



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:23 PM UTC

PDB ID : 2GN9 / pdb_00002gn9
Title : Crystal structure of UDP-GlcNAc inverting 4,6-dehydratase in complex with NADP and UDP-Glc
Authors : Ishiyama, N.; Creuzenet, C.; Lam, J.S.; Berghuis, A.M.
Deposited on : 2006-04-09
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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

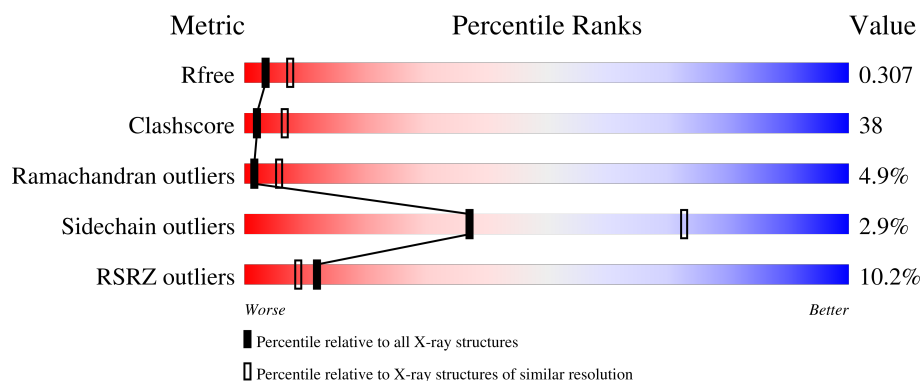
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	344	12% 38% 50% 7% .
1	B	344	8% 42% 46% 7% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5419 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 UDP-GlcNAc C6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2590	1656	440	479	15			
1	B	327	Total	C	N	O	S	0	0	0
			2573	1647	436	475	15			

There are 22 discrepancies between the modelled and reference sequences:

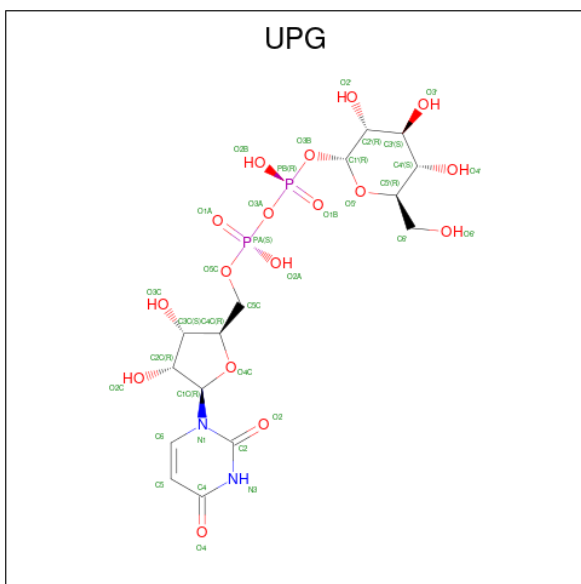
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	cloning artifact	UNP O25511
A	-9	HIS	-	expression tag	UNP O25511
A	-8	HIS	-	expression tag	UNP O25511
A	-7	HIS	-	expression tag	UNP O25511
A	-6	HIS	-	expression tag	UNP O25511
A	-5	HIS	-	expression tag	UNP O25511
A	-4	HIS	-	expression tag	UNP O25511
A	-3	GLY	-	cloning artifact	UNP O25511
A	-2	SER	-	cloning artifact	UNP O25511
A	-1	MET	-	cloning artifact	UNP O25511
A	0	SER	-	cloning artifact	UNP O25511
B	-10	MET	-	cloning artifact	UNP O25511
B	-9	HIS	-	expression tag	UNP O25511
B	-8	HIS	-	expression tag	UNP O25511
B	-7	HIS	-	expression tag	UNP O25511
B	-6	HIS	-	expression tag	UNP O25511
B	-5	HIS	-	expression tag	UNP O25511
B	-4	HIS	-	expression tag	UNP O25511
B	-3	GLY	-	cloning artifact	UNP O25511
B	-2	SER	-	cloning artifact	UNP O25511
B	-1	MET	-	cloning artifact	UNP O25511
B	0	SER	-	cloning artifact	UNP O25511

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



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

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $\text{C}_{15}\text{H}_{24}\text{N}_2\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 15	N 2	O 17	P 2	11	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	11	0
			36	15	2	17	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

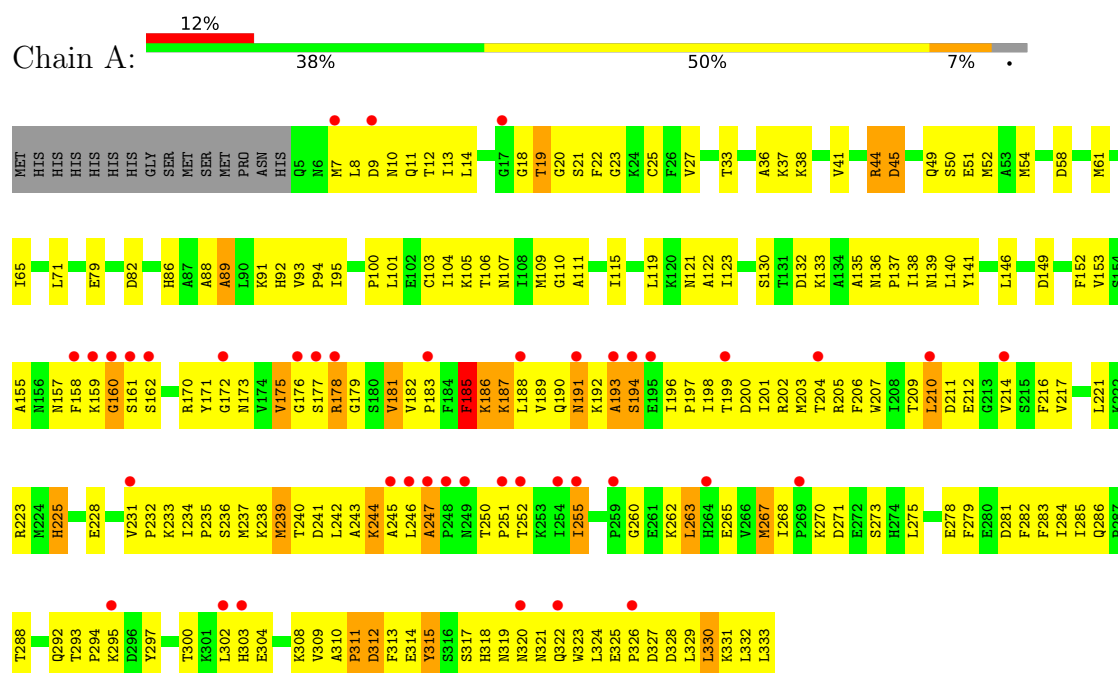
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		
5	B	42	Total	O	0	0
			42	42		

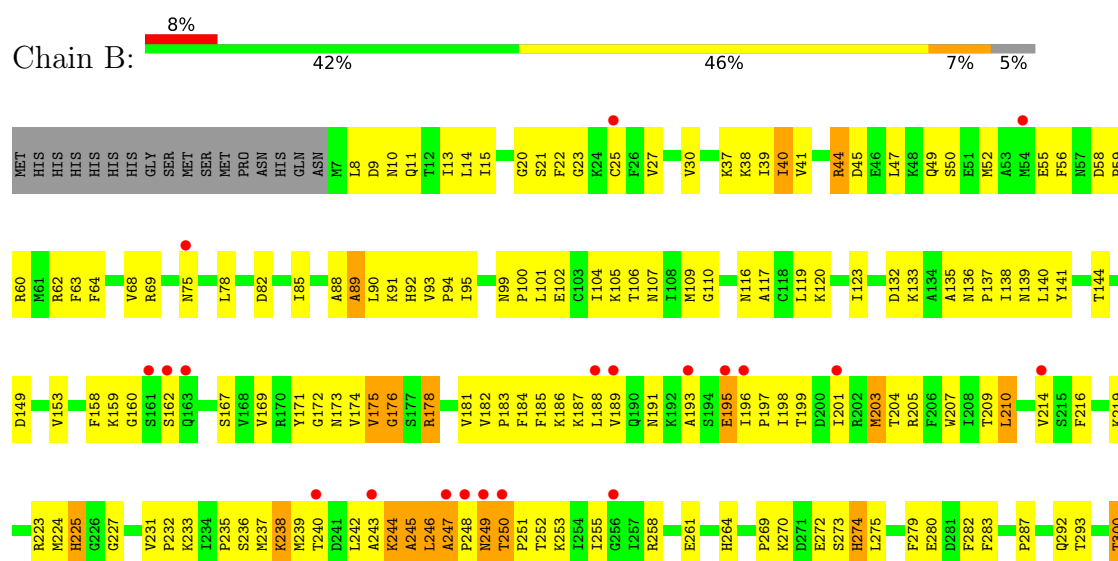
3 Residue-property plots

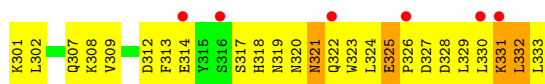
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UDP-GlcNAc C6 dehydratase



• Molecule 1: UDP-GlcNAc C6 dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	112.38Å 112.38Å 107.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.80) 96.9 (50.00-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.46 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.307 0.221 , 0.307	Depositor DCC
R_{free} test set	1852 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 82.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5419	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.40	0/2641	0.95	14/3568 (0.4%)
1	B	0.40	0/2624	0.95	10/3545 (0.3%)
All	All	0.40	0/5265	0.95	24/7113 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	PHE	N-CA-C	-7.22	105.00	113.88
1	B	225	HIS	N-CA-C	-7.09	104.89	113.97
1	A	225	HIS	N-CA-C	-6.25	105.67	113.55
1	B	44	ARG	N-CA-C	6.09	120.88	112.90
1	A	45	ASP	N-CA-C	6.01	118.42	109.59
1	A	330	LEU	N-CA-C	-5.99	104.82	111.71
1	A	58	ASP	CA-C-N	5.92	125.60	119.56
1	A	58	ASP	C-N-CA	5.92	125.60	119.56
1	A	71	LEU	N-CA-C	5.90	117.79	111.36
1	A	186	LYS	N-CA-C	-5.86	101.95	111.04
1	A	239	MET	N-CA-C	5.69	117.93	111.11
1	A	44	ARG	N-CA-C	5.68	118.68	111.69
1	B	40	ILE	N-CA-C	5.60	115.92	107.80
1	B	90	LEU	N-CA-C	-5.58	99.64	108.73
1	B	195	GLU	N-CA-C	5.50	115.38	108.45
1	B	107	ASN	N-CA-C	5.47	117.04	111.14
1	B	332	LEU	N-CA-C	-5.41	107.22	113.88
1	B	50	SER	N-CA-C	-5.40	105.05	111.69
1	B	330	LEU	N-CA-C	-5.37	105.86	112.90
1	A	160	GLY	N-CA-C	-5.34	103.34	111.14
1	B	331	LYS	N-CA-C	-5.34	106.02	112.54
1	A	267	MET	N-CA-C	-5.17	106.66	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ALA	N-CA-C	5.05	116.11	108.07
1	A	33	THR	N-CA-C	5.02	119.49	113.17

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	2590	0	2641	191	0
1	B	2573	0	2627	214	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
3	A	36	0	22	1	0
3	B	36	0	22	3	0
4	B	12	0	13	1	0
5	A	34	0	0	3	0
5	B	42	0	0	7	0
All	All	5419	0	5375	402	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 38.

All (402) 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:B:184:PHE:HA	1:B:187:LYS:HE2	1.39	1.03
1:A:189:VAL:HG21	1:A:247:ALA:HB2	1.38	1.02
1:B:321:ASN:HD22	1:B:322:GLN:N	1.73	0.87
1:A:223:ARG:HB2	1:A:300:THR:HB	1.56	0.85
1:B:269:PRO:HB2	1:B:272:GLU:HG2	1.57	0.85
1:B:159:LYS:NZ	1:B:292:GLN:HB2	1.90	0.85
1:B:250:THR:HG22	1:B:251:PRO:HD2	1.57	0.84
1:B:238:LYS:HE2	1:B:239:MET:H	1.43	0.84
1:B:38:LYS:HZ1	1:B:62:ARG:HH11	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ASP:OD2	1:B:172:GLY:HA2	1.81	0.81
1:B:38:LYS:NZ	1:B:62:ARG:HH11	1.78	0.81
1:B:270:LYS:HB2	1:B:314:GLU:OE1	1.82	0.80
1:A:209:THR:OG1	1:A:212:GLU:HB2	1.83	0.78
1:B:8:LEU:HD11	1:B:13:ILE:HD11	1.65	0.78
1:B:75:ASN:HD22	1:B:120:LYS:HD3	1.47	0.77
1:B:119:LEU:HD22	1:B:158:PHE:CD2	2.18	0.77
1:B:238:LYS:HD3	1:B:240:THR:H	1.50	0.77
1:A:194:SER:O	1:A:251:PRO:HG2	1.85	0.77
1:A:237:MET:HE1	1:A:329:LEU:HB2	1.67	0.76
1:B:20:GLY:HA2	1:B:178:ARG:NH1	2.00	0.76
1:B:174:VAL:HG11	1:B:210:LEU:HD22	1.67	0.76
1:B:75:ASN:ND2	1:B:120:LYS:HD3	2.01	0.75
1:B:325:GLU:HB2	1:B:328:ASP:OD2	1.85	0.75
1:A:25:CYS:SG	1:A:214:VAL:HG21	2.27	0.75
1:A:231:VAL:HB	1:A:283:PHE:HB2	1.68	0.75
1:B:38:LYS:HE2	1:B:40:ILE:HD11	1.67	0.74
1:B:237:MET:HE1	1:B:329:LEU:HB2	1.67	0.74
1:B:193:ALA:O	1:B:250:THR:HG21	1.87	0.74
1:B:225:HIS:HA	1:B:301:LYS:HE2	1.69	0.74
1:A:178:ARG:HD3	1:B:47:LEU:HG	1.67	0.74
1:A:7:MET:SD	1:A:9:ASP:HB3	2.28	0.74
1:A:51:GLU:HA	1:A:54:MET:HE2	1.68	0.73
1:B:198:ILE:HD11	1:B:243:ALA:HB2	1.70	0.73
1:A:7:MET:HE2	1:A:9:ASP:HA	1.70	0.72
1:B:238:LYS:HE2	1:B:239:MET:N	2.04	0.72
1:A:92:HIS:CE1	1:A:94:PRO:HG2	2.25	0.71
1:B:321:ASN:HD22	1:B:322:GLN:H	1.36	0.71
1:B:159:LYS:HZ1	1:B:293:THR:N	1.89	0.71
1:A:182:VAL:HG13	1:A:246:LEU:HD11	1.72	0.70
1:B:269:PRO:HD2	1:B:272:GLU:HG3	1.73	0.68
1:B:196:ILE:O	1:B:252:THR:HA	1.94	0.68
1:B:14:LEU:HD13	1:B:78:LEU:HD23	1.76	0.68
1:A:268:ILE:HG12	1:A:285:ILE:HD11	1.76	0.68
1:A:250:THR:HG23	1:A:251:PRO:HD2	1.76	0.67
1:B:88:ALA:O	1:B:89:ALA:HB2	1.93	0.67
1:A:109:MET:HE3	1:A:109:MET:HA	1.77	0.67
1:B:89:ALA:HB2	5:B:368:HOH:O	1.94	0.67
1:B:182:VAL:HG23	1:B:183:PRO:HD3	1.77	0.66
1:B:21:SER:HB3	1:B:210:LEU:HD21	1.78	0.66
1:B:149:ASP:O	1:B:153:VAL:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LEU:HD21	1:B:329:LEU:HD13	1.76	0.66
1:B:188:LEU:C	1:B:193:ALA:HB2	2.21	0.66
1:B:203:MET:O	1:B:239:MET:HB2	1.95	0.65
1:A:160:GLY:C	1:A:162:SER:H	2.04	0.65
1:B:58:ASP:OD1	1:B:60:ARG:HG2	1.97	0.65
1:B:159:LYS:HZ3	1:B:293:THR:HB	1.62	0.65
1:B:204:THR:O	1:B:205:ARG:HG2	1.97	0.65
1:A:7:MET:HG3	1:A:9:ASP:H	1.63	0.64
1:A:194:SER:C	1:A:251:PRO:HG2	2.22	0.64
1:B:264:HIS:HB3	1:B:317:SER:OG	1.97	0.64
1:A:237:MET:HE3	1:A:324:LEU:HB2	1.78	0.64
1:B:119:LEU:HD22	1:B:158:PHE:HD2	1.61	0.64
1:B:159:LYS:HZ1	1:B:292:GLN:HB2	1.59	0.64
1:B:184:PHE:HA	1:B:187:LYS:CE	2.22	0.64
1:B:236:SER:O	1:B:323:TRP:HA	1.98	0.63
1:A:186:LYS:HG2	1:A:246:LEU:HD22	1.81	0.63
1:B:68:VAL:HG22	2:B:334:NAP:N1A	2.14	0.62
1:A:241:ASP:HA	1:A:244:LYS:HD2	1.81	0.62
1:B:196:ILE:HB	1:B:252:THR:HG22	1.81	0.62
1:A:197:PRO:HB2	3:A:335:UPG:HN3	1.64	0.62
1:A:20:GLY:HA2	1:A:178:ARG:HH21	1.65	0.62
1:B:293:THR:O	1:B:293:THR:HG23	2.00	0.62
1:B:23:GLY:O	1:B:27:VAL:HG23	1.99	0.62
1:B:223:ARG:HG2	1:B:302:LEU:HD12	1.82	0.62
1:B:136:ASN:HD21	1:B:269:PRO:HB3	1.63	0.61
1:B:92:HIS:ND1	1:B:94:PRO:HD2	2.15	0.61
1:A:327:ASP:HA	1:A:330:LEU:HG	1.81	0.61
1:A:333:LEU:HD23	1:A:333:LEU:O	2.00	0.61
1:A:325:GLU:C	1:A:327:ASP:H	2.07	0.61
1:B:100:PRO:HA	1:B:140:LEU:CD2	2.30	0.61
1:B:242:LEU:HD13	1:B:329:LEU:HD23	1.82	0.61
1:A:9:ASP:O	1:A:11:GLN:HG3	2.00	0.61
1:B:197:PRO:HB2	1:B:255:ILE:HD13	1.81	0.61
1:A:27:VAL:HG11	1:A:61:MET:HE1	1.83	0.61
1:A:189:VAL:HA	1:A:193:ALA:HB2	1.82	0.61
1:A:188:LEU:C	1:A:190:GLN:H	2.07	0.61
1:B:13:ILE:HD12	1:B:30:VAL:HG11	1.83	0.61
1:A:18:GLY:HA2	1:A:23:GLY:HA3	1.83	0.60
1:A:133:LYS:HE3	5:A:366:HOH:O	2.01	0.60
1:A:300:THR:C	1:A:302:LEU:H	2.08	0.60
1:B:38:LYS:HE3	1:B:62:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:HG21	1:B:247:ALA:CB	2.31	0.60
1:A:122:ALA:HA	1:A:162:SER:OG	2.00	0.60
1:B:324:LEU:CD2	1:B:329:LEU:HD13	2.32	0.60
1:A:239:MET:SD	1:A:242:LEU:HD23	2.42	0.60
1:B:188:LEU:HB3	1:B:193:ALA:HB2	1.82	0.60
1:A:313:PHE:CZ	1:A:315:TYR:HB2	2.37	0.59
1:A:209:THR:C	1:A:211:ASP:H	2.10	0.59
1:A:327:ASP:O	1:A:331:LYS:HG3	2.03	0.59
1:A:238:LYS:HE2	1:A:240:THR:CG2	2.32	0.59
1:A:100:PRO:HA	1:A:140:LEU:CD2	2.33	0.58
1:A:206:PHE:HB3	1:A:234:ILE:CD1	2.33	0.58
1:A:235:PRO:HG3	1:A:322:GLN:NE2	2.19	0.58
1:B:239:MET:CE	1:B:242:LEU:HD23	2.34	0.58
1:B:160:GLY:C	1:B:162:SER:H	2.11	0.58
1:A:228:GLU:HG3	1:A:297:TYR:CD2	2.38	0.58
1:B:8:LEU:HD23	1:B:9:ASP:N	2.19	0.58
1:B:301:LYS:HD2	5:B:365:HOH:O	2.03	0.58
1:A:241:ASP:HA	1:A:244:LYS:CD	2.34	0.58
1:B:69:ARG:NH2	1:B:102:GLU:OE1	2.36	0.57
1:A:159:LYS:HD2	1:A:292:GLN:OE1	2.05	0.57
1:A:318:HIS:CE1	1:A:319:ASN:HB3	2.40	0.57
1:B:101:LEU:HG	1:B:105:LYS:HE3	1.86	0.57
1:A:88:ALA:O	1:A:89:ALA:HB2	2.04	0.57
1:A:225:HIS:HB3	1:A:295:LYS:HD3	1.86	0.56
1:B:258:ARG:HD3	1:B:261:GLU:OE2	2.04	0.56
1:B:60:ARG:HH11	1:B:60:ARG:HG3	1.71	0.56
1:A:8:LEU:HD23	1:A:13:ILE:HD11	1.88	0.56
1:A:12:THR:HG23	1:A:38:LYS:CG	2.36	0.56
1:B:181:VAL:HG23	3:B:335:UPG:O2A	2.06	0.56
1:B:38:LYS:NZ	1:B:62:ARG:NH1	2.51	0.55
1:A:22:PHE:CZ	1:A:217:VAL:HG21	2.40	0.55
1:A:130:SER:O	2:A:334:NAP:H6N	2.06	0.55
1:B:30:VAL:CG1	1:B:39:ILE:HD11	2.37	0.55
1:B:244:LYS:O	1:B:245:ALA:C	2.50	0.55
1:B:22:PHE:HA	1:B:210:LEU:HD11	1.89	0.54
1:B:173:ASN:HD22	1:B:173:ASN:N	2.04	0.54
1:B:199:THR:HG22	1:B:255:ILE:HG13	1.90	0.54
1:B:25:CYS:SG	1:B:214:VAL:HG21	2.48	0.54
1:B:237:MET:HE3	1:B:324:LEU:HD23	1.88	0.54
1:A:189:VAL:HG13	1:A:193:ALA:HB2	1.90	0.54
1:A:19:THR:HG22	2:A:334:NAP:O3B	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:O	1:A:110:GLY:HA3	2.08	0.54
1:A:278:GLU:HB2	1:A:309:VAL:HG12	1.90	0.54
1:B:244:LYS:C	1:B:248:PRO:HG3	2.33	0.54
1:A:242:LEU:HD13	1:A:329:LEU:CD2	2.38	0.54
1:A:240:THR:O	1:A:243:ALA:HB3	2.09	0.53
1:A:100:PRO:HB3	1:A:140:LEU:HD22	1.89	0.53
1:A:182:VAL:O	1:A:246:LEU:HD13	2.09	0.53
1:B:325:GLU:HB2	1:B:328:ASP:CG	2.32	0.53
1:A:235:PRO:HB2	1:A:324:LEU:HG	1.91	0.53
1:B:9:ASP:H	1:B:11:GLN:HG2	1.74	0.53
1:A:270:LYS:HB2	1:A:314:GLU:OE2	2.09	0.53
1:B:93:VAL:HB	1:B:94:PRO:HD3	1.90	0.53
1:B:167:SER:OG	1:B:224:MET:HE3	2.09	0.53
1:B:238:LYS:HD3	1:B:240:THR:HB	1.90	0.53
1:B:328:ASP:HA	1:B:331:LYS:HD2	1.89	0.53
1:B:245:ALA:HB2	1:B:326:PRO:O	2.09	0.53
1:B:309:VAL:HG21	1:B:313:PHE:CD2	2.43	0.53
1:B:30:VAL:HG12	1:B:39:ILE:HD11	1.90	0.52
1:B:207:TRP:CD1	1:B:237:MET:HB3	2.43	0.52
1:A:332:LEU:O	1:A:333:LEU:C	2.52	0.52
1:A:173:ASN:N	1:A:173:ASN:HD22	2.07	0.52
1:A:197:PRO:O	1:A:198:ILE:HD13	2.09	0.52
1:B:60:ARG:NH1	5:B:350:HOH:O	2.42	0.52
1:A:302:LEU:O	1:A:303:HIS:HB2	2.09	0.52
1:B:195:GLU:OE2	1:B:253:LYS:HD2	2.10	0.52
1:A:190:GLN:O	1:A:190:GLN:HG2	2.10	0.52
1:B:138:ILE:HG13	1:B:139:ASN:N	2.24	0.52
1:B:196:ILE:N	1:B:251:PRO:O	2.43	0.52
1:A:7:MET:HE2	1:A:9:ASP:CA	2.38	0.52
1:A:45:ASP:O	1:A:49:GLN:HG3	2.10	0.52
1:B:38:LYS:HE2	1:B:40:ILE:CD1	2.38	0.52
1:B:209:THR:CG2	1:B:332:LEU:HD21	2.40	0.52
1:B:209:THR:HG22	1:B:332:LEU:HD21	1.91	0.52
1:A:41:VAL:HG21	1:A:52:MET:HE2	1.92	0.51
1:A:198:ILE:HG22	1:A:199:THR:N	2.25	0.51
1:A:209:THR:C	1:A:211:ASP:N	2.67	0.51
1:B:91:LYS:HA	1:B:141:TYR:CE1	2.44	0.51
1:A:242:LEU:HD12	1:A:242:LEU:O	2.10	0.51
1:A:325:GLU:O	1:A:327:ASP:N	2.43	0.51
1:B:8:LEU:HD11	1:B:13:ILE:CD1	2.37	0.51
1:B:258:ARG:HD3	1:B:261:GLU:CD	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:VAL:HA	1:B:207:TRP:CZ3	2.46	0.51
1:A:149:ASP:O	1:A:153:VAL:HG23	2.10	0.51
1:B:246:LEU:O	1:B:247:ALA:HB2	2.09	0.51
1:B:49:GLN:OE1	1:B:63:PHE:HB3	2.11	0.51
1:A:329:LEU:O	1:A:332:LEU:HB2	2.10	0.51
1:B:189:VAL:HG21	1:B:247:ALA:HB2	1.93	0.51
1:B:237:MET:SD	1:B:329:LEU:HD22	2.50	0.51
1:B:318:HIS:C	1:B:320:ASN:H	2.18	0.51
1:B:11:GLN:HA	1:B:82:ASP:OD1	2.11	0.50
1:A:237:MET:HE3	1:A:324:LEU:CB	2.41	0.50
1:A:279:PHE:HB2	1:A:282:PHE:O	2.11	0.50
1:A:182:VAL:N	1:A:183:PRO:HD2	2.26	0.50
1:A:321:ASN:CG	1:A:322:GLN:N	2.69	0.50
1:A:235:PRO:HG3	1:A:322:GLN:HE21	1.76	0.50
1:B:182:VAL:CG2	1:B:183:PRO:HD3	2.41	0.50
1:B:133:LYS:O	1:B:137:PRO:HB3	2.11	0.50
1:A:7:MET:CG	1:A:9:ASP:HB3	2.42	0.50
1:B:181:VAL:HG21	3:B:335:UPG:O4C	2.11	0.50
1:A:91:LYS:HA	1:A:141:TYR:CE1	2.47	0.50
1:A:223:ARG:HB3	1:A:302:LEU:HG	1.94	0.50
1:B:116:ASN:HB2	4:B:336:MES:O1	2.12	0.50
1:B:250:THR:CG2	1:B:251:PRO:HD2	2.35	0.50
1:A:160:GLY:O	1:A:162:SER:N	2.43	0.50
1:A:188:LEU:C	1:A:190:GLN:N	2.70	0.50
1:A:216:PHE:CE2	1:A:232:PRO:HD3	2.46	0.50
1:A:171:TYR:HB3	1:A:232:PRO:CG	2.42	0.50
1:A:194:SER:HA	1:A:251:PRO:HD2	1.94	0.49
1:B:159:LYS:CE	1:B:292:GLN:HB2	2.40	0.49
1:A:115:ILE:HD13	1:A:155:ALA:HB2	1.95	0.49
1:B:38:LYS:HZ1	1:B:62:ARG:NH1	2.01	0.49
1:B:181:VAL:C	1:B:183:PRO:HD2	2.37	0.49
1:A:160:GLY:C	1:A:162:SER:N	2.70	0.49
1:A:171:TYR:HB3	1:A:232:PRO:HG3	1.95	0.49
1:A:333:LEU:HD23	1:A:333:LEU:C	2.36	0.49
1:B:78:LEU:HD12	1:B:117:ALA:CB	2.42	0.49
1:B:185:PHE:CB	1:B:246:LEU:HD13	2.43	0.49
1:A:186:LYS:O	1:A:190:GLN:N	2.45	0.49
1:A:327:ASP:HA	1:A:330:LEU:CG	2.43	0.49
1:B:8:LEU:HD23	1:B:8:LEU:C	2.38	0.49
1:A:187:LYS:O	1:A:191:ASN:ND2	2.41	0.49
1:A:206:PHE:HB3	1:A:234:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLY:CA	1:A:178:ARG:HH21	2.26	0.49
1:B:239:MET:HE3	1:B:242:LEU:HD23	1.94	0.49
1:B:201:ILE:C	1:B:238:LYS:HZ2	2.20	0.49
1:A:176:GLY:HA2	1:A:183:PRO:HD3	1.95	0.48
1:B:227:GLY:O	1:B:287:PRO:HG3	2.11	0.48
1:A:325:GLU:N	1:A:328:ASP:OD2	2.44	0.48
1:A:101:LEU:CD2	1:A:105:LYS:HE3	2.44	0.48
1:B:186:LYS:HZ1	1:B:333:LEU:HD12	1.78	0.48
1:B:293:THR:HG21	5:B:351:HOH:O	2.13	0.48
1:A:197:PRO:HB3	1:A:255:ILE:HD12	1.94	0.48
1:A:7:MET:HG3	1:A:9:ASP:HB3	1.96	0.48
1:B:105:LYS:O	1:B:109:MET:HB2	2.13	0.48
1:A:310:ALA:O	1:A:312:ASP:N	2.47	0.48
1:A:189:VAL:HG13	1:A:193:ALA:CB	2.44	0.48
1:B:88:ALA:O	1:B:89:ALA:CB	2.60	0.48
1:B:159:LYS:HZ3	1:B:293:THR:CB	2.26	0.48
1:B:189:VAL:N	1:B:193:ALA:HB2	2.28	0.48
1:B:160:GLY:C	1:B:162:SER:N	2.71	0.47
1:B:274:HIS:CD2	1:B:275:LEU:H	2.32	0.47
1:A:11:GLN:N	1:A:37:LYS:H	2.12	0.47
1:A:204:THR:O	1:A:205:ARG:HG2	2.13	0.47
1:A:11:GLN:O	1:A:36:ALA:HB1	2.14	0.47
1:A:191:ASN:C	1:A:192:LYS:HG3	2.39	0.47
1:B:159:LYS:NZ	1:B:293:THR:HG22	2.29	0.47
1:B:219:LYS:HB3	1:B:223:ARG:NH1	2.29	0.47
1:B:309:VAL:HG21	1:B:313:PHE:HD2	1.79	0.47
1:A:286:GLN:HG2	1:A:297:TYR:CD1	2.50	0.47
1:B:238:LYS:CE	1:B:239:MET:H	2.21	0.47
1:A:86:HIS:HE1	5:A:349:HOH:O	1.97	0.47
1:B:181:VAL:HG11	1:B:239:MET:CE	2.45	0.47
1:B:242:LEU:CD1	1:B:329:LEU:HD23	2.44	0.47
1:A:318:HIS:ND1	1:A:319:ASN:N	2.63	0.47
1:A:330:LEU:C	1:A:332:LEU:H	2.23	0.47
1:B:136:ASN:N	1:B:137:PRO:CD	2.77	0.47
1:B:216:PHE:CE2	1:B:232:PRO:HD3	2.50	0.47
1:B:238:LYS:CE	1:B:239:MET:N	2.75	0.47
1:A:92:HIS:HE1	1:A:94:PRO:HG2	1.76	0.47
1:B:188:LEU:HB3	1:B:193:ALA:CB	2.44	0.47
1:B:188:LEU:CB	1:B:193:ALA:HB2	2.45	0.47
1:B:325:GLU:CB	1:B:328:ASP:OD2	2.60	0.47
1:B:92:HIS:CE1	1:B:94:PRO:HD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLY:HA2	1:B:183:PRO:HD3	1.97	0.46
1:B:325:GLU:C	1:B:327:ASP:H	2.21	0.46
1:A:36:ALA:O	1:A:37:LYS:C	2.58	0.46
1:B:185:PHE:CD2	1:B:246:LEU:HD13	2.50	0.46
1:B:13:ILE:CD1	1:B:30:VAL:HG11	2.46	0.46
1:B:238:LYS:HE2	1:B:238:LYS:HA	1.96	0.46
1:A:132:ASP:OD2	1:A:172:GLY:HA2	2.15	0.46
1:B:203:MET:HE3	3:B:335:UPG:O2C	2.15	0.46
1:A:44:ARG:NH1	1:B:44:ARG:HB3	2.30	0.46
1:B:106:THR:O	1:B:110:GLY:HA3	2.16	0.46
1:B:172:GLY:O	2:B:334:NAP:H4N	2.15	0.46
1:B:237:MET:HE3	1:B:324:LEU:HB3	1.97	0.46
1:B:270:LYS:HE3	1:B:312:ASP:OD1	2.16	0.46
1:A:100:PRO:CB	1:A:140:LEU:HD22	2.46	0.46
1:B:300:THR:C	1:B:302:LEU:H	2.23	0.46
1:A:196:ILE:H	1:A:252:THR:HA	1.79	0.45
1:B:25:CYS:SG	1:B:210:LEU:HD12	2.56	0.45
1:B:55:GLU:HG3	1:B:56:PHE:CD1	2.51	0.45
1:A:14:LEU:C	1:A:14:LEU:HD23	2.42	0.45
1:A:231:VAL:CG1	1:A:267:MET:HG3	2.46	0.45
1:A:111:ALA:HB1	1:A:152:PHE:CE2	2.52	0.45
1:A:300:THR:C	1:A:302:LEU:N	2.71	0.45
1:A:186:LYS:O	1:A:188:LEU:N	2.49	0.45
1:A:12:THR:HG23	1:A:38:LYS:HG3	1.99	0.45
1:A:103:CYS:SG	1:A:107:ASN:ND2	2.89	0.45
1:A:278:GLU:HB2	1:A:309:VAL:CG1	2.46	0.45
1:A:281:ASP:OD1	1:A:281:ASP:N	2.49	0.45
1:B:274:HIS:CD2	1:B:274:HIS:N	2.83	0.45
1:A:284:ILE:O	1:A:284:ILE:HG22	2.15	0.45
1:A:322:GLN:C	1:A:323:TRP:CD1	2.94	0.45
1:B:185:PHE:HB2	1:B:246:LEU:HD22	1.98	0.45
1:A:22:PHE:HZ	1:A:217:VAL:HG21	1.82	0.45
1:A:157:ASN:O	1:A:158:PHE:C	2.60	0.45
1:B:45:ASP:HA	5:B:354:HOH:O	2.16	0.45
1:B:238:LYS:HD3	1:B:240:THR:CB	2.46	0.45
1:B:60:ARG:HG3	1:B:60:ARG:NH1	2.31	0.44
1:B:279:PHE:HB2	1:B:282:PHE:O	2.17	0.44
1:A:93:VAL:HG12	1:A:94:PRO:N	2.31	0.44
1:A:119:LEU:HD22	1:A:158:PHE:CE2	2.52	0.44
1:A:175:VAL:HA	1:A:207:TRP:CZ3	2.52	0.44
1:A:203:MET:HA	1:A:263:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PRO:CG	1:A:322:GLN:HE21	2.29	0.44
1:A:325:GLU:C	1:A:327:ASP:N	2.75	0.44
1:B:14:LEU:HD23	1:B:14:LEU:C	2.41	0.44
1:B:322:GLN:C	1:B:323:TRP:CD1	2.95	0.44
1:A:139:ASN:HB3	1:A:260:GLY:O	2.17	0.44
1:A:190:GLN:O	1:A:191:ASN:CG	2.60	0.44
1:A:236:SER:CB	1:A:320:ASN:HD22	2.30	0.44
1:B:173:ASN:N	1:B:173:ASN:ND2	2.65	0.44
1:A:137:PRO:HA	5:A:344:HOH:O	2.18	0.44
1:A:205:ARG:HD3	1:A:265:GLU:CG	2.47	0.44
1:A:206:PHE:CE1	1:A:317:SER:HB3	2.52	0.44
1:A:238:LYS:HE2	1:A:240:THR:HG23	1.99	0.44
1:B:320:ASN:ND2	1:B:322:GLN:O	2.50	0.44
1:A:202:ARG:O	1:A:204:THR:HG23	2.18	0.44
1:B:14:LEU:HD13	1:B:78:LEU:CD2	2.47	0.44
1:B:47:LEU:HD13	1:B:47:LEU:C	2.43	0.44
1:A:135:ALA:O	1:A:136:ASN:C	2.59	0.44
1:B:186:LYS:NZ	1:B:333:LEU:HD12	2.33	0.44
1:B:312:ASP:O	1:B:312:ASP:CG	2.61	0.44
1:B:95:ILE:HG23	1:B:99:ASN:HD22	1.83	0.44
1:A:177:SER:O	1:A:178:ARG:C	2.61	0.43
1:A:318:HIS:CG	1:A:319:ASN:N	2.86	0.43
1:A:173:ASN:N	1:A:173:ASN:ND2	2.66	0.43
1:A:235:PRO:HA	1:A:322:GLN:HG3	2.00	0.43
1:B:45:ASP:OD1	1:B:47:LEU:N	2.51	0.43
1:B:45:ASP:OD1	1:B:47:LEU:HB3	2.18	0.43
1:A:210:LEU:O	1:A:214:VAL:HG23	2.18	0.43
1:A:246:LEU:O	1:A:247:ALA:HB2	2.17	0.43
1:A:228:GLU:HG3	1:A:297:TYR:CE2	2.53	0.43
1:B:171:TYR:O	2:B:334:NAP:H5N	2.17	0.43
1:B:82:ASP:O	1:B:123:ILE:HG23	2.19	0.43
1:A:92:HIS:CE1	1:A:95:ILE:HG13	2.54	0.43
1:A:300:THR:CG2	1:A:304:GLU:HB2	2.47	0.43
1:B:328:ASP:HA	1:B:331:LYS:CD	2.48	0.43
1:A:275:LEU:CD1	1:A:288:THR:HG22	2.49	0.43
1:B:10:ASN:HA	1:B:37:LYS:HB2	1.99	0.43
1:B:140:LEU:O	1:B:144:THR:HG23	2.19	0.43
1:B:325:GLU:N	1:B:328:ASP:OD2	2.52	0.43
1:A:8:LEU:HD23	1:A:13:ILE:CD1	2.48	0.43
1:B:41:VAL:HG21	1:B:52:MET:CE	2.49	0.43
1:A:27:VAL:HG11	1:A:61:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:C	1:A:295:LYS:HG3	2.43	0.42
1:B:318:HIS:C	1:B:320:ASN:N	2.77	0.42
1:B:184:PHE:HD1	1:B:187:LYS:NZ	2.17	0.42
1:A:203:MET:SD	1:A:263:LEU:HA	2.59	0.42
1:A:159:LYS:NZ	1:A:293:THR:OG1	2.47	0.42
1:B:182:VAL:HG23	1:B:183:PRO:CD	2.47	0.42
1:A:235:PRO:CA	1:A:322:GLN:HE21	2.31	0.42
1:A:267:MET:HB3	1:A:315:TYR:CD2	2.55	0.42
1:B:101:LEU:HD12	1:B:101:LEU:HA	1.90	0.42
1:B:181:VAL:HG13	1:B:185:PHE:CE1	2.54	0.42
1:B:182:VAL:HG11	1:B:329:LEU:HD21	2.01	0.42
1:A:50:SER:C	1:A:52:MET:H	2.27	0.42
1:B:174:VAL:O	1:B:175:VAL:C	2.62	0.42
1:A:176:GLY:HA2	1:A:182:VAL:HB	2.02	0.42
1:B:58:ASP:HA	1:B:59:PRO:HD3	1.82	0.42
1:A:186:LYS:CG	1:A:246:LEU:HD22	2.47	0.42
1:A:200:ASP:HB3	1:A:203:MET:HB2	2.02	0.42
1:A:286:GLN:HE21	1:A:297:TYR:HD1	1.68	0.42
1:A:321:ASN:OD1	1:A:322:GLN:N	2.50	0.42
1:B:78:LEU:HD12	1:B:117:ALA:HB3	2.02	0.42
1:B:100:PRO:O	1:B:104:ILE:HD12	2.20	0.42
1:B:191:ASN:O	1:B:191:ASN:CG	2.61	0.42
1:B:235:PRO:HA	1:B:322:GLN:HB2	2.01	0.42
1:A:201:ILE:HG22	1:A:201:ILE:O	2.20	0.41
1:B:140:LEU:O	1:B:141:TYR:C	2.63	0.41
1:B:272:GLU:O	1:B:273:SER:C	2.62	0.41
1:A:194:SER:CA	1:A:251:PRO:HG2	2.49	0.41
1:A:275:LEU:HD11	1:A:288:THR:HG22	2.01	0.41
1:A:320:ASN:ND2	1:A:322:GLN:O	2.53	0.41
1:B:15:ILE:HA	1:B:85:ILE:O	2.19	0.41
1:B:174:VAL:HG21	5:B:360:HOH:O	2.19	0.41
1:B:182:VAL:N	1:B:183:PRO:HD2	2.35	0.41
1:B:231:VAL:HB	1:B:283:PHE:HB2	2.01	0.41
1:B:238:LYS:HE2	1:B:238:LYS:CA	2.50	0.41
1:A:130:SER:HB3	1:A:170:ARG:HB2	2.01	0.41
1:A:194:SER:HA	1:A:251:PRO:CG	2.51	0.41
1:A:241:ASP:C	1:A:243:ALA:N	2.77	0.41
1:B:58:ASP:OD1	1:B:58:ASP:C	2.63	0.41
1:B:321:ASN:ND2	1:B:322:GLN:HG3	2.35	0.41
1:B:20:GLY:HA2	1:B:178:ARG:HH12	1.82	0.41
1:A:65:ILE:HB	1:B:102:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ALA:C	1:A:247:ALA:H	2.28	0.41
1:A:273:SER:C	1:A:275:LEU:H	2.29	0.41
1:B:248:PRO:O	1:B:249:ASN:C	2.64	0.41
1:A:9:ASP:O	1:A:10:ASN:C	2.64	0.41
1:A:82:ASP:O	1:A:123:ILE:HG23	2.20	0.41
1:B:242:LEU:HD12	1:B:242:LEU:O	2.21	0.41
1:A:79:GLU:HA	1:A:121:ASN:OD1	2.21	0.41
1:A:185:PHE:CB	1:A:246:LEU:HD13	2.51	0.41
1:A:194:SER:HA	1:A:251:PRO:HG2	2.03	0.41
1:A:209:THR:O	1:A:211:ASP:N	2.54	0.41
1:B:40:ILE:CG2	1:B:64:PHE:HD2	2.33	0.41
1:B:325:GLU:C	1:B:327:ASP:N	2.79	0.41
1:A:239:MET:O	1:A:240:THR:C	2.62	0.41
1:B:201:ILE:O	1:B:238:LYS:HD2	2.21	0.41
1:B:237:MET:CE	1:B:324:LEU:HD23	2.50	0.41
1:B:321:ASN:ND2	1:B:322:GLN:N	2.55	0.41
1:B:68:VAL:HG21	5:B:344:HOH:O	2.21	0.40
1:B:135:ALA:O	1:B:136:ASN:C	2.64	0.40
1:B:159:LYS:NZ	1:B:293:THR:HB	2.35	0.40
1:A:233:LYS:HE2	1:A:283:PHE:CE2	2.57	0.40
1:A:311:PRO:O	1:A:312:ASP:HB3	2.22	0.40
1:B:159:LYS:HZ1	1:B:293:THR:H	1.64	0.40
1:A:181:VAL:O	1:A:185:PHE:HB2	2.22	0.40
1:B:233:LYS:HD2	1:B:280:GLU:O	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	327/344 (95%)	267 (82%)	40 (12%)	20 (6%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	325/344 (94%)	274 (84%)	39 (12%)	12 (4%)	2	9
All	All	652/688 (95%)	541 (83%)	79 (12%)	32 (5%)	1	6

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	VAL
1	A	255	ILE
1	A	312	ASP
1	B	244	LYS
1	A	21	SER
1	A	161	SER
1	A	179	GLY
1	A	187	LYS
1	A	193	ALA
1	A	308	LYS
1	A	315	TYR
1	B	175	VAL
1	B	176	GLY
1	B	178	ARG
1	B	203	MET
1	B	245	ALA
1	B	247	ALA
1	B	308	LYS
1	A	178	ARG
1	A	191	ASN
1	A	247	ALA
1	A	326	PRO
1	B	89	ALA
1	B	246	LEU
1	B	249	ASN
1	A	262	LYS
1	B	300	THR
1	A	194	SER
1	A	210	LEU
1	A	181	VAL
1	A	138	ILE
1	A	311	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	290/304 (95%)	282 (97%)	8 (3%)	38	73
1	B	288/304 (95%)	279 (97%)	9 (3%)	35	70
All	All	578/608 (95%)	561 (97%)	17 (3%)	37	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	104	ILE
1	A	146	LEU
1	A	185	PHE
1	A	221	LEU
1	A	244	LYS
1	A	263	LEU
1	A	271	ASP
1	B	169	VAL
1	B	210	LEU
1	B	238	LYS
1	B	250	THR
1	B	274	HIS
1	B	307	GLN
1	B	319	ASN
1	B	321	ASN
1	B	325	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	86	HIS
1	A	125	GLN
1	A	165	GLN
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	286	GLN
1	A	320	ASN
1	A	322	GLN
1	B	35	ASN
1	B	75	ASN
1	B	136	ASN
1	B	173	ASN
1	B	190	GLN
1	B	264	HIS
1	B	274	HIS
1	B	286	GLN
1	B	307	GLN
1	B	320	ASN
1	B	321	ASN
1	B	322	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](#)

5 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	B	334	-	50,52,52	1.71	11 (22%)	71,80,80	1.90	15 (21%)
2	NAP	A	334	-	50,52,52	1.70	11 (22%)	71,80,80	1.93	14 (19%)
3	UPG	B	335	-	37,38,38	1.15	3 (8%)	55,58,58	1.34	3 (5%)
4	MES	B	336	-	12,12,12	0.75	0	15,16,16	1.04	1 (6%)
3	UPG	A	335	-	37,38,38	1.14	3 (8%)	55,58,58	1.37	3 (5%)

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	B	334	-	-	17/35/67/67	0/5/5/5
2	NAP	A	334	-	-	10/35/67/67	0/5/5/5
3	UPG	B	335	-	-	5/23/59/59	0/3/3/3
4	MES	B	336	-	-	2/6/14/14	0/1/1/1
3	UPG	A	335	-	-	6/23/59/59	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	NAP	C2N-N1N	4.34	1.39	1.35
2	A	334	NAP	C2N-N1N	3.86	1.39	1.35
2	A	334	NAP	P2B-O1X	3.59	1.61	1.50
2	B	334	NAP	C2A-N1A	3.58	1.40	1.33
2	A	334	NAP	C2A-N1A	3.49	1.40	1.33
2	B	334	NAP	P2B-O1X	3.45	1.61	1.50
2	A	334	NAP	PN-O1N	3.42	1.62	1.50
2	B	334	NAP	PN-O1N	3.31	1.62	1.50
3	A	335	UPG	PB-O1B	3.22	1.62	1.50
3	B	335	UPG	PB-O1B	3.18	1.61	1.50
3	A	335	UPG	PA-O1A	3.16	1.61	1.50
2	B	334	NAP	PA-O1A	3.14	1.61	1.50
3	B	335	UPG	PA-O1A	3.10	1.61	1.50
3	A	335	UPG	C5-C4	3.03	1.50	1.43
3	B	335	UPG	C5-C4	3.01	1.50	1.43
2	A	334	NAP	C4N-C3N	2.97	1.43	1.39
2	A	334	NAP	PA-O1A	2.95	1.61	1.50
2	B	334	NAP	C4N-C3N	2.81	1.43	1.39
2	A	334	NAP	C5N-C4N	2.72	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	NAP	C7N-N7N	2.63	1.37	1.33
2	B	334	NAP	C5N-C4N	2.55	1.43	1.38
2	A	334	NAP	C4A-N9A	-2.51	1.32	1.37
2	B	334	NAP	C4A-N9A	-2.47	1.32	1.37
2	B	334	NAP	C4A-N3A	2.41	1.38	1.34
2	A	334	NAP	C7N-N7N	2.38	1.37	1.33
2	A	334	NAP	C4A-N3A	2.37	1.38	1.34
2	B	334	NAP	P2B-O2B	2.06	1.63	1.59
2	A	334	NAP	P2B-O3X	2.03	1.62	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	334	NAP	C4A-N9A-C8A	7.25	113.35	105.74
2	B	334	NAP	C4A-N9A-C8A	7.03	113.12	105.74
2	A	334	NAP	C6N-N1N-C2N	6.92	127.77	121.88
2	B	334	NAP	C6N-N1N-C2N	6.82	127.68	121.88
3	B	335	UPG	O5'-C1'-O3B	-6.77	102.52	111.36
3	A	335	UPG	O5'-C1'-O3B	-6.66	102.67	111.36
2	B	334	NAP	N3A-C4A-N9A	4.17	134.25	127.17
2	A	334	NAP	N3A-C4A-N9A	4.12	134.17	127.17
2	A	334	NAP	C3N-C7N-N7N	-3.84	113.01	117.74
2	A	334	NAP	N9A-C8A-N7A	-3.74	108.63	113.94
2	B	334	NAP	N9A-C8A-N7A	-3.62	108.79	113.94
2	A	334	NAP	O7N-C7N-C3N	3.50	123.88	119.60
2	B	334	NAP	O7N-C7N-C3N	3.17	123.47	119.60
2	B	334	NAP	C3N-C7N-N7N	-3.03	114.00	117.74
2	B	334	NAP	C5A-C4A-N3A	-2.92	122.70	126.72
2	A	334	NAP	C5A-C4A-N3A	-2.86	122.78	126.72
2	B	334	NAP	C5N-C6N-N1N	-2.75	116.64	120.38
3	A	335	UPG	C3C-C2C-C1C	2.71	106.59	101.46
2	B	334	NAP	C6N-N1N-C1D	-2.70	114.42	119.73
2	A	334	NAP	C6N-N1N-C1D	-2.69	114.45	119.73
2	B	334	NAP	C6A-C5A-C4A	2.62	120.75	117.18
2	A	334	NAP	C5N-C6N-N1N	-2.61	116.82	120.38
2	A	334	NAP	C6A-C5A-C4A	2.60	120.72	117.18
2	A	334	NAP	N6A-C6A-N1A	2.57	124.09	118.38
2	B	334	NAP	N6A-C6A-N1A	2.56	124.08	118.38
2	B	334	NAP	C5A-C4A-N9A	-2.54	103.05	105.81
2	A	334	NAP	C5A-C4A-N9A	-2.53	103.05	105.81
3	B	335	UPG	O4-C4-N3	2.26	122.55	119.27
3	A	335	UPG	O4-C4-N3	2.25	122.54	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	335	UPG	C3C-C2C-C1C	2.24	105.69	101.46
2	B	334	NAP	C6A-C5A-N7A	-2.22	127.81	132.09
2	A	334	NAP	O4B-C1B-N9A	2.16	112.23	108.09
2	B	334	NAP	O4B-C1B-N9A	2.14	112.20	108.09
2	A	334	NAP	C6A-C5A-N7A	-2.13	127.99	132.09
2	B	334	NAP	P2B-O2B-C2B	-2.10	117.82	123.43
4	B	336	MES	O1-C6-C5	-2.02	107.42	111.77

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	334	NAP	C5D-O5D-PN-O3
2	A	334	NAP	O4D-C1D-N1N-C2N
2	A	334	NAP	O4D-C1D-N1N-C6N
2	A	334	NAP	C2N-C3N-C7N-O7N
2	A	334	NAP	C2N-C3N-C7N-N7N
2	B	334	NAP	C5D-O5D-PN-O3
2	B	334	NAP	C5D-O5D-PN-O1N
2	B	334	NAP	O4D-C1D-N1N-C2N
2	B	334	NAP	O4D-C1D-N1N-C6N
3	A	335	UPG	C5C-O5C-PA-O3A
3	A	335	UPG	C1'-O3B-PB-O3A
3	B	335	UPG	C1'-O3B-PB-O3A
3	B	335	UPG	O5'-C1'-O3B-PB
2	A	334	NAP	C4N-C3N-C7N-O7N
2	A	334	NAP	C4N-C3N-C7N-N7N
3	A	335	UPG	O5'-C5'-C6'-O6'
3	A	335	UPG	C4'-C5'-C6'-O6'
2	B	334	NAP	C4N-C3N-C7N-N7N
2	B	334	NAP	C4N-C3N-C7N-O7N
2	B	334	NAP	C2N-C3N-C7N-O7N
2	B	334	NAP	C2N-C3N-C7N-N7N
4	B	336	MES	C8-C7-N4-C3
4	B	336	MES	C8-C7-N4-C5
3	B	335	UPG	C1'-O3B-PB-O2B
2	B	334	NAP	C5D-O5D-PN-O2N
2	A	334	NAP	C2B-O2B-P2B-O2X
2	B	334	NAP	C2D-C1D-N1N-C2N
2	B	334	NAP	C2D-C1D-N1N-C6N
2	B	334	NAP	PN-O3-PA-O5B
2	B	334	NAP	O4B-C4B-C5B-O5B

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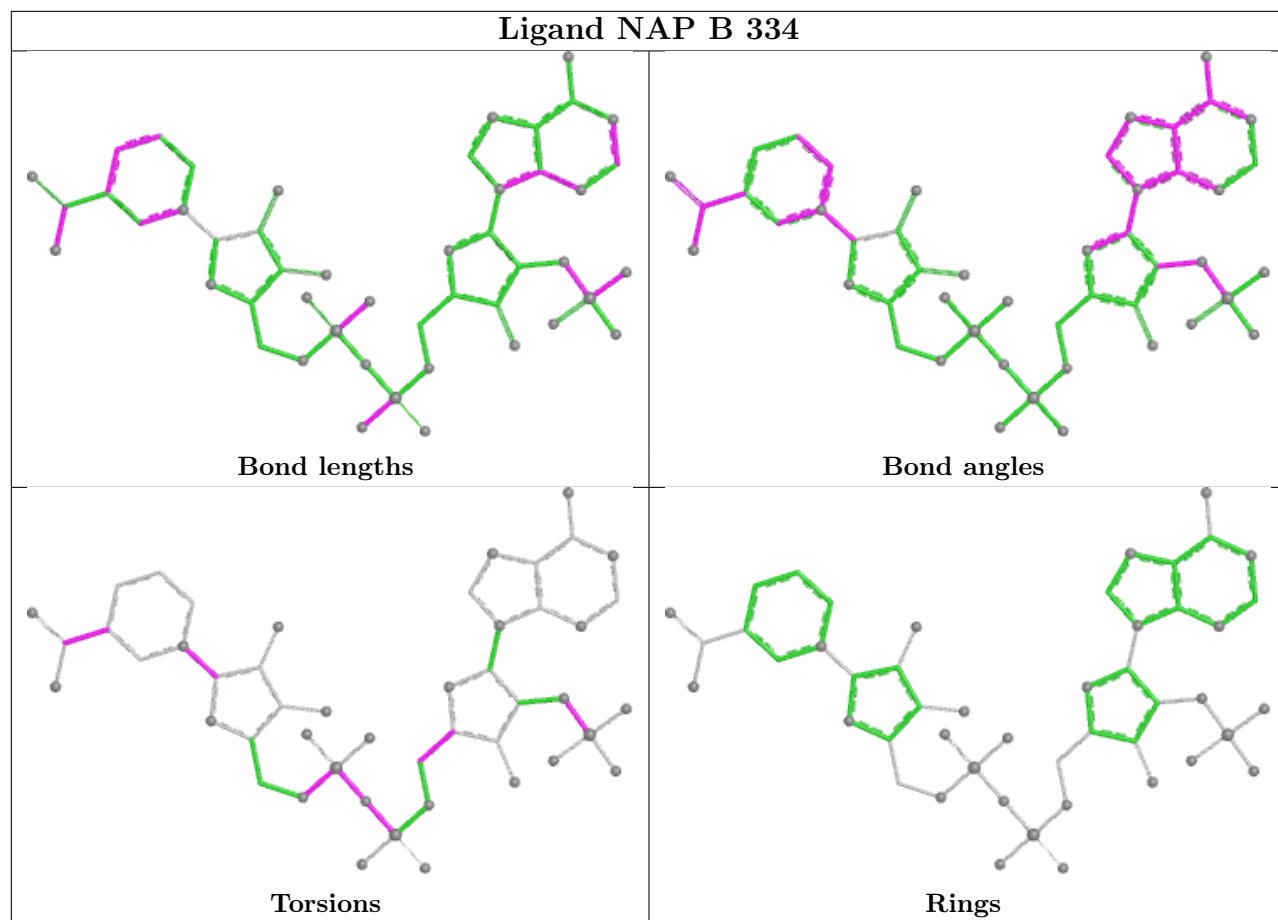
Mol	Chain	Res	Type	Atoms
3	A	335	UPG	C1'-O3B-PB-O1B
3	B	335	UPG	C1'-O3B-PB-O1B
2	B	334	NAP	PA-O3-PN-O2N
3	B	335	UPG	PA-O3A-PB-O2B
2	B	334	NAP	C2B-O2B-P2B-O2X
3	A	335	UPG	O4C-C1C-N1-C6
2	B	334	NAP	C3B-C4B-C5B-O5B
2	A	334	NAP	C2B-O2B-P2B-O1X
2	B	334	NAP	C2B-O2B-P2B-O1X
2	A	334	NAP	O4B-C4B-C5B-O5B

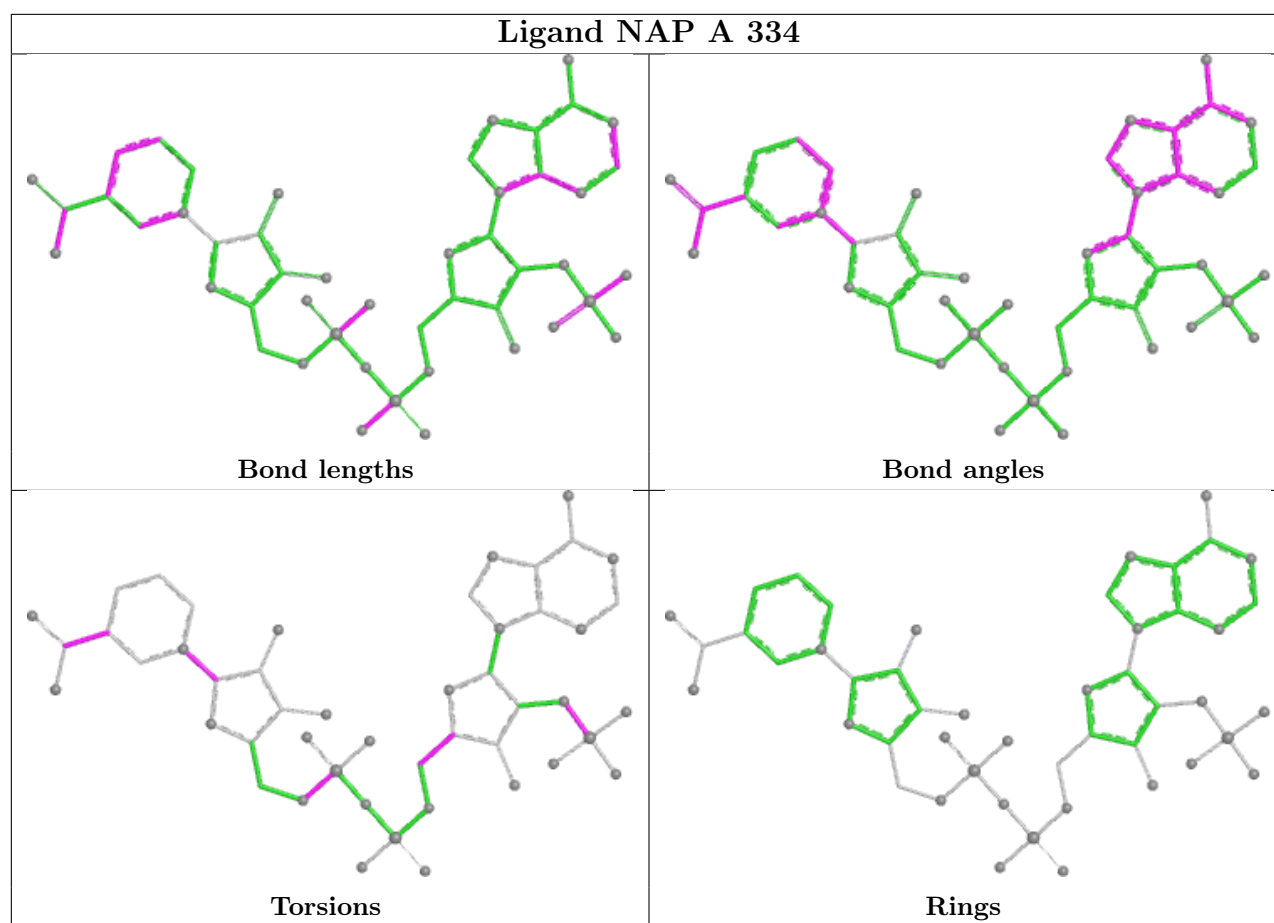
There are no ring outliers.

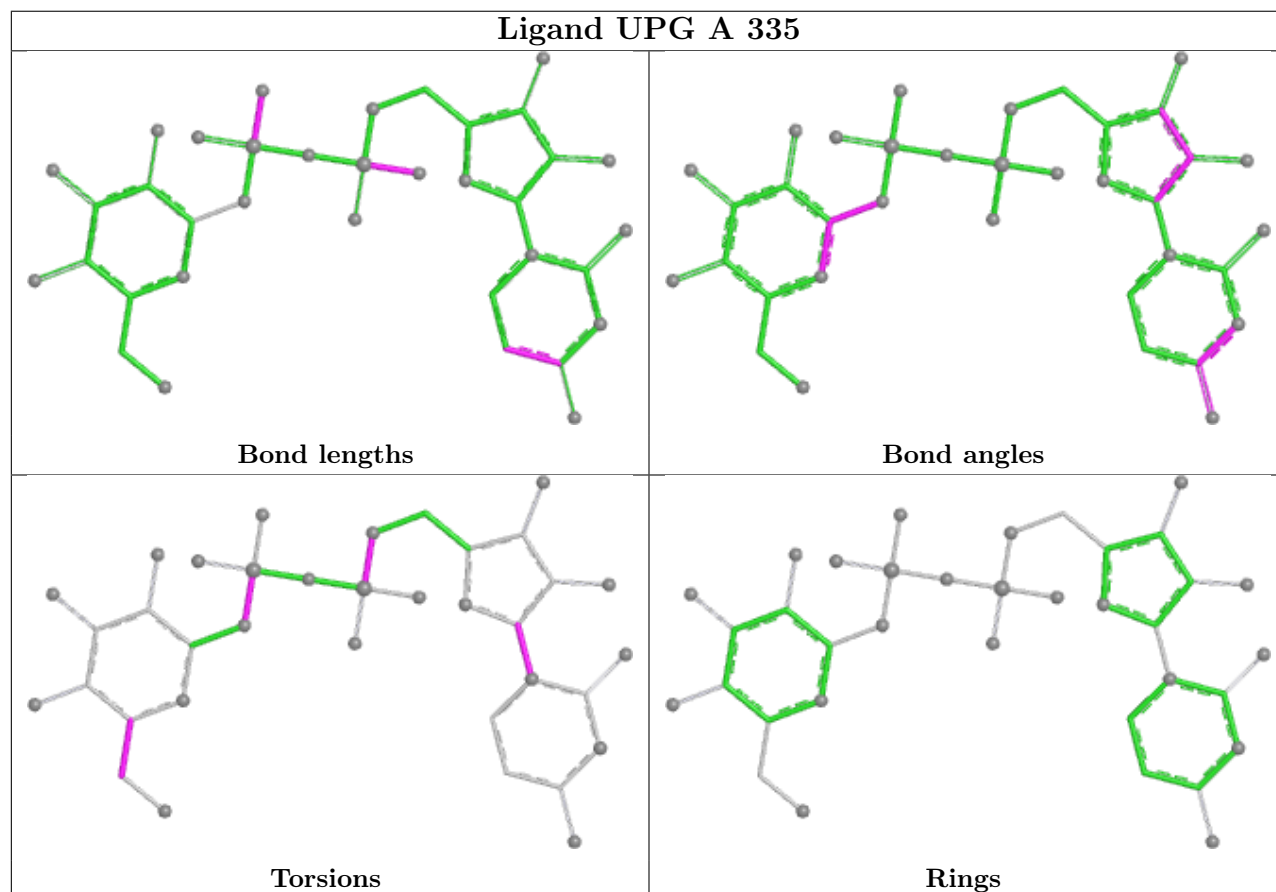
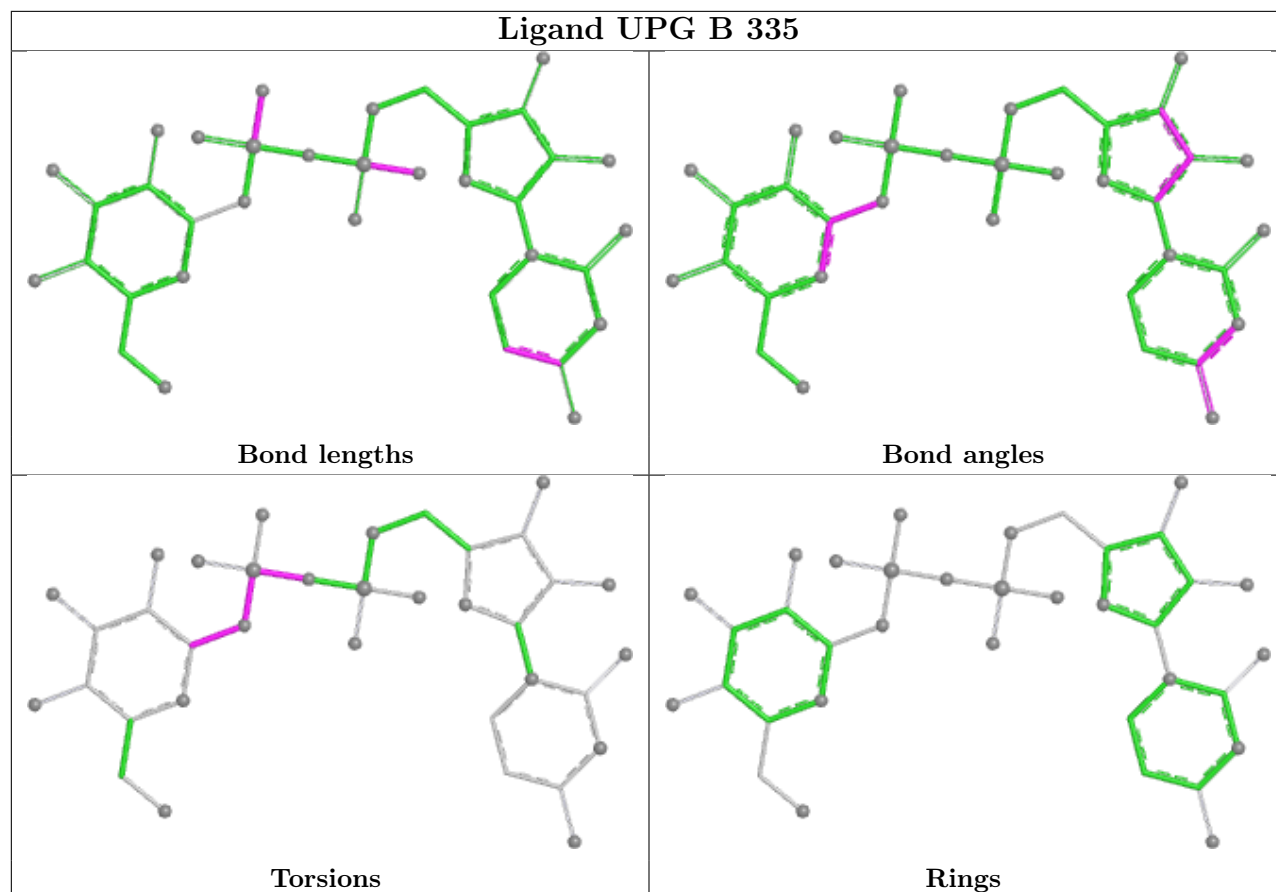
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	334	NAP	3	0
2	A	334	NAP	2	0
3	B	335	UPG	3	0
4	B	336	MES	1	0
3	A	335	UPG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	329/344 (95%)	0.64	41 (12%) 8 6	14, 48, 80, 80	0
1	B	327/344 (95%)	0.42	26 (7%) 18 13	12, 45, 79, 80	0
All	All	656/688 (95%)	0.53	67 (10%) 12 9	12, 46, 80, 80	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	GLY	5.1
1	A	17	GLY	4.7
1	B	201	ILE	4.5
1	A	162	SER	4.5
1	A	161	SER	4.5
1	A	303	HIS	4.4
1	A	159	LYS	4.1
1	B	326	PRO	3.9
1	A	204	THR	3.9
1	A	248	PRO	3.8
1	A	177	SER	3.7
1	B	54	MET	3.6
1	B	330	LEU	3.5
1	B	331	LYS	3.4
1	A	247	ALA	3.4
1	A	195	GLU	3.4
1	A	183	PRO	3.4
1	A	245	ALA	3.3
1	B	188	LEU	3.3
1	A	255	ILE	3.3
1	A	252	THR	3.3
1	B	25	CYS	3.1
1	B	189	VAL	3.0
1	A	322	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	250	THR	3.0
1	B	161	SER	2.9
1	A	320	ASN	2.9
1	A	176	GLY	2.9
1	A	254	ILE	2.9
1	B	195	GLU	2.8
1	B	314	GLU	2.8
1	A	160	GLY	2.7
1	A	259	PRO	2.6
1	A	199	THR	2.6
1	A	194	SER	2.6
1	B	162	SER	2.6
1	B	243	ALA	2.6
1	A	210	LEU	2.6
1	B	247	ALA	2.6
1	A	326	PRO	2.6
1	A	188	LEU	2.5
1	B	316	SER	2.5
1	B	196	ILE	2.5
1	A	158	PHE	2.5
1	A	9	ASP	2.5
1	B	322	GLN	2.5
1	A	214	VAL	2.4
1	A	7	MET	2.4
1	B	240	THR	2.3
1	A	193	ALA	2.2
1	A	264	HIS	2.2
1	A	295	LYS	2.2
1	A	231	VAL	2.2
1	B	75	ASN	2.2
1	B	249	ASN	2.2
1	A	269	PRO	2.2
1	A	246	LEU	2.1
1	B	163	GLN	2.1
1	A	251	PRO	2.1
1	B	214	VAL	2.1
1	A	302	LEU	2.1
1	B	193	ALA	2.1
1	B	248	PRO	2.0
1	A	191	ASN	2.0
1	B	256	GLY	2.0
1	A	178	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	249	ASN	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](#)

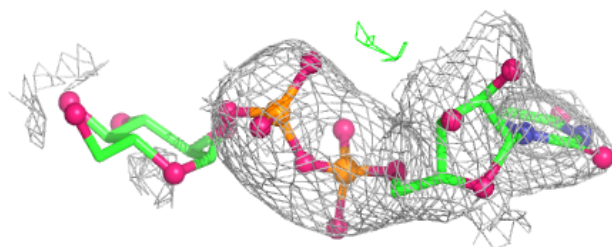
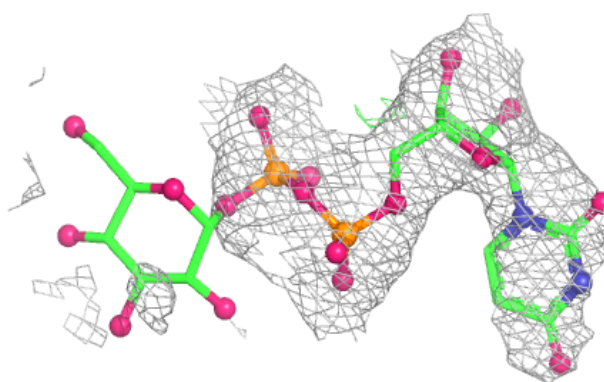
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MES	B	336	12/12	0.81	0.16	68,74,80,80	0
3	UPG	A	335	36/36	0.87	0.13	73,80,80,80	11
3	UPG	B	335	36/36	0.91	0.11	56,73,78,80	11
2	NAP	A	334	48/48	0.94	0.11	23,46,64,68	0
2	NAP	B	334	48/48	0.96	0.10	22,44,77,80	0

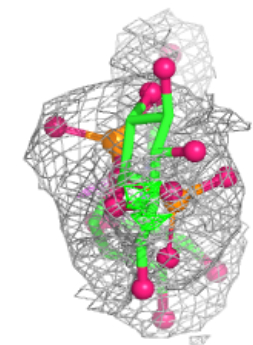
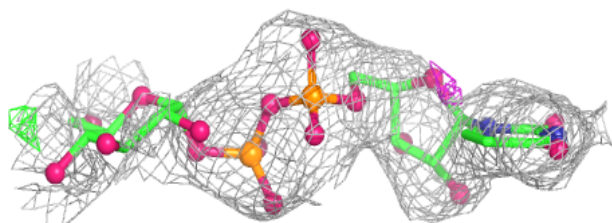
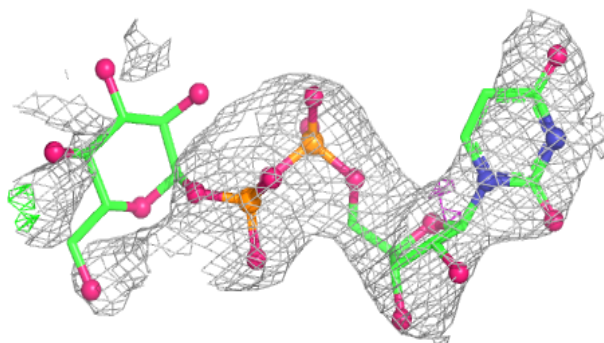
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UPG A 335:

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

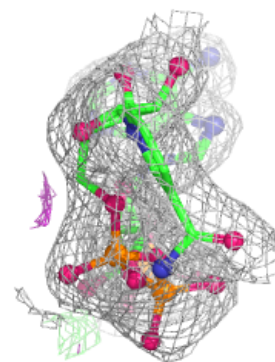
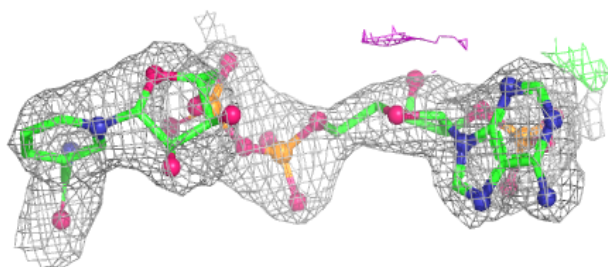
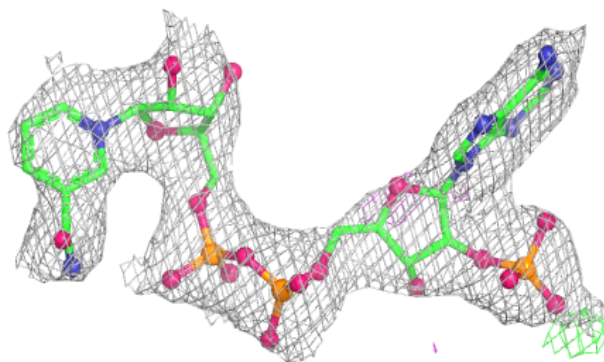
**Electron density around UPG B 335:**

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

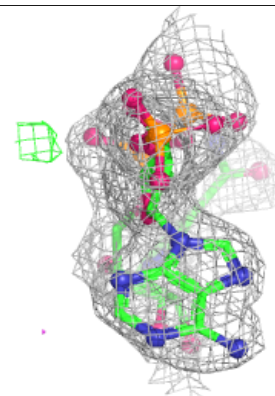
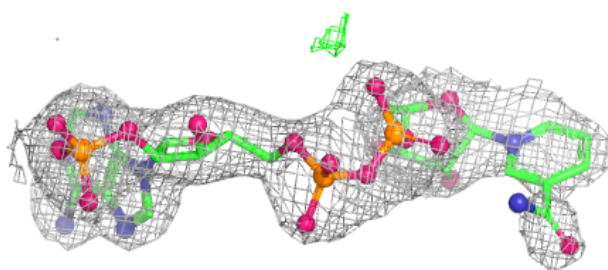
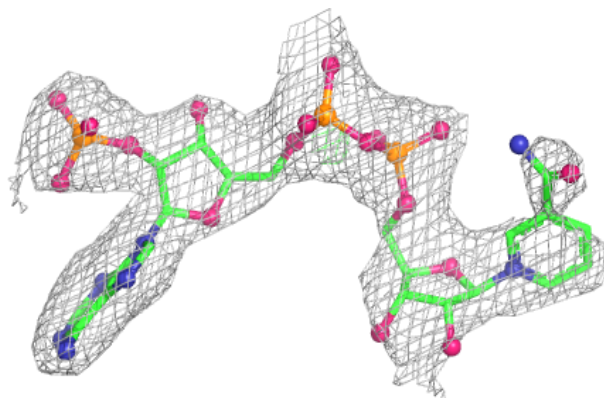


Electron density around NAP A 334:

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

**Electron density around NAP B 334:**

$2mF_o-DF_c$ (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.