Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 06:13 PM EDT

PDB ID	:	1NZZ
Title	:	Human mitochondrial aldehyde dehydrogenase complexed with NADH in the presence of low Mg2+
Authors	:	Perez-Miller, S.J.; Hurley, T.D.
Deposited on	:	2003-02-20
Resolution	:	2.45 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:

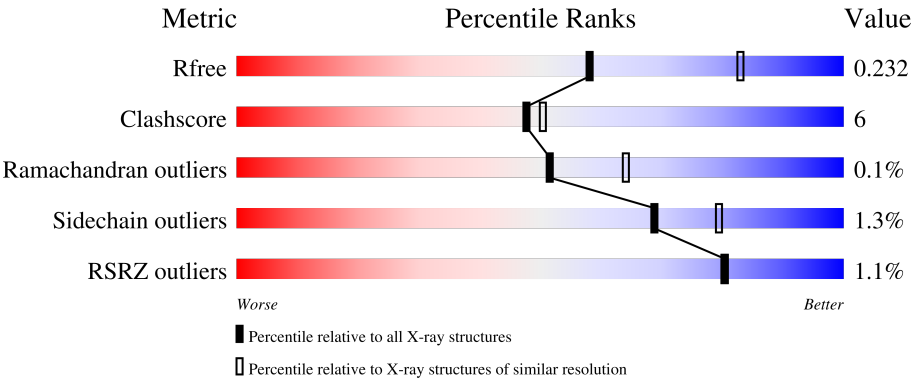
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	2% 83% 16%
1	B	500	84% 15%
1	C	500	84% 15%
1	D	500	2% 83% 16%
1	E	500	84% 14%

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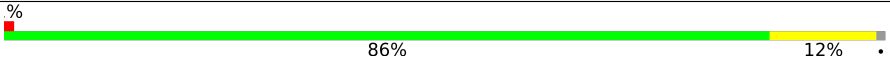
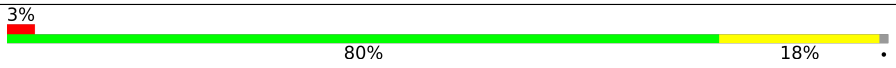
Mol	Chain	Length	Quality of chain
1	F	500	
1	G	500	
1	H	500	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32050 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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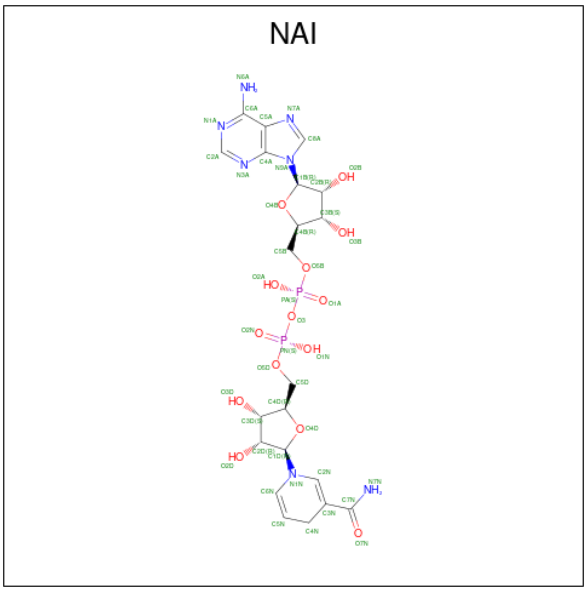
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

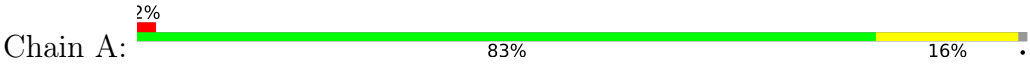
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total	O	0	0
			162	162		
5	B	164	Total	O	0	0
			164	164		
5	C	188	Total	O	0	0
			188	188		
5	D	137	Total	O	0	0
			137	137		
5	E	157	Total	O	0	0
			157	157		
5	F	206	Total	O	0	0
			206	206		
5	G	156	Total	O	0	0
			156	156		
5	H	128	Total	O	0	0
			128	128		

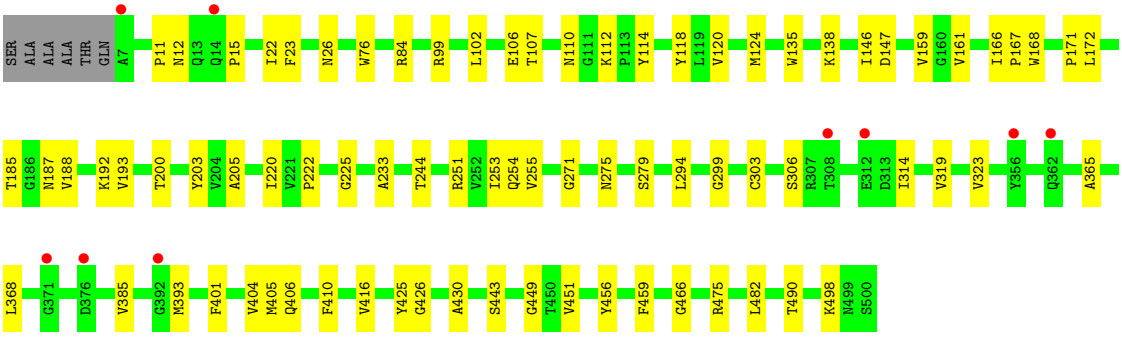
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Aldehyde dehydrogenase

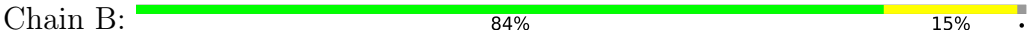
Chain A:

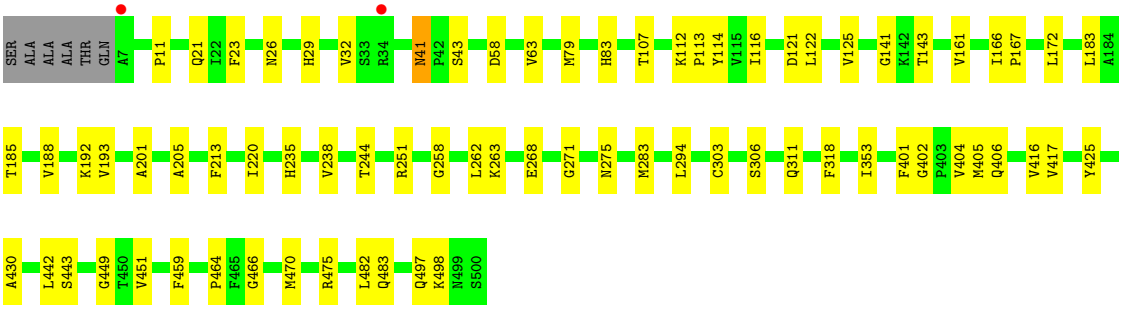




• Molecule 1: Aldehyde dehydrogenase

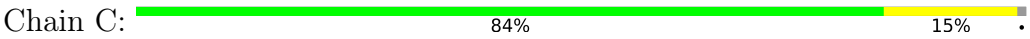
Chain B:

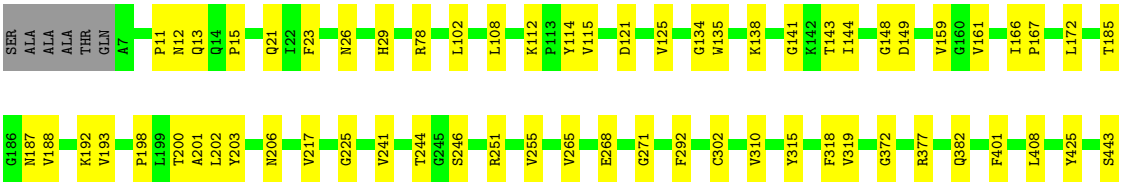




• Molecule 1: Aldehyde dehydrogenase

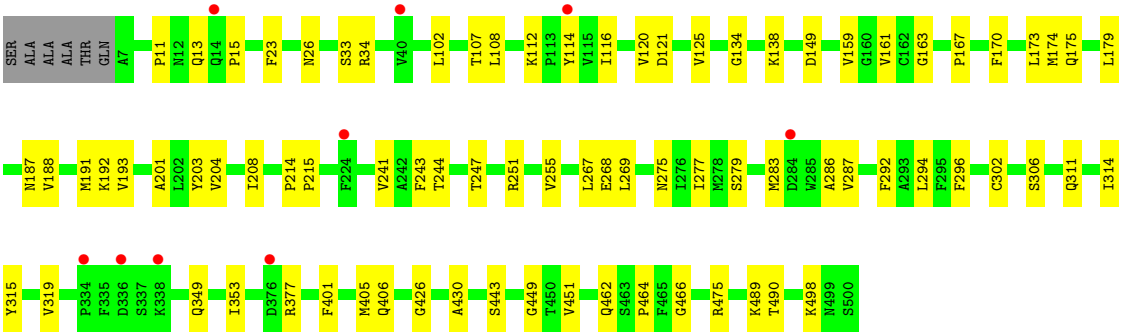
Chain C:





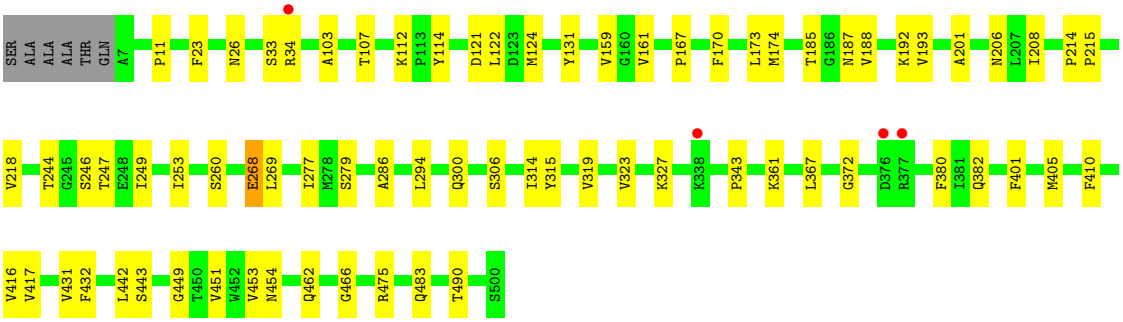
• Molecule 1: Aldehyde dehydrogenase

Chain D:



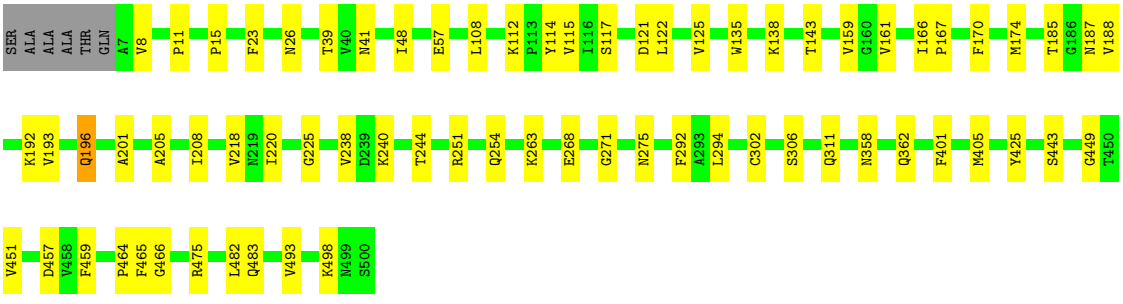
• Molecule 1: Aldehyde dehydrogenase

Chain E:



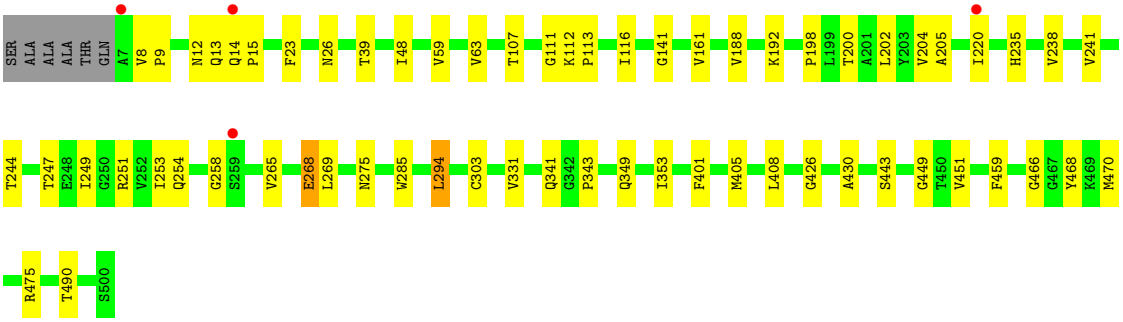
• Molecule 1: Aldehyde dehydrogenase

Chain F:



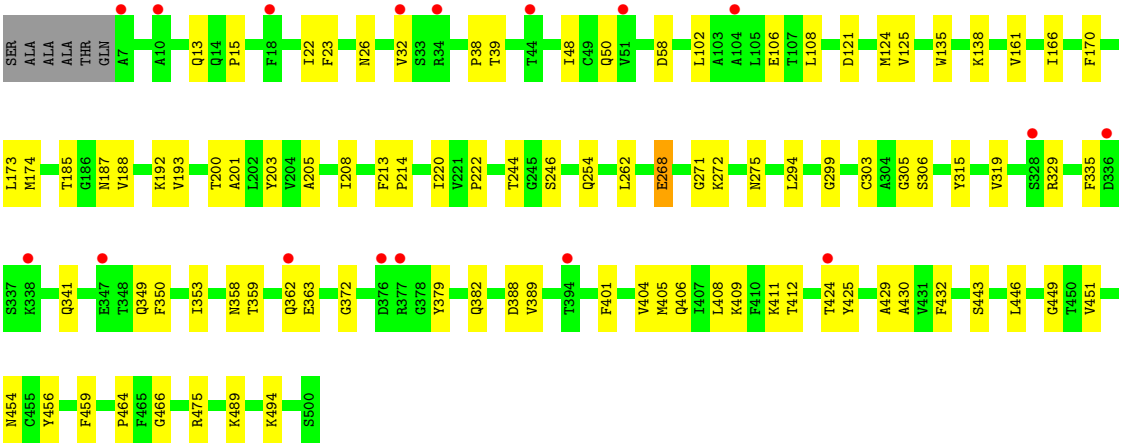
• Molecule 1: Aldehyde dehydrogenase

Chain G:



• Molecule 1: Aldehyde dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.31Å 150.90Å 177.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.45 21.99 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.0 (19.98-2.45) 94.1 (21.99-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.248 0.203 , 0.232	Depositor DCC
R_{free} test set	6568 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32050	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0271e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAI, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/3882	0.55	0/5267
1	B	0.37	0/3882	0.56	0/5267
1	C	0.39	0/3882	0.57	0/5267
1	D	0.36	0/3882	0.56	0/5267
1	E	0.38	0/3882	0.56	0/5267
1	F	0.39	0/3882	0.57	0/5267
1	G	0.38	0/3882	0.56	0/5267
1	H	0.39	0/3882	0.54	0/5267
All	All	0.38	0/31056	0.56	0/42136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3798	0	3745	49	0
1	B	3798	0	3745	49	0
1	C	3798	0	3745	49	0
1	D	3798	0	3745	46	0
1	E	3798	0	3745	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3745	50	0
1	G	3798	0	3745	39	0
1	H	3798	0	3745	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	27	1	0
4	B	44	0	27	1	0
4	C	44	0	27	4	0
4	D	44	0	27	1	0
4	E	44	0	27	2	0
4	F	44	0	27	3	0
4	G	44	0	27	0	0
4	H	44	0	27	1	0
5	A	162	0	0	0	0
5	B	164	0	0	2	0
5	C	188	0	0	2	0
5	D	137	0	0	2	0
5	E	157	0	0	0	0
5	F	206	0	0	4	0
5	G	156	0	0	0	0
5	H	128	0	0	1	0
All	All	32050	0	30176	370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (370) 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:F:196:GLN:H	1:F:196:GLN:HE21	1.19	0.90
1:A:404:VAL:HG12	1:A:406:GLN:HE22	1.47	0.78
1:D:311:GLN:HG3	5:D:4636:HOH:O	1.84	0.78
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.68	0.75
1:F:161:VAL:HA	1:F:188:VAL:HG23	1.69	0.75
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.69	0.75
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.69	0.73
1:H:358:ASN:O	1:H:362:GLN:HG2	1.89	0.73
1:H:38:PRO:HB3	1:H:50:GLN:HE22	1.55	0.72
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.72	0.71
1:A:102:LEU:HD21	1:A:203:TYR:HD2	1.54	0.71
1:E:361:LYS:HE2	1:E:367:LEU:HD22	1.74	0.70
1:D:294:LEU:HD12	1:D:306:SER:HA	1.74	0.69
1:G:275:ASN:ND2	1:G:430:ALA:HB3	2.09	0.67
1:D:283:MET:O	1:D:287:VAL:HG23	1.94	0.67
1:A:22:ILE:HG12	1:A:222:PRO:HD2	1.76	0.66
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.77	0.66
1:A:102:LEU:HD21	1:A:203:TYR:CD2	2.31	0.66
1:C:172:LEU:HD21	1:C:200:THR:HB	1.78	0.66
1:C:166:ILE:HD11	1:C:193:VAL:HG12	1.78	0.66
1:A:365:ALA:HB2	1:A:393:MET:HE2	1.78	0.65
1:A:294:LEU:HD12	1:A:306:SER:HA	1.79	0.65
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.78	0.65
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.80	0.64
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.27	0.64
1:D:161:VAL:HA	1:D:188:VAL:HG23	1.78	0.64
1:E:319:VAL:O	1:E:323:VAL:HG23	1.98	0.63
1:H:303:CYS:HG	1:H:459:PHE:HZ	1.47	0.63
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.79	0.63
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.35	0.62
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.34	0.62
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.80	0.62
1:G:470:MET:HE2	1:H:262:LEU:HD12	1.82	0.61
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.83	0.61
1:C:161:VAL:HA	1:C:188:VAL:HG23	1.83	0.60
1:A:365:ALA:HB2	1:A:393:MET:CE	2.31	0.60
1:B:275:ASN:ND2	1:B:430:ALA:HB3	2.16	0.60
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.37	0.60
1:D:247:THR:HA	1:D:269:LEU:HD13	1.83	0.59
1:H:15:PRO:HG2	1:H:108:LEU:HD22	1.84	0.59
1:A:319:VAL:O	1:A:323:VAL:HG23	2.02	0.59
1:F:166:ILE:HD11	1:F:193:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:MET:SD	1:B:83:HIS:HD2	2.26	0.58
1:C:292:PHE:HE1	1:C:457:ASP:HB2	1.69	0.58
1:C:167:PRO:HD3	1:C:244:THR:HB	1.85	0.57
1:A:172:LEU:HD21	1:A:200:THR:HB	1.86	0.57
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.27	0.57
1:G:258:GLY:CA	1:H:254:GLN:HG2	2.35	0.57
1:E:167:PRO:HD3	1:E:244:THR:HB	1.86	0.57
1:E:294:LEU:HD12	1:E:306:SER:HA	1.86	0.56
1:F:196:GLN:H	1:F:196:GLN:NE2	1.97	0.56
1:F:196:GLN:HE21	1:F:196:GLN:N	1.98	0.56
1:H:315:TYR:CG	1:H:409:LYS:HE2	2.40	0.56
1:G:59:VAL:O	1:G:63:VAL:HG23	2.06	0.56
1:G:443:SER:HA	1:G:451:VAL:HG11	1.88	0.56
1:D:121:ASP:O	1:D:125:VAL:HG23	2.06	0.56
1:H:166:ILE:HD11	1:H:193:VAL:HG12	1.88	0.56
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.88	0.56
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.88	0.56
1:A:225:GLY:HA3	4:A:1502:NAI:C8A	2.36	0.56
1:F:159:VAL:HG12	1:F:187:ASN:OD1	2.05	0.56
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.42	0.55
1:H:174:MET:HE1	5:H:8522:HOH:O	2.05	0.55
1:G:275:ASN:HD22	1:G:430:ALA:HB3	1.70	0.55
1:A:120:VAL:O	1:A:124:MET:HG3	2.06	0.55
1:F:167:PRO:HG3	1:F:244:THR:O	2.06	0.55
1:B:275:ASN:HD22	1:B:430:ALA:HB3	1.70	0.55
1:B:404:VAL:HG12	1:B:406:GLN:OE1	2.06	0.55
1:A:410:PHE:CD1	1:A:416:VAL:HB	2.41	0.55
1:C:241:VAL:HG12	1:C:265:VAL:HG22	1.87	0.55
1:C:271:GLY:HA2	1:C:425:TYR:CD2	2.41	0.55
1:H:294:LEU:HD12	1:H:306:SER:HA	1.89	0.55
1:G:247:THR:HA	1:G:269:LEU:HD13	1.88	0.55
1:C:449:GLY:HA3	1:C:466:GLY:O	2.07	0.55
1:G:241:VAL:CG1	1:G:265:VAL:HG22	2.37	0.54
1:A:404:VAL:HG12	1:A:406:GLN:NE2	2.19	0.54
1:B:63:VAL:HG21	1:B:235:HIS:CD2	2.42	0.54
1:E:161:VAL:HA	1:E:188:VAL:HG23	1.89	0.54
1:E:159:VAL:HG12	1:E:187:ASN:OD1	2.08	0.54
1:C:15:PRO:HG2	1:C:108:LEU:HD22	1.89	0.54
1:D:449:GLY:HA3	1:D:466:GLY:O	2.08	0.54
1:G:254:GLN:OE1	1:H:262:LEU:HD23	2.08	0.54
1:D:349:GLN:O	1:D:353:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:TRP:CZ2	1:H:494:LYS:HE3	2.43	0.54
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.43	0.54
1:G:449:GLY:HA3	1:G:466:GLY:O	2.08	0.53
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.43	0.53
1:B:41:ASN:C	1:B:41:ASN:HD22	2.12	0.53
1:B:483:GLN:HB3	5:B:2527:HOH:O	2.07	0.53
1:F:443:SER:HA	1:F:451:VAL:HG11	1.91	0.53
1:A:107:THR:HG23	1:A:112:LYS:O	2.09	0.53
1:E:279:SER:HA	1:E:314:ILE:HD13	1.90	0.53
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.44	0.53
1:B:107:THR:HG23	1:B:112:LYS:O	2.08	0.53
1:H:389:VAL:HB	1:H:408:LEU:HG	1.91	0.53
1:H:411:LYS:HG2	1:H:412:THR:HG23	1.91	0.53
1:C:148:GLY:O	1:C:498:LYS:HD3	2.08	0.52
1:H:161:VAL:HA	1:H:188:VAL:HG23	1.91	0.52
1:F:11:PRO:HB3	1:F:114:TYR:CE2	2.44	0.52
1:G:468:TYR:OH	1:H:489:LYS:HB2	2.09	0.52
1:F:117:SER:O	1:F:122:LEU:HD23	2.10	0.52
1:C:149:ASP:HA	1:C:498:LYS:HB2	1.91	0.52
1:E:372:GLY:O	1:E:382:GLN:HG3	2.10	0.52
1:F:449:GLY:HA3	1:F:466:GLY:O	2.10	0.52
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.10	0.52
1:H:430:ALA:HB2	1:H:456:TYR:CD1	2.44	0.52
1:B:294:LEU:CD1	1:B:405:MET:HA	2.39	0.51
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.45	0.51
1:F:225:GLY:HA3	4:F:6502:NAI:C8A	2.40	0.51
1:E:170:PHE:O	1:E:174:MET:HG2	2.09	0.51
1:F:483:GLN:HB3	5:F:6634:HOH:O	2.09	0.51
1:H:39:THR:HG23	1:H:48:ILE:HB	1.92	0.51
1:E:208:ILE:HD13	1:E:218:VAL:HG11	1.92	0.51
1:E:277:ILE:HD12	1:E:286:ALA:HB1	1.91	0.51
1:F:238:VAL:O	1:F:263:LYS:HE3	2.10	0.51
1:B:294:LEU:HD13	1:B:405:MET:HA	1.92	0.51
1:C:193:VAL:HG11	1:C:201:ALA:CB	2.41	0.51
1:G:303:CYS:SG	1:G:459:PHE:HZ	2.34	0.51
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.45	0.51
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.46	0.51
1:E:449:GLY:HA3	1:E:466:GLY:O	2.12	0.50
1:F:121:ASP:O	1:F:125:VAL:HG23	2.11	0.50
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.45	0.50
1:H:449:GLY:HA3	1:H:466:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:CYS:SG	1:A:459:PHE:HZ	2.34	0.50
1:F:170:PHE:O	1:F:174:MET:HG2	2.12	0.50
1:F:311:GLN:HG2	5:F:6525:HOH:O	2.10	0.50
1:D:15:PRO:HD2	1:D:108:LEU:HD22	1.92	0.50
1:E:174:MET:CE	1:E:244:THR:HG21	2.41	0.50
1:H:170:PHE:HB3	1:H:173:LEU:HB3	1.94	0.50
1:F:143:THR:OG1	1:G:141:GLY:HA3	2.12	0.50
1:G:113:PRO:HB2	1:G:116:ILE:HG12	1.94	0.50
1:D:134:GLY:O	1:D:138:LYS:HD2	2.12	0.50
1:B:238:VAL:HB	1:B:263:LYS:HE2	1.94	0.50
1:D:159:VAL:HG12	1:D:187:ASN:OD1	2.11	0.50
1:E:167:PRO:CB	4:E:5502:NAI:H4N	2.42	0.50
1:H:315:TYR:O	1:H:319:VAL:HG23	2.12	0.50
1:A:430:ALA:HB2	1:A:456:TYR:CD1	2.47	0.49
1:H:246:SER:HB3	4:H:8502:NAI:O4D	2.12	0.49
1:C:302:CYS:HB3	4:C:3502:NAI:O7N	2.12	0.49
1:B:449:GLY:HA3	1:B:466:GLY:O	2.11	0.49
1:B:183:LEU:HD13	1:B:213:PHE:CE2	2.48	0.49
1:E:247:THR:HA	1:E:269:LEU:HD13	1.94	0.49
1:F:185:THR:HG23	1:F:482:LEU:HD22	1.94	0.49
1:G:408:LEU:N	1:G:408:LEU:HD12	2.28	0.49
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.36	0.49
1:C:310:VAL:HG21	1:C:318:PHE:CD2	2.48	0.49
1:A:449:GLY:HA3	1:A:466:GLY:O	2.13	0.49
1:C:372:GLY:O	1:C:382:GLN:HG3	2.12	0.49
1:D:107:THR:HG23	1:D:112:LYS:O	2.13	0.49
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.13	0.49
1:B:497:GLN:CD	1:C:78:ARG:HD3	2.34	0.48
1:B:353:ILE:HD13	1:B:402:GLY:HA3	1.95	0.48
1:B:193:VAL:HG11	1:B:201:ALA:CB	2.43	0.48
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.48	0.48
1:G:349:GLN:O	1:G:353:ILE:HG13	2.13	0.48
1:B:41:ASN:ND2	1:B:43:SER:H	2.11	0.48
4:C:3502:NAI:H8A	5:C:3633:HOH:O	2.12	0.48
1:H:349:GLN:O	1:H:353:ILE:HG13	2.13	0.48
1:E:33:SER:O	1:E:34:ARG:HB2	2.14	0.48
1:F:292:PHE:HE1	1:F:457:ASP:HB2	1.79	0.48
1:H:121:ASP:O	1:H:125:VAL:HG23	2.14	0.48
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.14	0.48
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.48	0.48
1:C:134:GLY:O	1:C:138:LYS:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:MET:HE3	1:B:318:PHE:HD1	1.79	0.48
1:C:443:SER:HA	1:C:451:VAL:HG11	1.96	0.48
1:D:294:LEU:HD22	1:D:405:MET:HB2	1.96	0.48
1:D:466:GLY:HA3	1:D:475:ARG:HD3	1.96	0.47
1:B:271:GLY:HA2	1:B:425:TYR:CD2	2.49	0.47
1:D:251:ARG:O	1:D:255:VAL:HG23	2.14	0.47
1:A:466:GLY:HA3	1:A:475:ARG:HD3	1.97	0.47
1:F:294:LEU:CD1	1:F:405:MET:HA	2.44	0.47
1:E:174:MET:HE2	1:E:244:THR:HG21	1.97	0.47
1:E:431:VAL:HG21	1:E:442:LEU:HB3	1.97	0.47
1:F:193:VAL:HG11	1:F:201:ALA:CB	2.44	0.47
1:G:470:MET:CE	1:H:262:LEU:HD12	2.43	0.47
1:H:443:SER:HA	1:H:451:VAL:HG11	1.95	0.47
1:D:167:PRO:HD3	1:D:244:THR:HB	1.97	0.47
1:F:15:PRO:HG2	1:F:108:LEU:HD22	1.96	0.47
1:H:32:VAL:HG23	1:H:58:ASP:OD1	2.14	0.47
1:E:244:THR:HG23	1:E:268:GLU:HB3	1.97	0.47
1:E:294:LEU:CD1	1:E:405:MET:HA	2.45	0.47
1:F:167:PRO:HD3	1:F:244:THR:HB	1.97	0.47
1:B:498:LYS:HD2	1:B:498:LYS:C	2.35	0.47
1:D:243:PHE:HB3	1:D:267:LEU:HD23	1.97	0.47
1:A:443:SER:HA	1:A:451:VAL:HG11	1.96	0.46
1:C:21:GLN:HB3	1:C:29:HIS:O	2.15	0.46
1:C:121:ASP:O	1:C:125:VAL:HG23	2.15	0.46
1:A:368:LEU:HD12	1:A:385:VAL:HG12	1.96	0.46
1:F:302:CYS:HB3	4:F:6502:NAI:O7N	2.16	0.46
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.49	0.46
1:D:443:SER:HA	1:D:451:VAL:HG11	1.97	0.46
1:B:235:HIS:HB3	1:B:238:VAL:HG23	1.98	0.46
1:B:238:VAL:O	1:B:263:LYS:HE3	2.16	0.46
1:A:146:ILE:HG12	1:A:147:ASP:N	2.31	0.46
1:C:468:TYR:OH	1:D:489:LYS:HB2	2.15	0.46
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.98	0.46
1:F:115:VAL:HG23	5:F:6548:HOH:O	2.16	0.46
1:E:124:MET:HE3	1:E:173:LEU:HD22	1.98	0.45
1:H:408:LEU:HD12	1:H:408:LEU:N	2.31	0.45
1:C:225:GLY:HA3	4:C:3502:NAI:C8A	2.46	0.45
1:E:361:LYS:HE2	1:E:367:LEU:CD2	2.45	0.45
1:B:443:SER:HA	1:B:451:VAL:HG11	1.98	0.45
1:A:294:LEU:HD13	1:A:405:MET:HA	1.97	0.45
1:D:315:TYR:O	1:D:319:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:294:LEU:HD12	1:H:305:GLY:O	2.17	0.45
1:A:12:ASN:O	1:A:15:PRO:HD3	2.17	0.45
1:D:302:CYS:HB3	4:D:4502:NAI:O7N	2.17	0.45
1:E:443:SER:HA	1:E:451:VAL:HG11	1.99	0.45
1:B:167:PRO:HD3	1:B:244:THR:HB	1.99	0.45
1:C:408:LEU:HD12	1:C:408:LEU:N	2.32	0.45
1:E:410:PHE:CD1	1:E:416:VAL:HB	2.52	0.45
1:E:417:VAL:HG22	1:E:442:LEU:HD23	1.99	0.45
1:A:294:LEU:O	1:A:299:GLY:HA2	2.17	0.45
1:A:185:THR:HG23	1:A:482:LEU:HD22	2.00	0.44
1:B:258:GLY:HA2	1:B:262:LEU:HD23	1.98	0.44
1:C:292:PHE:CE1	1:C:457:ASP:HB2	2.51	0.44
1:D:193:VAL:HG11	1:D:201:ALA:CB	2.48	0.44
1:F:112:LYS:HB3	1:F:112:LYS:HE2	1.86	0.44
1:G:251:ARG:NH2	1:G:470:MET:HE3	2.31	0.44
1:B:113:PRO:HB2	1:B:116:ILE:HG12	1.99	0.44
1:B:122:LEU:HD21	1:B:172:LEU:CD1	2.47	0.44
1:D:125:VAL:HG22	1:D:173:LEU:HA	1.99	0.44
1:H:38:PRO:HB3	1:H:50:GLN:NE2	2.27	0.44
1:D:292:PHE:HE2	1:D:296:PHE:CD2	2.36	0.44
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.52	0.44
1:D:179:LEU:HD12	5:D:4616:HOH:O	2.17	0.44
1:D:204:VAL:O	1:D:208:ILE:HG13	2.18	0.44
1:F:8:VAL:HG21	1:F:115:VAL:HG13	2.00	0.44
1:D:294:LEU:CD1	1:D:405:MET:HA	2.48	0.44
1:D:294:LEU:HD13	1:D:405:MET:HA	1.98	0.44
1:A:279:SER:HA	1:A:314:ILE:HD13	1.99	0.43
1:G:12:ASN:C	1:G:14:GLN:H	2.21	0.43
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.53	0.43
1:E:260:SER:O	1:F:251:ARG:NH2	2.51	0.43
1:A:233:ALA:HB2	1:A:253:ILE:HD13	1.99	0.43
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.53	0.43
1:C:102:LEU:HD21	1:C:203:TYR:HD2	1.83	0.43
1:C:115:VAL:HG23	5:C:3516:HOH:O	2.17	0.43
1:D:279:SER:HA	1:D:314:ILE:HD13	2.00	0.43
1:F:41:ASN:ND2	1:F:108:LEU:HD12	2.33	0.43
1:H:185:THR:OG1	1:H:187:ASN:ND2	2.51	0.43
1:B:166:ILE:HD11	1:B:193:VAL:HG12	2.00	0.43
1:C:159:VAL:HG12	1:C:187:ASN:OD1	2.18	0.43
1:A:76:TRP:CH2	1:A:84:ARG:HG2	2.54	0.43
1:A:167:PRO:HD3	1:A:244:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLN:HE21	1:C:13:GLN:HB3	1.63	0.43
1:G:331:VAL:HG22	1:G:341:GLN:HB3	2.00	0.43
1:E:343:PRO:HD3	1:E:380:PHE:CE2	2.54	0.43
1:G:258:GLY:HA3	1:H:254:GLN:HG2	2.00	0.43
1:H:294:LEU:CD1	1:H:405:MET:HA	2.48	0.43
1:B:11:PRO:HB3	1:B:114:TYR:CE2	2.53	0.43
1:B:79:MET:SD	1:B:83:HIS:CD2	3.10	0.43
1:H:193:VAL:HG11	1:H:201:ALA:CB	2.49	0.43
1:H:315:TYR:CE1	1:H:319:VAL:HG21	2.54	0.43
1:D:170:PHE:HB2	1:D:174:MET:HG2	1.99	0.43
1:E:214:PRO:HA	1:E:215:PRO:HD3	1.93	0.43
1:C:188:VAL:HG12	1:C:217:VAL:HA	2.01	0.43
1:A:99:ARG:HG2	1:A:118:TYR:CE1	2.54	0.43
1:H:205:ALA:HA	1:H:208:ILE:HD12	2.01	0.43
1:H:272:LYS:HD2	1:H:272:LYS:HA	1.89	0.43
1:B:32:VAL:HG23	1:B:58:ASP:OD1	2.19	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CE2	2.53	0.42
1:F:271:GLY:HA2	1:F:425:TYR:CD2	2.54	0.42
1:F:294:LEU:HD11	1:F:405:MET:HA	2.00	0.42
1:G:12:ASN:O	1:G:15:PRO:HD3	2.19	0.42
1:G:111:GLY:O	1:G:343:PRO:HD2	2.18	0.42
1:H:294:LEU:O	1:H:299:GLY:HA2	2.19	0.42
1:A:251:ARG:O	1:A:255:VAL:HG23	2.19	0.42
1:F:57:GLU:HB2	5:F:6613:HOH:O	2.19	0.42
1:G:198:PRO:O	1:G:202:LEU:HG	2.19	0.42
1:G:269:LEU:HD12	1:G:470:MET:O	2.18	0.42
1:H:106:GLU:OE2	1:H:200:THR:HG21	2.19	0.42
1:H:244:THR:HA	1:H:268:GLU:O	2.19	0.42
1:H:432:PHE:HA	1:H:454:ASN:OD1	2.19	0.42
1:B:251:ARG:NH2	1:B:470:MET:HE1	2.34	0.42
1:B:294:LEU:HD12	1:B:306:SER:HA	2.02	0.42
1:C:144:ILE:CG2	1:D:462:GLN:HB3	2.49	0.42
1:C:459:PHE:HE2	1:C:465:PHE:CD1	2.37	0.42
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.19	0.42
1:F:208:ILE:HD13	1:F:218:VAL:HG11	2.01	0.42
1:A:106:GLU:OE2	1:A:171:PRO:HB2	2.19	0.42
1:A:254:GLN:NE2	1:B:262:LEU:CD2	2.82	0.42
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.54	0.42
1:E:323:VAL:O	1:E:327:LYS:HG3	2.18	0.42
1:F:294:LEU:HD12	1:F:306:SER:HA	2.01	0.42
1:H:329:ARG:HE	1:H:341:GLN:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:HG23	1:B:482:LEU:HD22	2.01	0.42
1:C:112:LYS:HB3	1:C:112:LYS:HE2	1.89	0.42
1:F:135:TRP:CE2	1:H:138:LYS:HD3	2.55	0.42
1:H:466:GLY:HA3	1:H:475:ARG:HD3	2.01	0.42
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.19	0.42
1:D:33:SER:O	1:D:34:ARG:HB2	2.20	0.42
1:A:294:LEU:HD22	1:A:405:MET:HB2	2.01	0.42
1:C:251:ARG:O	1:C:255:VAL:HG23	2.20	0.42
1:C:246:SER:HB3	4:C:3502:NAI:O4D	2.20	0.42
1:E:315:TYR:CZ	1:E:319:VAL:HG21	2.55	0.42
1:E:453:VAL:HB	1:F:493:VAL:HG13	2.02	0.42
1:F:498:LYS:HE2	1:F:498:LYS:HB3	1.90	0.42
1:H:359:THR:O	1:H:363:GLU:HG3	2.19	0.42
1:B:311:GLN:HG3	5:B:2579:HOH:O	2.19	0.42
1:D:306:SER:O	1:D:406:GLN:HB2	2.20	0.42
1:G:107:THR:HG23	1:G:112:LYS:O	2.19	0.42
1:E:131:TYR:CE1	1:E:462:GLN:HG3	2.55	0.41
1:G:39:THR:HG23	1:G:48:ILE:HB	2.01	0.41
1:A:161:VAL:HA	1:A:188:VAL:HG23	2.01	0.41
1:A:294:LEU:CD1	1:A:405:MET:HA	2.51	0.41
1:B:417:VAL:HG22	1:B:442:LEU:HD23	2.02	0.41
1:E:432:PHE:HA	1:E:454:ASN:OD1	2.20	0.41
1:H:22:ILE:HG12	1:H:222:PRO:HD2	2.02	0.41
1:H:404:VAL:HG12	1:H:406:GLN:OE1	2.20	0.41
1:A:166:ILE:HD11	1:A:193:VAL:HG12	2.02	0.41
1:D:214:PRO:HA	1:D:215:PRO:HD3	1.88	0.41
1:D:292:PHE:CE2	1:D:296:PHE:CD2	3.08	0.41
1:E:107:THR:HG23	1:E:112:LYS:O	2.20	0.41
1:F:459:PHE:HE2	1:F:465:PHE:CD1	2.38	0.41
1:H:124:MET:HE3	1:H:173:LEU:CD2	2.44	0.41
1:A:430:ALA:HB2	1:A:456:TYR:HD1	1.84	0.41
1:C:172:LEU:CD2	1:C:200:THR:HB	2.48	0.41
1:C:315:TYR:CE1	1:C:319:VAL:HG21	2.55	0.41
1:D:102:LEU:HD21	1:D:203:TYR:HD2	1.85	0.41
1:F:358:ASN:O	1:F:362:GLN:HG2	2.20	0.41
1:H:13:GLN:HA	1:H:335:PHE:CZ	2.55	0.41
1:C:185:THR:HG23	1:C:482:LEU:HD22	2.02	0.41
1:E:193:VAL:HG11	1:E:201:ALA:CB	2.50	0.41
1:E:208:ILE:CD1	1:E:218:VAL:HG11	2.51	0.41
1:G:200:THR:O	1:G:204:VAL:HG23	2.20	0.41
1:B:21:GLN:HB3	1:B:29:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:THR:OG1	1:C:141:GLY:HA3	2.20	0.41
1:D:116:ILE:O	1:D:120:VAL:HB	2.20	0.41
1:E:103:ALA:HB2	1:E:122:LEU:HD12	2.02	0.41
1:F:166:ILE:HA	1:F:167:PRO:HD3	1.90	0.41
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.85	0.41
1:H:271:GLY:HA2	1:H:425:TYR:CD2	2.56	0.41
1:D:11:PRO:HB3	1:D:114:TYR:CE2	2.55	0.41
1:H:372:GLY:O	1:H:382:GLN:HG3	2.20	0.41
1:B:141:GLY:HA3	1:C:143:THR:OG1	2.21	0.41
1:B:271:GLY:HA2	1:B:425:TYR:CG	2.56	0.41
1:D:149:ASP:HA	1:D:498:LYS:HB2	2.03	0.41
1:E:246:SER:HB3	4:E:5502:NAI:O4D	2.21	0.41
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.21	0.41
1:G:8:VAL:HA	1:G:9:PRO:HD3	1.90	0.41
1:G:235:HIS:HB3	1:G:238:VAL:HG23	2.03	0.41
1:H:213:PHE:HA	1:H:214:PRO:HD3	1.97	0.41
1:A:498:LYS:HE2	1:A:498:LYS:HB3	1.96	0.41
1:D:163:GLY:O	1:D:241:VAL:HA	2.21	0.41
1:E:23:PHE:HZ	1:E:26:ASN:HD22	1.68	0.41
1:F:167:PRO:HB3	4:F:6502:NAI:H4N	2.03	0.41
1:C:198:PRO:O	1:C:202:LEU:HG	2.20	0.40
1:D:175:GLN:HG3	1:D:191:MET:SD	2.61	0.40
1:E:294:LEU:HD13	1:E:405:MET:HA	2.02	0.40
1:E:300:GLN:HE21	1:E:300:GLN:HB2	1.74	0.40
1:F:459:PHE:HE2	1:F:465:PHE:CE1	2.39	0.40
1:G:249:ILE:O	1:G:253:ILE:HG12	2.21	0.40
1:H:429:ALA:HB1	1:H:446:LEU:HD13	2.03	0.40
1:A:110:ASN:ND2	1:A:168:TRP:O	2.54	0.40
1:G:244:THR:HA	1:G:268:GLU:O	2.21	0.40
1:H:350:PHE:CD2	1:H:379:TYR:HD2	2.38	0.40
1:A:135:TRP:CD1	1:C:138:LYS:HE3	2.56	0.40
1:D:275:ASN:OD1	1:D:430:ALA:HB3	2.21	0.40
1:E:185:THR:OG1	1:E:187:ASN:ND2	2.54	0.40
1:E:249:ILE:O	1:E:253:ILE:HG12	2.21	0.40
1:F:39:THR:HG23	1:F:48:ILE:HB	2.03	0.40
4:B:2502:NAI:H6N	4:B:2502:NAI:H3D	2.04	0.40
1:C:12:ASN:O	1:C:15:PRO:HD3	2.20	0.40
1:F:138:LYS:HE3	1:H:135:TRP:CD1	2.57	0.40
1:H:13:GLN:HA	1:H:335:PHE:CE2	2.57	0.40
1:B:121:ASP:O	1:B:125:VAL:HG23	2.21	0.40
1:D:277:ILE:HD12	1:D:286:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	492/500 (98%)	471 (96%)	20 (4%)	1 (0%)	47 57
1	B	492/500 (98%)	476 (97%)	16 (3%)	0	100 100
1	C	492/500 (98%)	471 (96%)	21 (4%)	0	100 100
1	D	492/500 (98%)	471 (96%)	19 (4%)	2 (0%)	34 41
1	E	492/500 (98%)	473 (96%)	19 (4%)	0	100 100
1	F	492/500 (98%)	475 (96%)	17 (4%)	0	100 100
1	G	492/500 (98%)	471 (96%)	19 (4%)	2 (0%)	34 41
1	H	492/500 (98%)	469 (95%)	23 (5%)	0	100 100
All	All	3936/4000 (98%)	3777 (96%)	154 (4%)	5 (0%)	51 64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	13	GLN
1	D	13	GLN
1	A	426	GLY
1	D	426	GLY
1	G	426	GLY

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	399/402 (99%)	396 (99%)	3 (1%)	81 88
1	B	399/402 (99%)	394 (99%)	5 (1%)	69 79
1	C	399/402 (99%)	393 (98%)	6 (2%)	65 76
1	D	399/402 (99%)	395 (99%)	4 (1%)	76 84
1	E	399/402 (99%)	393 (98%)	6 (2%)	65 76
1	F	399/402 (99%)	392 (98%)	7 (2%)	59 71
1	G	399/402 (99%)	395 (99%)	4 (1%)	76 84
1	H	399/402 (99%)	393 (98%)	6 (2%)	65 76
All	All	3192/3216 (99%)	3151 (99%)	41 (1%)	69 79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	275	ASN
1	A	401	PHE
1	B	41	ASN
1	B	192	LYS
1	B	268	GLU
1	B	401	PHE
1	B	416	VAL
1	C	192	LYS
1	C	206	ASN
1	C	268	GLU
1	C	377	ARG
1	C	401	PHE
1	C	471	SER
1	D	192	LYS
1	D	268	GLU
1	D	377	ARG
1	D	401	PHE
1	E	121	ASP
1	E	192	LYS
1	E	206	ASN
1	E	268	GLU
1	E	401	PHE
1	E	483	GLN
1	F	192	LYS
1	F	196	GLN
1	F	240	LYS

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Mol	Chain	Res	Type
1	F	254	GLN
1	F	268	GLU
1	F	275	ASN
1	F	401	PHE
1	G	192	LYS
1	G	268	GLU
1	G	294	LEU
1	G	401	PHE
1	H	192	LYS
1	H	268	GLU
1	H	275	ASN
1	H	388	ASP
1	H	401	PHE
1	H	424	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	254	GLN
1	A	275	ASN
1	A	406	GLN
1	B	41	ASN
1	B	83	HIS
1	B	254	GLN
1	B	275	ASN
1	B	390	GLN
1	B	483	GLN
1	C	13	GLN
1	C	26	ASN
1	C	83	HIS
1	C	175	GLN
1	D	390	GLN
1	D	440	ASN
1	E	13	GLN
1	E	50	GLN
1	E	254	GLN
1	F	13	GLN
1	F	14	GLN
1	F	71	GLN
1	F	196	GLN
1	F	275	ASN

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Mol	Chain	Res	Type
1	G	13	GLN
1	G	14	GLN
1	G	50	GLN
1	G	175	GLN
1	G	275	ASN
1	H	13	GLN
1	H	50	GLN
1	H	275	ASN
1	H	298	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	NAI	B	2502	3	42,48,48	2.23	8 (19%)	47,73,73	1.63	10 (21%)
4	NAI	C	3502	3	42,48,48	2.13	8 (19%)	47,73,73	1.41	6 (12%)
4	NAI	D	4502	3	42,48,48	2.37	8 (19%)	47,73,73	1.43	7 (14%)
4	NAI	F	6502	3	42,48,48	2.21	7 (16%)	47,73,73	1.39	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAI	E	5502	3	42,48,48	2.24	7 (16%)	47,73,73	1.55	11 (23%)
4	NAI	G	7502	3	42,48,48	2.19	8 (19%)	47,73,73	1.44	8 (17%)
4	NAI	A	1502	3	42,48,48	2.11	8 (19%)	47,73,73	1.52	7 (14%)
4	NAI	H	8502	3	42,48,48	2.28	8 (19%)	47,73,73	1.39	7 (14%)

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	NAI	B	2502	3	-	1/25/72/72	0/5/5/5
4	NAI	C	3502	3	-	2/25/72/72	0/5/5/5
4	NAI	D	4502	3	-	5/25/72/72	0/5/5/5
4	NAI	F	6502	3	-	2/25/72/72	0/5/5/5
4	NAI	E	5502	3	-	3/25/72/72	0/5/5/5
4	NAI	G	7502	3	-	3/25/72/72	0/5/5/5
4	NAI	A	1502	3	-	2/25/72/72	0/5/5/5
4	NAI	H	8502	3	-	4/25/72/72	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4502	NAI	C4N-C3N	-8.23	1.33	1.49
4	G	7502	NAI	C4N-C3N	-7.76	1.34	1.49
4	E	5502	NAI	C4N-C3N	-7.63	1.34	1.49
4	F	6502	NAI	C4N-C3N	-7.49	1.35	1.49
4	B	2502	NAI	C4N-C3N	-7.47	1.35	1.49
4	A	1502	NAI	C4N-C3N	-7.46	1.35	1.49
4	H	8502	NAI	C4N-C3N	-7.34	1.35	1.49
4	D	4502	NAI	C7N-C3N	-7.03	1.33	1.48
4	C	3502	NAI	C4N-C3N	-6.87	1.36	1.49
4	B	2502	NAI	C7N-C3N	-6.80	1.34	1.48
4	C	3502	NAI	C7N-C3N	-6.70	1.34	1.48
4	E	5502	NAI	C7N-C3N	-6.50	1.34	1.48
4	H	8502	NAI	C7N-C3N	-6.26	1.35	1.48
4	F	6502	NAI	C7N-C3N	-6.25	1.35	1.48
4	D	4502	NAI	C4N-C5N	-6.16	1.32	1.48
4	G	7502	NAI	C7N-C3N	-6.13	1.35	1.48
4	B	2502	NAI	C4N-C5N	-5.99	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	8502	NAI	C4N-C5N	-5.97	1.33	1.48
4	E	5502	NAI	C4N-C5N	-5.85	1.33	1.48
4	F	6502	NAI	C4N-C5N	-5.80	1.33	1.48
4	A	1502	NAI	C4N-C5N	-5.67	1.34	1.48
4	G	7502	NAI	C4N-C5N	-5.63	1.34	1.48
4	C	3502	NAI	C4N-C5N	-5.29	1.35	1.48
4	A	1502	NAI	C7N-C3N	-5.22	1.37	1.48
4	H	8502	NAI	C2A-N3A	5.18	1.40	1.32
4	F	6502	NAI	C2A-N3A	4.96	1.40	1.32
4	E	5502	NAI	C2A-N3A	4.84	1.39	1.32
4	B	2502	NAI	C2A-N3A	4.71	1.39	1.32
4	G	7502	NAI	C2A-N3A	4.64	1.39	1.32
4	D	4502	NAI	C2A-N3A	4.64	1.39	1.32
4	C	3502	NAI	C2A-N3A	4.58	1.39	1.32
4	A	1502	NAI	C2A-N3A	4.44	1.39	1.32
4	D	4502	NAI	C8A-N7A	3.65	1.41	1.34
4	H	8502	NAI	C2A-N1A	3.54	1.40	1.33
4	E	5502	NAI	C8A-N7A	3.45	1.40	1.34
4	C	3502	NAI	C6N-C5N	3.45	1.39	1.33
4	F	6502	NAI	C2A-N1A	3.45	1.40	1.33
4	D	4502	NAI	C2A-N1A	3.41	1.40	1.33
4	C	3502	NAI	C2A-N1A	3.37	1.40	1.33
4	H	8502	NAI	C6N-C5N	3.25	1.39	1.33
4	H	8502	NAI	C4A-N3A	3.24	1.40	1.35
4	F	6502	NAI	C6N-C5N	3.21	1.39	1.33
4	E	5502	NAI	C2A-N1A	3.20	1.39	1.33
4	A	1502	NAI	C2A-N1A	3.20	1.39	1.33
4	G	7502	NAI	C2A-N1A	3.13	1.39	1.33
4	B	2502	NAI	C8A-N7A	3.07	1.40	1.34
4	B	2502	NAI	C6N-C5N	3.06	1.38	1.33
4	E	5502	NAI	C6N-C5N	2.98	1.38	1.33
4	H	8502	NAI	C8A-N7A	2.96	1.40	1.34
4	G	7502	NAI	C6N-C5N	2.92	1.38	1.33
4	D	4502	NAI	C6N-C5N	2.85	1.38	1.33
4	B	2502	NAI	C2A-N1A	2.80	1.39	1.33
4	A	1502	NAI	C8A-N7A	2.69	1.39	1.34
4	F	6502	NAI	C8A-N7A	2.66	1.39	1.34
4	G	7502	NAI	C8A-N7A	2.63	1.39	1.34
4	A	1502	NAI	C4A-N3A	2.60	1.39	1.35
4	A	1502	NAI	C6N-C5N	2.36	1.37	1.33
4	G	7502	NAI	O4B-C1B	2.34	1.44	1.41
4	C	3502	NAI	C8A-N7A	2.25	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2502	NAI	C4A-N3A	2.13	1.38	1.35
4	D	4502	NAI	C4A-N3A	2.06	1.38	1.35
4	C	3502	NAI	C4A-N3A	2.01	1.38	1.35

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1502	NAI	N3A-C2A-N1A	-4.80	121.17	128.68
4	H	8502	NAI	N3A-C2A-N1A	-4.49	121.67	128.68
4	B	2502	NAI	C2B-C3B-C4B	-4.34	94.21	102.64
4	F	6502	NAI	N3A-C2A-N1A	-4.06	122.34	128.68
4	G	7502	NAI	O4B-C1B-C2B	-3.95	101.15	106.93
4	E	5502	NAI	O4B-C1B-C2B	-3.90	101.22	106.93
4	D	4502	NAI	O4B-C1B-C2B	-3.74	101.46	106.93
4	E	5502	NAI	N3A-C2A-N1A	-3.66	122.95	128.68
4	B	2502	NAI	O4B-C1B-C2B	-3.63	101.62	106.93
4	F	6502	NAI	O4B-C1B-C2B	-3.60	101.67	106.93
4	D	4502	NAI	PN-O3-PA	-3.57	120.58	132.83
4	C	3502	NAI	C1D-N1N-C2N	-3.57	115.17	121.11
4	C	3502	NAI	N3A-C2A-N1A	-3.52	123.18	128.68
4	E	5502	NAI	C2B-C3B-C4B	-3.40	96.03	102.64
4	D	4502	NAI	N3A-C2A-N1A	-3.37	123.40	128.68
4	B	2502	NAI	C2D-C3D-C4D	-3.36	96.11	102.64
4	A	1502	NAI	O4B-C1B-C2B	-3.33	102.06	106.93
4	B	2502	NAI	N3A-C2A-N1A	-3.33	123.48	128.68
4	C	3502	NAI	O4B-C1B-C2B	-3.23	102.20	106.93
4	C	3502	NAI	PN-O3-PA	-3.22	121.77	132.83
4	B	2502	NAI	C3N-C2N-N1N	-3.20	118.53	123.10
4	A	1502	NAI	C1D-N1N-C2N	-3.19	115.80	121.11
4	G	7502	NAI	N3A-C2A-N1A	-3.10	123.83	128.68
4	E	5502	NAI	PN-O3-PA	-3.09	122.21	132.83
4	G	7502	NAI	C1D-N1N-C2N	-3.07	115.99	121.11
4	B	2502	NAI	PN-O3-PA	-3.05	122.36	132.83
4	D	4502	NAI	C3N-C2N-N1N	-3.04	118.75	123.10
4	A	1502	NAI	C2B-C3B-C4B	-3.00	96.82	102.64
4	H	8502	NAI	C2B-C3B-C4B	-2.99	96.82	102.64
4	H	8502	NAI	C3N-C2N-N1N	-2.98	118.85	123.10
4	C	3502	NAI	C3D-C2D-C1D	-2.94	95.83	101.43
4	G	7502	NAI	PN-O3-PA	-2.93	122.77	132.83
4	B	2502	NAI	C1D-N1N-C2N	-2.90	116.28	121.11
4	D	4502	NAI	C2B-C3B-C4B	-2.84	97.13	102.64
4	D	4502	NAI	O4D-C4D-C3D	-2.78	99.61	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	7502	NAI	C2B-C3B-C4B	-2.78	97.24	102.64
4	E	5502	NAI	C3N-C2N-N1N	-2.74	119.18	123.10
4	G	7502	NAI	C2D-C3D-C4D	-2.74	97.32	102.64
4	B	2502	NAI	O4B-C4B-C3B	2.67	110.40	105.11
4	F	6502	NAI	PN-O3-PA	-2.64	123.78	132.83
4	F	6502	NAI	C1D-N1N-C2N	-2.63	116.73	121.11
4	A	1502	NAI	PN-O3-PA	-2.63	123.80	132.83
4	F	6502	NAI	C2B-C3B-C4B	-2.61	97.57	102.64
4	H	8502	NAI	O4D-C4D-C3D	-2.58	100.02	105.11
4	F	6502	NAI	C3N-C2N-N1N	-2.57	119.43	123.10
4	C	3502	NAI	C3N-C2N-N1N	-2.57	119.43	123.10
4	G	7502	NAI	C3N-C2N-N1N	-2.55	119.46	123.10
4	E	5502	NAI	C1D-N1N-C2N	-2.50	116.95	121.11
4	H	8502	NAI	O4B-C1B-C2B	-2.50	103.28	106.93
4	A	1502	NAI	C3D-C2D-C1D	-2.47	96.73	101.43
4	E	5502	NAI	C3N-C7N-N7N	2.46	122.04	117.67
4	B	2502	NAI	O4D-C4D-C3D	-2.45	100.27	105.11
4	E	5502	NAI	O7N-C7N-N7N	-2.34	117.42	122.88
4	E	5502	NAI	O4D-C4D-C3D	-2.33	100.50	105.11
4	G	7502	NAI	O7N-C7N-N7N	-2.30	117.50	122.88
4	H	8502	NAI	C3D-C2D-C1D	-2.26	97.13	101.43
4	E	5502	NAI	C2D-C3D-C4D	-2.25	98.27	102.64
4	A	1502	NAI	C3N-C2N-N1N	-2.22	119.92	123.10
4	F	6502	NAI	O4D-C4D-C3D	-2.10	100.95	105.11
4	H	8502	NAI	C1D-N1N-C2N	-2.10	117.61	121.11
4	D	4502	NAI	C2D-C3D-C4D	-2.04	98.67	102.64
4	E	5502	NAI	C5A-C6A-N6A	2.04	123.45	120.35
4	B	2502	NAI	C3D-C2D-C1D	-2.03	97.57	101.43

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1502	NAI	C2N-C3N-C7N-N7N
4	C	3502	NAI	C2N-C3N-C7N-N7N
4	E	5502	NAI	C2N-C3N-C7N-N7N
4	F	6502	NAI	C2N-C3N-C7N-N7N
4	G	7502	NAI	O4D-C1D-N1N-C2N
4	H	8502	NAI	C2N-C3N-C7N-N7N
4	A	1502	NAI	O4D-C1D-N1N-C2N
4	C	3502	NAI	O4D-C1D-N1N-C2N
4	D	4502	NAI	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	E	5502	NAI	O4D-C1D-N1N-C2N
4	H	8502	NAI	O4D-C1D-N1N-C2N
4	H	8502	NAI	O4B-C4B-C5B-O5B
4	B	2502	NAI	O4D-C1D-N1N-C2N
4	H	8502	NAI	C3B-C4B-C5B-O5B
4	F	6502	NAI	O4D-C1D-N1N-C2N
4	D	4502	NAI	C5B-O5B-PA-O2A
4	G	7502	NAI	C4D-C5D-O5D-PN
4	G	7502	NAI	O4D-C4D-C5D-O5D
4	D	4502	NAI	C5B-O5B-PA-O3
4	D	4502	NAI	C4B-C5B-O5B-PA
4	D	4502	NAI	C4D-C5D-O5D-PN
4	E	5502	NAI	C4D-C5D-O5D-PN

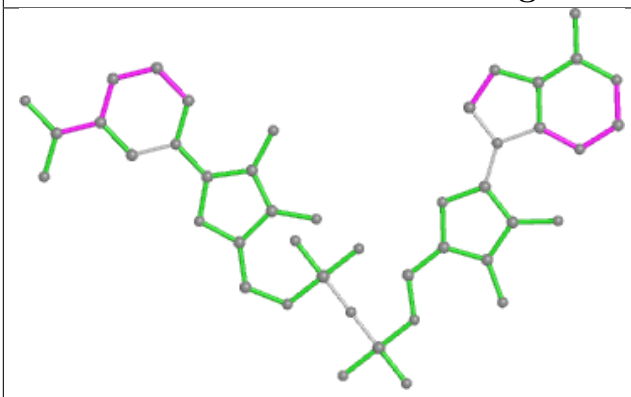
There are no ring outliers.

7 monomers are involved in 13 short contacts:

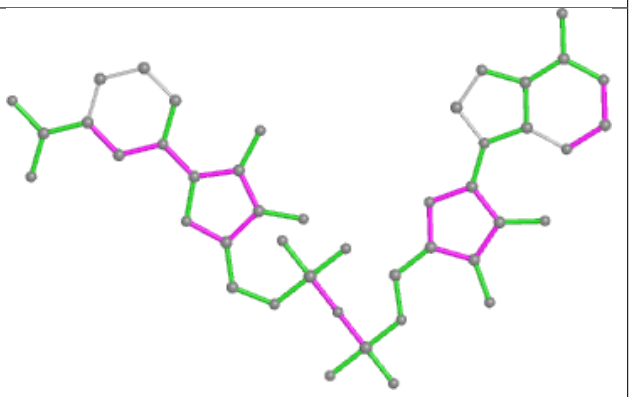
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2502	NAI	1	0
4	C	3502	NAI	4	0
4	D	4502	NAI	1	0
4	F	6502	NAI	3	0
4	E	5502	NAI	2	0
4	A	1502	NAI	1	0
4	H	8502	NAI	1	0

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

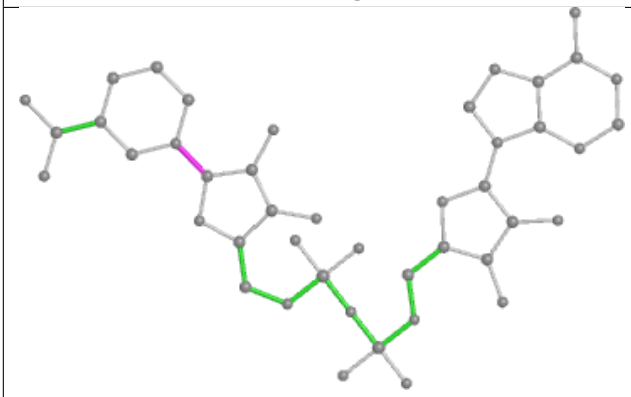
Ligand NAI B 2502



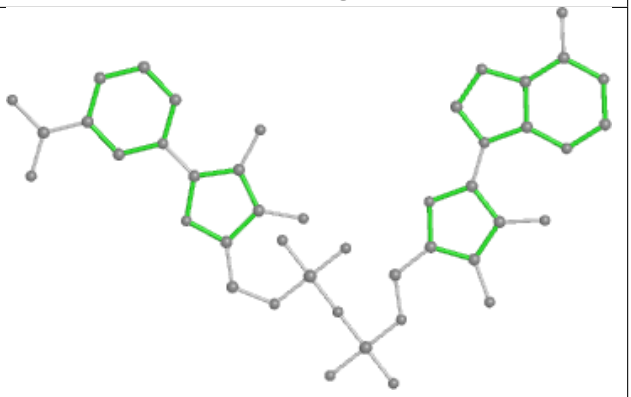
Bond lengths



Bond angles

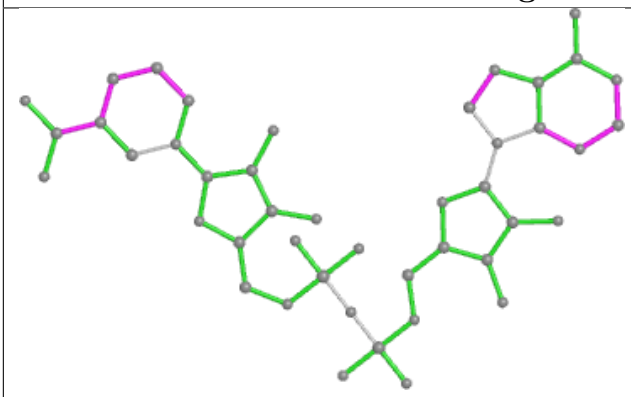


Torsions

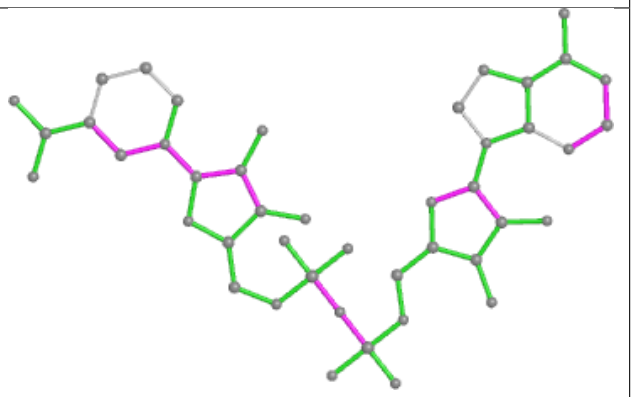


Rings

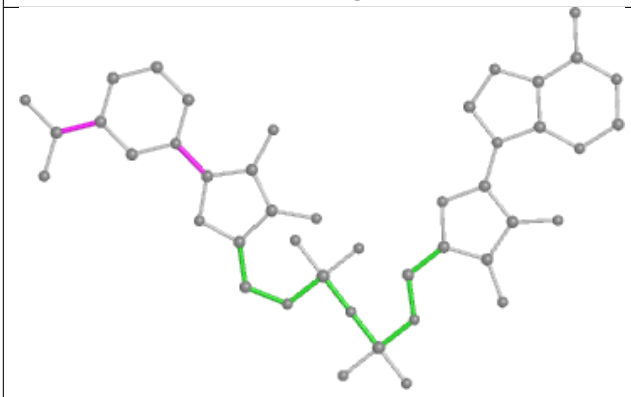
Ligand NAI C 3502



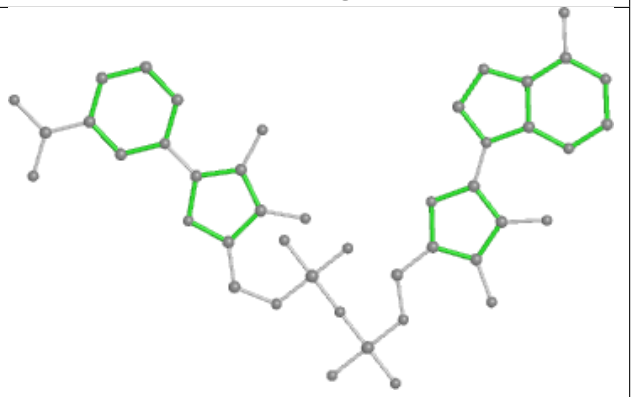
Bond lengths



Bond angles

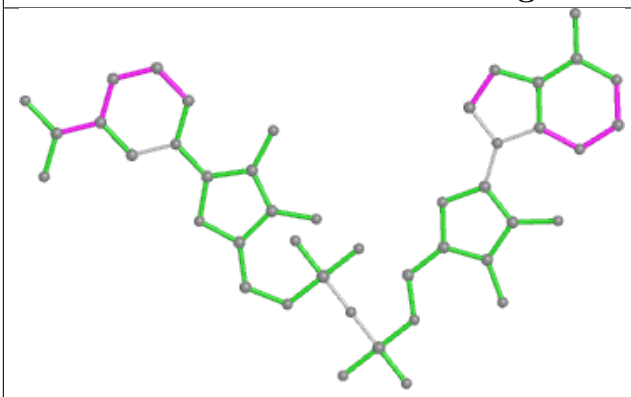


Torsions

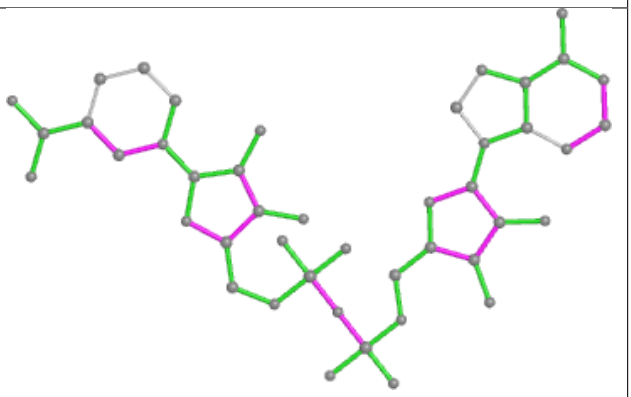


Rings

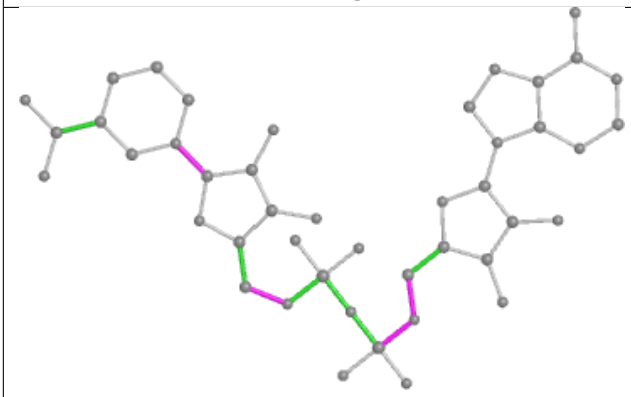
Ligand NAI D 4502



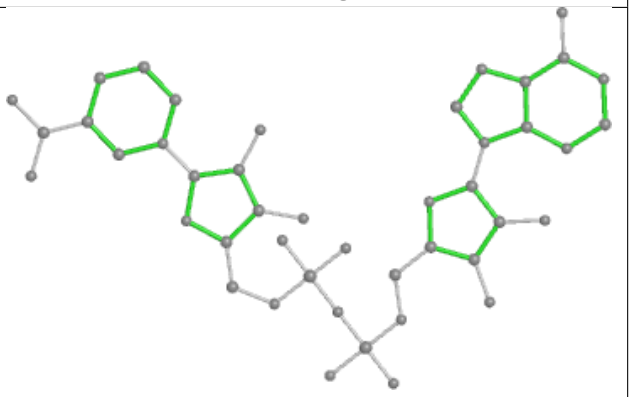
Bond lengths



Bond angles

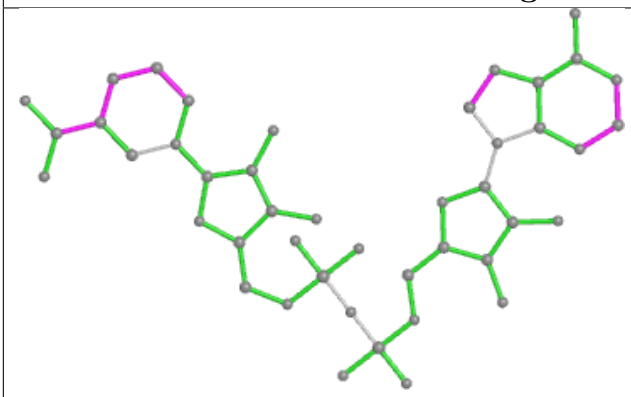


Torsions

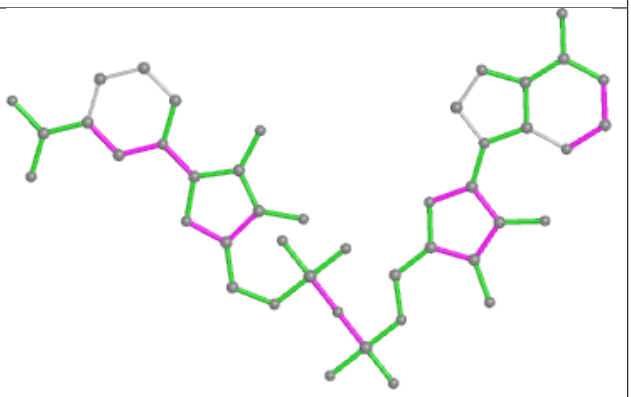


Rings

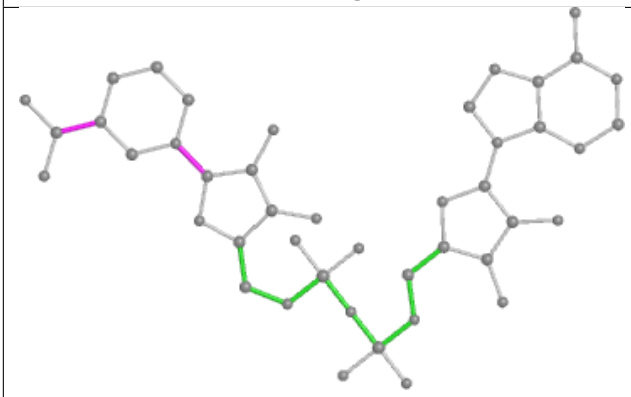
Ligand NAI F 6502



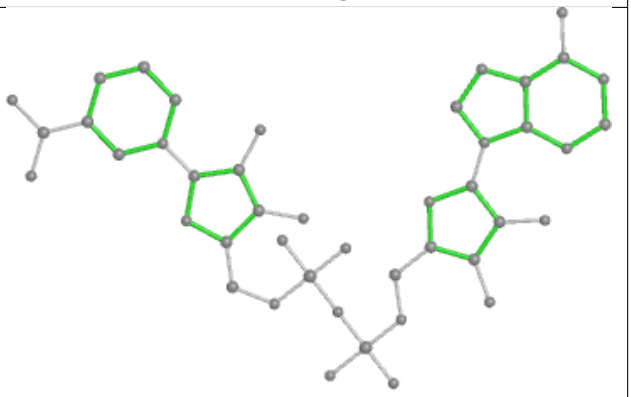
Bond lengths



Bond angles

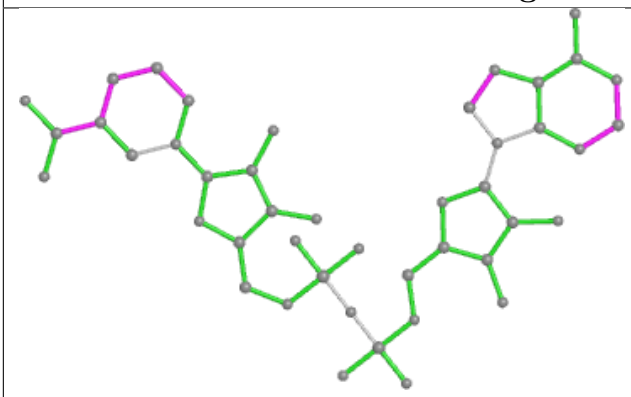


Torsions

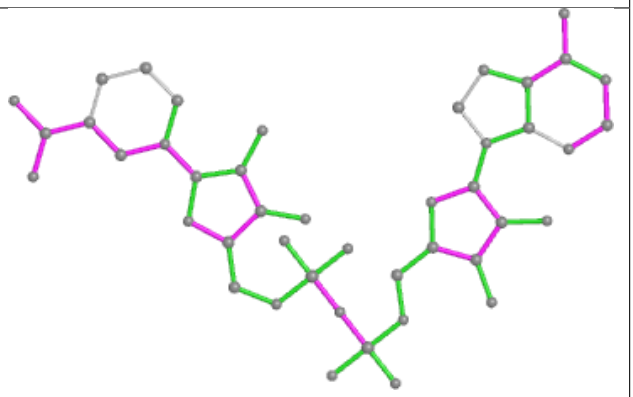


Rings

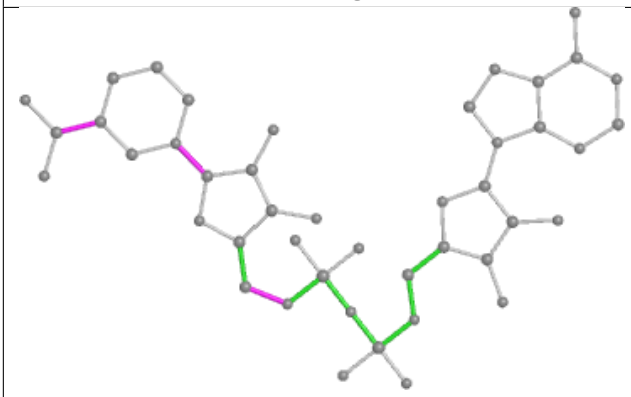
Ligand NAI E 5502



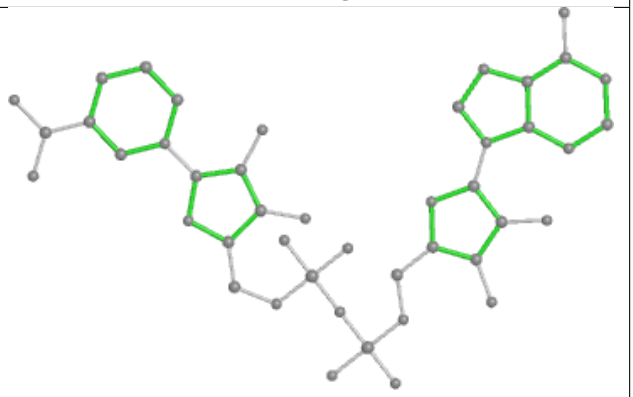
Bond lengths



Bond angles

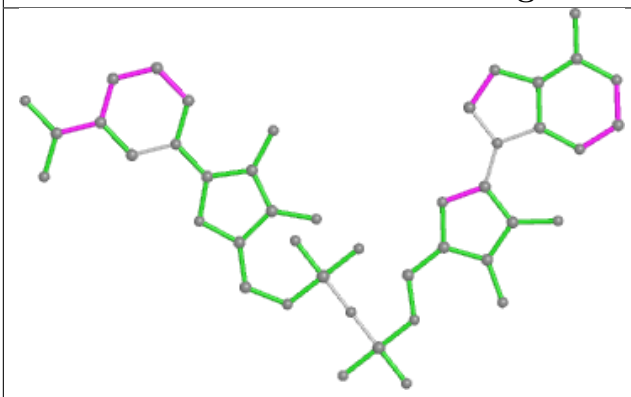


Torsions

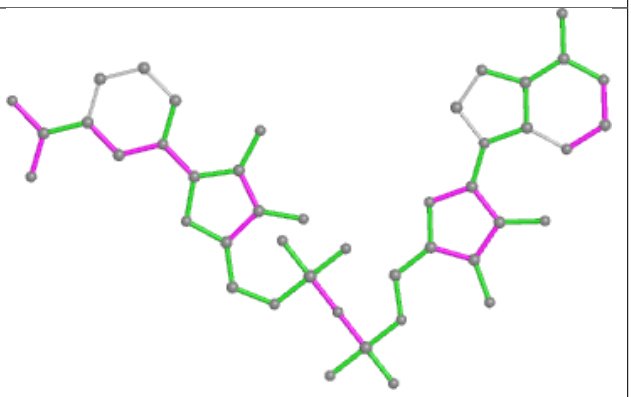


Rings

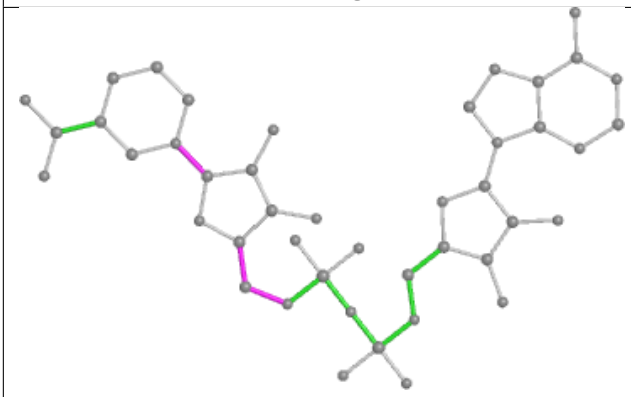
Ligand NAI G 7502



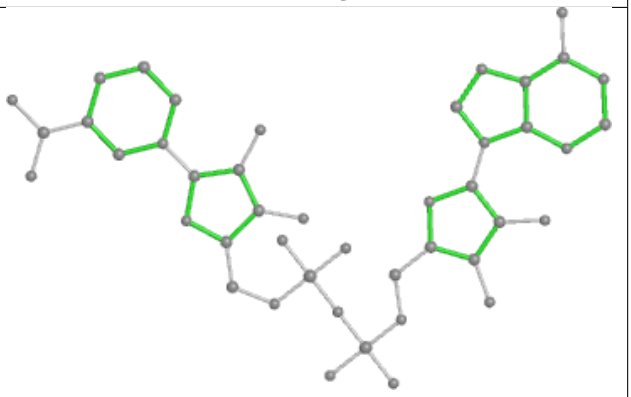
Bond lengths



Bond angles

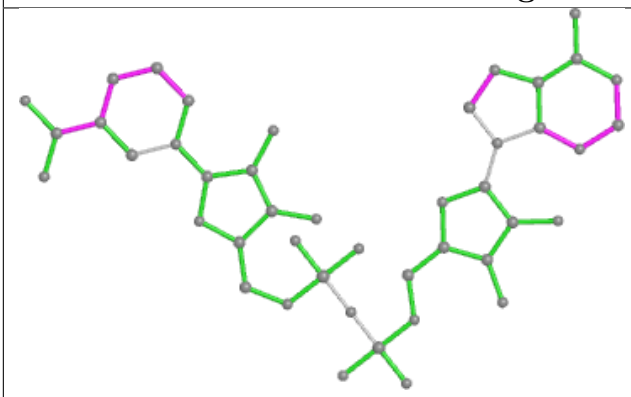


Torsions

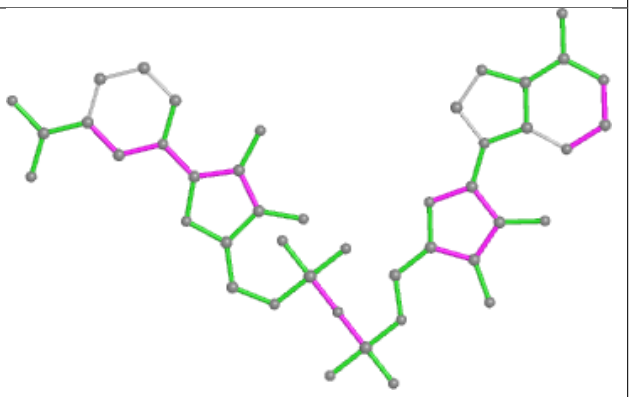


Rings

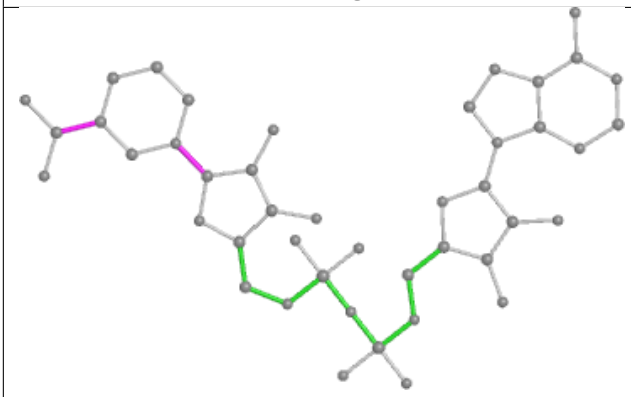
Ligand NAI A 1502



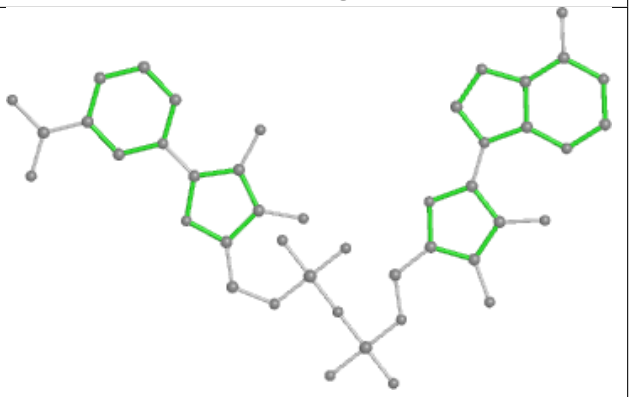
Bond lengths



Bond angles

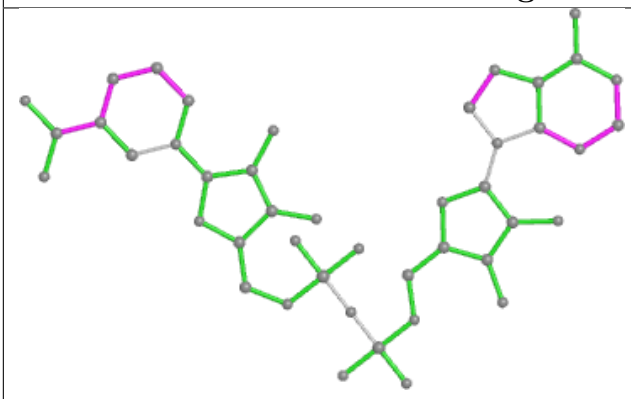


Torsions

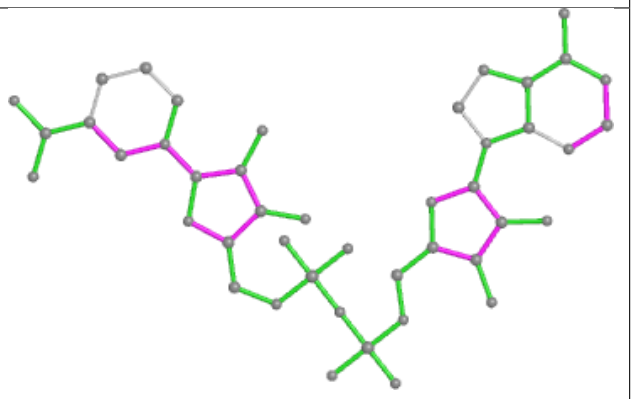


Rings

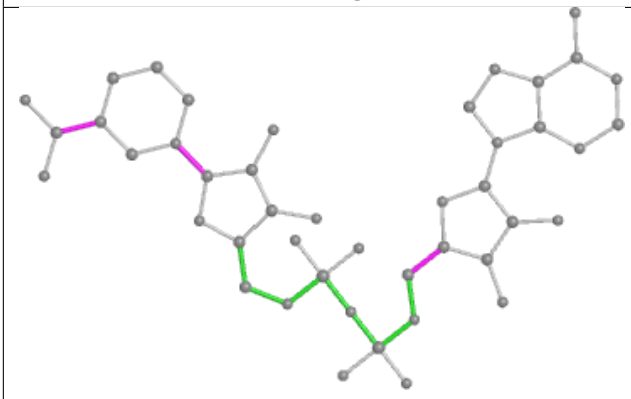
Ligand NAI H 8502



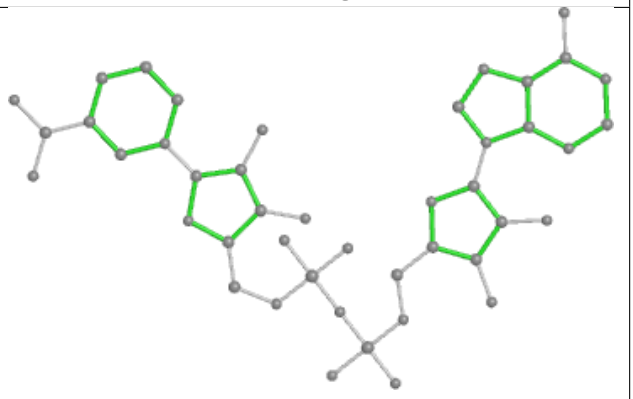
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	494/500 (98%)	-0.07	9 (1%) 68 65	19, 41, 55, 66	0
1	B	494/500 (98%)	-0.34	2 (0%) 92 93	22, 36, 51, 64	0
1	C	494/500 (98%)	-0.54	0 100 100	19, 29, 42, 54	0
1	D	494/500 (98%)	-0.04	9 (1%) 68 65	20, 43, 59, 71	0
1	E	494/500 (98%)	-0.38	4 (0%) 86 86	21, 36, 50, 64	0
1	F	494/500 (98%)	-0.59	0 100 100	18, 28, 40, 51	0
1	G	494/500 (98%)	-0.35	4 (0%) 86 86	21, 36, 50, 64	0
1	H	494/500 (98%)	0.13	17 (3%) 45 41	21, 44, 59, 71	0
All	All	3952/4000 (98%)	-0.27	45 (1%) 80 80	18, 36, 54, 71	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	376	ASP	4.9
1	E	376	ASP	4.4
1	H	376	ASP	3.9
1	H	377	ARG	3.7
1	A	356	TYR	3.4
1	G	7	ALA	3.2
1	D	40	VAL	3.1
1	A	362	GLN	3.0
1	A	371	GLY	2.9
1	B	34	ARG	2.9
1	A	14	GLN	2.9
1	B	7	ALA	2.8
1	H	32	VAL	2.8
1	H	336	ASP	2.7
1	H	7	ALA	2.7
1	D	336	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	44	THR	2.6
1	H	394	THR	2.6
1	H	424	THR	2.6
1	H	10	ALA	2.6
1	G	14	GLN	2.5
1	H	362	GLN	2.5
1	G	259	SER	2.4
1	E	34	ARG	2.4
1	A	392	GLY	2.4
1	E	338	LYS	2.3
1	H	18	PHE	2.3
1	H	51	VAL	2.3
1	E	377	ARG	2.3
1	A	376	ASP	2.3
1	A	312	GLU	2.2
1	D	338	LYS	2.2
1	H	34	ARG	2.2
1	H	338	LYS	2.1
1	A	7	ALA	2.1
1	D	334	PRO	2.1
1	G	220	ILE	2.1
1	H	328	SER	2.1
1	A	308	THR	2.1
1	H	347	GLU	2.1
1	H	104	ALA	2.1
1	D	284	ASP	2.1
1	D	224	PHE	2.1
1	D	14	GLN	2.0
1	D	114	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

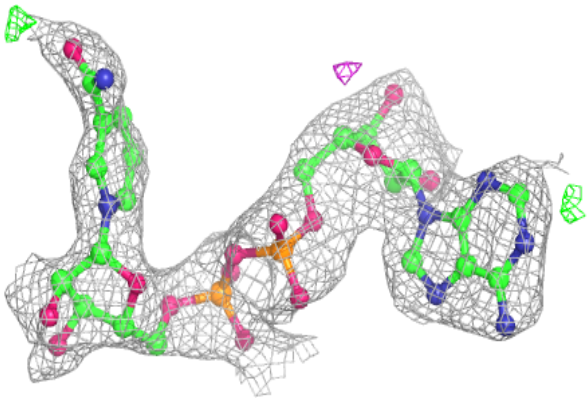
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

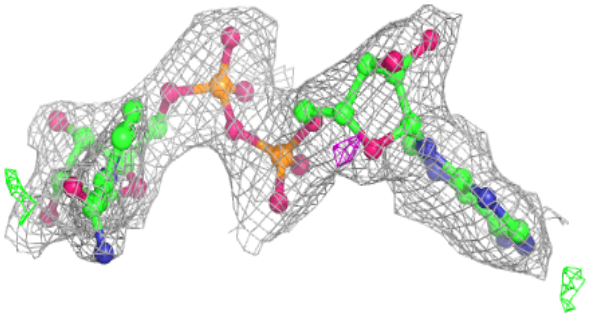
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	D	1704	1/1	0.44	0.39	88,88,88,88	0
3	MG	F	1606	1/1	0.52	0.15	52,52,52,52	0
3	MG	C	1603	1/1	0.64	0.15	64,64,64,64	0
3	MG	H	1608	1/1	0.67	0.18	62,62,62,62	0
2	NA	C	1703	1/1	0.76	0.19	37,37,37,37	0
2	NA	H	1708	1/1	0.78	0.18	60,60,60,60	0
3	MG	E	1605	1/1	0.79	0.12	58,58,58,58	0
3	MG	A	1601	1/1	0.81	0.11	54,54,54,54	0
2	NA	F	1706	1/1	0.84	0.13	31,31,31,31	0
2	NA	A	1701	1/1	0.88	0.14	46,46,46,46	0
2	NA	E	1705	1/1	0.89	0.19	44,44,44,44	0
2	NA	G	1707	1/1	0.89	0.10	51,51,51,51	0
3	MG	G	1607	1/1	0.90	0.11	57,57,57,57	0
4	NAI	H	8502	44/44	0.90	0.18	54,57,61,63	0
2	NA	B	1702	1/1	0.91	0.10	36,36,36,36	0
4	NAI	A	1502	44/44	0.92	0.18	46,50,54,55	0
4	NAI	G	7502	44/44	0.93	0.15	42,51,53,54	0
3	MG	D	1604	1/1	0.93	0.07	58,58,58,58	0
4	NAI	D	4502	44/44	0.94	0.16	40,49,57,59	0
3	MG	B	1602	1/1	0.94	0.08	44,44,44,44	0
4	NAI	B	2502	44/44	0.94	0.14	47,51,54,55	0
4	NAI	C	3502	44/44	0.96	0.17	26,37,41,42	0
4	NAI	E	5502	44/44	0.96	0.14	33,45,48,48	0
4	NAI	F	6502	44/44	0.97	0.13	26,34,42,42	0

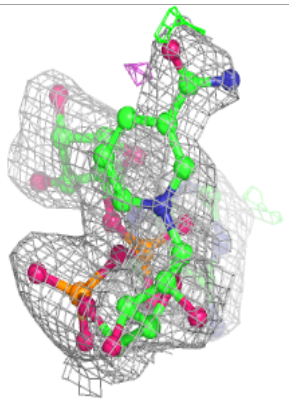
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI H 8502:

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

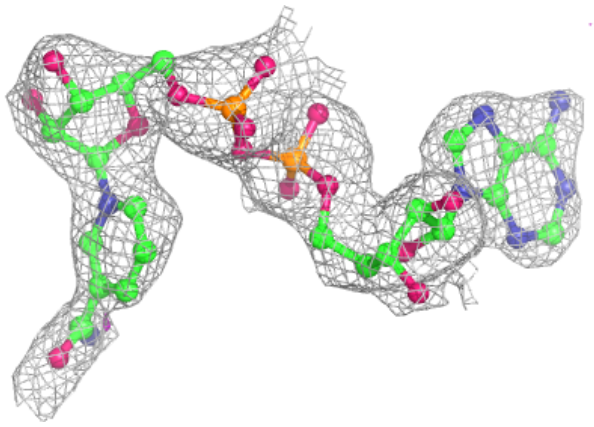


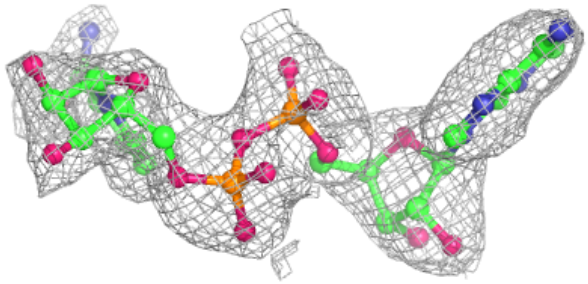


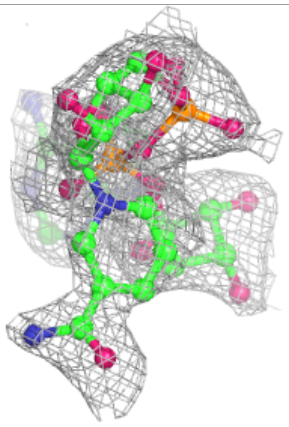


Electron density around NAI A 1502:

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

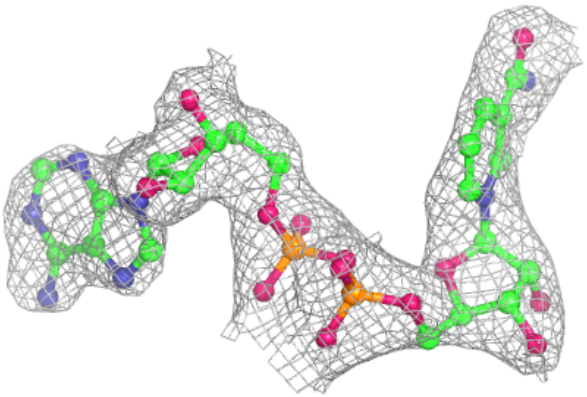


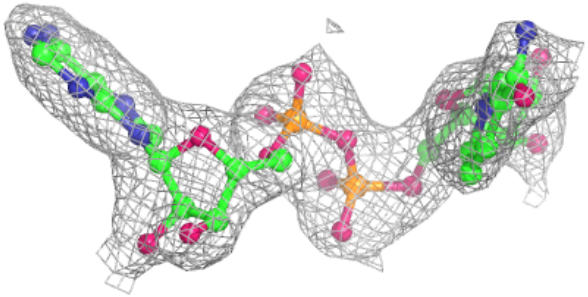


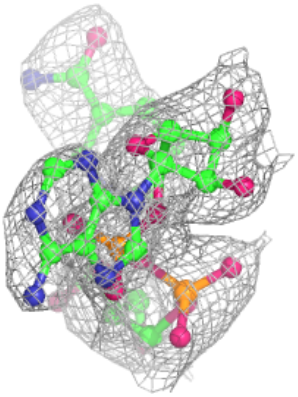


Electron density around NAI G 7502:

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

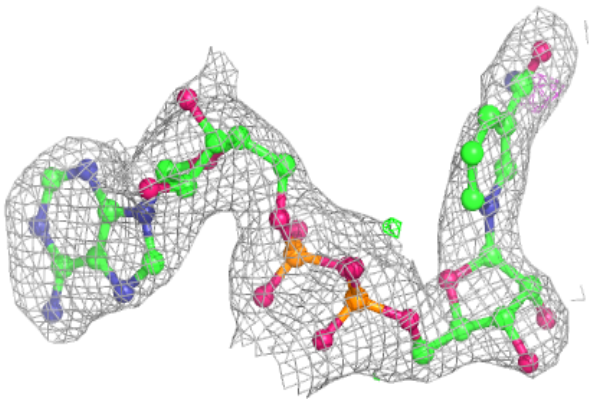


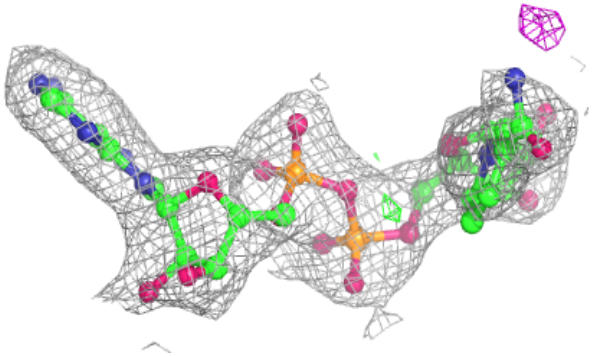


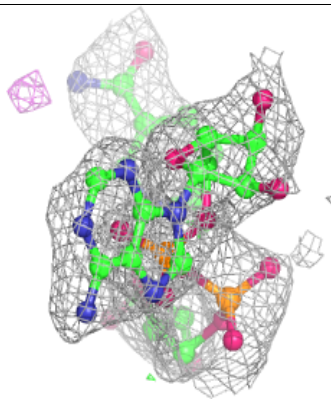


Electron density around NAI D 4502:

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

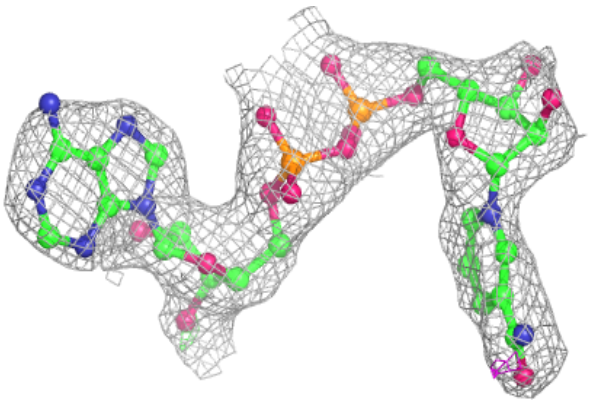


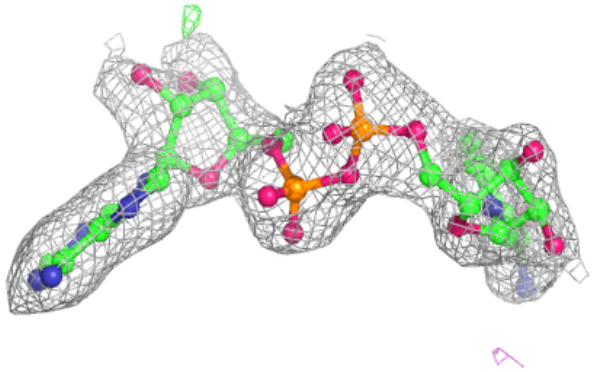


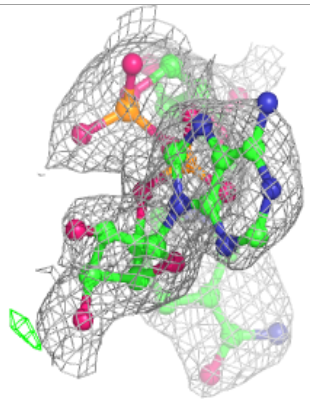


Electron density around NAI B 2502:

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

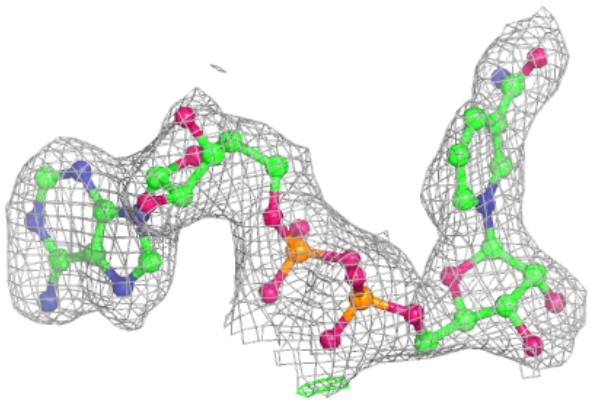


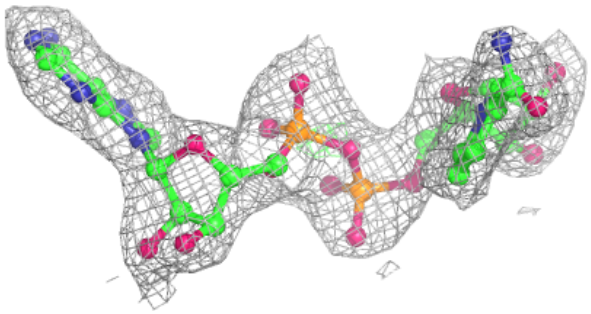


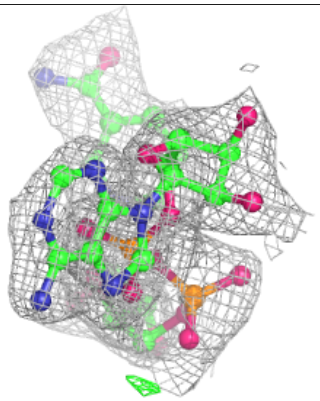


Electron density around NAI C 3502:

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

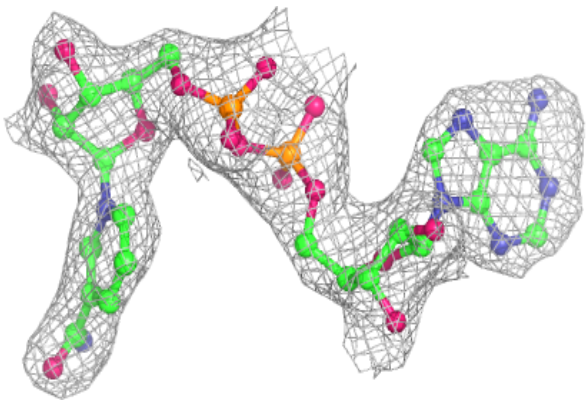


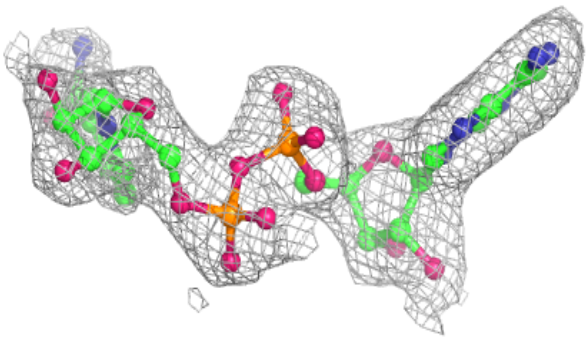


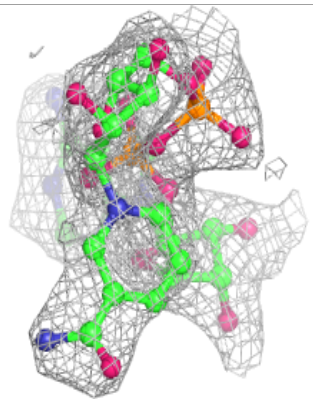


Electron density around NAI E 5502:

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

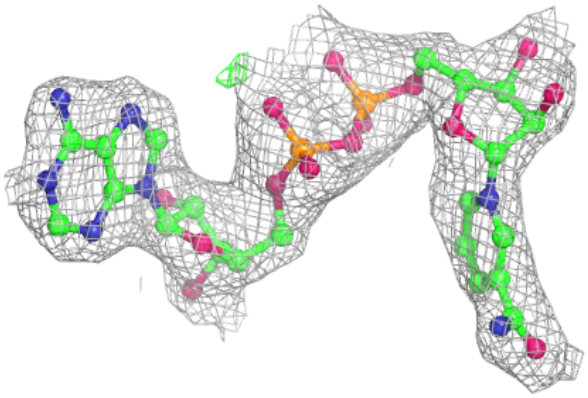


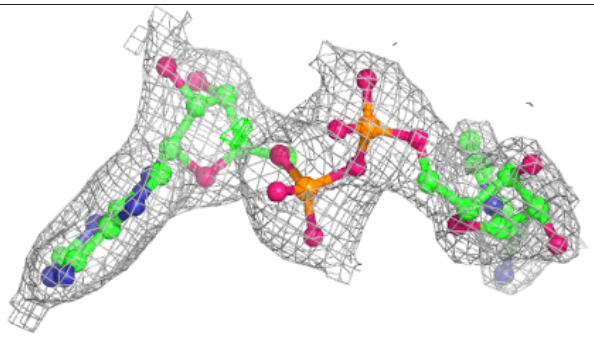


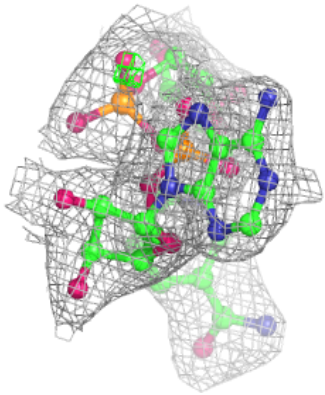


Electron density around NAI F 6502:

$2mF_o$-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.