Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 09:14 PM JST

PDB ID	:	6ADG
Title	:	Crystal Structures of IDH1 R132H in complex with AG-881
Authors	:	Ma, R.; Yun, C.H.
Deposited on	:	2018-08-01
Resolution	:	3.00 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:

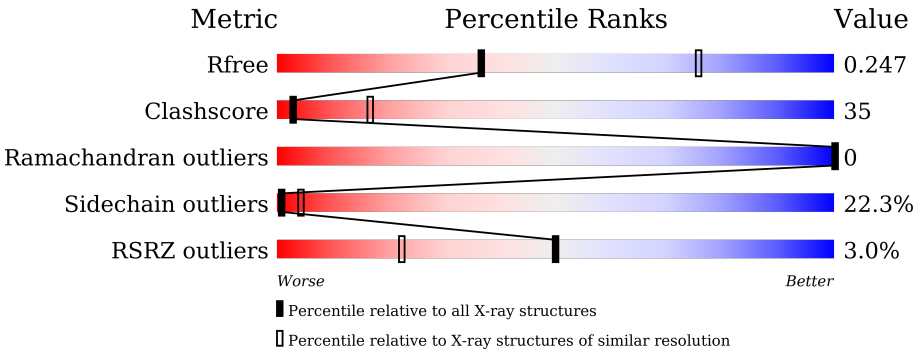
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	425	48% 43% 7% .
1	B	425	51% 37% 8% .
1	C	425	8% 42% 38% 12% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	502	-	-	-	X
3	MG	A	503	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9612 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3262	2074	553	617	18			
1	B	411	Total	C	N	O	S	0	0	0
			3255	2070	552	615	18			
1	C	390	Total	C	N	O	S	0	0	0
			2795	1760	485	535	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	HIS	ARG	engineered mutation	UNP O75874
A	415	SER	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
B	132	HIS	ARG	engineered mutation	UNP O75874
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874

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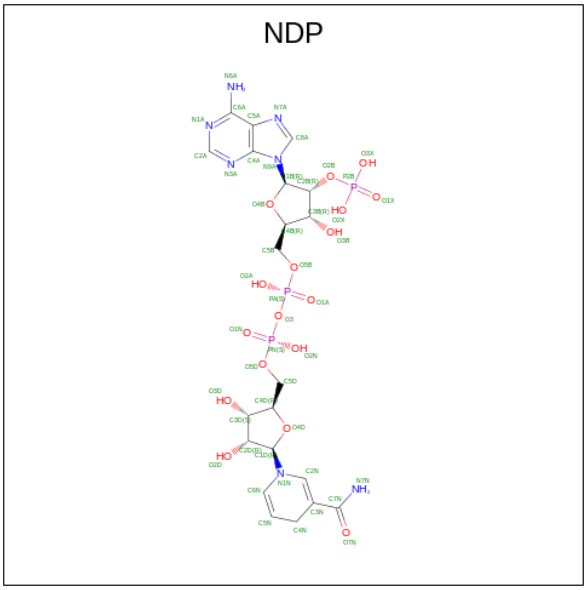
Chain	Residue	Modelled	Actual	Comment	Reference
B	425	HIS	-	expression tag	UNP O75874
C	132	HIS	ARG	engineered mutation	UNP O75874
C	415	SER	-	expression tag	UNP O75874
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

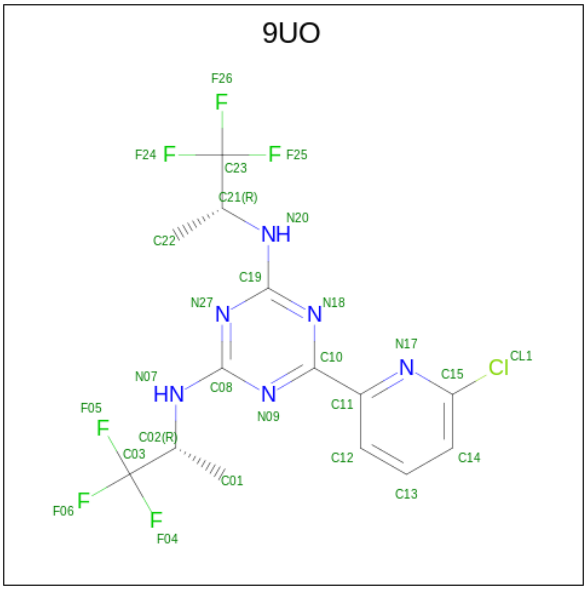


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0

- Molecule 4 is 6-(6-chloropyridin-2-yl)-N2,N4-bis[(2R)-1,1,1-trifluoropropan-2-yl]-1,3,5-triazine-2,4-diamine (three-letter code: 9UO) (formula: $C_{14}H_{13}ClF_6N_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl F N 54 28 2 12 12	0	1
4	C	1	Total C Cl F N 27 14 1 6 6	0	0

- Molecule 5 is water.

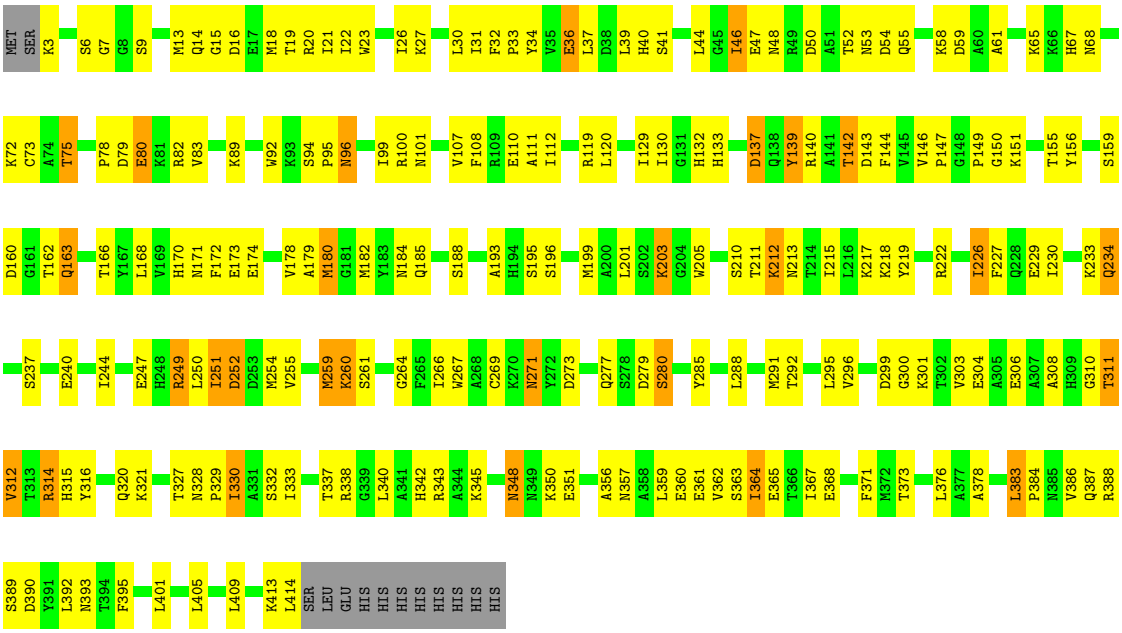
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	34	Total O 34 34	0	0
5	C	32	Total O 32 32	0	0

3 Residue-property plots (i)

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

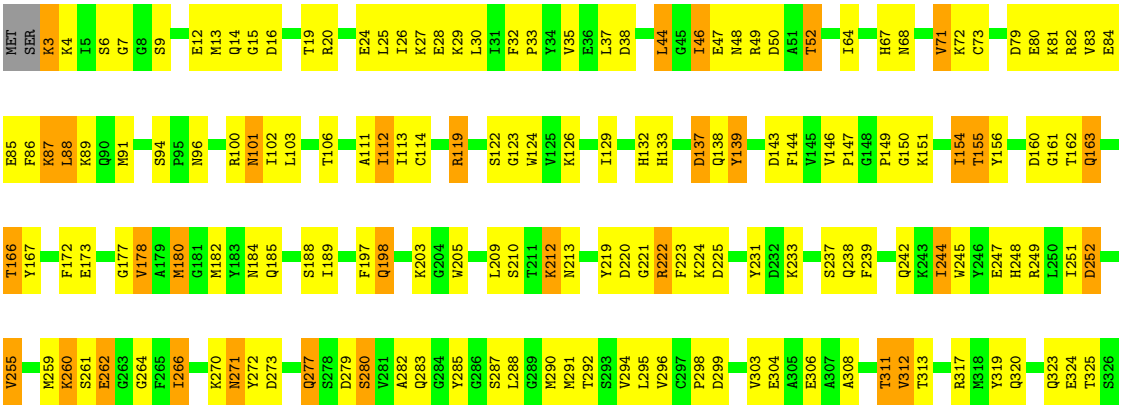
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

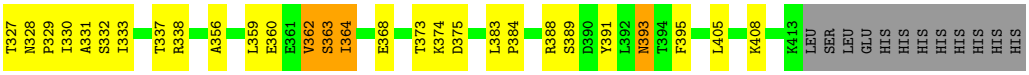
Chain A:



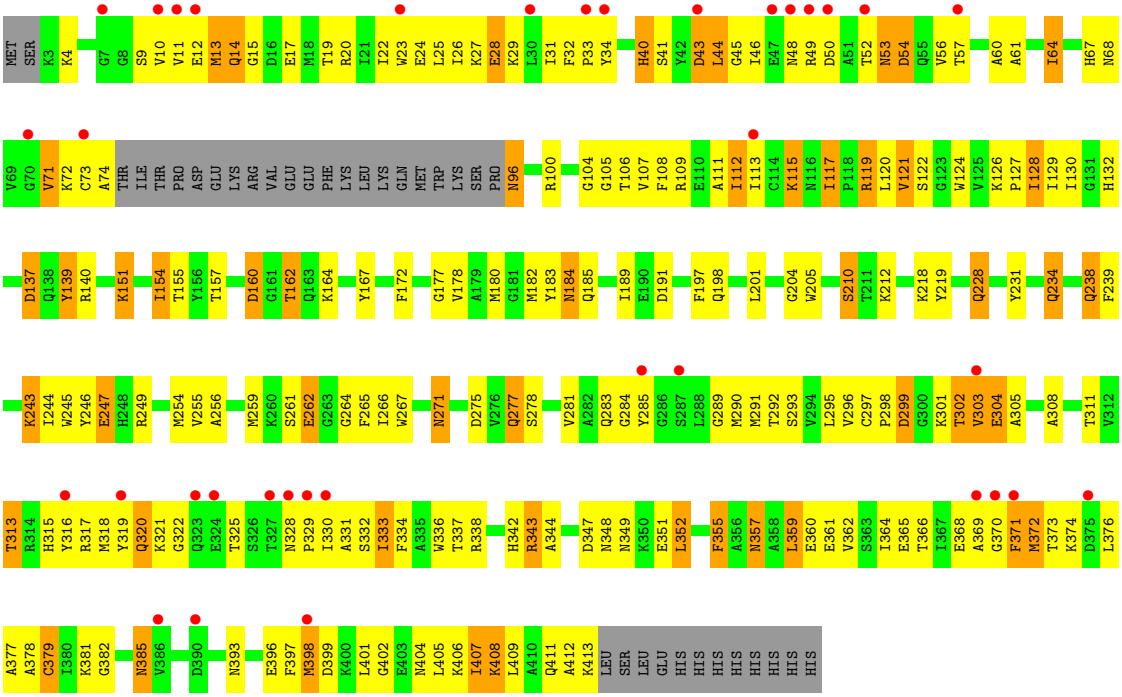
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:





• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.97Å 197.25Å 85.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.02 – 3.00 49.31 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.02-3.00) 99.9 (49.31-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.221 , 0.244 0.222 , 0.247	Depositor DCC
R_{free} test set	1607 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9612	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 12.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, NDP, 9UO

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	0.47	0/3331	0.52	0/4492
1	B	0.47	0/3324	0.52	0/4482
1	C	0.40	0/2852	0.54	0/3871
All	All	0.45	0/9507	0.53	0/12845

There are no bond length outliers.

There are no bond angle outliers.

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	3262	0	3224	182	0
1	B	3255	0	3217	190	0
1	C	2795	0	2437	288	0
2	A	48	0	26	5	0
2	B	48	0	26	5	0
3	A	2	0	0	0	0
4	A	54	0	0	10	0
4	C	27	0	0	2	0
5	A	55	0	0	5	0
5	B	34	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	0	2	0
All	All	9612	0	8930	642	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 35.

All (642) 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:112:ILE:HD12	1:C:113:ILE:N	1.34	1.39
1:B:239:PHE:CD2	1:B:244:ILE:HG22	1.68	1.28
1:C:119:ARG:HB3	1:C:119:ARG:NH1	1.43	1.28
1:C:352:LEU:O	1:C:352:LEU:HD13	1.34	1.27
1:C:277:GLN:O	1:C:281:VAL:HG23	1.36	1.23
1:B:111:ALA:HB2	1:B:291:MET:CE	1.73	1.19
1:C:48:ASN:O	1:C:52:THR:HG23	1.39	1.19
1:C:119:ARG:HB3	1:C:119:ARG:CZ	1.66	1.18
1:C:239:PHE:CD2	1:C:244:ILE:HG22	1.79	1.17
1:B:3:LYS:HG2	1:B:4:LYS:N	1.53	1.16
1:C:352:LEU:HD13	1:C:352:LEU:C	1.62	1.16
1:C:344:ALA:HB2	1:C:352:LEU:HD12	1.31	1.13
1:C:124:TRP:HB3	1:C:285:TYR:CE1	1.84	1.13
1:B:239:PHE:CD2	1:B:244:ILE:CG2	2.31	1.12
1:A:7:GLY:HA3	1:A:37:LEU:HD23	1.30	1.11
1:C:239:PHE:HD2	1:C:244:ILE:HG22	0.94	1.11
1:A:260:LYS:HG2	1:B:283:GLN:NE2	1.66	1.10
1:C:239:PHE:CD2	1:C:244:ILE:CG2	2.34	1.10
1:B:3:LYS:CG	1:B:4:LYS:H	1.63	1.10
1:C:96:ASN:C	1:C:96:ASN:HD22	1.54	1.09
1:C:115:LYS:HB3	1:C:368:GLU:OE2	1.52	1.09
1:C:277:GLN:NE2	1:C:277:GLN:HA	1.67	1.09
1:C:137:ASP:HB3	1:C:219:TYR:OH	1.55	1.05
1:C:119:ARG:HB2	1:C:285:TYR:O	1.54	1.05
1:C:124:TRP:HB3	1:C:285:TYR:HE1	1.11	1.04
1:B:46:ILE:O	1:B:46:ILE:HD12	1.59	1.02
1:A:155:THR:HG22	1:A:166:THR:HG23	1.05	1.01
1:C:352:LEU:C	1:C:352:LEU:CD1	2.30	0.99
1:C:137:ASP:O	1:C:182:MET:HG2	1.64	0.97
1:B:111:ALA:CB	1:B:291:MET:HE2	1.94	0.97
1:C:239:PHE:HD2	1:C:244:ILE:CG2	1.73	0.96
1:C:357:ASN:C	1:C:357:ASN:HD22	1.69	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:O	1:B:87:LYS:HE3	1.65	0.96
1:B:111:ALA:HB2	1:B:291:MET:HE2	0.97	0.96
1:C:119:ARG:NH1	1:C:119:ARG:CB	2.30	0.94
1:B:239:PHE:HD2	1:B:244:ILE:HG22	1.11	0.94
1:A:155:THR:HG22	1:A:166:THR:CG2	1.98	0.94
1:A:111:ALA:HB2	1:A:291:MET:HE2	1.50	0.94
1:C:334:PHE:CE2	1:C:360:GLU:HG2	2.03	0.93
1:B:7:GLY:HA3	1:B:37:LEU:HD23	1.51	0.93
1:C:317:ARG:HA	1:C:320:GLN:CG	1.99	0.93
1:A:137:ASP:HB3	1:A:219:TYR:OH	1.70	0.92
1:C:301:LYS:O	1:C:342:HIS:HE1	1.53	0.91
1:C:328:ASN:OD1	1:C:330:ILE:HD13	1.70	0.91
1:C:34:TYR:CD1	1:C:409:LEU:HD12	2.05	0.91
4:A:504[B]:9UO:CL1	1:B:273:ASP:OD1	2.26	0.90
1:B:112:ILE:N	1:B:112:ILE:HD12	1.84	0.90
1:A:142:THR:HG22	1:A:142:THR:O	1.71	0.90
1:C:112:ILE:HG22	1:C:290:MET:O	1.72	0.89
1:C:374:LYS:HA	1:C:377:ALA:HB3	1.54	0.89
1:C:112:ILE:CD1	1:C:113:ILE:N	2.30	0.87
1:A:155:THR:CG2	1:A:166:THR:HG23	1.99	0.86
1:C:112:ILE:CD1	1:C:113:ILE:H	1.88	0.86
1:A:110:GLU:HB2	1:A:129:ILE:HG12	1.56	0.86
1:A:46:ILE:HD12	1:A:46:ILE:O	1.74	0.86
1:B:112:ILE:H	1:B:112:ILE:CD1	1.89	0.86
1:A:111:ALA:HB2	1:A:291:MET:CE	2.06	0.85
1:C:15:GLY:N	1:C:73:CYS:SG	2.50	0.84
1:B:137:ASP:HB3	1:B:219:TYR:OH	1.76	0.84
1:B:84:GLU:O	1:B:87:LYS:HD3	1.76	0.84
1:C:239:PHE:CD2	1:C:244:ILE:HG21	2.11	0.84
1:C:290:MET:SD	1:C:328:ASN:ND2	2.51	0.84
1:A:277:GLN:NE2	4:A:504[B]:9UO:C12	2.41	0.83
1:C:366:THR:O	1:C:369:ALA:HB3	1.77	0.83
1:A:205:TRP:CE3	1:A:264:GLY:O	2.31	0.83
1:A:137:ASP:O	1:A:182:MET:HB2	1.77	0.83
1:B:364:ILE:O	1:B:368:GLU:HG3	1.78	0.83
1:B:112:ILE:N	1:B:112:ILE:CD1	2.39	0.83
1:C:25:LEU:O	1:C:29:LYS:HB2	1.78	0.82
1:C:117:ILE:CD1	1:C:117:ILE:N	2.42	0.82
1:C:184:ASN:HD22	1:C:185:GLN:H	1.25	0.82
1:C:112:ILE:HD12	1:C:112:ILE:C	1.98	0.82
1:B:3:LYS:HG2	1:B:4:LYS:H	0.73	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ARG:HA	1:C:320:GLN:HG3	1.60	0.82
1:C:205:TRP:CE3	1:C:264:GLY:O	2.33	0.82
1:A:280:SER:OG	1:B:255:VAL:HG23	1.80	0.81
1:B:374:LYS:HD2	1:B:391:TYR:CE2	2.14	0.81
1:A:50:ASP:O	1:A:89:LYS:HE3	1.81	0.81
1:C:112:ILE:HD12	1:C:113:ILE:H	0.98	0.81
1:C:96:ASN:C	1:C:96:ASN:ND2	2.30	0.80
1:C:301:LYS:O	1:C:342:HIS:CE1	2.35	0.80
1:C:210:SER:HG	1:C:267:TRP:HE1	0.80	0.80
1:B:84:GLU:O	1:B:87:LYS:CE	2.30	0.79
1:C:15:GLY:O	1:C:20:ARG:CB	2.30	0.79
1:B:84:GLU:OE2	1:B:87:LYS:HE2	1.82	0.79
1:C:349:ASN:OD1	1:C:352:LEU:CB	2.30	0.79
1:C:355:PHE:O	1:C:355:PHE:CD1	2.36	0.79
1:C:49:ARG:HA	1:C:52:THR:OG1	1.82	0.79
1:A:260:LYS:HG2	1:B:283:GLN:HE21	1.48	0.78
1:B:7:GLY:HA3	1:B:37:LEU:CD2	2.13	0.78
1:A:413:LYS:O	1:A:414:LEU:CB	2.30	0.78
1:C:119:ARG:HB3	1:C:119:ARG:HH11	1.49	0.78
1:C:17:GLU:CG	1:C:311:THR:CB	2.61	0.78
1:C:111:ALA:HA	1:C:291:MET:HA	1.65	0.78
1:B:239:PHE:HD2	1:B:244:ILE:CG2	1.84	0.78
1:C:119:ARG:CZ	1:C:119:ARG:CB	2.55	0.78
1:A:80:GLU:H	1:A:80:GLU:CD	1.85	0.77
1:C:124:TRP:CB	1:C:285:TYR:CE1	2.67	0.77
1:B:84:GLU:O	1:B:87:LYS:CD	2.32	0.77
1:C:316:TYR:O	1:C:320:GLN:HG2	1.84	0.77
1:C:349:ASN:OD1	1:C:352:LEU:HB2	1.85	0.77
1:C:60:ALA:O	1:C:64:ILE:CG1	2.34	0.75
1:A:23:TRP:O	1:A:27:LYS:HG3	1.85	0.75
1:B:291:MET:HB3	1:B:308:ALA:HB3	1.68	0.75
1:C:160:ASP:OD2	1:C:162:THR:CG2	2.35	0.75
1:C:60:ALA:O	1:C:64:ILE:HG12	1.87	0.75
1:C:61:ALA:HA	1:C:64:ILE:HG13	1.67	0.75
1:B:48:ASN:O	1:B:52:THR:HG23	1.86	0.75
1:A:79:ASP:O	1:A:83:VAL:HG23	1.86	0.74
1:A:367:ILE:HD13	1:A:376:LEU:CD1	2.18	0.74
1:C:137:ASP:O	1:C:182:MET:CG	2.36	0.74
1:C:344:ALA:CB	1:C:352:LEU:HD12	2.15	0.74
1:C:344:ALA:HB2	1:C:352:LEU:CD1	2.14	0.74
1:C:371:PHE:N	1:C:371:PHE:CD2	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLN:NE2	1:C:277:GLN:CA	2.49	0.74
1:B:296:VAL:HG22	1:B:303:VAL:HG22	1.68	0.74
1:A:52:THR:O	1:A:53:ASN:HB2	1.88	0.73
1:B:84:GLU:OE2	1:B:87:LYS:CE	2.37	0.72
1:B:72:LYS:HD3	1:B:306:GLU:OE2	1.90	0.72
1:A:321:LYS:HE3	5:A:647:HOH:O	1.87	0.72
1:A:72:LYS:NZ	1:A:75:THR:OG1	2.23	0.72
1:C:34:TYR:CD1	1:C:409:LEU:CD1	2.72	0.71
1:A:251:ILE:HD13	1:B:272:TYR:OH	1.89	0.71
1:C:72:LYS:HG3	1:C:73:CYS:N	2.04	0.71
1:C:204:GLY:HA2	1:C:244:ILE:HD11	1.70	0.71
4:A:504[A]:9UO:C12	1:B:277:GLN:NE2	2.53	0.71
1:B:311:THR:OG1	2:B:501:NDP:H4D	1.90	0.71
1:A:72:LYS:HD3	1:A:306:GLU:OE1	1.90	0.71
1:A:142:THR:O	1:A:142:THR:CG2	2.39	0.71
1:C:355:PHE:O	1:C:355:PHE:HD1	1.72	0.70
1:A:383:LEU:HB3	1:A:384:PRO:HD3	1.73	0.70
1:B:146:VAL:N	1:B:177:GLY:O	2.22	0.70
1:A:182:MET:SD	1:B:180:MET:HE3	2.31	0.70
1:A:273:ASP:OD1	4:A:504[A]:9UO:CL1	2.47	0.70
1:C:357:ASN:C	1:C:357:ASN:ND2	2.43	0.70
1:C:371:PHE:N	1:C:371:PHE:HD2	1.90	0.70
1:C:71:VAL:HG11	1:C:336:TRP:HA	1.74	0.69
1:C:14:GLN:O	1:C:44:LEU:HB2	1.91	0.69
1:B:13:MET:CE	1:B:64:ILE:HD11	2.23	0.69
1:B:101:ASN:OD1	1:B:101:ASN:C	2.30	0.69
1:A:14:GLN:HG2	5:A:608:HOH:O	1.92	0.69
1:A:144:PHE:CE2	1:A:179:ALA:HB3	2.28	0.69
1:A:280:SER:OG	1:B:255:VAL:CG2	2.41	0.69
1:C:73:CYS:O	1:C:74:ALA:C	2.30	0.69
1:C:112:ILE:CG2	1:C:290:MET:O	2.40	0.69
1:B:13:MET:HB3	1:B:44:LEU:HG	1.76	0.68
1:C:34:TYR:CG	1:C:409:LEU:CD1	2.76	0.68
1:A:133:HIS:O	1:A:271:ASN:HB2	1.93	0.68
1:C:10:VAL:O	1:C:40:HIS:HD2	1.77	0.68
1:B:35:VAL:HG11	1:B:37:LEU:HD21	1.74	0.68
1:B:222:ARG:NH1	5:B:601:HOH:O	2.26	0.68
1:C:29:LYS:CE	1:C:398:MET:O	2.41	0.68
1:C:29:LYS:CE	1:C:399:ASP:HA	2.23	0.68
1:C:277:GLN:O	1:C:281:VAL:CG2	2.30	0.68
1:A:156:TYR:CE1	1:B:150:GLY:HA3	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLY:HA3	5:B:609:HOH:O	1.94	0.67
1:C:364:ILE:O	1:C:368:GLU:HG3	1.94	0.67
1:A:219:TYR:HB2	1:B:143:ASP:HB2	1.76	0.67
1:C:333:ILE:O	1:C:337:THR:HG23	1.95	0.67
1:C:330:ILE:HA	1:C:333:ILE:HG22	1.77	0.67
1:C:317:ARG:CA	1:C:320:GLN:HG3	2.25	0.67
1:C:333:ILE:HD11	1:C:359:LEU:HG	1.77	0.67
1:A:260:LYS:HG2	1:B:283:GLN:HE22	1.57	0.67
1:A:314:ARG:NH2	2:A:501:NDP:O2X	2.28	0.67
1:C:14:GLN:C	1:C:73:CYS:SG	2.73	0.67
1:C:355:PHE:CD1	1:C:355:PHE:C	2.65	0.67
1:C:119:ARG:CG	1:C:121:VAL:O	2.44	0.66
1:A:277:GLN:HE21	4:A:504[B]:9UO:C12	2.07	0.66
1:C:198:GLN:CD	1:C:298:PRO:O	2.34	0.66
1:C:315:HIS:O	1:C:318:MET:HB2	1.94	0.66
1:C:393:ASN:O	1:C:397:PHE:N	2.27	0.66
1:C:299:ASP:OD1	1:C:299:ASP:C	2.33	0.66
1:C:52:THR:O	1:C:53:ASN:CG	2.34	0.66
1:C:128:ILE:HG13	1:C:285:TYR:OH	1.95	0.66
1:A:79:ASP:OD1	1:A:79:ASP:C	2.30	0.65
1:C:117:ILE:N	1:C:117:ILE:HD13	2.11	0.65
1:C:119:ARG:CB	1:C:119:ARG:HH11	2.06	0.65
1:B:139:TYR:CD1	1:B:139:TYR:N	2.62	0.65
1:C:378:ALA:O	1:C:382:GLY:N	2.30	0.65
1:A:132:HIS:NE2	1:A:271:ASN:ND2	2.45	0.65
1:B:247:GLU:OE2	1:B:249:ARG:NH2	2.30	0.65
1:C:48:ASN:O	1:C:52:THR:CG2	2.32	0.65
1:C:139:TYR:N	1:C:139:TYR:CD1	2.64	0.65
1:C:239:PHE:CE2	1:C:244:ILE:HG21	2.31	0.65
1:B:85:GLU:HG2	1:B:86:PHE:CD2	2.32	0.65
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.31	0.65
1:C:304:GLU:OE1	1:C:305:ALA:N	2.30	0.65
1:C:52:THR:O	1:C:53:ASN:ND2	2.30	0.65
1:C:160:ASP:HB2	1:C:162:THR:HG22	1.77	0.65
1:A:156:TYR:HE1	1:B:150:GLY:HA3	1.60	0.65
1:A:140:ARG:HG3	5:A:632:HOH:O	1.97	0.65
1:A:388:ARG:NH1	1:A:388:ARG:O	2.30	0.65
1:A:96:ASN:ND2	1:A:96:ASN:H	1.94	0.64
1:B:333:ILE:O	1:B:337:THR:HG23	1.98	0.64
1:C:244:ILE:CG2	1:C:245:TRP:N	2.60	0.64
1:B:112:ILE:H	1:B:112:ILE:HD13	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ILE:O	1:C:411:GLN:N	2.30	0.64
1:B:35:VAL:CG1	1:B:37:LEU:HD21	2.27	0.64
1:C:317:ARG:O	1:C:320:GLN:HG3	1.98	0.64
1:C:374:LYS:O	1:C:378:ALA:N	2.30	0.64
1:A:7:GLY:N	1:A:36:GLU:O	2.29	0.64
1:B:111:ALA:CB	1:B:291:MET:CE	2.64	0.64
1:C:128:ILE:HD13	1:C:265:PHE:CZ	2.32	0.64
1:B:317:ARG:NH1	1:B:320:GLN:OE1	2.30	0.64
1:B:155:THR:HG22	1:B:166:THR:HG23	1.80	0.64
1:A:80:GLU:N	1:A:80:GLU:OE1	2.30	0.63
1:B:133:HIS:O	1:B:271:ASN:HB2	1.99	0.63
1:C:317:ARG:CA	1:C:320:GLN:CG	2.74	0.63
1:C:23:TRP:CH2	1:C:336:TRP:NE1	2.67	0.63
1:A:160:ASP:OD1	1:A:160:ASP:C	2.37	0.63
1:C:277:GLN:OE1	4:C:501:9UO:C12	2.47	0.63
1:C:14:GLN:OE1	1:C:15:GLY:N	2.30	0.63
1:B:13:MET:HE1	1:B:64:ILE:HD11	1.81	0.63
1:C:29:LYS:CE	1:C:398:MET:C	2.67	0.63
1:C:277:GLN:HA	1:C:277:GLN:HE21	1.57	0.62
1:B:46:ILE:HD12	1:B:46:ILE:C	2.19	0.62
1:C:372:MET:SD	1:C:377:ALA:HA	2.39	0.62
1:A:210:SER:HA	1:A:249:ARG:O	1.98	0.62
1:C:289:GLY:O	1:C:331:ALA:HB2	1.99	0.62
1:C:184:ASN:HD22	1:C:185:GLN:N	1.97	0.62
1:C:49:ARG:O	1:C:53:ASN:N	2.30	0.62
1:A:13:MET:HB3	1:A:44:LEU:HG	1.80	0.62
1:A:112:ILE:HD13	1:A:330:ILE:HG22	1.82	0.62
1:A:67:HIS:O	1:A:68:ASN:HB2	2.00	0.62
1:C:19:THR:O	1:C:23:TRP:N	2.30	0.61
1:C:295:LEU:HB3	1:C:304:GLU:HB3	1.82	0.61
1:C:117:ILE:N	1:C:117:ILE:HD12	2.14	0.61
1:C:244:ILE:HG22	1:C:245:TRP:N	2.15	0.61
1:C:349:ASN:OD1	1:C:352:LEU:HB3	1.99	0.61
1:C:357:ASN:ND2	1:C:357:ASN:O	2.30	0.61
1:C:22:ILE:O	1:C:26:ILE:N	2.32	0.61
1:C:119:ARG:CB	1:C:285:TYR:O	2.42	0.61
1:C:374:LYS:HA	1:C:377:ALA:CB	2.30	0.61
1:A:160:ASP:OD1	1:A:162:THR:N	2.30	0.61
1:A:53:ASN:HA	1:A:92:TRP:CH2	2.36	0.61
1:A:142:THR:HG21	1:B:154:ILE:CG2	2.31	0.61
1:B:160:ASP:C	1:B:160:ASP:OD1	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASP:OD1	1:B:88:LEU:HB3	2.00	0.61
1:B:245:TRP:HD1	1:B:247:GLU:HG3	1.65	0.61
1:A:247:GLU:OE2	1:A:249:ARG:NH1	2.30	0.61
1:B:137:ASP:O	1:B:182:MET:HB2	2.00	0.61
1:B:137:ASP:HB2	1:B:182:MET:SD	2.41	0.60
1:C:160:ASP:OD2	1:C:162:THR:HG23	2.01	0.60
1:C:68:ASN:HA	1:C:302:THR:HG23	1.83	0.60
1:C:15:GLY:CA	1:C:73:CYS:SG	2.90	0.60
1:C:117:ILE:HD13	1:C:117:ILE:H	1.66	0.60
2:A:501:NDP:P2B	2:A:501:NDP:O3B	2.60	0.60
1:B:67:HIS:O	1:B:68:ASN:HB2	2.02	0.60
1:B:126:LYS:NZ	1:B:262:GLU:OE1	2.31	0.60
1:B:198:GLN:OE1	1:B:298:PRO:O	2.20	0.60
1:B:362:VAL:HG23	1:B:408:LYS:HD3	1.83	0.60
1:C:120:LEU:CB	1:C:284:GLY:HA2	2.32	0.60
1:C:317:ARG:HA	1:C:320:GLN:CD	2.20	0.60
1:B:271:ASN:O	1:B:271:ASN:ND2	2.30	0.60
1:A:14:GLN:O	1:A:44:LEU:HB2	2.02	0.59
1:B:86:PHE:HB2	1:B:88:LEU:HD21	1.83	0.59
1:A:277:GLN:HA	1:A:277:GLN:OE1	2.02	0.59
1:B:160:ASP:OD1	1:B:162:THR:N	2.30	0.59
1:C:60:ALA:O	1:C:64:ILE:HG13	2.01	0.59
1:C:362:VAL:HG21	1:C:405:LEU:HA	1.85	0.59
1:A:364:ILE:O	1:A:368:GLU:HG3	2.03	0.59
1:C:365:GLU:O	1:C:369:ALA:N	2.32	0.59
1:A:55:GLN:NE2	1:A:59:ASP:OD1	2.36	0.59
1:C:52:THR:C	1:C:53:ASN:CG	2.61	0.59
1:B:14:GLN:OE1	1:B:15:GLY:N	2.30	0.58
1:B:356:ALA:O	1:B:360:GLU:HG3	2.03	0.58
1:B:271:ASN:ND2	1:B:271:ASN:C	2.57	0.58
1:C:61:ALA:CA	1:C:64:ILE:HG13	2.34	0.58
1:B:139:TYR:N	1:B:139:TYR:HD1	2.00	0.58
1:B:149:PRO:HB3	1:B:172:PHE:O	2.03	0.58
1:B:311:THR:OG1	2:B:501:NDP:C4D	2.51	0.58
1:A:296:VAL:HG22	1:A:303:VAL:HG22	1.86	0.58
1:A:255:VAL:HG23	1:B:280:SER:HB3	1.85	0.58
1:B:15:GLY:O	1:B:20:ARG:NH1	2.30	0.58
1:B:291:MET:HB3	1:B:308:ALA:CB	2.33	0.58
1:C:27:LYS:O	1:C:32:PHE:CD2	2.56	0.58
1:C:29:LYS:HD2	1:C:398:MET:HB3	1.86	0.58
1:C:128:ILE:HD13	1:C:265:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:O	1:A:226:ILE:HG13	2.03	0.57
1:A:395:PHE:CD1	1:A:395:PHE:N	2.72	0.57
1:C:34:TYR:CE1	1:C:409:LEU:HD12	2.39	0.57
1:A:142:THR:HG21	1:B:154:ILE:HG21	1.86	0.57
2:A:501:NDP:P2B	2:A:501:NDP:HO3A	2.26	0.57
1:B:239:PHE:CE2	1:B:244:ILE:CG2	2.85	0.57
1:C:334:PHE:CE2	1:C:360:GLU:CG	2.83	0.57
1:A:361:GLU:O	1:A:365:GLU:HG3	2.04	0.57
4:A:504[A]:9UO:C12	1:B:277:GLN:HE22	2.18	0.57
1:C:29:LYS:CD	1:C:398:MET:HB3	2.33	0.57
1:C:366:THR:HA	1:C:369:ALA:HB3	1.85	0.57
1:C:46:ILE:O	1:C:50:ASP:N	2.30	0.57
1:C:119:ARG:NH1	1:C:119:ARG:N	2.53	0.57
1:A:280:SER:HB3	4:A:504[A]:9UO:C01	2.35	0.57
1:C:53:ASN:O	1:C:54:ASP:HB2	2.05	0.56
1:C:172:PHE:CE2	1:C:177:GLY:HA3	2.40	0.56
1:C:139:TYR:N	1:C:139:TYR:HD1	2.03	0.56
1:C:119:ARG:CD	1:C:121:VAL:O	2.54	0.56
1:B:282:ALA:CB	1:B:291:MET:HG3	2.35	0.56
1:C:330:ILE:O	1:C:333:ILE:HG22	2.05	0.56
1:B:72:LYS:CD	1:B:306:GLU:OE2	2.53	0.56
1:C:137:ASP:HB3	1:C:219:TYR:HH	1.69	0.56
1:A:9:SER:O	1:A:343:ARG:NH1	2.36	0.56
1:A:271:ASN:C	1:A:271:ASN:HD22	2.07	0.56
1:A:311:THR:C	1:A:312:VAL:HG23	2.26	0.56
1:C:120:LEU:N	1:C:284:GLY:O	2.39	0.56
1:B:132:HIS:NE2	1:B:271:ASN:ND2	2.54	0.55
1:C:137:ASP:O	1:C:182:MET:SD	2.64	0.55
1:C:316:TYR:O	1:C:319:TYR:N	2.39	0.55
1:B:239:PHE:CD2	1:B:244:ILE:HG21	2.36	0.55
1:C:185:GLN:NE2	5:C:603:HOH:O	2.39	0.55
1:C:10:VAL:O	1:C:40:HIS:CD2	2.59	0.55
1:A:212:LYS:CG	1:A:251:ILE:HD11	2.37	0.55
1:B:311:THR:C	1:B:312:VAL:HG23	2.26	0.55
1:A:31:ILE:HG22	1:A:32:PHE:HD1	1.71	0.55
1:A:139:TYR:CD1	1:A:139:TYR:N	2.74	0.55
1:B:255:VAL:O	1:B:259:MET:HG3	2.07	0.55
1:B:362:VAL:HG23	1:B:408:LYS:CD	2.36	0.55
1:B:3:LYS:CG	1:B:4:LYS:N	2.32	0.55
1:B:79:ASP:OD1	1:B:82:ARG:N	2.32	0.55
1:B:271:ASN:C	1:B:271:ASN:HD22	1.99	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:HA	1:B:88:LEU:HD12	1.88	0.54
1:A:130:ILE:HD13	1:A:267:TRP:HB3	1.87	0.54
1:A:359:LEU:HD13	1:A:405:LEU:HD22	1.88	0.54
1:B:324:GLU:OE2	1:B:388:ARG:NE	2.40	0.54
1:C:239:PHE:CE2	1:C:244:ILE:CG2	2.86	0.54
1:C:17:GLU:HB3	1:C:313:THR:HG23	1.89	0.54
1:C:330:ILE:HA	1:C:333:ILE:CG2	2.36	0.54
1:B:112:ILE:HD13	1:B:290:MET:O	2.08	0.54
1:A:357:ASN:O	1:A:361:GLU:HG3	2.08	0.54
1:A:15:GLY:O	1:A:20:ARG:NH1	2.39	0.54
1:A:255:VAL:O	1:A:259:MET:CG	2.56	0.54
1:C:385:ASN:OD1	1:C:385:ASN:N	2.39	0.53
1:A:393:ASN:C	1:A:393:ASN:OD1	2.47	0.53
1:C:374:LYS:CA	1:C:377:ALA:HB3	2.31	0.53
1:C:401:LEU:O	1:C:405:LEU:CB	2.56	0.53
1:C:344:ALA:O	1:C:348:ASN:N	2.40	0.53
1:C:124:TRP:HE3	1:C:285:TYR:CD1	2.25	0.53
1:C:245:TRP:CD1	1:C:247:GLU:OE1	2.62	0.53
1:C:370:GLY:C	1:C:371:PHE:HD2	2.11	0.53
1:A:16:ASP:HB2	1:A:311:THR:HG21	1.91	0.53
1:B:35:VAL:CG1	1:B:37:LEU:CD2	2.87	0.53
1:B:26:ILE:O	1:B:30:LEU:HB2	2.08	0.52
1:C:108:PHE:HA	1:C:130:ILE:O	2.08	0.52
1:B:84:GLU:OE2	1:B:87:LYS:HE3	2.09	0.52
1:C:259:MET:HG3	4:C:501:9UO:F04	1.98	0.52
1:B:83:VAL:HA	1:B:88:LEU:CD1	2.39	0.52
1:A:395:PHE:N	1:A:395:PHE:HD1	2.08	0.52
1:C:334:PHE:CZ	1:C:360:GLU:HG2	2.43	0.52
1:A:7:GLY:CA	1:A:37:LEU:HD23	2.20	0.52
1:A:32:PHE:N	1:A:33:PRO:CD	2.72	0.52
1:B:210:SER:HA	1:B:249:ARG:O	2.10	0.52
1:C:160:ASP:OD1	1:C:160:ASP:N	2.42	0.52
1:A:53:ASN:O	1:A:54:ASP:CB	2.58	0.52
1:C:333:ILE:HG23	1:C:334:PHE:N	2.24	0.52
1:B:96:ASN:O	1:B:100:ARG:HB2	2.08	0.52
1:B:160:ASP:OD1	1:B:161:GLY:N	2.43	0.52
1:C:45:GLY:O	1:C:49:ARG:N	2.39	0.52
1:A:120:LEU:HD11	1:B:260:LYS:HG2	1.91	0.52
1:C:120:LEU:CB	1:C:284:GLY:O	2.59	0.52
1:A:133:HIS:O	1:A:271:ASN:CB	2.58	0.51
1:C:40:HIS:CE1	1:C:67:HIS:NE2	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:GLU:OE2	1:C:408:LYS:NZ	2.42	0.51
1:A:316:TYR:O	1:A:320:GLN:HG3	2.11	0.51
1:C:10:VAL:CG1	1:C:11:VAL:N	2.73	0.51
1:C:13:MET:HG3	1:C:72:LYS:HB2	1.93	0.51
1:C:23:TRP:CZ2	1:C:336:TRP:NE1	2.79	0.51
1:A:277:GLN:HE22	4:A:504[B]:9UO:C12	2.23	0.51
1:A:299:ASP:OD1	1:A:300:GLY:N	2.44	0.51
1:A:387:GLN:O	1:A:390:ASP:HB2	2.11	0.51
1:B:13:MET:HE2	1:B:64:ILE:HD11	1.91	0.51
1:C:12:GLU:O	1:C:41:SER:HA	2.11	0.51
1:A:211:THR:O	1:A:250:LEU:HD23	2.11	0.51
1:B:185:GLN:O	1:B:189:ILE:HG13	2.10	0.51
1:B:114:CYS:O	1:B:119:ARG:NH2	2.43	0.51
1:C:254:MET:HG2	1:C:267:TRP:CZ2	2.46	0.51
1:C:373:THR:O	1:C:377:ALA:N	2.38	0.51
1:B:319:TYR:HB2	1:B:325:THR:HG21	1.92	0.51
1:C:137:ASP:C	1:C:182:MET:SD	2.90	0.51
1:C:376:LEU:O	1:C:379:CYS:SG	2.65	0.51
1:B:72:LYS:HB3	1:B:306:GLU:HB3	1.93	0.50
1:C:197:PHE:CZ	1:C:231:TYR:HB2	2.47	0.50
1:C:317:ARG:O	1:C:321:LYS:N	2.40	0.50
1:C:359:LEU:HD12	1:C:359:LEU:O	2.12	0.50
1:B:294:VAL:CG1	1:B:303:VAL:HG13	2.42	0.50
1:C:372:MET:CE	1:C:377:ALA:HA	2.42	0.50
1:B:9:SER:HA	1:B:38:ASP:HB3	1.94	0.50
1:C:43:ASP:OD2	1:C:43:ASP:N	2.30	0.50
1:B:44:LEU:O	1:B:49:ARG:NE	2.42	0.50
1:A:383:LEU:N	1:A:384:PRO:CD	2.75	0.50
1:C:45:GLY:O	1:C:49:ARG:CB	2.60	0.50
1:C:299:ASP:OD1	1:C:299:ASP:O	2.30	0.50
1:C:347:ASP:O	1:C:348:ASN:CB	2.59	0.50
1:B:3:LYS:HZ3	1:B:3:LYS:N	2.10	0.50
1:B:83:VAL:O	1:B:87:LYS:N	2.45	0.50
1:B:395:PHE:N	1:B:395:PHE:CD1	2.77	0.50
1:C:185:GLN:O	1:C:189:ILE:HG13	2.12	0.50
1:C:24:GLU:O	1:C:28:GLU:HG3	2.11	0.49
1:C:154:ILE:HG23	1:C:167:TYR:HB2	1.92	0.49
1:C:27:LYS:O	1:C:32:PHE:HD2	1.95	0.49
1:C:366:THR:HA	1:C:369:ALA:CB	2.42	0.49
1:C:330:ILE:CA	1:C:333:ILE:HG22	2.40	0.49
1:A:137:ASP:OD2	1:A:184:ASN:ND2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:OG1	2:A:501:NDP:H4D	2.13	0.49
1:A:371:PHE:HB3	1:A:392:LEU:HD11	1.95	0.49
1:B:87:LYS:HD3	1:B:87:LYS:N	2.27	0.49
1:B:221:GLY:O	1:B:225:ASP:N	2.32	0.49
1:C:67:HIS:O	1:C:68:ASN:CB	2.61	0.49
1:C:393:ASN:CB	1:C:396:GLU:CB	2.90	0.49
1:A:310:GLY:N	2:A:501:NDP:O1A	2.33	0.49
1:C:343:ARG:CD	1:C:343:ARG:O	2.59	0.49
1:A:218:LYS:HD3	1:B:144:PHE:HA	1.95	0.49
1:A:363:SER:HA	1:A:401:LEU:HD21	1.94	0.49
1:C:343:ARG:O	1:C:343:ARG:HD3	2.12	0.49
1:C:412:ALA:O	1:C:413:LYS:O	2.30	0.49
1:C:402:GLY:O	1:C:406:LYS:N	2.46	0.49
1:C:105:GLY:HA3	1:C:296:VAL:O	2.12	0.49
1:A:255:VAL:O	1:A:259:MET:HG3	2.13	0.48
2:B:501:NDP:O1X	2:B:501:NDP:O3B	2.30	0.48
1:A:356:ALA:O	1:A:360:GLU:HG3	2.13	0.48
1:C:73:CYS:O	1:C:74:ALA:O	2.30	0.48
1:B:16:ASP:O	1:B:311:THR:HG22	2.13	0.48
1:A:271:ASN:ND2	1:A:271:ASN:O	2.40	0.48
1:A:255:VAL:O	1:A:259:MET:HG2	2.14	0.48
1:B:137:ASP:OD2	1:B:184:ASN:ND2	2.44	0.48
1:C:349:ASN:O	1:C:351:GLU:OE1	2.31	0.48
1:C:366:THR:HG22	1:C:371:PHE:O	2.13	0.48
1:A:48:ASN:O	1:A:52:THR:OG1	2.30	0.48
1:A:143:ASP:CB	1:A:180:MET:HG3	2.44	0.48
1:B:24:GLU:OE1	1:B:27:LYS:CE	2.61	0.48
1:C:112:ILE:HG21	1:C:330:ILE:CG2	2.44	0.48
1:A:273:ASP:O	1:A:277:GLN:HG2	2.14	0.48
1:B:64:ILE:HG21	1:B:103:LEU:HD11	1.96	0.48
1:C:13:MET:HB3	1:C:44:LEU:HG	1.95	0.48
1:C:115:LYS:CB	1:C:368:GLU:OE2	2.44	0.48
1:C:234:GLN:O	1:C:238:GLN:NE2	2.47	0.48
1:A:251:ILE:O	1:A:255:VAL:HG13	2.14	0.48
1:C:124:TRP:CE3	1:C:285:TYR:CE1	3.02	0.48
1:B:282:ALA:HB2	1:B:291:MET:HG3	1.96	0.47
1:C:277:GLN:CA	1:C:277:GLN:HE21	2.23	0.47
1:C:366:THR:O	1:C:370:GLY:N	2.47	0.47
1:A:271:ASN:ND2	1:A:271:ASN:C	2.67	0.47
1:B:86:PHE:HB2	1:B:88:LEU:CD2	2.43	0.47
1:C:4:LYS:HE2	1:C:32:PHE:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PRO:O	1:C:264:GLY:HA2	2.14	0.47
1:A:251:ILE:H	1:A:251:ILE:HG13	1.35	0.47
1:B:88:LEU:H	1:B:88:LEU:HG	1.53	0.47
1:C:40:HIS:CD2	1:C:40:HIS:N	2.82	0.47
1:A:146:VAL:HA	1:A:147:PRO:HD3	1.75	0.47
1:A:212:LYS:NZ	1:A:252:ASP:OD2	2.47	0.47
1:B:282:ALA:HB1	1:B:291:MET:HG3	1.96	0.47
1:C:160:ASP:OD2	1:C:162:THR:HG22	2.15	0.47
1:A:201:LEU:HD23	1:A:244:ILE:HD11	1.96	0.47
1:B:162:THR:C	1:B:163:GLN:HG3	2.34	0.47
1:A:32:PHE:N	1:A:33:PRO:HD2	2.30	0.47
1:B:79:ASP:OD1	1:B:82:ARG:HG2	2.15	0.47
1:B:252:ASP:OD1	1:B:252:ASP:N	2.34	0.47
1:C:106:THR:HG23	1:C:132:HIS:O	2.14	0.47
1:C:334:PHE:HA	1:C:337:THR:HG23	1.97	0.47
1:B:154:ILE:HG23	1:B:167:TYR:HB2	1.96	0.46
1:B:383:LEU:N	1:B:384:PRO:CD	2.77	0.46
1:C:296:VAL:HG12	1:C:297:CYS:N	2.31	0.46
1:A:67:HIS:O	1:A:68:ASN:CB	2.63	0.46
1:B:251:ILE:O	1:B:255:VAL:HG13	2.16	0.46
1:A:260:LYS:CG	1:B:283:GLN:NE2	2.57	0.46
1:B:238:GLN:O	1:B:242:GLN:HG3	2.15	0.46
1:A:142:THR:CG2	1:B:154:ILE:HG21	2.45	0.46
1:A:150:GLY:HA3	1:B:156:TYR:CE1	2.49	0.46
1:A:314:ARG:HH21	1:A:315:HIS:CD2	2.34	0.46
1:C:357:ASN:HD21	1:C:361:GLU:HG3	1.80	0.46
1:A:203:LYS:HA	1:A:203:LYS:HD2	1.55	0.46
1:A:222:ARG:HG3	1:B:178:VAL:HG13	1.96	0.46
1:B:32:PHE:N	1:B:33:PRO:CD	2.79	0.46
1:C:32:PHE:N	1:C:33:PRO:HD2	2.31	0.46
1:A:72:LYS:CD	1:A:306:GLU:OE1	2.63	0.46
1:A:160:ASP:OD1	1:A:162:THR:OG1	2.32	0.46
1:A:212:LYS:HZ3	1:A:252:ASP:CG	2.19	0.46
1:C:56:VAL:HG13	1:C:57:THR:N	2.31	0.46
1:C:124:TRP:HA	1:C:262:GLU:O	2.16	0.46
1:C:381:LYS:O	1:C:385:ASN:HB2	2.16	0.46
1:C:151:LYS:HB2	1:C:151:LYS:HE2	1.30	0.46
1:B:337:THR:OG1	1:B:360:GLU:OE2	2.23	0.46
1:B:359:LEU:O	1:B:363:SER:OG	2.30	0.46
1:C:71:VAL:CG1	1:C:336:TRP:HA	2.44	0.46
1:A:260:LYS:CG	1:B:283:GLN:HE21	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LYS:O	1:A:342:HIS:NE2	2.34	0.45
1:B:101:ASN:OD1	1:B:102:ILE:N	2.49	0.45
1:B:124:TRP:HE3	1:B:285:TYR:CE1	2.34	0.45
1:C:330:ILE:HG23	1:C:334:PHE:CD1	2.50	0.45
1:A:7:GLY:HA3	1:A:37:LEU:CD2	2.22	0.45
1:B:327:THR:O	1:B:329:PRO:HD3	2.17	0.45
1:B:383:LEU:HB3	1:B:384:PRO:HD3	1.98	0.45
1:C:29:LYS:CE	1:C:399:ASP:CA	2.94	0.45
1:C:304:GLU:OE1	1:C:304:GLU:C	2.54	0.45
1:C:32:PHE:CB	1:C:33:PRO:HD3	2.46	0.45
1:C:34:TYR:CG	1:C:409:LEU:HD11	2.50	0.45
1:C:303:VAL:HG12	1:C:303:VAL:O	2.16	0.45
1:C:328:ASN:OD1	1:C:329:PRO:HD2	2.16	0.45
1:C:228:GLN:NE2	1:C:246:TYR:HE2	2.15	0.45
1:A:72:LYS:HB3	1:A:306:GLU:HB3	1.98	0.45
1:A:119:ARG:HG2	1:A:285:TYR:O	2.17	0.45
1:A:15:GLY:HA3	1:A:73:CYS:SG	2.56	0.45
1:C:349:ASN:O	1:C:351:GLU:N	2.45	0.45
1:A:53:ASN:O	1:A:54:ASP:HB2	2.17	0.45
1:A:108:PHE:HA	1:A:130:ILE:O	2.17	0.45
1:A:291:MET:HB3	1:A:308:ALA:HB3	1.99	0.45
1:C:53:ASN:O	1:C:54:ASP:CB	2.64	0.45
1:C:128:ILE:CG1	1:C:285:TYR:OH	2.63	0.45
1:C:343:ARG:HD3	1:C:343:ARG:HA	1.62	0.45
1:A:34:TYR:CD1	1:A:409:LEU:HD12	2.51	0.45
1:A:46:ILE:HD12	1:A:46:ILE:C	2.31	0.45
1:A:233:LYS:HB3	1:A:234:GLN:HG2	1.99	0.45
1:C:137:ASP:OD2	1:C:184:ASN:OD1	2.35	0.45
1:C:378:ALA:O	1:C:382:GLY:CA	2.65	0.45
1:C:317:ARG:C	1:C:320:GLN:HG3	2.36	0.44
1:C:320:GLN:HG2	1:C:320:GLN:H	1.44	0.44
1:A:333:ILE:O	1:A:337:THR:HG23	2.16	0.44
1:B:244:ILE:HA	1:B:244:ILE:HD12	1.66	0.44
1:B:393:ASN:C	1:B:393:ASN:OD1	2.56	0.44
1:C:56:VAL:CG1	1:C:57:THR:N	2.80	0.44
1:A:180:MET:HE3	1:A:180:MET:HB3	1.77	0.44
1:B:129:ILE:HD12	1:B:266:ILE:HD13	2.00	0.44
1:B:295:LEU:HB3	1:B:304:GLU:HB3	1.98	0.44
1:A:139:TYR:N	1:A:139:TYR:HD1	2.14	0.44
1:B:212:LYS:N	1:B:220:ASP:OD2	2.42	0.44
1:B:328:ASN:HA	1:B:373:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ILE:CD1	1:C:112:ILE:C	2.70	0.44
1:C:366:THR:C	1:C:369:ALA:HB3	2.37	0.44
1:C:31:ILE:HG13	1:C:32:PHE:N	2.33	0.44
1:C:40:HIS:CD2	1:C:40:HIS:H	2.36	0.44
1:C:49:ARG:CA	1:C:52:THR:OG1	2.61	0.44
1:A:359:LEU:CD1	1:A:405:LEU:HD22	2.49	0.43
1:B:14:GLN:OE1	1:B:14:GLN:CA	2.65	0.43
1:B:106:THR:HG23	1:B:132:HIS:O	2.18	0.43
1:A:107:VAL:HG22	1:A:295:LEU:CD1	2.47	0.43
1:B:96:ASN:ND2	1:B:306:GLU:OE1	2.51	0.43
1:C:100:ARG:O	1:C:104:GLY:N	2.45	0.43
1:C:330:ILE:C	1:C:333:ILE:HG22	2.38	0.43
1:B:32:PHE:N	1:B:33:PRO:HD2	2.34	0.43
1:C:254:MET:HG2	1:C:267:TRP:CE2	2.53	0.43
1:A:149:PRO:HB3	1:A:172:PHE:O	2.18	0.43
1:A:328:ASN:HA	1:A:373:THR:HG21	2.00	0.43
1:B:26:ILE:HG12	1:B:333:ILE:HG12	2.00	0.43
1:C:228:GLN:HE22	1:C:246:TYR:HE2	1.67	0.43
1:A:314:ARG:HH21	1:A:315:HIS:HE2	1.67	0.43
1:B:205:TRP:CE3	1:B:264:GLY:O	2.72	0.43
1:C:255:VAL:HG23	1:C:256:ALA:N	2.34	0.43
1:C:137:ASP:HB2	1:C:182:MET:SD	2.58	0.43
1:C:293:SER:HB3	1:C:308:ALA:HA	2.01	0.43
1:B:14:GLN:OE1	1:B:14:GLN:HA	2.18	0.43
1:C:343:ARG:CD	1:C:343:ARG:C	2.87	0.43
1:C:374:LYS:O	1:C:377:ALA:HB3	2.18	0.43
1:A:94:SER:HA	1:A:95:PRO:HD3	1.93	0.43
1:A:301:LYS:HE3	1:A:301:LYS:HB3	1.79	0.43
1:A:378:ALA:HA	1:A:386:VAL:CG2	2.48	0.43
1:A:383:LEU:N	1:A:384:PRO:HD2	2.34	0.43
1:B:220:ASP:O	1:B:223:PHE:HB2	2.18	0.43
1:A:47:GLU:OE2	1:A:47:GLU:N	2.30	0.42
1:C:317:ARG:HA	1:C:320:GLN:OE1	2.19	0.42
1:C:372:MET:SD	1:C:377:ALA:CA	3.06	0.42
1:A:328:ASN:HA	1:A:329:PRO:HD3	1.74	0.42
1:B:67:HIS:O	1:B:68:ASN:CB	2.64	0.42
1:B:79:ASP:H	1:B:82:ARG:HB2	1.84	0.42
1:C:366:THR:CA	1:C:369:ALA:HB3	2.49	0.42
1:A:33:PRO:HB2	1:A:34:TYR:CD2	2.55	0.42
1:A:383:LEU:CB	1:A:384:PRO:HD3	2.46	0.42
1:B:224:LYS:HG3	1:B:248:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.85	0.42
1:A:193:ALA:HA	1:A:227:PHE:CZ	2.53	0.42
1:C:49:ARG:C	1:C:52:THR:HG1	2.20	0.42
1:C:183:TYR:CD2	1:C:183:TYR:C	2.91	0.42
1:A:31:ILE:HG22	1:A:32:PHE:CD1	2.54	0.42
1:B:112:ILE:HD11	1:B:292:THR:HG23	2.01	0.42
1:B:146:VAL:HA	1:B:147:PRO:HD3	1.80	0.42
1:B:359:LEU:HD13	1:B:405:LEU:HD13	2.01	0.42
1:C:24:GLU:O	1:C:28:GLU:CG	2.67	0.42
1:C:247:GLU:CD	1:C:249:ARG:NH2	2.73	0.42
1:C:271:ASN:HD22	1:C:271:ASN:C	2.21	0.42
1:A:367:ILE:HD13	1:A:376:LEU:HD12	1.98	0.42
1:B:375:ASP:OD1	1:B:375:ASP:N	2.51	0.42
1:A:180:MET:HE2	1:B:182:MET:HG2	2.00	0.42
1:A:314:ARG:HE	1:A:314:ARG:HB3	1.69	0.42
2:B:501:NDP:HO3A	2:B:501:NDP:P2B	2.42	0.42
1:A:40:HIS:CD2	1:A:67:HIS:CD2	3.08	0.42
1:A:182:MET:CG	1:B:180:MET:CE	2.97	0.42
1:B:25:LEU:HD22	1:B:29:LYS:HD2	2.01	0.42
1:B:146:VAL:HB	1:B:177:GLY:O	2.20	0.42
1:B:154:ILE:CG2	1:B:167:TYR:HB2	2.50	0.42
1:B:383:LEU:N	1:B:384:PRO:HD3	2.35	0.42
1:C:365:GLU:CD	1:C:408:LYS:NZ	2.73	0.42
1:A:112:ILE:HD13	1:A:330:ILE:CG2	2.47	0.42
1:A:150:GLY:HA3	1:B:156:TYR:HE1	1.85	0.42
1:B:30:LEU:HD22	1:B:405:LEU:HD22	2.02	0.42
1:B:277:GLN:OE1	1:B:277:GLN:HA	2.20	0.42
2:B:501:NDP:H2D	2:B:501:NDP:H6N	1.83	0.42
1:C:333:ILE:HD11	1:C:359:LEU:CG	2.48	0.42
1:A:78:PRO:HG2	1:A:92:TRP:HB2	2.01	0.41
1:B:16:ASP:HB2	1:B:311:THR:HG21	2.01	0.41
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.86	0.41
1:A:348:ASN:ND2	5:A:607:HOH:O	2.49	0.41
1:B:291:MET:O	1:B:331:ALA:HB1	2.21	0.41
1:A:26:ILE:O	1:A:30:LEU:HB2	2.19	0.41
1:C:137:ASP:CB	1:C:219:TYR:OH	2.46	0.41
1:B:79:ASP:OD1	1:B:79:ASP:C	2.57	0.41
1:C:32:PHE:N	1:C:33:PRO:CD	2.83	0.41
1:B:87:LYS:CD	1:B:87:LYS:N	2.83	0.41
1:C:204:GLY:CA	1:C:244:ILE:HD11	2.44	0.41
1:A:18:MET:O	1:A:22:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ALA:HB2	1:A:99:ILE:HG12	2.00	0.41
1:A:230:ILE:O	1:A:234:GLN:HG3	2.20	0.41
1:A:254:MET:HG2	1:A:267:TRP:CE2	2.55	0.41
1:B:12:GLU:HA	1:B:71:VAL:HG23	2.02	0.41
1:B:14:GLN:O	1:B:44:LEU:HB2	2.19	0.41
1:A:39:LEU:HD12	1:A:39:LEU:HA	1.93	0.41
1:A:260:LYS:HD2	1:A:260:LYS:HA	1.36	0.41
1:B:15:GLY:N	1:B:73:CYS:HB3	2.36	0.41
1:C:119:ARG:HD3	1:C:121:VAL:O	2.21	0.41
1:C:201:LEU:HD23	1:C:201:LEU:HA	1.90	0.41
1:A:162:THR:HG22	1:A:163:GLN:N	2.34	0.41
1:C:366:THR:O	1:C:369:ALA:CB	2.60	0.41
1:B:46:ILE:HG23	1:B:47:GLU:N	2.36	0.41
1:B:213:ASN:HA	1:B:220:ASP:HB2	2.01	0.41
1:C:40:HIS:NE2	1:C:67:HIS:NE2	2.69	0.41
1:C:96:ASN:ND2	1:C:96:ASN:O	2.46	0.41
1:C:28:GLU:H	1:C:28:GLU:HG2	1.58	0.41
1:C:119:ARG:HH11	1:C:119:ARG:N	2.19	0.41
1:A:143:ASP:HB3	1:A:180:MET:HG3	2.03	0.40
1:C:126:LYS:HB3	1:C:264:GLY:N	2.36	0.40
1:A:79:ASP:H	1:A:82:ARG:HB2	1.87	0.40
1:A:199:MET:O	1:A:203:LYS:HB2	2.20	0.40
1:A:259:MET:SD	4:A:504[B]:9UO:F04	2.68	0.40
1:C:210:SER:OG	1:C:267:TRP:NE1	2.33	0.40
1:A:46:ILE:HD13	1:A:46:ILE:HA	1.91	0.40
1:A:168:LEU:HD11	1:A:170:HIS:O	2.21	0.40
1:A:371:PHE:CD2	1:A:371:PHE:N	2.89	0.40
1:C:105:GLY:CA	1:C:296:VAL:O	2.69	0.40
1:A:33:PRO:HB2	1:A:34:TYR:CE2	2.56	0.40
1:A:100:ARG:HG3	1:A:295:LEU:CD1	2.52	0.40
1:B:111:ALA:HB2	1:B:291:MET:HE1	1.86	0.40
1:C:32:PHE:HB2	1:C:33:PRO:HD3	2.03	0.40
1:C:243:LYS:NZ	5:C:608:HOH:O	2.53	0.40
1:C:318:MET:O	1:C:322:GLY:N	2.44	0.40
1:A:269:CYS:HA	5:A:606:HOH:O	2.21	0.40
4:A:504[A]:9UO:C12	1:B:277:GLN:HE21	2.29	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	410/425 (96%)	403 (98%)	7 (2%)	0	100	100
1	B	409/425 (96%)	401 (98%)	8 (2%)	0	100	100
1	C	386/425 (91%)	375 (97%)	11 (3%)	0	100	100
All	All	1205/1275 (94%)	1179 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	347/361 (96%)	281 (81%)	66 (19%)	1	8
1	B	346/361 (96%)	280 (81%)	66 (19%)	1	8
1	C	241/361 (67%)	165 (68%)	76 (32%)	0	1
All	All	934/1083 (86%)	726 (78%)	208 (22%)	1	4

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6	SER
1	A	19	THR
1	A	21	ILE
1	A	36	GLU

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Mol	Chain	Res	Type
1	A	41	SER
1	A	46	ILE
1	A	58	LYS
1	A	65	LYS
1	A	75	THR
1	A	80	GLU
1	A	96	ASN
1	A	101	ASN
1	A	137	ASP
1	A	139	TYR
1	A	142	THR
1	A	151	LYS
1	A	159	SER
1	A	163	GLN
1	A	171	ASN
1	A	173	GLU
1	A	174	GLU
1	A	178	VAL
1	A	180	MET
1	A	185	GLN
1	A	188	SER
1	A	195	SER
1	A	196	SER
1	A	203	LYS
1	A	212	LYS
1	A	213	ASN
1	A	215	ILE
1	A	217	LYS
1	A	226	ILE
1	A	229	GLU
1	A	234	GLN
1	A	237	SER
1	A	240	GLU
1	A	249	ARG
1	A	251	ILE
1	A	252	ASP
1	A	259	MET
1	A	260	LYS
1	A	261	SER
1	A	266	ILE
1	A	271	ASN
1	A	279	ASP

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Mol	Chain	Res	Type
1	A	280	SER
1	A	288	LEU
1	A	292	THR
1	A	304	GLU
1	A	311	THR
1	A	312	VAL
1	A	314	ARG
1	A	327	THR
1	A	330	ILE
1	A	332	SER
1	A	338	ARG
1	A	345	LYS
1	A	348	ASN
1	A	350	LYS
1	A	351	GLU
1	A	362	VAL
1	A	364	ILE
1	A	383	LEU
1	A	389	SER
1	B	3	LYS
1	B	6	SER
1	B	19	THR
1	B	28	GLU
1	B	44	LEU
1	B	46	ILE
1	B	52	THR
1	B	71	VAL
1	B	80	GLU
1	B	81	LYS
1	B	87	LYS
1	B	88	LEU
1	B	89	LYS
1	B	91	MET
1	B	94	SER
1	B	101	ASN
1	B	112	ILE
1	B	113	ILE
1	B	119	ARG
1	B	122	SER
1	B	137	ASP
1	B	138	GLN
1	B	139	TYR

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Mol	Chain	Res	Type
1	B	151	LYS
1	B	154	ILE
1	B	155	THR
1	B	163	GLN
1	B	166	THR
1	B	173	GLU
1	B	178	VAL
1	B	180	MET
1	B	188	SER
1	B	198	GLN
1	B	203	LYS
1	B	209	LEU
1	B	212	LYS
1	B	222	ARG
1	B	233	LYS
1	B	237	SER
1	B	244	ILE
1	B	252	ASP
1	B	255	VAL
1	B	260	LYS
1	B	261	SER
1	B	262	GLU
1	B	266	ILE
1	B	270	LYS
1	B	271	ASN
1	B	277	GLN
1	B	279	ASP
1	B	280	SER
1	B	287	SER
1	B	288	LEU
1	B	299	ASP
1	B	311	THR
1	B	312	VAL
1	B	313	THR
1	B	323	GLN
1	B	330	ILE
1	B	332	SER
1	B	338	ARG
1	B	362	VAL
1	B	363	SER
1	B	364	ILE
1	B	389	SER

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Mol	Chain	Res	Type
1	B	393	ASN
1	C	9	SER
1	C	13	MET
1	C	14	GLN
1	C	28	GLU
1	C	40	HIS
1	C	43	ASP
1	C	44	LEU
1	C	53	ASN
1	C	54	ASP
1	C	64	ILE
1	C	71	VAL
1	C	96	ASN
1	C	107	VAL
1	C	109	ARG
1	C	112	ILE
1	C	115	LYS
1	C	117	ILE
1	C	119	ARG
1	C	121	VAL
1	C	122	SER
1	C	128	ILE
1	C	129	ILE
1	C	137	ASP
1	C	139	TYR
1	C	140	ARG
1	C	151	LYS
1	C	154	ILE
1	C	155	THR
1	C	157	THR
1	C	160	ASP
1	C	162	THR
1	C	164	LYS
1	C	178	VAL
1	C	180	MET
1	C	184	ASN
1	C	191	ASP
1	C	210	SER
1	C	212	LYS
1	C	218	LYS
1	C	228	GLN
1	C	234	GLN

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Mol	Chain	Res	Type
1	C	238	GLN
1	C	243	LYS
1	C	247	GLU
1	C	261	SER
1	C	262	GLU
1	C	266	ILE
1	C	271	ASN
1	C	275	ASP
1	C	277	GLN
1	C	278	SER
1	C	283	GLN
1	C	292	THR
1	C	299	ASP
1	C	302	THR
1	C	303	VAL
1	C	304	GLU
1	C	313	THR
1	C	320	GLN
1	C	325	THR
1	C	332	SER
1	C	333	ILE
1	C	338	ARG
1	C	343	ARG
1	C	352	LEU
1	C	355	PHE
1	C	357	ASN
1	C	359	LEU
1	C	371	PHE
1	C	372	MET
1	C	379	CYS
1	C	385	ASN
1	C	398	MET
1	C	404	ASN
1	C	407	ILE
1	C	408	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	185	GLN
1	A	257	GLN

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Mol	Chain	Res	Type
1	A	271	ASN
1	A	277	GLN
1	A	348	ASN
1	B	90	GLN
1	B	96	ASN
1	B	198	GLN
1	B	234	GLN
1	B	271	ASN
1	B	277	GLN
1	B	283	GLN
1	B	357	ASN
1	C	40	HIS
1	C	96	ASN
1	C	101	ASN
1	C	133	HIS
1	C	163	GLN
1	C	184	ASN
1	C	228	GLN
1	C	234	GLN
1	C	342	HIS
1	C	357	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	B	501	-	45,52,52	0.99	2 (4%)	53,80,80	1.10	3 (5%)
4	9UO	A	504[A]	-	28,28,28	2.43	2 (7%)	32,42,42	3.05	11 (34%)
4	9UO	A	504[B]	-	28,28,28	2.43	2 (7%)	32,42,42	3.10	12 (37%)
2	NDP	A	501	-	45,52,52	1.00	2 (4%)	53,80,80	1.09	3 (5%)
4	9UO	C	501	-	28,28,28	2.41	2 (7%)	32,42,42	3.16	12 (37%)

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	NDP	B	501	-	-	17/30/77/77	0/5/5/5
4	9UO	A	504[A]	-	-	12/24/24/24	0/2/2/2
4	9UO	A	504[B]	-	-	12/24/24/24	0/2/2/2
2	NDP	A	501	-	-	18/30/77/77	0/5/5/5
4	9UO	C	501	-	-	10/24/24/24	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504[B]	9UO	C19-N20	8.52	1.45	1.34
4	A	504[A]	9UO	C19-N20	8.41	1.45	1.34
4	A	504[A]	9UO	C08-N07	8.36	1.45	1.34
4	C	501	9UO	C19-N20	8.36	1.45	1.34
4	C	501	9UO	C08-N07	8.29	1.45	1.34
4	A	504[B]	9UO	C08-N07	8.26	1.45	1.34
2	A	501	NDP	C6N-C5N	3.22	1.39	1.33
2	B	501	NDP	C6N-C5N	3.17	1.39	1.33
2	A	501	NDP	C5A-C4A	2.07	1.46	1.40
2	B	501	NDP	C5A-C4A	2.06	1.46	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504[A]	9UO	C19-N18-C10	8.98	120.32	114.60
4	A	504[B]	9UO	C08-N09-C10	8.84	120.23	114.60
4	C	501	9UO	C08-N09-C10	8.63	120.10	114.60
4	A	504[B]	9UO	C19-N18-C10	8.46	119.99	114.60
4	C	501	9UO	C19-N18-C10	8.36	119.93	114.60
4	A	504[A]	9UO	C08-N09-C10	8.16	119.80	114.60
4	C	501	9UO	C19-N20-C21	-5.85	119.73	124.53
4	C	501	9UO	C08-N07-C02	-5.56	119.96	124.53
4	A	504[A]	9UO	C08-N07-C02	-5.13	120.32	124.53
4	A	504[B]	9UO	C19-N20-C21	-4.96	120.46	124.53
4	A	504[B]	9UO	C08-N07-C02	-4.75	120.64	124.53
4	A	504[A]	9UO	C19-N20-C21	-4.21	121.08	124.53
4	C	501	9UO	N27-C08-N09	-4.02	119.88	126.23
4	A	504[B]	9UO	N27-C19-N18	-3.99	119.92	126.23
4	A	504[A]	9UO	N27-C19-N18	-3.99	119.93	126.23
4	C	501	9UO	N27-C19-N18	-3.95	119.98	126.23
4	A	504[B]	9UO	N27-C08-N09	-3.90	120.06	126.23
4	A	504[A]	9UO	N27-C08-N09	-3.79	120.23	126.23
4	C	501	9UO	C19-N27-C08	3.70	120.16	113.89
4	A	504[B]	9UO	C19-N27-C08	3.57	119.95	113.89
4	A	504[A]	9UO	C19-N27-C08	3.49	119.81	113.89
2	A	501	NDP	N3A-C2A-N1A	-3.39	123.37	128.68
4	A	504[B]	9UO	N18-C10-N09	-3.33	119.84	125.23
2	B	501	NDP	N3A-C2A-N1A	-3.30	123.52	128.68
4	A	504[A]	9UO	N18-C10-N09	-3.29	119.91	125.23
4	C	501	9UO	N18-C10-N09	-3.26	119.95	125.23
4	A	504[B]	9UO	C10-C11-N17	2.79	120.23	117.28
2	A	501	NDP	C4A-C5A-N7A	-2.74	106.55	109.40
4	A	504[B]	9UO	C11-C10-N18	2.73	121.19	117.48
4	A	504[A]	9UO	C11-C10-N09	2.72	121.17	117.48
4	A	504[A]	9UO	C10-C11-N17	2.66	120.10	117.28
4	A	504[A]	9UO	N20-C19-N27	2.61	121.09	117.18
4	C	501	9UO	C10-C11-N17	2.54	119.97	117.28
2	B	501	NDP	C4A-C5A-N7A	-2.44	106.86	109.40
4	A	504[B]	9UO	N07-C08-N27	2.34	120.69	117.18
2	A	501	NDP	PN-O3-PA	-2.26	125.06	132.83
4	C	501	9UO	C11-C10-N18	2.26	120.55	117.48
4	C	501	9UO	N20-C19-N18	2.11	120.35	117.18
2	B	501	NDP	O4D-C1D-N1N	2.11	112.18	108.06
4	C	501	9UO	N07-C08-N27	2.03	120.23	117.18
4	A	504[B]	9UO	N20-C19-N18	2.00	120.19	117.18

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	PA-O3-PN-O5D
2	A	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	O4D-C4D-C5D-O5D
2	A	501	NDP	C2N-C3N-C7N-O7N
2	B	501	NDP	C5B-O5B-PA-O1A
2	B	501	NDP	C5B-O5B-PA-O2A
2	B	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C5D-O5D-PN-O3
4	A	504[A]	9UO	C22-C21-C23-F24
4	A	504[A]	9UO	C22-C21-C23-F25
4	A	504[A]	9UO	C22-C21-C23-F26
4	A	504[A]	9UO	N20-C21-C23-F24
4	A	504[A]	9UO	N20-C21-C23-F25
4	A	504[A]	9UO	N20-C21-C23-F26
4	A	504[A]	9UO	C01-C02-C03-F04
4	A	504[A]	9UO	C01-C02-C03-F05
4	A	504[A]	9UO	C01-C02-C03-F06
4	A	504[A]	9UO	N07-C02-C03-F04
4	A	504[A]	9UO	N07-C02-C03-F05
4	A	504[A]	9UO	N07-C02-C03-F06
4	A	504[B]	9UO	C22-C21-C23-F24
4	A	504[B]	9UO	C22-C21-C23-F25
4	A	504[B]	9UO	C22-C21-C23-F26
4	A	504[B]	9UO	N20-C21-C23-F25
4	A	504[B]	9UO	C01-C02-C03-F04
4	A	504[B]	9UO	C01-C02-C03-F05
4	A	504[B]	9UO	C01-C02-C03-F06
4	A	504[B]	9UO	N07-C02-C03-F04
4	A	504[B]	9UO	N07-C02-C03-F05
4	A	504[B]	9UO	N07-C02-C03-F06
4	C	501	9UO	N09-C08-N07-C02
4	C	501	9UO	N27-C08-N07-C02
2	A	501	NDP	C3B-C4B-C5B-O5B
2	A	501	NDP	C3D-C4D-C5D-O5D
2	A	501	NDP	C1B-C2B-O2B-P2B
2	A	501	NDP	C3B-C2B-O2B-P2B
2	B	501	NDP	O4D-C4D-C5D-O5D
4	C	501	9UO	N09-C10-C11-N17
4	A	504[B]	9UO	N20-C21-C23-F24
4	C	501	9UO	N18-C10-C11-N17
4	C	501	9UO	N18-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	C	501	9UO	N09-C10-C11-C12
2	B	501	NDP	PA-O3-PN-O5D
4	C	501	9UO	C22-C21-C23-F24
2	A	501	NDP	C2B-O2B-P2B-O1X
2	B	501	NDP	C2D-C1D-N1N-C2N
2	B	501	NDP	PN-O3-PA-O2A
2	A	501	NDP	C2N-C3N-C7N-N7N
2	B	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	C2D-C1D-N1N-C2N
2	A	501	NDP	O4D-C1D-N1N-C2N
2	B	501	NDP	O4D-C1D-N1N-C2N
2	B	501	NDP	C2D-C1D-N1N-C6N
4	A	504[B]	9UO	N20-C21-C23-F26
4	C	501	9UO	N20-C21-C23-F26
2	A	501	NDP	PN-O3-PA-O2A
2	A	501	NDP	C2D-C1D-N1N-C6N
2	B	501	NDP	O4D-C1D-N1N-C6N
4	C	501	9UO	C22-C21-C23-F25
2	B	501	NDP	C3D-C4D-C5D-O5D
2	B	501	NDP	C2B-O2B-P2B-O1X
2	A	501	NDP	C5D-O5D-PN-O3
2	B	501	NDP	C2B-O2B-P2B-O3X
4	C	501	9UO	N20-C21-C23-F25
2	A	501	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	PN-O3-PA-O1A
2	B	501	NDP	C5D-O5D-PN-O2N
2	B	501	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

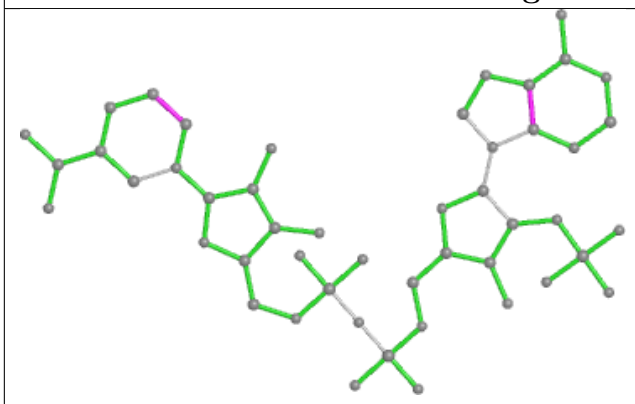
5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NDP	5	0
4	A	504[A]	9UO	5	0
4	A	504[B]	9UO	5	0
2	A	501	NDP	5	0
4	C	501	9UO	2	0

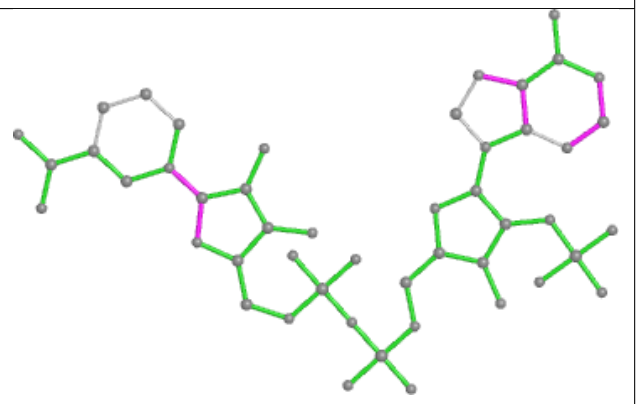
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

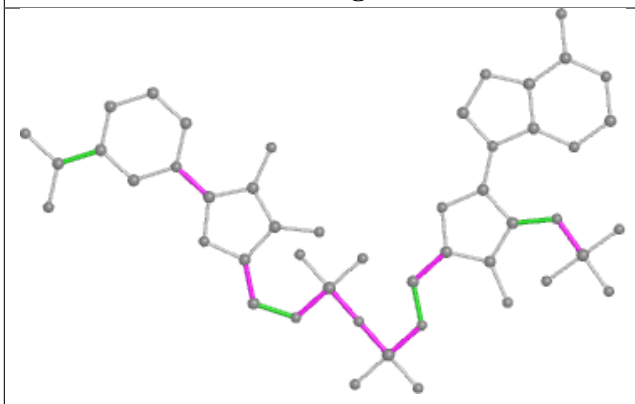
Ligand NDP B 501



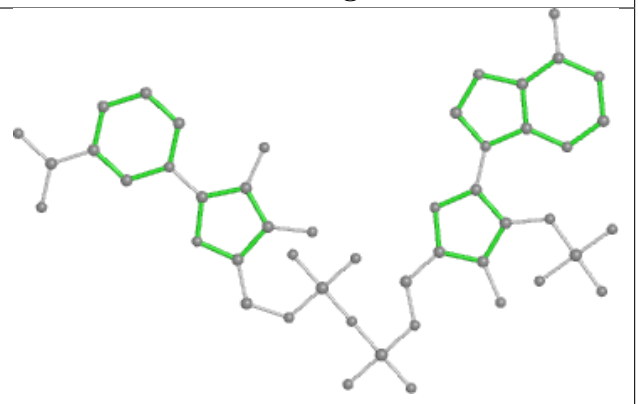
Bond lengths



Bond angles

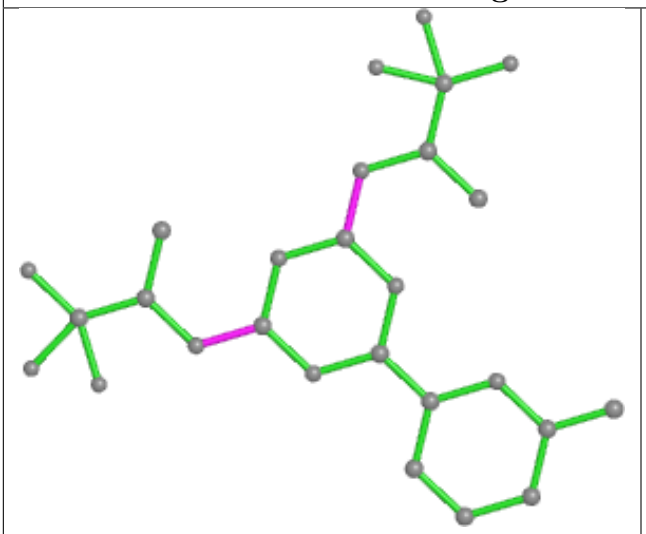


Torsions

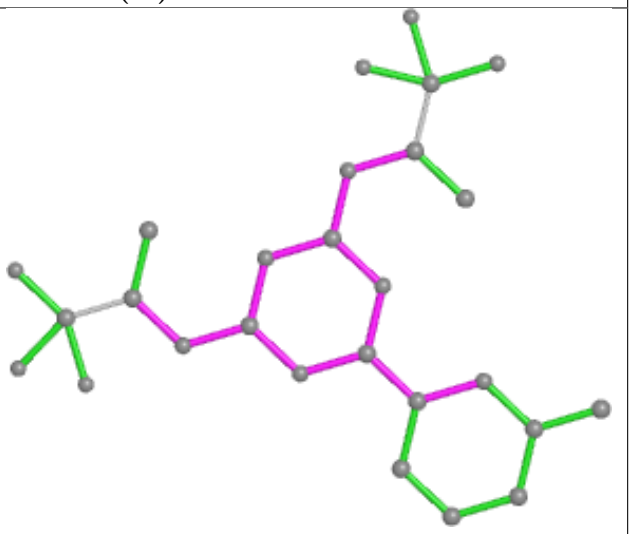


Rings

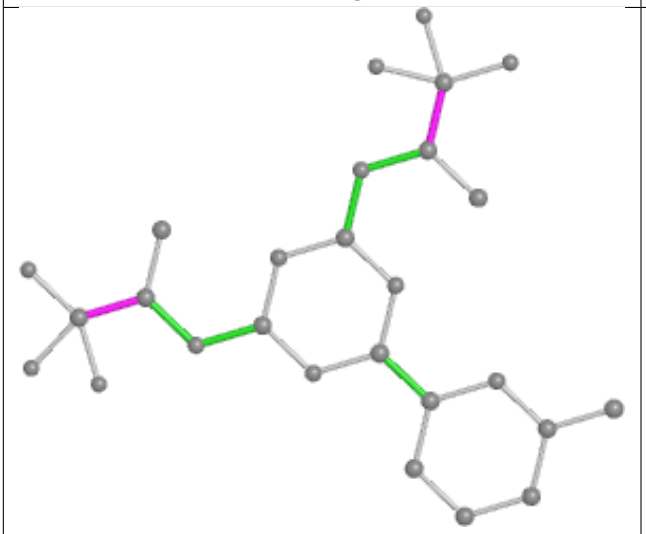
Ligand 9UO A 504 (A)



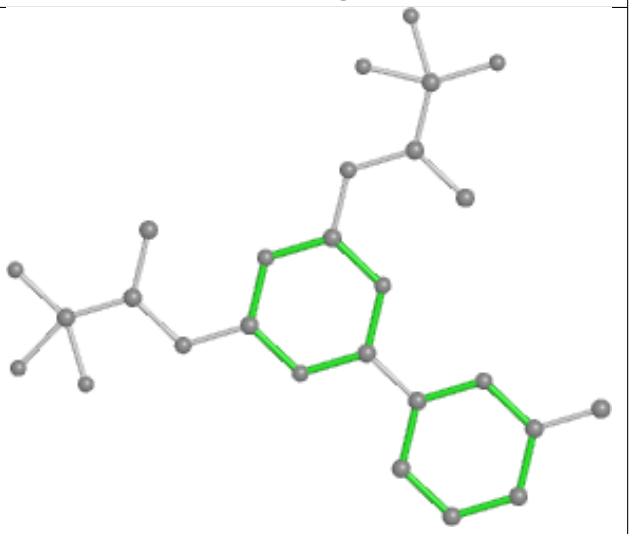
Bond lengths



Bond angles

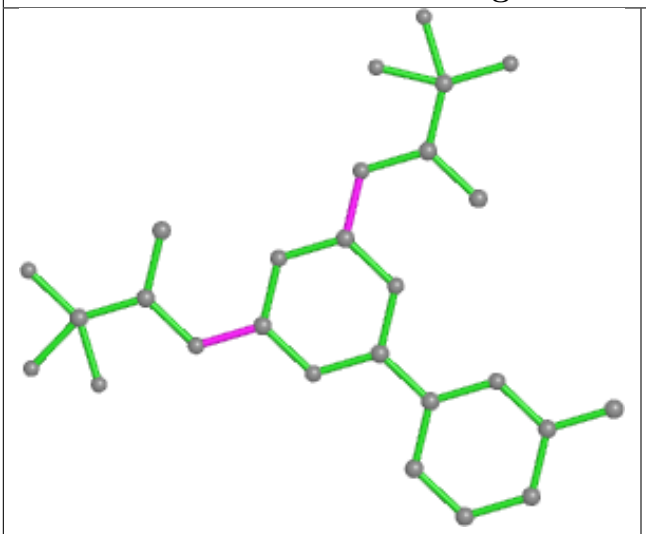


Torsions

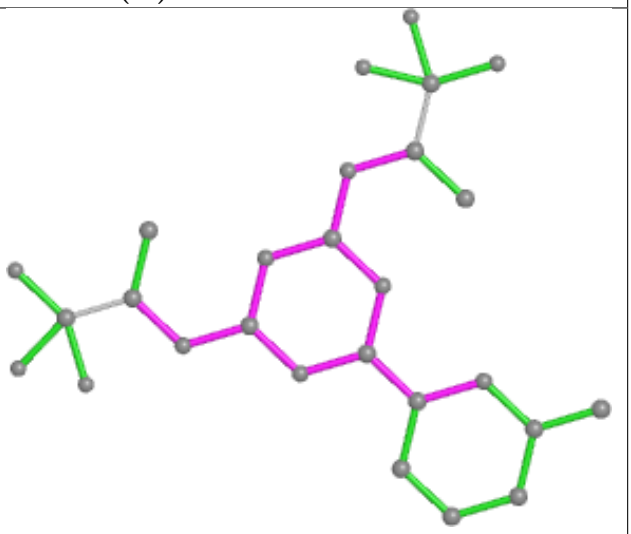


Rings

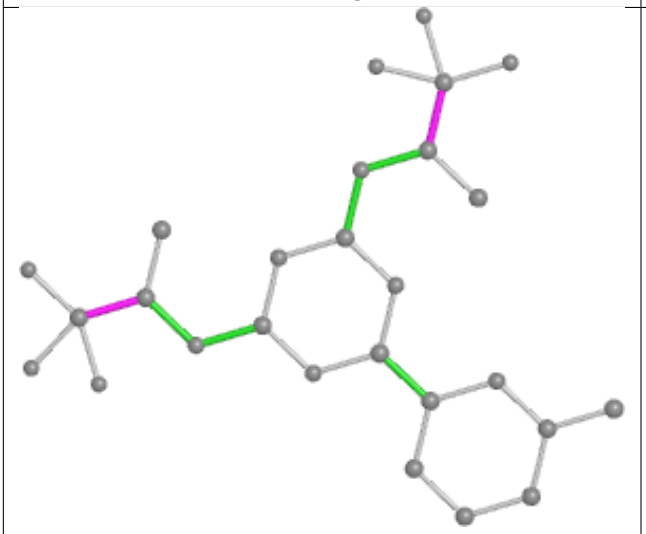
Ligand 9UO A 504 (B)



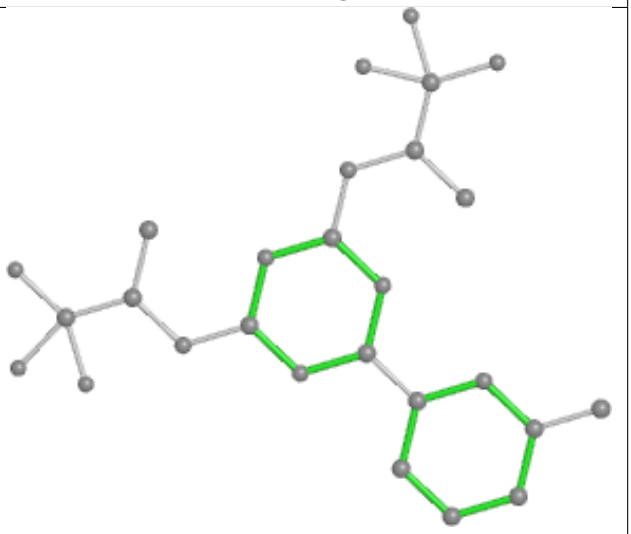
Bond lengths



Bond angles

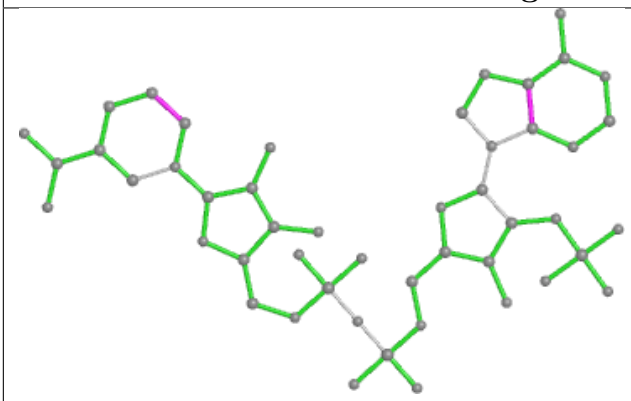


Torsions

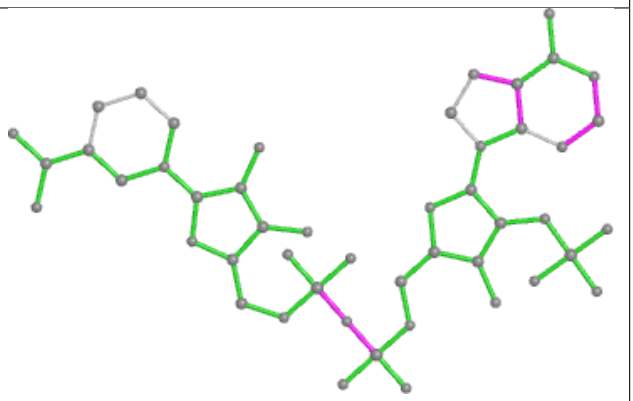


Rings

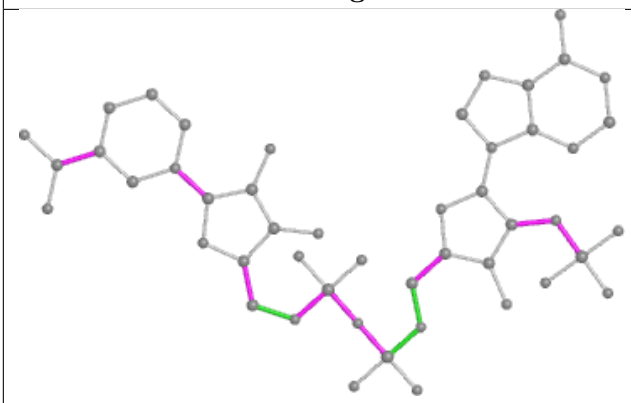
Ligand NDP A 501



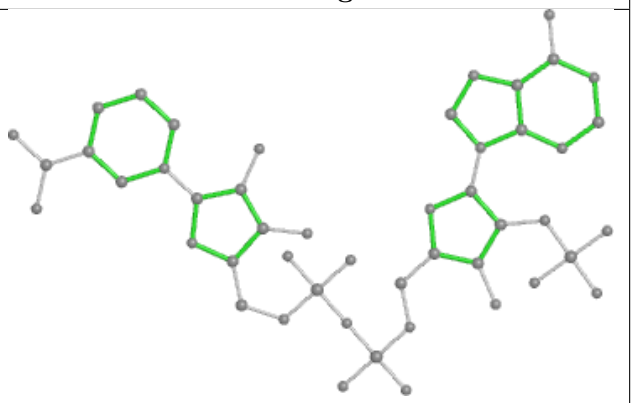
Bond lengths



Bond angles

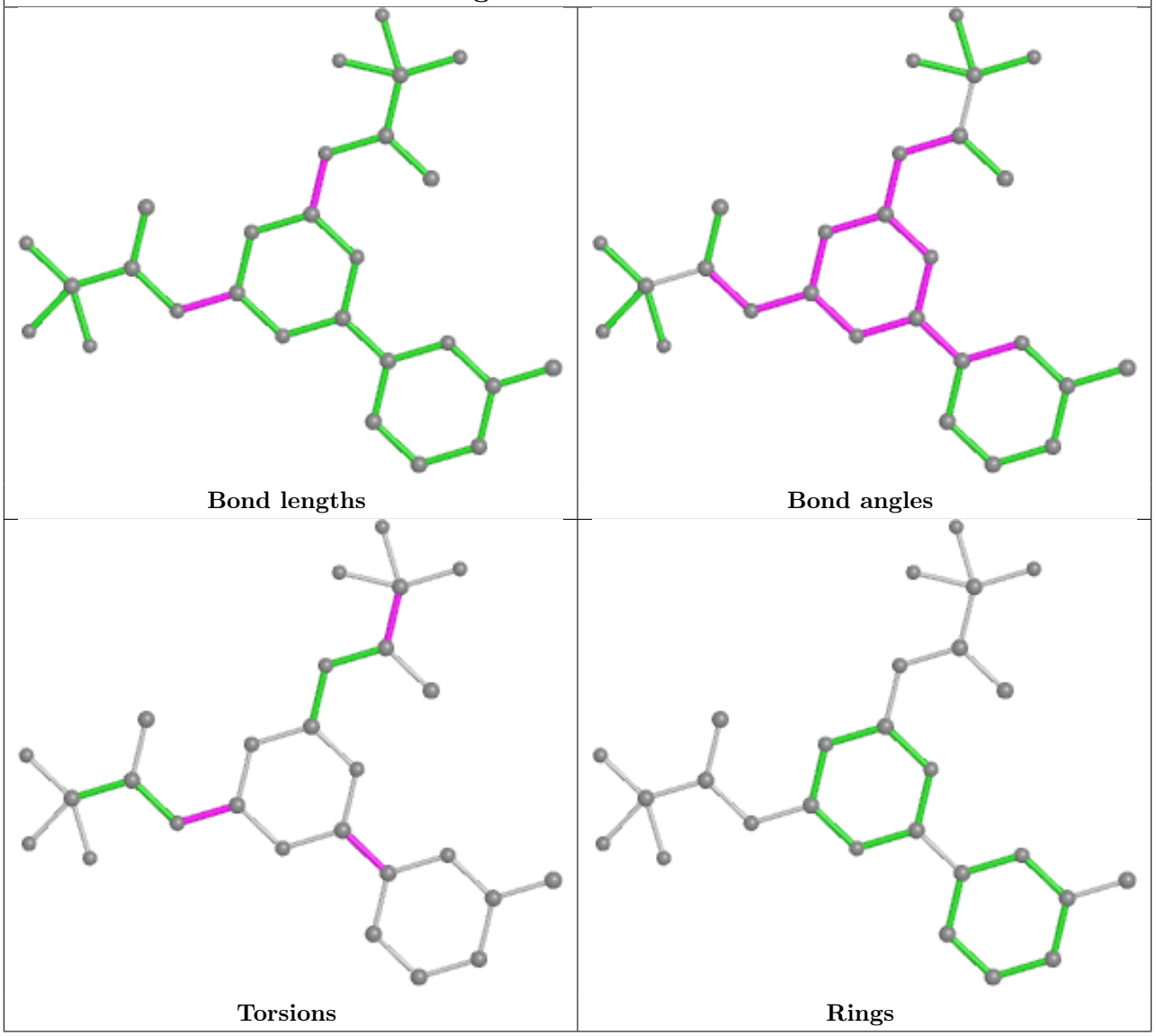


Torsions



Rings

Ligand 9UO C 501



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, 95^{th} 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	412/425 (96%)	-0.38	0 100 100	23, 36, 54, 74	0
1	B	411/425 (96%)	-0.39	0 100 100	24, 37, 57, 70	0
1	C	390/425 (91%)	0.34	36 (9%) 9 3	28, 89, 133, 154	0
All	All	1213/1275 (95%)	-0.15	36 (2%) 50 22	23, 40, 120, 154	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	327	THR	3.5
1	C	73	CYS	3.4
1	C	398	MET	3.4
1	C	324	GLU	3.1
1	C	50	ASP	3.1
1	C	70	GLY	3.1
1	C	47	GLU	3.1
1	C	319	TYR	3.0
1	C	49	ARG	2.9
1	C	323	GLN	2.8
1	C	390	ASP	2.8
1	C	329	PRO	2.6
1	C	11	VAL	2.6
1	C	7	GLY	2.6
1	C	316	TYR	2.5
1	C	285	TYR	2.3
1	C	386	VAL	2.3
1	C	52	THR	2.3
1	C	12	GLU	2.3
1	C	34	TYR	2.3
1	C	30	LEU	2.3
1	C	303	VAL	2.3
1	C	23	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	57	THR	2.2
1	C	113	ILE	2.2
1	C	330	ILE	2.1
1	C	287	SER	2.1
1	C	10	VAL	2.1
1	C	371	PHE	2.1
1	C	370	GLY	2.0
1	C	369	ALA	2.0
1	C	33	PRO	2.0
1	C	43	ASP	2.0
1	C	48	ASN	2.0
1	C	328	ASN	2.0
1	C	375	ASP	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

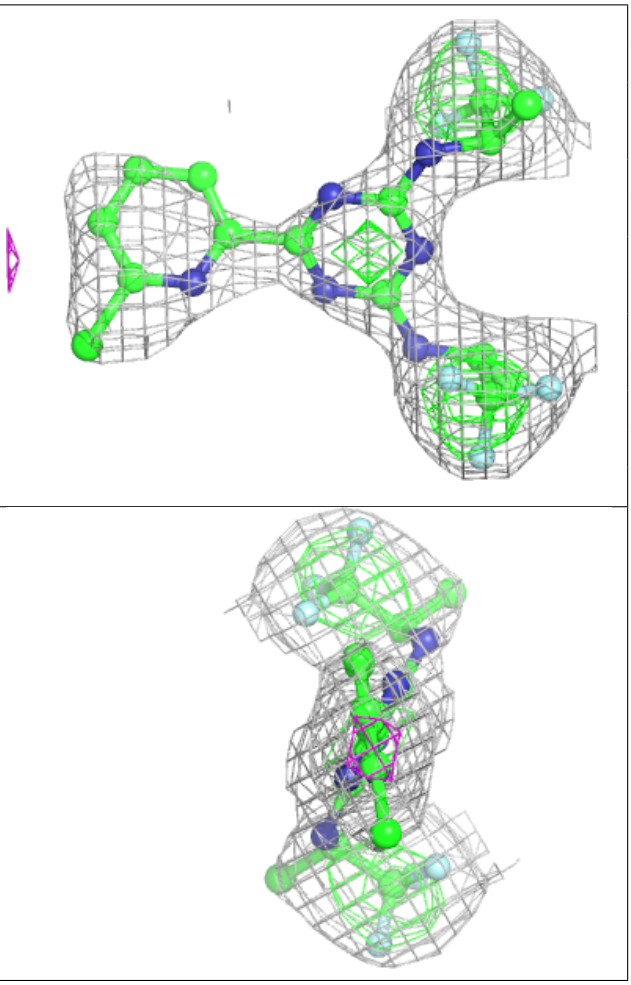
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	502	1/1	0.72	0.78	53,53,53,53	0
3	MG	A	503	1/1	0.74	0.72	53,53,53,53	0
4	9UO	C	501	27/27	0.84	0.44	108,154,159,191	27
4	9UO	A	504[B]	27/27	0.95	0.22	35,41,47,60	27
4	9UO	A	504[A]	27/27	0.95	0.22	30,41,47,68	27
2	NDP	B	501	48/48	0.96	0.15	24,31,43,46	0
2	NDP	A	501	48/48	0.96	0.14	23,32,39,43	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.

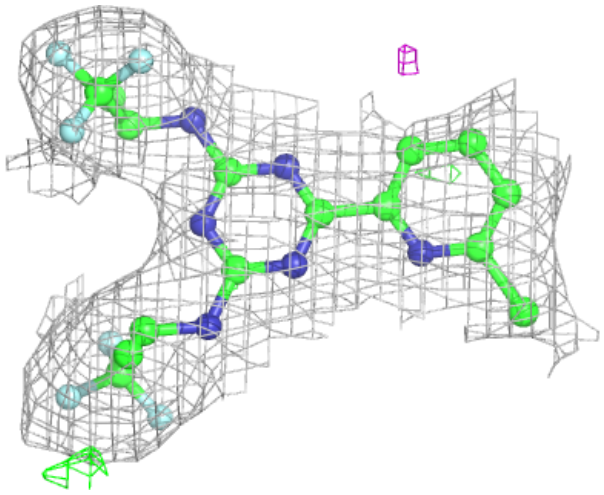
Electron density around 9UO C 501:

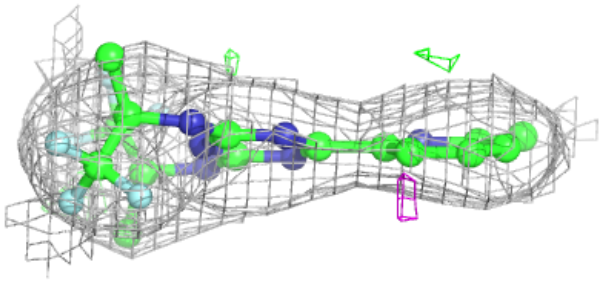
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

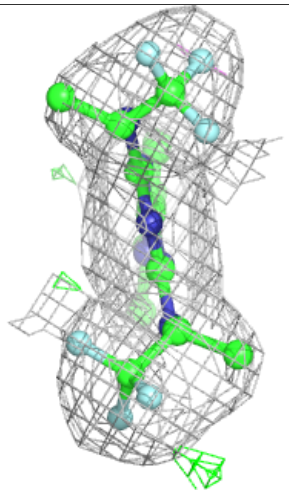


Electron density around 9UO A 504 (B):

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

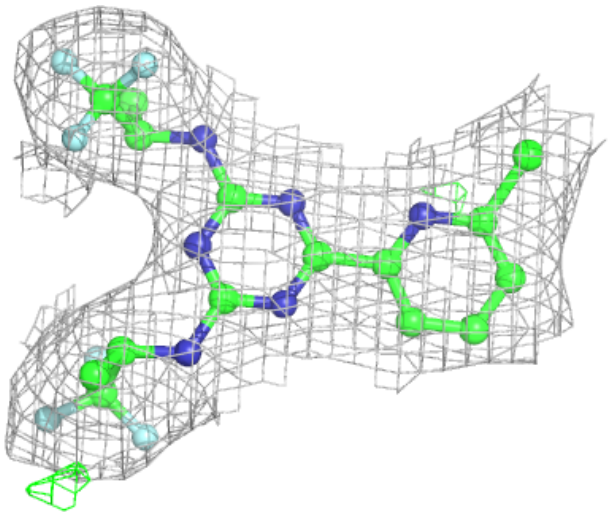


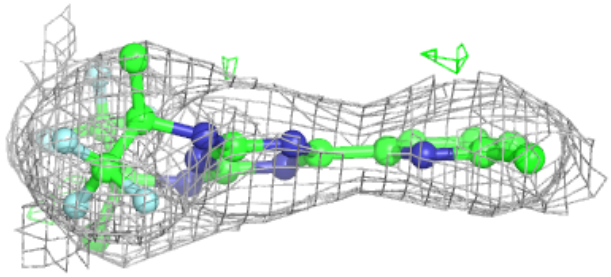


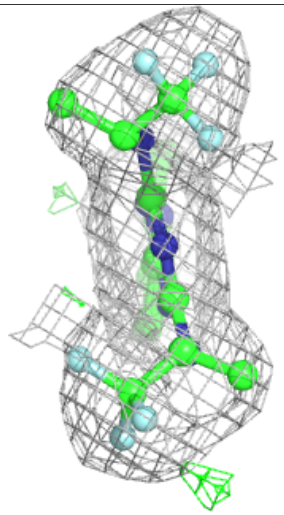


Electron density around 9UO A 504 (A):

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

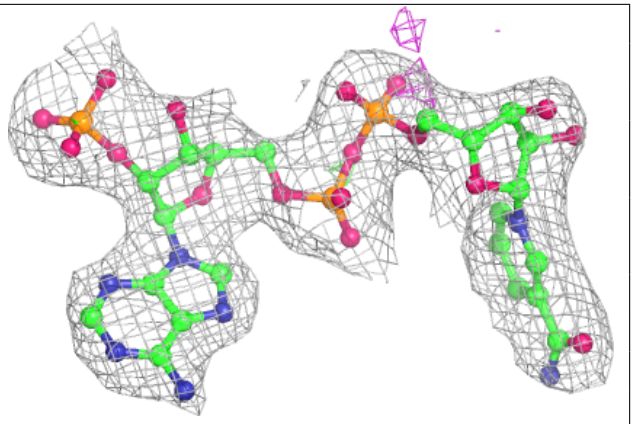


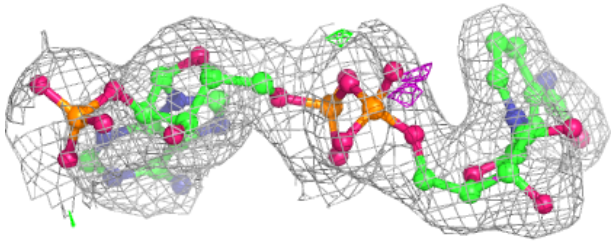


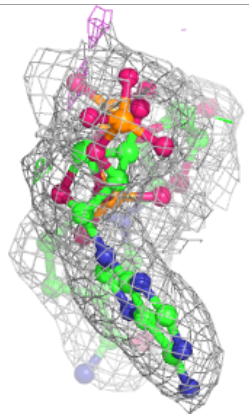


Electron density around NDP B 501:

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

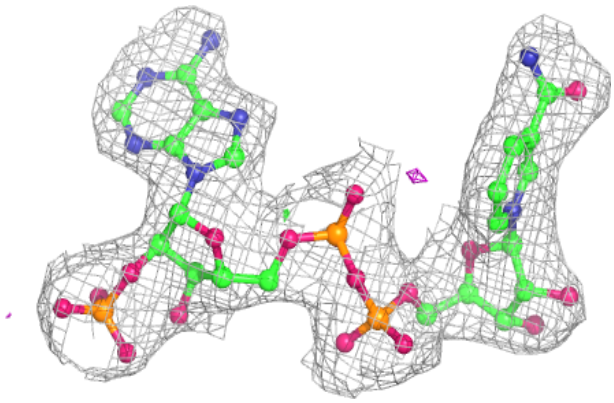


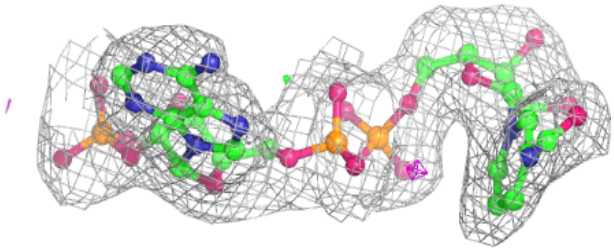


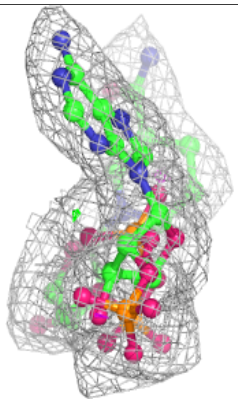


Electron density around NDP A 501:

$2mF_o$-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.