



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:01 PM UTC

PDB ID : 1OG6 / pdb_00001og6
Title : ydhF, an aldo-keto reductase from E.coli complexed with NADPH
Authors : Jeudy, S.; Abergel, C.; Claverie, J.M.
Deposited on : 2003-04-24
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

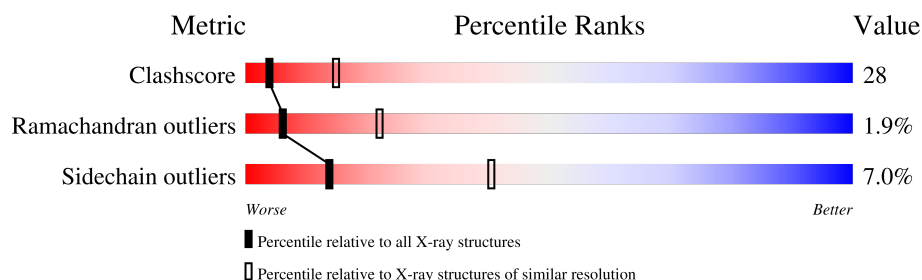
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	48% 46% 6%
1	B	298	46% 46% 6%
1	C	298	47% 47% 6%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7423 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.

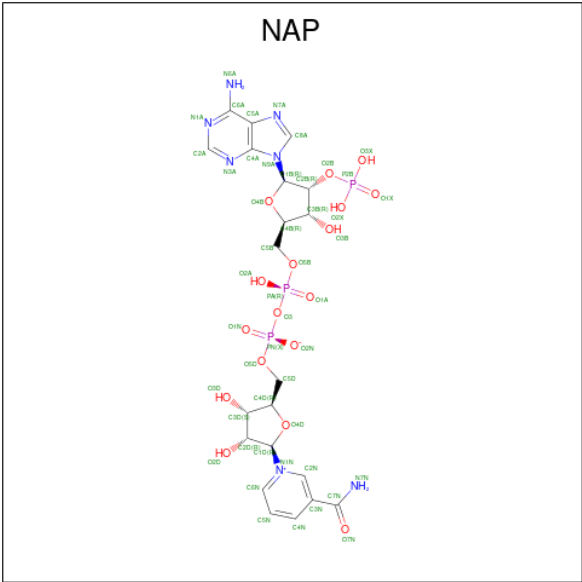
- Molecule 1 is a protein called HYPOTHETICAL OXIDOREDUCTASE YDHF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	1
			2362	1500	422	430	10			
1	B	294	Total	C	N	O	S	0	0	0
			2349	1493	418	428	10			
1	C	298	Total	C	N	O	S	0	0	0
			2369	1505	422	432	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	conflict	UNP P76187
B	1	LEU	MET	conflict	UNP P76187
C	1	LEU	MET	conflict	UNP P76187

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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		

- Molecule 3 is water.

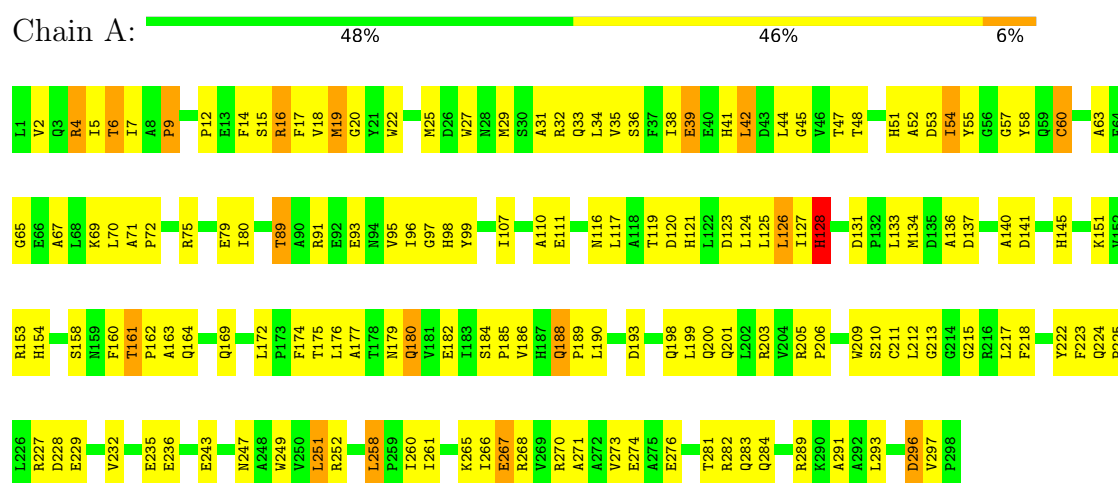
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	76	Total	O	0	0
			76	76		
3	C	53	Total	O	0	0
			53	53		

3 Residue-property plots

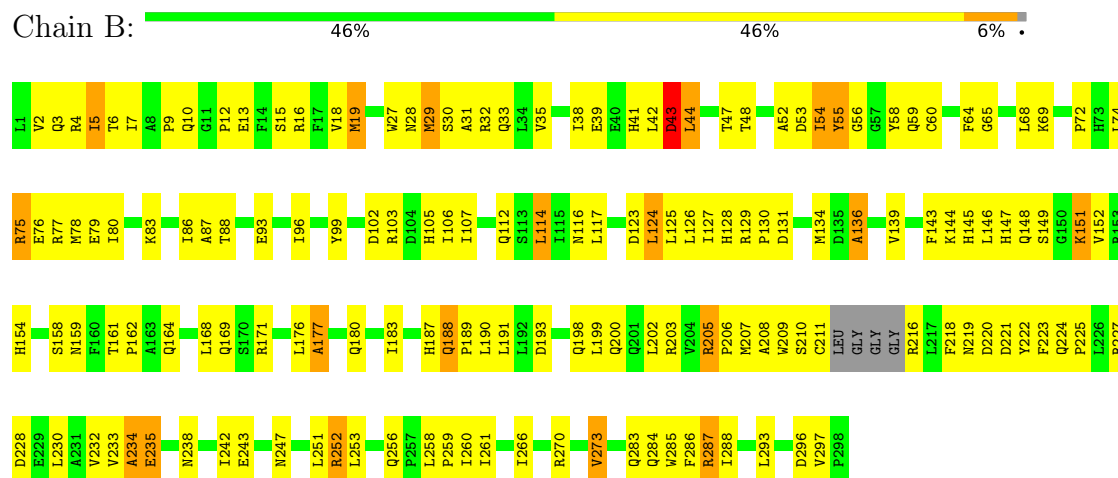
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: HYPOTHETICAL OXIDOREDUCTASE YDHF



• Molecule 1: HYPOTHETICAL OXIDOREDUCTASE YDHF



• Molecule 1: HYPOTHETICAL OXIDOREDUCTASE YDHF



L1	V2	Q3	R4	I5	T6	I7	A8	P9	Q10	G11	P12	E13	F14	S15	R16	M19	R23	L24	M25	D26	W27	N28	M29	S30	A31	Q32	Q33	L34	V35	I38	E39	E40	H41	L42	D43	H51	A52	D53	I54	Y55	G56	G57	Y58	Q59	C60	E61	A62	A63	F64	G65	F66	A67	L68	K69	L70
A71	E76	R77	M78	E79	I80	V81	S82	K83	C84	G85	I86	A87	T88	T89	A90	R91	E92	E93	N94	V95	H98	Y99	I100	R103	D104	H105	I106	I107	A110	E111	Q112	S113	L114	T115	N116	L117	H121	L124	L125	L126	I127	H128	R129	P130	D131	P132	L133	A136	A140	K144					
H147	Q148	S149	R153	G156	T161	P162	A163	Q164	Q169	S170	R171	L172	P173	F174	T175	L176	A177	Q180	V181	E182	I183	S184	P185	V186	H187	Q188	P189	L190	L191	L192	T195	Q198	L199	Q200	R203	V204	R205	P206	M207	A208	W209	S210	C211	L212	G213	R216	L217	F218	N219						
D220	Q224	P225	L226	L230	V233	L237	N238	I242	E243	V246	N247	A248	W249	V250	L251	R252	L253	P254	L258	P259	R270	A271	A272	V273	E274	T281	R282	Q283	Q284	W285	F286	R287	I288	R289	A292	Y295	D296	V297	F298																

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	174.53Å 174.53Å 97.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.80	Depositor
% Data completeness (in resolution range)	99.7 (29.91-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7423	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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	0.49	1/2414 (0.0%)	1.02	9/3278 (0.3%)
1	B	0.50	0/2401	1.01	6/3259 (0.2%)
1	C	0.47	0/2422	1.01	10/3288 (0.3%)
All	All	0.49	1/7237 (0.0%)	1.01	25/9825 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	VAL	C-N	-5.28	1.26	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ILE	N-CA-C	9.51	120.32	110.62
1	A	44	LEU	N-CA-C	-7.50	104.26	113.41
1	C	284	GLN	N-CA-C	-7.25	103.40	112.90
1	B	54	ILE	N-CA-C	7.07	119.07	111.58
1	A	7	ILE	N-CA-C	6.72	121.30	112.76
1	B	43	ASP	N-CA-C	-6.70	104.58	112.89
1	B	234	ALA	N-CA-C	-6.60	104.01	111.07
1	C	7	ILE	N-CA-C	6.55	119.23	111.05
1	C	55	TYR	N-CA-C	6.54	120.11	110.30
1	C	11	GLY	CA-C-N	6.10	127.50	120.98
1	C	11	GLY	C-N-CA	6.10	127.50	120.98
1	C	252	ARG	N-CA-C	6.01	120.31	112.92
1	C	43	ASP	N-CA-C	-5.80	106.25	113.38
1	C	54	ILE	N-CA-C	5.79	120.53	113.00
1	C	149	SER	N-CA-C	-5.74	106.14	114.12
1	B	60	CYS	N-CA-C	-5.62	105.55	112.90
1	A	60	CYS	N-CA-C	5.49	117.70	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ALA	N-CA-C	-5.46	104.74	111.40
1	B	222	TYR	N-CA-C	-5.42	106.37	112.87
1	A	188	GLN	N-CA-C	5.37	121.67	109.81
1	B	177	ALA	N-CA-C	5.33	118.01	111.82
1	C	90	ALA	N-CA-C	-5.32	106.86	113.19
1	A	161	THR	CA-C-N	-5.30	114.62	119.82
1	A	161	THR	C-N-CA	-5.30	114.62	119.82
1	A	177	ALA	N-CA-C	5.06	118.72	112.54

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	2362	0	2355	132	0
1	B	2349	0	2341	136	0
1	C	2369	0	2362	155	0
2	A	48	0	25	8	0
2	B	48	0	25	7	0
2	C	48	0	25	5	0
3	A	70	0	0	4	0
3	B	76	0	0	6	0
3	C	53	0	0	13	0
All	All	7423	0	7133	405	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 28.

All (405) 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:161:THR:HB	1:C:164:GLN:HG3	1.40	1.02
1:A:95:VAL:H	1:C:283:GLN:NE2	1.60	1.00
1:A:210:SER:H	2:A:1298:NAP:H51N	1.28	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:HD3	1:B:75:ARG:O	1.67	0.94
1:C:88:THR:HG22	1:C:90:ALA:H	1.33	0.92
1:A:127:ILE:HD11	1:A:160:PHE:HZ	1.35	0.89
1:C:210:SER:H	2:C:1299:NAP:H51N	1.38	0.89
1:B:162:PRO:HA	1:B:198:GLN:HE22	1.37	0.87
1:A:2:VAL:HG12	1:A:45:GLY:HA3	1.56	0.85
1:B:129:ARG:HG3	1:B:130:PRO:HD2	1.60	0.84
1:C:169:GLN:HE22	1:C:176:LEU:H	1.23	0.83
1:A:95:VAL:H	1:C:283:GLN:HE22	1.22	0.83
1:C:250:VAL:HB	3:C:2038:HOH:O	1.76	0.83
1:C:38:ILE:O	1:C:42:LEU:HG	1.77	0.83
1:C:247:ASN:C	3:C:2038:HOH:O	2.21	0.83
1:B:200:GLN:HE22	1:C:136:ALA:H	1.26	0.82
1:C:180:GLN:NE2	2:C:1299:NAP:H2N	1.94	0.81
1:C:112:GLN:HG3	1:C:116:ASN:HD21	1.45	0.81
1:A:18:VAL:CG2	1:A:260:ILE:HG12	2.10	0.80
1:B:149:SER:HB2	1:B:151:LYS:HG2	1.63	0.80
1:B:31:ALA:O	1:B:35:VAL:HG23	1.82	0.79
1:B:64:PHE:CE2	1:B:78:MET:HE1	2.17	0.79
1:B:54:ILE:HD11	3:B:2037:HOH:O	1.84	0.77
1:A:4:ARG:NH2	1:A:47:THR:OG1	2.17	0.77
1:A:162:PRO:HA	1:A:198:GLN:HE22	1.50	0.76
1:B:65:GLY:O	1:B:69:LYS:HG3	1.86	0.75
1:A:127:ILE:HD11	1:A:160:PHE:CZ	2.21	0.75
1:A:270:ARG:O	1:A:273:VAL:HG12	1.86	0.75
1:A:65:GLY:O	1:A:69:LYS:HG3	1.85	0.75
1:A:175:THR:HA	3:A:2036:HOH:O	1.86	0.74
1:B:284:GLN:O	1:B:288:ILE:HG12	1.87	0.74
1:C:218:PHE:HE2	1:C:243:GLU:HG2	1.53	0.74
1:C:25:MET:HE3	1:C:60:CYS:HA	1.70	0.74
1:B:38:ILE:O	1:B:42:LEU:HG	1.87	0.74
1:C:226:LEU:HD13	1:C:292:ALA:HB2	1.70	0.73
1:B:252:ARG:O	1:B:252:ARG:HD3	1.89	0.73
1:A:161:THR:HG22	1:A:163:ALA:H	1.52	0.72
1:C:144:LYS:HE2	1:C:173:PRO:HD3	1.69	0.71
1:A:121:HIS:CD2	1:A:153:ARG:HE	2.08	0.71
1:C:199:LEU:HD13	1:C:206:PRO:HB3	1.71	0.71
1:B:210:SER:H	2:B:1299:NAP:H51N	1.56	0.71
1:B:216:ARG:HA	1:B:219:ASN:HD22	1.55	0.71
1:C:103:ARG:HD3	1:C:104:ASP:N	2.06	0.71
1:B:224:GLN:HB3	1:B:225:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:HIS:CD2	1:C:153:ARG:HE	2.09	0.70
1:C:88:THR:HG22	1:C:90:ALA:N	2.06	0.70
1:B:162:PRO:HA	1:B:198:GLN:NE2	2.05	0.70
1:A:247:ASN:O	1:A:251:LEU:HD22	1.92	0.70
1:C:7:ILE:HD13	1:C:14:PHE:CE2	2.26	0.70
1:C:250:VAL:N	3:C:2038:HOH:O	2.24	0.70
1:A:169:GLN:HE22	1:A:176:LEU:H	1.38	0.70
1:C:23:ARG:HH21	1:C:23:ARG:HG2	1.54	0.69
1:C:111:GLU:HA	1:C:114:LEU:HD23	1.72	0.69
1:B:209:TRP:HB2	2:B:1299:NAP:O4D	1.93	0.69
1:B:180:GLN:NE2	2:B:1299:NAP:H2N	2.06	0.69
1:A:161:THR:HB	1:A:164:GLN:HG3	1.76	0.68
1:C:65:GLY:O	1:C:69:LYS:HG3	1.94	0.68
1:A:119:THR:HG22	1:A:120:ASP:N	2.08	0.68
1:A:121:HIS:HD2	1:A:153:ARG:HE	1.39	0.68
1:B:220:ASP:HB3	1:B:223:PHE:HD1	1.58	0.68
1:A:75:ARG:HH11	1:A:80:ILE:HD12	1.58	0.68
1:C:216:ARG:O	1:C:220:ASP:HB2	1.94	0.67
1:A:99:TYR:HB2	1:A:131:ASP:OD1	1.94	0.67
1:B:260:ILE:HG21	2:B:1299:NAP:O3D	1.95	0.67
1:A:18:VAL:HG21	1:A:260:ILE:HG12	1.76	0.66
1:B:64:PHE:HE2	1:B:78:MET:HE1	1.59	0.66
1:A:119:THR:HG22	1:A:121:HIS:H	1.61	0.65
1:C:34:LEU:HD23	1:C:67:ALA:HB2	1.79	0.65
1:B:114:LEU:HD21	1:B:151:LYS:HB2	1.79	0.65
1:A:119:THR:HG22	1:A:120:ASP:H	1.62	0.64
1:C:25:MET:HE1	1:C:63:ALA:CB	2.26	0.64
1:A:27:TRP:HB3	1:A:29:MET:HE3	1.80	0.64
1:B:251:LEU:HD13	1:B:259:PRO:HG2	1.80	0.64
1:C:144:LYS:HE2	1:C:173:PRO:CD	2.27	0.64
1:C:25:MET:HE1	1:C:63:ALA:HB2	1.81	0.63
1:C:91:ARG:HB3	1:C:93:GLU:OE1	1.99	0.63
1:C:180:GLN:HE21	2:C:1299:NAP:H2N	1.63	0.63
1:C:189:PRO:O	1:C:192:LEU:HD23	1.99	0.63
1:A:127:ILE:HG13	1:A:127:ILE:O	1.97	0.63
1:A:39:GLU:O	1:A:42:LEU:HD12	1.98	0.63
1:B:189:PRO:HG2	1:B:190:LEU:HD22	1.80	0.63
1:A:128:HIS:O	1:A:158:SER:HB3	1.99	0.62
1:B:297:VAL:HG22	3:C:2014:HOH:O	1.99	0.62
1:C:16:ARG:HH21	1:C:16:ARG:HG3	1.64	0.62
1:C:121:HIS:HD2	1:C:153:ARG:HE	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLN:HE22	1:B:136:ALA:H	1.48	0.61
1:C:218:PHE:CE2	1:C:243:GLU:HG2	2.35	0.61
1:B:169:GLN:HE22	1:B:176:LEU:H	1.49	0.61
1:B:158:SER:O	1:B:159:ASN:HB2	2.01	0.61
1:C:53:ASP:HB2	1:C:84:CYS:HA	1.83	0.61
1:A:2:VAL:HG12	1:A:45:GLY:CA	2.31	0.61
1:C:181:VAL:HB	1:C:190:LEU:CD1	2.31	0.61
1:C:283:GLN:O	1:C:287:ARG:HB2	2.01	0.60
1:B:180:GLN:HE21	2:B:1299:NAP:H2N	1.64	0.60
1:C:103:ARG:HD3	1:C:103:ARG:C	2.27	0.60
1:C:212:LEU:HD13	1:C:218:PHE:HZ	1.67	0.60
1:B:233:VAL:HG21	1:B:288:ILE:HD11	1.85	0.59
1:C:281:THR:OG1	1:C:284:GLN:HB2	2.03	0.59
1:B:235:GLU:HG2	3:B:2062:HOH:O	2.02	0.59
1:B:3:GLN:HG2	1:B:4:ARG:N	2.16	0.58
1:C:199:LEU:CD1	1:C:206:PRO:HB3	2.33	0.58
1:B:183:ILE:HD12	1:B:208:ALA:HB2	1.86	0.58
1:A:14:PHE:CD2	1:A:48:THR:HG21	2.38	0.58
1:A:31:ALA:O	1:A:35:VAL:HG23	2.02	0.58
1:A:210:SER:N	2:A:1298:NAP:H51N	2.10	0.58
1:A:265:LYS:HB3	1:A:267:GLU:OE1	2.03	0.58
1:A:51:HIS:O	1:A:52:ALA:HB2	2.04	0.58
1:C:140:ALA:O	1:C:144:LYS:HG2	2.04	0.58
1:A:12:PRO:HB3	1:A:154:HIS:CD2	2.38	0.58
1:A:140:ALA:HA	1:A:172:LEU:HD21	1.85	0.58
1:A:79:GLU:HA	1:A:123:ASP:OD2	2.03	0.58
1:B:4:ARG:NH2	1:B:47:THR:OG1	2.36	0.57
1:B:64:PHE:CZ	1:B:78:MET:HE1	2.38	0.57
1:A:217:LEU:O	1:A:217:LEU:HD23	2.05	0.57
1:A:229:GLU:HG3	1:A:291:ALA:HB2	1.86	0.57
1:A:184:SER:HB2	1:A:211:CYS:O	2.04	0.57
1:B:52:ALA:HB3	1:B:55:TYR:CD2	2.40	0.57
1:A:69:LYS:O	1:A:72:PRO:HD3	2.05	0.56
1:B:260:ILE:HB	2:B:1299:NAP:H4D	1.87	0.56
1:C:27:TRP:HE3	1:C:29:MET:HE2	1.70	0.56
1:B:29:MET:HA	1:B:33:GLN:NE2	2.21	0.56
1:B:80:ILE:HG21	1:B:117:LEU:HD13	1.87	0.56
1:A:34:LEU:HD23	1:A:67:ALA:HB2	1.87	0.56
1:C:110:ALA:O	1:C:114:LEU:HD22	2.06	0.56
1:C:162:PRO:HA	1:C:198:GLN:HE22	1.70	0.56
1:A:91:ARG:HD3	1:A:93:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASP:C	1:B:193:ASP:OD2	2.48	0.55
1:A:35:VAL:O	1:A:39:GLU:HB2	2.05	0.55
1:C:64:PHE:HD2	1:C:117:LEU:HD22	1.71	0.55
1:A:35:VAL:HG21	1:A:70:LEU:HD11	1.89	0.55
1:B:12:PRO:HB3	1:B:154:HIS:CD2	2.42	0.55
1:A:212:LEU:HD23	1:A:218:PHE:CE1	2.42	0.55
1:C:226:LEU:O	1:C:230:LEU:HG	2.07	0.55
1:A:162:PRO:HA	1:A:198:GLN:NE2	2.21	0.54
1:B:18:VAL:HG13	1:B:48:THR:HG22	1.89	0.54
1:A:45:GLY:O	1:A:47:THR:HG23	2.07	0.54
1:A:16:ARG:CZ	1:A:251:LEU:HD12	2.37	0.54
1:A:89:THR:HG22	3:A:2019:HOH:O	2.07	0.54
1:A:91:ARG:HB3	1:A:93:GLU:OE1	2.06	0.54
1:C:23:ARG:HG2	1:C:23:ARG:NH2	2.21	0.54
1:B:200:GLN:NE2	1:C:136:ALA:H	2.02	0.53
1:C:16:ARG:HG3	1:C:16:ARG:NH2	2.20	0.53
1:C:32:ARG:HG2	1:C:32:ARG:HH11	1.73	0.53
1:C:270:ARG:O	1:C:273:VAL:HG22	2.08	0.53
1:A:199:LEU:CD1	1:A:206:PRO:HB3	2.37	0.53
1:B:5:ILE:HG23	1:B:5:ILE:O	2.08	0.53
1:B:149:SER:CB	1:B:151:LYS:HG2	2.37	0.53
1:B:149:SER:HB3	1:B:151:LYS:HE2	1.90	0.53
1:B:247:ASN:O	1:B:251:LEU:HB2	2.09	0.53
1:C:195:THR:HG23	3:C:2026:HOH:O	2.07	0.53
1:A:124:LEU:HA	1:A:154:HIS:O	2.09	0.53
1:C:297:VAL:HG22	3:C:2051:HOH:O	2.08	0.53
1:A:70:LEU:HD12	1:A:70:LEU:O	2.09	0.53
1:A:282:ARG:HH12	1:B:102:ASP:HB3	1.72	0.53
1:C:273:VAL:HG23	1:C:274:GLU:OE2	2.09	0.53
1:A:15:SER:O	1:A:17:PHE:N	2.43	0.52
1:C:250:VAL:CA	3:C:2038:HOH:O	2.57	0.52
1:B:5:ILE:HG21	1:B:258:LEU:HD21	1.91	0.52
1:C:213:GLY:O	1:C:216:ARG:HG2	2.08	0.52
1:A:96:ILE:HG22	1:C:283:GLN:HG2	1.92	0.52
1:C:161:THR:HG22	1:C:163:ALA:H	1.75	0.52
1:C:103:ARG:HE	1:C:107:ILE:HD12	1.74	0.52
1:A:38:ILE:HA	1:A:41:HIS:CD2	2.45	0.52
1:A:57:GLY:O	1:A:58:TYR:HB2	2.11	0.52
1:A:212:LEU:N	1:A:212:LEU:HD12	2.24	0.52
1:B:286:PHE:CD1	1:C:98:HIS:HB2	2.45	0.51
1:B:56:GLY:O	1:B:59:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:O	1:C:70:LEU:HD12	2.10	0.51
1:B:32:ARG:HA	1:B:32:ARG:NE	2.26	0.51
1:B:53:ASP:HB2	1:B:83:LYS:O	2.10	0.51
1:A:268:ARG:HH11	2:A:1298:NAP:P2B	2.34	0.51
1:B:283:GLN:O	1:B:287:ARG:HB2	2.11	0.51
1:A:184:SER:OG	1:A:186:VAL:HG22	2.11	0.51
1:C:181:VAL:HB	1:C:190:LEU:HD13	1.93	0.51
1:A:96:ILE:HG12	1:A:97:GLY:N	2.26	0.51
1:A:218:PHE:CZ	1:A:243:GLU:HG3	2.46	0.51
1:C:192:LEU:HD23	1:C:192:LEU:H	1.75	0.51
1:A:18:VAL:HG23	1:A:260:ILE:HG23	1.91	0.51
1:B:3:GLN:HG2	1:B:4:ARG:O	2.11	0.50
1:C:247:ASN:O	1:C:251:LEU:HB2	2.11	0.50
1:C:271:ALA:O	1:C:274:GLU:HB2	2.11	0.50
1:A:20:GLY:HA3	2:A:1298:NAP:O3D	2.11	0.50
1:A:201:GLN:HA	1:B:171:ARG:NH2	2.25	0.50
1:B:127:ILE:HG12	1:B:143:PHE:HZ	1.76	0.50
1:B:27:TRP:HB3	1:B:29:MET:HE3	1.94	0.50
1:B:228:ASP:O	1:B:232:VAL:HG23	2.11	0.50
1:B:205:ARG:HD3	3:B:2061:HOH:O	2.10	0.50
1:C:112:GLN:HG3	1:C:116:ASN:ND2	2.23	0.50
1:A:95:VAL:HG22	3:A:2017:HOH:O	2.10	0.50
1:B:79:GLU:HA	1:B:123:ASP:OD2	2.12	0.50
1:C:147:HIS:C	1:C:149:SER:H	2.18	0.50
1:A:98:HIS:CE1	1:C:283:GLN:HG3	2.47	0.50
1:B:52:ALA:HB3	1:B:55:TYR:CG	2.47	0.50
1:C:289:ARG:NH2	1:C:295:TYR:O	2.45	0.50
1:A:124:LEU:HG	1:A:126:LEU:HD13	1.94	0.50
1:B:42:LEU:HD13	1:B:77:ARG:CZ	2.42	0.50
1:B:54:ILE:HG22	1:B:58:TYR:CZ	2.47	0.49
1:B:183:ILE:O	1:B:211:CYS:HA	2.12	0.49
1:C:126:LEU:HA	1:C:156:GLY:O	2.11	0.49
1:A:22:TRP:HB2	2:A:1298:NAP:H2D	1.94	0.49
1:A:203:ARG:HG2	1:A:203:ARG:HH11	1.77	0.49
1:B:42:LEU:HD12	1:B:43:ASP:N	2.27	0.49
1:C:27:TRP:HE3	1:C:29:MET:CE	2.25	0.49
1:C:107:ILE:O	1:C:111:GLU:HG3	2.12	0.49
1:C:180:GLN:HE22	2:C:1299:NAP:H2N	1.76	0.49
1:B:161:THR:OG1	1:B:164:GLN:HG3	2.12	0.49
1:A:18:VAL:HG12	1:A:48:THR:HB	1.94	0.49
1:B:296:ASP:HB3	3:C:2014:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:PHE:CE2	1:C:78:MET:HE1	2.48	0.48
1:C:180:GLN:HG2	1:C:209:TRP:HD1	1.78	0.48
1:B:2:VAL:HG12	1:B:273:VAL:HG13	1.95	0.48
1:A:95:VAL:N	1:C:283:GLN:NE2	2.44	0.48
1:B:54:ILE:O	1:B:55:TYR:C	2.56	0.48
1:B:190:LEU:HD23	3:B:2056:HOH:O	2.13	0.48
1:A:5:ILE:HD11	1:A:205:ARG:HG2	1.95	0.48
1:A:218:PHE:CE2	1:A:243:GLU:HG3	2.48	0.48
1:C:4:ARG:HD3	1:C:13:GLU:OE1	2.14	0.48
1:A:54:ILE:HG13	1:A:55:TYR:N	2.27	0.48
1:A:217:LEU:HD23	1:A:217:LEU:C	2.38	0.48
1:B:200:GLN:HE22	1:C:136:ALA:N	2.04	0.48
1:A:281:THR:OG1	1:A:284:GLN:HG3	2.13	0.48
1:C:32:ARG:HG2	1:C:32:ARG:NH1	2.28	0.47
1:A:268:ARG:NH1	2:A:1298:NAP:P2B	2.87	0.47
1:C:188:GLN:HE22	1:C:289:ARG:HG3	1.79	0.47
1:C:233:VAL:HG13	1:C:284:GLN:HG2	1.96	0.47
1:C:51:HIS:O	1:C:83:LYS:NZ	2.47	0.47
1:C:242:ILE:O	1:C:246:VAL:HG23	2.14	0.47
1:A:32:ARG:HG3	1:A:33:GLN:N	2.30	0.47
1:A:119:THR:CG2	1:A:120:ASP:N	2.76	0.47
1:A:161:THR:HG21	3:C:2030:HOH:O	2.14	0.47
1:A:212:LEU:HD23	1:A:218:PHE:CZ	2.49	0.47
1:B:42:LEU:HD13	1:B:77:ARG:NH2	2.30	0.47
1:C:282:ARG:O	1:C:286:PHE:HD1	1.98	0.47
1:A:107:ILE:HD13	1:A:145:HIS:CD2	2.50	0.47
1:B:221:ASP:C	1:B:223:PHE:H	2.23	0.47
1:A:136:ALA:H	1:C:200:GLN:HE22	1.61	0.46
1:C:162:PRO:HA	1:C:198:GLN:NE2	2.30	0.46
1:C:192:LEU:HD23	1:C:192:LEU:N	2.30	0.46
1:C:86:ILE:HG13	1:C:128:HIS:HB3	1.98	0.46
1:C:91:ARG:HB2	1:C:94:ASN:ND2	2.30	0.46
1:B:99:TYR:HB2	1:B:131:ASP:OD1	2.15	0.46
1:B:199:LEU:HD13	1:B:206:PRO:HB3	1.96	0.46
1:B:216:ARG:HA	1:B:219:ASN:ND2	2.26	0.46
1:B:107:ILE:HD13	1:B:145:HIS:CD2	2.50	0.46
1:C:61:GLU:O	1:C:117:LEU:HD23	2.16	0.46
1:C:237:LEU:O	1:C:238:ASN:HB2	2.15	0.46
1:A:235:GLU:HG3	1:A:236:GLU:N	2.30	0.46
1:C:7:ILE:HD13	1:C:14:PHE:CD2	2.50	0.46
1:C:250:VAL:CB	3:C:2038:HOH:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:N	1:A:258:LEU:HD23	2.31	0.46
1:B:220:ASP:HB3	1:B:223:PHE:CD1	2.46	0.46
1:A:80:ILE:HG21	1:A:117:LEU:HD13	1.98	0.46
1:A:189:PRO:O	1:A:193:ASP:HB3	2.15	0.46
1:B:124:LEU:HD22	1:B:126:LEU:HD12	1.96	0.46
1:B:188:GLN:N	1:B:189:PRO:CD	2.79	0.46
1:C:52:ALA:HB2	1:C:83:LYS:NZ	2.31	0.46
1:C:52:ALA:HB2	1:C:83:LYS:HZ2	1.81	0.46
1:C:87:ALA:HB2	1:C:100:ILE:CD1	2.46	0.46
1:A:25:MET:HE3	1:A:60:CYS:HA	1.98	0.45
1:B:221:ASP:C	1:B:223:PHE:N	2.73	0.45
1:B:285:TRP:CE2	1:C:133:LEU:HD21	2.52	0.45
1:C:7:ILE:HG21	1:C:14:PHE:CD2	2.51	0.45
1:A:137:ASP:O	1:A:141:ASP:HB2	2.17	0.45
1:B:147:HIS:HD2	1:B:147:HIS:O	1.99	0.45
1:B:168:LEU:O	1:B:169:GLN:C	2.59	0.45
1:B:218:PHE:HA	1:B:227:ARG:HD3	1.98	0.45
1:A:267:GLU:CD	1:A:267:GLU:H	2.23	0.45
1:C:51:HIS:O	1:C:82:SER:HA	2.15	0.45
1:A:12:PRO:HD3	1:A:154:HIS:CG	2.52	0.45
1:A:223:PHE:O	1:A:227:ARG:HG3	2.17	0.45
1:A:133:LEU:HA	1:C:254:PRO:HD3	1.99	0.45
1:B:58:TYR:CE2	1:B:88:THR:OG1	2.70	0.45
1:B:266:ILE:O	1:B:266:ILE:HG13	2.16	0.45
1:A:19:MET:HE2	1:A:261:ILE:HB	1.98	0.45
1:A:252:ARG:HH21	1:A:252:ARG:HG3	1.80	0.45
1:B:9:PRO:O	1:B:10:GLN:HB2	2.17	0.45
1:A:127:ILE:O	1:A:127:ILE:CG1	2.64	0.45
1:A:199:LEU:HD13	1:A:206:PRO:HB3	1.99	0.45
1:A:15:SER:O	1:A:16:ARG:C	2.60	0.45
1:C:2:VAL:HG23	1:C:2:VAL:O	2.16	0.45
1:C:121:HIS:CD2	1:C:153:ARG:NE	2.81	0.45
1:C:284:GLN:O	1:C:288:ILE:HG13	2.17	0.45
1:B:58:TYR:HE2	1:B:88:THR:OG1	2.00	0.44
1:B:210:SER:O	1:B:211:CYS:C	2.60	0.44
1:B:105:HIS:HE1	3:B:2029:HOH:O	1.99	0.44
1:B:188:GLN:HB3	1:B:191:LEU:HD22	1.99	0.44
1:C:103:ARG:HG3	1:C:103:ARG:HH11	1.81	0.44
1:A:185:PRO:HG3	1:A:249:TRP:CE3	2.53	0.44
1:B:30:SER:O	1:B:31:ALA:C	2.60	0.44
1:B:253:LEU:HD21	1:B:285:TRP:HZ2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HB3	1:A:199:LEU:HD11	2.00	0.44
1:C:84:CYS:SG	1:C:106:ILE:HG23	2.57	0.44
1:A:180:GLN:OE1	2:A:1298:NAP:H2N	2.18	0.44
1:A:205:ARG:HD2	1:A:205:ARG:N	2.32	0.44
1:B:131:ASP:HB3	1:B:134:MET:HB2	2.00	0.44
1:B:190:LEU:HD22	1:B:190:LEU:N	2.33	0.44
1:C:42:LEU:HD13	1:C:77:ARG:CZ	2.48	0.44
1:C:224:GLN:N	1:C:225:PRO:CD	2.80	0.44
1:C:203:ARG:HG2	1:C:203:ARG:HH11	1.83	0.44
1:A:182:GLU:HB2	1:A:209:TRP:CE2	2.52	0.44
1:B:16:ARG:HH22	1:B:256:GLN:HB3	1.83	0.44
1:B:7:ILE:HD11	1:B:177:ALA:HB1	2.00	0.44
1:B:103:ARG:NH1	1:B:103:ARG:HG2	2.33	0.43
1:C:7:ILE:HG21	1:C:14:PHE:HD2	1.83	0.43
1:A:228:ASP:O	1:A:232:VAL:HG23	2.17	0.43
1:B:146:LEU:HD13	1:B:152:VAL:HG21	2.00	0.43
1:A:175:THR:HB	3:A:2004:HOH:O	2.18	0.43
1:C:41:HIS:ND1	1:C:41:HIS:C	2.76	0.43
1:B:12:PRO:HD3	1:B:154:HIS:CG	2.53	0.43
1:C:182:GLU:HG2	1:C:187:HIS:CD2	2.53	0.43
1:A:69:LYS:C	1:A:71:ALA:H	2.27	0.43
1:C:251:LEU:HD13	1:C:259:PRO:HG3	2.00	0.43
1:B:64:PHE:O	1:B:68:LEU:HD13	2.18	0.43
1:B:124:LEU:HD22	1:B:126:LEU:CD1	2.49	0.43
1:A:54:ILE:O	1:A:55:TYR:C	2.61	0.43
1:B:6:THR:HA	1:B:13:GLU:HA	1.99	0.43
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.87	0.43
1:C:129:ARG:HD3	1:C:130:PRO:HD2	2.01	0.43
1:A:252:ARG:HG3	1:A:252:ARG:NH2	2.34	0.43
1:B:42:LEU:HD12	1:B:42:LEU:C	2.44	0.43
1:B:144:LYS:O	1:B:148:GLN:HG3	2.19	0.43
1:B:74:LEU:O	1:B:76:GLU:N	2.52	0.43
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.84	0.43
1:B:230:LEU:HB3	1:B:242:ILE:HB	2.01	0.43
1:C:83:LYS:HA	1:C:126:LEU:O	2.19	0.43
1:C:140:ALA:HB2	1:C:171:ARG:HB3	2.01	0.43
1:A:65:GLY:HA3	1:A:116:ASN:O	2.19	0.42
1:A:271:ALA:O	1:A:274:GLU:HB2	2.19	0.42
1:A:282:ARG:NH1	1:B:102:ASP:HB3	2.34	0.42
1:C:271:ALA:O	1:C:272:ALA:C	2.62	0.42
1:C:5:ILE:O	1:C:5:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:CG	1:C:130:PRO:HD2	2.49	0.42
1:A:266:ILE:O	1:A:270:ARG:HG3	2.18	0.42
1:C:25:MET:HG2	1:C:60:CYS:SG	2.60	0.42
1:C:35:VAL:HG11	1:C:71:ALA:HB2	2.01	0.42
1:C:129:ARG:HG3	1:C:130:PRO:HD2	2.00	0.42
1:B:180:GLN:HE21	2:B:1299:NAP:H71N	1.67	0.42
1:C:129:ARG:CD	1:C:130:PRO:HD2	2.50	0.42
1:A:33:GLN:O	1:A:36:SER:N	2.51	0.42
1:B:86:ILE:HG22	1:B:87:ALA:N	2.33	0.42
1:C:30:SER:OG	1:C:33:GLN:HG3	2.19	0.42
1:C:99:TYR:HD2	1:C:131:ASP:OD1	2.02	0.42
1:C:243:GLU:H	1:C:243:GLU:HG3	1.47	0.42
1:B:39:GLU:O	1:B:43:ASP:HB2	2.20	0.42
1:C:88:THR:CG2	1:C:89:THR:N	2.82	0.42
1:C:112:GLN:O	1:C:116:ASN:ND2	2.53	0.42
1:C:212:LEU:HB2	2:C:1299:NAP:H52A	2.02	0.42
1:C:246:VAL:C	1:C:248:ALA:N	2.78	0.42
1:B:286:PHE:HZ	1:C:131:ASP:OD1	2.03	0.42
1:A:213:GLY:C	1:A:215:GLY:H	2.28	0.42
1:A:289:ARG:NH2	1:A:296:ASP:O	2.53	0.42
1:B:28:ASN:ND2	3:B:2010:HOH:O	2.52	0.42
1:B:44:LEU:HD21	1:B:270:ARG:HB2	2.01	0.42
1:C:184:SER:OG	1:C:186:VAL:HG22	2.20	0.42
1:A:111:GLU:OE2	1:A:151:LYS:HE3	2.19	0.42
1:A:188:GLN:N	1:A:189:PRO:HD2	2.35	0.42
1:B:202:LEU:O	1:B:203:ARG:HB2	2.20	0.42
1:A:119:THR:CG2	1:A:120:ASP:H	2.30	0.41
1:A:161:THR:HG22	1:A:162:PRO:N	2.35	0.41
1:B:19:MET:HG3	1:B:41:HIS:CD2	2.55	0.41
1:B:180:GLN:HG3	1:B:207:MET:O	2.19	0.41
1:C:8:ALA:HB2	1:C:177:ALA:HA	2.02	0.41
1:C:124:LEU:HD13	1:C:126:LEU:CD1	2.51	0.41
1:C:181:VAL:O	1:C:208:ALA:HA	2.20	0.41
1:C:246:VAL:C	1:C:248:ALA:H	2.29	0.41
1:B:187:HIS:C	1:B:189:PRO:HD2	2.44	0.41
1:B:188:GLN:CD	1:B:293:LEU:HD11	2.45	0.41
1:B:5:ILE:HD11	1:B:205:ARG:HG2	2.02	0.41
1:B:19:MET:HE2	1:B:261:ILE:HB	2.02	0.41
1:B:65:GLY:HA3	1:B:116:ASN:O	2.21	0.41
1:C:233:VAL:HG22	1:C:287:ARG:NH2	2.35	0.41
1:A:283:GLN:HG3	1:B:96:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:THR:HG22	1:C:8:ALA:O	2.21	0.41
1:C:88:THR:HG22	1:C:89:THR:N	2.36	0.41
1:C:6:THR:HA	1:C:12:PRO:O	2.20	0.41
1:C:8:ALA:HB1	1:C:9:PRO:CD	2.51	0.41
1:A:75:ARG:NH1	1:A:80:ILE:HD12	2.29	0.41
1:C:52:ALA:HB3	1:C:55:TYR:CD2	2.56	0.41
1:A:274:GLU:C	1:A:276:GLU:H	2.29	0.41
1:B:32:ARG:HA	1:B:32:ARG:HE	1.83	0.41
1:B:74:LEU:C	1:B:76:GLU:H	2.29	0.41
1:C:40:GLU:HG3	3:C:2006:HOH:O	2.20	0.41
1:C:55:TYR:HB2	3:C:2008:HOH:O	2.20	0.41
1:A:131:ASP:HB3	1:A:134:MET:HB2	2.03	0.41
1:C:218:PHE:CD1	1:C:218:PHE:N	2.88	0.41
1:A:6:THR:O	1:A:6:THR:HG22	2.21	0.40
1:B:4:ARG:HD2	1:B:13:GLU:OE1	2.22	0.40
1:B:15:SER:O	1:B:16:ARG:C	2.64	0.40
1:C:203:ARG:HG2	1:C:203:ARG:NH1	2.37	0.40
1:C:259:PRO:HD3	3:C:2039:HOH:O	2.20	0.40
1:B:234:ALA:O	1:B:238:ASN:N	2.52	0.40
1:C:57:GLY:O	1:C:58:TYR:HB2	2.21	0.40
1:B:112:GLN:HG3	1:B:116:ASN:HD21	1.87	0.40
1:A:124:LEU:HD12	1:A:154:HIS:C	2.46	0.40
1:A:224:GLN:N	1:A:225:PRO:CD	2.84	0.40
1:B:106:ILE:CD1	1:B:139:VAL:HG22	2.51	0.40
1:B:151:LYS:NZ	1:B:151:LYS:HB3	2.35	0.40
1:C:2:VAL:O	1:C:2:VAL:CG2	2.69	0.40
1:C:25:MET:CE	1:C:60:CYS:HA	2.46	0.40
1:C:78:MET:HE2	1:C:80:ILE:HD11	2.03	0.40
1:A:22:TRP:CE3	2:A:1298:NAP:H6N	2.56	0.40
1:A:25:MET:HE1	1:A:63:ALA:CB	2.52	0.40
1:B:52:ALA:HB3	1:B:55:TYR:CE2	2.57	0.40
1:C:30:SER:C	1:C:32:ARG:N	2.77	0.40
1:C:216:ARG:HD2	1:C:220:ASP:OD2	2.21	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	296/298 (99%)	266 (90%)	24 (8%)	6 (2%)	6	21
1	B	290/298 (97%)	258 (89%)	26 (9%)	6 (2%)	5	20
1	C	296/298 (99%)	260 (88%)	31 (10%)	5 (2%)	7	25
All	All	882/894 (99%)	784 (89%)	81 (9%)	17 (2%)	6	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	53	ASP
1	B	75	ARG
1	B	136	ALA
1	C	3	GLN
1	C	28	ASN
1	A	296	ASP
1	B	55	TYR
1	C	53	ASP
1	C	272	ALA
1	C	273	VAL
1	A	128	HIS
1	B	72	PRO
1	A	222	TYR
1	B	5	ILE
1	B	188	GLN
1	A	9	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/253 (100%)	235 (93%)	17 (7%)	15	42
1	B	252/253 (100%)	236 (94%)	16 (6%)	16	45
1	C	253/253 (100%)	233 (92%)	20 (8%)	11	35
All	All	757/759 (100%)	704 (93%)	53 (7%)	14	40

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	6	THR
1	A	9	PRO
1	A	19	MET
1	A	39	GLU
1	A	42	LEU
1	A	89	THR
1	A	125	LEU
1	A	126	LEU
1	A	128	HIS
1	A	174	PHE
1	A	180	GLN
1	A	190	LEU
1	A	251	LEU
1	A	258	LEU
1	A	267	GLU
1	A	293	LEU
1	B	19	MET
1	B	29	MET
1	B	43	ASP
1	B	44	LEU
1	B	93	GLU
1	B	114	LEU
1	B	124	LEU
1	B	125	LEU
1	B	128	HIS
1	B	151	LYS
1	B	205	ARG
1	B	235	GLU
1	B	243	GLU
1	B	252	ARG

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	287	ARG
1	C	2	VAL
1	C	9	PRO
1	C	19	MET
1	C	41	HIS
1	C	76	GLU
1	C	95	VAL
1	C	104	ASP
1	C	114	LEU
1	C	124	LEU
1	C	125	LEU
1	C	126	LEU
1	C	175	THR
1	C	192	LEU
1	C	205	ARG
1	C	218	PHE
1	C	220	ASP
1	C	247	ASN
1	C	258	LEU
1	C	284	GLN
1	C	287	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	59	GLN
1	A	121	HIS
1	A	145	HIS
1	A	147	HIS
1	A	148	GLN
1	A	154	HIS
1	A	169	GLN
1	A	188	GLN
1	A	198	GLN
1	A	200	GLN
1	A	201	GLN
1	A	219	ASN
1	B	28	ASN
1	B	33	GLN
1	B	105	HIS

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Mol	Chain	Res	Type
1	B	112	GLN
1	B	116	ASN
1	B	128	HIS
1	B	145	HIS
1	B	147	HIS
1	B	148	GLN
1	B	154	HIS
1	B	169	GLN
1	B	180	GLN
1	B	198	GLN
1	B	200	GLN
1	B	219	ASN
1	B	244	GLN
1	C	3	GLN
1	C	10	GLN
1	C	28	ASN
1	C	51	HIS
1	C	94	ASN
1	C	105	HIS
1	C	116	ASN
1	C	121	HIS
1	C	148	GLN
1	C	154	HIS
1	C	169	GLN
1	C	180	GLN
1	C	187	HIS
1	C	188	GLN
1	C	198	GLN
1	C	200	GLN
1	C	201	GLN
1	C	238	ASN
1	C	244	GLN
1	C	247	ASN
1	C	283	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	A	1298	-	50,52,52	2.11	12 (24%)	71,80,80	2.29	19 (26%)
2	NAP	C	1299	-	50,52,52	1.99	11 (22%)	71,80,80	2.31	20 (28%)
2	NAP	B	1299	-	50,52,52	1.99	11 (22%)	71,80,80	2.30	21 (29%)

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	A	1298	-	-	8/35/67/67	0/5/5/5
2	NAP	C	1299	-	-	12/35/67/67	0/5/5/5
2	NAP	B	1299	-	-	6/35/67/67	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1298	NAP	C2N-N1N	7.97	1.43	1.35
2	C	1299	NAP	C2N-N1N	6.75	1.42	1.35
2	B	1299	NAP	C2N-N1N	6.49	1.42	1.35
2	B	1299	NAP	C4N-C3N	5.57	1.47	1.39
2	A	1298	NAP	C4N-C3N	5.26	1.47	1.39
2	C	1299	NAP	C4N-C3N	5.18	1.47	1.39
2	A	1298	NAP	O4D-C1D	4.38	1.46	1.40
2	C	1299	NAP	O4D-C1D	4.37	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1299	NAP	O4D-C1D	4.18	1.46	1.40
2	B	1299	NAP	C2A-N1A	4.12	1.41	1.33
2	A	1298	NAP	C2A-N1A	4.09	1.41	1.33
2	C	1299	NAP	C2A-N1A	4.02	1.41	1.33
2	C	1299	NAP	C6N-N1N	3.98	1.44	1.35
2	A	1298	NAP	C6N-N1N	3.75	1.43	1.35
2	B	1299	NAP	C6N-N1N	3.60	1.43	1.35
2	C	1299	NAP	C2A-N3A	3.01	1.39	1.33
2	B	1299	NAP	C2A-N3A	2.92	1.39	1.33
2	A	1298	NAP	C2A-N3A	2.85	1.39	1.33
2	A	1298	NAP	C3N-C7N	2.82	1.54	1.50
2	A	1298	NAP	PA-O1A	-2.79	1.41	1.50
2	A	1298	NAP	C4A-N3A	2.72	1.39	1.34
2	C	1299	NAP	PA-O1A	-2.68	1.41	1.50
2	C	1299	NAP	C4A-N3A	2.54	1.39	1.34
2	B	1299	NAP	PA-O1A	-2.44	1.42	1.50
2	B	1299	NAP	C4A-N3A	2.43	1.39	1.34
2	C	1299	NAP	C5N-C4N	2.38	1.43	1.38
2	A	1298	NAP	P2B-O2B	2.31	1.63	1.59
2	B	1299	NAP	C5N-C4N	2.29	1.42	1.38
2	C	1299	NAP	C3N-C7N	2.24	1.53	1.50
2	B	1299	NAP	C6N-C5N	2.17	1.43	1.38
2	C	1299	NAP	C6N-C5N	2.16	1.43	1.38
2	B	1299	NAP	C3N-C7N	2.09	1.53	1.50
2	A	1298	NAP	C5B-C4B	2.09	1.57	1.51
2	A	1298	NAP	C6N-C5N	2.03	1.42	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1299	NAP	O3X-P2B-O1X	-7.85	80.25	110.83
2	B	1299	NAP	O3X-P2B-O1X	-7.80	80.45	110.83
2	A	1298	NAP	O5D-PN-O1N	-7.59	78.86	108.94
2	C	1299	NAP	O5D-PN-O1N	-7.53	79.07	108.94
2	B	1299	NAP	O5D-PN-O1N	-7.38	79.67	108.94
2	A	1298	NAP	O3X-P2B-O1X	-7.34	82.24	110.83
2	B	1299	NAP	O3X-P2B-O2B	-6.84	79.19	105.85
2	C	1299	NAP	O3X-P2B-O2B	-6.82	79.28	105.85
2	A	1298	NAP	O3X-P2B-O2B	-6.73	79.64	105.85
2	C	1299	NAP	O2B-P2B-O1X	5.26	128.09	109.33
2	B	1299	NAP	O2B-P2B-O1X	5.19	127.85	109.33
2	A	1298	NAP	O2B-P2B-O1X	4.78	126.36	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1298	NAP	O3X-P2B-O2X	-4.37	91.43	107.80
2	C	1299	NAP	O2N-PN-O5D	-4.11	88.94	107.57
2	A	1298	NAP	O2N-PN-O5D	-4.09	89.01	107.57
2	B	1299	NAP	O3X-P2B-O2X	-4.09	92.45	107.80
2	B	1299	NAP	O2N-PN-O5D	-4.03	89.28	107.57
2	C	1299	NAP	O3X-P2B-O2X	-4.00	92.80	107.80
2	C	1299	NAP	O3-PN-O1N	3.87	122.34	110.70
2	B	1299	NAP	O3-PN-O1N	3.80	122.14	110.70
2	A	1298	NAP	O3-PN-O1N	3.78	122.07	110.70
2	C	1299	NAP	N3A-C2A-N1A	-3.70	122.98	128.58
2	A	1298	NAP	N3A-C2A-N1A	-3.68	123.01	128.58
2	B	1299	NAP	N3A-C2A-N1A	-3.63	123.08	128.58
2	A	1298	NAP	C3N-C7N-N7N	3.45	121.99	117.74
2	C	1299	NAP	C3N-C7N-N7N	3.08	121.53	117.74
2	B	1299	NAP	O2A-PA-O1A	3.02	126.51	112.44
2	B	1299	NAP	C3N-C7N-N7N	2.92	121.34	117.74
2	C	1299	NAP	O2A-PA-O1A	2.89	125.91	112.44
2	B	1299	NAP	C4D-O4D-C1D	-2.84	107.33	109.92
2	A	1298	NAP	O2A-PA-O1A	2.79	125.42	112.44
2	C	1299	NAP	C2N-C3N-C4N	2.76	121.47	118.26
2	B	1299	NAP	C2N-C3N-C4N	2.69	121.39	118.26
2	A	1298	NAP	O7N-C7N-C3N	-2.68	116.33	119.60
2	C	1299	NAP	O7N-C7N-C3N	-2.67	116.34	119.60
2	A	1298	NAP	O4B-C4B-C5B	-2.66	100.81	109.33
2	B	1299	NAP	O7N-C7N-C3N	-2.57	116.46	119.60
2	B	1299	NAP	C5N-C4N-C3N	-2.52	117.89	120.36
2	A	1298	NAP	C2N-C3N-C4N	2.51	121.18	118.26
2	A	1298	NAP	O2X-P2B-O1X	2.48	120.51	110.83
2	A	1298	NAP	C4B-O4B-C1B	2.48	114.95	109.47
2	C	1299	NAP	C2B-C3B-C4B	2.48	107.33	101.99
2	B	1299	NAP	O4B-C4B-C5B	-2.47	101.42	109.33
2	C	1299	NAP	C5N-C4N-C3N	-2.46	117.94	120.36
2	A	1298	NAP	O3B-C3B-C4B	-2.46	104.03	111.08
2	C	1299	NAP	O2X-P2B-O1X	2.44	120.33	110.83
2	B	1299	NAP	O2X-P2B-O1X	2.41	120.24	110.83
2	B	1299	NAP	C4B-O4B-C1B	2.40	114.77	109.47
2	C	1299	NAP	C4B-O4B-C1B	2.39	114.74	109.47
2	A	1298	NAP	O2N-PN-O1N	2.36	123.41	112.44
2	C	1299	NAP	O2N-PN-O1N	2.34	123.35	112.44
2	A	1298	NAP	C2B-C3B-C4B	2.29	106.91	101.99
2	B	1299	NAP	O2N-PN-O1N	2.21	122.71	112.44
2	C	1299	NAP	O4B-C4B-C5B	-2.19	102.32	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1299	NAP	C2B-C1B-N9A	-2.14	110.24	113.75
2	A	1298	NAP	C6N-N1N-C1D	-2.11	115.58	119.73
2	B	1299	NAP	C2B-C3B-C4B	2.11	106.53	101.99
2	B	1299	NAP	O3B-C3B-C4B	-2.11	105.03	111.08
2	B	1299	NAP	C2B-C1B-N9A	-2.08	110.33	113.75
2	C	1299	NAP	C1B-N9A-C8A	2.04	131.63	127.09

There are no chirality outliers.

All (26) torsion outliers are listed below:

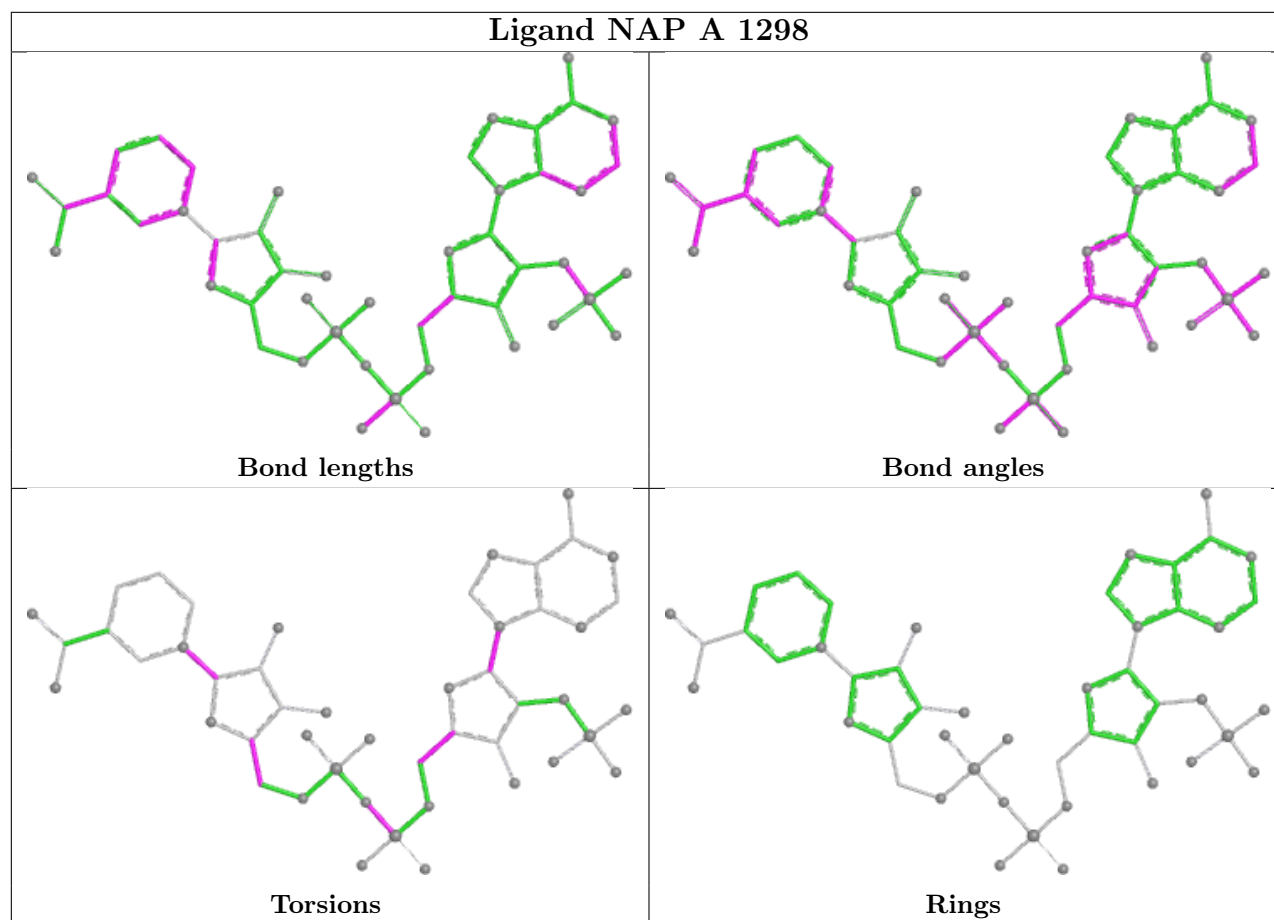
Mol	Chain	Res	Type	Atoms
2	A	1298	NAP	O4D-C1D-N1N-C2N
2	A	1298	NAP	O4D-C1D-N1N-C6N
2	A	1298	NAP	C2D-C1D-N1N-C2N
2	A	1298	NAP	C2D-C1D-N1N-C6N
2	B	1299	NAP	O4D-C1D-N1N-C2N
2	B	1299	NAP	O4D-C1D-N1N-C6N
2	B	1299	NAP	C2D-C1D-N1N-C2N
2	B	1299	NAP	C2D-C1D-N1N-C6N
2	C	1299	NAP	C5B-O5B-PA-O2A
2	C	1299	NAP	O4D-C1D-N1N-C2N
2	C	1299	NAP	O4D-C1D-N1N-C6N
2	C	1299	NAP	C2D-C1D-N1N-C2N
2	C	1299	NAP	C2D-C1D-N1N-C6N
2	C	1299	NAP	O4D-C4D-C5D-O5D
2	A	1298	NAP	O4D-C4D-C5D-O5D
2	A	1298	NAP	PN-O3-PA-O5B
2	C	1299	NAP	PN-O3-PA-O5B
2	C	1299	NAP	C3D-C4D-C5D-O5D
2	B	1299	NAP	PA-O3-PN-O2N
2	A	1298	NAP	O4B-C4B-C5B-O5B
2	A	1298	NAP	C2B-C1B-N9A-C8A
2	C	1299	NAP	C4D-C5D-O5D-PN
2	C	1299	NAP	PN-O3-PA-O2A
2	C	1299	NAP	PA-O3-PN-O1N
2	B	1299	NAP	O4B-C4B-C5B-O5B
2	C	1299	NAP	O4B-C4B-C5B-O5B

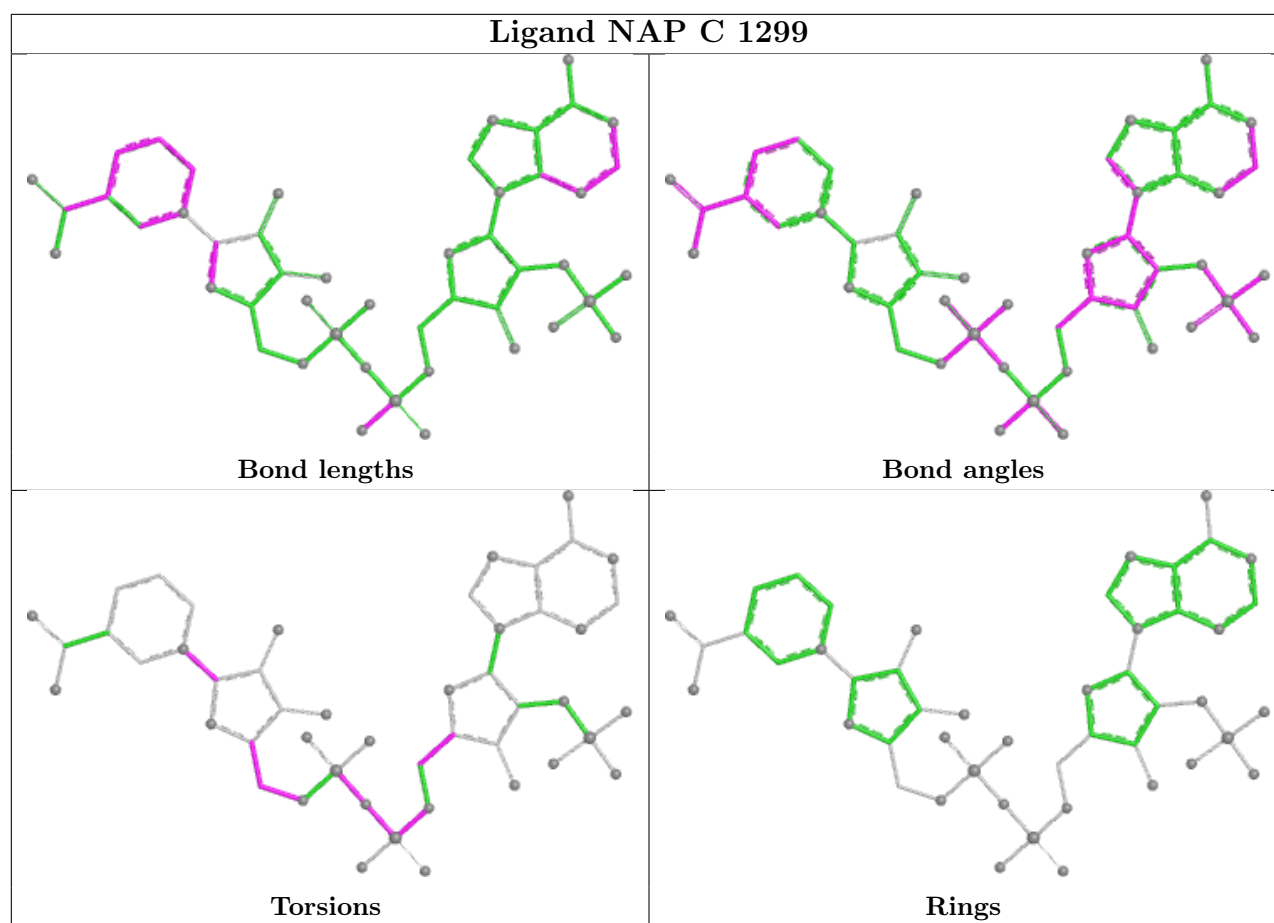
There are no ring outliers.

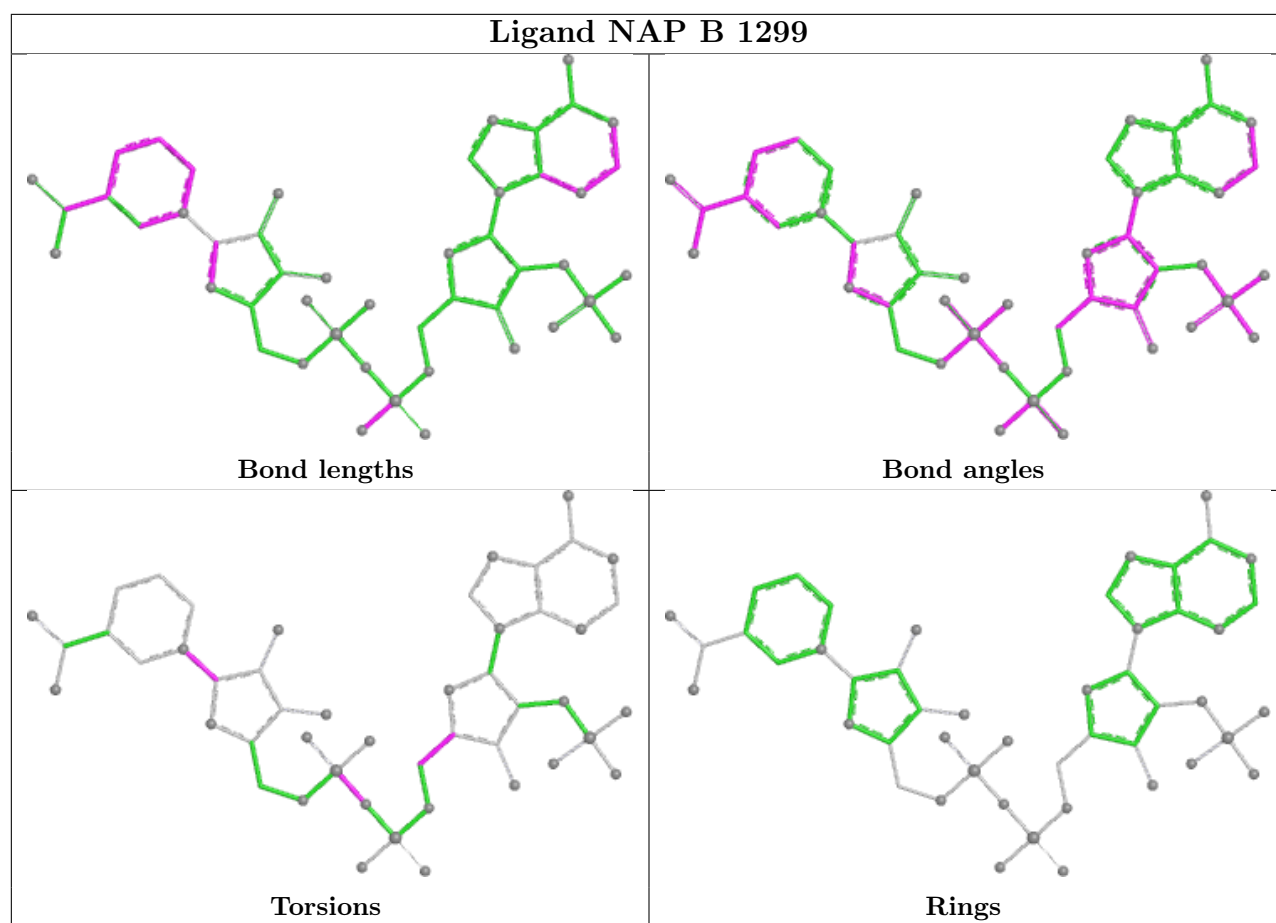
3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1298	NAP	8	0
2	C	1299	NAP	5	0
2	B	1299	NAP	7	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.