



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:40 AM UTC

PDB ID : 2RIR / pdb_00002rir
Title : Crystal structure of dipicolinate synthase, A chain, from *Bacillus subtilis*
Authors : Osipiuk, J.; Quartey, P.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-10-12
Resolution : 2.79 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:

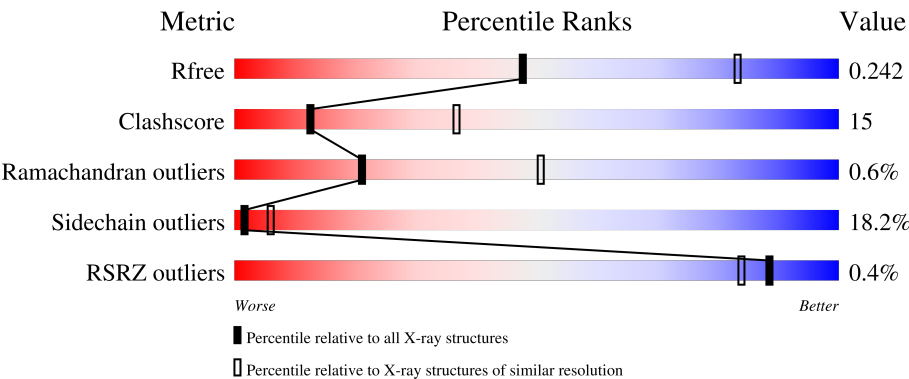
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	300	65%26%7% ..
1	B	300	64%28%7% .
1	C	300	68%23%8% ..
1	D	300	% 64%27%7% ..
1	E	300	% 63%30%7% .

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Mol	Chain	Length	Quality of chain
1	F	300	67%25%7%•
1	G	300	63%29%6%•
1	H	300	63%27%9%••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18495 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 Dipicolinate synthase, A chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	B	296	Total	C	N	O	S	Se	0	1	0
			2240	1424	381	425	3	7			
1	C	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	D	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	E	298	Total	C	N	O	S	Se	0	1	0
			2254	1431	384	429	3	7			
1	F	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	G	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	H	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q04809
A	-1	ASN	-	expression tag	UNP Q04809
A	0	ALA	-	expression tag	UNP Q04809
A	1	MSE	-	expression tag	UNP Q04809
A	297	LEU	-	expression tag	UNP Q04809
B	-2	SER	-	expression tag	UNP Q04809
B	-1	ASN	-	expression tag	UNP Q04809
B	0	ALA	-	expression tag	UNP Q04809
B	1	MSE	-	expression tag	UNP Q04809
B	297	LEU	-	expression tag	UNP Q04809
C	-2	SER	-	expression tag	UNP Q04809
C	-1	ASN	-	expression tag	UNP Q04809
C	0	ALA	-	expression tag	UNP Q04809

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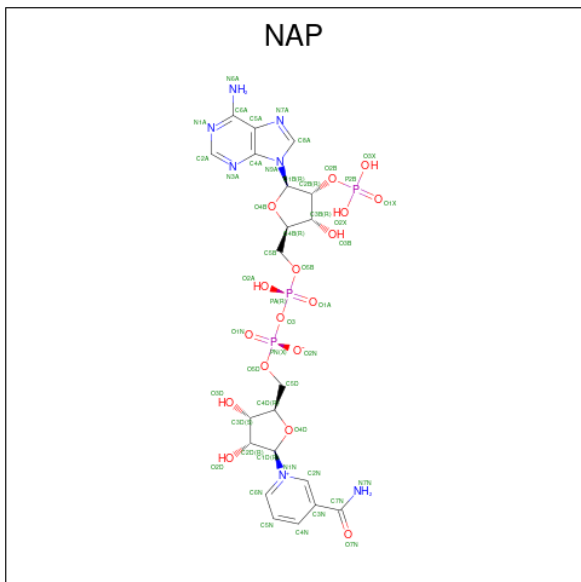
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	expression tag	UNP Q04809
C	297	LEU	-	expression tag	UNP Q04809
D	-2	SER	-	expression tag	UNP Q04809
D	-1	ASN	-	expression tag	UNP Q04809
D	0	ALA	-	expression tag	UNP Q04809
D	1	MSE	-	expression tag	UNP Q04809
D	297	LEU	-	expression tag	UNP Q04809
E	-2	SER	-	expression tag	UNP Q04809
E	-1	ASN	-	expression tag	UNP Q04809
E	0	ALA	-	expression tag	UNP Q04809
E	1	MSE	-	expression tag	UNP Q04809
E	297	LEU	-	expression tag	UNP Q04809
F	-2	SER	-	expression tag	UNP Q04809
F	-1	ASN	-	expression tag	UNP Q04809
F	0	ALA	-	expression tag	UNP Q04809
F	1	MSE	-	expression tag	UNP Q04809
F	297	LEU	-	expression tag	UNP Q04809
G	-2	SER	-	expression tag	UNP Q04809
G	-1	ASN	-	expression tag	UNP Q04809
G	0	ALA	-	expression tag	UNP Q04809
G	1	MSE	-	expression tag	UNP Q04809
G	297	LEU	-	expression tag	UNP Q04809
H	-2	SER	-	expression tag	UNP Q04809
H	-1	ASN	-	expression tag	UNP Q04809
H	0	ALA	-	expression tag	UNP Q04809
H	1	MSE	-	expression tag	UNP Q04809
H	297	LEU	-	expression tag	UNP Q04809

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	2	Total Cl 2 2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	H	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	25	Total O 26 26	0	1

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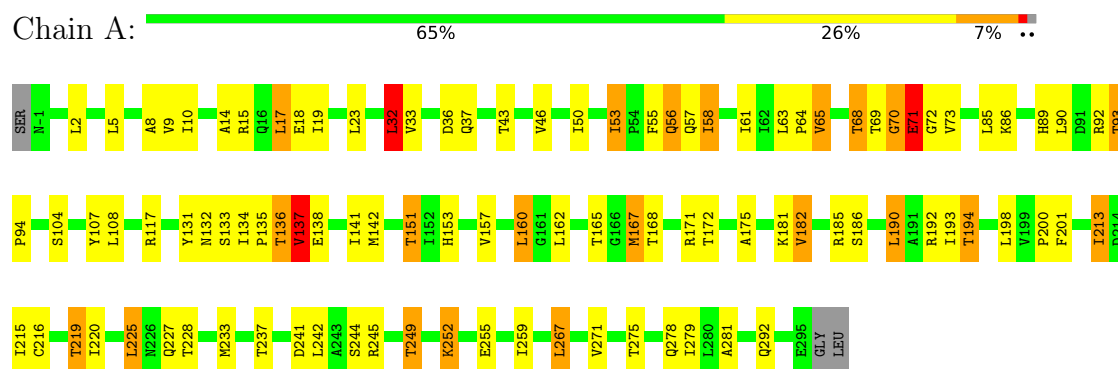
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	23	Total 23	O 23	0	0
4	D	15	Total 15	O 15	0	0
4	E	6	Total 6	O 6	0	0
4	F	5	Total 5	O 5	0	0
4	G	20	Total 20	O 20	0	0
4	H	10	Total 10	O 10	0	0

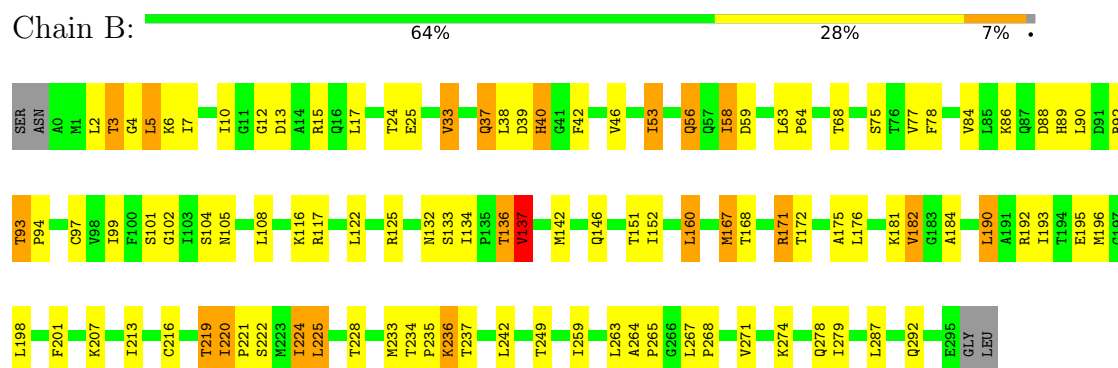
3 Residue-property plots [i](#)

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.

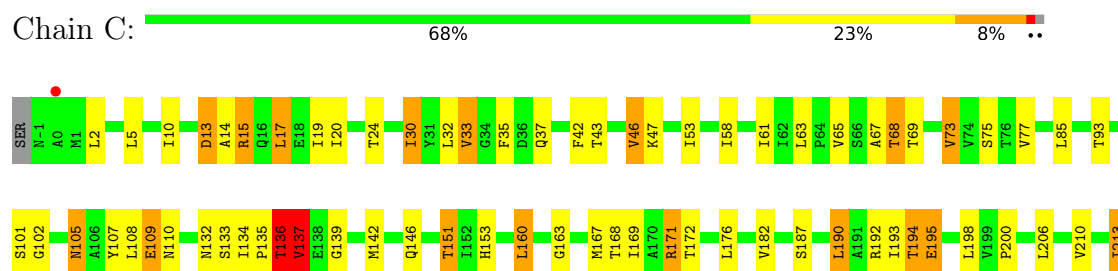
- Molecule 1: Dipicolinate synthase, A chain



- Molecule 1: Dipicolinate synthase, A chain

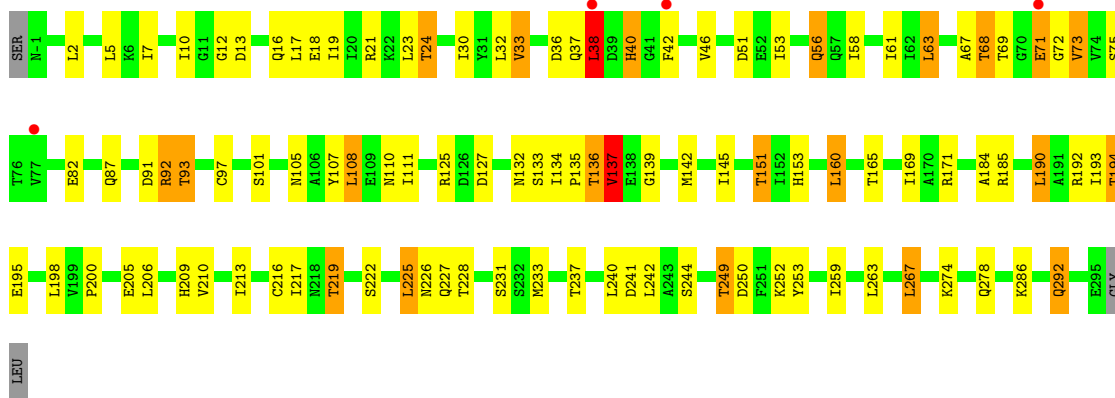


- Molecule 1: Dipicolinate synthase, A chain

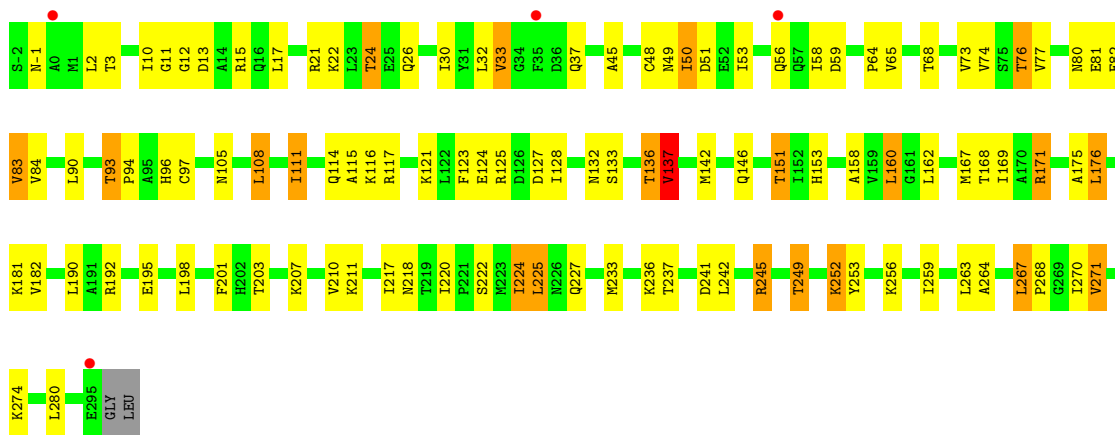




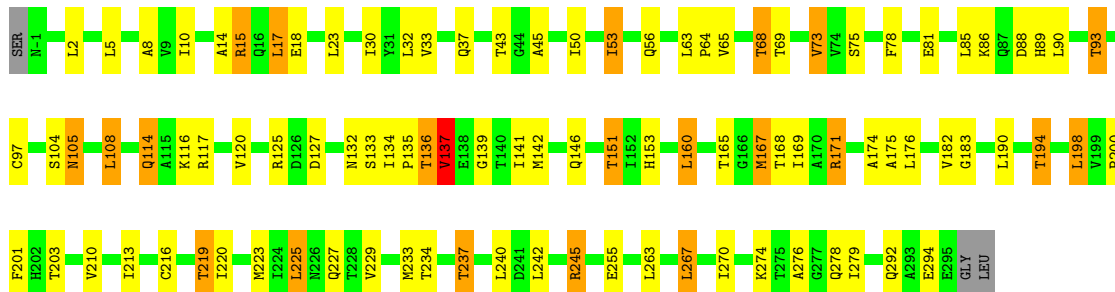
• Molecule 1: Dipicolinate synthase, A chain



• Molecule 1: Dipicolinate synthase, A chain

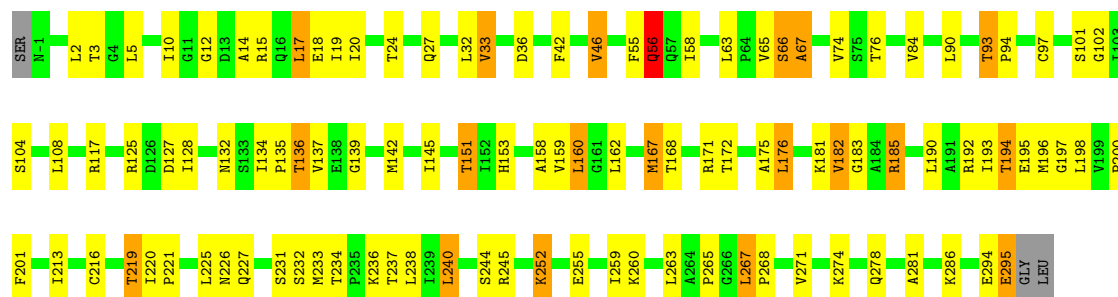


• Molecule 1: Dipicolinate synthase, A chain



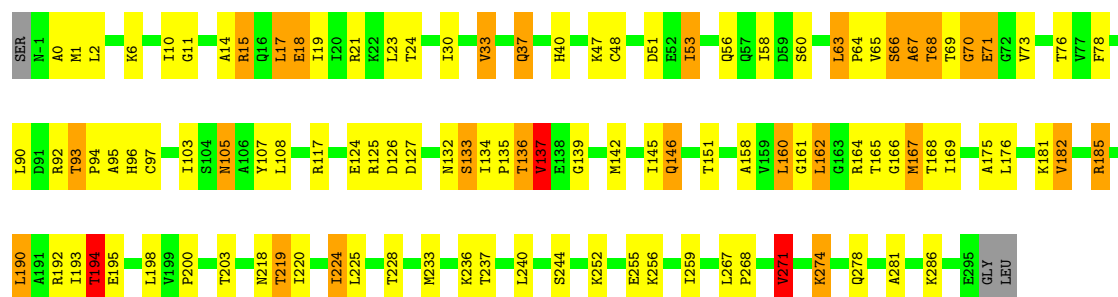
• Molecule 1: Dipicolinate synthase, A chain

Chain G:  63% 29% 6%



• Molecule 1: Dipicolinate synthase, A chain

Chain H:  63% 27% 9% 1%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.58Å 75.11Å 200.46Å 90.00° 119.74° 90.00°	Depositor
Resolution (Å)	40.00 – 2.79 40.00 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.00-2.79) 96.3 (40.00-2.79)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.249 0.193 , 0.242	Depositor DCC
R_{free} test set	4079 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18495	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.82	0/2277	1.08	4/3078 (0.1%)
1	B	0.77	0/2269	1.08	5/3067 (0.2%)
1	C	0.82	0/2277	1.10	8/3078 (0.3%)
1	D	0.78	1/2277 (0.0%)	1.06	4/3078 (0.1%)
1	E	0.70	0/2283	1.01	5/3086 (0.2%)
1	F	0.70	0/2277	1.05	4/3078 (0.1%)
1	G	0.79	0/2277	1.08	2/3078 (0.1%)
1	H	0.80	0/2277	1.03	3/3078 (0.1%)
All	All	0.77	1/18214 (0.0%)	1.06	35/24621 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	24	THR	CA-CB	6.38	1.63	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	137	VAL	CB-CA-C	-8.65	100.89	111.97
1	B	137	VAL	CB-CA-C	-8.61	100.52	112.14
1	C	137	VAL	CB-CA-C	-8.46	100.71	112.14
1	A	137	VAL	CB-CA-C	-7.96	101.39	112.14
1	G	12	GLY	N-CA-C	7.87	120.68	111.63
1	H	137	VAL	CB-CA-C	-7.67	102.00	112.04
1	D	137	VAL	CB-CA-C	-7.45	102.28	112.04
1	C	46	VAL	CB-CA-C	-7.04	101.05	110.98
1	E	12	GLY	N-CA-C	6.83	120.07	110.38
1	F	220	ILE	N-CA-C	6.71	114.54	107.76
1	E	137	VAL	CB-CA-C	-6.67	103.01	112.22
1	D	137	VAL	N-CA-CB	6.65	118.78	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	ILE	N-CA-C	6.55	114.38	107.76
1	D	12	GLY	N-CA-C	6.47	119.07	111.63
1	G	46	VAL	CB-CA-C	-6.33	102.25	111.68
1	C	30	ILE	N-CA-C	6.21	117.54	108.53
1	F	137	VAL	N-CA-CB	6.21	117.82	110.55
1	B	77	VAL	N-CA-C	-6.14	106.24	113.42
1	C	136	THR	N-CA-C	6.03	118.81	111.82
1	B	137	VAL	N-CA-CB	5.61	118.17	110.54
1	H	271	VAL	N-CA-C	5.57	116.35	110.72
1	A	32	LEU	N-CA-C	5.55	117.69	108.20
1	E	264	ALA	CA-C-N	-5.52	114.89	120.85
1	E	264	ALA	C-N-CA	-5.52	114.89	120.85
1	B	279	ILE	N-CA-C	-5.51	104.95	110.30
1	F	270	ILE	N-CA-C	5.45	115.65	110.53
1	C	13	ASP	CB-CA-C	-5.44	100.87	112.63
1	B	220	ILE	N-CA-C	5.43	113.30	108.63
1	A	220	ILE	N-CA-C	5.40	113.27	108.63
1	C	137	VAL	N-CA-CB	5.33	117.79	110.54
1	C	110	ASN	N-CA-C	5.22	116.65	111.07
1	E	76	THR	N-CA-C	5.21	116.51	109.11
1	D	38	LEU	N-CA-C	5.15	117.68	109.96
1	A	141	ILE	N-CA-C	-5.10	105.53	110.42
1	H	194	THR	N-CA-CB	5.06	118.13	110.28

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	2248	0	2328	77	0
1	B	2240	0	2322	80	0
1	C	2248	0	2328	76	0
1	D	2248	0	2328	78	0
1	E	2254	0	2333	69	0
1	F	2248	0	2328	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2248	0	2328	77	0
1	H	2248	0	2328	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
3	A	48	0	25	5	0
3	B	48	0	25	4	0
3	C	48	0	25	3	0
3	D	48	0	25	4	0
3	E	48	0	25	1	0
3	F	48	0	25	4	0
3	G	48	0	25	3	0
3	H	48	0	25	5	0
4	A	17	0	0	1	0
4	B	26	0	0	1	0
4	C	23	0	0	6	0
4	D	15	0	0	2	0
4	E	6	0	0	1	0
4	F	5	0	0	1	0
4	G	20	0	0	2	0
4	H	10	0	0	2	0
All	All	18495	0	18823	568	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 15.

All (568) 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:C:171:ARG:HG3	1:C:171:ARG:HH11	1.08	1.17
4:E:511:HOH:O	1:F:194:THR:HG21	1.40	1.16
1:E:245:ARG:HB2	1:E:245:ARG:HH21	0.99	1.09
1:C:142[B]:MSE:HE1	1:D:142[B]:MSE:HA	1.27	1.06
1:H:68:THR:HG22	1:H:105:ASN:HD21	1.16	1.05
1:H:219:THR:HG21	4:H:511:HOH:O	1.59	1.02
1:E:245:ARG:HB2	1:E:245:ARG:NH2	1.78	0.97
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.30	0.95
1:D:194:THR:HG22	1:D:200:PRO:HG3	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:THR:HG22	1:C:105:ASN:HD21	1.32	0.94
1:B:40:HIS:HB3	4:B:505:HOH:O	1.68	0.92
1:G:233:MSE:HE3	1:G:237:THR:HB	1.51	0.91
1:E:245:ARG:HH21	1:E:245:ARG:CB	1.84	0.91
1:C:233:MSE:HE3	1:C:237:THR:HB	1.52	0.90
1:H:95:ALA:HA	1:H:117:ARG:NH2	1.89	0.86
1:H:194:THR:HG22	1:H:200:PRO:HG3	1.57	0.86
1:G:93:THR:HG22	1:G:117:ARG:HE	1.40	0.85
1:D:233:MSE:HE3	1:D:237:THR:HB	1.58	0.84
1:B:86:LYS:H	1:B:89:HIS:CD2	1.94	0.83
1:E:133:SER:HA	1:E:136:THR:HG23	1.60	0.83
1:D:24:THR:HG22	1:D:30:ILE:HD12	1.60	0.82
1:E:33:VAL:HG11	1:E:53:ILE:HD11	1.60	0.82
1:C:223:MSE:HE2	1:C:226:ASN:HA	1.60	0.82
1:G:185:ARG:HD3	3:G:407:NAP:O1X	1.79	0.82
1:E:132:ASN:O	1:E:136:THR:HG22	1.79	0.82
1:B:196:MSE:HG2	1:C:171:ARG:HH21	1.45	0.81
1:C:171:ARG:HH11	1:C:171:ARG:CG	1.90	0.81
1:B:93:THR:HG22	1:B:117:ARG:HE	1.45	0.80
1:A:93:THR:HG22	1:A:117:ARG:HE	1.46	0.79
1:B:171:ARG:HH11	1:B:171:ARG:CG	1.95	0.79
1:H:40:HIS:HE2	1:H:47:LYS:HD3	1.46	0.79
1:B:53:ILE:HD11	1:B:58:ILE:HG12	1.64	0.79
1:H:11:GLY:HA2	1:H:76:THR:HG22	1.62	0.79
1:D:92:ARG:HG2	1:D:92:ARG:HH11	1.48	0.78
1:C:142[B]:MSE:HE3	1:D:145:ILE:HB	1.66	0.77
1:D:24:THR:CG2	1:D:30:ILE:HD12	2.14	0.77
1:D:38:LEU:HD21	1:D:40:HIS:HB3	1.67	0.77
1:C:151:THR:HG22	1:C:153:HIS:O	1.83	0.77
1:G:93:THR:HG23	1:G:97:CYS:HB3	1.66	0.76
1:F:171:ARG:HG3	1:F:171:ARG:HH11	1.50	0.76
1:B:86:LYS:H	1:B:89:HIS:HD2	1.31	0.76
1:C:68:THR:HG22	1:C:105:ASN:ND2	2.01	0.76
1:A:233:MSE:HE3	1:A:237:THR:HB	1.67	0.75
1:D:5:LEU:HD11	1:D:292:GLN:HB2	1.66	0.75
1:F:2:LEU:HA	1:F:292:GLN:HE22	1.52	0.75
1:H:0:ALA:O	1:H:1:MSE:HE2	1.86	0.75
1:G:245:ARG:HH11	1:G:265:PRO:HG2	1.51	0.75
1:H:68:THR:HG22	1:H:105:ASN:ND2	1.97	0.75
1:H:160:LEU:O	1:H:219:THR:HB	1.87	0.74
1:D:40:HIS:CD2	1:D:42:PHE:HB2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:O	1:A:93:THR:HB	1.88	0.74
1:A:160:LEU:O	1:A:219:THR:HB	1.87	0.73
1:H:18:GLU:OE1	1:H:21:ARG:NH1	2.21	0.73
1:C:142[B]:MSE:CE	1:D:142[B]:MSE:HA	2.14	0.73
1:G:132:ASN:O	1:G:136:THR:HG23	1.89	0.73
1:H:185:ARG:HD2	3:H:408:NAP:C2A	2.19	0.73
1:C:233:MSE:HE3	1:C:237:THR:CB	2.19	0.72
1:C:233:MSE:CE	1:C:237:THR:HB	2.18	0.72
1:G:132:ASN:O	1:G:136:THR:CG2	2.36	0.72
1:H:68:THR:HG23	1:H:69:THR:N	2.03	0.72
1:B:196:MSE:HG2	1:C:171:ARG:NH2	2.04	0.72
1:E:245:ARG:NH2	1:E:245:ARG:CB	2.48	0.72
1:E:220:ILE:HB	1:E:224:ILE:HD11	1.71	0.72
1:A:133:SER:HA	1:A:136:THR:HG23	1.72	0.72
1:G:252:LYS:O	1:G:255:GLU:HB3	1.89	0.72
1:E:59:ASP:O	1:E:97:CYS:HA	1.89	0.71
1:A:132:ASN:O	1:A:136:THR:HG22	1.90	0.71
1:F:133:SER:HA	1:F:136:THR:HG23	1.71	0.71
1:G:136:THR:HG22	1:G:268:PRO:HG3	1.73	0.71
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.55	0.71
1:B:142[A]:MSE:HE2	1:B:146:GLN:NE2	2.05	0.70
1:H:233:MSE:HE3	1:H:237:THR:HB	1.73	0.70
1:C:245:ARG:CD	1:C:245:ARG:H	2.04	0.69
1:F:69:THR:OG1	1:F:73:VAL:HG13	1.92	0.69
1:H:219:THR:CG2	4:H:511:HOH:O	2.28	0.69
1:F:132:ASN:O	1:F:135:PRO:HD2	1.92	0.69
1:F:146:GLN:HE21	1:H:142[B]:MSE:HE1	1.57	0.69
1:E:171:ARG:HH11	1:E:171:ARG:HB3	1.58	0.68
1:C:132:ASN:O	1:C:136:THR:HG22	1.94	0.68
1:B:171:ARG:NH2	1:C:195:GLU:OE2	2.23	0.68
1:B:213:ILE:HD11	1:B:216:CYS:HB2	1.75	0.68
1:F:242:LEU:O	3:F:406:NAP:H2N	1.94	0.68
1:H:68:THR:HG23	1:H:69:THR:H	1.58	0.68
1:F:194:THR:HG22	1:F:200:PRO:HG3	1.76	0.68
1:H:68:THR:HG21	1:H:107:TYR:HD1	1.59	0.68
1:G:194:THR:HG22	1:G:200:PRO:HG3	1.76	0.67
1:E:24:THR:HG23	1:E:30:ILE:HD12	1.76	0.67
1:E:252:LYS:H	1:E:252:LYS:HD3	1.58	0.67
1:F:105:ASN:OD1	1:F:108:LEU:HB2	1.94	0.67
1:F:132:ASN:O	1:F:136:THR:HG22	1.93	0.67
1:C:192:ARG:HD2	4:C:424:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:GLU:O	1:G:295:GLU:HG2	1.94	0.67
1:G:255:GLU:HA	1:G:255:GLU:OE1	1.94	0.66
1:B:160:LEU:HB3	1:B:220:ILE:HD12	1.77	0.66
1:E:146:GLN:HB3	1:G:142[A]:MSE:CE	2.24	0.66
1:C:132:ASN:O	1:C:136:THR:CG2	2.43	0.66
1:B:233:MSE:HE3	1:B:237:THR:HB	1.77	0.66
1:C:75:SER:HB3	4:C:425:HOH:O	1.95	0.66
1:B:171:ARG:CG	1:B:171:ARG:NH1	2.56	0.66
1:C:171:ARG:HG3	1:C:171:ARG:NH1	1.90	0.66
1:A:233:MSE:CE	1:A:237:THR:HB	2.26	0.66
1:E:142[B]:MSE:HE1	1:G:142[B]:MSE:HA	1.77	0.66
1:B:160:LEU:O	1:B:219:THR:HB	1.96	0.65
1:F:93:THR:HG22	1:F:117:ARG:HE	1.61	0.65
1:C:219:THR:HG21	4:C:404:HOH:O	1.96	0.65
1:A:142[A]:MSE:HG3	1:B:142[A]:MSE:HE1	1.78	0.65
1:B:24:THR:HG21	1:B:42:PHE:HB3	1.79	0.65
1:A:194:THR:HG22	1:A:200:PRO:HG3	1.77	0.64
1:G:171:ARG:NH2	1:H:195:GLU:OE2	2.23	0.64
1:D:213:ILE:HD11	1:D:216:CYS:HB2	1.78	0.64
1:B:265:PRO:HA	3:B:402:NAP:H72N	1.62	0.64
1:E:252:LYS:H	1:E:252:LYS:CD	2.07	0.64
1:F:86:LYS:H	1:F:89:HIS:CD2	2.15	0.64
1:H:68:THR:HG21	1:H:107:TYR:CD1	2.33	0.64
1:C:218:ASN:OD1	1:C:224:ILE:HD11	1.98	0.64
1:A:69:THR:OG1	1:A:73:VAL:HG12	1.97	0.63
1:H:66:SER:O	1:H:67:ALA:HB3	1.97	0.63
1:F:213:ILE:O	1:F:237:THR:HG23	1.99	0.63
1:A:132:ASN:O	1:A:136:THR:CG2	2.47	0.63
1:A:69:THR:HG1	1:A:73:VAL:HG12	1.63	0.63
1:A:241:ASP:OD2	1:A:249:THR:CG2	2.47	0.63
1:H:70:GLY:HA2	1:H:107:TYR:CB	2.28	0.63
1:H:133:SER:HA	1:H:136:THR:HG23	1.80	0.63
1:A:162:LEU:HD22	1:A:193:ILE:HG13	1.82	0.62
1:B:59:ASP:O	1:B:97:CYS:HA	1.99	0.62
1:H:70:GLY:HA2	1:H:107:TYR:HB3	1.82	0.62
1:E:146:GLN:HE21	1:G:142[A]:MSE:HE1	1.64	0.62
1:D:16:GLN:HA	1:D:19:ILE:HD12	1.81	0.61
1:A:134:ILE:O	1:A:137:VAL:HG23	2.00	0.61
1:E:10:ILE:HG22	1:E:74:VAL:HG11	1.80	0.61
1:G:233:MSE:HE3	1:G:237:THR:CB	2.29	0.61
1:H:66:SER:O	1:H:67:ALA:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:ASN:O	1:H:135:PRO:HD2	2.01	0.61
1:B:68:THR:HG23	1:B:105:ASN:HD21	1.66	0.61
1:H:48:CYS:SG	1:H:53:ILE:HG22	2.40	0.61
1:D:38:LEU:CD2	1:D:40:HIS:HB3	2.30	0.61
1:E:132:ASN:O	1:E:136:THR:CG2	2.49	0.61
1:C:133:SER:HA	1:C:136:THR:HG23	1.82	0.61
1:B:220:ILE:HD13	1:B:224:ILE:HD11	1.84	0.60
1:F:93:THR:HG23	1:F:97:CYS:HB3	1.83	0.60
1:D:233:MSE:HE3	1:D:237:THR:CB	2.29	0.60
1:A:157:VAL:HG22	1:A:215:ILE:HB	1.83	0.60
1:E:142[B]:MSE:CE	1:G:145:ILE:HB	2.32	0.60
1:H:69:THR:C	1:H:71:GLU:H	2.10	0.60
1:C:142[B]:MSE:HE1	1:D:142[B]:MSE:CA	2.18	0.60
1:B:132:ASN:O	1:B:136:THR:CG2	2.49	0.60
1:D:68:THR:HG23	1:D:72:GLY:HA2	1.84	0.60
1:F:160:LEU:O	1:F:219:THR:HB	2.01	0.60
1:E:76:THR:HG21	1:E:83:VAL:CG1	2.32	0.59
1:H:190:LEU:HA	1:H:193:ILE:HD12	1.83	0.59
1:B:133:SER:HA	1:B:136:THR:HG23	1.85	0.59
1:B:192:ARG:HH21	1:B:195:GLU:HG2	1.66	0.59
1:D:10:ILE:HD12	1:D:61:ILE:HG23	1.83	0.59
1:A:131:TYR:HB3	1:A:279:ILE:HD13	1.84	0.59
1:A:93:THR:HG22	1:A:117:ARG:NE	2.18	0.58
1:C:192:ARG:HH21	1:C:195:GLU:HG2	1.67	0.58
1:A:168:THR:OG1	1:D:192:ARG:NH2	2.36	0.58
1:C:242:LEU:O	3:C:403:NAP:H2N	2.03	0.58
1:D:184:ALA:HB3	1:D:190:LEU:HD13	1.85	0.58
1:E:252:LYS:HD3	1:E:252:LYS:N	2.18	0.58
1:F:132:ASN:O	1:F:136:THR:CG2	2.51	0.58
1:D:33:VAL:CG1	1:D:53:ILE:HD11	2.32	0.58
1:H:136:THR:HG22	1:H:268:PRO:HG3	1.83	0.58
1:G:234:THR:HG23	1:G:236:LYS:HB2	1.86	0.58
1:H:23:LEU:HB2	1:H:30:ILE:HD11	1.86	0.58
1:H:14:ALA:HA	1:H:17:LEU:HD22	1.86	0.58
1:A:241:ASP:OD2	1:A:249:THR:HG22	2.04	0.57
1:F:90:LEU:O	1:F:93:THR:HB	2.04	0.57
1:A:134:ILE:HB	1:A:135:PRO:HD3	1.85	0.57
1:G:183:GLY:HA2	1:G:201:PHE:O	2.05	0.57
1:G:93:THR:CG2	1:G:97:CYS:HB3	2.33	0.57
1:A:9:VAL:HB	1:A:32:LEU:HD12	1.86	0.57
1:C:105:ASN:O	1:C:109:GLU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:THR:OG1	1:C:192:ARG:NH2	2.38	0.57
1:B:225:LEU:HB3	1:B:249:THR:HG23	1.86	0.57
1:E:121:LYS:O	1:E:124:GLU:HB2	2.04	0.57
1:A:133:SER:HB3	1:A:165:THR:HG22	1.87	0.57
1:D:132:ASN:O	1:D:136:THR:CG2	2.52	0.57
1:D:68:THR:HG21	1:D:107:TYR:HD1	1.70	0.56
1:H:94:PRO:HB2	1:H:96:HIS:ND1	2.20	0.56
1:A:56:GLN:OE1	1:A:57:GLN:HG2	2.04	0.56
1:F:213:ILE:CD1	1:F:216:CYS:HB2	2.35	0.56
1:A:86:LYS:H	1:A:89:HIS:CD2	2.24	0.56
1:B:68:THR:HG22	1:B:105:ASN:ND2	2.19	0.56
1:B:234:THR:OG1	1:B:235:PRO:HD2	2.05	0.56
1:E:267:LEU:O	1:E:271:VAL:HG23	2.05	0.56
1:C:151:THR:CG2	1:C:153:HIS:HB3	2.36	0.56
1:H:203:THR:HG21	3:H:408:NAP:H2A	1.87	0.56
1:C:146:GLN:HB3	1:D:142[A]:MSE:HE1	1.88	0.56
1:C:223:MSE:HE2	1:C:226:ASN:CA	2.32	0.56
1:D:160:LEU:O	1:D:219:THR:HB	2.06	0.56
1:F:137:VAL:HG13	1:F:169:ILE:HA	1.88	0.56
1:G:192:ARG:HH21	1:G:195:GLU:HG2	1.70	0.56
1:H:37:GLN:HB2	1:H:78:PHE:O	2.06	0.56
1:B:233:MSE:HE2	1:B:259:ILE:HD13	1.88	0.55
1:G:24:THR:HG21	1:G:42:PHE:HB3	1.88	0.55
1:G:90:LEU:O	1:G:93:THR:HB	2.05	0.55
1:D:225:LEU:CB	1:D:249:THR:HB	2.36	0.55
1:F:171:ARG:HH11	1:F:171:ARG:CG	2.20	0.55
1:H:15:ARG:NH1	1:H:65:VAL:HG21	2.21	0.55
1:A:171:ARG:HG3	1:A:171:ARG:NH1	2.21	0.55
1:B:122:LEU:O	1:B:125:ARG:HG3	2.07	0.55
1:D:67:ALA:HB2	1:D:101:SER:OG	2.06	0.55
1:G:67:ALA:HB2	1:G:101:SER:OG	2.07	0.55
1:C:142[B]:MSE:HE2	1:D:145:ILE:HD12	1.88	0.55
1:D:16:GLN:HG2	4:D:509:HOH:O	2.07	0.55
1:E:137:VAL:HG21	1:E:168:THR:HG22	1.87	0.55
1:H:68:THR:CG2	1:H:69:THR:N	2.69	0.55
1:G:192:ARG:NH2	1:H:168:THR:OG1	2.40	0.55
1:C:160:LEU:HB2	1:C:218:ASN:HA	1.89	0.55
1:H:134:ILE:O	1:H:137:VAL:HG23	2.07	0.55
1:H:10:ILE:HG12	1:H:33:VAL:HG13	1.90	0.54
1:F:183:GLY:HA2	1:F:201:PHE:O	2.07	0.54
1:D:56:GLN:CD	1:D:56:GLN:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ILE:HB	1:F:135:PRO:HD3	1.88	0.54
1:H:125:ARG:NH1	1:H:127:ASP:OD2	2.40	0.54
1:B:68:THR:CG2	1:B:105:ASN:HD21	2.21	0.54
1:D:134:ILE:HB	1:D:135:PRO:HD3	1.89	0.54
1:B:192:ARG:NH2	1:B:195:GLU:HG2	2.22	0.54
1:D:226:ASN:C	1:D:226:ASN:OD1	2.50	0.54
1:E:48:CYS:SG	1:E:49:ASN:N	2.81	0.54
1:G:213:ILE:HD11	1:G:216:CYS:HB2	1.90	0.54
1:H:95:ALA:HA	1:H:117:ARG:HH21	1.71	0.54
1:C:233:MSE:HE2	1:C:259:ILE:HD13	1.90	0.54
1:H:94:PRO:HB2	1:H:96:HIS:CE1	2.43	0.54
1:C:75:SER:CB	4:C:425:HOH:O	2.53	0.54
1:A:175:ALA:HB1	1:B:175:ALA:HB1	1.90	0.53
1:C:219:THR:CG2	4:C:404:HOH:O	2.53	0.53
1:H:95:ALA:HA	1:H:117:ARG:HH22	1.72	0.53
1:D:63:LEU:HD23	1:D:108:LEU:HD11	1.89	0.53
1:E:233:MSE:HE3	1:E:237:THR:HB	1.90	0.53
1:G:151:THR:HG23	1:G:153:HIS:O	2.08	0.53
1:C:19:ILE:HA	1:C:281:ALA:HB2	1.90	0.53
1:D:190:LEU:HA	1:D:193:ILE:HD12	1.91	0.53
1:D:213:ILE:CD1	1:D:216:CYS:HB2	2.38	0.53
1:H:233:MSE:HE2	1:H:259:ILE:HD13	1.90	0.53
1:E:133:SER:CA	1:E:136:THR:HG23	2.37	0.53
1:E:192:ARG:NH2	1:F:168:THR:OG1	2.42	0.53
1:A:56:GLN:HA	1:A:92:ARG:O	2.08	0.53
1:D:33:VAL:HG11	1:D:53:ILE:HD11	1.91	0.53
1:C:210:VAL:HA	1:C:213:ILE:HG12	1.90	0.53
1:E:222:SER:O	1:E:224:ILE:HG12	2.09	0.53
1:F:125:ARG:NH1	1:F:127:ASP:OD1	2.41	0.53
1:A:185:ARG:HD3	3:A:401:NAP:O1X	2.08	0.53
1:B:68:THR:CG2	1:B:105:ASN:ND2	2.71	0.53
1:B:137:VAL:HG11	1:B:172:THR:HB	1.89	0.53
1:D:132:ASN:O	1:D:136:THR:HG23	2.09	0.53
1:B:213:ILE:CD1	1:B:216:CYS:HB2	2.38	0.52
1:C:206:LEU:O	1:C:210:VAL:HG22	2.10	0.52
1:D:5:LEU:HD11	1:D:292:GLN:OE1	2.10	0.52
1:E:160:LEU:HB3	1:E:220:ILE:HD12	1.92	0.52
1:G:233:MSE:HE2	1:G:259:ILE:HD13	1.91	0.52
1:D:91:ASP:C	1:D:93:THR:H	2.17	0.52
1:H:69:THR:O	1:H:71:GLU:N	2.32	0.52
1:D:5:LEU:HD11	1:D:292:GLN:CD	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ALA:HB2	1:C:101:SER:OG	2.10	0.52
1:G:14:ALA:HA	1:G:17:LEU:HD22	1.92	0.52
1:A:70:GLY:O	1:A:72:GLY:N	2.42	0.52
1:G:65:VAL:HA	1:G:102:GLY:HA3	1.92	0.52
1:C:134:ILE:HB	1:C:135:PRO:CD	2.40	0.52
1:F:50:ILE:HD11	1:F:85:LEU:HD12	1.91	0.52
1:B:5:LEU:HD23	1:B:7:ILE:HD11	1.91	0.51
1:F:233:MSE:HE2	1:F:237:THR:HB	1.92	0.51
1:B:220:ILE:HD13	1:B:224:ILE:CD1	2.40	0.51
1:B:233:MSE:HE1	1:B:259:ILE:HG21	1.91	0.51
1:E:175:ALA:HB1	1:G:175:ALA:HB1	1.92	0.51
1:F:165:THR:HG23	3:F:406:NAP:O1N	2.10	0.51
1:G:167:MSE:CE	1:G:171:ARG:HH22	2.24	0.51
1:C:43:THR:HG22	4:C:419:HOH:O	2.11	0.51
1:A:233:MSE:HE3	1:A:237:THR:CB	2.38	0.51
1:D:136:THR:HG21	3:D:404:NAP:H4N	1.91	0.51
1:F:68:THR:HG23	1:F:105:ASN:OD1	2.10	0.51
1:G:245:ARG:HH11	1:G:265:PRO:CG	2.23	0.51
1:H:90:LEU:O	1:H:93:THR:HB	2.10	0.51
1:A:167:MSE:CE	1:A:171:ARG:NH2	2.74	0.51
1:B:132:ASN:O	1:B:136:THR:HG23	2.09	0.51
1:B:265:PRO:HA	3:B:402:NAP:N7N	2.26	0.51
1:G:93:THR:HG23	1:G:97:CYS:CB	2.37	0.51
1:A:244:SER:O	1:A:245:ARG:C	2.54	0.50
1:B:93:THR:HG23	1:B:97:CYS:HB3	1.93	0.50
1:G:132:ASN:O	1:G:136:THR:HG22	2.11	0.50
1:B:132:ASN:O	1:B:136:THR:HG22	2.10	0.50
1:B:181:LYS:HG3	1:B:201:PHE:CE2	2.47	0.50
1:A:151:THR:CG2	1:A:153:HIS:O	2.60	0.50
1:D:133:SER:HA	1:D:136:THR:HG23	1.93	0.50
1:G:55:PHE:HA	1:G:58:ILE:HD13	1.93	0.50
1:D:139:GLY:HA3	1:D:267:LEU:HG	1.92	0.50
1:D:225:LEU:HB3	1:D:249:THR:HB	1.94	0.50
1:B:12:GLY:HA2	1:B:64:PRO:HB3	1.93	0.50
1:C:69:THR:HG23	1:C:73:VAL:HG12	1.94	0.50
1:D:233:MSE:HE2	1:D:259:ILE:HD13	1.93	0.50
1:F:8:ALA:HB2	1:F:53:ILE:CD1	2.42	0.50
1:G:20:ILE:CD1	1:G:32:LEU:HD11	2.42	0.50
1:H:94:PRO:CB	1:H:96:HIS:CE1	2.94	0.50
1:B:182:VAL:HG22	1:B:193:ILE:CD1	2.42	0.49
1:E:146:GLN:HE21	1:G:142[A]:MSE:CE	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:MSE:CE	1:F:237:THR:HB	2.42	0.49
1:G:10:ILE:HA	1:G:33:VAL:HG13	1.94	0.49
1:E:90:LEU:O	1:E:93:THR:HG22	2.12	0.49
1:E:32:LEU:HD22	1:E:45:ALA:HB1	1.95	0.49
1:F:146:GLN:HB3	1:H:142[B]:MSE:CE	2.42	0.49
1:A:14:ALA:O	1:A:17:LEU:HB2	2.13	0.49
1:A:55:PHE:HA	1:A:58:ILE:HD13	1.95	0.49
1:E:158:ALA:HA	1:E:181:LYS:O	2.13	0.49
1:A:151:THR:HG23	1:A:153:HIS:O	2.12	0.49
1:D:2:LEU:HA	1:D:292:GLN:HE22	1.78	0.49
1:D:5:LEU:CD1	1:D:292:GLN:OE1	2.61	0.49
1:D:219:THR:O	3:D:404:NAP:H52N	2.11	0.49
1:G:3:THR:HA	1:G:27:GLN:O	2.13	0.49
1:G:219:THR:HG21	4:G:508:HOH:O	2.12	0.49
1:G:219:THR:O	3:G:407:NAP:H52N	2.13	0.49
1:B:192:ARG:NH2	1:C:168:THR:OG1	2.46	0.48
1:C:142[B]:MSE:CE	1:D:145:ILE:HD12	2.43	0.48
1:C:194:THR:HG22	1:C:200:PRO:HG3	1.94	0.48
1:E:80:ASN:O	1:E:81:GLU:HG2	2.13	0.48
1:E:160:LEU:HB2	1:E:218:ASN:HA	1.95	0.48
1:D:24:THR:HG23	1:D:30:ILE:HD12	1.94	0.48
1:F:142[A]:MSE:HE2	1:H:145:ILE:HG22	1.94	0.48
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.11	0.48
1:A:242:LEU:O	3:A:401:NAP:H2N	2.14	0.48
1:C:134:ILE:O	1:C:137:VAL:HG23	2.14	0.48
1:C:146:GLN:HB3	1:D:142[A]:MSE:CE	2.42	0.48
1:A:68:THR:HG21	1:A:107:TYR:CD1	2.48	0.48
1:B:220:ILE:CD1	1:B:224:ILE:HD11	2.43	0.48
1:C:15:ARG:NH1	1:C:65:VAL:HG21	2.29	0.48
1:D:93:THR:HG23	1:D:97:CYS:HB3	1.95	0.48
1:D:227:GLN:HG3	1:D:253:TYR:CD1	2.49	0.48
1:E:137:VAL:CG2	1:E:168:THR:HG22	2.43	0.48
1:F:23:LEU:HB3	1:F:30:ILE:HD11	1.96	0.48
1:C:14:ALA:HA	1:C:17:LEU:HD22	1.94	0.48
1:C:245:ARG:H	1:C:245:ARG:HD2	1.79	0.48
1:H:158:ALA:HA	1:H:181:LYS:HG2	1.95	0.48
1:C:33:VAL:CG1	1:C:53:ILE:HD11	2.43	0.47
1:C:137:VAL:HG13	1:C:169:ILE:HA	1.95	0.47
1:D:40:HIS:HD2	1:D:42:PHE:HB2	1.78	0.47
1:D:185:ARG:HD2	3:D:404:NAP:C2A	2.44	0.47
1:E:210:VAL:O	1:E:211:LYS:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:GLN:HB2	1:F:78:PHE:C	2.39	0.47
1:F:276:ALA:HA	1:F:279:ILE:HD12	1.95	0.47
1:G:185:ARG:NH1	3:G:407:NAP:O3X	2.47	0.47
1:D:125:ARG:NH1	1:D:127:ASP:OD2	2.47	0.47
1:A:56:GLN:O	1:A:94:PRO:HG3	2.14	0.47
1:A:233:MSE:HE2	1:A:259:ILE:HD13	1.95	0.47
1:B:136:THR:HG22	1:B:268:PRO:HG3	1.95	0.47
1:F:133:SER:CA	1:F:136:THR:HG23	2.40	0.47
4:F:410:HOH:O	1:H:274:LYS:HE2	2.13	0.47
1:H:233:MSE:HE3	1:H:237:THR:CB	2.41	0.47
1:E:10:ILE:O	1:E:64:PRO:HD3	2.14	0.47
1:F:225:LEU:HD12	1:F:229:VAL:HG11	1.97	0.47
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.66	0.47
1:B:171:ARG:NH1	1:B:171:ARG:CB	2.78	0.47
1:F:30:ILE:O	1:F:45:ALA:HA	2.15	0.47
1:F:151:THR:CG2	1:F:153:HIS:O	2.63	0.47
1:F:151:THR:HG22	1:F:153:HIS:O	2.15	0.47
1:A:190:LEU:HD12	1:A:190:LEU:HA	1.72	0.47
1:C:151:THR:CG2	1:C:153:HIS:O	2.58	0.47
1:D:206:LEU:O	1:D:210:VAL:HG22	2.15	0.47
1:F:137:VAL:CG1	1:F:169:ILE:HA	2.45	0.47
1:G:134:ILE:O	1:G:137:VAL:HG12	2.13	0.47
1:G:139:GLY:HA3	1:G:267:LEU:HG	1.97	0.47
1:H:162:LEU:HG	1:H:167:MSE:HG3	1.97	0.47
1:B:93:THR:HG23	1:B:97:CYS:CB	2.44	0.47
1:C:132:ASN:O	1:C:136:THR:HG23	2.14	0.47
1:E:50:ILE:O	1:E:50:ILE:CG1	2.63	0.47
1:A:61:ILE:HG22	1:A:63:LEU:HD22	1.97	0.47
1:F:219:THR:O	3:F:406:NAP:H52N	2.15	0.47
1:H:93:THR:HG23	1:H:97:CYS:HB3	1.97	0.47
1:D:40:HIS:ND1	1:D:40:HIS:N	2.63	0.47
1:A:19:ILE:HA	1:A:281:ALA:HB2	1.97	0.46
1:C:10:ILE:HD12	1:C:61:ILE:HG23	1.98	0.46
1:D:105:ASN:OD1	1:D:108:LEU:HB2	2.16	0.46
1:E:242:LEU:O	3:E:405:NAP:H2N	2.14	0.46
1:F:14:ALA:HA	1:F:17:LEU:HD22	1.97	0.46
1:F:175:ALA:HB1	1:H:175:ALA:HB1	1.97	0.46
1:G:219:THR:CG2	4:G:508:HOH:O	2.63	0.46
1:G:220:ILE:HA	1:G:221:PRO:HD3	1.76	0.46
1:H:69:THR:C	1:H:71:GLU:N	2.72	0.46
1:A:137:VAL:HG11	1:A:172:THR:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HG23	1:B:236:LYS:HG2	1.98	0.46
1:B:134:ILE:O	1:B:137:VAL:HG23	2.16	0.46
1:B:171:ARG:NH1	1:B:171:ARG:HB2	2.31	0.46
1:E:108:LEU:HA	1:E:111:ILE:HD13	1.97	0.46
1:D:217:ILE:HG22	1:D:242:LEU:HD12	1.98	0.46
1:E:94:PRO:HB2	1:E:96:HIS:CE1	2.50	0.46
1:G:213:ILE:CD1	1:G:216:CYS:HB2	2.46	0.46
1:E:49:ASN:C	1:E:51:ASP:H	2.22	0.46
1:G:134:ILE:HB	1:G:135:PRO:HD3	1.97	0.46
1:H:70:GLY:HA2	1:H:107:TYR:HB2	1.97	0.46
1:B:10:ILE:HG23	1:B:33:VAL:HG22	1.98	0.46
1:H:11:GLY:CA	1:H:76:THR:HG22	2.38	0.46
1:B:101:SER:OG	1:B:102:GLY:N	2.46	0.46
1:B:196:MSE:CG	1:C:171:ARG:HH21	2.22	0.46
1:A:252:LYS:H	1:A:252:LYS:HG2	1.45	0.46
1:B:167:MSE:HE2	1:B:167:MSE:HB3	1.88	0.46
1:F:142[A]:MSE:CE	1:H:146:GLN:HE21	2.28	0.46
1:G:19:ILE:HA	1:G:281:ALA:HB2	1.98	0.46
1:F:32:LEU:HD13	1:F:45:ALA:HB1	1.98	0.46
1:C:137:VAL:HG11	1:C:172:THR:HB	1.97	0.45
1:H:19:ILE:HA	1:H:281:ALA:HB2	1.96	0.45
1:D:171:ARG:HG2	1:D:171:ARG:HH11	1.80	0.45
1:E:233:MSE:HE2	1:E:259:ILE:HD13	1.99	0.45
1:G:162:LEU:HD22	1:G:193:ILE:HG13	1.97	0.45
1:D:21:ARG:HH11	1:D:42:PHE:HZ	1.64	0.45
1:E:105:ASN:HB3	1:E:108:LEU:HB2	1.98	0.45
1:E:225:LEU:CB	1:E:249:THR:HB	2.47	0.45
1:A:71:GLU:H	1:A:71:GLU:HG2	1.33	0.45
1:D:68:THR:HG22	1:D:105:ASN:OD1	2.16	0.45
1:C:101:SER:OG	1:C:102:GLY:N	2.49	0.45
1:C:223:MSE:HE1	1:C:250:ASP:N	2.32	0.45
1:G:127:ASP:OD1	1:G:128:ILE:N	2.49	0.45
1:B:167:MSE:HE2	1:C:192:ARG:CZ	2.47	0.45
1:A:86:LYS:H	1:A:89:HIS:HD2	1.64	0.45
1:A:132:ASN:C	1:A:135:PRO:HD2	2.43	0.45
1:D:132:ASN:O	1:D:136:THR:HG22	2.16	0.45
1:F:167:MSE:HE2	1:F:167:MSE:HB3	1.89	0.45
1:H:219:THR:O	3:H:408:NAP:H52N	2.16	0.45
1:A:85:LEU:HD12	1:A:89:HIS:HD2	1.81	0.44
1:C:13:ASP:HB2	1:C:15:ARG:HB2	1.99	0.44
1:C:24:THR:HG21	1:C:42:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:THR:HG21	1:D:107:TYR:CD1	2.50	0.44
1:F:245:ARG:H	1:F:245:ARG:CD	2.30	0.44
1:E:22:LYS:O	1:E:26:GLN:HG3	2.17	0.44
1:F:203:THR:HG21	3:F:406:NAP:H2A	1.98	0.44
1:A:181:LYS:HG3	1:A:201:PHE:HE2	1.82	0.44
1:G:20:ILE:HD13	1:G:32:LEU:HD11	1.99	0.44
1:G:158:ALA:HA	1:G:181:LYS:O	2.17	0.44
1:A:70:GLY:C	1:A:72:GLY:H	2.26	0.44
1:G:66:SER:O	1:G:67:ALA:C	2.61	0.44
1:E:128:ILE:O	1:E:132:ASN:HB2	2.17	0.44
1:C:20:ILE:CD1	1:C:32:LEU:HD11	2.48	0.44
1:C:223:MSE:HE1	1:C:250:ASP:H	1.83	0.44
1:F:86:LYS:H	1:F:89:HIS:HD2	1.64	0.44
1:F:114:GLN:HE21	1:F:114:GLN:HB2	1.65	0.44
1:G:74:VAL:O	1:G:76:THR:HG23	2.17	0.44
1:G:238:LEU:HG	1:G:240:LEU:HD13	1.99	0.44
1:H:233:MSE:HE3	1:H:237:THR:CG2	2.48	0.44
1:E:176:LEU:HD13	1:G:176:LEU:HD13	2.00	0.44
1:F:213:ILE:HD11	1:F:216:CYS:HB2	2.00	0.44
1:A:8:ALA:HB2	1:A:53:ILE:CD1	2.48	0.44
1:A:241:ASP:OD2	1:A:249:THR:HG23	2.18	0.44
1:A:267:LEU:HB2	3:A:401:NAP:O7N	2.17	0.44
1:G:125:ARG:NH1	1:G:127:ASP:OD2	2.51	0.44
1:F:171:ARG:CG	1:F:171:ARG:NH1	2.79	0.44
1:B:90:LEU:O	1:B:93:THR:HB	2.17	0.43
1:B:94:PRO:HD2	1:B:97:CYS:HB2	2.00	0.43
1:D:92:ARG:HH11	1:D:92:ARG:CG	2.25	0.43
1:H:69:THR:HG23	1:H:73:VAL:O	2.17	0.43
3:A:401:NAP:H1B	4:A:504:HOH:O	2.17	0.43
1:B:264:ALA:O	3:B:402:NAP:N7N	2.51	0.43
1:C:171:ARG:CG	1:C:171:ARG:NH1	2.59	0.43
1:D:137:VAL:CG1	1:D:169:ILE:HA	2.48	0.43
1:D:205:GLU:HB2	1:D:209:HIS:HD2	1.82	0.43
1:A:225:LEU:HB2	1:A:249:THR:HB	2.00	0.43
1:F:210:VAL:HA	1:F:213:ILE:HG12	2.01	0.43
1:G:93:THR:HG22	1:G:117:ARG:NE	2.20	0.43
1:H:126:ASP:HA	1:H:164:ARG:HH21	1.84	0.43
1:C:242:LEU:O	3:C:403:NAP:C2N	2.66	0.43
1:E:10:ILE:HG12	1:E:33:VAL:HG22	2.01	0.43
1:E:181:LYS:HG3	1:E:201:PHE:CE2	2.53	0.43
1:F:68:THR:OG1	1:F:69:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:VAL:HG21	1:F:168:THR:HG22	2.01	0.43
1:G:171:ARG:HG3	1:G:171:ARG:HH11	1.81	0.43
1:G:233:MSE:CE	1:G:237:THR:HB	2.36	0.43
1:H:24:THR:HG23	1:H:30:ILE:HD12	2.01	0.43
1:A:185:ARG:HG2	1:A:186:SER:N	2.33	0.43
1:D:267:LEU:HD12	1:D:267:LEU:HA	1.86	0.43
1:E:151:THR:CG2	1:E:153:HIS:O	2.67	0.43
1:G:195:GLU:C	1:G:197:GLY:H	2.27	0.43
1:H:161:GLY:O	1:H:166:GLY:HA3	2.18	0.43
1:A:275:THR:O	1:A:279:ILE:HG13	2.19	0.43
1:G:171:ARG:HH21	1:H:195:GLU:CD	2.22	0.43
1:G:192:ARG:HH21	1:G:195:GLU:CG	2.30	0.43
1:G:219:THR:O	1:G:219:THR:HG23	2.17	0.43
1:A:10:ILE:HD12	1:A:61:ILE:HG23	2.01	0.43
1:A:50:ILE:O	1:A:53:ILE:HG23	2.19	0.43
1:A:165:THR:HG23	3:A:401:NAP:O1N	2.19	0.43
1:A:213:ILE:HD11	1:A:216:CYS:HB2	2.00	0.43
1:G:160:LEU:O	1:G:219:THR:HG22	2.19	0.43
1:B:242:LEU:O	3:B:402:NAP:H2N	2.19	0.43
1:E:142[B]:MSE:HE3	1:G:145:ILE:HB	2.01	0.43
1:C:139:GLY:HA3	1:C:267:LEU:HG	2.00	0.43
1:E:136:THR:HG22	1:E:268:PRO:HG3	2.00	0.43
1:E:241:ASP:OD2	1:E:249:THR:HG22	2.18	0.43
1:F:10:ILE:O	1:F:64:PRO:HD3	2.19	0.43
1:H:182:VAL:HG13	1:H:193:ILE:CG2	2.49	0.43
1:B:3:THR:HG22	1:B:4:GLY:N	2.34	0.43
1:B:63:LEU:CD2	1:B:99:ILE:HG23	2.49	0.43
1:B:93:THR:HG22	1:B:117:ARG:NE	2.25	0.43
1:C:85:LEU:O	1:C:107:TYR:OH	2.33	0.43
1:A:14:ALA:HA	1:A:17:LEU:HD22	2.01	0.42
1:D:18:GLU:OE1	1:D:21:ARG:NH2	2.51	0.42
1:E:15:ARG:NH1	1:E:65:VAL:HG21	2.34	0.42
1:G:151:THR:CG2	1:G:153:HIS:O	2.67	0.42
1:H:133:SER:HB2	1:H:165:THR:HA	2.02	0.42
1:A:132:ASN:O	1:A:135:PRO:HD2	2.19	0.42
1:D:87:GLN:HE22	1:D:111:ILE:HA	1.85	0.42
1:G:168:THR:OG1	1:H:192:ARG:NH2	2.52	0.42
1:A:182:VAL:HG22	1:A:193:ILE:CD1	2.50	0.42
1:C:190:LEU:HA	1:C:193:ILE:HD12	2.01	0.42
1:D:133:SER:HB3	1:D:165:THR:HG22	2.01	0.42
1:G:137:VAL:HG21	1:G:172:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:THR:CG2	3:H:408:NAP:H2A	2.50	0.42
1:F:93:THR:HG22	1:F:117:ARG:NE	2.32	0.42
1:C:234:THR:OG1	1:C:235:PRO:HD2	2.19	0.42
1:E:169:ILE:HG21	1:E:217:ILE:HG21	2.00	0.42
1:B:181:LYS:HG3	1:B:201:PHE:HE2	1.83	0.42
1:E:123:PHE:HE1	1:E:280:LEU:HD21	1.85	0.42
1:E:162:LEU:HG	1:E:167:MSE:HG3	2.02	0.42
1:H:139:GLY:HA2	1:H:271:VAL:HG21	2.01	0.42
1:A:64:PRO:O	1:A:65:VAL:C	2.63	0.42
1:C:35:PHE:O	1:C:47:LYS:HE2	2.19	0.42
1:E:50:ILE:O	1:E:50:ILE:HG13	2.19	0.42
1:A:181:LYS:HG3	1:A:201:PHE:CE2	2.55	0.42
1:E:227:GLN:HG3	1:E:253:TYR:CD1	2.55	0.42
1:F:174:ALA:HB2	1:F:198:LEU:HD11	2.01	0.41
1:H:10:ILE:HG23	1:H:33:VAL:HG22	2.01	0.41
1:C:160:LEU:HB3	1:C:220:ILE:HD12	2.01	0.41
1:E:11:GLY:C	1:E:64:PRO:HG3	2.45	0.41
1:G:101:SER:OG	1:G:102:GLY:N	2.52	0.41
1:H:137:VAL:HG13	1:H:169:ILE:HA	2.03	0.41
1:A:85:LEU:HD12	1:A:89:HIS:CD2	2.55	0.41
1:H:219:THR:HG23	3:H:408:NAP:H52N	2.02	0.41
1:B:37:GLN:HB2	1:B:78:PHE:C	2.45	0.41
1:B:184:ALA:HB3	1:B:190:LEU:HD13	2.03	0.41
3:D:404:NAP:H5N	4:D:506:HOH:O	2.19	0.41
1:G:56:GLN:H	1:G:56:GLN:HG3	1.51	0.41
1:A:2:LEU:HA	1:A:292:GLN:HE22	1.86	0.41
1:B:220:ILE:HA	1:B:221:PRO:HD3	1.94	0.41
1:D:2:LEU:HA	1:D:292:GLN:NE2	2.36	0.41
1:G:226:ASN:OD1	1:G:226:ASN:C	2.63	0.41
1:H:63:LEU:HB3	1:H:64:PRO:CD	2.50	0.41
1:B:56:GLN:HA	1:B:92:ARG:O	2.20	0.41
1:E:133:SER:HA	1:E:136:THR:CG2	2.39	0.41
1:H:15:ARG:HH11	1:H:65:VAL:HG21	1.85	0.41
1:H:134:ILE:HB	1:H:135:PRO:HD3	2.02	0.41
1:C:163:GLY:HA3	3:C:403:NAP:H4B	2.03	0.41
1:D:69:THR:OG1	1:D:73:VAL:HG13	2.21	0.41
1:E:267:LEU:HD12	1:E:267:LEU:HA	1.90	0.41
1:F:139:GLY:HA3	1:F:267:LEU:HG	2.03	0.41
1:H:160:LEU:HB2	1:H:218:ASN:HA	2.02	0.41
1:H:220:ILE:HD12	1:H:224:ILE:HD13	2.02	0.41
1:A:225:LEU:CB	1:A:249:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ARG:HH21	1:B:195:GLU:CG	2.30	0.41
1:C:245:ARG:H	1:C:245:ARG:NE	2.18	0.41
1:D:93:THR:HG23	1:D:97:CYS:CB	2.51	0.41
1:F:15:ARG:NH1	1:F:65:VAL:HG21	2.36	0.41
1:G:56:GLN:O	1:G:94:PRO:HG3	2.21	0.41
1:B:88:ASP:O	1:B:92:ARG:HG3	2.21	0.41
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.86	0.40
1:D:7:ILE:HD13	1:D:23:LEU:HD13	2.02	0.40
1:E:125:ARG:NH1	1:E:127:ASP:OD2	2.54	0.40
1:H:133:SER:O	1:H:137:VAL:HG22	2.21	0.40
1:B:5:LEU:HD13	1:B:292:GLN:HG3	2.03	0.40
1:F:213:ILE:HD12	1:F:216:CYS:HB2	2.02	0.40
1:E:115:ALA:O	1:E:117:ARG:NH2	2.54	0.40
1:A:56:GLN:H	1:A:56:GLN:HG3	1.52	0.40
1:A:61:ILE:HG22	1:A:63:LEU:CD2	2.52	0.40
1:A:171:ARG:NH1	1:A:171:ARG:CG	2.80	0.40
1:B:10:ILE:HG12	1:B:33:VAL:HG13	2.03	0.40
1:D:151:THR:HG23	1:D:153:HIS:HB3	2.02	0.40
1:E:76:THR:HG21	1:E:83:VAL:HG11	2.02	0.40
1:F:125:ARG:NH1	1:F:127:ASP:CG	2.80	0.40
1:A:138:GLU:CD	1:B:152:ILE:H	2.30	0.40
1:D:241:ASP:OD2	1:D:249:THR:CG2	2.70	0.40
1:G:159:VAL:HB	1:G:182:VAL:HB	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	296/300 (99%)	282 (95%)	12 (4%)	2 (1%)	18	47
1	B	295/300 (98%)	281 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	296/300 (99%)	280 (95%)	15 (5%)	1 (0%)	36	66
1	D	296/300 (99%)	277 (94%)	16 (5%)	3 (1%)	12	38
1	E	297/300 (99%)	278 (94%)	17 (6%)	2 (1%)	18	47
1	F	296/300 (99%)	274 (93%)	21 (7%)	1 (0%)	36	66
1	G	296/300 (99%)	277 (94%)	16 (5%)	3 (1%)	12	38
1	H	296/300 (99%)	270 (91%)	24 (8%)	2 (1%)	18	47
All	All	2368/2400 (99%)	2219 (94%)	135 (6%)	14 (1%)	21	51

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	H	67	ALA
1	A	70	GLY
1	C	223	MSE
1	D	110	ASN
1	G	56	GLN
1	G	196	MSE
1	D	71	GLU
1	D	250	ASP
1	E	-1	ASN
1	E	50	ILE
1	G	67	ALA
1	F	223	MSE
1	H	70	GLY

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	245/240 (102%)	204 (83%)	41 (17%)	2	8
1	B	244/240 (102%)	199 (82%)	45 (18%)	1	6
1	C	245/240 (102%)	203 (83%)	42 (17%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	245/240 (102%)	201 (82%)	44 (18%)	2	6
1	E	246/240 (102%)	201 (82%)	45 (18%)	2	6
1	F	245/240 (102%)	199 (81%)	46 (19%)	1	5
1	G	245/240 (102%)	204 (83%)	41 (17%)	2	8
1	H	245/240 (102%)	194 (79%)	51 (21%)	1	4
All	All	1960/1920 (102%)	1605 (82%)	355 (18%)	2	6

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	15	ARG
1	A	17	LEU
1	A	18	GLU
1	A	23	LEU
1	A	32	LEU
1	A	33	VAL
1	A	36	ASP
1	A	37	GLN
1	A	43	THR
1	A	46	VAL
1	A	53	ILE
1	A	56	GLN
1	A	58	ILE
1	A	65	VAL
1	A	68	THR
1	A	71	GLU
1	A	93	THR
1	A	104	SER
1	A	108	LEU
1	A	136	THR
1	A	137	VAL
1	A	151	THR
1	A	160	LEU
1	A	167	MSE
1	A	182	VAL
1	A	190	LEU
1	A	192	ARG
1	A	194	THR
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	213	ILE
1	A	219	THR
1	A	225	LEU
1	A	227	GLN
1	A	228	THR
1	A	249	THR
1	A	252	LYS
1	A	255	GLU
1	A	267	LEU
1	A	271	VAL
1	A	278	GLN
1	B	2	LEU
1	B	3	THR
1	B	5	LEU
1	B	6	LYS
1	B	13	ASP
1	B	15	ARG
1	B	17	LEU
1	B	25	GLU
1	B	33	VAL
1	B	37	GLN
1	B	38	LEU
1	B	39	ASP
1	B	40	HIS
1	B	46	VAL
1	B	53	ILE
1	B	56	GLN
1	B	58	ILE
1	B	75	SER
1	B	84	VAL
1	B	93	THR
1	B	104	SER
1	B	108	LEU
1	B	116	LYS
1	B	136	THR
1	B	137	VAL
1	B	151	THR
1	B	160	LEU
1	B	167	MSE
1	B	171	ARG
1	B	176	LEU
1	B	182	VAL

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Mol	Chain	Res	Type
1	B	190	LEU
1	B	198	LEU
1	B	207	LYS
1	B	219	THR
1	B	222	SER
1	B	224	ILE
1	B	225	LEU
1	B	228	THR
1	B	236	LYS
1	B	263	LEU
1	B	267	LEU
1	B	271	VAL
1	B	274	LYS
1	B	278	GLN
1	C	2	LEU
1	C	5	LEU
1	C	15	ARG
1	C	17	LEU
1	C	30	ILE
1	C	33	VAL
1	C	37	GLN
1	C	46	VAL
1	C	58	ILE
1	C	63	LEU
1	C	68	THR
1	C	73	VAL
1	C	77	VAL
1	C	93	THR
1	C	105	ASN
1	C	108	LEU
1	C	109	GLU
1	C	136	THR
1	C	137	VAL
1	C	151	THR
1	C	160	LEU
1	C	167	MSE
1	C	171	ARG
1	C	176	LEU
1	C	182	VAL
1	C	187	SER
1	C	190	LEU
1	C	194	THR

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Mol	Chain	Res	Type
1	C	195	GLU
1	C	198	LEU
1	C	213	ILE
1	C	219	THR
1	C	224	ILE
1	C	225	LEU
1	C	228	THR
1	C	240	LEU
1	C	244	SER
1	C	245	ARG
1	C	263	LEU
1	C	267	LEU
1	C	274	LYS
1	C	278	GLN
1	D	13	ASP
1	D	17	LEU
1	D	32	LEU
1	D	33	VAL
1	D	36	ASP
1	D	37	GLN
1	D	38	LEU
1	D	40	HIS
1	D	46	VAL
1	D	51	ASP
1	D	56	GLN
1	D	58	ILE
1	D	63	LEU
1	D	68	THR
1	D	71	GLU
1	D	73	VAL
1	D	75	SER
1	D	82	GLU
1	D	92	ARG
1	D	93	THR
1	D	108	LEU
1	D	136	THR
1	D	137	VAL
1	D	151	THR
1	D	160	LEU
1	D	190	LEU
1	D	194	THR
1	D	195	GLU

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Mol	Chain	Res	Type
1	D	198	LEU
1	D	219	THR
1	D	222	SER
1	D	225	LEU
1	D	228	THR
1	D	231	SER
1	D	240	LEU
1	D	244	SER
1	D	249	THR
1	D	252	LYS
1	D	263	LEU
1	D	267	LEU
1	D	274	LYS
1	D	278	GLN
1	D	286	LYS
1	D	292	GLN
1	E	2	LEU
1	E	3	THR
1	E	13	ASP
1	E	17	LEU
1	E	21	ARG
1	E	24	THR
1	E	33	VAL
1	E	37	GLN
1	E	56	GLN
1	E	58	ILE
1	E	68	THR
1	E	73	VAL
1	E	77	VAL
1	E	82	GLU
1	E	83	VAL
1	E	84	VAL
1	E	93	THR
1	E	108	LEU
1	E	111	ILE
1	E	114	GLN
1	E	116	LYS
1	E	136	THR
1	E	137	VAL
1	E	151	THR
1	E	160	LEU
1	E	171	ARG

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Mol	Chain	Res	Type
1	E	176	LEU
1	E	182	VAL
1	E	190	LEU
1	E	195	GLU
1	E	198	LEU
1	E	203	THR
1	E	207	LYS
1	E	224	ILE
1	E	225	LEU
1	E	236	LYS
1	E	245	ARG
1	E	249	THR
1	E	252	LYS
1	E	256	LYS
1	E	263	LEU
1	E	267	LEU
1	E	270	ILE
1	E	271	VAL
1	E	274	LYS
1	F	5	LEU
1	F	15	ARG
1	F	17	LEU
1	F	18	GLU
1	F	33	VAL
1	F	43	THR
1	F	53	ILE
1	F	56	GLN
1	F	63	LEU
1	F	68	THR
1	F	73	VAL
1	F	75	SER
1	F	81	GLU
1	F	88	ASP
1	F	93	THR
1	F	104	SER
1	F	105	ASN
1	F	108	LEU
1	F	114	GLN
1	F	116	LYS
1	F	120	VAL
1	F	136	THR
1	F	137	VAL

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Mol	Chain	Res	Type
1	F	141	ILE
1	F	151	THR
1	F	160	LEU
1	F	167	MSE
1	F	171	ARG
1	F	176	LEU
1	F	182	VAL
1	F	190	LEU
1	F	194	THR
1	F	198	LEU
1	F	219	THR
1	F	225	LEU
1	F	227	GLN
1	F	234	THR
1	F	237	THR
1	F	240	LEU
1	F	245	ARG
1	F	255	GLU
1	F	263	LEU
1	F	267	LEU
1	F	274	LYS
1	F	278	GLN
1	F	294	GLU
1	G	2	LEU
1	G	5	LEU
1	G	15	ARG
1	G	17	LEU
1	G	18	GLU
1	G	33	VAL
1	G	36	ASP
1	G	46	VAL
1	G	56	GLN
1	G	63	LEU
1	G	66	SER
1	G	84	VAL
1	G	93	THR
1	G	104	SER
1	G	108	LEU
1	G	136	THR
1	G	151	THR
1	G	160	LEU
1	G	167	MSE

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Mol	Chain	Res	Type
1	G	176	LEU
1	G	182	VAL
1	G	185	ARG
1	G	190	LEU
1	G	194	THR
1	G	198	LEU
1	G	219	THR
1	G	225	LEU
1	G	227	GLN
1	G	231	SER
1	G	232	SER
1	G	240	LEU
1	G	244	SER
1	G	252	LYS
1	G	260	LYS
1	G	263	LEU
1	G	267	LEU
1	G	271	VAL
1	G	274	LYS
1	G	278	GLN
1	G	286	LYS
1	G	295	GLU
1	H	2	LEU
1	H	6	LYS
1	H	15	ARG
1	H	17	LEU
1	H	18	GLU
1	H	33	VAL
1	H	37	GLN
1	H	51	ASP
1	H	53	ILE
1	H	56	GLN
1	H	58	ILE
1	H	60	SER
1	H	63	LEU
1	H	66	SER
1	H	68	THR
1	H	71	GLU
1	H	92	ARG
1	H	93	THR
1	H	103	ILE
1	H	105	ASN

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Mol	Chain	Res	Type
1	H	108	LEU
1	H	124	GLU
1	H	133	SER
1	H	136	THR
1	H	137	VAL
1	H	146	GLN
1	H	151	THR
1	H	160	LEU
1	H	162	LEU
1	H	167	MSE
1	H	176	LEU
1	H	182	VAL
1	H	185	ARG
1	H	190	LEU
1	H	194	THR
1	H	198	LEU
1	H	219	THR
1	H	224	ILE
1	H	225	LEU
1	H	228	THR
1	H	236	LYS
1	H	240	LEU
1	H	244	SER
1	H	252	LYS
1	H	255	GLU
1	H	256	LYS
1	H	267	LEU
1	H	271	VAL
1	H	274	LYS
1	H	278	GLN
1	H	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	49	ASN
1	A	87	GLN
1	A	89	HIS
1	A	114	GLN
1	A	132	ASN

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Mol	Chain	Res	Type
1	A	156	GLN
1	A	209	HIS
1	A	292	GLN
1	B	37	GLN
1	B	49	ASN
1	B	57	GLN
1	B	80	ASN
1	B	89	HIS
1	B	105	ASN
1	B	114	GLN
1	B	146	GLN
1	B	292	GLN
1	C	37	GLN
1	C	49	ASN
1	C	57	GLN
1	C	105	ASN
1	C	146	GLN
1	C	209	HIS
1	C	227	GLN
1	C	292	GLN
1	D	37	GLN
1	D	49	ASN
1	D	57	GLN
1	D	87	GLN
1	D	209	HIS
1	D	257	GLN
1	D	292	GLN
1	E	-1	ASN
1	E	26	GLN
1	E	37	GLN
1	E	87	GLN
1	E	96	HIS
1	E	146	GLN
1	E	209	HIS
1	E	278	GLN
1	E	292	GLN
1	F	26	GLN
1	F	37	GLN
1	F	49	ASN
1	F	89	HIS
1	F	114	GLN
1	F	146	GLN

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Mol	Chain	Res	Type
1	F	156	GLN
1	F	227	GLN
1	F	257	GLN
1	F	292	GLN
1	G	26	GLN
1	G	49	ASN
1	G	114	GLN
1	G	146	GLN
1	G	189	HIS
1	G	227	GLN
1	H	27	GLN
1	H	37	GLN
1	H	49	ASN
1	H	56	GLN
1	H	105	ASN
1	H	114	GLN
1	H	146	GLN
1	H	292	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 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$
3	NAP	D	404	-	50,52,52	1.76	4 (8%)	71,80,80	1.50	10 (14%)
3	NAP	A	401	-	50,52,52	1.75	6 (12%)	71,80,80	1.54	13 (18%)
3	NAP	C	403	-	50,52,52	1.68	5 (10%)	71,80,80	1.61	10 (14%)
3	NAP	F	406	-	50,52,52	1.64	4 (8%)	71,80,80	1.66	12 (16%)
3	NAP	G	407	-	50,52,52	1.68	5 (10%)	71,80,80	1.58	13 (18%)
3	NAP	E	405	-	50,52,52	1.68	5 (10%)	71,80,80	1.57	11 (15%)
3	NAP	H	408	-	50,52,52	1.73	4 (8%)	71,80,80	1.61	14 (19%)
3	NAP	B	402	-	50,52,52	1.76	7 (14%)	71,80,80	1.62	15 (21%)

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
3	NAP	D	404	-	-	20/35/67/67	0/5/5/5
3	NAP	A	401	-	-	13/35/67/67	0/5/5/5
3	NAP	C	403	-	-	15/35/67/67	0/5/5/5
3	NAP	F	406	-	-	18/35/67/67	0/5/5/5
3	NAP	G	407	-	-	17/35/67/67	0/5/5/5
3	NAP	E	405	-	-	14/35/67/67	0/5/5/5
3	NAP	H	408	-	-	13/35/67/67	0/5/5/5
3	NAP	B	402	-	-	12/35/67/67	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	NAP	O7N-C7N	9.65	1.42	1.24
3	H	408	NAP	O7N-C7N	9.30	1.41	1.24
3	B	402	NAP	O7N-C7N	9.29	1.41	1.24
3	C	403	NAP	O7N-C7N	8.84	1.40	1.24
3	G	407	NAP	O7N-C7N	8.80	1.40	1.24
3	A	401	NAP	O7N-C7N	8.75	1.40	1.24
3	E	405	NAP	O7N-C7N	8.70	1.40	1.24
3	F	406	NAP	O7N-C7N	8.62	1.40	1.24
3	D	404	NAP	C2A-N1A	3.37	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	407	NAP	C2A-N1A	3.28	1.39	1.33
3	F	406	NAP	C2A-N3A	3.28	1.39	1.33
3	C	403	NAP	C2A-N1A	3.18	1.39	1.33
3	A	401	NAP	C2N-N1N	3.15	1.38	1.35
3	G	407	NAP	C2A-N3A	3.15	1.39	1.33
3	E	405	NAP	C2A-N1A	3.13	1.39	1.33
3	B	402	NAP	C2A-N3A	3.11	1.39	1.33
3	F	406	NAP	C2A-N1A	3.11	1.39	1.33
3	B	402	NAP	C2A-N1A	3.09	1.39	1.33
3	C	403	NAP	C2A-N3A	3.04	1.39	1.33
3	A	401	NAP	C2A-N1A	2.96	1.39	1.33
3	A	401	NAP	C2A-N3A	2.96	1.39	1.33
3	D	404	NAP	C2A-N3A	2.95	1.39	1.33
3	H	408	NAP	C2A-N3A	2.83	1.39	1.33
3	H	408	NAP	C2A-N1A	2.79	1.38	1.33
3	A	401	NAP	C8A-N7A	2.61	1.36	1.31
3	E	405	NAP	C2A-N3A	2.48	1.38	1.33
3	G	407	NAP	C2N-N1N	2.44	1.37	1.35
3	B	402	NAP	C8A-N7A	2.43	1.36	1.31
3	E	405	NAP	O4D-C1D	2.32	1.43	1.40
3	E	405	NAP	C8A-N7A	2.29	1.36	1.31
3	G	407	NAP	C8A-N7A	2.28	1.36	1.31
3	F	406	NAP	C8A-N7A	2.25	1.36	1.31
3	A	401	NAP	PA-O3	-2.19	1.57	1.59
3	C	403	NAP	C8A-N7A	2.17	1.35	1.31
3	H	408	NAP	C5A-N7A	-2.15	1.35	1.39
3	C	403	NAP	O4B-C4B	-2.10	1.40	1.45
3	B	402	NAP	O4B-C4B	-2.09	1.40	1.45
3	B	402	NAP	O4D-C1D	2.07	1.43	1.40
3	B	402	NAP	C2N-N1N	2.03	1.37	1.35
3	D	404	NAP	O4B-C4B	-2.01	1.40	1.45

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	NAP	N3A-C2A-N1A	-6.42	118.86	128.58
3	F	406	NAP	N3A-C2A-N1A	-5.98	119.53	128.58
3	G	407	NAP	N3A-C2A-N1A	-5.54	120.19	128.58
3	B	402	NAP	N3A-C2A-N1A	-5.54	120.20	128.58
3	D	404	NAP	N3A-C2A-N1A	-5.53	120.21	128.58
3	E	405	NAP	N3A-C2A-N1A	-5.48	120.29	128.58
3	A	401	NAP	N3A-C2A-N1A	-5.30	120.55	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	408	NAP	N3A-C2A-N1A	-5.05	120.94	128.58
3	A	401	NAP	C5A-C4A-N3A	-4.57	120.42	126.72
3	G	407	NAP	N9A-C8A-N7A	-4.54	107.49	113.94
3	B	402	NAP	N9A-C8A-N7A	-4.42	107.66	113.94
3	F	406	NAP	C5A-C4A-N3A	-4.31	120.78	126.72
3	C	403	NAP	N9A-C8A-N7A	-4.22	107.95	113.94
3	F	406	NAP	N9A-C8A-N7A	-4.15	108.05	113.94
3	E	405	NAP	C5A-C4A-N3A	-4.12	121.05	126.72
3	H	408	NAP	N9A-C8A-N7A	-4.02	108.23	113.94
3	H	408	NAP	C5A-C4A-N3A	-4.02	121.19	126.72
3	D	404	NAP	N9A-C8A-N7A	-4.00	108.26	113.94
3	B	402	NAP	C5A-C4A-N3A	-3.83	121.45	126.72
3	G	407	NAP	C5A-C4A-N3A	-3.79	121.50	126.72
3	A	401	NAP	N9A-C8A-N7A	-3.78	108.57	113.94
3	D	404	NAP	C5A-C4A-N3A	-3.75	121.56	126.72
3	F	406	NAP	C2A-N3A-C4A	3.67	120.80	111.83
3	E	405	NAP	N9A-C8A-N7A	-3.62	108.80	113.94
3	G	407	NAP	C5A-N7A-C8A	3.43	108.84	103.45
3	D	404	NAP	C5A-N7A-C8A	3.40	108.80	103.45
3	F	406	NAP	C5A-N7A-C8A	3.40	108.80	103.45
3	C	403	NAP	C5A-C4A-N3A	-3.38	122.06	126.72
3	A	401	NAP	C2A-N3A-C4A	3.35	120.01	111.83
3	C	403	NAP	O2A-PA-O3	3.33	116.27	107.27
3	A	401	NAP	N3A-C4A-N9A	3.29	132.75	127.17
3	H	408	NAP	C5A-N7A-C8A	3.21	108.49	103.45
3	H	408	NAP	O7N-C7N-C3N	3.21	123.52	119.60
3	E	405	NAP	C2A-N3A-C4A	3.18	119.60	111.83
3	A	401	NAP	C5A-N7A-C8A	3.16	108.42	103.45
3	E	405	NAP	C5A-N7A-C8A	3.16	108.42	103.45
3	B	402	NAP	C5A-N7A-C8A	3.15	108.40	103.45
3	B	402	NAP	C4A-N9A-C8A	3.14	109.04	105.74
3	G	407	NAP	C2A-N3A-C4A	3.14	119.50	111.83
3	B	402	NAP	C2A-N3A-C4A	3.13	119.48	111.83
3	F	406	NAP	N3A-C4A-N9A	3.12	132.47	127.17
3	C	403	NAP	C5A-N7A-C8A	3.10	108.32	103.45
3	C	403	NAP	C2A-N3A-C4A	3.09	119.38	111.83
3	E	405	NAP	C6N-N1N-C2N	-3.09	119.25	121.88
3	D	404	NAP	C2A-N3A-C4A	3.08	119.36	111.83
3	G	407	NAP	C4A-N9A-C8A	3.08	108.97	105.74
3	B	402	NAP	N3A-C4A-N9A	3.07	132.38	127.17
3	B	402	NAP	C6N-N1N-C2N	-3.04	119.29	121.88
3	H	408	NAP	N3A-C4A-N9A	3.04	132.33	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	408	NAP	C2A-N3A-C4A	2.97	119.09	111.83
3	H	408	NAP	O7N-C7N-N7N	-2.96	118.34	122.62
3	E	405	NAP	N3A-C4A-N9A	2.95	132.19	127.17
3	C	403	NAP	C4A-N9A-C8A	2.90	108.78	105.74
3	A	401	NAP	C3N-C7N-N7N	2.89	121.30	117.74
3	C	403	NAP	N3A-C4A-N9A	2.86	132.03	127.17
3	G	407	NAP	N3A-C4A-N9A	2.81	131.94	127.17
3	H	408	NAP	O5D-C5D-C4D	2.73	118.27	108.99
3	F	406	NAP	O5D-C5D-C4D	2.71	118.24	108.99
3	D	404	NAP	N3A-C4A-N9A	2.70	131.76	127.17
3	G	407	NAP	C4N-C3N-C7N	-2.65	113.85	121.06
3	C	403	NAP	C2B-C1B-N9A	-2.61	109.46	113.75
3	D	404	NAP	C4A-N9A-C8A	2.53	108.40	105.74
3	E	405	NAP	C6N-N1N-C1D	2.53	124.68	119.73
3	F	406	NAP	C4A-N9A-C8A	2.52	108.39	105.74
3	G	407	NAP	O2B-C2B-C1B	-2.46	101.41	110.05
3	A	401	NAP	O3-PN-O1N	-2.45	103.35	110.70
3	G	407	NAP	O2N-PN-O1N	2.39	123.57	112.44
3	D	404	NAP	C4A-C5A-N7A	-2.38	107.86	110.58
3	B	402	NAP	O3-PN-O1N	-2.38	103.55	110.70
3	B	402	NAP	O2N-PN-O1N	2.37	123.46	112.44
3	D	404	NAP	C2B-C3B-C4B	2.34	107.03	101.99
3	G	407	NAP	O3-PA-O1A	-2.31	103.75	110.70
3	H	408	NAP	C4A-N9A-C8A	2.29	108.14	105.74
3	B	402	NAP	C4D-O4D-C1D	2.25	111.99	109.92
3	F	406	NAP	C4A-C5A-N7A	-2.24	108.02	110.58
3	C	403	NAP	O3-PA-O1A	-2.22	104.02	110.70
3	F	406	NAP	C2B-C1B-N9A	-2.21	110.11	113.75
3	H	408	NAP	C6N-N1N-C1D	2.20	124.05	119.73
3	B	402	NAP	C2B-C3B-C4B	2.20	106.72	101.99
3	G	407	NAP	O2N-PN-O3	-2.19	101.36	107.27
3	A	401	NAP	P2B-O2B-C2B	-2.19	117.59	123.43
3	H	408	NAP	C2D-C3D-C4D	2.17	106.81	102.61
3	H	408	NAP	O3D-C3D-C2D	-2.16	104.89	111.82
3	G	407	NAP	C4A-C5A-N7A	-2.15	108.13	110.58
3	E	405	NAP	O2N-PN-O1N	2.13	122.37	112.44
3	A	401	NAP	O7N-C7N-N7N	-2.12	119.55	122.62
3	A	401	NAP	C6A-C5A-C4A	2.11	120.06	117.18
3	F	406	NAP	O3X-P2B-O2X	2.08	115.59	107.80
3	E	405	NAP	C4D-O4D-C1D	2.07	111.83	109.92
3	E	405	NAP	C2B-C3B-C4B	2.05	106.41	101.99
3	A	401	NAP	C4A-N9A-C8A	2.04	107.88	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	O3-PA-O1A	-2.04	104.56	110.70
3	B	402	NAP	O2A-PA-O3	2.04	112.79	107.27
3	B	402	NAP	O5D-C5D-C4D	2.04	115.93	108.99
3	F	406	NAP	C6N-N1N-C1D	2.03	123.72	119.73
3	H	408	NAP	O3-PN-O1N	-2.03	104.59	110.70
3	D	404	NAP	O2A-PA-O3	2.02	112.74	107.27
3	A	401	NAP	C4A-C5A-N7A	-2.00	108.29	110.58

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAP	C5B-O5B-PA-O1A
3	A	401	NAP	PA-O3-PN-O5D
3	A	401	NAP	C5D-O5D-PN-O3
3	A	401	NAP	C5D-O5D-PN-O1N
3	A	401	NAP	C5D-O5D-PN-O2N
3	A	401	NAP	O4D-C1D-N1N-C2N
3	A	401	NAP	O4D-C1D-N1N-C6N
3	B	402	NAP	C5B-O5B-PA-O3
3	B	402	NAP	O4D-C1D-N1N-C2N
3	B	402	NAP	O4D-C1D-N1N-C6N
3	B	402	NAP	C2D-C1D-N1N-C2N
3	B	402	NAP	C2D-C1D-N1N-C6N
3	C	403	NAP	C5B-O5B-PA-O3
3	C	403	NAP	O4D-C1D-N1N-C2N
3	C	403	NAP	O4D-C1D-N1N-C6N
3	D	404	NAP	C5B-O5B-PA-O2A
3	D	404	NAP	C5B-O5B-PA-O3
3	D	404	NAP	PN-O3-PA-O5B
3	D	404	NAP	C5D-O5D-PN-O3
3	D	404	NAP	C5D-O5D-PN-O2N
3	D	404	NAP	O4D-C4D-C5D-O5D
3	D	404	NAP	O4D-C1D-N1N-C2N
3	D	404	NAP	O4D-C1D-N1N-C6N
3	D	404	NAP	C2D-C1D-N1N-C2N
3	D	404	NAP	C2D-C1D-N1N-C6N
3	E	405	NAP	C5B-O5B-PA-O2A
3	E	405	NAP	C5B-O5B-PA-O3
3	E	405	NAP	PN-O3-PA-O5B
3	E	405	NAP	O4D-C1D-N1N-C2N
3	E	405	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	E	405	NAP	C2D-C1D-N1N-C2N
3	E	405	NAP	C2D-C1D-N1N-C6N
3	F	406	NAP	C5B-O5B-PA-O3
3	F	406	NAP	C5D-O5D-PN-O3
3	F	406	NAP	C5D-O5D-PN-O2N
3	F	406	NAP	O4D-C1D-N1N-C2N
3	F	406	NAP	O4D-C1D-N1N-C6N
3	F	406	NAP	C2D-C1D-N1N-C2N
3	F	406	NAP	C2D-C1D-N1N-C6N
3	G	407	NAP	C5B-O5B-PA-O2A
3	G	407	NAP	C5B-O5B-PA-O3
3	G	407	NAP	PN-O3-PA-O5B
3	G	407	NAP	C5D-O5D-PN-O3
3	G	407	NAP	C5D-O5D-PN-O1N
3	G	407	NAP	C5D-O5D-PN-O2N
3	G	407	NAP	O4D-C1D-N1N-C6N
3	H	408	NAP	C5B-O5B-PA-O1A
3	H	408	NAP	PA-O3-PN-O5D
3	H	408	NAP	C5D-O5D-PN-O3
3	H	408	NAP	C5D-O5D-PN-O2N
3	H	408	NAP	O4D-C4D-C5D-O5D
3	H	408	NAP	O4D-C1D-N1N-C2N
3	H	408	NAP	O4D-C1D-N1N-C6N
3	A	401	NAP	C3D-C4D-C5D-O5D
3	D	404	NAP	C3D-C4D-C5D-O5D
3	F	406	NAP	C3D-C4D-C5D-O5D
3	G	407	NAP	C3D-C4D-C5D-O5D
3	A	401	NAP	O4D-C4D-C5D-O5D
3	F	406	NAP	O4D-C4D-C5D-O5D
3	G	407	NAP	O4D-C4D-C5D-O5D
3	H	408	NAP	C3D-C4D-C5D-O5D
3	A	401	NAP	O4B-C4B-C5B-O5B
3	A	401	NAP	C3B-C4B-C5B-O5B
3	B	402	NAP	O4D-C4D-C5D-O5D
3	C	403	NAP	C3B-C4B-C5B-O5B
3	C	403	NAP	O4D-C4D-C5D-O5D
3	D	404	NAP	O4B-C4B-C5B-O5B
3	D	404	NAP	C3B-C4B-C5B-O5B
3	E	405	NAP	O4B-C4B-C5B-O5B
3	E	405	NAP	C3B-C4B-C5B-O5B
3	G	407	NAP	O4B-C4B-C5B-O5B
3	G	407	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	H	408	NAP	O4B-C4B-C5B-O5B
3	H	408	NAP	C3B-C4B-C5B-O5B
3	C	403	NAP	O4B-C4B-C5B-O5B
3	E	405	NAP	O4D-C4D-C5D-O5D
3	F	406	NAP	O4B-C4B-C5B-O5B
3	D	404	NAP	C2B-O2B-P2B-O1X
3	H	408	NAP	C2B-O2B-P2B-O1X
3	B	402	NAP	O4B-C4B-C5B-O5B
3	F	406	NAP	C3B-C4B-C5B-O5B
3	C	403	NAP	PN-O3-PA-O1A
3	B	402	NAP	C3B-C4B-C5B-O5B
3	B	402	NAP	PN-O3-PA-O5B
3	B	402	NAP	PA-O3-PN-O5D
3	C	403	NAP	PN-O3-PA-O5B
3	C	403	NAP	PA-O3-PN-O5D
3	D	404	NAP	PA-O3-PN-O5D
3	F	406	NAP	PN-O3-PA-O5B
3	C	403	NAP	C4B-C5B-O5B-PA
3	F	406	NAP	C2B-O2B-P2B-O1X
3	G	407	NAP	C2B-O2B-P2B-O1X
3	B	402	NAP	C5B-O5B-PA-O1A
3	C	403	NAP	C5B-O5B-PA-O1A
3	C	403	NAP	C5D-O5D-PN-O2N
3	D	404	NAP	C5B-O5B-PA-O1A
3	E	405	NAP	C5B-O5B-PA-O1A
3	E	405	NAP	C5D-O5D-PN-O1N
3	F	406	NAP	C5B-O5B-PA-O1A
3	G	407	NAP	C5B-O5B-PA-O1A
3	D	404	NAP	C4B-C5B-O5B-PA
3	E	405	NAP	C4B-C5B-O5B-PA
3	A	401	NAP	C2D-C1D-N1N-C2N
3	C	403	NAP	C2D-C1D-N1N-C2N
3	C	403	NAP	C2D-C1D-N1N-C6N
3	H	408	NAP	C2D-C1D-N1N-C2N
3	G	407	NAP	C4B-C5B-O5B-PA
3	G	407	NAP	O4D-C1D-N1N-C2N
3	A	401	NAP	C2B-O2B-P2B-O1X
3	F	406	NAP	PA-O3-PN-O5D
3	F	406	NAP	C4B-C5B-O5B-PA
3	B	402	NAP	C3D-C4D-C5D-O5D
3	D	404	NAP	C4N-C3N-C7N-N7N
3	C	403	NAP	C3D-C4D-C5D-O5D

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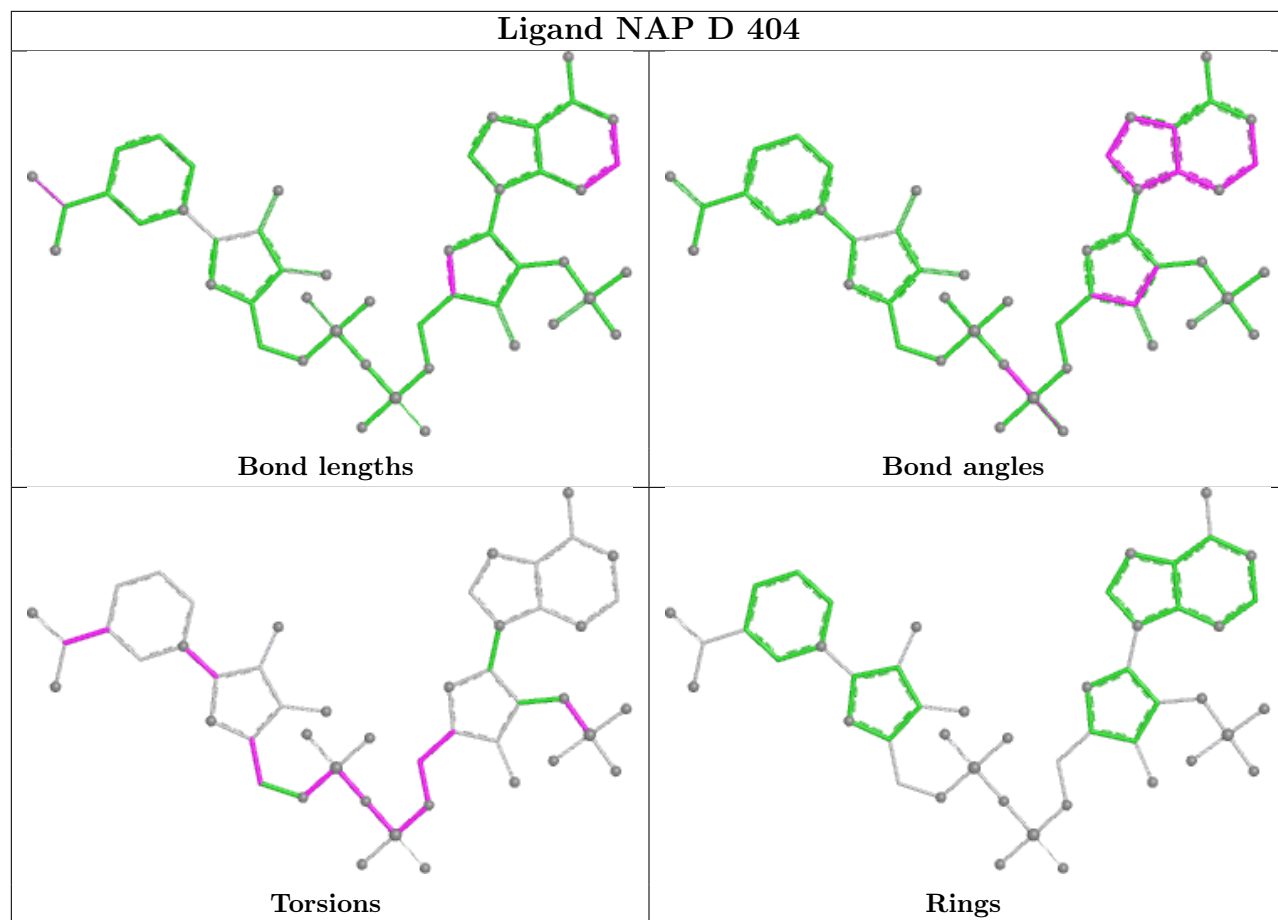
Mol	Chain	Res	Type	Atoms
3	D	404	NAP	C4N-C3N-C7N-O7N
3	D	404	NAP	PN-O3-PA-O1A
3	E	405	NAP	PN-O3-PA-O2A
3	F	406	NAP	C2B-O2B-P2B-O3X
3	H	408	NAP	C4B-C5B-O5B-PA
3	F	406	NAP	PA-O3-PN-O2N
3	G	407	NAP	PN-O3-PA-O1A
3	G	407	NAP	PN-O3-PA-O2A

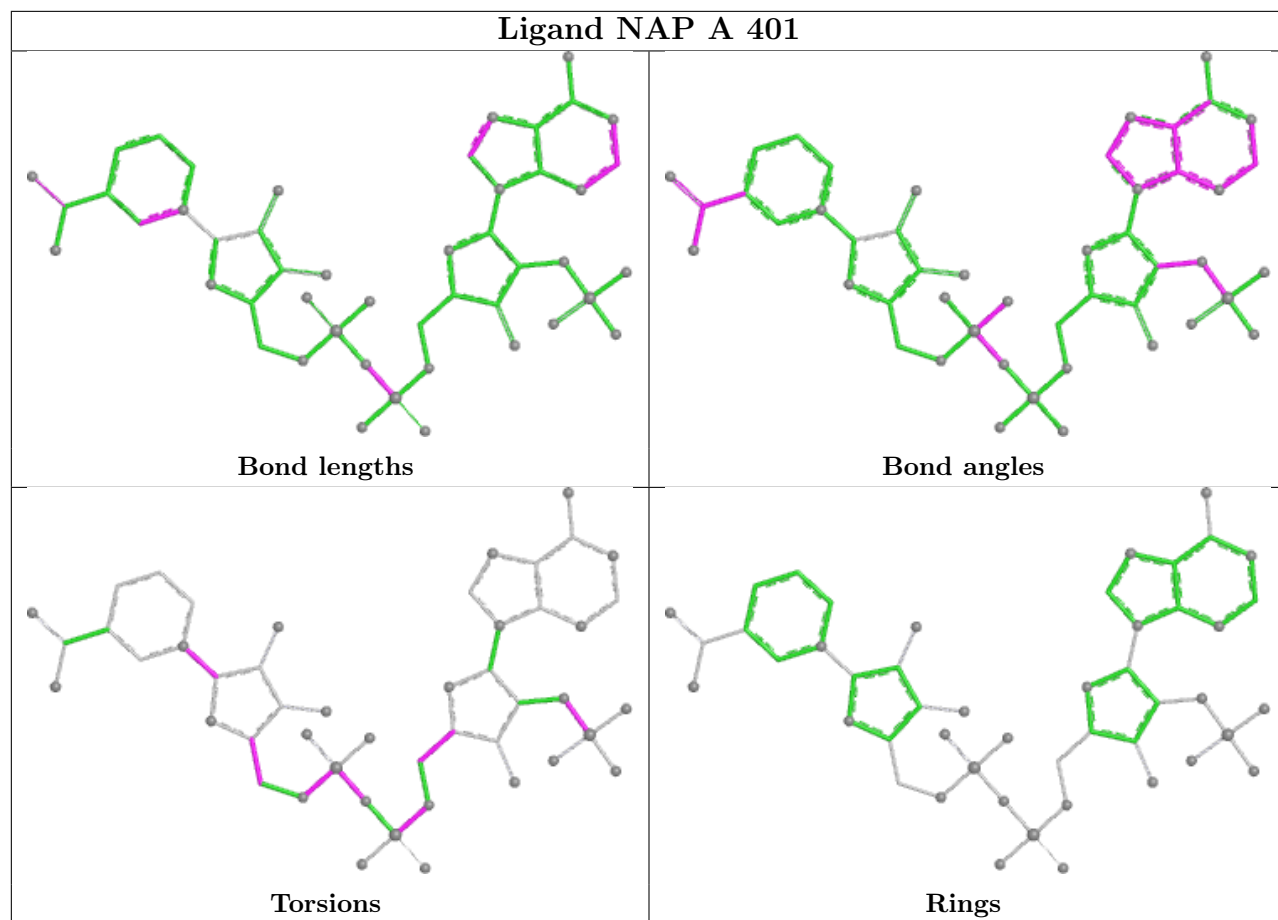
There are no ring outliers.

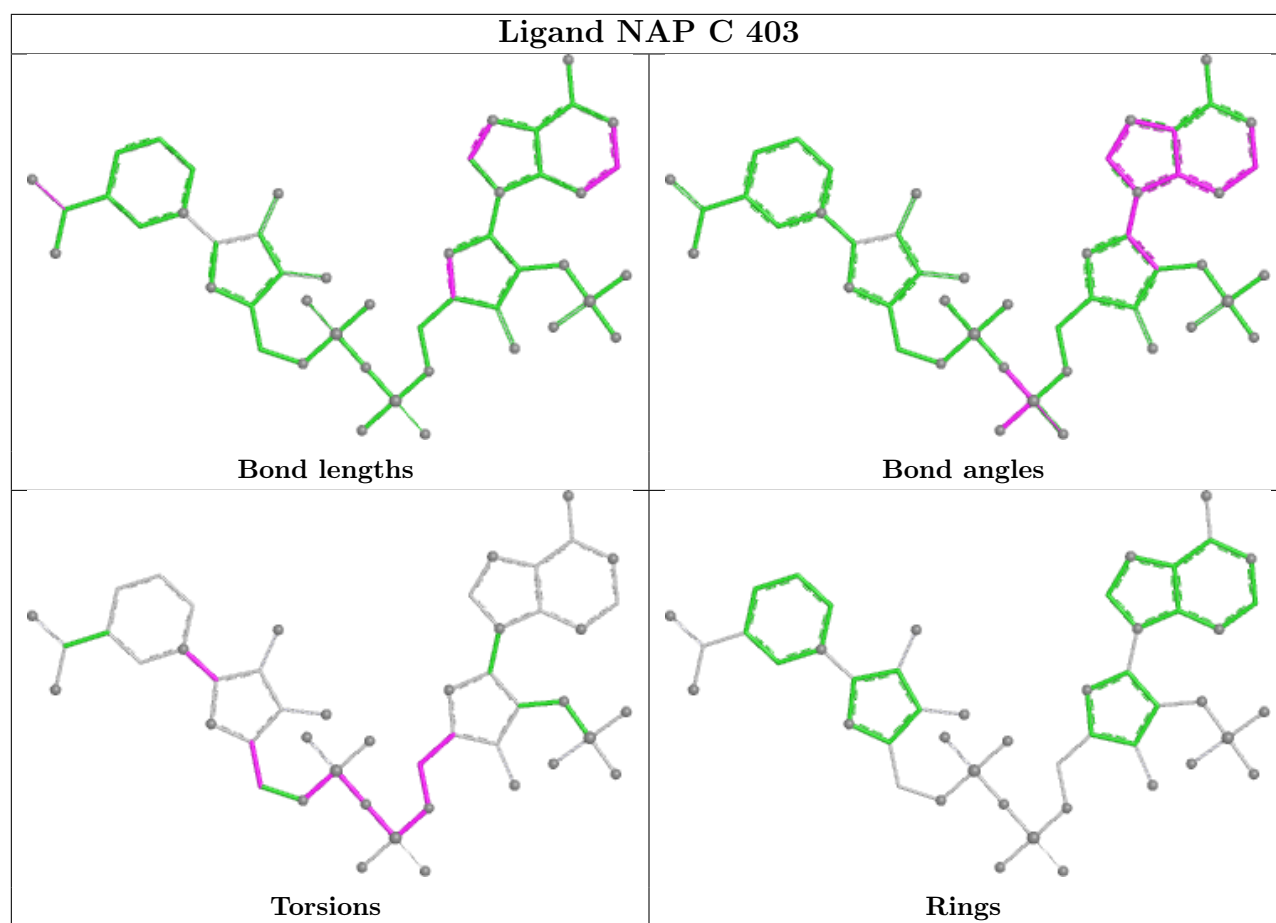
8 monomers are involved in 29 short contacts:

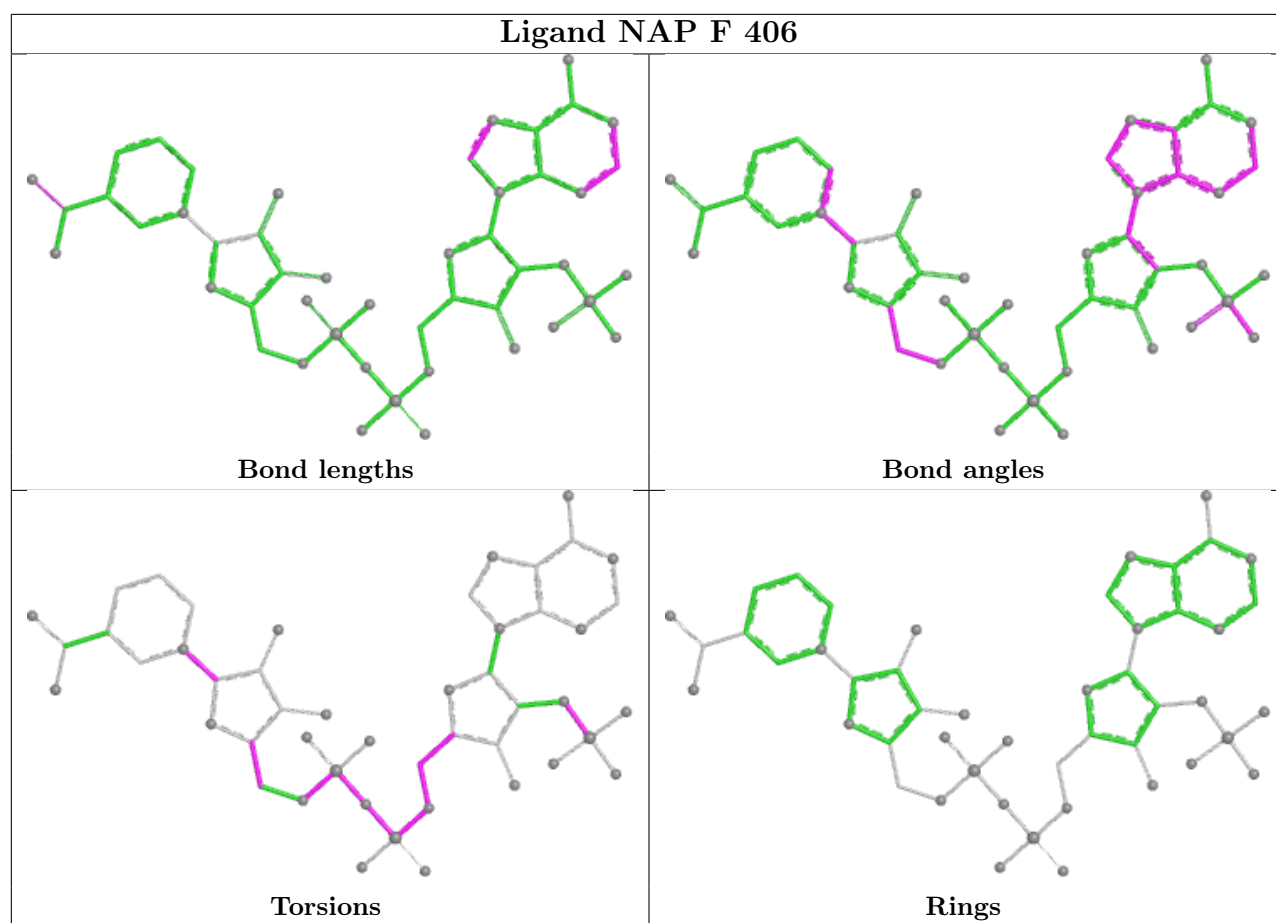
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	NAP	4	0
3	A	401	NAP	5	0
3	C	403	NAP	3	0
3	F	406	NAP	4	0
3	G	407	NAP	3	0
3	E	405	NAP	1	0
3	H	408	NAP	5	0
3	B	402	NAP	4	0

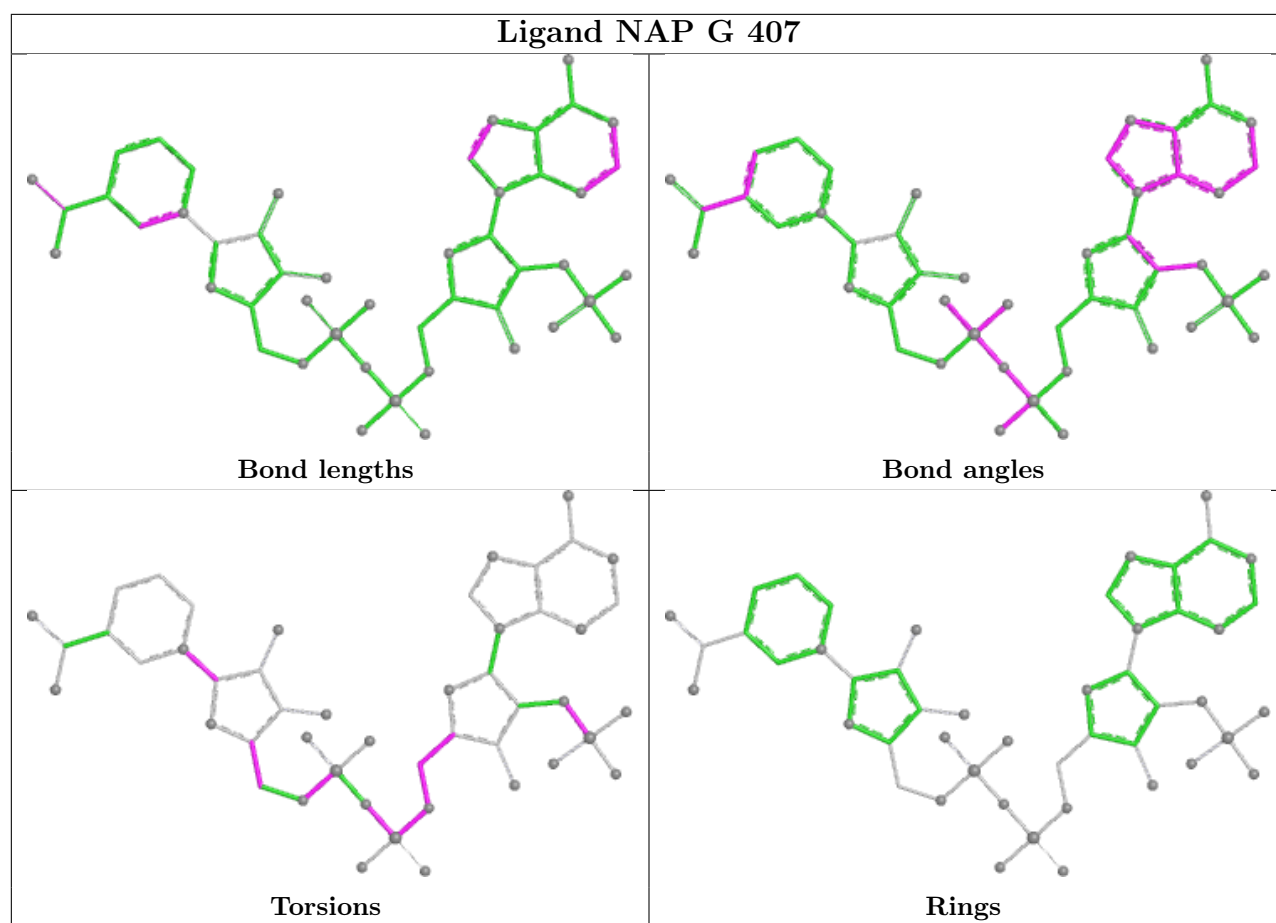
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

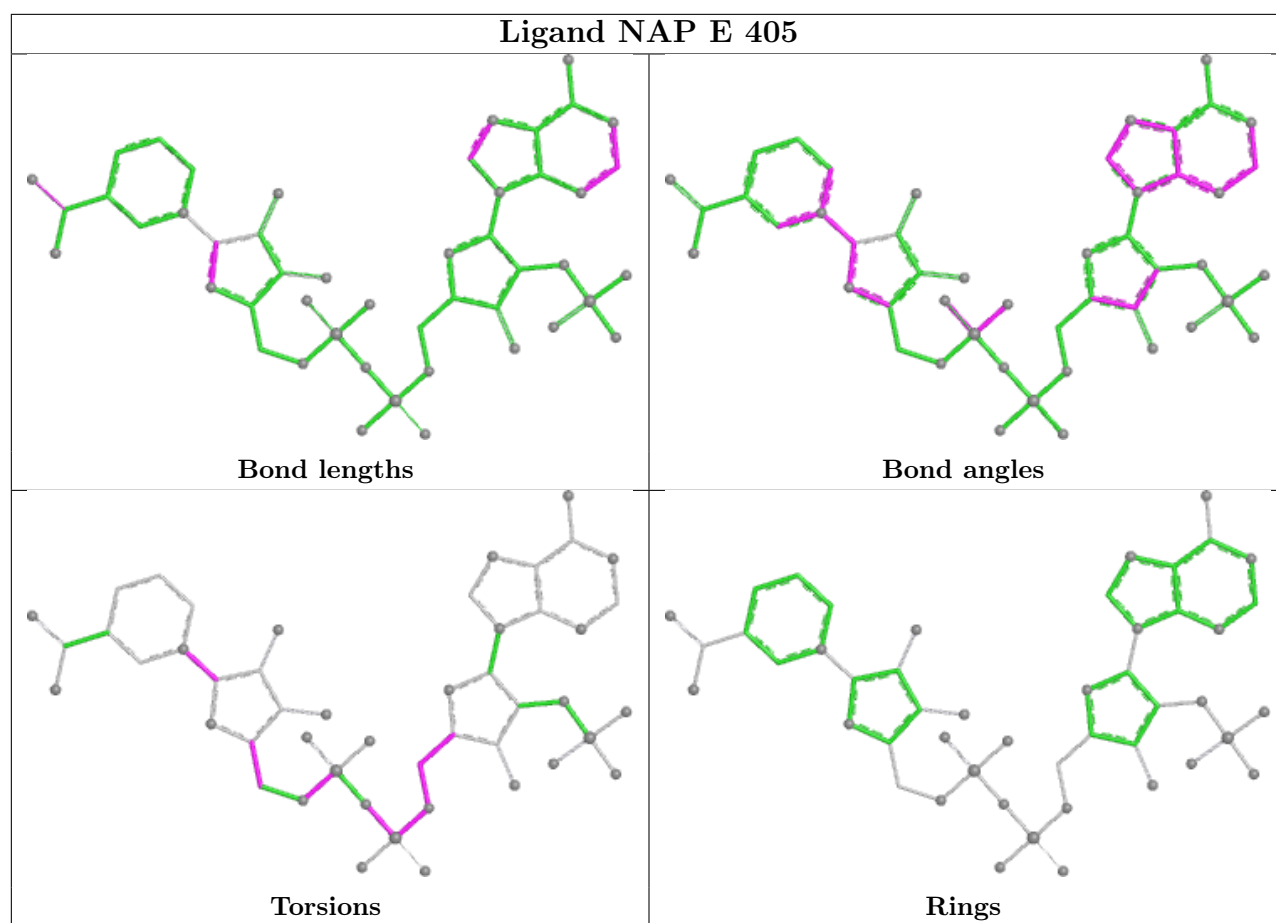


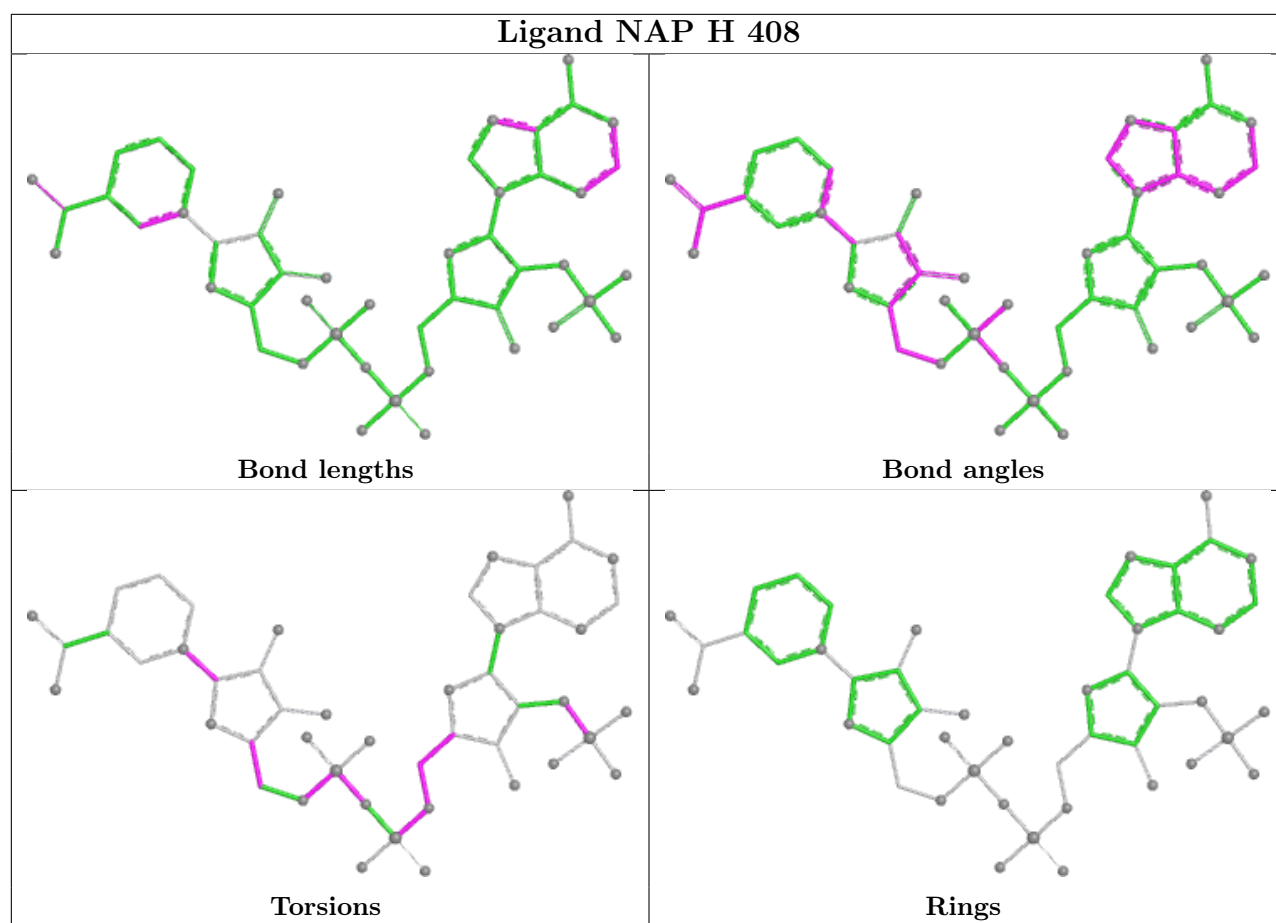


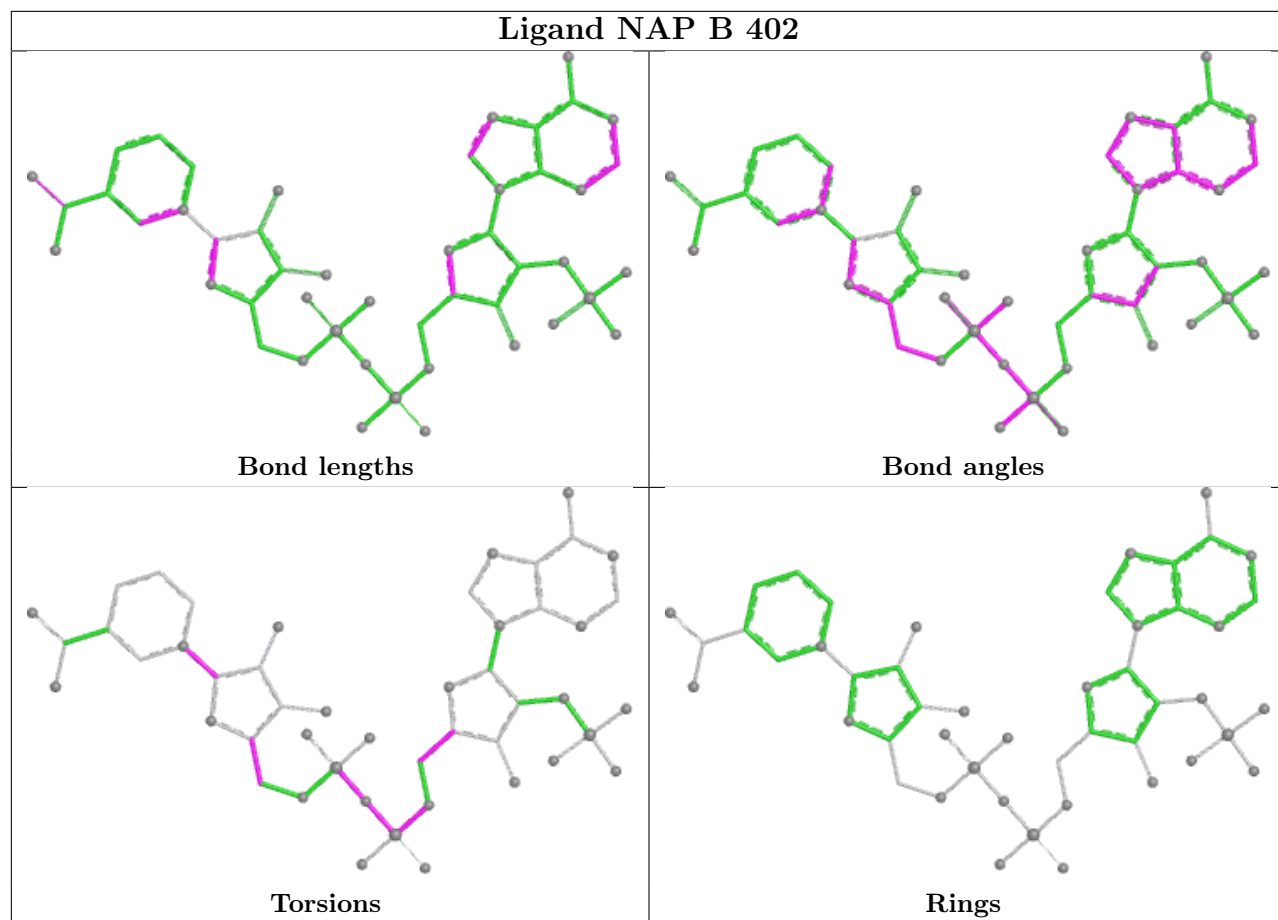












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	291/300 (97%)	-0.40	0 100 100	19, 32, 50, 59	0
1	B	290/300 (96%)	-0.07	0 100 100	22, 39, 57, 65	0
1	C	291/300 (97%)	-0.35	1 (0%) 90 86	18, 28, 42, 50	0
1	D	291/300 (97%)	0.07	4 (1%) 73 64	19, 41, 60, 63	0
1	E	292/300 (97%)	0.13	4 (1%) 73 64	20, 42, 59, 64	0
1	F	291/300 (97%)	-0.19	0 100 100	17, 33, 46, 50	0
1	G	291/300 (97%)	-0.50	0 100 100	18, 28, 43, 50	0
1	H	291/300 (97%)	-0.31	0 100 100	15, 30, 45, 56	0
All	All	2328/2400 (97%)	-0.20	9 (0%) 88 84	15, 34, 55, 65	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	LEU	2.7
1	E	0	ALA	2.7
1	D	42	PHE	2.5
1	E	56	GLN	2.4
1	E	295	GLU	2.4
1	C	0	ALA	2.3
1	D	71	GLU	2.3
1	E	35	PHE	2.1
1	D	77	VAL	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

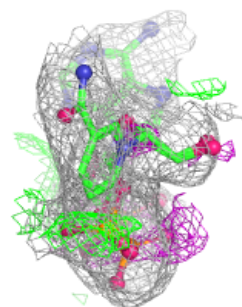
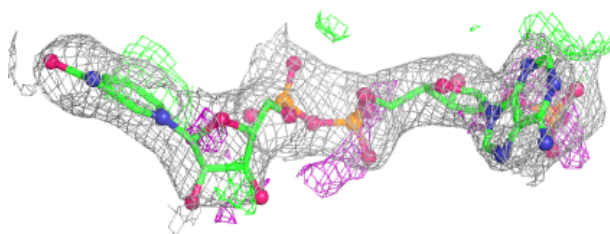
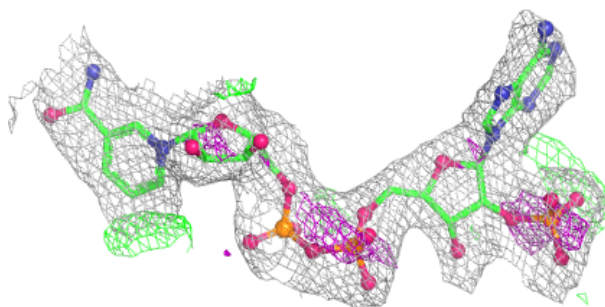
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	E	405	48/48	0.86	0.14	65,71,80,81	0
3	NAP	F	406	48/48	0.91	0.10	62,67,71,72	0
3	NAP	A	401	48/48	0.92	0.10	53,59,61,62	0
3	NAP	C	403	48/48	0.93	0.10	44,50,55,55	0
3	NAP	D	404	48/48	0.93	0.10	48,58,65,67	0
2	CL	B	502	1/1	0.93	0.07	46,46,46,46	0
3	NAP	B	402	48/48	0.93	0.10	52,60,67,67	0
2	CL	G	507	1/1	0.94	0.07	51,51,51,51	0
2	CL	H	509	1/1	0.94	0.08	42,42,42,42	0
2	CL	A	501	1/1	0.94	0.07	44,44,44,44	0
2	CL	D	504	1/1	0.94	0.09	39,39,39,39	0
3	NAP	G	407	48/48	0.94	0.09	42,54,58,59	0
3	NAP	H	408	48/48	0.94	0.09	43,51,66,67	0
2	CL	E	505	1/1	0.95	0.06	44,44,44,44	0
2	CL	H	508	1/1	0.98	0.05	37,37,37,37	0

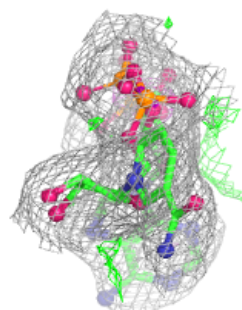
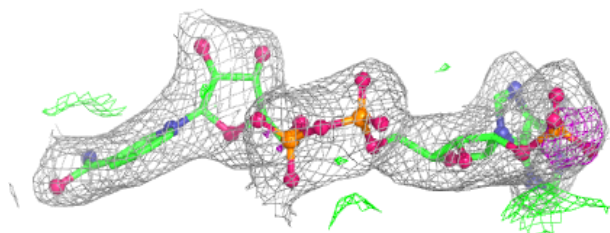
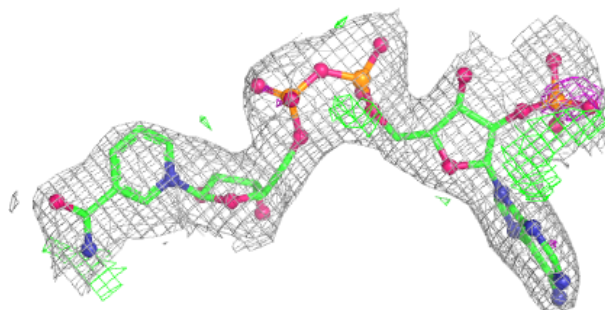
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP E 405:

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

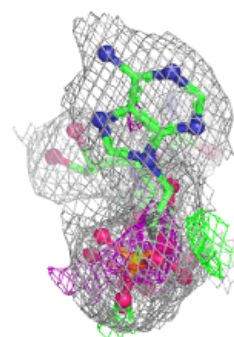
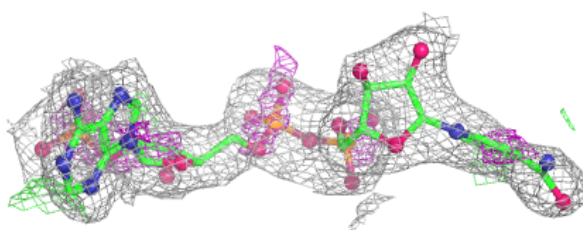
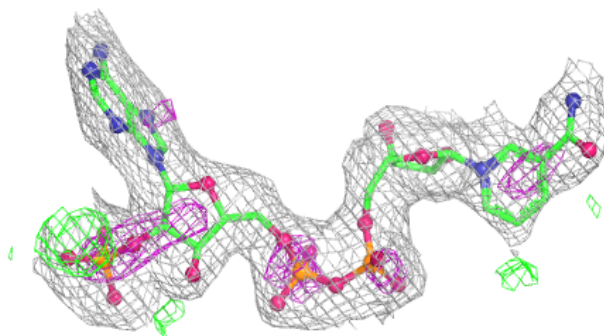
**Electron density around NAP F 406:**

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

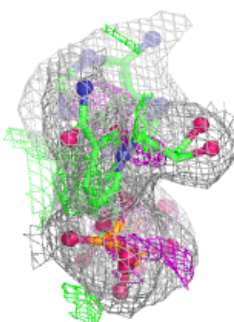
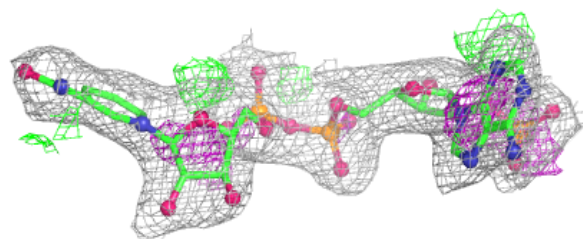
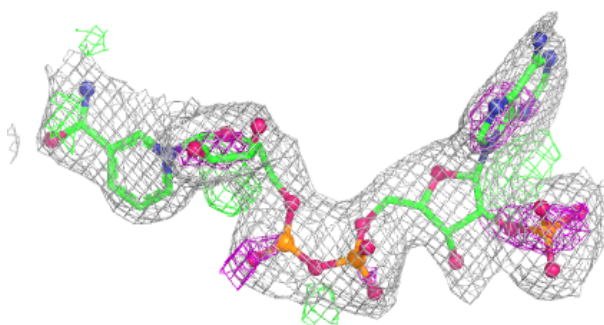


Electron density around NAP A 401:

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

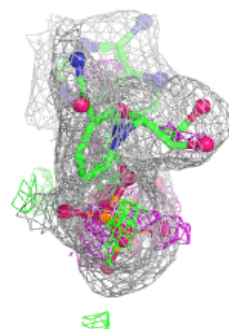
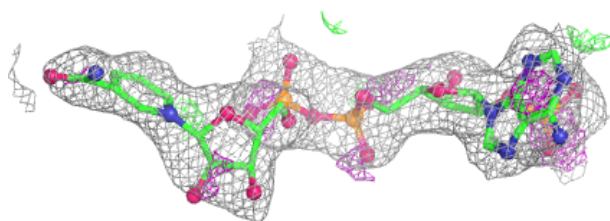
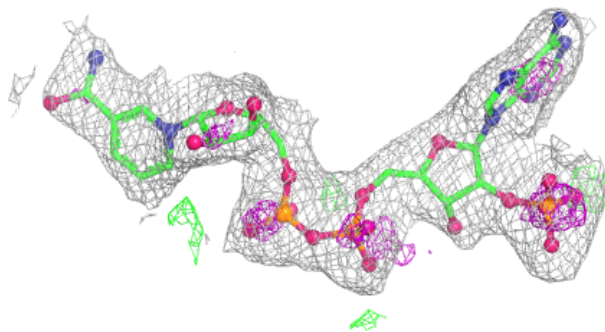
**Electron density around NAP C 403:**

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

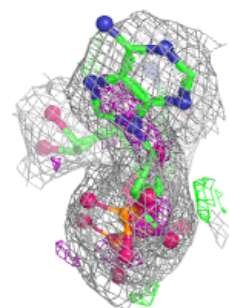
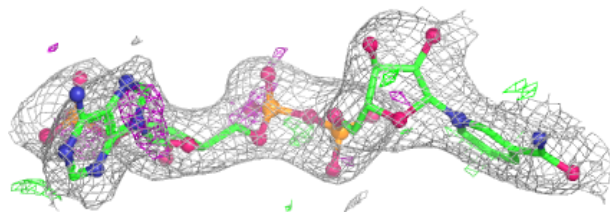
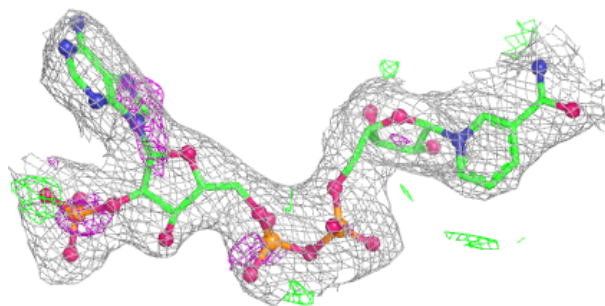


Electron density around NAP D 404:

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

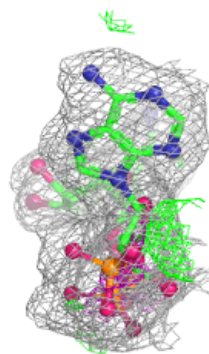
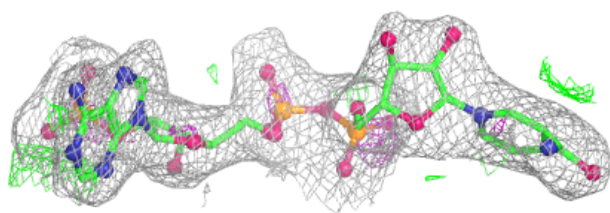
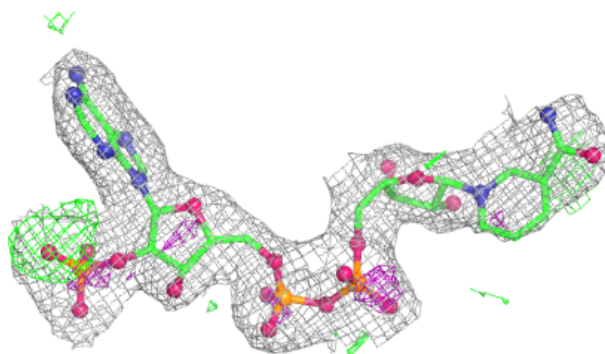
**Electron density around NAP B 402:**

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

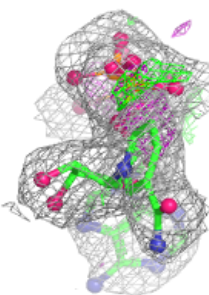
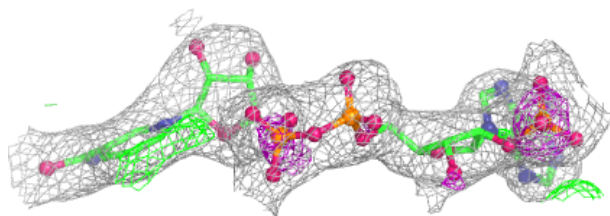
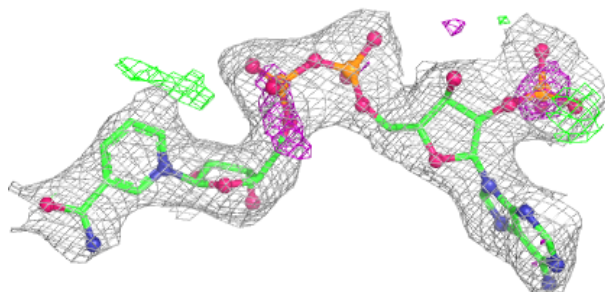


Electron density around NAP G 407:

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

**Electron density around NAP H 408:**

$2mF_o-DF_c$ (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.