



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:50 AM UTC

PDB ID : 7JSO / pdb_00007jso
Title : P. syringae AldA Indole-3-Acetaldehyde Dehydrogenase C302A mutant in complex with NAD⁺ and IAA
Authors : Jez, J.M.
Deposited on : 2020-08-15
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

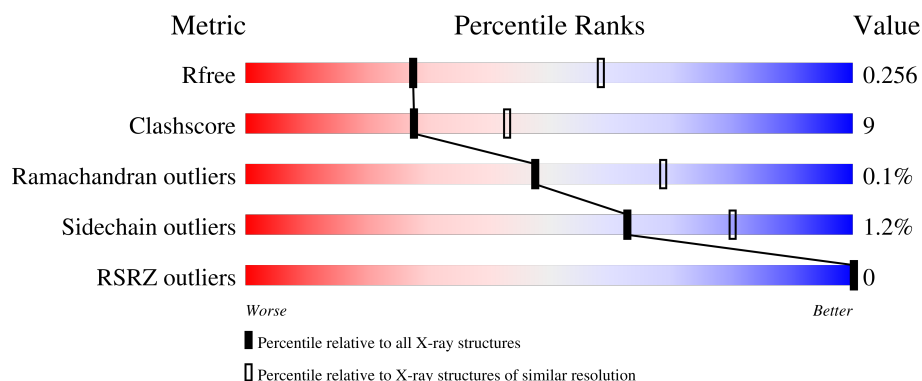
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	497	82% 18%
1	B	497	81% 18%
1	C	497	80% 19%
1	D	497	80% 19%
1	E	497	78% 21%

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Mol	Chain	Length	Quality of chain
1	F	497	 78%21%
1	G	497	 80%19%.
1	H	497	 78%21%.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAI	A	700	X	-	-	-
2	NAI	B	700	X	-	-	-
2	NAI	C	700	X	-	-	-
2	NAI	D	700	X	-	-	-
2	NAI	E	700	X	-	-	-
2	NAI	F	700	X	-	-	-
2	NAI	G	700	X	-	-	-
2	NAI	H	700	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29992 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.

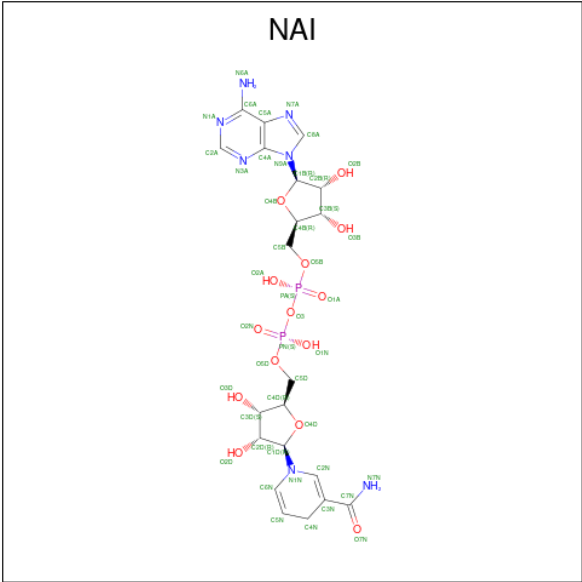
- Molecule 1 is a protein called Aldehyde dehydrogenase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			
1	B	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			
1	C	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			
1	D	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			
1	E	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			
1	F	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			
1	G	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			
1	H	495	Total	C	N	O	S	0	0	0
			3692	2333	638	707	14			

There are 8 discrepancies between the modelled and reference sequences:

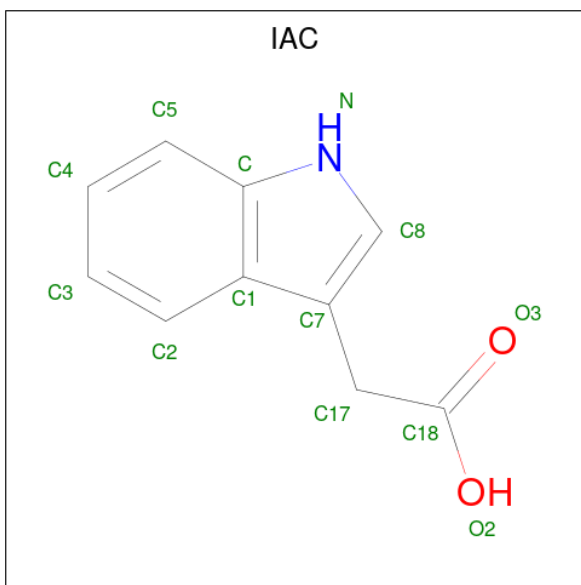
Chain	Residue	Modelled	Actual	Comment	Reference
A	302	ALA	CYS	engineered mutation	UNP Q88BC5
B	302	ALA	CYS	engineered mutation	UNP Q88BC5
C	302	ALA	CYS	engineered mutation	UNP Q88BC5
D	302	ALA	CYS	engineered mutation	UNP Q88BC5
E	302	ALA	CYS	engineered mutation	UNP Q88BC5
F	302	ALA	CYS	engineered mutation	UNP Q88BC5
G	302	ALA	CYS	engineered mutation	UNP Q88BC5
H	302	ALA	CYS	engineered mutation	UNP Q88BC5

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 1H-INDOL-3-YLACETIC ACID (CCD ID: IAC) (formula: C₁₀H₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	10	1	2		
3	B	1	Total	C	N	O	0	0
			13	10	1	2		
3	C	1	Total	C	N	O	0	0
			13	10	1	2		
3	D	1	Total	C	N	O	0	0
			13	10	1	2		
3	E	1	Total	C	N	O	0	0
			13	10	1	2		
3	F	1	Total	C	N	O	0	0
			13	10	1	2		
3	G	1	Total	C	N	O	0	0
			13	10	1	2		
3	H	1	Total	C	N	O	0	0
			13	10	1	2		

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.

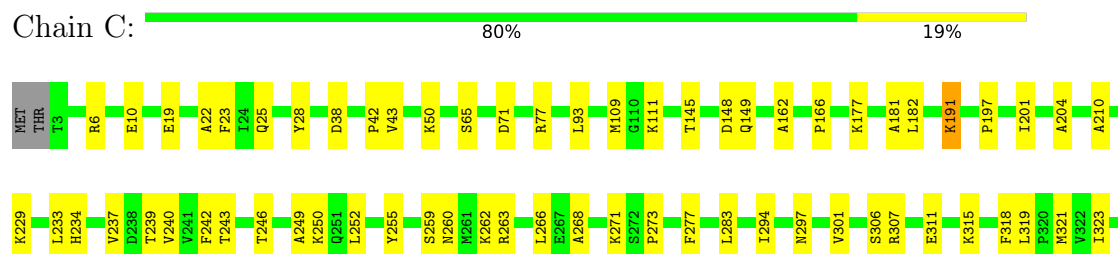
- Molecule 1: Aldehyde dehydrogenase family protein



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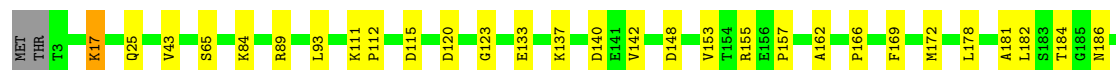
- Molecule 1: Aldehyde dehydrogenase family protein

Chain D: 80% 19%



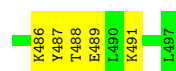
- Molecule 1: Aldehyde dehydrogenase family protein

Chain E: 78% 21%



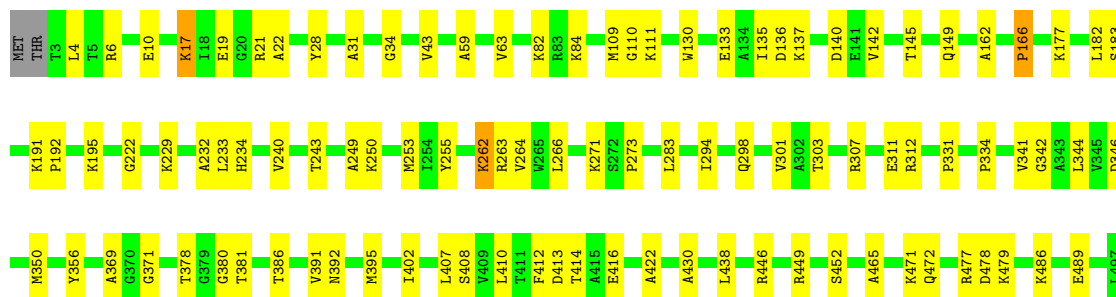
- Molecule 1: Aldehyde dehydrogenase family protein

Chain F: 78% 21%



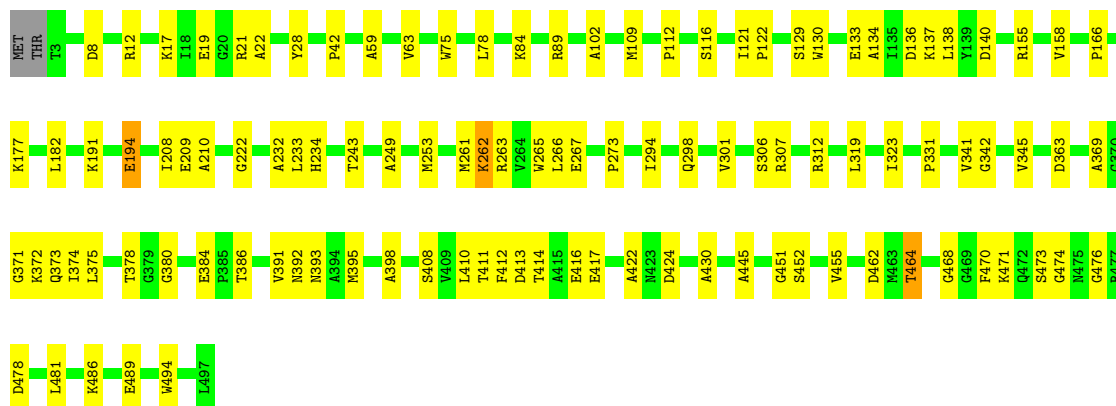
- Molecule 1: Aldehyde dehydrogenase family protein

Chain G:  80% 19% .



• Molecule 1: Aldehyde dehydrogenase family protein

Chain H:  78% 21% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	333.82Å 161.09Å 85.00Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	47.89 – 2.85 47.89 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.89-2.85) 98.3 (47.89-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.216 , 0.254 0.217 , 0.256	Depositor DCC
R_{free} test set	2006 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.438 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29992	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 94.87 % 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 2.1084e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/3764	0.63	1/5120 (0.0%)
1	B	0.40	0/3764	0.56	0/5120
1	C	0.41	0/3764	0.60	0/5120
1	D	0.57	1/3764 (0.0%)	0.61	1/5120 (0.0%)
1	E	0.46	1/3764 (0.0%)	0.64	1/5120 (0.0%)
1	F	0.47	1/3764 (0.0%)	0.58	0/5120
1	G	0.46	2/3764 (0.1%)	0.63	2/5120 (0.0%)
1	H	0.44	0/3764	0.60	0/5120
All	All	0.46	5/30112 (0.0%)	0.61	5/40960 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	259	SER	CA-C	-22.42	1.41	1.52
1	F	226	THR	CA-C	-14.29	1.43	1.52
1	G	17	LYS	CD-CE	-8.11	1.28	1.52
1	E	17	LYS	CG-CD	6.57	1.72	1.52
1	G	192	PRO	C-O	-6.02	1.16	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	LYS	CD-CE-NZ	-8.24	85.54	111.90
1	G	17	LYS	CB-CG-CD	7.75	129.14	111.30
1	D	259	SER	O-C-N	-6.13	116.29	120.83
1	A	235	MET	CA-CB-CG	-5.98	102.14	114.10
1	G	17	LYS	CA-CB-CG	-5.25	103.59	114.10

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	3692	0	3689	71	0
1	B	3692	0	3689	67	0
1	C	3692	0	3689	61	0
1	D	3692	0	3689	65	0
1	E	3692	0	3689	74	3
1	F	3692	0	3689	70	0
1	G	3692	0	3689	64	3
1	H	3692	0	3689	83	0
2	A	44	0	24	4	0
2	B	44	0	24	4	0
2	C	44	0	26	2	0
2	D	44	0	25	2	0
2	E	44	0	26	4	0
2	F	44	0	26	4	0
2	G	44	0	25	1	0
2	H	44	0	26	3	0
3	A	13	0	8	4	0
3	B	13	0	8	3	0
3	C	13	0	8	3	0
3	D	13	0	8	3	0
3	E	13	0	8	3	0
3	F	13	0	8	3	0
3	G	13	0	8	1	0
3	H	13	0	8	1	0
All	All	29992	0	29778	535	3

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 9.

All (535) 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:H:312:ARG:HH22	1:H:413:ASP:HB2	1.22	1.04
1:G:312:ARG:HH22	1:G:413:ASP:HB2	1.22	1.00
1:E:350:MET:HE2	1:E:381:THR:HG22	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:VAL:HG13	3:A:701:IAC:H172	1.51	0.92
1:E:191:LYS:HD2	1:E:220:LEU:O	1.70	0.91
1:G:19:GLU:OE1	1:G:21:ARG:NH1	2.06	0.88
1:H:84:LYS:NZ	1:H:136:ASP:OD2	2.06	0.87
1:H:312:ARG:NH2	1:H:413:ASP:HB2	1.90	0.86
1:F:392:ASN:HD22	1:F:394:ALA:H	1.22	0.83
1:A:350:MET:HE1	1:A:382:TYR:H	1.46	0.80
1:F:109:MET:SD	1:F:111:LYS:HE2	2.22	0.79
1:F:109:MET:SD	1:F:111:LYS:CE	2.73	0.77
1:F:240:VAL:HG23	1:F:262:LYS:HD2	1.65	0.76
1:H:298:GLN:HE21	1:H:342:GLY:H	1.33	0.76
1:F:17:LYS:HG2	1:H:17:LYS:HG3	1.68	0.75
1:C:25:GLN:NE2	1:C:65:SER:OG	2.18	0.75
1:B:301:VAL:HG13	3:B:701:IAC:H172	1.67	0.75
1:E:123:GLY:HA3	1:E:172:MET:HE2	1.68	0.75
1:G:84:LYS:NZ	1:G:136:ASP:OD2	2.14	0.75
1:G:312:ARG:NH2	1:G:413:ASP:HB2	1.99	0.74
1:A:25:GLN:NE2	1:A:65:SER:OG	2.21	0.74
1:F:274:ASN:HB3	1:F:308:LEU:HD12	1.69	0.74
1:F:263:ARG:NH2	1:F:489:GLU:OE1	2.21	0.73
1:A:274:ASN:HB3	1:A:308:LEU:HD12	1.70	0.73
1:E:240:VAL:HG23	1:E:262:LYS:HD2	1.71	0.72
1:A:166:PRO:HD3	1:A:243:THR:HB	1.72	0.72
1:F:301:VAL:HG13	3:F:701:IAC:H172	1.72	0.71
1:G:271:LYS:O	1:G:307:ARG:NH1	2.24	0.71
1:H:391:VAL:HA	1:H:395:MET:CE	2.21	0.70
1:E:274:ASN:HB3	1:E:308:LEU:HD12	1.74	0.70
1:F:111:LYS:NZ	1:F:168:ASN:O	2.22	0.70
1:E:169:PHE:CZ	3:E:701:IAC:H2	2.27	0.69
1:E:438:LEU:HD12	1:G:438:LEU:HD12	1.74	0.69
1:F:318:PHE:HA	1:F:321:MET:HE3	1.72	0.69
1:A:350:MET:HE2	1:A:381:THR:CB	2.22	0.69
1:H:462:ASP:OD1	1:H:464:THR:OG1	2.11	0.69
2:C:700:NAI:O5D	2:C:700:NAI:H6N	1.94	0.68
1:E:350:MET:HE2	1:E:381:THR:CG2	2.19	0.68
1:H:476:GLY:HA3	1:H:486:LYS:HE3	1.76	0.68
1:D:43:VAL:HG22	1:D:334:PRO:HG2	1.76	0.68
1:A:350:MET:HE1	1:A:382:TYR:N	2.07	0.68
2:E:700:NAI:O5D	2:E:700:NAI:H6N	1.94	0.67
1:G:109:MET:SD	1:G:111:LYS:HE3	2.34	0.67
1:G:311:GLU:HG3	1:G:412:PHE:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:HG22	1:B:334:PRO:HG2	1.77	0.67
2:H:700:NAI:O5D	2:H:700:NAI:H6N	1.94	0.67
1:G:249:ALA:HB1	1:G:266:LEU:HD13	1.77	0.67
1:E:157:PRO:HG3	1:E:184:THR:O	1.96	0.66
1:A:350:MET:HE2	1:A:381:THR:HB	1.75	0.66
1:C:43:VAL:HG22	1:C:334:PRO:HG2	1.78	0.66
1:D:162:ALA:HB3	1:D:240:VAL:HG22	1.79	0.65
1:H:89:ARG:NH1	1:H:210:ALA:O	2.30	0.64
1:B:477:ARG:O	1:B:486:LYS:HE2	1.97	0.64
1:D:177:LYS:NZ	1:D:478:ASP:OD2	2.30	0.64
1:D:234:HIS:O	1:D:262:LYS:NZ	2.30	0.64
1:B:129:SER:O	1:B:133:GLU:HG3	1.97	0.64
1:B:449:ARG:NH2	1:D:157:PRO:O	2.30	0.64
1:E:467:PHE:CZ	3:E:701:IAC:H8	2.33	0.64
2:F:700:NAI:O5D	2:F:700:NAI:H6N	1.97	0.64
1:B:166:PRO:HD3	1:B:243:THR:HB	1.80	0.64
1:F:109:MET:SD	1:F:111:LYS:HE3	2.37	0.63
1:E:89:ARG:NH1	1:E:210:ALA:O	2.31	0.63
1:F:156:GLU:OE1	1:F:491:LYS:HE3	1.98	0.63
1:F:467:PHE:CZ	3:F:701:IAC:H8	2.33	0.63
1:G:253:MET:HG2	1:G:264:VAL:HG11	1.81	0.63
1:F:166:PRO:HD3	1:F:243:THR:HB	1.80	0.63
1:G:477:ARG:O	1:G:486:LYS:NZ	2.32	0.63
1:H:378:THR:HB	1:H:380:GLY:H	1.64	0.63
1:H:301:VAL:HG13	3:H:701:IAC:H172	1.81	0.62
1:F:315:LYS:NZ	1:F:389:ASP:OD2	2.32	0.62
1:H:234:HIS:O	1:H:262:LYS:NZ	2.32	0.62
1:B:350:MET:HE1	1:B:381:THR:HA	1.79	0.62
1:F:366:ARG:NH1	1:F:389:ASP:OD2	2.33	0.62
1:F:392:ASN:ND2	1:F:394:ALA:H	1.95	0.61
1:E:301:VAL:HG13	3:E:701:IAC:H172	1.81	0.61
1:E:162:ALA:HB3	1:E:240:VAL:HG22	1.81	0.61
1:G:234:HIS:O	1:G:262:LYS:NZ	2.33	0.61
1:B:350:MET:HE2	1:B:381:THR:HG22	1.83	0.61
1:H:8:ASP:O	1:H:12:ARG:HD3	2.01	0.61
1:C:301:VAL:HG13	3:C:701:IAC:H172	1.81	0.61
1:C:162:ALA:HB3	1:C:240:VAL:HG22	1.82	0.60
1:F:89:ARG:NH1	1:F:210:ALA:O	2.35	0.60
1:G:191:LYS:HE2	1:G:222:GLY:O	2.01	0.60
1:E:415:ALA:O	1:E:419:ILE:HG13	2.02	0.60
1:G:250:LYS:NZ	1:G:472:GLN:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:PRO:HG3	1:B:184:THR:O	2.02	0.60
1:A:318:PHE:HA	1:A:321:MET:HE3	1.84	0.59
1:B:166:PRO:HD2	1:B:173:MET:HG2	1.84	0.59
1:D:273:PRO:HG3	1:D:422:ALA:HB1	1.84	0.59
1:A:93:LEU:HB3	1:A:206:LEU:HD22	1.84	0.59
1:F:169:PHE:CZ	3:F:701:IAC:H2	2.36	0.59
1:E:372:LYS:O	1:E:384:GLU:HG3	2.02	0.59
1:B:350:MET:CE	1:B:381:THR:HA	2.31	0.59
1:B:312:ARG:HG2	1:B:411:THR:HB	1.84	0.59
1:D:166:PRO:HD3	1:D:243:THR:HB	1.84	0.59
1:B:13:ALA:HA	1:B:103:LEU:HD21	1.85	0.58
1:B:467:PHE:CZ	3:B:701:IAC:H8	2.38	0.58
1:E:302:ALA:HB2	2:E:700:NAI:C7N	2.33	0.58
1:F:415:ALA:O	1:F:419:ILE:HG13	2.03	0.58
1:C:166:PRO:HD3	1:C:243:THR:HB	1.85	0.58
1:G:232:ALA:O	1:G:262:LYS:HE3	2.04	0.58
1:C:249:ALA:HB1	1:C:266:LEU:HD13	1.85	0.58
1:F:157:PRO:HG3	1:F:184:THR:O	2.03	0.58
1:B:93:LEU:HB3	1:B:206:LEU:HD22	1.85	0.58
1:F:350:MET:HE1	1:F:373:GLN:NE2	2.19	0.58
1:H:298:GLN:HE21	1:H:342:GLY:N	1.99	0.57
1:E:142:VAL:HB	1:G:140:ASP:HB2	1.87	0.57
2:A:700:NAI:O5D	2:A:700:NAI:H6N	2.04	0.57
1:B:241:VAL:HG12	1:B:265:TRP:HB2	1.87	0.57
1:C:318:PHE:HA	1:C:321:MET:HE3	1.85	0.57
1:A:374:ILE:HG23	1:A:375:LEU:HG	1.87	0.57
2:B:700:NAI:O5D	2:B:700:NAI:H6N	2.05	0.57
1:G:301:VAL:HG13	3:G:701:IAC:H172	1.87	0.57
1:D:392:ASN:ND2	1:D:395:MET:HG3	2.20	0.57
1:E:25:GLN:OE1	1:E:65:SER:OG	2.22	0.56
2:G:700:NAI:O5D	2:G:700:NAI:H6N	2.04	0.56
1:A:157:PRO:HG3	1:A:184:THR:O	2.06	0.56
1:A:312:ARG:HG2	1:A:411:THR:HB	1.87	0.56
1:H:392:ASN:H	1:H:395:MET:HE2	1.70	0.56
1:A:350:MET:HE2	1:A:381:THR:CA	2.36	0.56
1:E:268:ALA:O	2:E:700:NAI:N7N	2.38	0.56
1:F:372:LYS:O	1:F:384:GLU:HG3	2.05	0.56
1:C:385:PRO:HA	1:C:405:PRO:HB2	1.86	0.56
1:A:169:PHE:CE2	3:A:701:IAC:H171	2.41	0.56
1:A:350:MET:CE	1:A:381:THR:HA	2.35	0.56
1:B:302:ALA:HB2	2:B:700:NAI:C7N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:LEU:HB2	1:F:407:LEU:HD11	1.86	0.56
2:D:700:NAI:O5D	2:D:700:NAI:H6N	2.06	0.56
1:H:261:MET:O	1:H:261:MET:HG2	2.06	0.56
1:H:391:VAL:HA	1:H:395:MET:HE2	1.88	0.56
1:B:282:ASP:HB3	1:B:285:ALA:HB3	1.89	0.55
1:F:232:ALA:O	1:F:262:LYS:HE3	2.06	0.55
1:C:177:LYS:NZ	1:C:478:ASP:OD1	2.32	0.55
1:H:121:ILE:HB	1:H:122:PRO:HD3	1.88	0.55
1:G:298:GLN:HE21	1:G:342:GLY:H	1.53	0.55
1:C:38:ASP:OD1	1:C:50:LYS:HE2	2.06	0.55
1:E:289:SER:O	1:E:293:ALA:N	2.38	0.55
1:A:19:GLU:HG2	1:D:17:LYS:HB3	1.89	0.55
1:B:356:TYR:HB3	1:B:402:ILE:HD13	1.87	0.55
1:C:391:VAL:HG11	1:C:408:SER:HB3	1.89	0.55
1:F:312:ARG:NH1	1:F:411:THR:OG1	2.39	0.55
1:C:480:SER:OG	1:C:481:LEU:N	2.39	0.55
1:E:260:ASN:OD1	1:E:262:LYS:HG3	2.07	0.55
1:F:155:ARG:NH1	1:F:488:THR:OG1	2.40	0.54
1:D:191:LYS:C	1:D:191:LYS:HD2	2.31	0.54
1:C:374:ILE:HD12	1:C:375:LEU:HG	1.88	0.54
1:B:350:MET:HE2	1:B:381:THR:CB	2.37	0.54
1:H:414:THR:HB	1:H:416:GLU:HG2	1.88	0.54
1:B:162:ALA:HB3	1:B:240:VAL:HG23	1.90	0.54
1:G:414:THR:HB	1:G:416:GLU:HG2	1.90	0.54
1:H:294:ILE:HD13	1:H:306:SER:HA	1.89	0.54
1:B:13:ALA:HB1	1:B:107:LEU:HD11	1.89	0.54
1:B:21:ARG:HB3	1:B:29:THR:O	2.08	0.54
1:B:33:SER:OG	1:B:35:GLU:HG3	2.08	0.54
1:B:169:PHE:CZ	3:B:701:IAC:H2	2.43	0.54
1:A:162:ALA:HB3	1:A:240:VAL:HG23	1.90	0.53
1:A:392:ASN:H	1:A:395:MET:HE3	1.73	0.53
1:F:240:VAL:CG2	1:F:262:LYS:HD2	2.37	0.53
1:C:294:ILE:HD13	1:C:306:SER:HA	1.91	0.53
1:D:191:LYS:NZ	1:D:192:PRO:O	2.40	0.53
1:A:232:ALA:O	1:A:262:LYS:CE	2.57	0.53
1:D:301:VAL:HG13	3:D:701:IAC:H172	1.91	0.53
1:H:249:ALA:HB1	1:H:266:LEU:HD13	1.89	0.53
1:C:315:LYS:HD3	1:C:411:THR:HG22	1.89	0.53
1:G:195:LYS:HE2	1:G:346:ASP:OD2	2.09	0.53
1:D:480:SER:OG	1:D:481:LEU:N	2.42	0.53
1:E:166:PRO:HD3	1:E:243:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:LYS:HD3	1:E:227:VAL:HG13	1.90	0.53
1:A:301:VAL:CG1	3:A:701:IAC:H172	2.34	0.52
1:B:89:ARG:NH1	1:B:210:ALA:O	2.42	0.52
1:C:315:LYS:HD3	1:C:411:THR:CG2	2.38	0.52
1:E:43:VAL:HG22	1:E:334:PRO:HG2	1.91	0.52
1:G:177:LYS:NZ	1:G:243:THR:OG1	2.28	0.52
1:H:191:LYS:HE2	1:H:222:GLY:O	2.08	0.52
1:A:392:ASN:HD21	1:A:394:ALA:HB3	1.75	0.52
1:C:350:MET:HE2	1:C:381:THR:HG22	1.91	0.52
1:D:467:PHE:CE2	3:D:701:IAC:H8	2.44	0.52
1:A:302:ALA:HB2	2:A:700:NAI:C7N	2.40	0.52
1:C:469:GLY:HA3	1:C:473:SER:HB3	1.92	0.52
1:B:311:GLU:HG3	1:B:412:PHE:CE1	2.44	0.52
1:F:268:ALA:O	2:F:700:NAI:N7N	2.42	0.52
1:D:169:PHE:CE2	3:D:701:IAC:H171	2.45	0.52
1:D:93:LEU:HD12	1:D:210:ALA:HB2	1.91	0.51
1:D:294:ILE:HD13	1:D:306:SER:HA	1.92	0.51
1:G:43:VAL:HG22	1:G:334:PRO:HG2	1.93	0.51
1:E:133:GLU:O	1:E:137:LYS:NZ	2.44	0.51
1:F:294:ILE:HD13	1:F:306:SER:HA	1.92	0.51
1:C:392:ASN:N	1:C:395:MET:HE3	2.26	0.51
1:F:302:ALA:HB2	2:F:700:NAI:C7N	2.41	0.51
1:A:375:LEU:O	1:A:378:THR:OG1	2.24	0.51
1:C:6:ARG:O	1:C:10:GLU:HG3	2.11	0.51
1:H:19:GLU:OE2	1:H:21:ARG:NH2	2.32	0.51
1:H:232:ALA:O	1:H:262:LYS:HE3	2.11	0.51
1:H:470:PHE:HB3	1:H:471:LYS:HG3	1.92	0.51
1:A:336:ASP:HB3	1:A:339:THR:OG1	2.11	0.51
1:D:263:ARG:NH2	1:D:489:GLU:OE1	2.35	0.51
1:F:17:LYS:HE2	1:H:19:GLU:HG2	1.91	0.51
1:A:186:ASN:ND2	1:A:487:TYR:HB3	2.25	0.50
1:A:243:THR:HG23	1:A:267:GLU:HB3	1.92	0.50
1:C:319:LEU:O	1:C:323:ILE:HG13	2.10	0.50
1:E:244:GLY:HA2	2:E:700:NAI:H4N	1.92	0.50
1:E:273:PRO:HG3	1:E:422:ALA:HB1	1.93	0.50
1:H:476:GLY:HA3	1:H:486:LYS:CE	2.41	0.50
1:E:250:LYS:HG3	1:H:261:MET:HB2	1.94	0.50
1:B:191:LYS:NZ	1:B:192:PRO:O	2.33	0.50
1:B:385:PRO:HA	1:B:405:PRO:HB2	1.92	0.50
1:G:137:LYS:HD2	1:H:134:ALA:HB2	1.94	0.50
1:H:273:PRO:HG3	1:H:422:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:470:PHE:O	1:H:473:SER:HB2	2.11	0.50
1:C:467:PHE:CZ	3:C:701:IAC:H8	2.47	0.50
1:D:476:GLY:O	1:D:477:ARG:NH1	2.43	0.50
1:G:430:ALA:HA	1:G:452:SER:O	2.12	0.50
1:B:489:GLU:HG2	1:D:470:PHE:CE1	2.46	0.49
1:F:250:LYS:NZ	1:F:472:GLN:OE1	2.45	0.49
1:H:265:TRP:HB3	1:H:486:LYS:HE2	1.94	0.49
1:E:140:ASP:HB3	1:E:153:VAL:O	2.13	0.49
1:E:241:VAL:HG12	1:E:265:TRP:HB2	1.95	0.49
1:G:229:LYS:HG3	1:G:255:TYR:CZ	2.48	0.49
1:H:75:TRP:CE3	1:H:78:LEU:HD23	2.48	0.49
1:G:130:TRP:CZ2	1:H:137:LYS:HD3	2.48	0.49
1:B:391:VAL:HG11	1:B:408:SER:HB3	1.94	0.49
1:C:23:PHE:CD2	1:C:204:ALA:HB1	2.48	0.49
1:A:261:MET:HG3	1:C:250:LYS:HG2	1.94	0.49
1:H:363:ASP:HB3	1:H:395:MET:SD	2.53	0.49
1:A:385:PRO:HA	1:A:405:PRO:HB2	1.95	0.48
1:D:392:ASN:H	1:D:395:MET:HE3	1.78	0.48
1:G:294:ILE:HG12	1:G:407:LEU:HB2	1.95	0.48
1:E:468:GLY:HA3	1:E:477:ARG:HD3	1.95	0.48
1:C:311:GLU:HG3	1:C:412:PHE:CE1	2.48	0.48
1:C:467:PHE:CE2	3:C:701:IAC:H8	2.48	0.48
2:C:700:NAI:O5B	2:C:700:NAI:H1B	2.12	0.48
1:E:311:GLU:HG3	1:E:412:PHE:CE1	2.49	0.48
1:H:177:LYS:HZ1	1:H:243:THR:HG1	1.59	0.48
1:A:43:VAL:HG22	1:A:334:PRO:HG2	1.95	0.48
1:D:22:ALA:O	1:D:28:TYR:HA	2.13	0.48
1:G:350:MET:HG3	1:G:381:THR:HB	1.95	0.48
1:G:391:VAL:HG11	1:G:408:SER:HB3	1.96	0.48
1:C:271:LYS:NZ	1:C:397:ILE:O	2.47	0.48
1:E:120:ASP:HA	1:E:172:MET:HE3	1.94	0.48
1:C:181:ALA:HB2	1:C:487:TYR:CE1	2.49	0.48
1:C:283:LEU:HD23	1:C:283:LEU:HA	1.59	0.48
2:D:700:NAI:O5B	2:D:700:NAI:H1B	2.13	0.48
1:F:25:GLN:OE1	1:F:65:SER:OG	2.31	0.48
1:H:312:ARG:HG2	1:H:411:THR:HB	1.96	0.48
1:B:181:ALA:HB2	1:B:487:TYR:CE1	2.49	0.47
1:B:195:LYS:HD3	1:B:346:ASP:OD2	2.14	0.47
1:C:22:ALA:O	1:C:28:TYR:HA	2.14	0.47
1:C:111:LYS:HE3	1:C:297:ASN:OD1	2.13	0.47
1:H:166:PRO:HD3	1:H:243:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:700:NAI:H6N	2:H:700:NAI:C5D	2.43	0.47
1:G:22:ALA:O	1:G:28:TYR:HA	2.14	0.47
1:G:136:ASP:HB2	1:G:137:LYS:HZ2	1.78	0.47
1:B:158:VAL:O	1:D:449:ARG:NH2	2.47	0.47
1:D:312:ARG:HG3	1:D:412:PHE:O	2.14	0.47
1:H:392:ASN:O	1:H:395:MET:HG3	2.14	0.47
1:B:243:THR:HG23	1:B:267:GLU:HB3	1.97	0.47
1:G:130:TRP:CE2	1:H:137:LYS:HE3	2.50	0.47
1:H:369:ALA:O	1:H:386:THR:HA	2.14	0.47
1:D:63:VAL:HG11	1:D:234:HIS:CE1	2.49	0.47
1:E:263:ARG:NH2	1:H:474:GLY:O	2.48	0.47
1:F:181:ALA:HB2	1:F:487:TYR:CE1	2.49	0.47
1:F:283:LEU:HA	1:F:283:LEU:HD23	1.69	0.47
1:G:135:ILE:HD11	1:G:183:SER:HB3	1.96	0.47
1:B:25:GLN:OE1	1:B:65:SER:OG	2.29	0.47
1:B:350:MET:HE2	1:B:381:THR:CG2	2.43	0.47
1:C:273:PRO:HG3	1:C:422:ALA:HB1	1.97	0.47
1:D:414:THR:OG1	1:D:417:GLU:HG3	2.14	0.47
1:E:191:LYS:NZ	1:E:222:GLY:O	2.47	0.47
1:E:263:ARG:HG3	1:E:263:ARG:HH11	1.80	0.47
1:H:430:ALA:HA	1:H:452:SER:O	2.15	0.47
1:A:265:TRP:CE2	1:A:486:LYS:HB3	2.50	0.47
1:E:181:ALA:HB2	1:E:487:TYR:CE1	2.50	0.47
1:F:241:VAL:HG12	1:F:265:TRP:HB2	1.97	0.47
1:G:378:THR:HB	1:G:380:GLY:H	1.79	0.47
1:H:391:VAL:HG11	1:H:408:SER:HB3	1.97	0.47
1:D:176:TRP:CZ2	1:D:479:LYS:HD3	2.50	0.47
1:E:178:LEU:O	1:E:182:LEU:HB2	2.15	0.47
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.75	0.46
1:A:282:ASP:HB3	1:A:285:ALA:HB3	1.97	0.46
1:D:242:PHE:CD1	1:D:252:LEU:HD11	2.50	0.46
1:A:13:ALA:HB1	1:A:107:LEU:HD11	1.97	0.46
1:B:13:ALA:CA	1:B:103:LEU:HD21	2.46	0.46
1:B:392:ASN:HD21	1:B:394:ALA:HB3	1.80	0.46
1:G:145:THR:HB	1:G:149:GLN:HB3	1.96	0.46
1:H:158:VAL:HG12	1:H:489:GLU:HG2	1.98	0.46
1:A:259:SER:HB2	1:A:260:ASN:H	1.48	0.46
1:D:283:LEU:HA	1:D:283:LEU:HD23	1.58	0.46
1:D:350:MET:HE1	1:D:373:GLN:HE22	1.79	0.46
1:E:155:ARG:HB3	1:E:488:THR:HG21	1.98	0.46
1:F:483:ALA:O	1:F:486:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:344:LEU:HD13	1:G:350:MET:HA	1.98	0.46
1:H:102:ALA:HB1	1:H:116:SER:HB3	1.98	0.46
1:H:319:LEU:O	1:H:323:ILE:HG13	2.15	0.46
1:A:308:LEU:HB2	1:A:407:LEU:HD11	1.97	0.46
1:C:197:PRO:O	1:C:201:ILE:HG13	2.15	0.46
1:F:249:ALA:HB1	1:F:266:LEU:HD22	1.98	0.46
1:G:331:PRO:HA	1:G:341:VAL:HB	1.98	0.46
1:A:181:ALA:HB2	1:A:487:TYR:CE1	2.51	0.46
1:A:184:THR:OG1	1:A:186:ASN:ND2	2.49	0.46
1:A:212:ILE:HD13	1:A:212:ILE:HA	1.77	0.46
1:A:432:ALA:HA	1:A:454:TRP:O	2.16	0.46
1:C:250:LYS:NZ	1:C:472:GLN:OE1	2.48	0.46
1:D:84:LYS:HG3	1:D:132:GLY:O	2.15	0.46
1:F:123:GLY:HA3	1:F:172:MET:HE3	1.97	0.46
1:G:465:ALA:O	1:G:479:LYS:HE3	2.15	0.46
1:B:263:ARG:HH21	1:B:489:GLU:CD	2.24	0.46
1:C:148:ASP:OD1	1:C:148:ASP:N	2.48	0.46
1:E:184:THR:OG1	1:E:186:ASN:ND2	2.49	0.46
1:A:451:GLY:HA3	1:A:468:GLY:O	2.16	0.46
1:D:312:ARG:HD3	1:D:413:ASP:OD1	2.16	0.46
1:G:137:LYS:HE3	1:H:130:TRP:CE2	2.51	0.46
1:B:191:LYS:C	1:B:191:LYS:HD2	2.41	0.46
1:D:109:MET:HE2	1:D:109:MET:HB2	1.88	0.46
1:D:208:ILE:HD13	1:D:208:ILE:HA	1.77	0.46
1:E:308:LEU:HB2	1:E:407:LEU:HD11	1.98	0.46
1:H:8:ASP:O	1:H:12:ARG:CD	2.63	0.46
1:C:392:ASN:H	1:C:395:MET:HE3	1.80	0.45
1:D:129:SER:O	1:D:133:GLU:HG3	2.16	0.45
1:A:465:ALA:HB2	1:C:494:TRP:CZ2	2.50	0.45
1:E:253:MET:HE2	1:E:253:MET:HB3	1.81	0.45
1:E:366:ARG:NH1	1:E:389:ASP:OD2	2.49	0.45
1:F:392:ASN:H	1:F:395:MET:HE3	1.82	0.45
1:H:412:PHE:HB2	1:H:417:GLU:HG2	1.99	0.45
1:H:451:GLY:HA3	1:H:468:GLY:O	2.15	0.45
1:B:108:ASP:OD2	1:B:196:SER:HA	2.16	0.45
1:B:246:THR:HG23	1:D:261:MET:HE1	1.98	0.45
1:C:242:PHE:CD2	1:C:252:LEU:HD11	2.51	0.45
1:F:311:GLU:HG3	1:F:412:PHE:CE1	2.52	0.45
1:F:317:ARG:HG2	1:F:321:MET:HE2	1.98	0.45
1:H:253:MET:HE2	1:H:253:MET:HB3	1.87	0.45
1:F:326:LEU:HD22	1:F:387:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:LEU:O	1:B:378:THR:OG1	2.27	0.45
1:D:109:MET:SD	1:D:111:LYS:HB3	2.57	0.45
1:G:177:LYS:NZ	1:G:478:ASP:OD2	2.50	0.45
1:H:22:ALA:O	1:H:28:TYR:HA	2.16	0.45
1:H:391:VAL:O	1:H:410:LEU:HD13	2.17	0.45
1:B:286:ALA:HB2	1:B:434:TRP:CE3	2.52	0.45
1:G:449:ARG:HH12	1:G:471:LYS:NZ	2.15	0.45
1:A:167:TRP:CD1	1:A:195:LYS:HD2	2.51	0.45
1:A:260:ASN:OD1	1:A:262:LYS:HB3	2.17	0.45
1:H:243:THR:HA	1:H:267:GLU:O	2.17	0.45
1:A:141:GLU:OE1	1:C:482:HIS:NE2	2.33	0.45
1:A:350:MET:CE	1:A:381:THR:CA	2.94	0.45
1:C:229:LYS:HG3	1:C:255:TYR:CZ	2.52	0.45
1:D:237:VAL:O	1:D:260:ASN:ND2	2.49	0.45
1:E:148:ASP:OD1	1:E:148:ASP:N	2.50	0.45
1:F:234:HIS:O	1:F:262:LYS:NZ	2.50	0.45
1:H:129:SER:O	1:H:133:GLU:HG3	2.17	0.45
1:B:46:ARG:HE	1:B:46:ARG:HB3	1.47	0.45
1:D:369:ALA:O	1:D:386:THR:HA	2.17	0.45
1:H:372:LYS:O	1:H:384:GLU:HG2	2.17	0.45
1:A:145:THR:HB	1:A:149:GLN:HB2	1.98	0.44
1:C:237:VAL:O	1:C:260:ASN:ND2	2.43	0.44
1:A:241:VAL:HG12	1:A:265:TRP:HB2	1.99	0.44
1:F:425:THR:HG23	1:F:427:TYR:H	1.82	0.44
1:B:184:THR:OG1	1:B:186:ASN:ND2	2.50	0.44
1:B:403:PHE:HB2	2:B:700:NAI:O2D	2.18	0.44
1:C:479:LYS:O	1:C:480:SER:HB3	2.16	0.44
1:D:307:ARG:HD3	1:D:398:ALA:O	2.17	0.44
1:D:312:ARG:HG2	1:D:411:THR:HB	1.98	0.44
1:F:90:PHE:CD2	1:F:128:LEU:HD13	2.53	0.44
1:D:6:ARG:O	1:D:10:GLU:HG3	2.17	0.44
1:A:208:ILE:HD13	1:A:208:ILE:HA	1.85	0.44
1:D:38:ASP:HB3	1:D:40:ILE:HD11	1.98	0.44
1:E:432:ALA:HA	1:E:454:TRP:O	2.17	0.44
1:H:59:ALA:O	1:H:63:VAL:HG23	2.17	0.44
1:H:182:LEU:HD23	1:H:182:LEU:HA	1.65	0.44
2:A:700:NAI:O5B	2:A:700:NAI:H1B	2.17	0.44
1:B:492:SER:OG	1:D:466:PRO:HD2	2.18	0.44
1:H:177:LYS:NZ	1:H:478:ASP:OD2	2.50	0.44
1:C:410:LEU:HD12	1:C:410:LEU:N	2.33	0.44
1:B:59:ALA:O	1:B:63:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:THR:HB	1:C:149:GLN:HB2	2.00	0.44
1:D:208:ILE:HD13	1:D:212:ILE:O	2.18	0.44
1:E:491:LYS:NZ	1:H:445:ALA:O	2.50	0.44
1:F:195:LYS:HE3	1:F:346:ASP:OD2	2.17	0.44
1:G:6:ARG:O	1:G:10:GLU:HG3	2.18	0.44
1:H:371:GLY:N	1:H:386:THR:OG1	2.50	0.44
1:B:9:TRP:CE3	1:B:103:LEU:HD13	2.52	0.44
1:E:385:PRO:HA	1:E:405:PRO:HB2	2.00	0.44
1:F:13:ALA:N	1:F:103:LEU:HD21	2.33	0.44
1:B:169:PHE:O	1:B:173:MET:HB2	2.17	0.43
1:D:391:VAL:HG11	1:D:408:SER:HB3	1.99	0.43
1:F:263:ARG:NE	1:F:489:GLU:OE1	2.50	0.43
1:G:273:PRO:HG3	1:G:422:ALA:HB1	2.00	0.43
1:H:476:GLY:CA	1:H:486:LYS:HE3	2.47	0.43
2:H:700:NAI:O5B	2:H:700:NAI:H1B	2.18	0.43
1:B:253:MET:HB3	1:B:253:MET:HE2	1.87	0.43
1:D:331:PRO:HA	1:D:341:VAL:HB	1.99	0.43
1:E:430:ALA:HA	1:E:452:SER:O	2.19	0.43
1:F:112:PRO:O	1:F:115:ASP:HB2	2.19	0.43
1:C:277:PHE:HB2	1:C:434:TRP:O	2.18	0.43
1:G:133:GLU:O	1:G:137:LYS:NZ	2.50	0.43
1:D:249:ALA:HB1	1:D:266:LEU:HD13	2.01	0.43
1:G:392:ASN:H	1:G:395:MET:HE3	1.83	0.43
1:G:478:ASP:O	1:G:479:LYS:HB2	2.18	0.43
1:H:109:MET:HE2	1:H:109:MET:HB2	1.78	0.43
1:B:374:ILE:HG23	1:B:375:LEU:HG	2.00	0.43
1:E:495:ILE:HA	1:H:455:VAL:HB	2.00	0.43
1:E:182:LEU:HD23	1:E:182:LEU:HA	1.74	0.43
1:E:451:GLY:HA3	1:E:468:GLY:O	2.19	0.43
1:F:17:LYS:HD3	1:H:19:GLU:N	2.34	0.43
1:F:109:MET:CE	1:F:111:LYS:HE2	2.48	0.43
1:A:302:ALA:HB3	3:A:701:IAC:O3	2.18	0.43
1:A:312:ARG:CG	1:A:411:THR:HB	2.49	0.43
1:A:374:ILE:HG22	1:A:382:TYR:CB	2.48	0.43
1:C:239:THR:OG1	1:C:263:ARG:HB2	2.17	0.43
1:C:271:LYS:HE3	1:C:400:GLU:O	2.18	0.43
1:D:189:VAL:HG11	1:D:231:LEU:HD21	2.01	0.43
1:E:181:ALA:HB2	1:E:487:TYR:CD1	2.52	0.43
1:F:273:PRO:HG3	1:F:422:ALA:HB1	2.00	0.43
1:F:385:PRO:HA	1:F:405:PRO:HB2	2.01	0.43
1:G:369:ALA:O	1:G:386:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:LYS:HB3	1:H:84:LYS:HE2	1.86	0.43
1:F:78:LEU:O	1:F:83:ARG:NH1	2.52	0.43
1:G:263:ARG:NE	1:G:489:GLU:OE2	2.52	0.43
1:H:331:PRO:HA	1:H:341:VAL:HB	2.00	0.43
1:A:232:ALA:O	1:A:262:LYS:NZ	2.52	0.43
1:C:259:SER:OG	1:C:260:ASN:N	2.50	0.43
1:C:430:ALA:HA	1:C:452:SER:O	2.19	0.43
1:A:112:PRO:O	1:A:115:ASP:HB2	2.19	0.42
1:B:9:TRP:HE3	1:B:103:LEU:HD13	1.84	0.42
1:B:109:MET:HE2	1:B:109:MET:HB2	1.81	0.42
1:F:6:ARG:NH1	1:F:336:ASP:OD2	2.49	0.42
1:F:468:GLY:HA3	1:F:477:ARG:HD3	2.01	0.42
1:B:465:ALA:HB2	1:D:494:TRP:CZ2	2.54	0.42
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.81	0.42
1:D:158:VAL:HG13	1:D:487:TYR:C	2.44	0.42
1:D:253:MET:HG3	1:D:266:LEU:HD11	2.01	0.42
1:F:244:GLY:HA2	2:F:700:NAI:H4N	2.01	0.42
1:G:162:ALA:HB3	1:G:240:VAL:HG23	2.01	0.42
1:H:194:GLU:H	1:H:194:GLU:HG3	1.19	0.42
1:E:166:PRO:HG3	1:E:243:THR:HG22	2.00	0.42
1:G:59:ALA:O	1:G:63:VAL:HG23	2.19	0.42
1:G:301:VAL:HG12	1:G:303:THR:H	1.85	0.42
1:D:235:MET:HE3	1:D:235:MET:HB3	1.91	0.42
1:D:391:VAL:HG21	1:D:408:SER:HB3	2.00	0.42
1:E:140:ASP:HB2	1:G:142:VAL:HB	2.01	0.42
1:H:140:ASP:OD1	1:H:155:ARG:HG3	2.19	0.42
1:C:42:PRO:HG3	1:C:345:VAL:O	2.19	0.42
1:C:234:HIS:O	1:C:262:LYS:NZ	2.46	0.42
1:E:298:GLN:OE1	1:E:342:GLY:N	2.47	0.42
1:F:141:GLU:HB2	1:F:153:VAL:HB	2.01	0.42
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.68	0.42
1:E:208:ILE:HD13	1:E:208:ILE:HA	1.85	0.42
1:F:178:LEU:O	1:F:182:LEU:HB2	2.19	0.42
1:F:350:MET:HE3	1:F:381:THR:HB	2.02	0.42
1:G:31:ALA:O	1:G:34:GLY:N	2.35	0.42
1:G:137:LYS:HD3	1:H:130:TRP:CZ2	2.54	0.42
1:A:486:LYS:H	1:A:486:LYS:HG2	1.64	0.42
1:G:371:GLY:N	1:G:386:THR:OG1	2.52	0.42
1:A:403:PHE:HB2	2:A:700:NAI:O2D	2.19	0.42
1:E:155:ARG:HB3	1:E:488:THR:CG2	2.49	0.42
1:E:309:LEU:HD12	1:E:410:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:PRO:HA	1:F:341:VAL:O	2.20	0.42
1:A:391:VAL:HG11	1:A:408:SER:HB3	2.01	0.42
1:B:491:LYS:NZ	1:D:445:ALA:O	2.45	0.42
1:E:93:LEU:HB3	1:E:206:LEU:HD22	2.01	0.42
1:B:203:ILE:HA	1:B:206:LEU:HB2	2.02	0.42
1:B:336:ASP:HB3	1:B:339:THR:OG1	2.20	0.42
1:C:109:MET:HE2	1:C:109:MET:HB2	1.70	0.42
1:D:178:LEU:O	1:D:182:LEU:HB2	2.20	0.42
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.81	0.41
1:B:302:ALA:HB2	2:B:700:NAI:O7N	2.20	0.41
1:E:350:MET:HB3	1:E:350:MET:HE3	1.78	0.41
1:G:4:LEU:N	1:G:4:LEU:HD23	2.35	0.41
1:G:109:MET:HG3	1:G:110:GLY:N	2.31	0.41
1:G:166:PRO:HD3	1:G:243:THR:HB	2.02	0.41
1:E:283:LEU:HD23	1:E:283:LEU:HA	1.72	0.41
1:F:40:ILE:HD13	1:F:40:ILE:HA	1.83	0.41
1:D:59:ALA:O	1:D:63:VAL:HG23	2.20	0.41
1:E:246:THR:OG1	1:E:268:ALA:HB1	2.20	0.41
1:H:393:ASN:ND2	1:H:424:ASP:OD2	2.54	0.41
1:A:41:SER:HA	1:A:42:PRO:HD3	1.97	0.41
1:B:356:TYR:OH	1:B:400:GLU:OE1	2.26	0.41
1:C:71:ASP:O	1:C:77:ARG:NH2	2.53	0.41
1:D:430:ALA:HA	1:D:452:SER:O	2.20	0.41
1:E:251:GLN:HG3	1:E:255:TYR:CZ	2.55	0.41
1:E:261:MET:HE3	1:H:266:LEU:HD12	2.02	0.41
1:G:233:LEU:HD23	1:G:233:LEU:HA	1.86	0.41
1:H:42:PRO:HG3	1:H:345:VAL:O	2.19	0.41
1:A:474:GLY:O	1:C:263:ARG:NH2	2.53	0.41
1:G:136:ASP:CB	1:G:137:LYS:HZ2	2.33	0.41
1:H:138:LEU:HD21	1:H:481:LEU:HD22	2.02	0.41
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.80	0.41
1:A:265:TRP:CD2	1:A:486:LYS:HB3	2.56	0.41
1:C:273:PRO:HD3	1:C:307:ARG:HH21	1.86	0.41
1:G:283:LEU:HD23	1:G:283:LEU:HA	1.74	0.41
1:H:133:GLU:O	1:H:137:LYS:NZ	2.53	0.41
1:H:208:ILE:HD13	1:H:208:ILE:HA	1.81	0.41
1:A:27:GLU:OE1	1:D:14:GLN:HG2	2.21	0.41
1:A:303:THR:HG22	1:A:430:ALA:HB2	2.02	0.41
1:B:369:ALA:HB3	1:B:387:ILE:HG13	2.02	0.41
1:H:374:ILE:HG13	1:H:375:LEU:HG	2.02	0.41
1:D:182:LEU:HD23	1:D:182:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:LEU:HD11	1:D:386:THR:HG23	2.02	0.41
1:F:432:ALA:HA	1:F:454:TRP:O	2.20	0.41
1:H:112:PRO:HD3	1:H:298:GLN:HE22	1.86	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.93	0.41
1:A:111:LYS:HE3	1:A:297:ASN:OD1	2.20	0.41
1:A:249:ALA:HB1	1:A:266:LEU:HD22	2.02	0.41
1:A:294:ILE:HD12	1:A:294:ILE:HA	1.96	0.41
1:D:108:ASP:CG	1:D:196:SER:HA	2.46	0.41
1:E:111:LYS:HB2	1:E:111:LYS:HE3	1.94	0.41
1:E:294:ILE:HD13	1:E:306:SER:HA	2.03	0.41
1:G:391:VAL:O	1:G:410:LEU:HD13	2.20	0.41
1:B:173:MET:HE3	1:B:173:MET:HA	2.03	0.41
1:C:246:THR:OG1	1:C:268:ALA:HB1	2.21	0.41
1:H:233:LEU:HD23	1:H:233:LEU:HA	1.73	0.41
1:D:65:SER:HB3	1:D:218:ASN:ND2	2.36	0.40
1:E:433:VAL:HG12	1:E:435:THR:HG22	2.03	0.40
1:E:465:ALA:HB2	1:H:494:TRP:CH2	2.56	0.40
1:F:16:LEU:HD21	1:F:100:GLU:HG3	2.02	0.40
1:A:465:ALA:HB2	1:C:494:TRP:CH2	2.56	0.40
1:E:112:PRO:O	1:E:115:ASP:HB2	2.22	0.40
1:E:326:LEU:HD22	1:E:387:ILE:HD11	2.02	0.40
1:F:17:LYS:HB3	1:F:17:LYS:HE3	1.73	0.40
1:F:244:GLY:O	1:F:268:ALA:HA	2.21	0.40
1:E:93:LEU:HD23	1:E:93:LEU:HA	1.78	0.40
1:E:474:GLY:O	1:H:263:ARG:NH2	2.54	0.40
1:F:208:ILE:HD13	1:F:208:ILE:HA	1.82	0.40
1:G:182:LEU:HA	1:G:182:LEU:HD23	1.90	0.40
1:B:208:ILE:HD13	1:B:208:ILE:HA	1.90	0.40
1:B:392:ASN:HB3	1:B:395:MET:HE3	2.03	0.40
1:B:494:TRP:CH2	1:D:465:ALA:HB2	2.57	0.40
1:C:191:LYS:C	1:C:191:LYS:HD2	2.47	0.40
1:E:234:HIS:HB3	1:E:237:VAL:HG23	2.03	0.40
1:F:283:LEU:HD12	1:F:317:ARG:NH1	2.36	0.40
1:H:307:ARG:HD3	1:H:398:ALA:O	2.22	0.40
1:A:19:GLU:CD	1:A:21:ARG:HE	2.29	0.40
1:A:109:MET:SD	1:A:111:LYS:HD2	2.61	0.40
1:C:93:LEU:HD12	1:C:210:ALA:HB2	2.03	0.40
1:D:108:ASP:OD2	1:D:196:SER:HA	2.21	0.40
1:E:278:ALA:HA	1:E:314:ILE:HD13	2.04	0.40
1:G:356:TYR:CD2	1:G:402:ILE:HG23	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:LYS:CE	1:G:17:LYS:NZ[4_747]	1.85	0.35
1:E:17:LYS:CD	1:G:17:LYS:CE[4_747]	2.01	0.19
1:E:17:LYS:CE	1:G:17:LYS:CE[4_747]	2.14	0.06

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	493/497 (99%)	472 (96%)	21 (4%)	0	100	100
1	B	493/497 (99%)	471 (96%)	22 (4%)	0	100	100
1	C	493/497 (99%)	476 (97%)	17 (3%)	0	100	100
1	D	493/497 (99%)	474 (96%)	18 (4%)	1 (0%)	43	62
1	E	493/497 (99%)	469 (95%)	22 (4%)	2 (0%)	30	48
1	F	493/497 (99%)	472 (96%)	21 (4%)	0	100	100
1	G	493/497 (99%)	471 (96%)	21 (4%)	1 (0%)	43	62
1	H	493/497 (99%)	472 (96%)	21 (4%)	0	100	100
All	All	3944/3976 (99%)	3777 (96%)	163 (4%)	4 (0%)	48	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	262	LYS
1	G	166	PRO
1	E	428	GLY
1	D	166	PRO

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	377/379 (100%)	372 (99%)	5 (1%)	61	79
1	B	377/379 (100%)	373 (99%)	4 (1%)	65	81
1	C	377/379 (100%)	373 (99%)	4 (1%)	65	81
1	D	377/379 (100%)	370 (98%)	7 (2%)	50	73
1	E	377/379 (100%)	374 (99%)	3 (1%)	73	86
1	F	377/379 (100%)	372 (99%)	5 (1%)	61	79
1	G	377/379 (100%)	374 (99%)	3 (1%)	73	86
1	H	377/379 (100%)	372 (99%)	5 (1%)	61	79
All	All	3016/3032 (100%)	2980 (99%)	36 (1%)	63	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	141	GLU
1	A	173	MET
1	A	191	LYS
1	A	486	LYS
1	B	111	LYS
1	B	120	ASP
1	B	141	GLU
1	B	191	LYS
1	C	19	GLU
1	C	191	LYS
1	C	373	GLN
1	C	473	SER
1	D	3	THR
1	D	19	GLU
1	D	111	LYS
1	D	191	LYS
1	D	262	LYS
1	D	373	GLN

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Mol	Chain	Res	Type
1	D	496	LYS
1	E	84	LYS
1	E	195	LYS
1	E	263	ARG
1	F	84	LYS
1	F	116	SER
1	F	191	LYS
1	F	262	LYS
1	F	324	GLU
1	G	82	LYS
1	G	262	LYS
1	G	446	ARG
1	H	194	GLU
1	H	209	GLU
1	H	262	LYS
1	H	373	GLN
1	H	464	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	251	GLN
1	A	373	GLN
1	A	392	ASN
1	A	442	HIS
1	B	251	GLN
1	B	284	GLN
1	B	392	ASN
1	C	97	ASN
1	C	351	ASN
1	C	373	GLN
1	D	373	GLN
1	E	399	GLN
1	F	392	ASN
1	G	333	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	NAI	B	700	-	47,48,48	3.66	25 (53%)	64,73,73	2.50	27 (42%)
3	IAC	B	701	-	14,14,14	1.60	3 (21%)	19,19,19	1.69	6 (31%)
3	IAC	C	701	-	14,14,14	1.84	4 (28%)	19,19,19	2.02	5 (26%)
3	IAC	E	701	-	14,14,14	1.58	3 (21%)	19,19,19	1.54	4 (21%)
2	NAI	G	700	-	47,48,48	3.62	25 (53%)	64,73,73	2.35	22 (34%)
3	IAC	H	701	-	14,14,14	1.83	4 (28%)	19,19,19	1.75	5 (26%)
2	NAI	E	700	-	47,48,48	3.64	26 (55%)	64,73,73	2.47	24 (37%)
2	NAI	C	700	-	47,48,48	3.60	25 (53%)	64,73,73	2.24	18 (28%)
3	IAC	G	701	-	14,14,14	1.97	5 (35%)	19,19,19	1.67	4 (21%)
3	IAC	A	701	-	14,14,14	1.78	5 (35%)	19,19,19	2.02	3 (15%)
2	NAI	A	700	-	47,48,48	3.67	27 (57%)	64,73,73	2.49	24 (37%)
3	IAC	D	701	-	14,14,14	1.71	3 (21%)	19,19,19	1.52	5 (26%)
3	IAC	F	701	-	14,14,14	1.53	4 (28%)	19,19,19	1.29	2 (10%)
2	NAI	H	700	-	47,48,48	3.60	25 (53%)	64,73,73	2.38	20 (31%)
2	NAI	D	700	-	47,48,48	3.60	25 (53%)	64,73,73	2.31	18 (28%)
2	NAI	F	700	-	47,48,48	3.63	25 (53%)	64,73,73	2.50	26 (40%)

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	NAI	B	700	-	3/3/13/16	7/29/72/72	0/5/5/5
3	IAC	B	701	-	-	2/4/4/4	0/2/2/2
3	IAC	C	701	-	-	2/4/4/4	0/2/2/2
3	IAC	E	701	-	-	2/4/4/4	0/2/2/2
2	NAI	G	700	-	3/3/13/16	4/29/72/72	0/5/5/5
3	IAC	H	701	-	-	0/4/4/4	0/2/2/2
2	NAI	E	700	-	3/3/13/16	10/29/72/72	0/5/5/5
2	NAI	C	700	-	3/3/13/16	9/29/72/72	0/5/5/5
3	IAC	G	701	-	-	2/4/4/4	0/2/2/2
3	IAC	A	701	-	-	2/4/4/4	0/2/2/2
2	NAI	A	700	-	3/3/13/16	6/29/72/72	0/5/5/5
3	IAC	D	701	-	-	0/4/4/4	0/2/2/2
3	IAC	F	701	-	-	2/4/4/4	0/2/2/2
2	NAI	H	700	-	3/3/13/16	8/29/72/72	0/5/5/5
2	NAI	D	700	-	3/3/13/16	7/29/72/72	0/5/5/5
2	NAI	F	700	-	3/3/13/16	11/29/72/72	0/5/5/5

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	700	NAI	C3B-C4B	-9.84	1.28	1.53
2	E	700	NAI	C3B-C4B	-9.75	1.28	1.53
2	F	700	NAI	C3B-C4B	-9.65	1.28	1.53
2	H	700	NAI	C3B-C4B	-9.60	1.28	1.53
2	B	700	NAI	C3B-C4B	-9.60	1.28	1.53
2	A	700	NAI	C3B-C4B	-9.33	1.29	1.53
2	D	700	NAI	C3B-C4B	-9.30	1.29	1.53
2	C	700	NAI	C3B-C4B	-9.20	1.29	1.53
2	B	700	NAI	PA-O3	7.90	1.68	1.59
2	C	700	NAI	PA-O3	7.77	1.67	1.59
2	A	700	NAI	PA-O3	7.73	1.67	1.59
2	D	700	NAI	PA-O3	7.66	1.67	1.59
2	H	700	NAI	PA-O3	7.18	1.67	1.59
2	G	700	NAI	PA-O3	7.14	1.67	1.59
2	E	700	NAI	PA-O3	7.07	1.67	1.59
2	G	700	NAI	O4B-C4B	6.98	1.60	1.45
2	C	700	NAI	O4B-C4B	6.94	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	700	NAI	PA-O3	6.91	1.67	1.59
2	D	700	NAI	O4B-C4B	6.87	1.60	1.45
2	E	700	NAI	O4B-C4B	6.79	1.60	1.45
2	H	700	NAI	O4B-C4B	6.78	1.60	1.45
2	B	700	NAI	C7N-N7N	6.76	1.53	1.33
2	F	700	NAI	O4B-C4B	6.75	1.60	1.45
2	G	700	NAI	O4D-C4D	6.72	1.59	1.45
2	A	700	NAI	C7N-N7N	6.70	1.52	1.33
2	A	700	NAI	O4B-C4B	6.60	1.59	1.45
2	B	700	NAI	O4D-C4D	6.48	1.59	1.45
2	B	700	NAI	O4B-C4B	6.43	1.59	1.45
2	F	700	NAI	O4D-C4D	6.38	1.59	1.45
2	H	700	NAI	O4D-C4D	6.36	1.59	1.45
2	A	700	NAI	O4D-C4D	6.30	1.59	1.45
2	E	700	NAI	O4D-C4D	6.29	1.59	1.45
2	H	700	NAI	C4N-C3N	-6.26	1.38	1.50
2	B	700	NAI	C4N-C3N	-6.25	1.38	1.50
2	E	700	NAI	C4N-C3N	-6.24	1.38	1.50
2	A	700	NAI	C7N-C3N	6.23	1.62	1.48
2	A	700	NAI	C2D-C3D	-6.19	1.36	1.53
2	D	700	NAI	C7N-N7N	6.16	1.51	1.33
2	G	700	NAI	C7N-N7N	6.13	1.51	1.33
2	C	700	NAI	O4D-C4D	6.13	1.58	1.45
2	C	700	NAI	C7N-N7N	6.10	1.51	1.33
2	D	700	NAI	C4N-C3N	-6.10	1.38	1.50
2	F	700	NAI	C7N-C3N	6.08	1.61	1.48
2	G	700	NAI	C2D-C3D	-6.08	1.36	1.53
2	A	700	NAI	C4N-C3N	-6.05	1.38	1.50
2	D	700	NAI	O4D-C4D	6.01	1.58	1.45
2	B	700	NAI	C2D-C3D	-5.99	1.37	1.53
2	F	700	NAI	C4N-C3N	-5.99	1.38	1.50
2	F	700	NAI	C7N-N7N	5.95	1.50	1.33
2	C	700	NAI	C4N-C3N	-5.94	1.38	1.50
2	H	700	NAI	C7N-N7N	5.93	1.50	1.33
2	E	700	NAI	C7N-N7N	5.92	1.50	1.33
2	D	700	NAI	C2D-C3D	-5.91	1.37	1.53
2	E	700	NAI	C2D-C3D	-5.90	1.37	1.53
2	G	700	NAI	C4N-C3N	-5.84	1.39	1.50
2	F	700	NAI	C2D-C3D	-5.83	1.37	1.53
2	H	700	NAI	C2D-C3D	-5.80	1.37	1.53
2	C	700	NAI	C2D-C3D	-5.76	1.37	1.53
2	G	700	NAI	C7N-C3N	5.69	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	NAI	C7N-C3N	5.69	1.60	1.48
2	B	700	NAI	C7N-C3N	5.59	1.60	1.48
2	E	700	NAI	O4B-C1B	-5.50	1.29	1.42
2	B	700	NAI	O4B-C1B	-5.47	1.29	1.42
2	F	700	NAI	O4B-C1B	-5.46	1.29	1.42
2	A	700	NAI	O4B-C1B	-5.33	1.29	1.42
2	C	700	NAI	C7N-C3N	5.14	1.59	1.48
2	D	700	NAI	C5D-C4D	-5.09	1.36	1.51
2	D	700	NAI	PN-O3	5.07	1.65	1.59
2	C	700	NAI	PN-O3	5.06	1.65	1.59
2	C	700	NAI	C5D-C4D	-5.05	1.36	1.51
2	A	700	NAI	C6A-N6A	5.01	1.47	1.34
2	D	700	NAI	C7N-C3N	5.00	1.59	1.48
2	E	700	NAI	C6A-N6A	4.99	1.46	1.34
2	H	700	NAI	C7N-C3N	4.97	1.59	1.48
2	G	700	NAI	O4B-C1B	-4.97	1.30	1.42
2	H	700	NAI	C5D-C4D	-4.89	1.36	1.51
2	F	700	NAI	C6A-N6A	4.89	1.46	1.34
2	D	700	NAI	O4B-C1B	-4.86	1.30	1.42
2	C	700	NAI	O4B-C1B	-4.85	1.30	1.42
2	H	700	NAI	O4B-C1B	-4.81	1.30	1.42
2	H	700	NAI	C6A-N6A	4.73	1.46	1.34
2	H	700	NAI	C2D-C1D	4.73	1.68	1.53
2	B	700	NAI	C6A-N6A	4.72	1.46	1.34
2	G	700	NAI	C2D-C1D	4.72	1.68	1.53
2	G	700	NAI	C5D-C4D	-4.60	1.37	1.51
2	E	700	NAI	PN-O3	4.59	1.64	1.59
2	A	700	NAI	C5D-C4D	-4.59	1.37	1.51
2	B	700	NAI	C2D-C1D	4.56	1.67	1.53
2	D	700	NAI	C2D-C1D	4.55	1.67	1.53
2	C	700	NAI	C2D-C1D	4.55	1.67	1.53
2	H	700	NAI	PN-O3	4.51	1.64	1.59
2	G	700	NAI	C6A-N6A	4.51	1.45	1.34
2	F	700	NAI	PN-O3	4.47	1.64	1.59
2	A	700	NAI	C2D-C1D	4.46	1.67	1.53
2	F	700	NAI	C2D-C1D	4.41	1.67	1.53
2	E	700	NAI	C2D-C1D	4.39	1.67	1.53
2	C	700	NAI	C6A-N6A	4.38	1.45	1.34
2	F	700	NAI	C5D-C4D	-4.35	1.38	1.51
2	B	700	NAI	C5D-C4D	-4.35	1.38	1.51
2	E	700	NAI	C5D-C4D	-4.32	1.38	1.51
2	D	700	NAI	C6A-N6A	4.32	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	700	NAI	PN-O3	4.25	1.64	1.59
3	G	701	IAC	C17-C7	4.22	1.55	1.50
2	A	700	NAI	O3B-C3B	4.19	1.53	1.43
3	H	701	IAC	C17-C7	3.99	1.55	1.50
2	B	700	NAI	PN-O3	3.98	1.63	1.59
3	C	701	IAC	C17-C7	3.86	1.55	1.50
2	F	700	NAI	O3B-C3B	3.78	1.52	1.43
2	F	700	NAI	C1B-N9A	3.75	1.56	1.46
2	D	700	NAI	O3B-C3B	3.72	1.52	1.43
2	G	700	NAI	C1B-N9A	3.71	1.56	1.46
2	E	700	NAI	O3B-C3B	3.70	1.52	1.43
2	H	700	NAI	C1B-N9A	3.68	1.56	1.46
2	A	700	NAI	PN-O3	3.67	1.63	1.59
2	E	700	NAI	C1B-N9A	3.63	1.56	1.46
2	F	700	NAI	C2N-C3N	3.63	1.45	1.35
2	H	700	NAI	O3B-C3B	3.61	1.51	1.43
2	B	700	NAI	O3B-C3B	3.54	1.51	1.43
2	C	700	NAI	O3B-C3B	3.53	1.51	1.43
2	H	700	NAI	C2N-C3N	3.52	1.44	1.35
2	E	700	NAI	C2N-C3N	3.51	1.44	1.35
2	G	700	NAI	O3B-C3B	3.46	1.51	1.43
2	G	700	NAI	C2N-C3N	3.45	1.44	1.35
2	B	700	NAI	O4D-C1D	-3.42	1.34	1.42
2	D	700	NAI	O4D-C1D	-3.40	1.34	1.42
2	A	700	NAI	C1B-N9A	3.37	1.55	1.46
2	A	700	NAI	O4D-C1D	-3.37	1.34	1.42
2	D	700	NAI	C2N-C3N	3.37	1.44	1.35
2	C	700	NAI	C2N-C3N	3.37	1.44	1.35
3	D	701	IAC	C17-C7	3.36	1.54	1.50
2	G	700	NAI	O4D-C1D	-3.36	1.34	1.42
2	A	700	NAI	C2N-C3N	3.33	1.44	1.35
2	C	700	NAI	O4D-C1D	-3.31	1.34	1.42
2	B	700	NAI	C1B-N9A	3.29	1.55	1.46
3	C	701	IAC	C17-C18	3.27	1.56	1.51
2	H	700	NAI	O4D-C1D	-3.27	1.34	1.42
3	G	701	IAC	C17-C18	3.25	1.56	1.51
3	A	701	IAC	C17-C7	3.25	1.54	1.50
2	D	700	NAI	C1B-N9A	3.24	1.55	1.46
2	B	700	NAI	C2N-C3N	3.13	1.43	1.35
2	F	700	NAI	O4D-C1D	-3.13	1.34	1.42
2	E	700	NAI	O4D-C1D	-3.12	1.34	1.42
2	E	700	NAI	C4N-C5N	-3.12	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	700	NAI	C4N-C5N	-3.11	1.40	1.49
2	C	700	NAI	C1B-N9A	3.09	1.54	1.46
2	G	700	NAI	O3D-C3D	3.08	1.50	1.43
2	B	700	NAI	O3D-C3D	3.07	1.50	1.43
2	B	700	NAI	C8A-N9A	-3.06	1.32	1.37
2	C	700	NAI	C5B-C4B	3.03	1.60	1.51
3	H	701	IAC	C17-C18	3.02	1.55	1.51
2	F	700	NAI	C4N-C5N	-3.01	1.41	1.49
2	G	700	NAI	C6N-C5N	3.00	1.42	1.33
2	D	700	NAI	O7N-C7N	-2.99	1.17	1.24
2	F	700	NAI	C5B-C4B	2.99	1.60	1.51
2	F	700	NAI	O7N-C7N	-2.98	1.17	1.24
2	H	700	NAI	O3D-C3D	2.96	1.50	1.43
2	H	700	NAI	O7N-C7N	-2.94	1.17	1.24
2	E	700	NAI	O3D-C3D	2.93	1.50	1.43
2	E	700	NAI	O7N-C7N	-2.90	1.17	1.24
2	D	700	NAI	C4N-C5N	-2.90	1.41	1.49
2	A	700	NAI	C5B-C4B	2.90	1.60	1.51
2	C	700	NAI	O3D-C3D	2.89	1.50	1.43
2	E	700	NAI	C5B-C4B	2.88	1.60	1.51
3	B	701	IAC	C17-C7	2.87	1.53	1.50
2	H	700	NAI	C5B-C4B	2.87	1.60	1.51
2	F	700	NAI	O3D-C3D	2.86	1.50	1.43
3	E	701	IAC	C1-C	-2.83	1.37	1.41
2	C	700	NAI	O2D-C2D	2.82	1.49	1.43
2	D	700	NAI	C5B-C4B	2.82	1.60	1.51
2	D	700	NAI	O3D-C3D	2.82	1.49	1.43
2	C	700	NAI	C6N-C5N	2.80	1.41	1.33
2	B	700	NAI	C4N-C5N	-2.79	1.41	1.49
2	B	700	NAI	O7N-C7N	-2.78	1.17	1.24
2	C	700	NAI	O7N-C7N	-2.76	1.18	1.24
2	C	700	NAI	C4N-C5N	-2.76	1.41	1.49
2	B	700	NAI	C5B-C4B	2.76	1.59	1.51
2	G	700	NAI	O7N-C7N	-2.75	1.18	1.24
2	A	700	NAI	C6N-C5N	2.75	1.41	1.33
3	F	701	IAC	C1-C	-2.74	1.38	1.41
2	D	700	NAI	C6N-C5N	2.73	1.41	1.33
2	A	700	NAI	C4N-C5N	-2.72	1.41	1.49
2	B	700	NAI	C6N-C5N	2.68	1.41	1.33
3	D	701	IAC	C17-C18	2.67	1.55	1.51
2	H	700	NAI	C6N-C5N	2.67	1.41	1.33
2	G	700	NAI	C5B-C4B	2.66	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	NAI	O3D-C3D	2.64	1.49	1.43
3	E	701	IAC	C17-C7	2.62	1.53	1.50
2	A	700	NAI	C8A-N9A	-2.57	1.33	1.37
2	F	700	NAI	O2D-C2D	2.56	1.49	1.43
3	B	701	IAC	C1-C	-2.55	1.38	1.41
2	D	700	NAI	O2D-C2D	2.54	1.49	1.43
2	A	700	NAI	O7N-C7N	-2.54	1.18	1.24
2	G	700	NAI	O2D-C2D	2.53	1.49	1.43
3	A	701	IAC	C5-C	2.53	1.43	1.39
2	H	700	NAI	O2D-C2D	2.52	1.49	1.43
2	G	700	NAI	C4N-C5N	-2.51	1.42	1.49
2	E	700	NAI	O2D-C2D	2.47	1.49	1.43
3	F	701	IAC	C5-C	2.46	1.43	1.39
2	C	700	NAI	C8A-N9A	-2.45	1.33	1.37
3	G	701	IAC	C1-C	-2.44	1.38	1.41
3	E	701	IAC	C5-C	2.44	1.43	1.39
2	B	700	NAI	O2D-C2D	2.44	1.49	1.43
3	C	701	IAC	C1-C	-2.43	1.38	1.41
3	A	701	IAC	C1-C	-2.43	1.38	1.41
3	B	701	IAC	C5-C	2.42	1.43	1.39
3	D	701	IAC	C1-C	-2.42	1.38	1.41
3	H	701	IAC	C1-C	-2.41	1.38	1.41
2	G	700	NAI	C8A-N9A	-2.41	1.33	1.37
3	A	701	IAC	C17-C18	2.38	1.54	1.51
3	F	701	IAC	C17-C7	2.35	1.53	1.50
2	D	700	NAI	C8A-N9A	-2.33	1.33	1.37
2	F	700	NAI	C6N-C5N	2.32	1.40	1.33
2	A	700	NAI	O2D-C2D	2.29	1.48	1.43
2	F	700	NAI	C8A-N9A	-2.28	1.33	1.37
2	H	700	NAI	C8A-N9A	-2.26	1.33	1.37
3	A	701	IAC	C2-C1	2.25	1.43	1.39
2	E	700	NAI	C6N-C5N	2.24	1.39	1.33
2	E	700	NAI	C8A-N9A	-2.17	1.33	1.37
2	B	700	NAI	C5A-N7A	-2.16	1.35	1.39
2	A	700	NAI	C5A-N7A	-2.10	1.35	1.39
2	A	700	NAI	C4A-N3A	2.09	1.38	1.34
2	F	700	NAI	C5A-N7A	-2.08	1.35	1.39
3	G	701	IAC	C5-C	2.07	1.43	1.39
2	G	700	NAI	PA-O1A	2.06	1.58	1.50
2	C	700	NAI	C4A-N3A	2.06	1.38	1.34
3	F	701	IAC	C2-C1	2.05	1.43	1.39
3	C	701	IAC	C5-C	2.04	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	NAI	C5A-N7A	-2.03	1.35	1.39
2	D	700	NAI	PA-O1A	2.03	1.57	1.50
3	G	701	IAC	C2-C1	2.02	1.43	1.39
2	A	700	NAI	PA-O1A	2.01	1.57	1.50
2	E	700	NAI	C6N-N1N	-2.01	1.32	1.37
2	H	700	NAI	PA-O1A	2.01	1.57	1.50
3	H	701	IAC	C5-C	2.00	1.43	1.39

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	NAI	C2D-C1D-N1N	7.96	132.87	113.31
2	H	700	NAI	C2D-C1D-N1N	7.49	131.73	113.31
2	E	700	NAI	C2D-C1D-N1N	7.38	131.46	113.31
2	F	700	NAI	C2D-C1D-N1N	7.37	131.44	113.31
2	B	700	NAI	C2D-C1D-N1N	7.34	131.36	113.31
2	G	700	NAI	C2D-C1D-N1N	7.29	131.23	113.31
3	A	701	IAC	C18-C17-C7	7.20	125.98	114.93
2	B	700	NAI	C5A-C4A-N3A	-6.48	117.80	126.72
2	D	700	NAI	C2D-C1D-N1N	6.44	129.13	113.31
2	C	700	NAI	C2D-C1D-N1N	6.24	128.66	113.31
2	B	700	NAI	N3A-C4A-N9A	5.98	137.34	127.17
2	D	700	NAI	C5A-C4A-N3A	-5.93	118.56	126.72
2	A	700	NAI	C5A-C4A-N3A	-5.88	118.62	126.72
2	H	700	NAI	C5A-C4A-N3A	-5.86	118.65	126.72
2	D	700	NAI	C4B-O4B-C1B	-5.83	96.60	109.47
2	G	700	NAI	C5A-C4A-N3A	-5.77	118.77	126.72
2	G	700	NAI	C3D-C2D-C1D	5.74	112.32	101.46
2	A	700	NAI	C3D-C2D-C1D	5.74	112.32	101.46
2	B	700	NAI	C3D-C2D-C1D	5.67	112.18	101.46
2	C	700	NAI	C5A-C4A-N3A	-5.66	118.92	126.72
2	F	700	NAI	C5A-C4A-N3A	-5.66	118.93	126.72
2	E	700	NAI	C3D-C2D-C1D	5.60	112.06	101.46
2	F	700	NAI	C3D-C2D-C1D	5.57	112.00	101.46
2	A	700	NAI	N3A-C4A-N9A	5.56	136.63	127.17
2	E	700	NAI	C5A-C4A-N3A	-5.49	119.15	126.72
2	H	700	NAI	C3D-C2D-C1D	5.40	111.68	101.46
3	C	701	IAC	C18-C17-C7	5.38	123.18	114.93
2	C	700	NAI	C4B-O4B-C1B	-5.30	97.75	109.47
2	B	700	NAI	C4B-O4B-C1B	-5.24	97.90	109.47
2	F	700	NAI	N3A-C4A-N9A	5.21	136.02	127.17
2	A	700	NAI	C4B-O4B-C1B	-5.18	98.02	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	NAI	N3A-C4A-N9A	5.01	135.69	127.17
2	G	700	NAI	N3A-C4A-N9A	5.00	135.66	127.17
2	H	700	NAI	C4B-O4B-C1B	-4.99	98.45	109.47
2	F	700	NAI	C4B-O4B-C1B	-4.99	98.46	109.47
2	H	700	NAI	N3A-C4A-N9A	4.96	135.60	127.17
2	E	700	NAI	O4B-C1B-N9A	4.90	117.50	108.09
2	E	700	NAI	C4B-O4B-C1B	-4.89	98.68	109.47
2	C	700	NAI	N3A-C4A-N9A	4.87	135.44	127.17
2	G	700	NAI	C4B-O4B-C1B	-4.82	98.83	109.47
2	E	700	NAI	N3A-C4A-N9A	4.80	135.33	127.17
2	C	700	NAI	C3D-C2D-C1D	4.73	110.41	101.46
2	D	700	NAI	C3D-C2D-C1D	4.62	110.21	101.46
2	E	700	NAI	C3N-C2N-N1N	-4.62	116.43	123.20
2	D	700	NAI	C2B-C1B-N9A	4.57	124.65	113.30
2	F	700	NAI	C3N-C2N-N1N	-4.56	116.52	123.20
2	E	700	NAI	C1D-N1N-C6N	-4.55	111.16	120.77
2	H	700	NAI	O4B-C1B-N9A	4.53	116.78	108.09
2	F	700	NAI	C1D-N1N-C6N	-4.46	111.34	120.77
2	H	700	NAI	C2B-C1B-N9A	4.45	124.35	113.30
2	F	700	NAI	O4B-C1B-N9A	4.35	116.45	108.09
2	A	700	NAI	N3A-C2A-N1A	-4.26	122.14	128.58
3	G	701	IAC	C18-C17-C7	4.24	121.42	114.93
2	G	700	NAI	C2B-C1B-N9A	4.23	123.80	113.30
2	B	700	NAI	O4B-C1B-N9A	4.18	116.12	108.09
2	G	700	NAI	N3A-C2A-N1A	-4.17	122.27	128.58
2	H	700	NAI	N3A-C2A-N1A	-4.10	122.37	128.58
3	C	701	IAC	O2-C18-O3	-4.04	112.94	123.33
2	B	700	NAI	N3A-C2A-N1A	-3.99	122.55	128.58
2	B	700	NAI	C1B-N9A-C8A	-3.96	118.32	127.09
2	C	700	NAI	C4A-N9A-C8A	3.94	109.87	105.74
2	C	700	NAI	C2B-C1B-N9A	3.92	123.04	113.30
2	C	700	NAI	O4B-C1B-N9A	3.91	115.61	108.09
2	G	700	NAI	O4B-C1B-N9A	3.90	115.58	108.09
2	A	700	NAI	O4B-C1B-N9A	3.88	115.55	108.09
2	E	700	NAI	N3A-C2A-N1A	-3.87	122.72	128.58
2	D	700	NAI	O4B-C1B-N9A	3.79	115.37	108.09
2	B	700	NAI	C2A-N3A-C4A	3.72	120.92	111.83
3	H	701	IAC	C18-C17-C7	3.71	120.61	114.93
2	E	700	NAI	C1D-N1N-C2N	3.70	127.23	121.14
2	C	700	NAI	C5A-N7A-C8A	3.67	109.21	103.45
2	D	700	NAI	C4A-N9A-C8A	3.64	109.56	105.74
2	C	700	NAI	C4A-C5A-N7A	-3.62	106.44	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	700	NAI	C2A-N3A-C4A	3.61	120.65	111.83
2	C	700	NAI	N9A-C8A-N7A	-3.61	108.82	113.94
2	D	700	NAI	C5A-N7A-C8A	3.58	109.08	103.45
3	H	701	IAC	O2-C18-O3	-3.58	114.13	123.33
3	E	701	IAC	C17-C7-C1	3.54	131.04	126.43
2	A	700	NAI	C2B-C1B-N9A	3.53	122.08	113.30
2	D	700	NAI	C3N-C2N-N1N	-3.52	118.03	123.20
2	C	700	NAI	C3N-C2N-N1N	-3.51	118.05	123.20
2	H	700	NAI	C3N-C2N-N1N	-3.49	118.08	123.20
2	D	700	NAI	N9A-C8A-N7A	-3.49	108.99	113.94
2	D	700	NAI	C4A-C5A-N7A	-3.47	106.61	110.58
2	A	700	NAI	C2A-N3A-C4A	3.47	120.30	111.83
2	F	700	NAI	N3A-C2A-N1A	-3.44	123.37	128.58
2	G	700	NAI	C2A-N3A-C4A	3.44	120.24	111.83
2	F	700	NAI	C1B-N9A-C8A	-3.42	119.50	127.09
2	F	700	NAI	O4D-C1D-N1N	-3.39	101.62	108.08
2	B	700	NAI	C3N-C2N-N1N	-3.36	118.27	123.20
2	D	700	NAI	C2A-N3A-C4A	3.36	120.03	111.83
2	A	700	NAI	C1B-N9A-C8A	-3.35	119.66	127.09
2	B	700	NAI	O4D-C1D-N1N	-3.35	101.70	108.08
3	H	701	IAC	O2-C18-C17	3.34	124.86	114.51
3	B	701	IAC	C17-C7-C1	3.34	130.78	126.43
2	E	700	NAI	C1B-N9A-C8A	-3.33	119.70	127.09
2	D	700	NAI	N3A-C2A-N1A	-3.33	123.54	128.58
2	H	700	NAI	N9A-C8A-N7A	-3.32	109.22	113.94
2	C	700	NAI	C2A-N3A-C4A	3.32	119.93	111.83
2	F	700	NAI	C1D-N1N-C2N	3.31	126.59	121.14
2	C	700	NAI	N3A-C2A-N1A	-3.30	123.59	128.58
3	D	701	IAC	O2-C18-O3	-3.29	114.88	123.33
3	D	701	IAC	C18-C17-C7	3.29	119.97	114.93
2	H	700	NAI	C5A-N7A-C8A	3.23	108.53	103.45
2	G	700	NAI	C5A-N7A-C8A	3.23	108.52	103.45
2	E	700	NAI	O4D-C1D-N1N	-3.22	101.95	108.08
2	F	700	NAI	C2B-C1B-N9A	3.21	121.27	113.30
3	G	701	IAC	O2-C18-O3	-3.20	115.09	123.33
2	A	700	NAI	C4A-N9A-C8A	3.20	109.10	105.74
2	H	700	NAI	C4A-N9A-C8A	3.13	109.03	105.74
2	E	700	NAI	C2A-N3A-C4A	3.08	119.34	111.83
2	A	700	NAI	C5A-N7A-C8A	3.06	108.26	103.45
2	G	700	NAI	N9A-C8A-N7A	-3.04	109.62	113.94
2	A	700	NAI	N9A-C8A-N7A	-3.01	109.67	113.94
2	B	700	NAI	C2B-C1B-N9A	3.01	120.78	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	NAI	O4D-C1D-C2D	-2.99	100.21	106.62
3	E	701	IAC	C17-C7-C8	-2.98	122.77	126.84
2	A	700	NAI	O4D-C1D-N1N	-2.95	102.47	108.08
3	B	701	IAC	C18-C17-C7	2.91	119.39	114.93
2	G	700	NAI	C4A-N9A-C8A	2.90	108.78	105.74
2	B	700	NAI	C4A-N9A-C8A	2.87	108.75	105.74
2	F	700	NAI	C2A-N3A-C4A	2.86	118.81	111.83
2	D	700	NAI	C1B-N9A-C8A	-2.82	120.84	127.09
2	B	700	NAI	C5A-N7A-C8A	2.81	107.87	103.45
2	E	700	NAI	C2B-C1B-N9A	2.81	120.28	113.30
3	B	701	IAC	O2-C18-O3	-2.80	116.14	123.33
2	D	700	NAI	C1D-N1N-C6N	-2.77	114.91	120.77
2	H	700	NAI	C4A-C5A-N7A	-2.73	107.46	110.58
2	G	700	NAI	C4A-C5A-N7A	-2.71	107.48	110.58
2	F	700	NAI	C3N-C7N-N7N	2.70	122.47	117.67
2	H	700	NAI	C1D-N1N-C2N	2.68	125.55	121.14
2	A	700	NAI	C3N-C2N-N1N	-2.67	119.28	123.20
3	D	701	IAC	O2-C18-C17	2.67	122.79	114.51
2	E	700	NAI	C5A-N7A-C8A	2.67	107.64	103.45
2	G	700	NAI	C1B-N9A-C8A	-2.67	121.18	127.09
2	A	700	NAI	N6A-C6A-N1A	2.62	124.21	118.38
2	B	700	NAI	C4A-N9A-C1B	2.61	132.73	126.63
2	B	700	NAI	N9A-C8A-N7A	-2.60	110.24	113.94
2	F	700	NAI	O4D-C1D-C2D	-2.60	101.06	106.62
2	G	700	NAI	O2B-C2B-C1B	2.59	119.01	110.10
2	C	700	NAI	C1D-N1N-C6N	-2.59	115.31	120.77
2	G	700	NAI	O4D-C1D-C2D	-2.58	101.09	106.62
3	C	701	IAC	C17-C7-C1	2.58	129.79	126.43
2	H	700	NAI	C1D-N1N-C6N	-2.56	115.35	120.77
3	G	701	IAC	C-C1-C7	2.56	109.75	107.17
2	G	700	NAI	O2D-C2D-C1D	2.55	118.89	110.10
2	A	700	NAI	C5A-C6A-N6A	-2.54	117.01	123.29
3	B	701	IAC	C17-C7-C8	-2.52	123.39	126.84
2	H	700	NAI	C1B-N9A-C8A	-2.52	121.51	127.09
2	C	700	NAI	C1B-N9A-C8A	-2.50	121.56	127.09
3	F	701	IAC	C17-C7-C1	2.48	129.66	126.43
2	E	700	NAI	O4D-C1D-C2D	-2.48	101.32	106.62
2	F	700	NAI	C5A-N7A-C8A	2.47	107.33	103.45
2	B	700	NAI	C5A-C6A-N6A	-2.47	117.18	123.29
2	F	700	NAI	C4A-N9A-C1B	2.44	132.35	126.63
3	H	701	IAC	C-C1-C7	2.42	109.61	107.17
2	B	700	NAI	O4D-C1D-C2D	-2.42	101.44	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	IAC	C-C1-C7	2.40	109.59	107.17
3	B	701	IAC	O2-C18-C17	2.39	121.91	114.51
3	H	701	IAC	C17-C7-C1	2.37	129.52	126.43
2	F	700	NAI	C6A-C5A-C4A	2.37	120.42	117.18
2	B	700	NAI	O4D-C4D-C5D	2.37	116.93	109.33
2	E	700	NAI	C4A-N9A-C1B	2.36	132.16	126.63
2	B	700	NAI	O3D-C3D-C2D	2.34	119.33	111.82
2	F	700	NAI	O7N-C7N-N7N	-2.34	117.64	122.89
3	A	701	IAC	C-C1-C7	2.31	109.51	107.17
3	A	701	IAC	O2-C18-O3	-2.30	117.41	123.33
2	H	700	NAI	O2D-C2D-C1D	2.29	118.00	110.10
2	G	700	NAI	C3N-C2N-N1N	-2.29	119.84	123.20
3	C	701	IAC	O2-C18-C17	2.26	121.51	114.51
2	B	700	NAI	N6A-C6A-N1A	2.25	123.39	118.38
2	D	700	NAI	C1D-N1N-C2N	2.25	124.85	121.14
3	F	701	IAC	C17-C7-C8	-2.24	123.77	126.84
2	F	700	NAI	N6A-C6A-N1A	2.24	123.37	118.38
3	D	701	IAC	C-N-C8	-2.23	107.09	109.08
2	E	700	NAI	C4A-C5A-N7A	-2.22	108.04	110.58
2	F	700	NAI	O3D-C3D-C2D	2.22	118.93	111.82
2	F	700	NAI	O4D-C4D-C5D	2.22	116.44	109.33
2	B	700	NAI	C3N-C7N-N7N	2.20	121.58	117.67
2	E	700	NAI	O5D-C5D-C4D	2.20	116.49	108.99
2	G	700	NAI	C2B-C3B-C4B	2.20	106.86	102.61
2	C	700	NAI	C2B-C3B-C4B	2.19	106.84	102.61
2	E	700	NAI	N9A-C8A-N7A	-2.19	110.83	113.94
2	B	700	NAI	C6A-C5A-C4A	2.19	120.16	117.18
3	E	701	IAC	O2-C18-O3	-2.18	117.72	123.33
3	G	701	IAC	C17-C7-C1	2.17	129.26	126.43
2	H	700	NAI	O4D-C1D-C2D	-2.17	101.97	106.62
2	E	700	NAI	O4D-C4D-C5D	2.17	116.28	109.33
3	B	701	IAC	C2-C1-C	-2.16	116.60	118.84
3	E	701	IAC	C2-C1-C	-2.16	116.60	118.84
2	B	700	NAI	O5D-C5D-C4D	2.16	116.34	108.99
3	D	701	IAC	C-C1-C7	2.15	109.34	107.17
2	B	700	NAI	O2D-C2D-C1D	2.15	117.50	110.10
2	A	700	NAI	O2D-C2D-C1D	2.14	117.48	110.10
2	A	700	NAI	O4D-C4D-C5D	2.13	116.15	109.33
2	A	700	NAI	C6A-C5A-C4A	2.13	120.08	117.18
2	H	700	NAI	O2B-C2B-C1B	2.12	117.40	110.10
2	F	700	NAI	O5D-C5D-C4D	2.11	116.19	108.99
2	G	700	NAI	O4D-C1D-N1N	-2.11	104.06	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	700	NAI	O3D-C3D-C2D	2.11	118.57	111.82
2	B	700	NAI	C1D-N1N-C6N	-2.10	116.32	120.77
2	E	700	NAI	C4A-N9A-C8A	2.10	107.94	105.74
2	E	700	NAI	C6A-C5A-C4A	2.10	120.05	117.18
2	A	700	NAI	C3N-C7N-N7N	2.10	121.39	117.67
2	F	700	NAI	C6N-N1N-C2N	2.10	121.56	119.32
2	A	700	NAI	C4A-C5A-N7A	-2.09	108.19	110.58
2	F	700	NAI	C4A-N9A-C8A	2.08	107.92	105.74
2	D	700	NAI	O2D-C2D-C1D	2.08	117.25	110.10
2	C	700	NAI	C2D-C3D-C4D	2.05	106.56	102.61
2	G	700	NAI	O4D-C4D-C5D	2.04	115.88	109.33
2	B	700	NAI	C4A-C5A-N7A	-2.03	108.26	110.58
2	E	700	NAI	O3D-C3D-C2D	2.01	118.27	111.82
2	A	700	NAI	O3D-C3D-C2D	2.00	118.23	111.82

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	700	NAI	C2D
2	A	700	NAI	C1B
2	A	700	NAI	C3D
2	B	700	NAI	C2D
2	B	700	NAI	C1B
2	B	700	NAI	C3D
2	C	700	NAI	C2D
2	C	700	NAI	C1B
2	C	700	NAI	C3D
2	D	700	NAI	C2D
2	D	700	NAI	C1B
2	D	700	NAI	C3D
2	E	700	NAI	C2D
2	E	700	NAI	C1B
2	E	700	NAI	C3D
2	F	700	NAI	C2D
2	F	700	NAI	C1B
2	F	700	NAI	C3D
2	G	700	NAI	C2D
2	G	700	NAI	C1B
2	G	700	NAI	C3D
2	H	700	NAI	C2D
2	H	700	NAI	C1B
2	H	700	NAI	C3D

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	NAI	O4B-C1B-N9A-C4A
2	B	700	NAI	O4B-C1B-N9A-C4A
2	C	700	NAI	C4D-C5D-O5D-PN
2	C	700	NAI	O4D-C1D-N1N-C2N
2	C	700	NAI	C2N-C3N-C7N-N7N
2	D	700	NAI	C4D-C5D-O5D-PN
2	D	700	NAI	O4D-C1D-N1N-C2N
2	D	700	NAI	C2N-C3N-C7N-N7N
2	E	700	NAI	O4D-C1D-N1N-C2N
2	E	700	NAI	C2N-C3N-C7N-N7N
2	F	700	NAI	C5B-O5B-PA-O1A
2	F	700	NAI	O4B-C1B-N9A-C4A
2	G	700	NAI	C2N-C3N-C7N-N7N
2	H	700	NAI	C4D-C5D-O5D-PN
2	H	700	NAI	O4D-C1D-N1N-C2N
2	H	700	NAI	C2N-C3N-C7N-N7N
2	E	700	NAI	O4D-C4D-C5D-O5D
2	B	700	NAI	O4B-C1B-N9A-C8A
2	F	700	NAI	O4D-C1D-N1N-C2N
2	C	700	NAI	O4D-C4D-C5D-O5D
2	F	700	NAI	O4D-C4D-C5D-O5D
2	C	700	NAI	O4B-C1B-N9A-C4A
2	D	700	NAI	O4B-C1B-N9A-C4A
2	E	700	NAI	O4B-C1B-N9A-C4A
2	G	700	NAI	O4B-C1B-N9A-C4A
2	H	700	NAI	O4B-C1B-N9A-C4A
2	C	700	NAI	C3D-C4D-C5D-O5D
2	H	700	NAI	O4D-C4D-C5D-O5D
2	H	700	NAI	C3D-C4D-C5D-O5D
2	E	700	NAI	C3D-C4D-C5D-O5D
2	F	700	NAI	C3D-C4D-C5D-O5D
2	A	700	NAI	O4B-C1B-N9A-C8A
2	F	700	NAI	O4B-C1B-N9A-C8A
2	G	700	NAI	O4D-C1D-N1N-C2N
2	G	700	NAI	O4B-C1B-N9A-C8A
3	E	701	IAC	C7-C17-C18-O2
3	E	701	IAC	C7-C17-C18-O3
2	B	700	NAI	C3D-C4D-C5D-O5D
2	C	700	NAI	PN-O3-PA-O5B
2	E	700	NAI	PN-O3-PA-O5B
2	F	700	NAI	PN-O3-PA-O5B
2	H	700	NAI	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	E	700	NAI	O4B-C1B-N9A-C8A
3	A	701	IAC	C7-C17-C18-O3
3	B	701	IAC	C7-C17-C18-O2
3	B	701	IAC	C7-C17-C18-O3
3	F	701	IAC	C7-C17-C18-O2
3	F	701	IAC	C7-C17-C18-O3
2	C	700	NAI	O4B-C1B-N9A-C8A
2	H	700	NAI	O4B-C1B-N9A-C8A
2	A	700	NAI	O4D-C1D-N1N-C2N
2	B	700	NAI	O4D-C1D-N1N-C2N
2	B	700	NAI	O4D-C4D-C5D-O5D
2	C	700	NAI	C5D-O5D-PN-O2N
2	D	700	NAI	C5D-O5D-PN-O2N
2	E	700	NAI	C5B-O5B-PA-O1A
2	E	700	NAI	C5B-O5B-PA-O2A
2	F	700	NAI	C5B-O5B-PA-O2A
2	F	700	NAI	C5B-O5B-PA-O3
3	G	701	IAC	C7-C17-C18-O2
3	G	701	IAC	C7-C17-C18-O3
2	D	700	NAI	O4B-C1B-N9A-C8A
3	A	701	IAC	C7-C17-C18-O2
2	F	700	NAI	C4D-C5D-O5D-PN
2	A	700	NAI	O4D-C4D-C5D-O5D
2	F	700	NAI	C2N-C3N-C7N-N7N
2	E	700	NAI	C4D-C5D-O5D-PN
3	C	701	IAC	C7-C17-C18-O2
2	A	700	NAI	PA-O3-PN-O1N
2	B	700	NAI	PA-O3-PN-O1N
3	C	701	IAC	C7-C17-C18-O3
2	A	700	NAI	C3D-C4D-C5D-O5D
2	B	700	NAI	PA-O3-PN-O2N
2	D	700	NAI	C3D-C4D-C5D-O5D

There are no ring outliers.

16 monomers are involved in 45 short contacts:

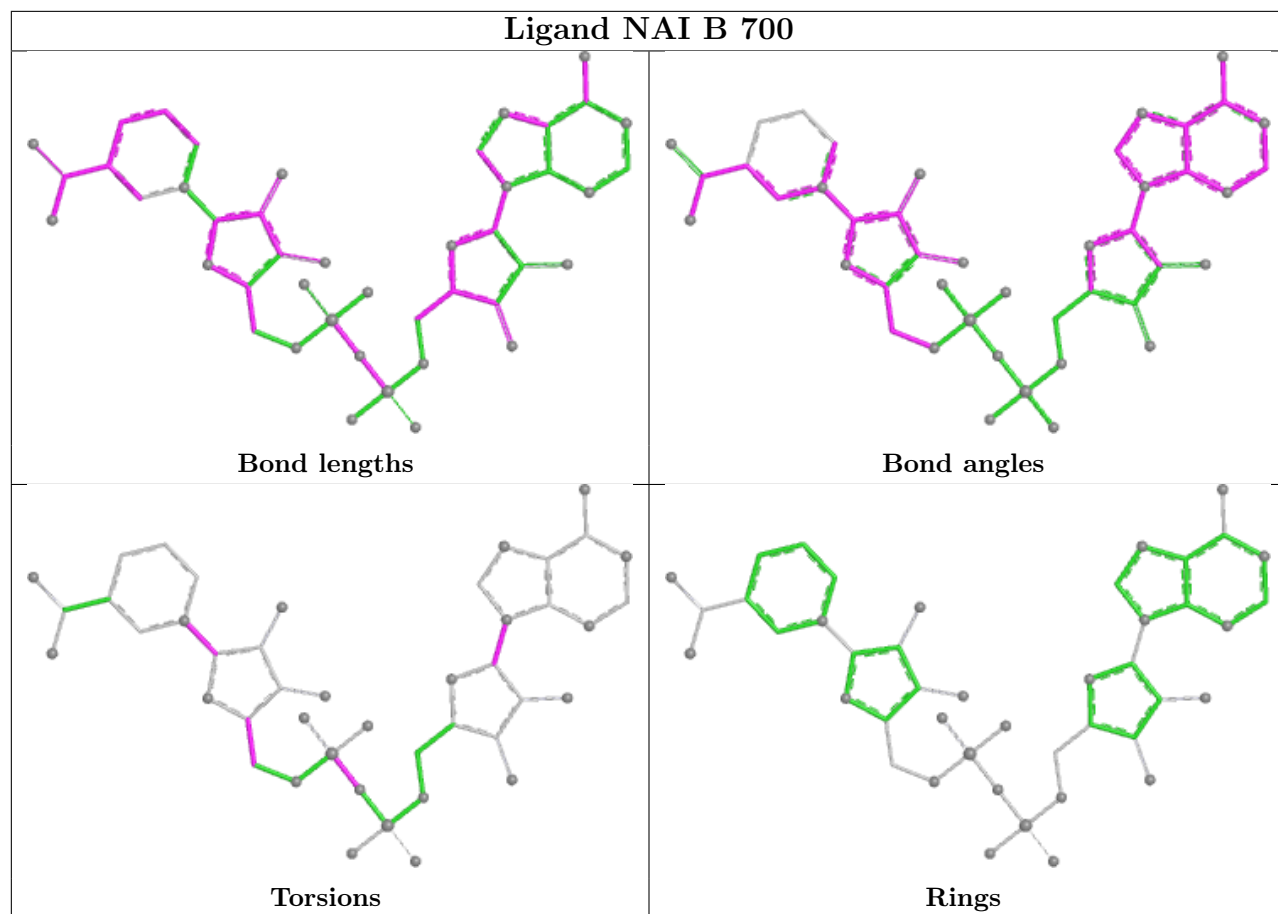
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	NAI	4	0
3	B	701	IAC	3	0
3	C	701	IAC	3	0
3	E	701	IAC	3	0
2	G	700	NAI	1	0

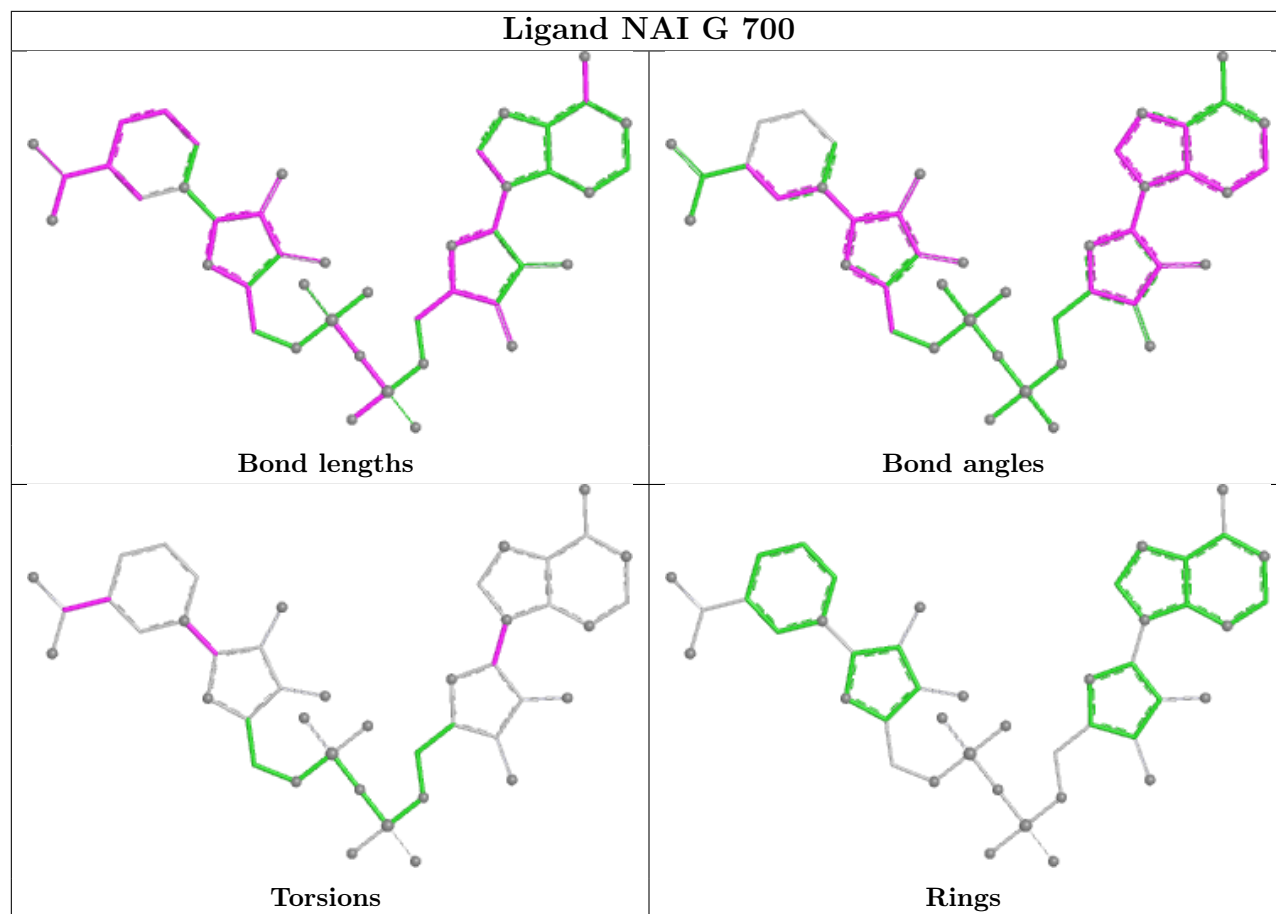
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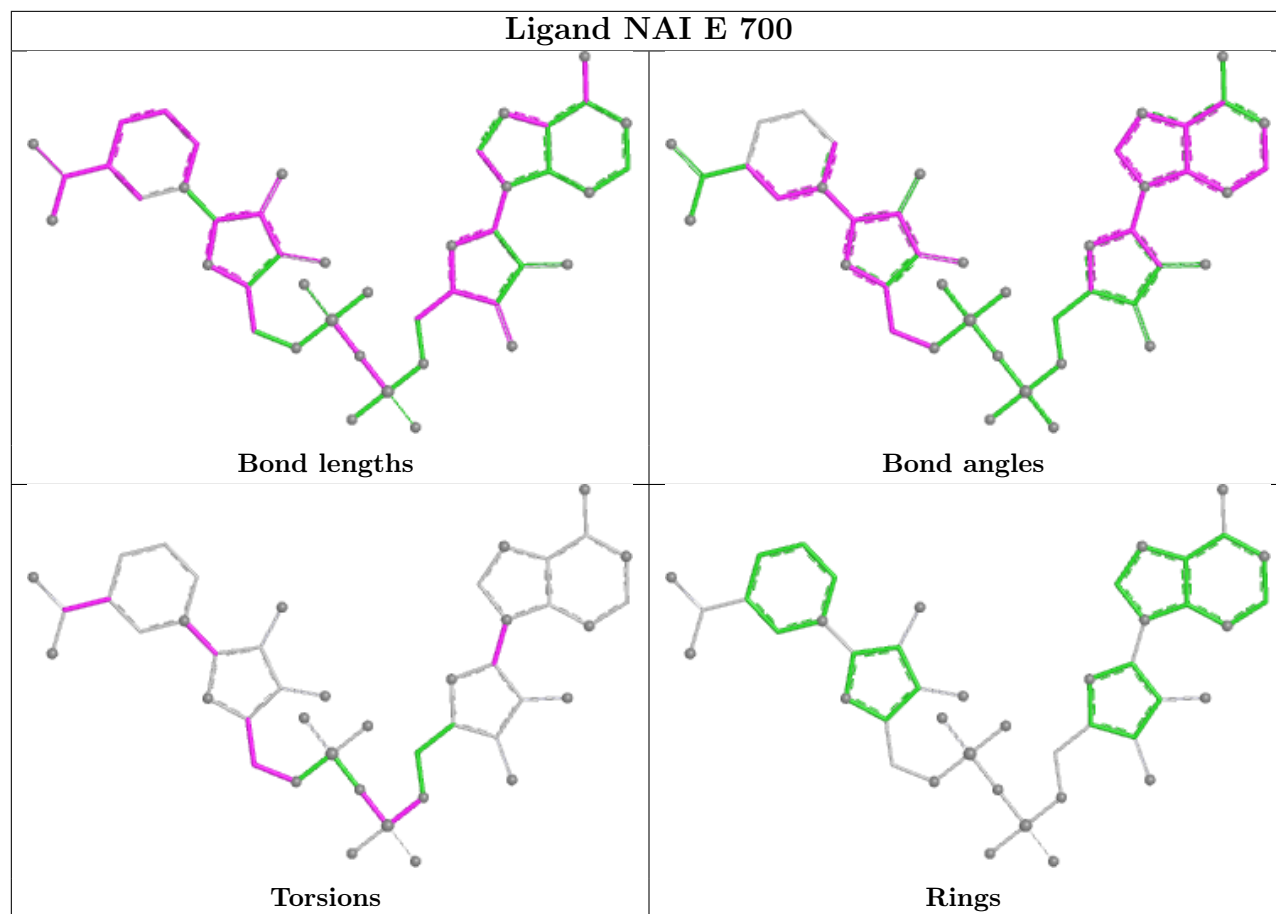
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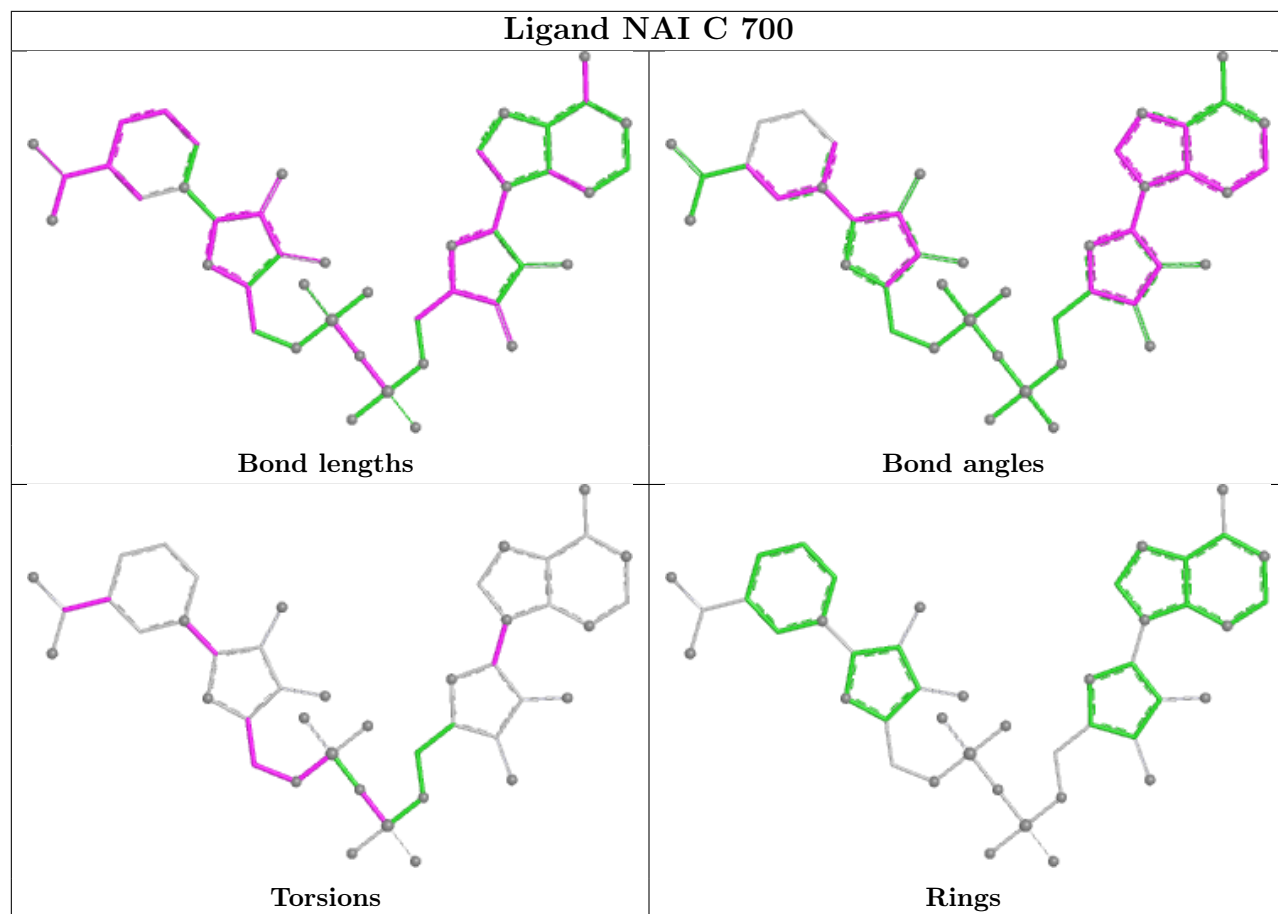
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	701	IAC	1	0
2	E	700	NAI	4	0
2	C	700	NAI	2	0
3	G	701	IAC	1	0
3	A	701	IAC	4	0
2	A	700	NAI	4	0
3	D	701	IAC	3	0
3	F	701	IAC	3	0
2	H	700	NAI	3	0
2	D	700	NAI	2	0
2	F	700	NAI	4	0

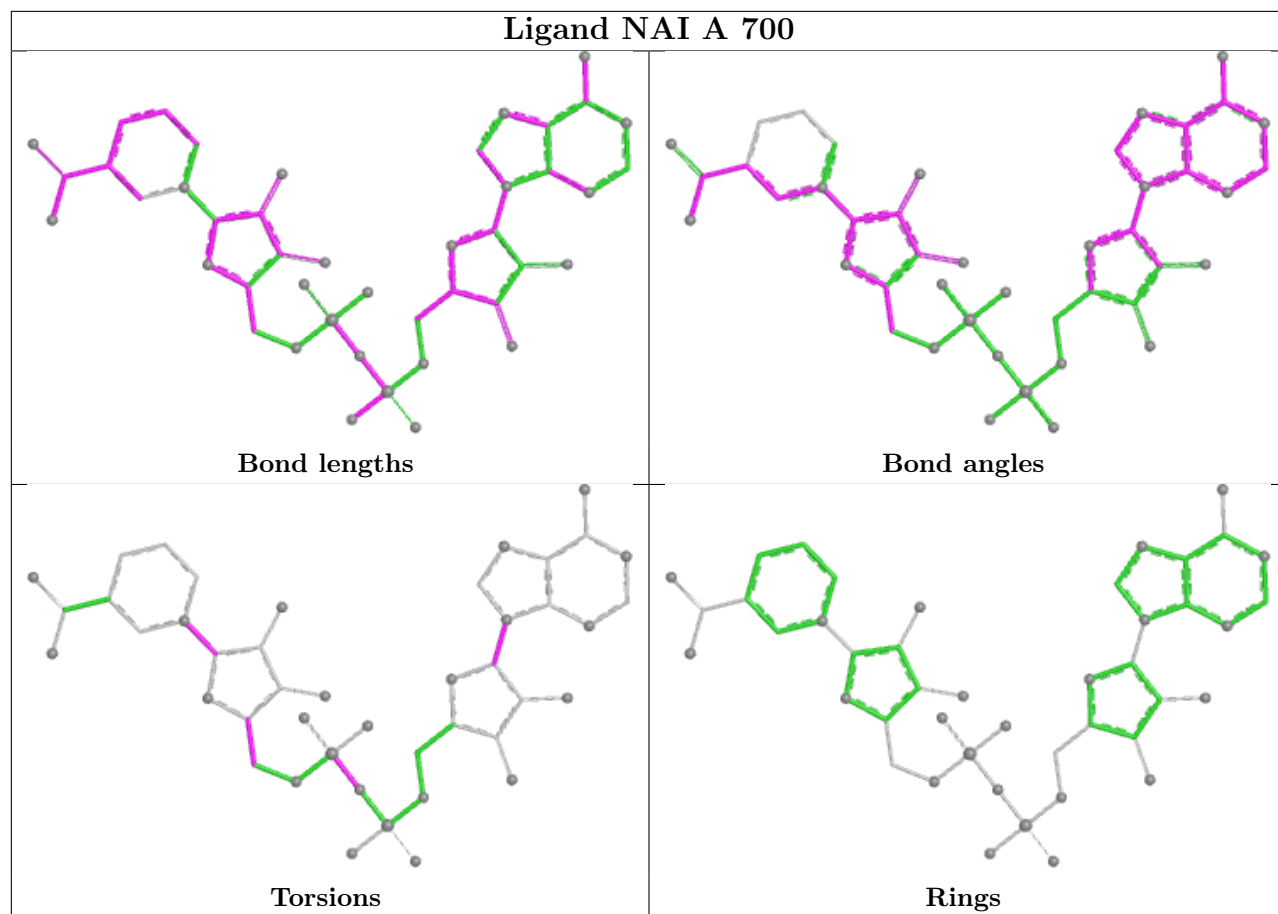
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

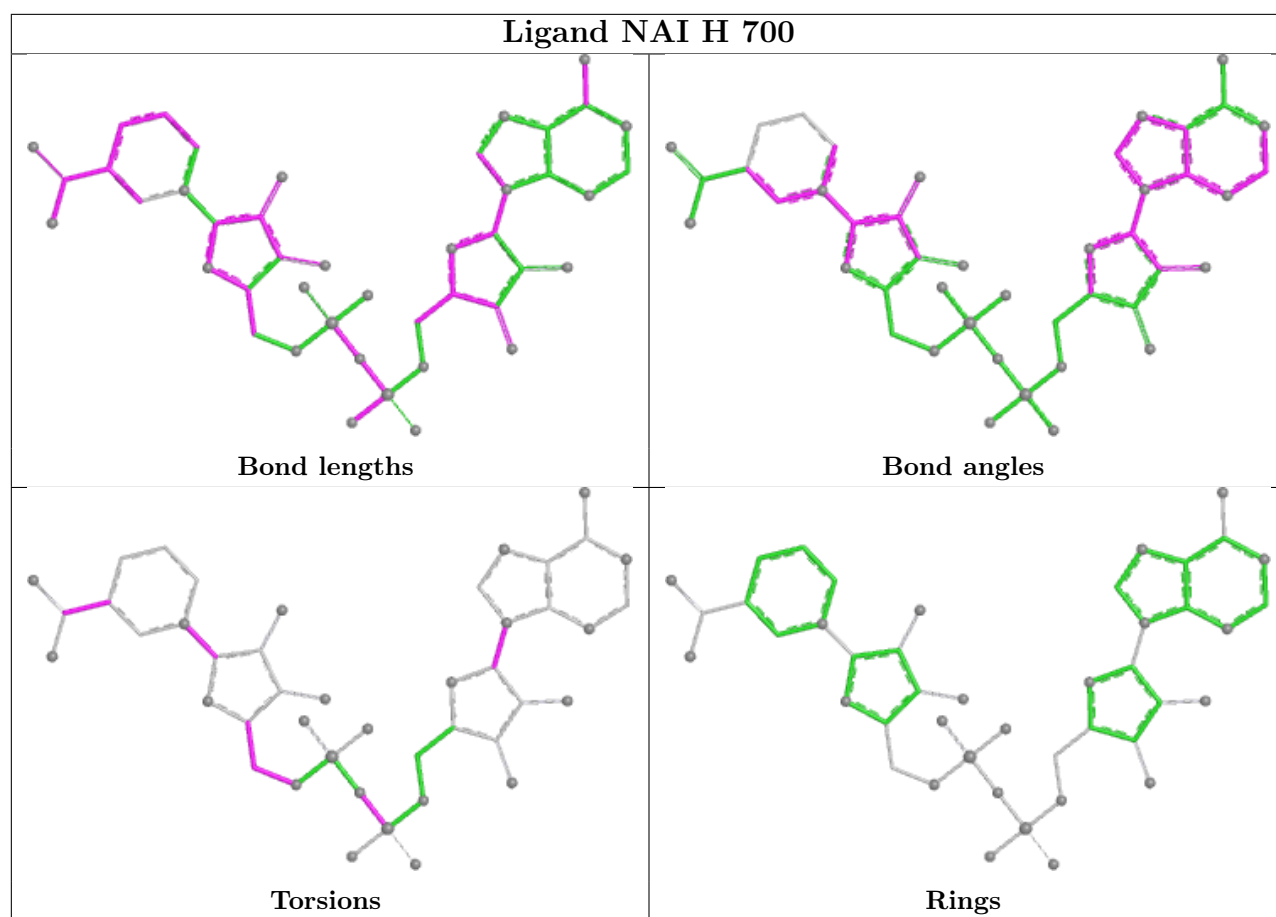


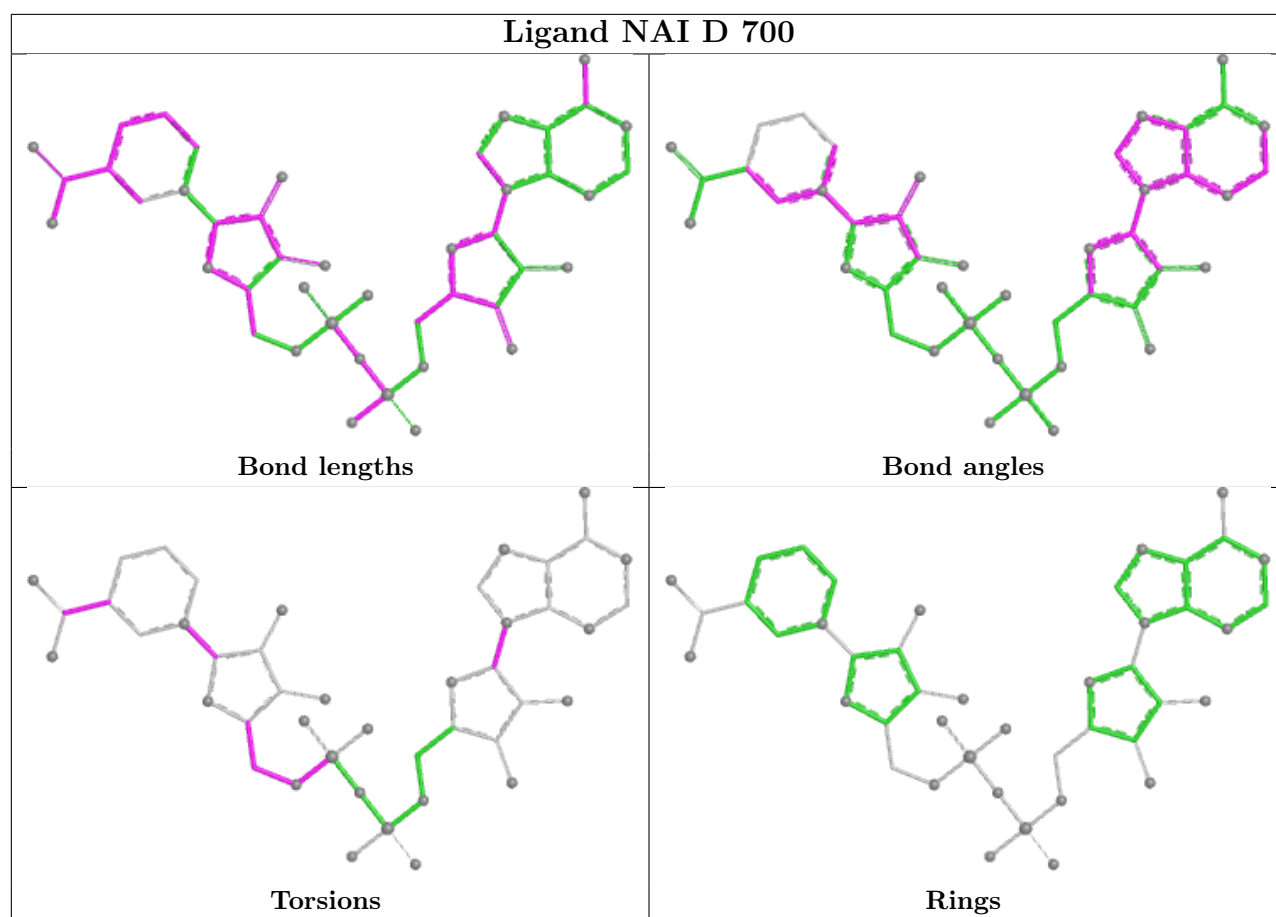


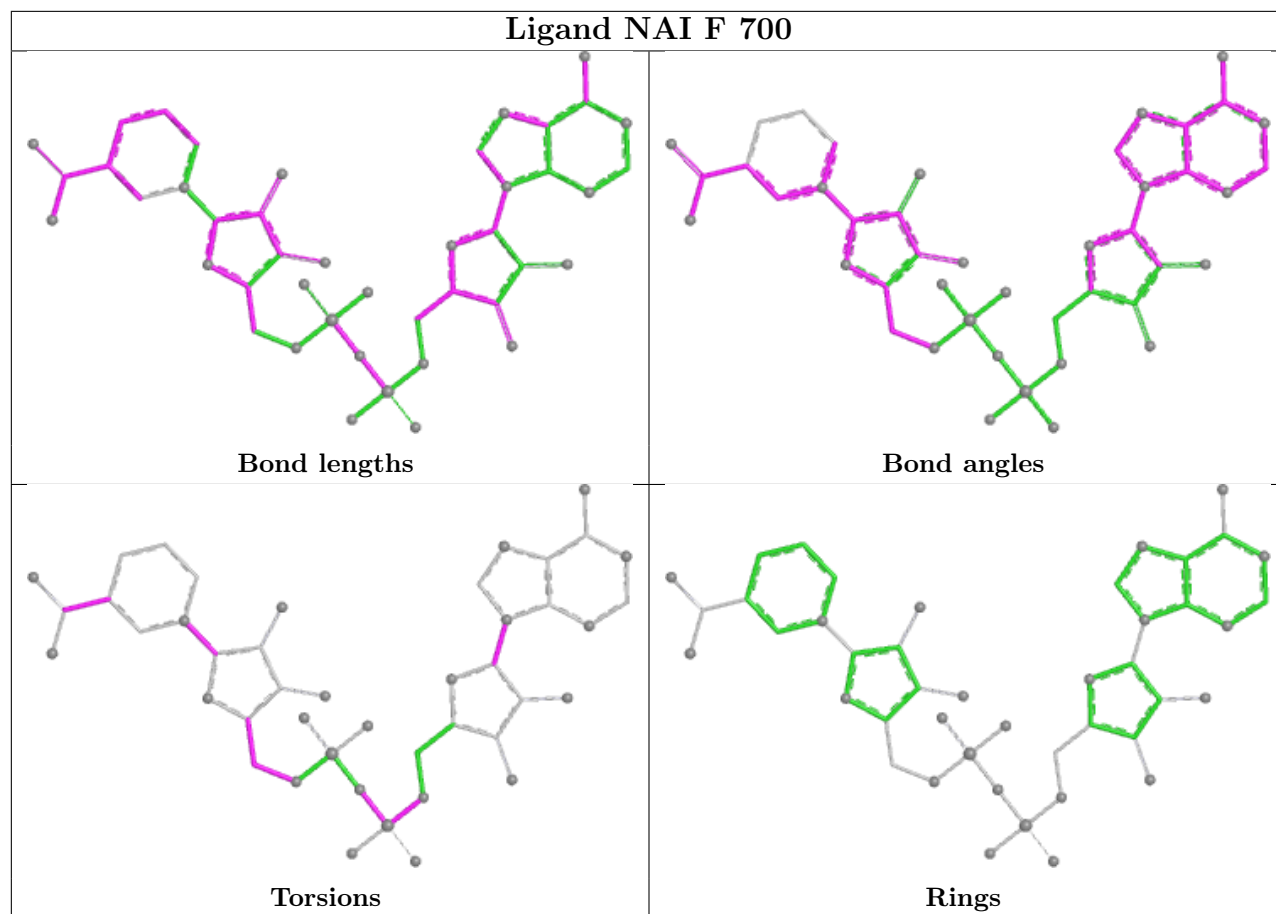












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/497 (99%)	-1.22	0 100 100	12, 28, 49, 66	0
1	B	495/497 (99%)	-0.68	0 100 100	19, 46, 77, 94	0
1	C	495/497 (99%)	-1.26	0 100 100	17, 31, 51, 77	0
1	D	495/497 (99%)	-1.23	0 100 100	13, 29, 49, 72	0
1	E	495/497 (99%)	-1.25	0 100 100	12, 29, 51, 69	0
1	F	495/497 (99%)	-0.86	0 100 100	14, 41, 68, 96	0
1	G	495/497 (99%)	-1.09	0 100 100	17, 38, 61, 88	0
1	H	495/497 (99%)	-1.27	0 100 100	14, 29, 50, 69	0
All	All	3960/3976 (99%)	-1.11	0 100 100	12, 33, 62, 96	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

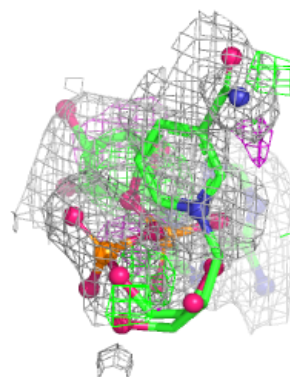
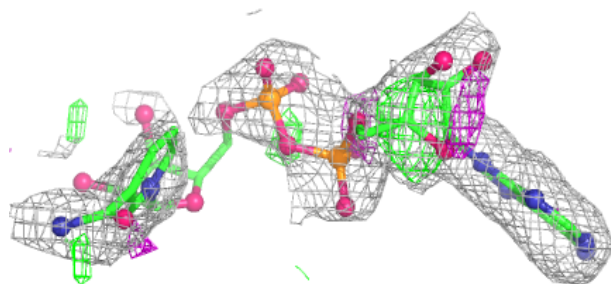
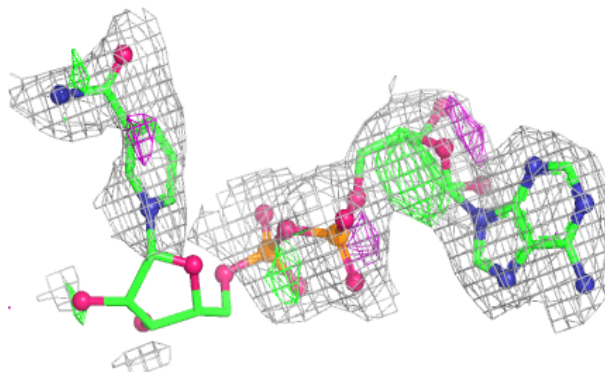
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAI	G	700	44/44	0.97	0.09	38,66,102,104	0
3	IAC	B	701	13/13	0.97	0.10	36,73,82,84	0
2	NAI	B	700	44/44	0.98	0.09	36,56,91,92	0
2	NAI	H	700	44/44	0.98	0.08	16,72,115,117	0
3	IAC	A	701	13/13	0.98	0.09	17,70,74,77	0
2	NAI	F	700	44/44	0.98	0.07	24,66,103,112	0
3	IAC	C	701	13/13	0.98	0.09	48,62,72,73	0
3	IAC	D	701	13/13	0.98	0.10	56,73,82,83	0
3	IAC	E	701	13/13	0.98	0.10	28,69,76,78	0
3	IAC	F	701	13/13	0.98	0.09	41,72,83,87	0
2	NAI	C	700	44/44	0.99	0.07	17,63,107,119	0
2	NAI	D	700	44/44	0.99	0.07	10,56,107,116	0
2	NAI	E	700	44/44	0.99	0.07	20,65,101,107	0
2	NAI	A	700	44/44	0.99	0.07	14,50,104,106	0
3	IAC	G	701	13/13	0.99	0.07	45,70,76,77	0
3	IAC	H	701	13/13	0.99	0.08	46,74,82,83	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.

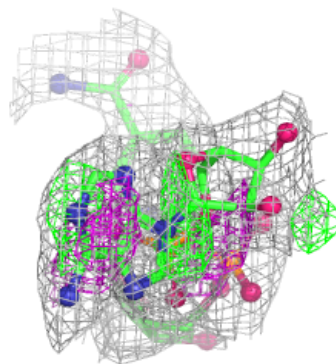
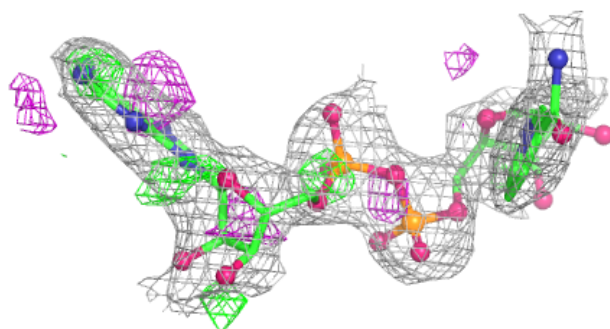
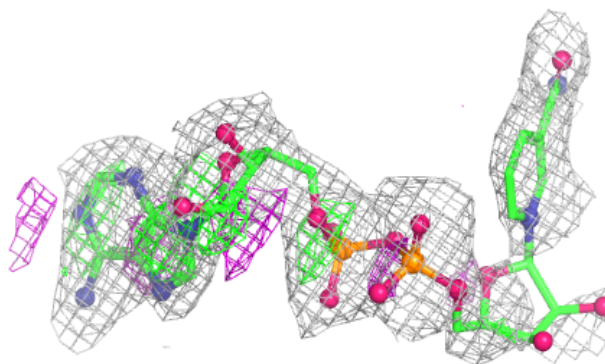
Electron density around NAI G 700:

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

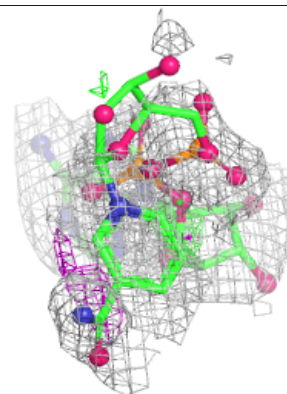
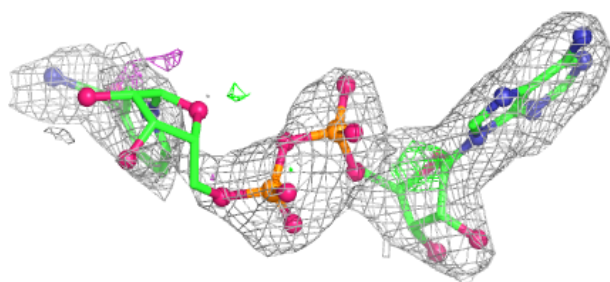
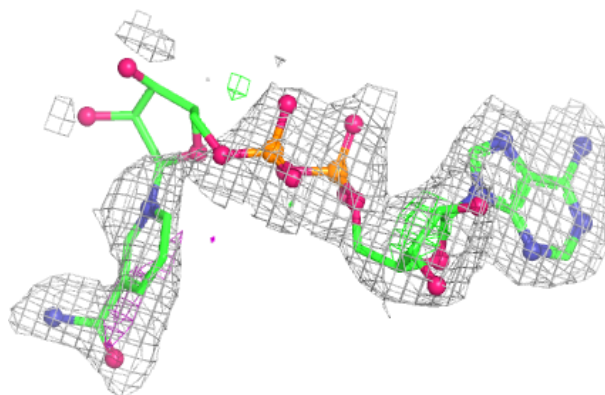


Electron density around NAI B 700:

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

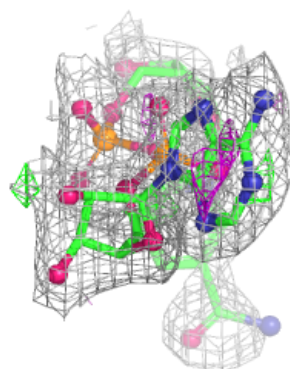
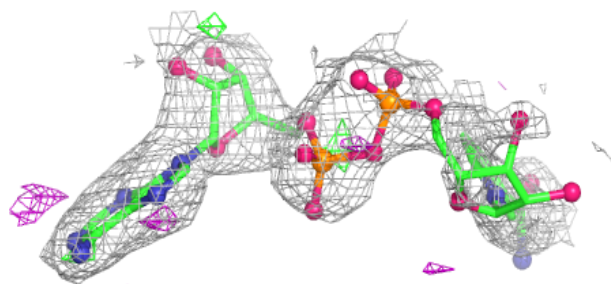
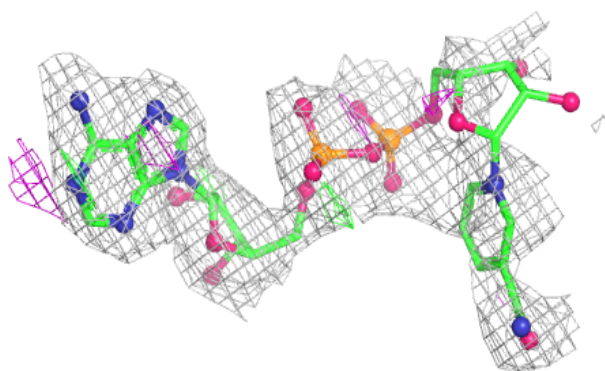
**Electron density around NAI H 700:**

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

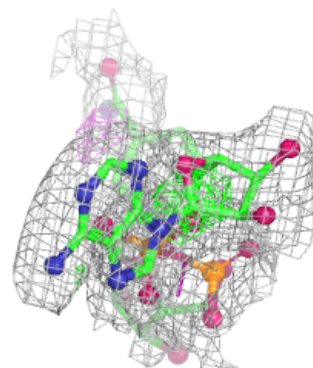
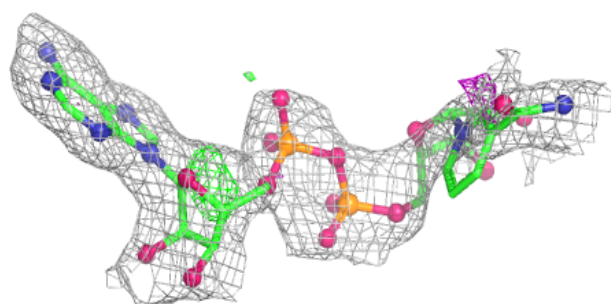


Electron density around NAI F 700:

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

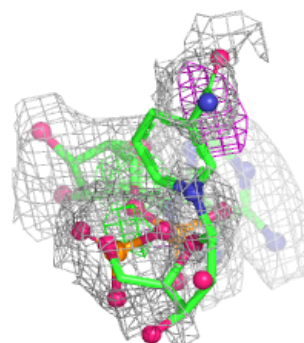
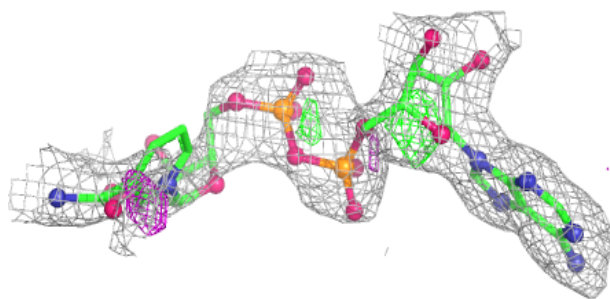
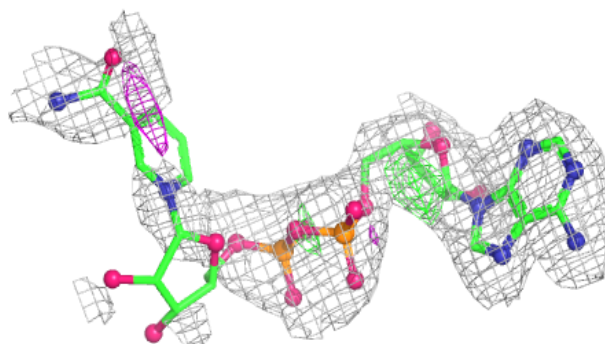
**Electron density around NAI C 700:**

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

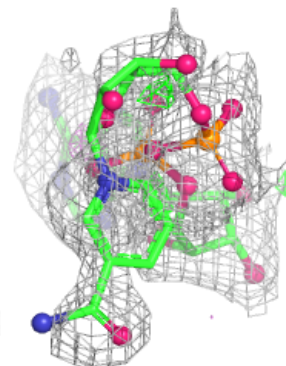
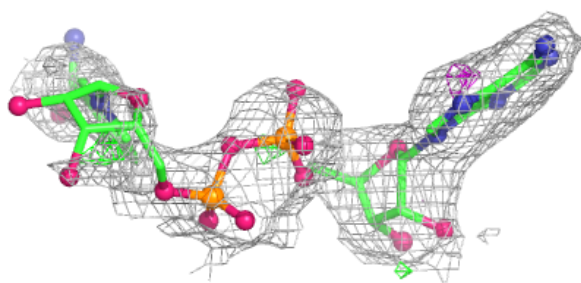
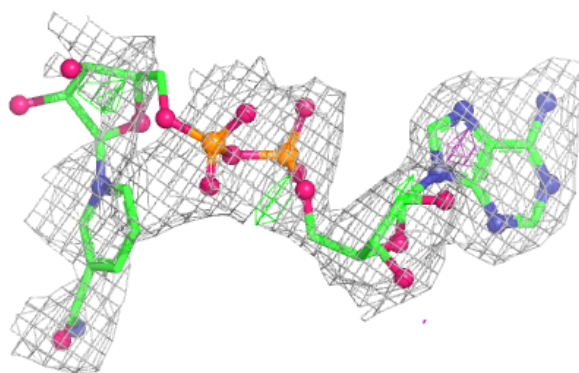


Electron density around NAI D 700:

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

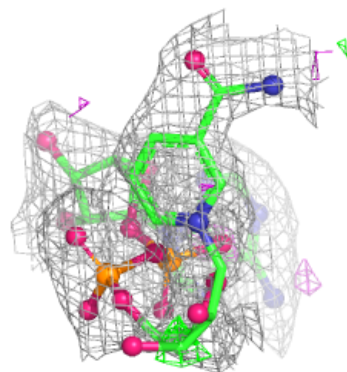
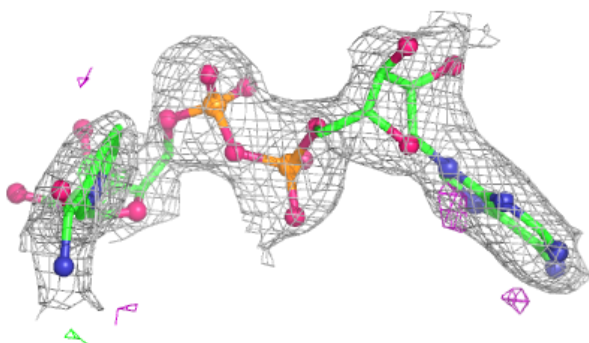
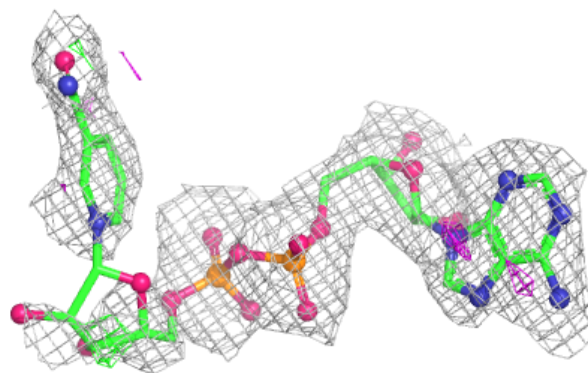
**Electron density around NAI E 700:**

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



Electron density around NAI A 700:

$2mF_o-DF_c$ (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.