	2.9
1	B	592	GLY	2.7
1	A	470	HIS	2.6
1	A	127	THR	2.5
1	B	449	PHE	2.5
1	B	465	PHE	2.5
1	A	452	GLY	2.5
1	A	471	THR	2.4
1	B	451	ASN	2.3
1	B	386	GLU	2.3
1	B	466	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	384	MET	2.3
1	A	421	ALA	2.2
1	B	472	TYR	2.2
1	A	472	TYR	2.2
1	B	351	GLU	2.1
1	B	355	ASN	2.1
1	B	471	THR	2.1
1	A	466	GLU	2.0
1	B	378	VAL	2.0
1	B	347	GLY	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

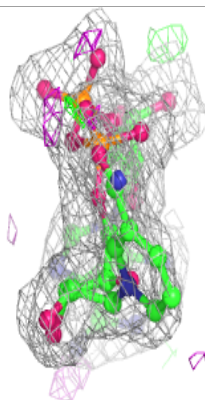
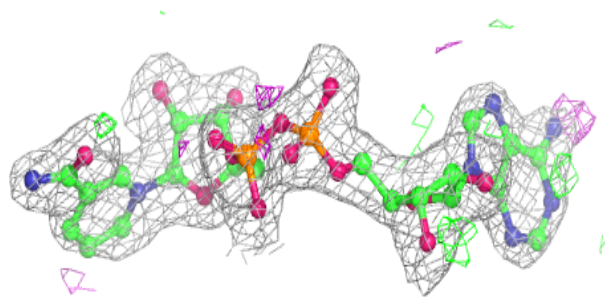
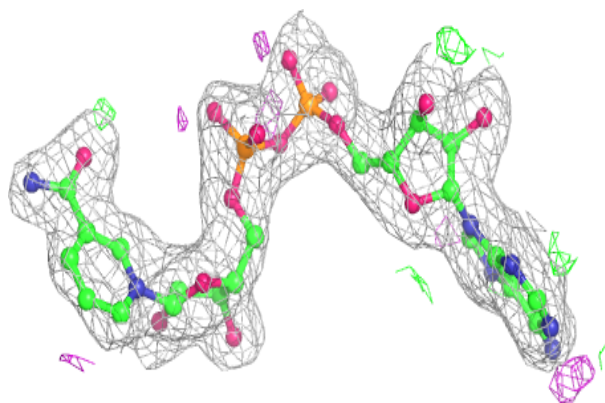
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	NAI	A	920	44/44	0.96	0.09	27,44,56,59	0
3	NAI	B	930	44/44	0.96	0.09	27,38,51,59	0
2	TTN	A	810	8/8	0.97	0.07	29,36,40,44	0
2	TTN	B	815	8/8	0.98	0.12	27,31,34,36	0

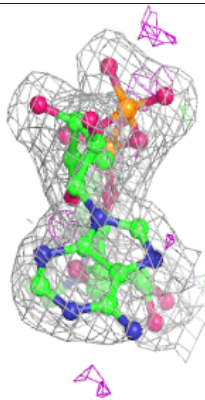
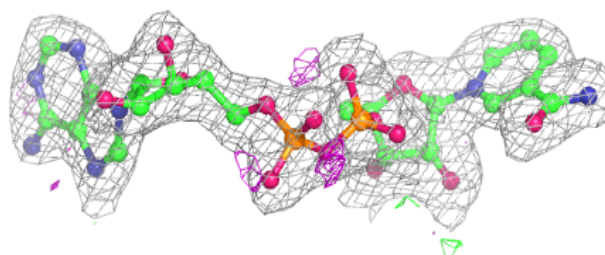
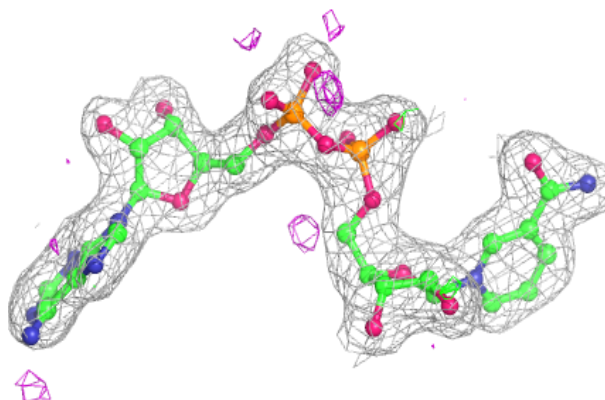
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAI A 920:**

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

**Electron density around NAI B 930:**

$2mF_o-DF_c$  (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.