



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 6SLE / pdb_00006sle
Title : Structure of Reductive Aminase from Neosartorya fumigata in complex with NADP+
Authors : Sharma, M.; Mangas-Sanchez, J.; Turner, N.J.; Grogan, G.
Deposited on : 2019-08-19
Resolution : 2.77 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

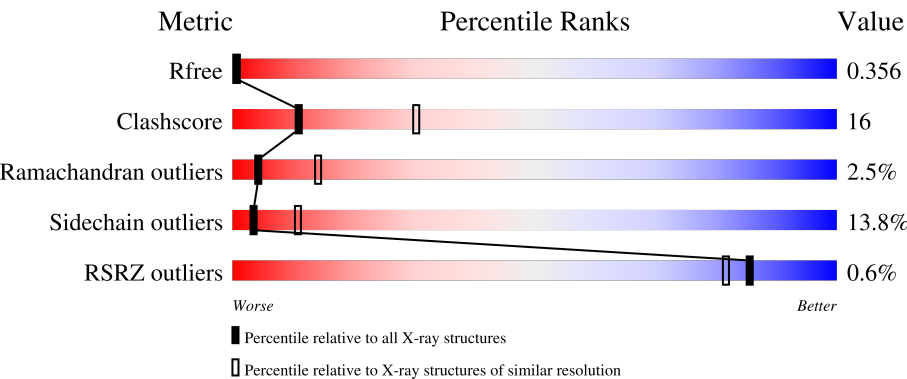
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	285	62%31%5%.
1	B	285	2% 69%18%.8%
1	C	285	% 72%21%. .
1	D	285	% 62%30%5%.
1	E	285	68%22%.6%

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Mol	Chain	Length	Quality of chain
1	F	285	63%32%
1	G	285	% 71%24%
1	H	285	66%28%

2 Entry composition

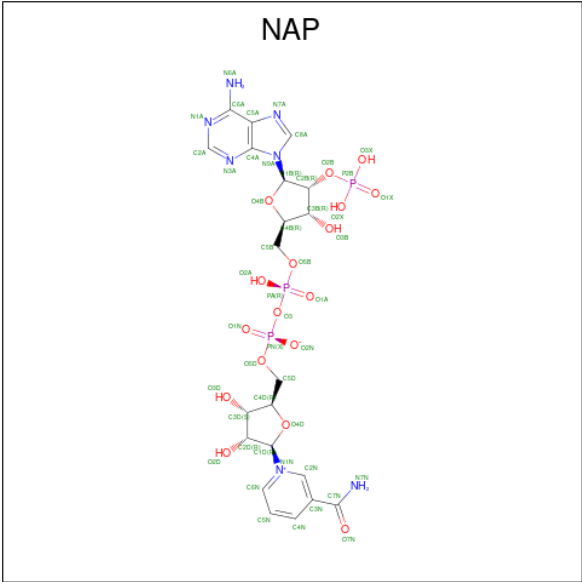
There are 3 unique types of molecules in this entry. The entry contains 15201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Oxidoreductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	1	0
			1951	1234	332	374	11			
1	B	261	Total	C	N	O	S	0	1	0
			1648	1032	286	320	10			
1	C	273	Total	C	N	O	S	0	0	0
			1820	1152	315	340	13			
1	D	278	Total	C	N	O	S	0	0	0
			1920	1222	320	367	11			
1	E	268	Total	C	N	O	S	0	0	0
			1708	1070	300	328	10			
1	F	280	Total	C	N	O	S	0	0	0
			1930	1221	326	372	11			
1	G	279	Total	C	N	O	S	0	0	0
			1820	1137	317	353	13			
1	H	278	Total	C	N	O	S	0	0	0
			1915	1210	322	372	11			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	15	Total	O	0	0
			15	15		
3	C	8	Total	O	0	0
			8	8		
3	D	11	Total	O	0	0
			11	11		

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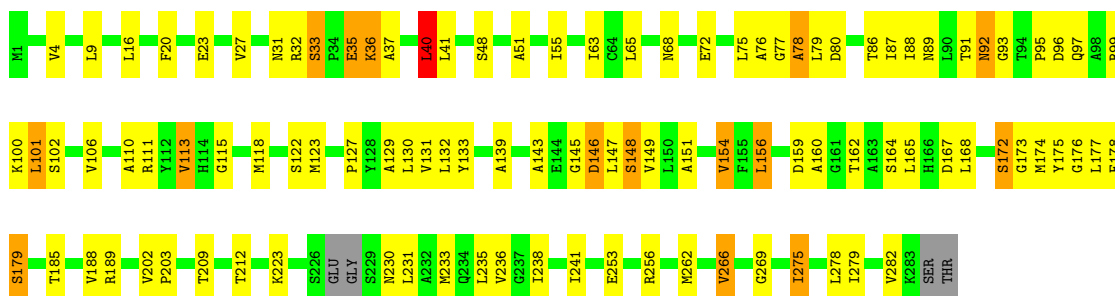
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	15	Total	O	0	0
			15	15		
3	F	14	Total	O	0	0
			14	14		
3	G	13	Total	O	0	0
			13	13		
3	H	14	Total	O	0	0
			14	14		

3 Residue-property plots

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

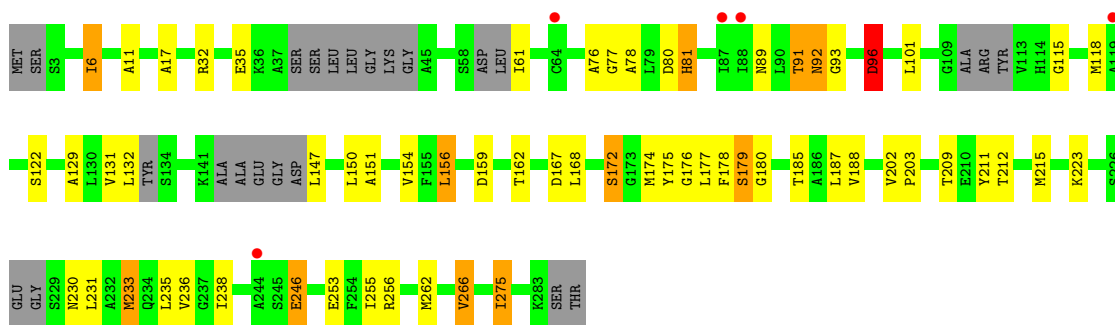
- Molecule 1: Oxidoreductase, putative

Chain A: 



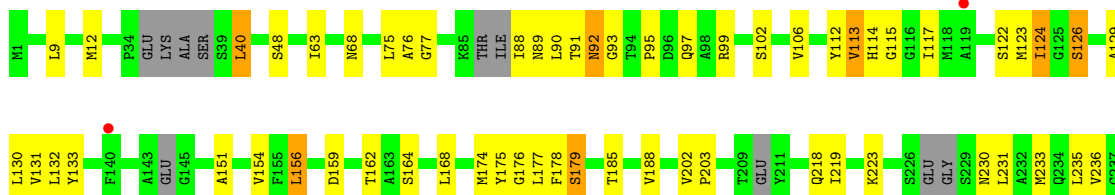
- Molecule 1: Oxidoreductase, putative

Chain B: 



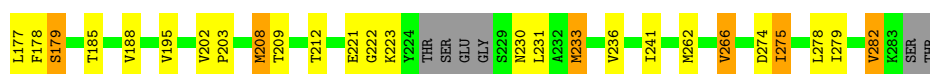
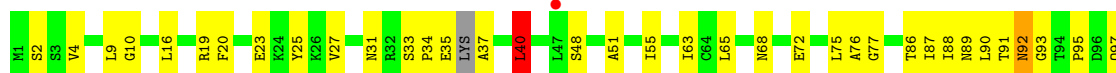
- Molecule 1: Oxidoreductase, putative

Chain C: 

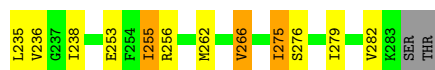
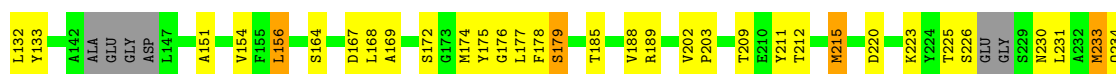
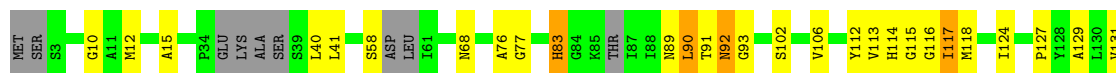




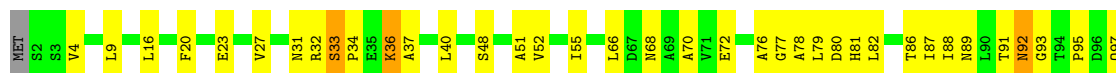
- Molecule 1: Oxidoreductase, putative



- Molecule 1: Oxidoreductase, putative

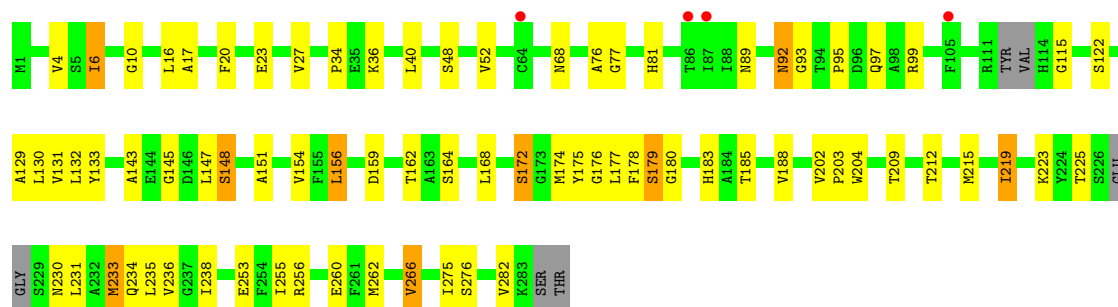


- Molecule 1: Oxidoreductase, putative



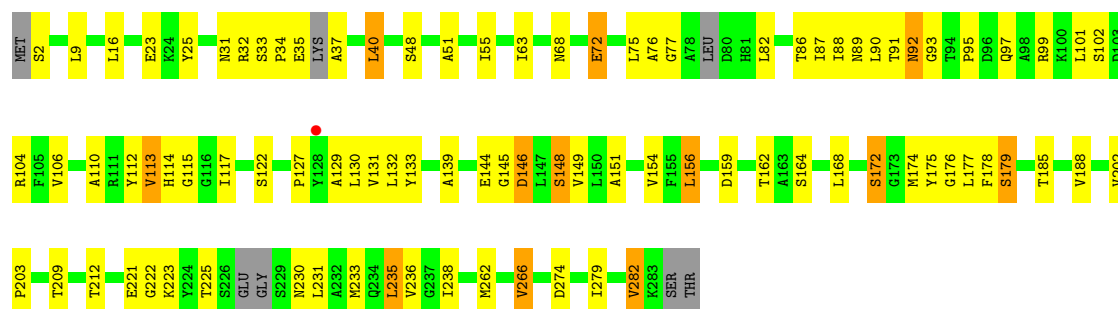
- Molecule 1: Oxidoreductase, putative





- Molecule 1: Oxidoreductase, putative

Chain H: 66% 28%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.39Å 89.31Å 97.93Å 105.56° 90.00° 93.99°	Depositor
Resolution (Å)	48.28 – 2.77 48.28 – 2.77	Depositor EDS
% Data completeness (in resolution range)	79.0 (48.28-2.77) 79.1 (48.28-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.286 , 0.357 0.287 , 0.356	Depositor DCC
R_{free} test set	2666 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.0	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
Reported twinning fraction	0.866 for H, K, L 0.134 for h,-k,-l	Depositor
Outliers	0 of 53895 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15201	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 40.99 % 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 2.5207e-04. 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

5.1 Standard geometry

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

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	1.15	0/1986	1.60	2/2701 (0.1%)
1	B	1.20	0/1671	1.65	4/2281 (0.2%)
1	C	1.15	0/1846	1.57	0/2510
1	D	1.16	0/1952	1.58	3/2658 (0.1%)
1	E	1.17	0/1729	1.63	4/2359 (0.2%)
1	F	1.16	1/1962 (0.1%)	1.59	1/2673 (0.0%)
1	G	1.18	0/1848	1.62	0/2521
1	H	1.16	0/1945	1.60	3/2647 (0.1%)
All	All	1.16	1/14939 (0.0%)	1.60	17/20350 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	HIS	CE1-NE2	5.45	1.38	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ASP	CA-CB-CG	7.30	119.90	112.60
1	B	81	HIS	CA-CB-CG	6.44	120.24	113.80
1	H	221	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	41	LEU	CA-C-N	5.73	126.45	120.03
1	A	41	LEU	C-N-CA	5.73	126.45	120.03
1	D	40	LEU	CA-C-O	-5.66	112.41	120.51
1	E	41	LEU	CA-C-N	5.37	126.05	120.03
1	E	41	LEU	C-N-CA	5.37	126.05	120.03
1	H	144	GLU	CB-CG-CD	5.35	121.69	112.60
1	H	282	VAL	N-CA-C	-5.35	107.60	113.43
1	F	135	GLY	CA-C-O	-5.33	116.83	122.01
1	E	83	HIS	CA-CB-CG	5.28	119.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	VAL	N-CA-C	-5.21	107.76	113.43
1	E	83	HIS	CB-CA-C	5.17	117.60	110.16
1	B	78	ALA	CA-C-N	5.09	127.06	120.44
1	B	78	ALA	C-N-CA	5.09	127.06	120.44
1	D	221	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1951	0	1816	79	0
1	B	1648	0	1353	48	0
1	C	1820	0	1620	40	0
1	D	1920	0	1801	67	0
1	E	1708	0	1434	70	0
1	F	1930	0	1782	74	0
1	G	1820	0	1555	59	0
1	H	1915	0	1779	57	0
2	A	48	0	25	4	0
2	B	48	0	25	3	0
2	C	48	0	25	1	0
2	D	48	0	25	5	0
2	E	48	0	25	4	0
2	F	48	0	25	5	0
2	G	48	0	25	4	0
2	H	48	0	25	2	0
3	A	15	0	0	3	0
3	B	15	0	0	2	0
3	C	8	0	0	3	0
3	D	11	0	0	2	0
3	E	15	0	0	5	0
3	F	14	0	0	6	0
3	G	13	0	0	3	0
3	H	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15201	0	13340	468	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 16.

All (468) 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:D:127:PRO:HA	1:F:127:PRO:HA	1.20	1.16
1:A:127:PRO:HA	1:H:127:PRO:HA	1.26	1.09
1:A:40:LEU:HD23	1:A:40:LEU:O	1.58	1.02
1:A:111:ARG:CD	1:A:139:ALA:HB2	1.92	1.00
1:E:12:MET:SD	1:E:124:ILE:HD11	2.04	0.98
1:A:145:GLY:O	1:A:148:SER:OG	1.89	0.90
1:F:79:LEU:O	1:F:81:HIS:N	2.04	0.90
1:G:145:GLY:O	1:G:148:SER:OG	1.89	0.90
1:H:145:GLY:O	1:H:148:SER:OG	1.89	0.89
1:D:145:GLY:O	1:D:148:SER:OG	1.90	0.88
1:B:167:ASP:OD1	3:B:401:HOH:O	1.91	0.88
1:F:145:GLY:O	1:F:148:SER:OG	1.89	0.88
1:D:127:PRO:HA	1:F:127:PRO:CA	2.04	0.86
1:E:118:MET:HE1	1:E:167:ASP:OD1	1.76	0.85
1:D:118:MET:HE1	1:D:167:ASP:OD1	1.75	0.84
1:F:233:MET:HE3	2:G:301:NAP:O2D	1.77	0.84
1:D:127:PRO:CA	1:F:127:PRO:HA	2.04	0.84
1:E:90:LEU:HD12	1:E:117:ILE:HG12	1.57	0.84
1:C:12:MET:SD	1:C:124:ILE:HD11	2.17	0.83
1:A:118:MET:HE1	1:A:167:ASP:OD1	1.77	0.83
1:B:118:MET:HE1	1:B:167:ASP:OD1	1.79	0.83
1:B:246[A]:GLU:OE1	1:B:246[A]:GLU:HA	1.78	0.83
1:D:19:ARG:HB2	3:D:401:HOH:O	1.81	0.79
1:F:233:MET:HE3	2:G:301:NAP:C2D	2.13	0.78
3:F:409:HOH:O	1:G:282:VAL:CB	2.32	0.77
1:A:127:PRO:HA	1:H:127:PRO:CA	2.12	0.76
1:A:92:ASN:HB2	3:A:1102:HOH:O	1.85	0.76
1:A:127:PRO:CA	1:H:127:PRO:HA	2.11	0.75
1:F:233:MET:HE3	2:G:301:NAP:H2D	1.69	0.74
1:D:63:ILE:HD11	1:D:75:LEU:HD11	1.70	0.73
1:E:234:GLN:NE2	3:E:401:HOH:O	1.91	0.73
1:A:32[B]:ARG:HG2	1:A:32[B]:ARG:HH21	1.53	0.73
1:H:63:ILE:HD11	1:H:75:LEU:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:LEU:CD1	1:E:117:ILE:HG12	2.20	0.70
1:E:118:MET:HE1	1:E:167:ASP:CG	2.16	0.70
1:F:4:VAL:HG11	1:F:20:PHE:CD2	2.26	0.70
1:D:118:MET:HE1	1:D:167:ASP:CG	2.16	0.70
1:D:4:VAL:HG11	1:D:20:PHE:CD2	2.26	0.70
1:F:175:TYR:O	1:F:179:SER:OG	2.09	0.70
1:D:90:LEU:HD13	1:D:117:ILE:HD11	1.74	0.69
1:B:118:MET:HE1	1:B:167:ASP:CG	2.16	0.69
1:B:253:GLU:OE1	1:B:256:ARG:NH1	2.24	0.69
1:C:63:ILE:HD11	1:C:75:LEU:HD11	1.75	0.69
1:D:145:GLY:HA3	3:D:410:HOH:O	1.92	0.69
1:D:175:TYR:O	1:D:179:SER:OG	2.10	0.68
1:H:90:LEU:HD13	1:H:117:ILE:HD11	1.75	0.68
1:H:82:LEU:HD22	1:H:87:ILE:HD11	1.76	0.68
1:D:175:TYR:CZ	1:E:238:ILE:HD11	2.28	0.67
1:A:175:TYR:O	1:A:179:SER:OG	2.10	0.67
1:A:63:ILE:HD11	1:A:75:LEU:HD11	1.75	0.67
1:B:238:ILE:HD12	1:B:262:MET:HE2	1.75	0.67
1:A:118:MET:HE1	1:A:167:ASP:CG	2.19	0.67
1:A:4:VAL:HG11	1:A:20:PHE:CD2	2.29	0.67
1:D:72:GLU:HG3	1:D:101:LEU:HD11	1.77	0.67
1:F:238:ILE:HD12	1:F:262:MET:HE2	1.75	0.67
1:C:238:ILE:HD12	1:C:262:MET:HE2	1.76	0.67
1:C:90:LEU:HD13	1:C:117:ILE:HD11	1.76	0.67
1:G:4:VAL:HG11	1:G:20:PHE:CD2	2.31	0.66
1:E:175:TYR:O	1:E:179:SER:OG	2.10	0.66
1:F:82:LEU:HD22	1:F:87:ILE:HD11	1.76	0.66
1:F:175:TYR:CZ	1:G:238:ILE:HD11	2.31	0.65
1:B:175:TYR:O	1:B:179:SER:OG	2.11	0.65
1:G:81:HIS:HB2	3:G:410:HOH:O	1.96	0.65
1:E:215:MET:HG3	1:E:276:SER:HB3	1.79	0.65
1:C:175:TYR:O	1:C:179:SER:OG	2.11	0.65
1:B:92:ASN:HB3	2:B:301:NAP:O2D	1.98	0.64
1:G:175:TYR:O	1:G:179:SER:OG	2.11	0.64
1:A:253:GLU:OE2	1:A:256:ARG:NH1	2.31	0.63
1:F:9:LEU:HD12	1:F:31:ASN:HB2	1.81	0.63
1:E:169:ALA:O	1:E:172:SER:OG	2.13	0.63
1:F:253:GLU:OE2	1:F:256:ARG:NH1	2.32	0.63
1:H:9:LEU:HD12	1:H:31:ASN:HB2	1.81	0.63
1:A:9:LEU:HD12	1:A:31:ASN:HB2	1.81	0.63
1:G:52:VAL:HA	3:G:410:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:TYR:O	1:H:179:SER:OG	2.11	0.61
1:C:253:GLU:OE2	1:C:256:ARG:NH1	2.33	0.61
1:E:15:ALA:CB	1:E:124:ILE:HD12	2.30	0.61
1:H:235:LEU:HD22	1:H:262:MET:HB3	1.83	0.61
1:A:262:MET:HG3	1:A:278:LEU:HD21	1.82	0.61
1:G:253:GLU:OE2	1:G:256:ARG:NH1	2.32	0.61
1:E:253:GLU:OE2	1:E:256:ARG:NH1	2.34	0.61
1:D:9:LEU:HD12	1:D:31:ASN:HB2	1.83	0.60
1:G:238:ILE:HD13	1:G:262:MET:HE1	1.82	0.60
1:D:168:LEU:O	1:D:172:SER:OG	2.19	0.60
1:A:168:LEU:O	1:A:172:SER:OG	2.20	0.60
1:E:238:ILE:HD13	1:E:262:MET:HE1	1.83	0.60
1:G:260:GLU:HG2	3:G:412:HOH:O	2.02	0.60
2:A:1000:NAP:O2D	1:B:233:MET:HE1	2.02	0.59
1:F:168:LEU:O	1:F:172:SER:OG	2.20	0.59
1:H:168:LEU:O	1:H:172:SER:OG	2.20	0.59
1:A:72:GLU:HG3	1:A:101:LEU:HD11	1.84	0.59
1:F:72:GLU:HG3	1:F:101:LEU:HD11	1.85	0.59
1:B:96:ASP:OD1	1:B:96:ASP:C	2.45	0.58
1:D:31:ASN:ND2	1:D:37:ALA:HB3	2.18	0.58
1:D:51:ALA:O	1:D:55:ILE:HG12	2.03	0.58
1:A:51:ALA:O	1:A:55:ILE:HG12	2.02	0.58
1:F:33:SER:OG	2:F:301:NAP:O3X	2.22	0.58
1:F:51:ALA:O	1:F:55:ILE:HG12	2.02	0.58
1:G:168:LEU:O	1:G:172:SER:OG	2.21	0.58
1:G:215:MET:O	1:G:219:ILE:HD13	2.04	0.58
1:B:89:ASN:HD21	1:B:91:THR:HB	1.69	0.58
1:H:51:ALA:O	1:H:55:ILE:HG12	2.03	0.58
1:H:112:TYR:OH	1:H:114:HIS:HD2	1.87	0.58
1:H:115:GLY:HA2	1:H:132:LEU:O	2.04	0.57
1:C:112:TYR:OH	1:C:114:HIS:HD2	1.88	0.57
1:C:115:GLY:HA2	1:C:132:LEU:O	2.04	0.57
1:D:115:GLY:HA2	1:D:132:LEU:O	2.04	0.57
1:D:112:TYR:OH	1:D:114:HIS:HD2	1.87	0.57
1:H:72:GLU:CD	1:H:104:ARG:HH22	2.11	0.57
1:F:31:ASN:ND2	2:F:301:NAP:O2X	2.31	0.57
1:A:35:GLU:OE1	1:A:36:LYS:N	2.38	0.57
1:H:235:LEU:HD22	1:H:262:MET:HE3	1.86	0.57
1:D:130:LEU:HD21	1:D:154:VAL:HG21	1.87	0.57
1:B:115:GLY:HA2	1:B:132:LEU:O	2.05	0.57
1:E:115:GLY:HA2	1:E:132:LEU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:MET:HE2	1:G:233:MET:O	2.05	0.57
1:E:112:TYR:OH	1:E:114:HIS:HD2	1.88	0.56
1:E:234:GLN:O	1:E:238:ILE:HD13	2.05	0.56
1:F:87:ILE:HD12	1:F:110:ALA:HB1	1.86	0.56
1:A:160:ALA:HB3	3:A:1105:HOH:O	2.06	0.56
1:B:233:MET:HE2	1:B:233:MET:O	2.05	0.56
1:B:168:LEU:O	1:B:172:SER:OG	2.22	0.56
1:G:115:GLY:HA2	1:G:132:LEU:O	2.05	0.56
1:A:65:LEU:HD22	2:A:1000:NAP:N3A	2.21	0.56
1:A:130:LEU:HD21	1:A:154:VAL:HG21	1.88	0.56
1:F:115:GLY:HA2	1:F:132:LEU:O	2.05	0.56
1:E:102:SER:O	1:E:106:VAL:HG13	2.06	0.55
1:E:211:TYR:CE1	1:E:215:MET:HE1	2.41	0.55
1:C:92:ASN:N	3:C:402:HOH:O	2.39	0.55
1:C:92:ASN:CA	3:C:402:HOH:O	2.55	0.55
1:H:130:LEU:HD23	1:H:131:VAL:N	2.22	0.55
2:D:301:NAP:O2D	1:E:233:MET:HE1	2.07	0.55
1:H:31:ASN:ND2	1:H:37:ALA:HB3	2.22	0.55
1:A:40:LEU:HD23	1:A:40:LEU:C	2.30	0.55
1:H:68:ASN:O	1:H:72:GLU:HG3	2.07	0.55
1:D:208:MET:HG3	1:E:174:MET:HG3	1.89	0.54
1:E:12:MET:HE3	2:E:301:NAP:C4N	2.37	0.54
1:E:233:MET:HE2	1:E:233:MET:O	2.06	0.54
1:A:115:GLY:HA2	1:A:132:LEU:O	2.06	0.54
1:B:61:ILE:HD12	1:B:61:ILE:N	2.23	0.54
1:F:33:SER:HB2	1:F:36:LYS:CB	2.37	0.54
1:G:234:GLN:O	1:G:238:ILE:HD13	2.08	0.54
1:H:238:ILE:HD12	1:H:262:MET:HE2	1.90	0.54
1:F:79:LEU:C	1:F:81:HIS:H	2.12	0.54
1:B:147:LEU:O	1:B:150:LEU:HG	2.08	0.54
1:A:87:ILE:HD12	1:A:110:ALA:HB1	1.90	0.54
1:A:33:SER:HB2	1:A:36:LYS:CB	2.39	0.53
2:A:1000:NAP:O2D	1:B:233:MET:CE	2.56	0.53
1:F:130:LEU:HD23	1:F:131:VAL:N	2.24	0.53
1:G:183:HIS:HD1	1:G:183:HIS:C	2.16	0.53
1:A:235:LEU:HD12	1:A:266:VAL:HG11	1.91	0.53
1:C:130:LEU:HD23	1:C:131:VAL:N	2.24	0.53
1:G:130:LEU:HD23	1:G:131:VAL:N	2.23	0.53
1:F:118:MET:HE3	1:G:204:TRP:CZ3	2.44	0.53
1:G:219:ILE:CD1	1:G:276:SER:HB2	2.39	0.53
1:H:235:LEU:HD23	1:H:266:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:ASP:OD1	1:H:146:ASP:N	2.43	0.52
1:A:269:GLY:O	1:E:225:THR:CB	2.57	0.52
1:E:234:GLN:HG3	3:E:401:HOH:O	2.08	0.52
1:G:174:MET:HG2	1:G:178:PHE:CE2	2.45	0.52
1:H:87:ILE:HD12	1:H:110:ALA:HB1	1.92	0.52
1:C:9:LEU:N	2:C:301:NAP:O3B	2.42	0.51
1:E:15:ALA:HB3	1:E:124:ILE:HD12	1.90	0.51
1:H:93:GLY:O	1:H:168:LEU:HD11	2.11	0.51
1:A:146:ASP:OD1	1:A:146:ASP:N	2.43	0.51
1:F:268:ALA:HA	3:F:404:HOH:O	2.10	0.51
1:B:89:ASN:ND2	1:B:91:THR:HB	2.25	0.51
1:B:235:LEU:HD12	1:B:266:VAL:HG11	1.92	0.51
1:E:15:ALA:HB1	1:E:124:ILE:HD12	1.92	0.51
1:A:32[B]:ARG:HG2	1:A:32[B]:ARG:NH2	2.24	0.51
1:A:174:MET:HG2	1:A:178:PHE:CE2	2.45	0.51
1:D:146:ASP:OD1	1:D:146:ASP:N	2.42	0.51
1:A:129:ALA:HB1	1:A:151:ALA:HB2	1.93	0.51
1:F:173:GLY:HA2	1:G:180:GLY:HA3	1.93	0.51
1:B:93:GLY:O	1:B:168:LEU:HD11	2.11	0.51
1:C:93:GLY:O	1:C:168:LEU:HD11	2.11	0.51
1:F:174:MET:HG2	1:F:178:PHE:CE2	2.46	0.51
1:A:102:SER:O	1:A:106:VAL:HG23	2.11	0.51
1:E:230:ASN:O	1:E:233:MET:HG3	2.11	0.51
1:B:174:MET:HG2	1:B:178:PHE:CE2	2.46	0.51
1:E:174:MET:HG2	1:E:178:PHE:CE2	2.46	0.51
1:D:174:MET:HG2	1:D:178:PHE:CE2	2.46	0.50
1:C:174:MET:HG2	1:C:178:PHE:CE2	2.46	0.50
1:D:95:PRO:O	1:D:99:ARG:HG3	2.12	0.50
1:G:230:ASN:O	1:G:233:MET:HG3	2.12	0.50
1:C:218:GLN:NE2	3:C:401:HOH:O	2.06	0.50
1:F:20:PHE:HB3	1:F:27:VAL:HG22	1.93	0.50
1:G:93:GLY:O	1:G:168:LEU:HD11	2.12	0.50
1:D:20:PHE:HB3	1:D:27:VAL:HG22	1.92	0.50
1:F:102:SER:O	1:F:106:VAL:HG23	2.12	0.50
1:D:93:GLY:O	1:D:168:LEU:HD11	2.10	0.50
1:D:130:LEU:HD23	1:D:131:VAL:N	2.27	0.50
1:H:174:MET:HG2	1:H:178:PHE:CE2	2.47	0.50
1:C:102:SER:O	1:C:106:VAL:HG23	2.12	0.50
1:F:93:GLY:O	1:F:168:LEU:HD11	2.12	0.50
1:H:95:PRO:O	1:H:99:ARG:HG3	2.12	0.50
1:A:20:PHE:HB3	1:A:27:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:HB1	1:B:151:ALA:HB2	1.94	0.49
1:B:233:MET:HE2	1:B:233:MET:C	2.37	0.49
1:D:102:SER:O	1:D:106:VAL:HG23	2.12	0.49
1:B:230:ASN:O	1:B:233:MET:HG3	2.12	0.49
1:D:241:ILE:HG13	1:E:168:LEU:HD22	1.94	0.49
1:D:262:MET:HG3	1:D:278:LEU:HD21	1.93	0.49
1:G:20:PHE:HB3	1:G:27:VAL:CG2	2.42	0.49
1:G:20:PHE:HB3	1:G:27:VAL:HG22	1.93	0.49
1:H:102:SER:O	1:H:106:VAL:HG23	2.13	0.49
1:H:230:ASN:O	1:H:233:MET:HG3	2.13	0.49
1:A:95:PRO:O	1:A:99:ARG:HG3	2.13	0.49
1:F:95:PRO:O	1:F:99:ARG:HG3	2.12	0.49
1:A:78:ALA:O	1:A:80:ASP:N	2.40	0.49
1:E:90:LEU:HB3	1:E:117:ILE:HD11	1.95	0.49
1:F:204:TRP:HE1	1:G:174:MET:HB2	1.78	0.49
1:E:226:SER:HA	3:E:406:HOH:O	2.13	0.49
1:F:129:ALA:HB1	1:F:151:ALA:HB2	1.95	0.49
1:G:129:ALA:HB1	1:G:151:ALA:HB2	1.95	0.49
1:G:6:ILE:HD12	1:G:17:ALA:HB2	1.95	0.49
1:G:95:PRO:O	1:G:99:ARG:HG3	2.12	0.49
1:C:230:ASN:O	1:C:233:MET:HG3	2.13	0.49
1:A:20:PHE:HB3	1:A:27:VAL:CG2	2.43	0.48
1:C:95:PRO:O	1:C:99:ARG:HG3	2.13	0.48
1:D:146:ASP:O	1:D:149:VAL:HG22	2.13	0.48
1:E:129:ALA:HB1	1:E:151:ALA:HB2	1.94	0.48
1:E:238:ILE:N	1:E:238:ILE:HD12	2.27	0.48
1:E:235:LEU:HD12	1:E:266:VAL:HG11	1.94	0.48
1:F:88:ILE:CD1	1:F:113:VAL:HG13	2.43	0.48
1:F:146:ASP:O	1:F:149:VAL:HG22	2.14	0.48
1:H:92:ASN:OD1	1:H:92:ASN:C	2.56	0.48
1:A:159:ASP:HB3	1:A:162:THR:OG1	2.14	0.48
1:B:211:TYR:CD2	1:B:215:MET:HE3	2.49	0.48
1:C:92:ASN:OD1	1:C:92:ASN:C	2.56	0.48
1:D:129:ALA:HB1	1:D:151:ALA:HB2	1.95	0.48
1:E:233:MET:HE2	1:E:233:MET:C	2.39	0.48
1:F:176:GLY:O	1:F:179:SER:OG	2.32	0.48
1:D:92:ASN:OD1	1:D:92:ASN:C	2.56	0.48
1:H:176:GLY:O	1:H:179:SER:OG	2.31	0.48
1:E:93:GLY:O	1:E:168:LEU:HD11	2.13	0.48
1:F:146:ASP:OD1	1:F:146:ASP:N	2.42	0.48
1:A:93:GLY:O	1:A:168:LEU:HD11	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:O	1:A:149:VAL:HG22	2.14	0.48
1:C:123:MET:O	1:C:126:SER:OG	2.32	0.48
1:C:176:GLY:O	1:C:179:SER:OG	2.32	0.48
1:E:92:ASN:OD1	1:E:92:ASN:C	2.56	0.48
1:A:32[B]:ARG:HA	1:A:32[B]:ARG:NE	2.29	0.48
1:A:130:LEU:HD23	1:A:131:VAL:N	2.29	0.48
1:F:20:PHE:HB3	1:F:27:VAL:CG2	2.44	0.48
1:A:230:ASN:O	1:A:233:MET:HG3	2.14	0.48
1:B:176:GLY:O	1:B:179:SER:OG	2.31	0.48
1:C:129:ALA:HB1	1:C:151:ALA:HB2	1.96	0.48
1:C:185:THR:O	1:C:188:VAL:HG12	2.14	0.47
1:D:175:TYR:CB	1:E:255:ILE:HD11	2.44	0.47
1:G:92:ASN:OD1	1:G:92:ASN:C	2.57	0.47
1:A:173:GLY:HA2	1:B:180:GLY:HA3	1.97	0.47
1:B:92:ASN:OD1	1:B:92:ASN:C	2.57	0.47
1:G:176:GLY:O	1:G:179:SER:OG	2.32	0.47
1:A:92:ASN:C	1:A:92:ASN:OD1	2.57	0.47
1:D:159:ASP:HB3	1:D:162:THR:OG1	2.14	0.47
1:D:20:PHE:HB3	1:D:27:VAL:CG2	2.44	0.47
1:D:176:GLY:O	1:D:179:SER:OG	2.33	0.47
1:H:129:ALA:HB1	1:H:151:ALA:HB2	1.97	0.47
1:H:146:ASP:O	1:H:149:VAL:HG22	2.14	0.47
1:B:6:ILE:HD12	1:B:17:ALA:HB2	1.96	0.47
1:D:175:TYR:HB3	1:E:255:ILE:HD11	1.96	0.47
1:F:92:ASN:C	1:F:92:ASN:OD1	2.57	0.47
1:F:159:ASP:HB3	1:F:162:THR:OG1	2.15	0.47
1:F:185:THR:CG2	1:F:189:ARG:NH2	2.78	0.47
1:G:233:MET:HE2	1:G:233:MET:C	2.39	0.47
1:G:238:ILE:N	1:G:238:ILE:HD12	2.29	0.47
1:H:32:ARG:HB3	2:H:1001:NAP:O3X	2.15	0.47
1:H:159:ASP:HB3	1:H:162:THR:OG1	2.15	0.47
1:H:174:MET:O	1:H:177:LEU:HB3	2.15	0.47
1:E:176:GLY:O	1:E:179:SER:OG	2.32	0.47
1:H:235:LEU:CD2	1:H:262:MET:HB3	2.45	0.47
1:C:88:ILE:HD13	1:C:113:VAL:HG13	1.97	0.47
1:E:234:GLN:O	1:E:238:ILE:CD1	2.63	0.47
1:E:230:ASN:C	3:E:401:HOH:O	2.58	0.46
1:F:174:MET:O	1:F:177:LEU:HB3	2.15	0.46
1:D:208:MET:CG	1:E:174:MET:HG3	2.45	0.46
1:F:258:MET:HE2	1:G:179:SER:HB3	1.95	0.46
1:A:176:GLY:O	1:A:179:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:MET:O	1:C:177:LEU:HB3	2.15	0.46
1:E:185:THR:O	1:E:188:VAL:HG12	2.15	0.46
2:F:301:NAP:O2D	1:G:233:MET:HE1	2.15	0.46
1:E:174:MET:O	1:E:177:LEU:HB3	2.16	0.46
1:F:265:ALA:HB2	3:F:406:HOH:O	2.15	0.46
1:G:235:LEU:HD23	1:G:262:MET:HE3	1.97	0.46
1:A:31:ASN:ND2	1:A:37:ALA:HB3	2.31	0.46
1:F:86:THR:HG23	1:F:139:ALA:HB1	1.97	0.46
1:G:174:MET:O	1:G:177:LEU:HB3	2.16	0.46
1:G:185:THR:O	1:G:188:VAL:HG12	2.15	0.46
1:B:185:THR:O	1:B:188:VAL:HG12	2.15	0.46
1:A:86:THR:HG23	1:A:139:ALA:HB1	1.98	0.46
1:B:159:ASP:HB3	1:B:162:THR:OG1	2.15	0.46
1:D:65:LEU:O	2:D:301:NAP:C3D	2.64	0.46
1:D:130:LEU:HD21	1:D:154:VAL:CG2	2.46	0.46
1:C:159:ASP:HB3	1:C:162:THR:OG1	2.16	0.45
1:C:230:ASN:ND2	1:C:233:MET:H	2.15	0.45
1:D:174:MET:O	1:D:177:LEU:HB3	2.15	0.45
1:F:79:LEU:C	1:F:81:HIS:N	2.73	0.45
1:H:88:ILE:CD1	1:H:113:VAL:HG13	2.46	0.45
1:A:174:MET:O	1:A:177:LEU:HB3	2.16	0.45
1:C:235:LEU:HD12	1:C:266:VAL:HG11	1.97	0.45
1:E:102:SER:O	1:E:106:VAL:HG22	2.15	0.45
1:F:31:ASN:ND2	1:F:37:ALA:HB3	2.31	0.45
1:F:70:ALA:HB1	2:F:301:NAP:C2A	2.46	0.45
1:G:159:ASP:HB3	1:G:162:THR:OG1	2.16	0.45
1:A:88:ILE:CD1	1:A:113:VAL:HG13	2.46	0.45
1:H:185:THR:O	1:H:188:VAL:HG12	2.16	0.45
1:A:173:GLY:HA2	1:B:180:GLY:CA	2.46	0.45
1:F:202:VAL:N	1:F:203:PRO:HD2	2.32	0.45
1:F:230:ASN:ND2	1:F:233:MET:H	2.15	0.45
1:G:225:THR:CB	1:H:225:THR:CB	2.94	0.45
1:G:230:ASN:ND2	1:G:233:MET:H	2.15	0.45
1:G:235:LEU:HD12	1:G:266:VAL:HG11	1.98	0.45
1:F:265:ALA:CB	3:F:406:HOH:O	2.63	0.45
1:B:174:MET:O	1:B:177:LEU:HB3	2.16	0.45
1:D:87:ILE:HD12	1:D:110:ALA:HB1	1.97	0.45
1:D:230:ASN:ND2	1:D:233:MET:H	2.15	0.45
1:F:52:VAL:HG23	3:F:410:HOH:O	2.17	0.45
1:G:10:GLY:HA3	2:G:301:NAP:O1A	2.17	0.45
1:A:160:ALA:CB	3:A:1105:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:ND2	1:A:233:MET:H	2.15	0.45
1:E:12:MET:HG2	1:E:117:ILE:HD12	1.98	0.45
1:E:230:ASN:ND2	1:E:233:MET:H	2.15	0.45
1:A:55:ILE:HD11	1:A:75:LEU:HD21	1.99	0.45
1:B:230:ASN:ND2	1:B:233:MET:H	2.15	0.45
1:H:230:ASN:ND2	1:H:233:MET:H	2.15	0.45
1:B:266:VAL:HG21	3:B:413:HOH:O	2.16	0.45
1:E:202:VAL:N	1:E:203:PRO:HD2	2.32	0.45
1:F:143:ALA:O	1:F:147:LEU:HD12	2.17	0.45
1:H:86:THR:HG23	1:H:139:ALA:HB1	1.99	0.45
1:D:55:ILE:HD11	1:D:75:LEU:CD2	2.47	0.44
1:A:165:LEU:HD11	1:B:187:LEU:O	2.17	0.44
1:C:202:VAL:N	1:C:203:PRO:HD2	2.32	0.44
1:D:143:ALA:O	1:D:147:LEU:HD12	2.17	0.44
1:D:68:ASN:ND2	1:D:89:ASN:HD21	2.16	0.44
1:B:202:VAL:N	1:B:203:PRO:HD2	2.33	0.44
1:F:131:VAL:HG23	1:F:151:ALA:HB3	2.00	0.44
1:F:173:GLY:HA2	1:G:180:GLY:CA	2.47	0.44
1:H:202:VAL:N	1:H:203:PRO:HD2	2.33	0.44
1:D:88:ILE:CD1	1:D:113:VAL:HG13	2.47	0.44
1:D:86:THR:HG23	1:D:139:ALA:HB1	1.98	0.44
1:D:202:VAL:N	1:D:203:PRO:HD2	2.33	0.44
1:G:234:GLN:O	1:G:238:ILE:CD1	2.65	0.44
1:H:68:ASN:ND2	1:H:89:ASN:HD21	2.16	0.44
1:A:131:VAL:HG23	1:A:151:ALA:HB3	2.00	0.43
1:H:2:SER:HB3	1:H:25:TYR:CE2	2.53	0.43
1:A:202:VAL:N	1:A:203:PRO:HD2	2.33	0.43
1:F:101:LEU:HD12	1:F:101:LEU:HA	1.88	0.43
1:H:92:ASN:HB3	2:H:1001:NAP:O2D	2.18	0.43
1:C:235:LEU:HD23	1:C:262:MET:HE3	2.00	0.43
1:D:185:THR:O	1:D:188:VAL:HG12	2.17	0.43
1:D:195:VAL:HG23	1:E:220:ASP:OD2	2.18	0.43
1:D:40:LEU:N	1:D:40:LEU:CD1	2.82	0.43
1:H:156:LEU:N	1:H:156:LEU:CD2	2.82	0.43
1:B:131:VAL:HG23	1:B:151:ALA:HB3	2.00	0.43
1:H:72:GLU:HB3	1:H:104:ARG:NH1	2.34	0.43
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.89	0.43
1:D:275:ILE:HD13	1:D:275:ILE:O	2.19	0.43
1:E:131:VAL:HG23	1:E:151:ALA:HB3	2.00	0.43
1:D:262:MET:O	1:D:266:VAL:HG13	2.19	0.43
1:F:118:MET:HE3	1:G:204:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:THR:HG22	1:F:189:ARG:NH2	2.33	0.43
1:F:209:THR:O	1:F:212:THR:OG1	2.36	0.43
1:F:279:ILE:O	1:F:282:VAL:HG22	2.19	0.43
1:H:72:GLU:HG2	1:H:104:ARG:NH2	2.34	0.43
1:A:88:ILE:HD13	1:A:113:VAL:HG13	2.01	0.43
1:F:68:ASN:ND2	1:F:89:ASN:HD21	2.17	0.43
1:F:265:ALA:HA	3:F:406:HOH:O	2.18	0.43
1:A:241:ILE:HG13	1:B:168:LEU:HD22	2.01	0.43
1:B:235:LEU:HD23	1:B:262:MET:HE3	2.01	0.43
1:C:88:ILE:CD1	1:C:113:VAL:HG13	2.49	0.43
1:F:88:ILE:HD13	1:F:113:VAL:HG13	2.00	0.42
1:G:68:ASN:ND2	1:G:89:ASN:HD21	2.17	0.42
1:A:174:MET:CG	1:A:178:PHE:CE2	3.02	0.42
1:A:262:MET:O	1:A:266:VAL:HG13	2.20	0.42
1:D:174:MET:CG	1:D:178:PHE:CE2	3.02	0.42
1:E:211:TYR:CE1	1:E:215:MET:CE	3.01	0.42
1:F:32:ARG:HB3	2:F:301:NAP:O3X	2.19	0.42
1:F:156:LEU:N	1:F:156:LEU:CD2	2.82	0.42
1:A:131:VAL:HB	1:A:133:TYR:CE1	2.54	0.42
1:A:209:THR:O	1:A:212:THR:OG1	2.37	0.42
1:D:65:LEU:HD22	2:D:301:NAP:N3A	2.34	0.42
1:G:202:VAL:N	1:G:203:PRO:HD2	2.34	0.42
1:G:209:THR:O	1:G:212:THR:OG1	2.37	0.42
1:A:130:LEU:HD21	1:A:154:VAL:CG2	2.49	0.42
1:C:68:ASN:ND2	1:C:89:ASN:HD21	2.17	0.42
1:D:2:SER:HB3	1:D:25:TYR:CE1	2.55	0.42
1:E:10:GLY:HA3	2:E:301:NAP:O1A	2.19	0.42
1:E:279:ILE:O	1:E:282:VAL:HG22	2.19	0.42
1:H:235:LEU:HD13	1:H:235:LEU:HA	1.82	0.42
1:A:185:THR:O	1:A:188:VAL:HG12	2.19	0.42
1:B:11:ALA:N	2:B:301:NAP:O2N	2.52	0.42
1:H:279:ILE:O	1:H:282:VAL:HG22	2.20	0.42
1:A:275:ILE:HD13	1:A:275:ILE:O	2.20	0.42
1:B:32:ARG:CB	2:B:301:NAP:O1X	2.67	0.42
1:D:156:LEU:CD2	1:D:156:LEU:N	2.82	0.42
1:D:10:GLY:HA3	2:D:301:NAP:O1A	2.20	0.42
1:H:55:ILE:HD11	1:H:75:LEU:CD2	2.50	0.42
1:C:68:ASN:HD22	1:C:89:ASN:HD21	1.68	0.42
1:E:238:ILE:HD12	1:E:238:ILE:H	1.84	0.42
1:F:36:LYS:O	1:F:37:ALA:C	2.62	0.42
1:H:131:VAL:HG23	1:H:151:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:N	1:A:156:LEU:CD2	2.82	0.42
1:C:131:VAL:HG23	1:C:151:ALA:HB3	2.01	0.42
1:E:90:LEU:HD12	1:E:117:ILE:CG1	2.38	0.42
1:A:68:ASN:ND2	1:A:89:ASN:HD21	2.18	0.41
1:A:279:ILE:O	1:A:282:VAL:HG22	2.19	0.41
1:C:219:ILE:HD13	1:C:279:ILE:HD13	2.01	0.41
1:E:127:PRO:HG3	3:E:412:HOH:O	2.19	0.41
1:E:209:THR:O	1:E:212:THR:OG1	2.37	0.41
1:F:131:VAL:HB	1:F:133:TYR:CE1	2.55	0.41
1:G:143:ALA:O	1:G:147:LEU:HD12	2.20	0.41
1:A:31:ASN:ND2	2:A:1000:NAP:O2X	2.41	0.41
2:D:301:NAP:O2D	1:E:233:MET:CE	2.67	0.41
1:E:275:ILE:O	1:E:275:ILE:HD13	2.20	0.41
1:A:32[B]:ARG:NE	1:A:32[B]:ARG:CA	2.83	0.41
1:B:209:THR:O	1:B:212:THR:OG1	2.38	0.41
1:D:209:THR:O	1:D:212:THR:OG1	2.38	0.41
1:E:92:ASN:HB3	2:E:301:NAP:O2D	2.19	0.41
1:G:131:VAL:HG23	1:G:151:ALA:HB3	2.01	0.41
1:B:156:LEU:N	1:B:156:LEU:CD2	2.83	0.41
1:B:262:MET:O	1:B:266:VAL:HG13	2.21	0.41
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.88	0.41
1:E:156:LEU:N	1:E:156:LEU:CD2	2.83	0.41
1:E:262:MET:O	1:E:266:VAL:HG13	2.21	0.41
1:E:68:ASN:ND2	1:E:89:ASN:HD21	2.17	0.41
1:E:174:MET:CG	1:E:178:PHE:CE2	3.04	0.41
1:G:233:MET:HE3	1:G:233:MET:HB2	1.97	0.41
1:H:174:MET:CG	1:H:178:PHE:CE2	3.04	0.41
1:H:262:MET:O	1:H:266:VAL:HG13	2.20	0.41
1:A:143:ALA:O	1:A:147:LEU:HD12	2.19	0.41
1:C:131:VAL:HB	1:C:133:TYR:CE1	2.56	0.41
1:E:68:ASN:HD22	1:E:89:ASN:HD21	1.68	0.41
1:G:156:LEU:N	1:G:156:LEU:CD2	2.83	0.41
1:F:235:LEU:HD23	1:F:262:MET:HE3	2.01	0.41
1:A:36:LYS:O	1:A:37:ALA:C	2.64	0.41
1:G:174:MET:CG	1:G:178:PHE:CE2	3.04	0.41
1:A:123:MET:O	1:A:129:ALA:HB2	2.20	0.41
1:B:275:ILE:HD13	1:B:275:ILE:O	2.21	0.41
1:D:131:VAL:HG23	1:D:151:ALA:HB3	2.02	0.41
1:D:279:ILE:O	1:D:282:VAL:HG22	2.21	0.41
1:E:116:GLY:C	1:E:118:MET:HE2	2.45	0.41
1:E:131:VAL:HB	1:E:133:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:LEU:HD23	1:E:262:MET:HE3	2.03	0.41
1:H:209:THR:O	1:H:212:THR:OG1	2.39	0.41
1:C:156:LEU:N	1:C:156:LEU:CD2	2.83	0.41
1:D:40:LEU:HD13	1:D:40:LEU:H	1.86	0.41
1:F:174:MET:CG	1:F:178:PHE:CE2	3.03	0.41
1:G:131:VAL:HB	1:G:133:TYR:CE1	2.56	0.41
1:C:279:ILE:O	1:C:282:VAL:HG22	2.22	0.40
1:F:87:ILE:HD12	1:F:110:ALA:CB	2.51	0.40
1:H:131:VAL:HB	1:H:133:TYR:CE1	2.56	0.40
1:C:129:ALA:C	1:C:151:ALA:HB1	2.47	0.40
1:E:117:ILE:HB	2:E:301:NAP:H5N	2.03	0.40
1:F:129:ALA:C	1:F:151:ALA:HB1	2.46	0.40
1:H:88:ILE:HD13	1:H:113:VAL:HG13	2.03	0.40
1:D:88:ILE:HD13	1:D:113:VAL:HG13	2.03	0.40
1:G:68:ASN:HD22	1:G:89:ASN:HD21	1.70	0.40
1:A:87:ILE:HD12	1:A:110:ALA:CB	2.52	0.40
1:D:123:MET:O	1:D:129:ALA:HB2	2.21	0.40
1:F:68:ASN:HD22	1:F:89:ASN:HD21	1.69	0.40
1:G:129:ALA:C	1:G:151:ALA:HB1	2.47	0.40
1:G:262:MET:O	1:G:266:VAL:HG13	2.21	0.40
1:B:174:MET:CG	1:B:178:PHE:CE2	3.04	0.40
1:G:183:HIS:C	1:G:183:HIS:ND1	2.80	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	278/285 (98%)	244 (88%)	26 (9%)	8 (3%)	3	11
1	B	248/285 (87%)	220 (89%)	22 (9%)	6 (2%)	4	15
1	C	261/285 (92%)	233 (89%)	23 (9%)	5 (2%)	6	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	272/285 (95%)	245 (90%)	20 (7%)	7 (3%)	4	13
1	E	256/285 (90%)	229 (90%)	22 (9%)	5 (2%)	6	18
1	F	276/285 (97%)	243 (88%)	24 (9%)	9 (3%)	3	9
1	G	273/285 (96%)	243 (89%)	23 (8%)	7 (3%)	4	13
1	H	270/285 (95%)	244 (90%)	19 (7%)	7 (3%)	4	13
All	All	2134/2280 (94%)	1901 (89%)	179 (8%)	54 (2%)	4	14

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	GLU
1	E	40	LEU
1	F	80	ASP
1	G	40	LEU
1	H	40	LEU
1	A	40	LEU
1	C	40	LEU
1	D	40	LEU
1	F	40	LEU
1	H	77	GLY
1	A	36	LYS
1	A	78	ALA
1	B	77	GLY
1	C	76	ALA
1	E	76	ALA
1	F	36	LYS
1	F	78	ALA
1	G	76	ALA
1	A	76	ALA
1	A	154	VAL
1	B	76	ALA
1	B	154	VAL
1	B	223	LYS
1	C	154	VAL
1	D	76	ALA
1	D	154	VAL
1	D	223	LYS
1	E	154	VAL
1	F	76	ALA
1	F	154	VAL

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Mol	Chain	Res	Type
1	F	223	LYS
1	G	36	LYS
1	G	154	VAL
1	G	223	LYS
1	H	76	ALA
1	H	154	VAL
1	H	223	LYS
1	A	79	LEU
1	A	223	LYS
1	C	223	LYS
1	E	223	LYS
1	B	80	ASP
1	E	77	GLY
1	C	77	GLY
1	D	77	GLY
1	D	34	PRO
1	G	77	GLY
1	H	34	PRO
1	A	77	GLY
1	D	222	GLY
1	F	34	PRO
1	F	77	GLY
1	H	222	GLY
1	G	34	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	177/221 (80%)	151 (85%)	26 (15%)	3	9
1	B	116/221 (52%)	98 (84%)	18 (16%)	2	8
1	C	147/221 (66%)	129 (88%)	18 (12%)	5	14
1	D	176/221 (80%)	150 (85%)	26 (15%)	3	9
1	E	125/221 (57%)	107 (86%)	18 (14%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	173/221 (78%)	151 (87%)	22 (13%)	4	13
1	G	142/221 (64%)	123 (87%)	19 (13%)	4	12
1	H	176/221 (80%)	152 (86%)	24 (14%)	3	11
All	All	1232/1768 (70%)	1061 (86%)	171 (14%)	3	11

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	23	GLU
1	A	33	SER
1	A	35	GLU
1	A	40	LEU
1	A	48	SER
1	A	91	THR
1	A	92	ASN
1	A	96	ASP
1	A	97	GLN
1	A	100	LYS
1	A	101	LEU
1	A	113	VAL
1	A	122	SER
1	A	146	ASP
1	A	148	SER
1	A	156	LEU
1	A	164	SER
1	A	172	SER
1	A	179	SER
1	A	189	ARG
1	A	231	LEU
1	A	236	VAL
1	A	238	ILE
1	A	266	VAL
1	A	275	ILE
1	B	6	ILE
1	B	81	HIS
1	B	91	THR
1	B	92	ASN
1	B	96	ASP
1	B	101	LEU
1	B	122	SER

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Mol	Chain	Res	Type
1	B	156	LEU
1	B	172	SER
1	B	179	SER
1	B	231	LEU
1	B	233	MET
1	B	236	VAL
1	B	246[A]	GLU
1	B	246[B]	GLU
1	B	255	ILE
1	B	266	VAL
1	B	275	ILE
1	C	40	LEU
1	C	48	SER
1	C	91	THR
1	C	92	ASN
1	C	97	GLN
1	C	113	VAL
1	C	122	SER
1	C	124	ILE
1	C	126	SER
1	C	156	LEU
1	C	164	SER
1	C	179	SER
1	C	231	LEU
1	C	236	VAL
1	C	255	ILE
1	C	266	VAL
1	C	274	ASP
1	C	275	ILE
1	D	16	LEU
1	D	23	GLU
1	D	33	SER
1	D	35	GLU
1	D	40	LEU
1	D	48	SER
1	D	91	THR
1	D	92	ASN
1	D	97	GLN
1	D	101	LEU
1	D	104	ARG
1	D	113	VAL
1	D	122	SER

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Mol	Chain	Res	Type
1	D	146	ASP
1	D	148	SER
1	D	156	LEU
1	D	164	SER
1	D	172	SER
1	D	179	SER
1	D	208	MET
1	D	231	LEU
1	D	233	MET
1	D	236	VAL
1	D	266	VAL
1	D	274	ASP
1	D	275	ILE
1	E	58	SER
1	E	83	HIS
1	E	90	LEU
1	E	91	THR
1	E	92	ASN
1	E	113	VAL
1	E	117	ILE
1	E	156	LEU
1	E	164	SER
1	E	179	SER
1	E	189	ARG
1	E	215	MET
1	E	231	LEU
1	E	233	MET
1	E	236	VAL
1	E	255	ILE
1	E	266	VAL
1	E	275	ILE
1	F	16	LEU
1	F	23	GLU
1	F	33	SER
1	F	48	SER
1	F	66	LEU
1	F	91	THR
1	F	92	ASN
1	F	97	GLN
1	F	101	LEU
1	F	113	VAL
1	F	122	SER

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Mol	Chain	Res	Type
1	F	146	ASP
1	F	148	SER
1	F	156	LEU
1	F	164	SER
1	F	172	SER
1	F	179	SER
1	F	225	THR
1	F	231	LEU
1	F	236	VAL
1	F	255	ILE
1	F	275	ILE
1	G	6	ILE
1	G	16	LEU
1	G	23	GLU
1	G	48	SER
1	G	92	ASN
1	G	97	GLN
1	G	122	SER
1	G	148	SER
1	G	156	LEU
1	G	164	SER
1	G	172	SER
1	G	179	SER
1	G	219	ILE
1	G	231	LEU
1	G	233	MET
1	G	236	VAL
1	G	255	ILE
1	G	266	VAL
1	G	275	ILE
1	H	16	LEU
1	H	23	GLU
1	H	33	SER
1	H	35	GLU
1	H	40	LEU
1	H	48	SER
1	H	72	GLU
1	H	91	THR
1	H	92	ASN
1	H	97	GLN
1	H	101	LEU
1	H	113	VAL

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Mol	Chain	Res	Type
1	H	122	SER
1	H	146	ASP
1	H	148	SER
1	H	156	LEU
1	H	164	SER
1	H	172	SER
1	H	179	SER
1	H	231	LEU
1	H	235	LEU
1	H	236	VAL
1	H	266	VAL
1	H	274	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	81	HIS
1	A	108	HIS
1	A	218	GLN
1	A	230	ASN
1	B	89	ASN
1	B	218	GLN
1	B	230	ASN
1	B	248	GLN
1	C	56	ASN
1	C	68	ASN
1	C	108	HIS
1	C	114	HIS
1	C	230	ASN
1	D	56	ASN
1	D	68	ASN
1	D	114	HIS
1	D	218	GLN
1	D	230	ASN
1	D	248	GLN
1	E	56	ASN
1	E	68	ASN
1	E	81	HIS
1	E	114	HIS
1	E	218	GLN
1	E	230	ASN

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Mol	Chain	Res	Type
1	E	248	GLN
1	F	56	ASN
1	F	68	ASN
1	F	81	HIS
1	F	108	HIS
1	F	218	GLN
1	F	230	ASN
1	F	240	ASN
1	G	56	ASN
1	G	68	ASN
1	G	89	ASN
1	G	114	HIS
1	G	230	ASN
1	G	248	GLN
1	H	56	ASN
1	H	81	HIS
1	H	89	ASN
1	H	114	HIS
1	H	218	GLN
1	H	230	ASN
1	H	248	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](#)

8 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	NAP	C	301	-	50,52,52	1.22	4 (8%)	71,80,80	1.75	15 (21%)
2	NAP	H	1001	-	50,52,52	1.75	7 (14%)	71,80,80	2.12	19 (26%)
2	NAP	B	301	-	50,52,52	1.49	7 (14%)	71,80,80	1.74	16 (22%)
2	NAP	G	301	-	50,52,52	1.37	6 (12%)	71,80,80	1.78	15 (21%)
2	NAP	F	301	-	50,52,52	1.47	11 (22%)	71,80,80	2.19	23 (32%)
2	NAP	A	1000	-	50,52,52	1.64	9 (18%)	71,80,80	2.06	24 (33%)
2	NAP	D	301	-	50,52,52	1.57	9 (18%)	71,80,80	2.25	22 (30%)
2	NAP	E	301	-	50,52,52	1.30	5 (10%)	71,80,80	1.61	11 (15%)

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	NAP	C	301	-	-	12/35/67/67	0/5/5/5
2	NAP	H	1001	-	-	11/35/67/67	0/5/5/5
2	NAP	B	301	-	-	11/35/67/67	0/5/5/5
2	NAP	G	301	-	-	7/35/67/67	0/5/5/5
2	NAP	F	301	-	-	14/35/67/67	0/5/5/5
2	NAP	A	1000	-	-	7/35/67/67	0/5/5/5
2	NAP	D	301	-	-	2/35/67/67	0/5/5/5
2	NAP	E	301	-	-	14/35/67/67	0/5/5/5

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C5A-C4A	5.81	1.49	1.39
2	H	1001	NAP	C5A-C4A	5.75	1.49	1.39
2	E	301	NAP	C5A-C4A	5.17	1.48	1.39
2	C	301	NAP	C5A-C4A	5.00	1.48	1.39
2	D	301	NAP	C5A-C4A	4.83	1.47	1.39
2	G	301	NAP	C5A-C4A	4.68	1.47	1.39
2	A	1000	NAP	C5A-C4A	4.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	NAP	PN-O3	4.32	1.64	1.59
2	F	301	NAP	C5A-C4A	4.22	1.46	1.39
2	H	1001	NAP	C8A-N7A	4.08	1.39	1.31
2	A	1000	NAP	O4D-C1D	4.06	1.46	1.40
2	F	301	NAP	O4D-C1D	4.04	1.46	1.40
2	D	301	NAP	C5A-C6A	3.95	1.52	1.41
2	H	1001	NAP	C2N-N1N	-3.86	1.30	1.35
2	H	1001	NAP	C5A-C6A	3.82	1.51	1.41
2	D	301	NAP	C8A-N7A	3.81	1.39	1.31
2	B	301	NAP	O4D-C1D	3.70	1.45	1.40
2	H	1001	NAP	O4D-C1D	3.29	1.45	1.40
2	G	301	NAP	C5A-C6A	3.22	1.50	1.41
2	D	301	NAP	C4N-C3N	-3.20	1.34	1.39
2	B	301	NAP	C8A-N7A	3.18	1.37	1.31
2	A	1000	NAP	PA-O3	3.15	1.62	1.59
2	E	301	NAP	C5A-C6A	3.11	1.49	1.41
2	H	1001	NAP	P2B-O2B	3.06	1.64	1.59
2	B	301	NAP	C5A-C6A	3.04	1.49	1.41
2	E	301	NAP	C8A-N7A	2.96	1.37	1.31
2	F	301	NAP	C8A-N7A	2.89	1.37	1.31
2	A	1000	NAP	C2N-N1N	2.89	1.38	1.35
2	H	1001	NAP	C3N-C7N	-2.87	1.46	1.50
2	C	301	NAP	C5A-C6A	2.86	1.49	1.41
2	F	301	NAP	C5A-N7A	-2.79	1.34	1.39
2	E	301	NAP	O4D-C1D	2.70	1.44	1.40
2	B	301	NAP	PN-O3	-2.63	1.56	1.59
2	G	301	NAP	C5A-N7A	-2.59	1.34	1.39
2	A	1000	NAP	C8A-N7A	2.58	1.36	1.31
2	G	301	NAP	P2B-O2B	2.50	1.63	1.59
2	C	301	NAP	C8A-N7A	2.49	1.36	1.31
2	G	301	NAP	C8A-N7A	2.49	1.36	1.31
2	F	301	NAP	C5A-C6A	2.37	1.47	1.41
2	D	301	NAP	O4D-C1D	2.37	1.44	1.40
2	F	301	NAP	O4B-C1B	2.36	1.47	1.42
2	A	1000	NAP	C5A-C6A	2.36	1.47	1.41
2	D	301	NAP	PN-O3	2.33	1.62	1.59
2	A	1000	NAP	PA-O1A	2.30	1.58	1.50
2	C	301	NAP	P2B-O2B	2.25	1.63	1.59
2	B	301	NAP	P2B-O2B	2.21	1.63	1.59
2	F	301	NAP	C6A-N6A	2.19	1.39	1.34
2	F	301	NAP	C7N-N7N	2.18	1.37	1.33
2	A	1000	NAP	C5A-N7A	-2.12	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	PA-O3	2.10	1.61	1.59
2	E	301	NAP	C5A-N7A	-2.10	1.35	1.39
2	F	301	NAP	C4A-N9A	-2.07	1.33	1.37
2	F	301	NAP	C2D-C3D	-2.07	1.47	1.53
2	F	301	NAP	P2B-O1X	2.05	1.56	1.50
2	D	301	NAP	C4A-N9A	-2.05	1.33	1.37
2	D	301	NAP	C6A-N6A	2.02	1.39	1.34
2	B	301	NAP	C5A-N7A	-2.02	1.35	1.39
2	G	301	NAP	PA-O3	2.01	1.61	1.59

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1001	NAP	O4B-C1B-N9A	6.74	121.03	108.09
2	D	301	NAP	O3B-C3B-C4B	-6.43	92.60	111.08
2	E	301	NAP	C5A-C4A-N3A	-6.35	117.98	126.72
2	G	301	NAP	C5A-C4A-N3A	-6.03	118.42	126.72
2	H	1001	NAP	C4D-O4D-C1D	-6.00	104.43	109.92
2	B	301	NAP	C5A-C4A-N3A	-5.91	118.58	126.72
2	C	301	NAP	C5A-C4A-N3A	-5.84	118.68	126.72
2	D	301	NAP	C5A-C4A-N3A	-5.83	118.69	126.72
2	H	1001	NAP	C5A-C4A-N3A	-5.55	119.08	126.72
2	D	301	NAP	O4B-C1B-N9A	5.49	118.63	108.09
2	F	301	NAP	C6N-N1N-C2N	-5.25	117.41	121.88
2	F	301	NAP	C5A-C4A-N3A	-5.07	119.74	126.72
2	E	301	NAP	N3A-C4A-N9A	4.74	135.23	127.17
2	A	1000	NAP	C5A-C4A-N3A	-4.73	120.21	126.72
2	H	1001	NAP	C2B-C1B-N9A	-4.73	105.97	113.75
2	D	301	NAP	C2A-N3A-C4A	4.70	123.31	111.83
2	C	301	NAP	N3A-C4A-N9A	4.64	135.06	127.17
2	F	301	NAP	N3A-C2A-N1A	-4.59	121.63	128.58
2	B	301	NAP	N3A-C4A-N9A	4.58	134.96	127.17
2	F	301	NAP	C4A-C5A-N7A	-4.50	105.44	110.58
2	G	301	NAP	N3A-C4A-N9A	4.41	134.67	127.17
2	A	1000	NAP	N3A-C2A-N1A	-4.40	121.91	128.58
2	H	1001	NAP	C5N-C4N-C3N	-4.38	116.06	120.36
2	D	301	NAP	O3-PN-O1N	-4.34	97.65	110.70
2	A	1000	NAP	O2N-PN-O1N	4.30	132.46	112.44
2	F	301	NAP	P2B-O2B-C2B	-4.23	112.12	123.43
2	H	1001	NAP	C4A-C5A-N7A	-4.23	105.74	110.58
2	F	301	NAP	O4B-C1B-N9A	4.17	116.10	108.09
2	G	301	NAP	C4A-C5A-N7A	-4.12	105.87	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	NAP	O4B-C1B-N9A	4.09	115.95	108.09
2	D	301	NAP	C6N-N1N-C2N	-4.07	118.42	121.88
2	C	301	NAP	C2A-N3A-C4A	4.05	121.72	111.83
2	D	301	NAP	C4A-C5A-N7A	-4.04	105.97	110.58
2	B	301	NAP	C4A-C5A-N7A	-3.98	106.03	110.58
2	A	1000	NAP	O2A-PA-O3	3.98	118.02	107.27
2	A	1000	NAP	N3A-C4A-N9A	3.95	133.88	127.17
2	C	301	NAP	N3A-C2A-N1A	-3.91	122.67	128.58
2	F	301	NAP	C2A-N1A-C6A	3.89	125.12	118.73
2	F	301	NAP	C2A-N3A-C4A	3.86	121.25	111.83
2	E	301	NAP	C4A-C5A-N7A	-3.85	106.19	110.58
2	D	301	NAP	N3A-C2A-N1A	-3.84	122.77	128.58
2	H	1001	NAP	C2A-N3A-C4A	3.84	121.20	111.83
2	A	1000	NAP	O2D-C2D-C3D	-3.80	99.64	111.82
2	G	301	NAP	C2A-N3A-C4A	3.79	121.08	111.83
2	E	301	NAP	C2A-N3A-C4A	3.74	120.97	111.83
2	A	1000	NAP	O4B-C1B-C2B	-3.74	100.15	106.59
2	A	1000	NAP	C2A-N3A-C4A	3.72	120.91	111.83
2	F	301	NAP	C4D-O4D-C1D	-3.71	106.53	109.92
2	F	301	NAP	O3X-P2B-O2X	3.69	121.64	107.80
2	D	301	NAP	C5N-C4N-C3N	-3.65	116.78	120.36
2	D	301	NAP	C5B-C4B-C3B	-3.59	102.30	115.21
2	C	301	NAP	C4A-C5A-N7A	-3.58	106.49	110.58
2	B	301	NAP	C2A-N3A-C4A	3.52	120.43	111.83
2	H	1001	NAP	O3-PA-O1A	-3.40	100.48	110.70
2	G	301	NAP	C5A-N7A-C8A	3.30	108.64	103.45
2	F	301	NAP	C5A-N7A-C8A	3.23	108.53	103.45
2	A	1000	NAP	O5B-PA-O1A	3.21	121.66	108.94
2	A	1000	NAP	P2B-O2B-C2B	-3.21	114.86	123.43
2	B	301	NAP	O2D-C2D-C3D	-3.18	101.62	111.82
2	A	1000	NAP	O3B-C3B-C4B	-3.14	102.07	111.08
2	G	301	NAP	N3A-C2A-N1A	-3.11	123.87	128.58
2	F	301	NAP	C5N-C4N-C3N	-3.11	117.31	120.36
2	D	301	NAP	C6A-C5A-N7A	3.11	138.08	132.09
2	D	301	NAP	O2N-PN-O1N	3.10	126.86	112.44
2	F	301	NAP	O4D-C4D-C3D	3.10	111.30	105.15
2	D	301	NAP	N3A-C4A-N9A	3.09	132.43	127.17
2	B	301	NAP	N3A-C2A-N1A	-3.09	123.90	128.58
2	G	301	NAP	O7N-C7N-N7N	-3.07	118.17	122.62
2	B	301	NAP	C5A-N7A-C8A	3.03	108.21	103.45
2	H	1001	NAP	N3A-C4A-N9A	3.01	132.29	127.17
2	D	301	NAP	O3B-C3B-C2B	3.00	119.58	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1001	NAP	N3A-C2A-N1A	-2.96	124.10	128.58
2	B	301	NAP	O7N-C7N-N7N	-2.95	118.35	122.62
2	C	301	NAP	C5A-N7A-C8A	2.94	108.06	103.45
2	D	301	NAP	O4B-C4B-C5B	2.93	118.72	109.33
2	B	301	NAP	O7N-C7N-C3N	2.92	123.17	119.60
2	A	1000	NAP	O2X-P2B-O2B	-2.92	94.47	105.85
2	E	301	NAP	C6N-N1N-C2N	-2.89	119.42	121.88
2	F	301	NAP	N3A-C4A-N9A	2.86	132.03	127.17
2	B	301	NAP	O4D-C4D-C5D	-2.82	100.31	109.33
2	G	301	NAP	C3N-C7N-N7N	2.81	121.21	117.74
2	D	301	NAP	C5A-C4A-N9A	2.81	108.88	105.81
2	F	301	NAP	C2B-C1B-N9A	-2.81	109.13	113.75
2	A	1000	NAP	O2X-P2B-O1X	2.81	121.77	110.83
2	H	1001	NAP	O7N-C7N-C3N	-2.77	116.22	119.60
2	A	1000	NAP	C4D-O4D-C1D	-2.76	107.40	109.92
2	E	301	NAP	N3A-C2A-N1A	-2.73	124.45	128.58
2	F	301	NAP	C6A-C5A-N7A	2.71	137.32	132.09
2	F	301	NAP	O3B-C3B-C4B	-2.68	103.37	111.08
2	A	1000	NAP	O3X-P2B-O2X	2.66	117.77	107.80
2	E	301	NAP	C5A-N7A-C8A	2.65	107.62	103.45
2	G	301	NAP	O4B-C1B-N9A	2.65	113.17	108.09
2	C	301	NAP	O4D-C4D-C3D	2.63	110.38	105.15
2	C	301	NAP	C6A-C5A-N7A	2.63	137.16	132.09
2	F	301	NAP	O2D-C2D-C3D	-2.59	103.53	111.82
2	A	1000	NAP	C5D-C4D-C3D	-2.59	105.90	115.21
2	H	1001	NAP	C5A-C4A-N9A	2.59	108.63	105.81
2	B	301	NAP	C4A-N9A-C8A	2.57	108.44	105.74
2	A	1000	NAP	N6A-C6A-N1A	2.56	124.07	118.38
2	H	1001	NAP	C6A-C5A-N7A	2.55	137.01	132.09
2	F	301	NAP	O3B-C3B-C2B	-2.55	104.06	111.19
2	C	301	NAP	O3D-C3D-C2D	2.53	119.93	111.82
2	A	1000	NAP	O3-PN-O1N	-2.53	103.11	110.70
2	F	301	NAP	N9A-C8A-N7A	-2.52	110.35	113.94
2	C	301	NAP	O4B-C1B-C2B	-2.52	102.25	106.59
2	H	1001	NAP	O4D-C4D-C3D	2.52	110.16	105.15
2	H	1001	NAP	O5B-C5B-C4B	2.50	117.52	108.99
2	F	301	NAP	O2X-P2B-O2B	-2.50	96.10	105.85
2	G	301	NAP	N9A-C8A-N7A	-2.46	110.44	113.94
2	C	301	NAP	O7N-C7N-N7N	-2.45	119.08	122.62
2	A	1000	NAP	C2A-N1A-C6A	2.44	122.75	118.73
2	E	301	NAP	O4B-C1B-N9A	2.43	112.75	108.09
2	G	301	NAP	C2B-C3B-C4B	2.41	107.17	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	O2A-PA-O3	2.40	113.76	107.27
2	H	1001	NAP	C5A-N7A-C8A	2.39	107.20	103.45
2	C	301	NAP	C4A-N9A-C8A	2.38	108.24	105.74
2	D	301	NAP	O3X-P2B-O2B	-2.38	96.59	105.85
2	D	301	NAP	C6N-C5N-C4N	2.31	122.77	119.45
2	C	301	NAP	C4D-O4D-C1D	-2.30	107.81	109.92
2	G	301	NAP	C4A-N9A-C8A	2.28	108.14	105.74
2	B	301	NAP	P2B-O2B-C2B	-2.26	117.38	123.43
2	E	301	NAP	C6A-C5A-N7A	2.22	136.38	132.09
2	F	301	NAP	C5A-C4A-N9A	2.22	108.23	105.81
2	D	301	NAP	C2B-C1B-N9A	-2.20	110.14	113.75
2	B	301	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
2	G	301	NAP	C6A-C5A-N7A	2.17	136.28	132.09
2	B	301	NAP	N9A-C8A-N7A	-2.17	110.86	113.94
2	D	301	NAP	O2D-C2D-C3D	2.16	118.74	111.82
2	G	301	NAP	O2X-P2B-O1X	2.16	119.24	110.83
2	H	1001	NAP	O2N-PN-O1N	2.15	122.43	112.44
2	G	301	NAP	O4B-C4B-C3B	-2.12	100.94	105.15
2	A	1000	NAP	C4A-N9A-C8A	2.12	107.96	105.74
2	E	301	NAP	O3X-P2B-O2X	2.11	115.73	107.80
2	C	301	NAP	N9A-C8A-N7A	-2.10	110.95	113.94
2	F	301	NAP	O7N-C7N-C3N	-2.10	117.03	119.60
2	D	301	NAP	O3X-P2B-O2X	2.09	115.65	107.80
2	E	301	NAP	C4A-N9A-C8A	2.08	107.92	105.74
2	B	301	NAP	C6A-C5A-N7A	2.08	136.09	132.09
2	B	301	NAP	C3B-C2B-C1B	2.07	106.77	102.81
2	H	1001	NAP	O2N-PN-O3	2.07	112.87	107.27
2	C	301	NAP	C2A-N1A-C6A	2.06	122.12	118.73
2	H	1001	NAP	O7N-C7N-N7N	2.05	125.58	122.62
2	A	1000	NAP	O2B-P2B-O1X	-2.02	102.13	109.33
2	A	1000	NAP	C4A-C5A-N7A	-2.02	108.28	110.58
2	A	1000	NAP	C5A-C6A-N6A	-2.01	118.31	123.29

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	NAP	C5B-O5B-PA-O1A
2	A	1000	NAP	C5B-O5B-PA-O2A
2	A	1000	NAP	C5B-O5B-PA-O3
2	A	1000	NAP	O4D-C1D-N1N-C2N
2	A	1000	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C5B-O5B-PA-O1A
2	B	301	NAP	C5B-O5B-PA-O2A
2	B	301	NAP	C5B-O5B-PA-O3
2	B	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	C5B-O5B-PA-O1A
2	C	301	NAP	C5B-O5B-PA-O3
2	C	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	C3B-C4B-C5B-O5B
2	C	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	O4D-C1D-N1N-C2N
2	D	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	C5B-O5B-PA-O3
2	E	301	NAP	C5D-O5D-PN-O3
2	E	301	NAP	C5D-O5D-PN-O1N
2	E	301	NAP	C5D-O5D-PN-O2N
2	E	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	O4D-C1D-N1N-C6N
2	E	301	NAP	C2D-C1D-N1N-C2N
2	E	301	NAP	C2D-C1D-N1N-C6N
2	F	301	NAP	C5B-O5B-PA-O3
2	F	301	NAP	PN-O3-PA-O5B
2	F	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	C5D-O5D-PN-O3
2	F	301	NAP	O4D-C1D-N1N-C2N
2	G	301	NAP	C5B-O5B-PA-O1A
2	G	301	NAP	C5B-O5B-PA-O2A
2	G	301	NAP	O4D-C1D-N1N-C2N
2	H	1001	NAP	C5B-O5B-PA-O1A
2	H	1001	NAP	C5B-O5B-PA-O2A
2	H	1001	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C4D-C5D-O5D
2	F	301	NAP	C3B-C4B-C5B-O5B
2	A	1000	NAP	O4B-C4B-C5B-O5B
2	A	1000	NAP	C3B-C4B-C5B-O5B
2	H	1001	NAP	C3B-C2B-O2B-P2B
2	E	301	NAP	C3B-C4B-C5B-O5B
2	E	301	NAP	O4B-C4B-C5B-O5B
2	H	1001	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	C3B-C4B-C5B-O5B
2	G	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	H	1001	NAP	C1B-C2B-O2B-P2B
2	F	301	NAP	O4D-C4D-C5D-O5D
2	E	301	NAP	PN-O3-PA-O5B
2	B	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O1N
2	E	301	NAP	C5B-O5B-PA-O1A
2	F	301	NAP	C5B-O5B-PA-O1A
2	F	301	NAP	C5D-O5D-PN-O1N
2	G	301	NAP	C5B-O5B-PA-O3
2	H	1001	NAP	C5B-O5B-PA-O3
2	B	301	NAP	PA-O3-PN-O2N
2	C	301	NAP	PA-O3-PN-O2N
2	F	301	NAP	PA-O3-PN-O2N
2	H	1001	NAP	C3B-C4B-C5B-O5B
2	C	301	NAP	C2B-O2B-P2B-O3X
2	F	301	NAP	C3B-C2B-O2B-P2B
2	B	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	O4D-C1D-N1N-C6N
2	D	301	NAP	O4D-C1D-N1N-C6N
2	F	301	NAP	O4D-C1D-N1N-C6N
2	H	1001	NAP	O4D-C1D-N1N-C6N
2	E	301	NAP	PA-O3-PN-O2N
2	G	301	NAP	O4D-C4D-C5D-O5D
2	C	301	NAP	PA-O3-PN-O1N
2	F	301	NAP	PA-O3-PN-O1N
2	H	1001	NAP	C2B-O2B-P2B-O3X
2	F	301	NAP	C1B-C2B-O2B-P2B
2	E	301	NAP	PA-O3-PN-O1N
2	G	301	NAP	PN-O3-PA-O2A
2	H	1001	NAP	PN-O3-PA-O2A

There are no ring outliers.

8 monomers are involved in 28 short contacts:

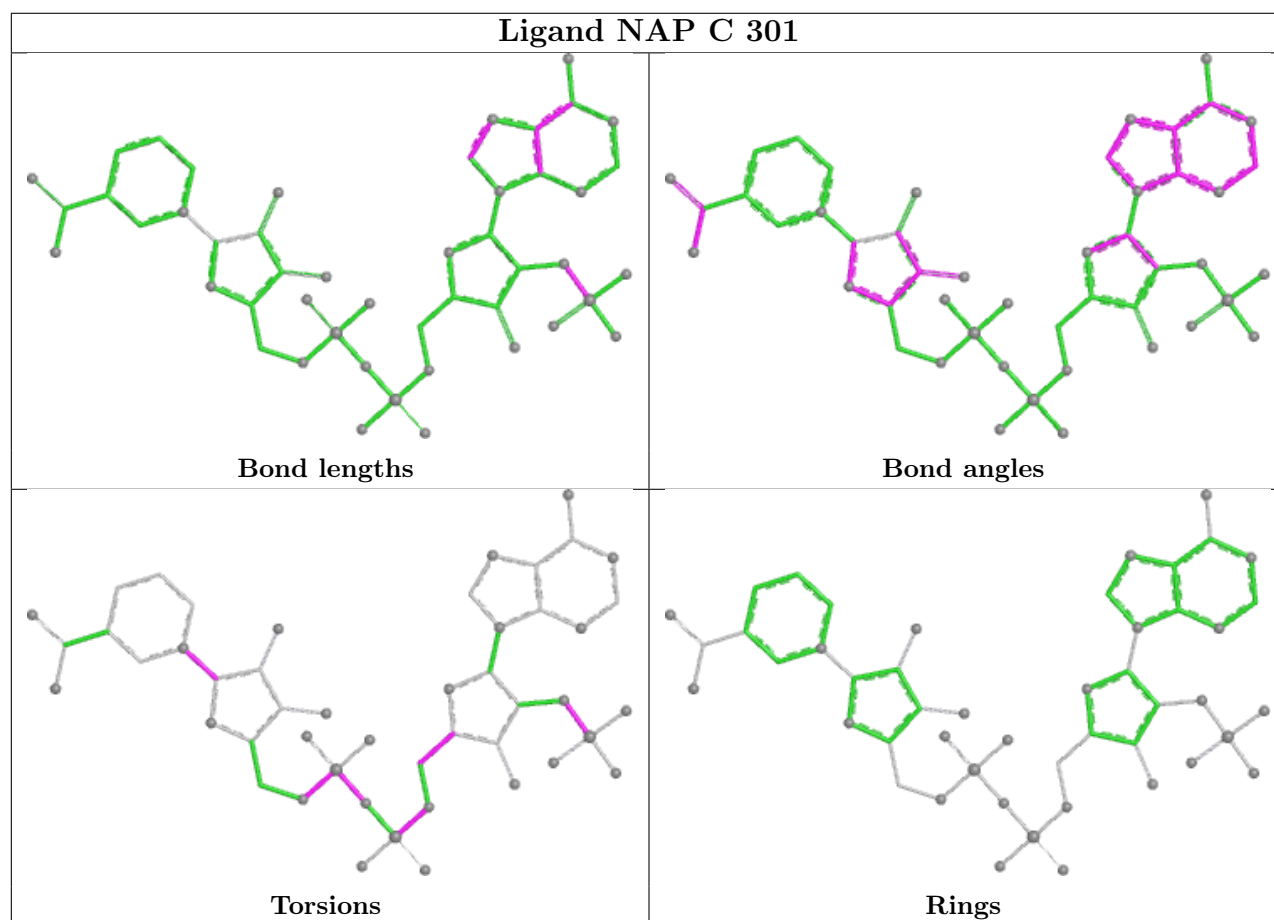
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NAP	1	0
2	H	1001	NAP	2	0
2	B	301	NAP	3	0
2	G	301	NAP	4	0
2	F	301	NAP	5	0
2	A	1000	NAP	4	0

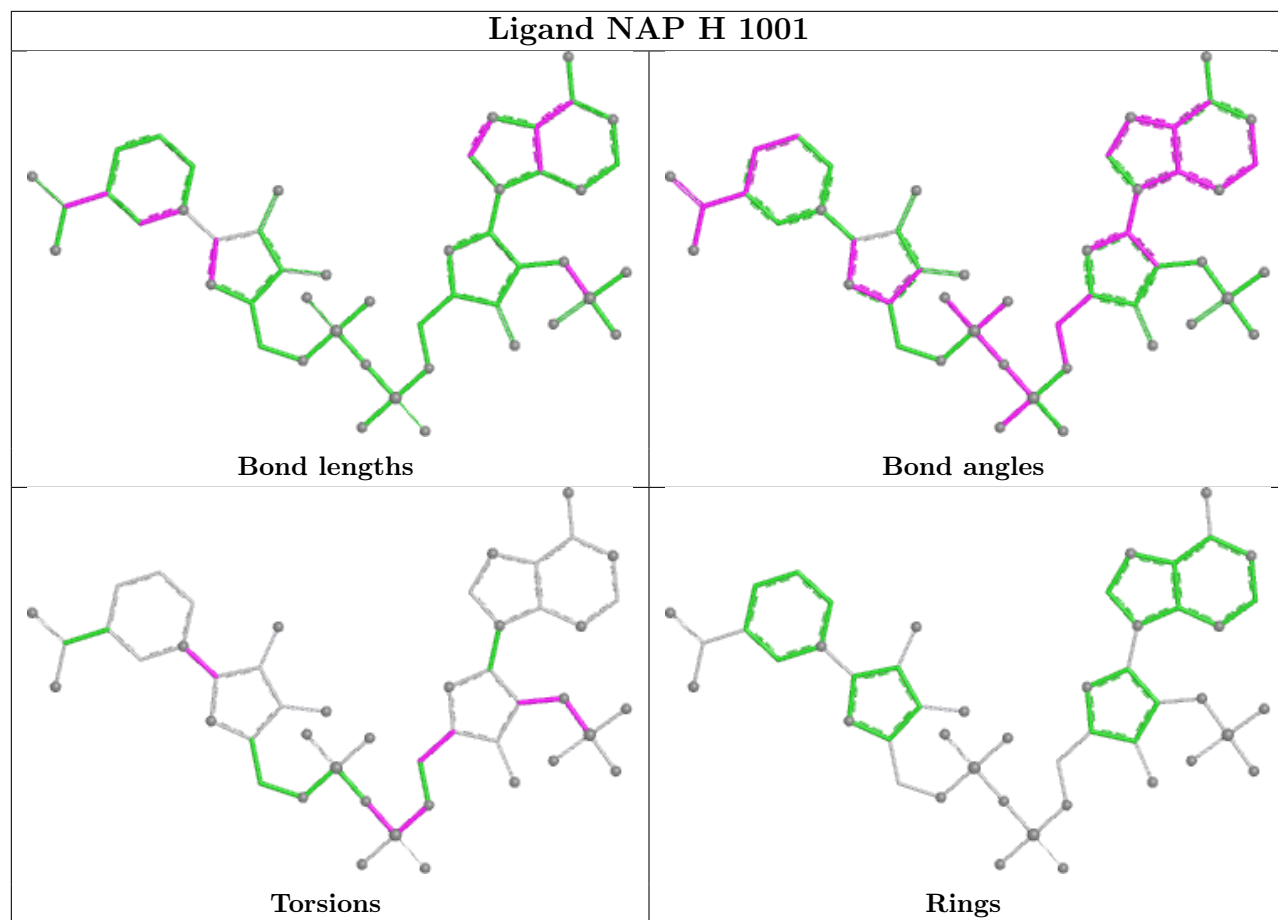
Continued on next page...

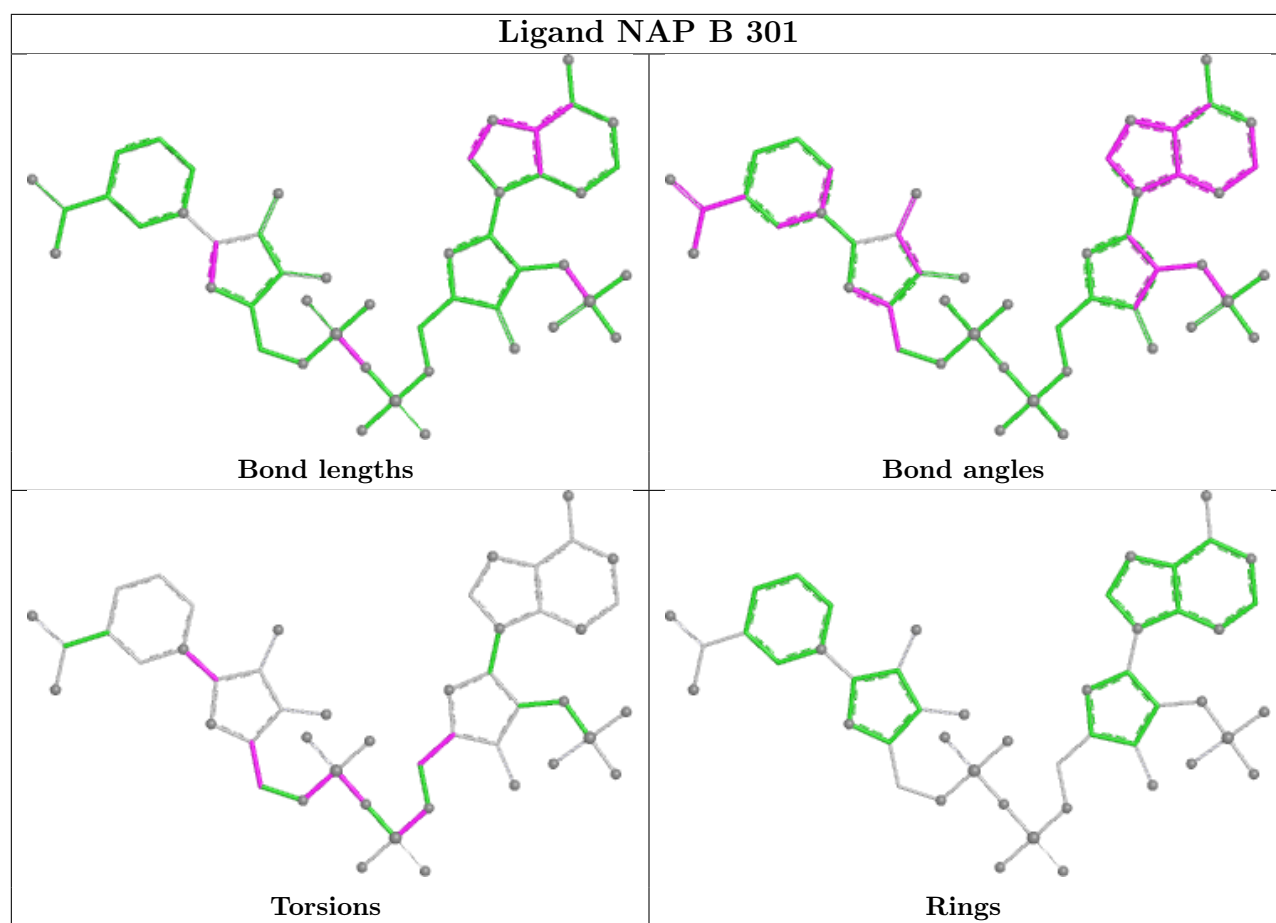
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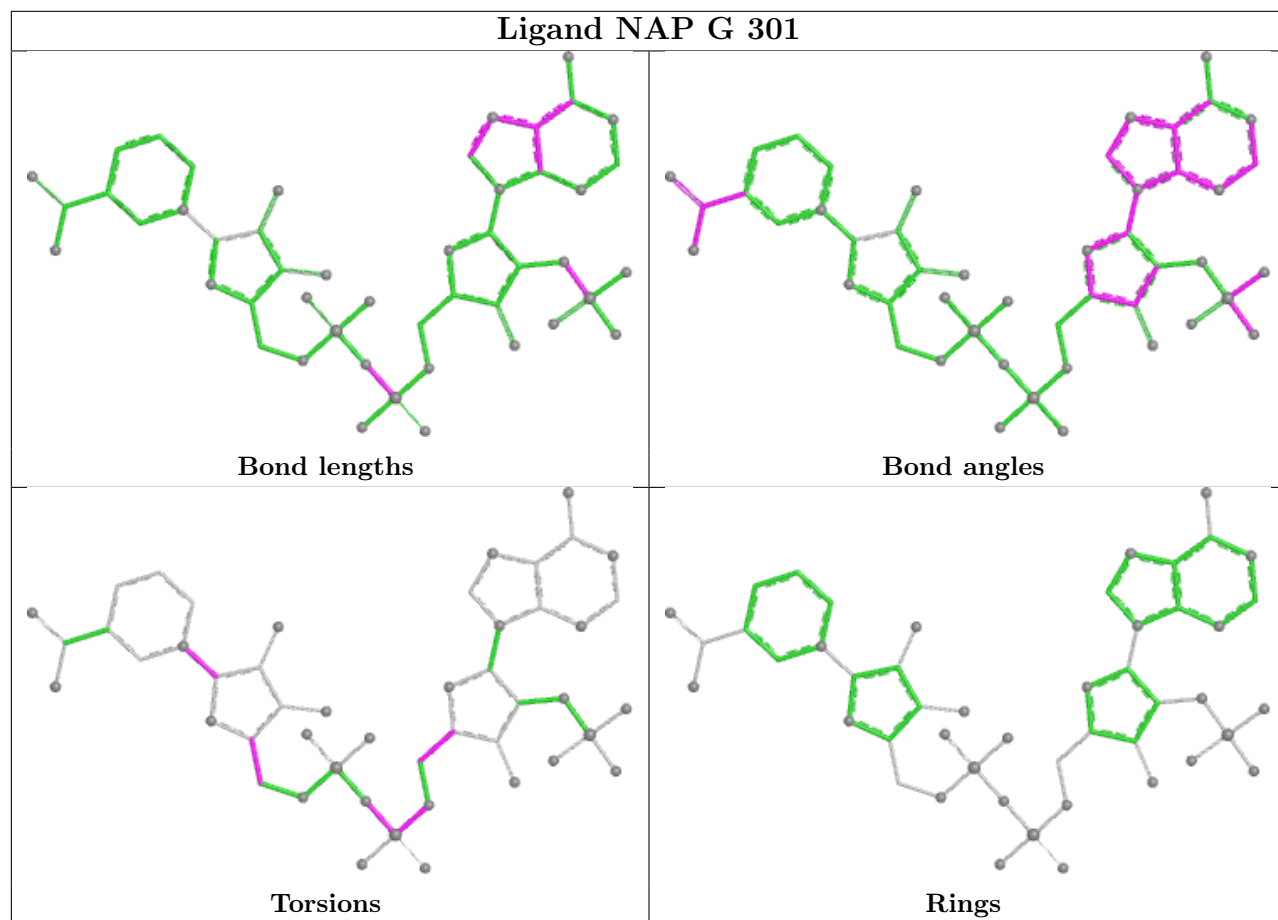
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	NAP	5	0
2	E	301	NAP	4	0

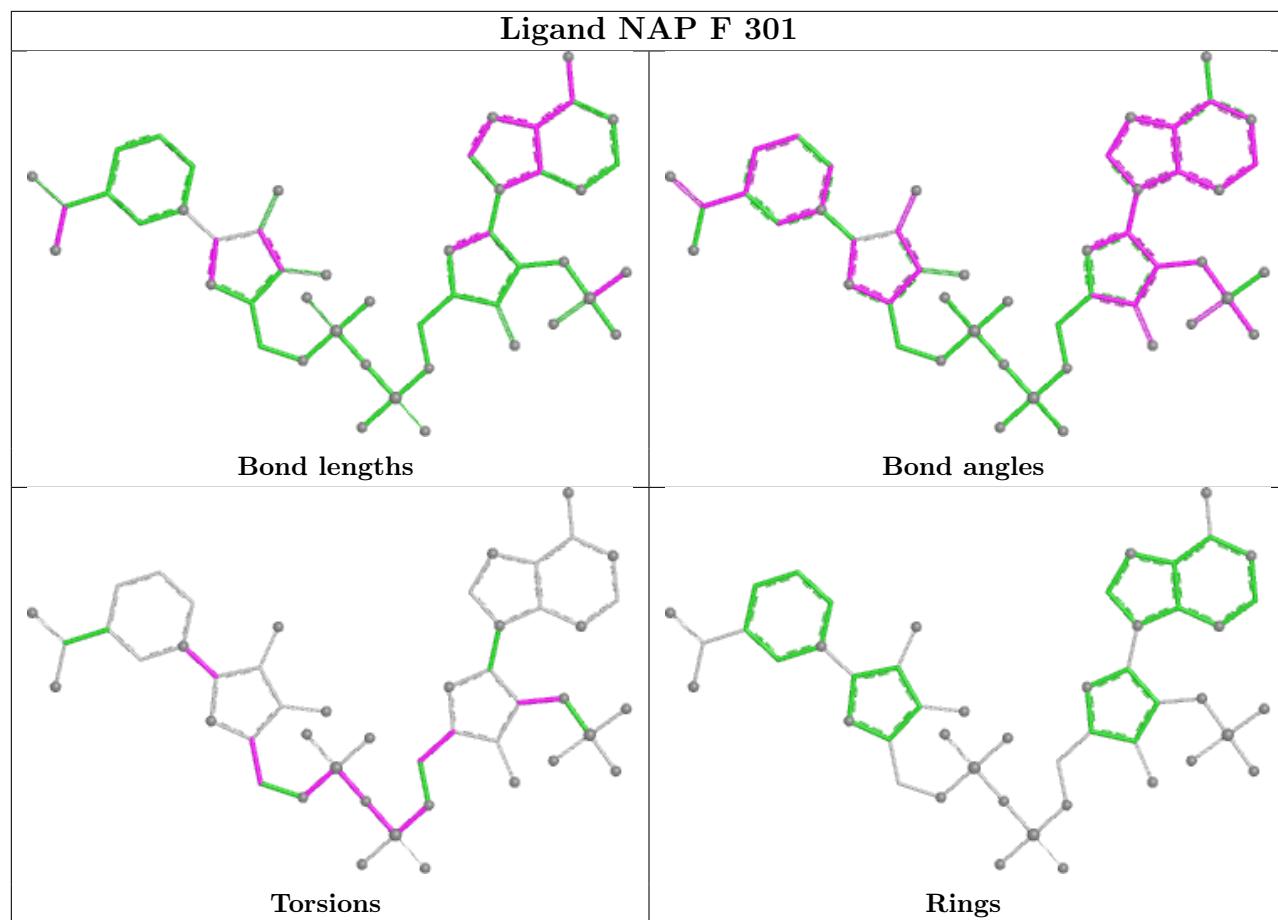
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

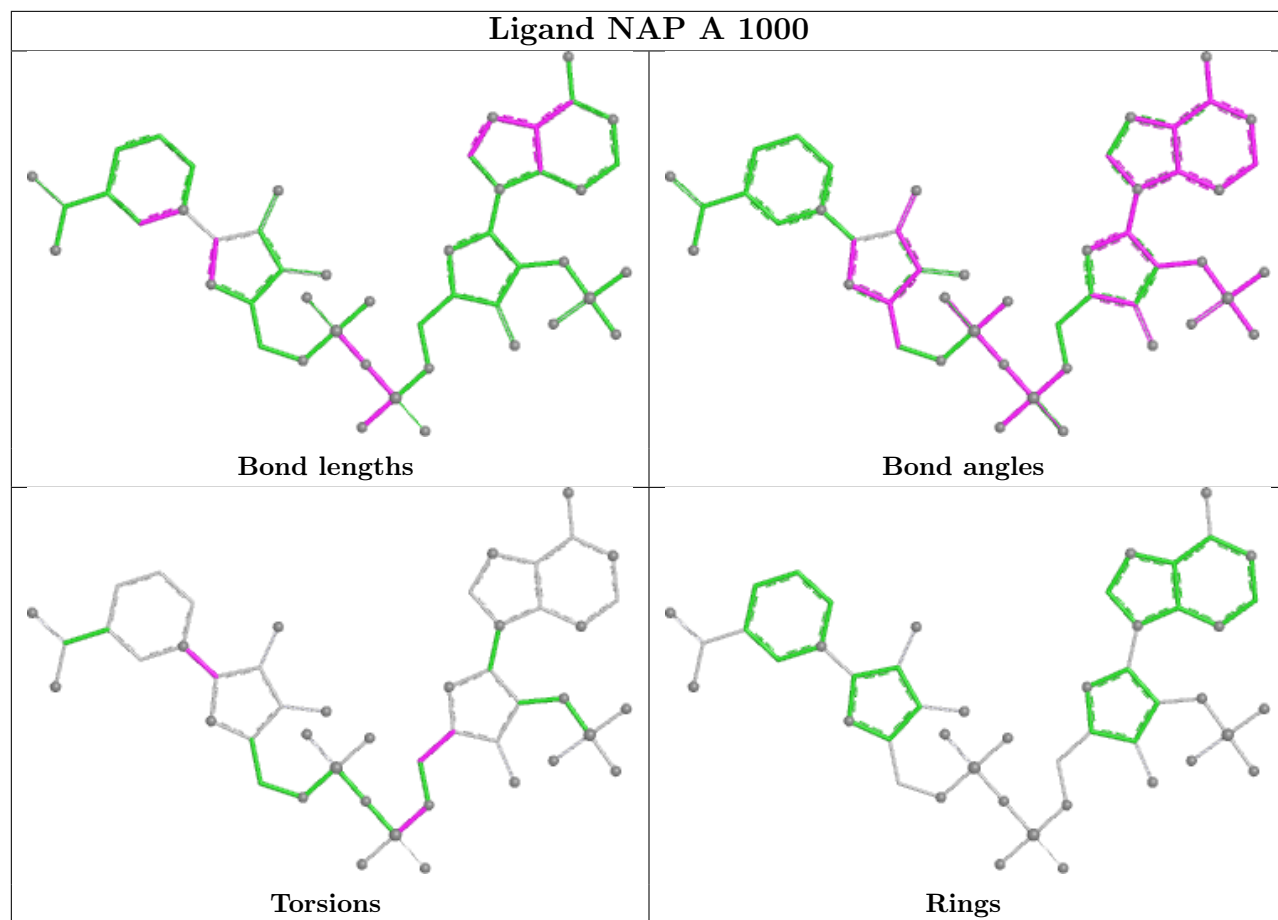


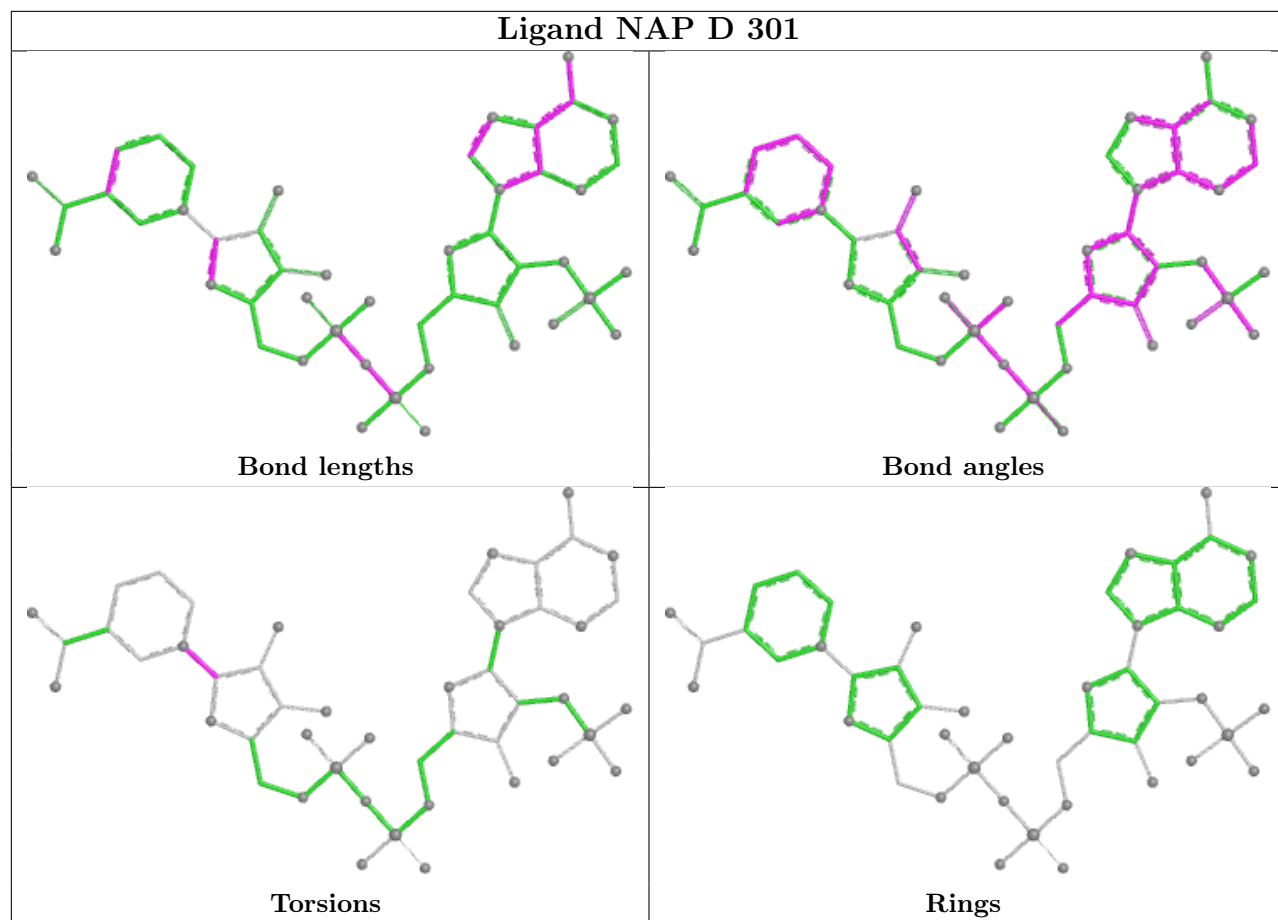


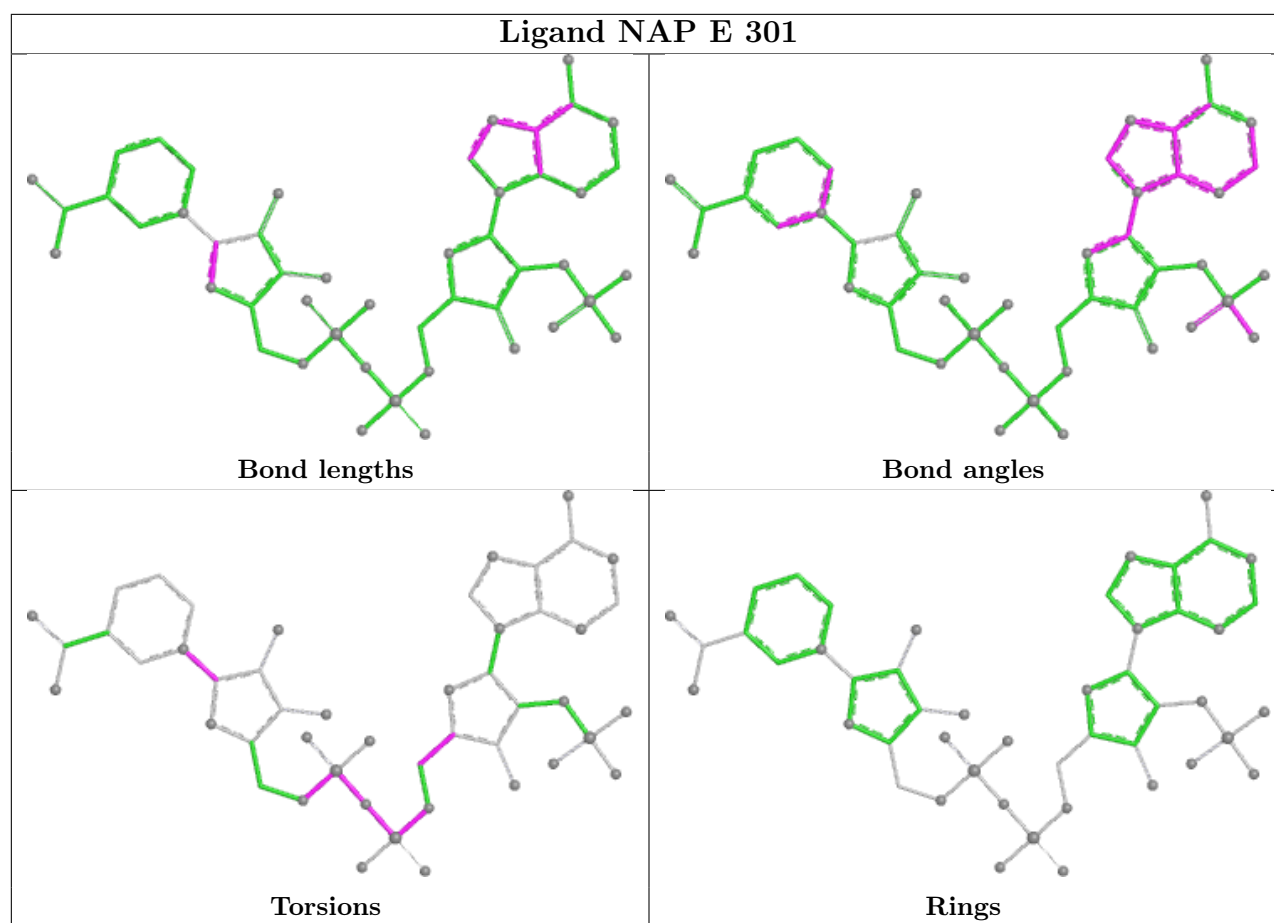












5.7 Other polymers [i](#)

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	281/285 (98%)	-0.92	0 100 100	13, 46, 76, 100	1 (0%)
1	B	261/285 (91%)	-0.67	5 (1%) 66 59	17, 74, 118, 152	1 (0%)
1	C	273/285 (95%)	-0.73	2 (0%) 84 79	23, 71, 107, 126	0
1	D	278/285 (97%)	-0.85	2 (0%) 84 79	17, 45, 70, 99	0
1	E	268/285 (94%)	-0.75	0 100 100	22, 69, 111, 134	0
1	F	280/285 (98%)	-0.90	0 100 100	16, 47, 79, 101	0
1	G	279/285 (97%)	-0.71	4 (1%) 73 67	23, 68, 106, 127	0
1	H	278/285 (97%)	-0.86	1 (0%) 88 85	18, 46, 76, 100	0
All	All	2198/2280 (96%)	-0.80	14 (0%) 85 81	13, 53, 104, 152	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	87	ILE	8.0
1	G	86	THR	4.5
1	B	87	ILE	4.0
1	D	47	LEU	3.6
1	B	88	ILE	3.2
1	B	64	CYS	3.1
1	G	64	CYS	3.0
1	H	128	TYR	2.9
1	C	140	PHE	2.9
1	C	119	ALA	2.8
1	B	244	ALA	2.4
1	G	105	PHE	2.4
1	B	119	ALA	2.1
1	D	128	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

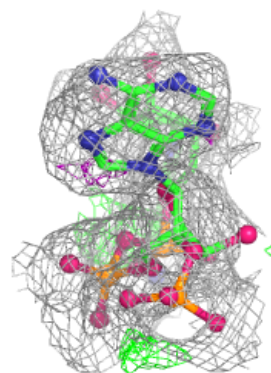
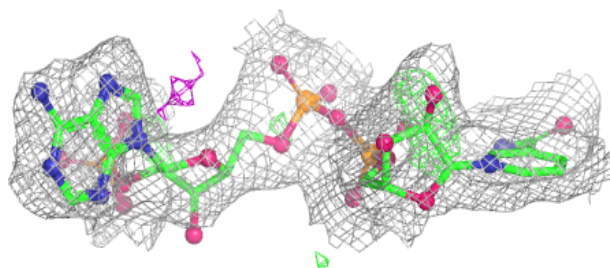
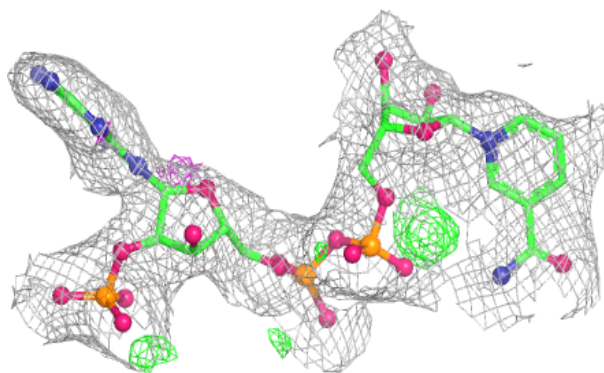
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAP	A	1000	48/48	0.98	0.05	19,25,35,45	0
2	NAP	B	301	48/48	0.98	0.04	26,51,66,68	0
2	NAP	C	301	48/48	0.98	0.04	26,51,81,93	0
2	NAP	D	301	48/48	0.98	0.04	12,19,29,33	0
2	NAP	E	301	48/48	0.98	0.04	35,66,93,100	0
2	NAP	F	301	48/48	0.98	0.05	17,32,36,46	0
2	NAP	G	301	48/48	0.98	0.04	31,47,56,67	0
2	NAP	H	1001	48/48	0.99	0.04	16,21,37,40	0

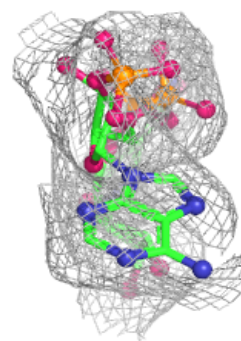
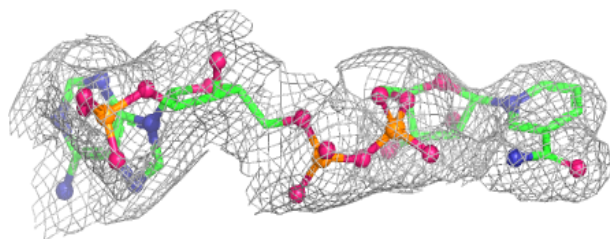
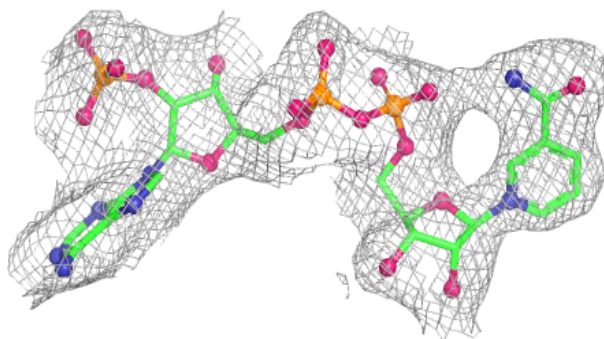
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 1000:

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

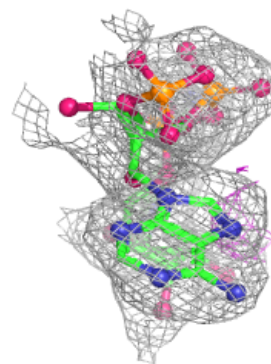
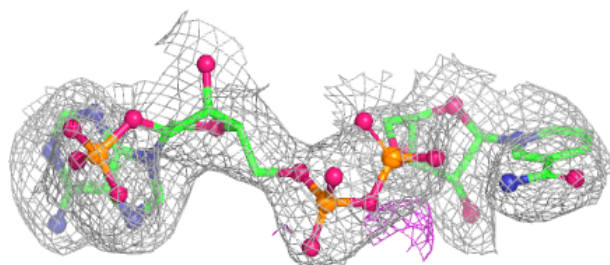
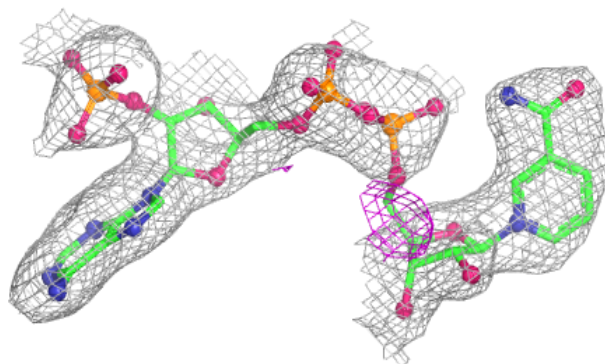
**Electron density around NAP B 301:**

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

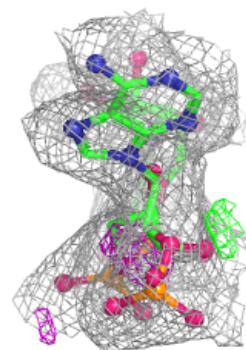
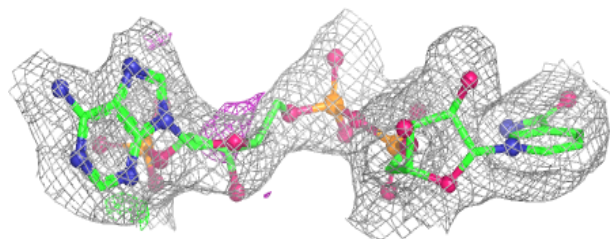
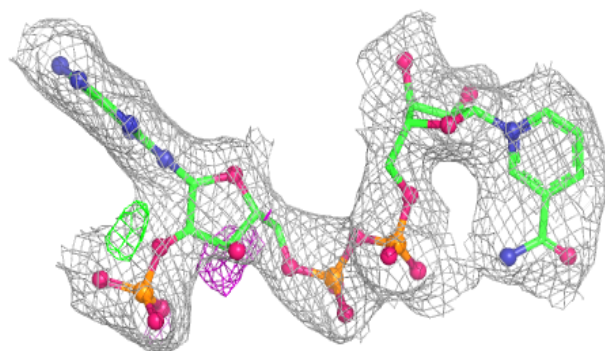


Electron density around NAP C 301:

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

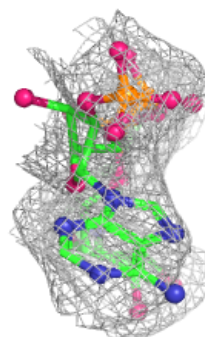
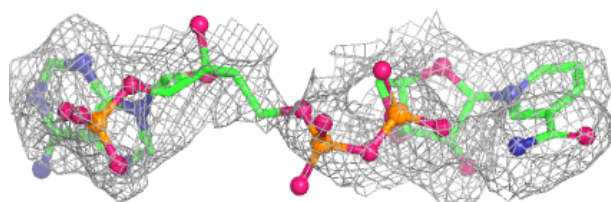
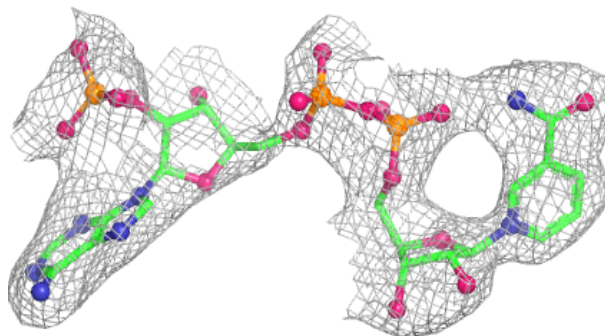
**Electron density around NAP D 301:**

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

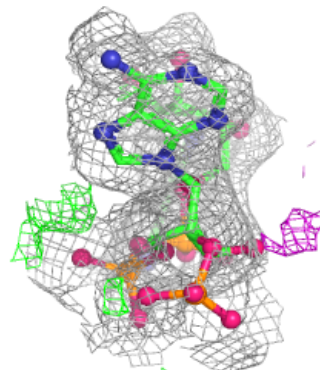
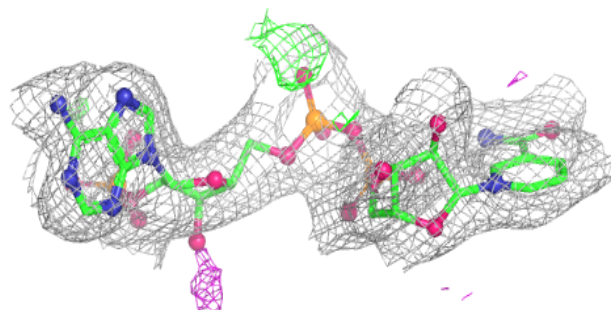
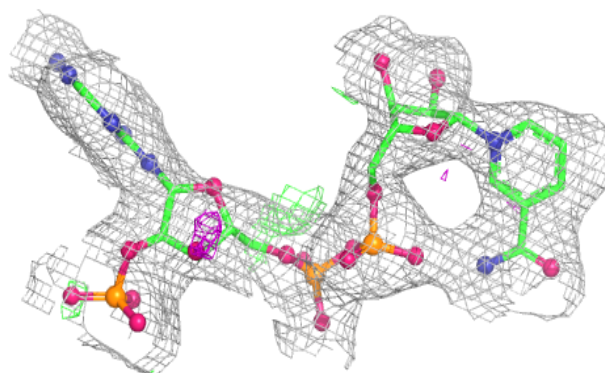


Electron density around NAP E 301:

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

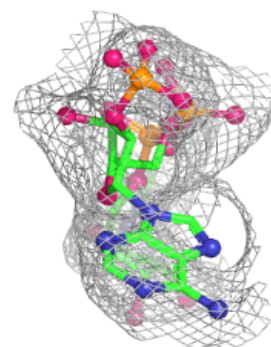
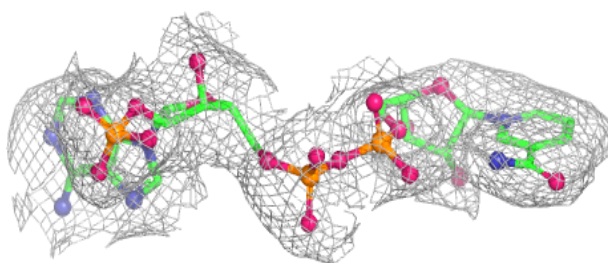
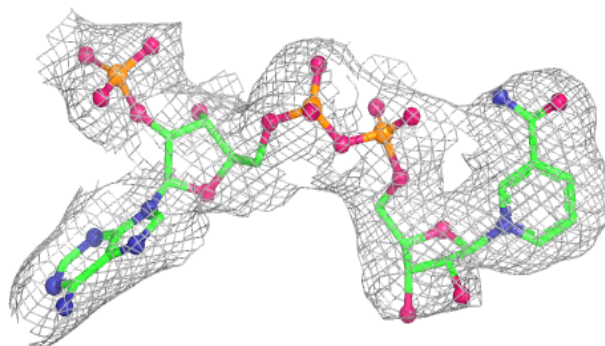
**Electron density around NAP F 301:**

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

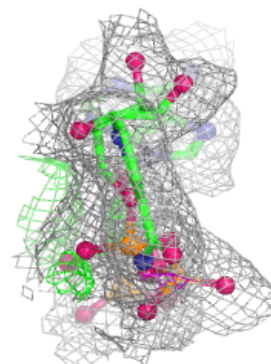
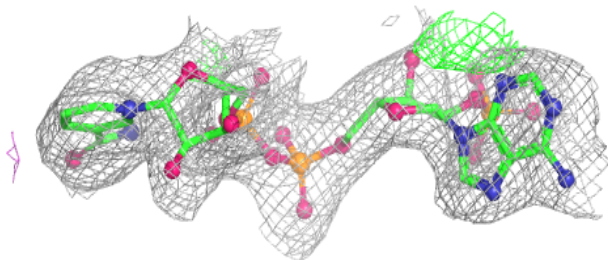
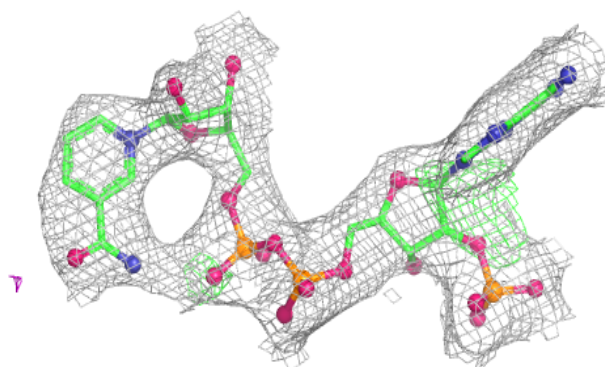


Electron density around NAP G 301:

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

**Electron density around NAP H 1001:**

$2mF_o-DF_c$ (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.