Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2021 – 01:17 PM EDT

PDB ID	:	3D5Q
Title	:	Crystal Structure of 11b-HSD1 in Complex with Triazole Inhibitor
Authors	:	Wang, Z.; Liu, J.; Sudom, A.; Walker, N.P.C.
Deposited on	:	2008-05-16
Resolution	:	2.55 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

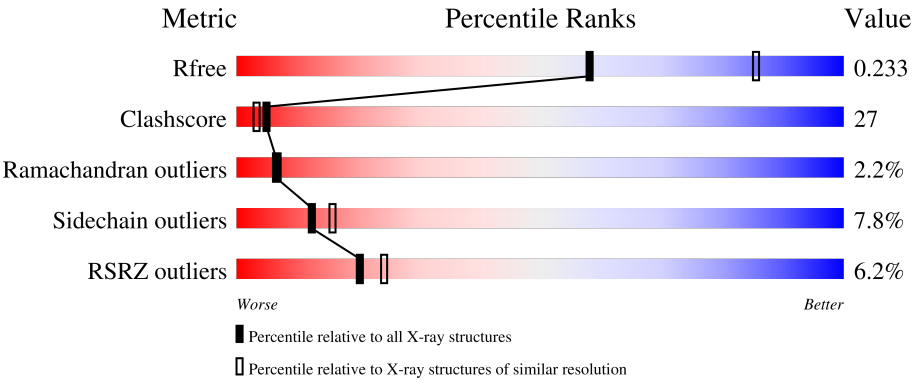
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	272	3% 53% 40%
1	B	272	4% 61% 32%
1	C	272	4% 54% 35% 7%
1	D	272	12% 43% 43% 8% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8311 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.

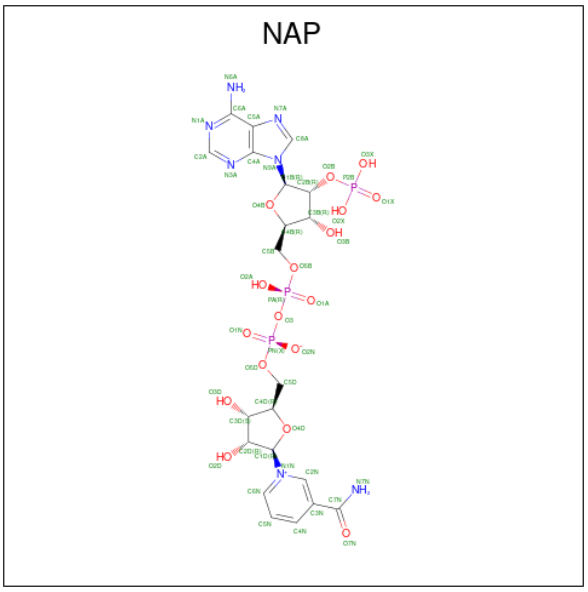
- Molecule 1 is a protein called Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	1	0
			2039	1300	344	379	16			
1	B	264	Total	C	N	O	S	0	5	0
			2042	1306	343	378	15			
1	C	253	Total	C	N	O	S	0	1	0
			1946	1242	329	361	14			
1	D	257	Total	C	N	O	S	0	1	0
			1976	1261	333	366	16			

There are 16 discrepancies between the modelled and reference sequences:

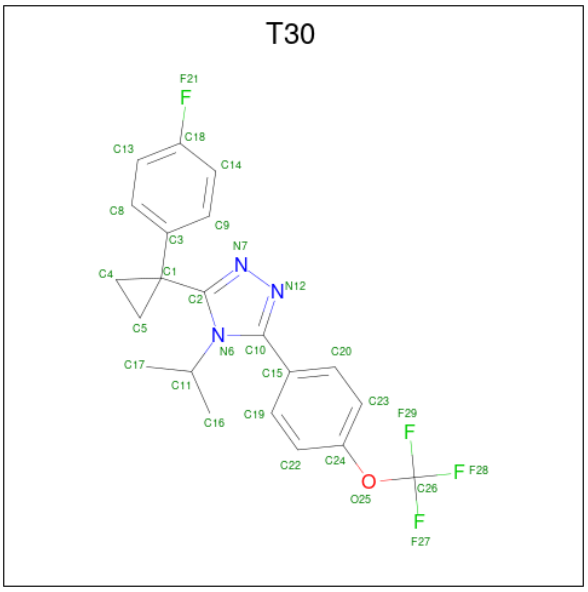
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLN	-	expression tag	UNP P28845
A	22	PRO	-	expression tag	UNP P28845
A	23	LEU	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	21	GLN	-	expression tag	UNP P28845
B	22	PRO	-	expression tag	UNP P28845
B	23	LEU	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	21	GLN	-	expression tag	UNP P28845
C	22	PRO	-	expression tag	UNP P28845
C	23	LEU	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845
D	23	LEU	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3-[1-(4-fluorophenyl)cyclopropyl]-4-(1-methylethyl)-5-[4-(trifluoromethoxy)phenyl]-4H-1,2,4-triazole (three-letter code: T30) (formula: $C_{21}H_{19}F_4N_3O$).



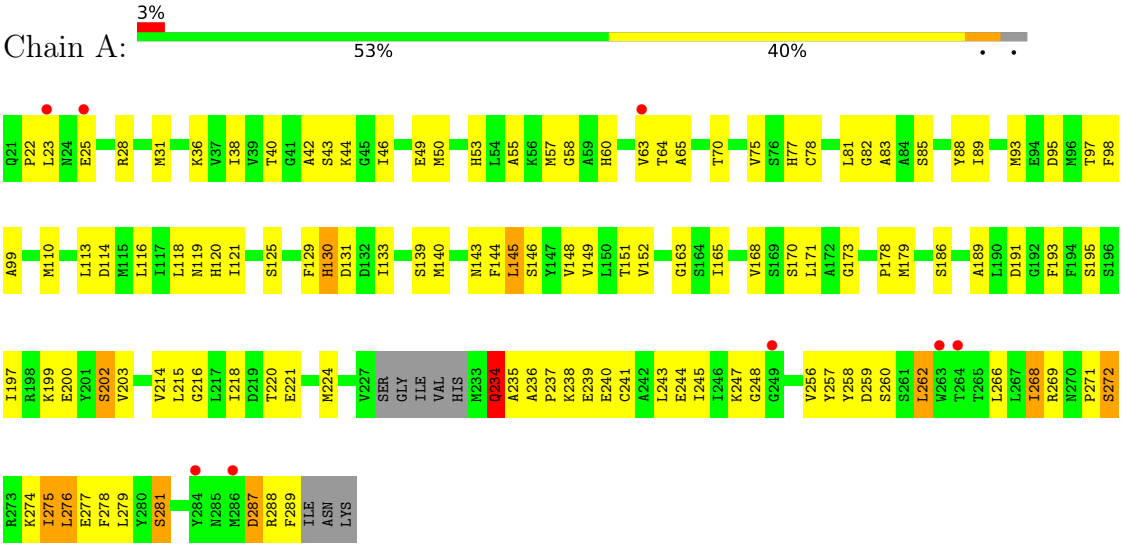
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			29	21	4	3	1		
3	B	1	Total	C	F	N	O	0	0
			29	21	4	3	1		
3	C	1	Total	C	F	N	O	0	0
			29	21	4	3	1		
3	D	1	Total	C	F	N	O	0	0
			29	21	4	3	1		

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.

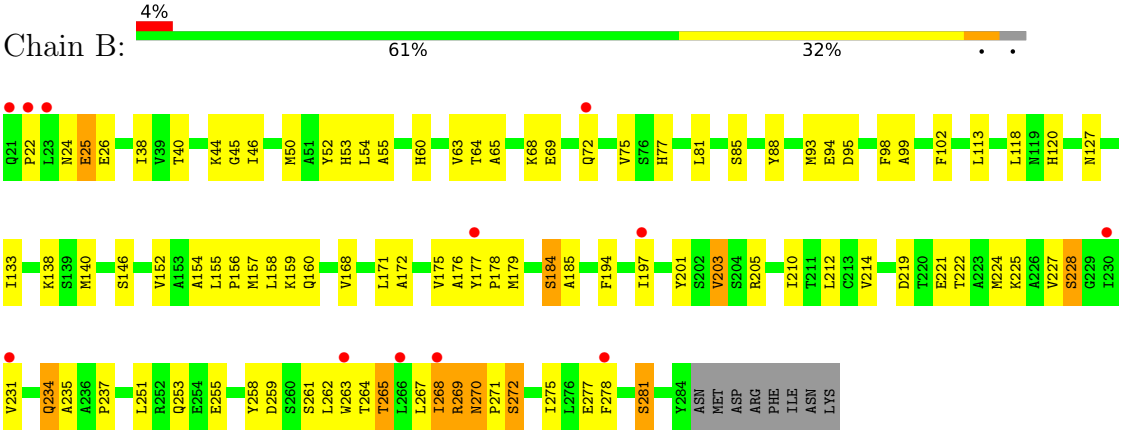
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain A:



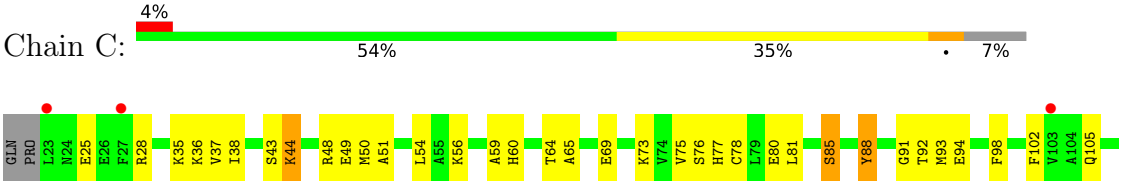
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

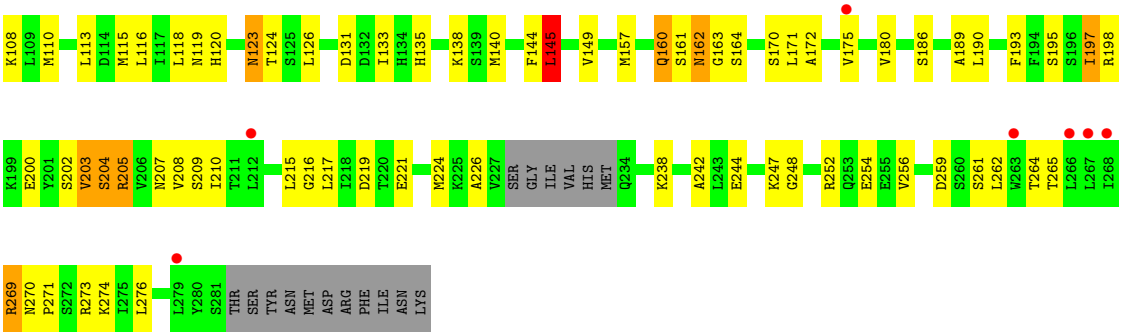
Chain B:



• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

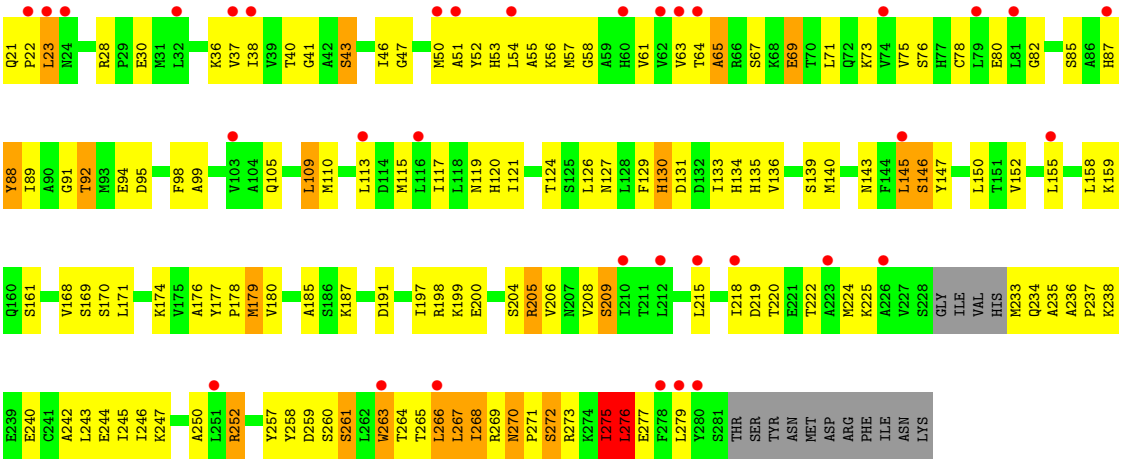
Chain C:





• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.67Å 153.32Å 73.60Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 76.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.55) 99.7 (76.66-2.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.230 , 0.265 0.223 , 0.233	Depositor DCC
R_{free} test set	2045 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8311	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: T30, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/2077	0.63	1/2802 (0.0%)
1	B	0.47	0/2099	0.67	0/2836
1	C	0.49	0/1981	0.66	1/2673 (0.0%)
1	D	0.42	0/2012	0.65	1/2714 (0.0%)
All	All	0.46	0/8169	0.65	3/11025 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	145	LEU	CA-CB-CG	-5.69	102.22	115.30
1	A	145	LEU	CA-CB-CG	-5.42	102.85	115.30
1	D	276	LEU	CA-CB-CG	-5.27	103.18	115.30

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	2039	0	2078	96	0
1	B	2042	0	2096	95	0
1	C	1946	0	1993	95	0
1	D	1976	0	2025	175	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	4	0
2	D	48	0	25	3	0
3	A	29	0	19	5	0
3	B	29	0	19	5	0
3	C	29	0	19	2	0
3	D	29	0	19	6	0
All	All	8311	0	8368	457	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 27.

All (457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:THR:HG22	1:D:135:HIS:CE1	1.61	1.35
1:D:273:ARG:HA	1:D:276:LEU:CD1	1.73	1.17
1:D:124:THR:HG22	1:D:135:HIS:NE2	1.63	1.14
1:D:219:ASP:OD1	1:D:237:PRO:HA	1.47	1.13
1:D:124:THR:CG2	1:D:135:HIS:CE1	2.39	1.05
1:D:269:ARG:HB2	1:D:269:ARG:HH21	1.20	1.04
1:D:219:ASP:HA	1:D:224:MET:CE	1.87	1.03
1:D:219:ASP:HA	1:D:224:MET:HE3	1.35	1.03
1:D:269:ARG:HB2	1:D:269:ARG:NH2	1.73	1.03
1:D:273:ARG:CA	1:D:276:LEU:HD11	1.88	1.02
1:D:92:THR:CG2	1:D:94:GLU:HB2	1.91	1.00
1:D:264:THR:O	1:D:267:LEU:HD12	1.61	1.00
1:D:264:THR:O	1:D:268:ILE:HG23	1.62	0.98
1:D:261:SER:O	1:D:265:THR:HG23	1.62	0.98
1:A:171:LEU:HD12	3:A:293:T30:H22	1.46	0.97
1:D:272:SER:O	1:D:276:LEU:HD21	1.64	0.97
1:D:273:ARG:HA	1:D:276:LEU:HD11	0.97	0.95
1:D:92:THR:HG23	1:D:94:GLU:H	1.35	0.91
1:C:224:MET:HE2	1:C:224:MET:HA	1.52	0.90
1:B:267:LEU:HD23	1:B:267:LEU:H	1.37	0.90
1:A:272:SER:O	1:A:276:LEU:HD23	1.73	0.89
1:A:224:MET:CE	1:A:235:ALA:HB2	2.03	0.88
3:A:293:T30:C20	3:A:293:T30:H16B	2.04	0.88
1:A:28:ARG:O	1:A:31:MET:HG3	1.72	0.87
1:D:261:SER:HB3	1:D:264:THR:HG23	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:MET:HE3	1:B:140:MET:HA	1.57	0.87
1:B:46:ILE:HG22	1:B:50:MET:CE	2.04	0.87
1:C:269:ARG:NH1	1:C:274:LYS:HG3	1.89	0.86
1:D:252:ARG:CG	1:D:252:ARG:HH11	1.89	0.85
1:D:124:THR:CG2	1:D:135:HIS:NE2	2.39	0.84
1:B:194:PHE:CD2	1:B:197[A]:ILE:HD11	2.12	0.84
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.61	0.83
1:D:269:ARG:HH21	1:D:269:ARG:CB	1.92	0.82
1:D:95:ASP:HB3	1:D:98:PHE:HB3	1.60	0.81
1:D:124:THR:HG22	1:D:135:HIS:HE1	1.43	0.81
1:D:105:GLN:NE2	1:D:109:LEU:HD13	1.95	0.81
1:B:22:PRO:HG3	1:B:253:GLN:HA	1.62	0.81
1:A:276:LEU:HD23	1:A:276:LEU:H	1.46	0.80
1:C:203:VAL:C	1:C:205:ARG:H	1.81	0.80
1:B:222:THR:HA	1:B:225:LYS:HD2	1.63	0.79
1:B:46:ILE:HG22	1:B:50:MET:HE2	1.64	0.78
1:A:38:ILE:HG13	1:A:113:LEU:HD11	1.65	0.78
1:D:243:LEU:HG	1:D:247:LYS:CE	2.14	0.77
3:B:1:T30:C15	3:B:1:T30:H16B	2.16	0.76
1:B:270:ASN:C	1:B:270:ASN:HD22	1.88	0.75
1:D:50:MET:HG2	1:D:242:ALA:HB1	1.66	0.75
1:C:124:THR:HG22	1:C:135:HIS:CE1	2.22	0.75
1:A:38:ILE:HG13	1:A:113:LEU:CD1	2.16	0.75
1:D:92:THR:HG21	1:D:94:GLU:HB2	1.67	0.74
1:B:194:PHE:HA	1:B:197[A]:ILE:HG12	1.68	0.74
1:D:252:ARG:HH11	1:D:252:ARG:HG3	1.52	0.74
1:A:224:MET:HE1	1:A:235:ALA:HB2	1.67	0.74
1:B:234:GLN:HA	1:B:234:GLN:HE21	1.50	0.74
1:C:124:THR:HG22	1:C:135:HIS:NE2	2.03	0.73
1:D:178:PRO:C	1:D:179:MET:HG2	2.06	0.73
1:C:44:LYS:HE2	2:C:3:NAP:H3B	1.70	0.73
1:B:268:ILE:O	1:B:268:ILE:HD12	1.89	0.73
1:D:257:TYR:CD2	1:D:268:ILE:HD11	2.25	0.72
1:D:124:THR:CG2	1:D:135:HIS:HE1	1.96	0.72
1:A:224:MET:HE3	1:A:235:ALA:CB	2.19	0.72
1:B:46:ILE:HG22	1:B:50:MET:HE1	1.72	0.72
1:A:197:ILE:HA	1:A:200:GLU:HB2	1.71	0.71
1:C:25:GLU:HG3	1:C:28:ARG:HH22	1.53	0.71
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.72	0.71
1:D:219:ASP:CA	1:D:224:MET:HE3	2.18	0.71
1:C:224:MET:HA	1:C:224:MET:CE	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ARG:HH11	1:C:274:LYS:HG3	1.54	0.70
1:D:50:MET:CE	1:D:117:ILE:HG21	2.22	0.70
1:D:261:SER:OG	1:D:263:TRP:HD1	1.73	0.70
1:D:243:LEU:HG	1:D:247:LYS:HE2	1.73	0.70
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.74	0.70
1:A:130:HIS:ND1	1:A:130:HIS:N	2.40	0.70
3:D:1:T30:H16B	3:D:1:T30:C15	2.22	0.70
1:D:36:LYS:HB3	1:D:110:MET:HE3	1.74	0.69
1:D:273:ARG:NE	1:D:277:GLU:OE1	2.21	0.69
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.75	0.69
1:B:94:GLU:OE2	1:B:138:LYS:HE2	1.92	0.69
1:D:119:ASN:HD22	1:D:168:VAL:HG21	1.57	0.69
1:D:197:ILE:O	1:D:198:ARG:C	2.32	0.69
1:B:270:ASN:HD22	1:B:271:PRO:N	1.92	0.68
1:D:92:THR:HG23	1:D:94:GLU:HB2	1.74	0.68
1:A:257:TYR:CG	1:A:268:ILE:HG21	2.29	0.68
1:A:60:HIS:HD1	1:A:85:SER:HG	1.33	0.68
1:D:219:ASP:HA	1:D:224:MET:HE2	1.72	0.68
1:B:219:ASP:OD1	1:B:237:PRO:HA	1.94	0.67
1:D:261:SER:HG	1:D:263:TRP:HD1	1.40	0.67
1:D:50:MET:HE3	1:D:117:ILE:HG21	1.74	0.67
1:A:199:LYS:O	1:A:202:SER:HB3	1.94	0.67
1:B:224:MET:HE2	1:B:235:ALA:CB	2.24	0.67
1:B:277:GLU:O	1:B:281:SER:HB2	1.94	0.66
1:C:123:ASN:HD22	1:C:124:THR:N	1.93	0.66
1:C:119:ASN:ND2	2:C:3:NAP:H4D	2.11	0.66
1:A:287:ASP:C	1:A:289:PHE:H	1.99	0.66
1:B:22:PRO:HA	1:B:251:LEU:O	1.96	0.66
1:A:224:MET:HE3	1:A:235:ALA:HB2	1.74	0.66
1:D:69:GLU:O	1:D:73:LYS:HG3	1.95	0.66
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.76	0.66
1:D:261:SER:OG	1:D:263:TRP:CD1	2.48	0.65
3:A:293:T30:H16B	3:A:293:T30:C15	2.27	0.65
1:C:203:VAL:C	1:C:205:ARG:N	2.45	0.65
1:D:261:SER:HB3	1:D:264:THR:CG2	2.26	0.64
1:C:244:GLU:OE1	1:C:247:LYS:HD2	1.96	0.64
1:B:24:ASN:O	1:B:25:GLU:HB3	1.97	0.64
1:C:276:LEU:HD11	1:D:268:ILE:HA	1.78	0.64
1:D:120:HIS:CE1	1:D:146:SER:OG	2.51	0.64
1:D:92:THR:CG2	1:D:94:GLU:H	2.09	0.64
3:A:293:T30:H20	3:A:293:T30:H17A	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:SER:O	1:D:265:THR:CG2	2.42	0.63
1:D:204:SER:C	1:D:206:VAL:H	2.00	0.63
1:D:270:ASN:ND2	1:D:273:ARG:H	1.96	0.63
1:B:275:ILE:HD11	1:D:266:LEU:HB3	1.81	0.63
1:D:120:HIS:O	1:D:121:ILE:HG23	1.98	0.63
1:A:148:VAL:O	1:A:152:VAL:HG23	1.99	0.62
1:D:271:PRO:O	1:D:275:ILE:HG12	1.99	0.62
1:B:262:LEU:HA	1:B:265:THR:HG23	1.79	0.62
1:A:129:PHE:HB3	1:B:197[B]:ILE:HD11	1.80	0.62
1:A:53:HIS:HB3	1:A:57:MET:HE3	1.82	0.62
1:C:270:ASN:OD1	1:C:273:ARG:HB2	1.99	0.62
1:D:37:VAL:HG11	1:D:54:LEU:HD13	1.82	0.62
1:D:264:THR:HA	1:D:267:LEU:HD11	1.81	0.62
1:A:93:MET:HG2	2:A:1:NAP:H2A	1.82	0.61
1:B:221:GLU:O	1:B:225:LYS:HG3	2.00	0.61
1:B:259:ASP:HB3	1:B:265:THR:HG22	1.81	0.61
1:B:77:HIS:CE1	1:B:81:LEU:HG	2.35	0.61
1:C:157:MET:O	1:C:160:GLN:HB3	2.00	0.61
1:A:214:VAL:C	1:A:215:LEU:HD23	2.20	0.61
1:C:261:SER:O	1:C:265:THR:HG23	1.99	0.61
1:A:60:HIS:ND1	1:A:85:SER:OG	2.30	0.61
1:D:275:ILE:HG22	1:D:279:LEU:HD11	1.83	0.61
1:A:116:LEU:HD11	1:A:118:LEU:HD21	1.82	0.61
1:C:37:VAL:HG11	1:C:54:LEU:HD13	1.83	0.61
1:C:48:ARG:O	1:C:51:ALA:N	2.34	0.61
1:D:180:VAL:O	1:D:180:VAL:HG23	2.01	0.60
1:D:234:GLN:HG3	1:D:260:SER:HB2	1.82	0.60
1:B:224:MET:CE	1:B:235:ALA:CB	2.79	0.60
1:B:270:ASN:C	1:B:270:ASN:ND2	2.53	0.60
1:C:259:ASP:OD2	1:C:264:THR:HG21	2.00	0.60
1:C:60:HIS:HD1	1:C:85:SER:HG	1.49	0.60
1:A:53:HIS:HB3	1:A:57:MET:CE	2.32	0.60
1:A:278:PHE:HA	1:A:281:SER:HB3	1.84	0.60
1:A:262:LEU:HD13	1:A:266:LEU:HD23	1.84	0.60
1:C:144:PHE:HD1	1:C:190:LEU:HD23	1.67	0.60
1:A:257:TYR:CD2	1:A:268:ILE:HG21	2.36	0.60
1:D:37:VAL:HG22	1:D:115:MET:HB3	1.83	0.60
1:D:252:ARG:CG	1:D:252:ARG:NH1	2.54	0.60
1:C:170:SER:HA	1:C:215:LEU:H	1.67	0.60
1:D:120:HIS:HE1	1:D:146:SER:OG	1.85	0.60
1:D:273:ARG:CA	1:D:276:LEU:CD1	2.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ILE:HG13	1:D:220:THR:HG21	1.84	0.59
1:C:77:HIS:HA	1:C:80:GLU:OE2	2.02	0.59
1:D:85:SER:HB2	1:D:87:HIS:HE1	1.66	0.59
1:C:276:LEU:HD21	1:D:268:ILE:HG22	1.85	0.59
1:D:130:HIS:CD2	1:D:131:ASP:HB2	2.37	0.59
1:D:270:ASN:HD22	1:D:273:ARG:H	1.51	0.59
1:B:172:ALA:O	1:B:184:SER:OG	2.21	0.59
1:C:123:ASN:HD22	1:C:124:THR:H	1.49	0.59
1:C:170:SER:HB2	2:C:3:NAP:H5N	1.85	0.59
1:C:126:LEU:HD12	1:C:226:ALA:O	2.03	0.58
1:D:28:ARG:HB3	1:D:30:GLU:OE2	2.04	0.58
1:B:38:ILE:HG13	1:B:113:LEU:CD1	2.34	0.58
1:B:140:MET:HE3	1:B:140:MET:CA	2.29	0.58
1:D:270:ASN:HD22	1:D:270:ASN:C	2.07	0.58
1:D:43:SER:HB3	1:D:65:ALA:CB	2.34	0.58
1:A:236:ALA:HB2	1:A:260:SER:HB3	1.85	0.58
1:D:89:ILE:HD11	1:D:105:GLN:HG3	1.86	0.58
1:C:94:GLU:OE2	1:C:138:LYS:HE2	2.04	0.57
1:D:197:ILE:O	1:D:200:GLU:N	2.37	0.57
1:A:49:GLU:HG3	1:A:238:LYS:HG3	1.85	0.57
1:D:113:LEU:HD23	1:D:158:LEU:HG	1.86	0.57
1:A:218:ILE:CG2	1:A:238:LYS:HA	2.35	0.57
1:B:237:PRO:HD2	1:B:258:TYR:OH	2.05	0.57
1:B:94:GLU:OE2	1:B:138:LYS:CE	2.52	0.56
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.86	0.56
1:D:242:ALA:HA	1:D:245:ILE:HD12	1.86	0.56
1:D:264:THR:C	1:D:268:ILE:HG23	2.26	0.56
1:D:264:THR:OG1	1:D:265:THR:N	2.35	0.56
1:D:50:MET:HG2	1:D:242:ALA:CB	2.35	0.56
1:C:131:ASP:O	1:C:133:ILE:HD12	2.05	0.56
1:C:217:LEU:HD11	1:C:224:MET:HE1	1.87	0.56
1:D:85:SER:HB2	1:D:87:HIS:CE1	2.41	0.55
1:D:50:MET:CE	1:D:117:ILE:CG2	2.84	0.55
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.87	0.55
1:D:145:LEU:O	1:D:146:SER:C	2.44	0.55
1:D:276:LEU:HA	1:D:279:LEU:HB2	1.88	0.55
1:B:224:MET:O	1:B:225:LYS:C	2.44	0.55
1:C:180:VAL:HG23	1:C:180:VAL:O	2.05	0.55
1:B:267:LEU:H	1:B:267:LEU:CD2	2.16	0.55
1:C:69:GLU:O	1:C:73:LYS:HG2	2.07	0.55
1:C:124:THR:CG2	1:C:135:HIS:CE1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:HIS:CE1	1:D:243:LEU:HB2	2.42	0.55
1:C:116:LEU:HG	1:C:118:LEU:HD21	1.88	0.54
1:B:24:ASN:O	1:B:25:GLU:CB	2.56	0.54
1:A:120:HIS:HE1	1:A:146:SER:OG	1.90	0.54
1:B:178:PRO:O	1:B:179:MET:HG3	2.08	0.54
1:A:202:SER:OG	1:A:203:VAL:HG13	2.07	0.54
1:A:272:SER:O	1:A:276:LEU:CD2	2.51	0.53
1:D:105:GLN:HE21	1:D:109:LEU:HD13	1.71	0.53
1:A:272:SER:O	1:A:275:ILE:HB	2.08	0.53
3:B:1:T30:H20	3:B:1:T30:H17A	1.90	0.53
1:C:164:SER:HG	1:C:209:SER:HG	1.49	0.53
1:D:199:LYS:HE3	1:D:277:GLU:HB3	1.89	0.53
1:B:194:PHE:HA	1:B:197[A]:ILE:CG1	2.37	0.53
1:C:38:ILE:HG13	1:C:113:LEU:HD11	1.91	0.53
1:B:38:ILE:HG13	1:B:113:LEU:HD11	1.91	0.53
1:D:204:SER:O	1:D:206:VAL:N	2.41	0.53
1:D:105:GLN:NE2	1:D:109:LEU:CD1	2.70	0.53
1:A:240:GLU:O	1:A:241:CYS:C	2.48	0.53
1:B:177:TYR:CD1	3:B:1:T30:F27	2.52	0.53
1:B:234:GLN:HA	1:B:234:GLN:NE2	2.23	0.52
1:D:234:GLN:HE21	1:D:235:ALA:H	1.57	0.52
1:A:271:PRO:HA	1:A:274:LYS:HD2	1.90	0.52
1:B:127:ASN:O	1:B:179:MET:HA	2.10	0.52
1:D:267:LEU:O	1:D:269:ARG:O	2.28	0.52
1:D:268:ILE:HD12	1:D:268:ILE:O	2.09	0.52
1:A:58:GLY:HA2	1:A:82:GLY:O	2.10	0.52
1:C:50:MET:HG2	1:C:242:ALA:HB1	1.90	0.52
1:D:171:LEU:CD1	3:D:1:T30:H22	2.39	0.52
1:A:98:PHE:O	1:A:99:ALA:C	2.44	0.52
1:D:105:GLN:HE22	1:D:109:LEU:HD13	1.70	0.52
1:D:246:ILE:O	1:D:247:LYS:C	2.48	0.52
1:A:257:TYR:HE1	1:A:269:ARG:NH2	2.08	0.51
1:A:42:ALA:HB3	1:A:63:VAL:HB	1.92	0.51
1:A:40:THR:HG1	1:A:119:ASN:H	1.56	0.51
1:B:72[B]:GLN:HG2	1:B:88:TYR:CE2	2.46	0.51
1:B:140:MET:HA	1:B:140:MET:CE	2.37	0.51
3:C:1:T30:C19	3:C:1:T30:H16B	2.41	0.51
1:D:204:SER:C	1:D:206:VAL:N	2.64	0.51
1:D:99:ALA:HB1	1:D:150:LEU:HD21	1.93	0.51
1:A:149:VAL:HG22	1:B:133:ILE:HD13	1.92	0.51
1:C:38:ILE:HG13	1:C:113:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:TYR:CD1	1:D:52:TYR:N	2.78	0.51
1:A:114:ASP:O	1:A:163:GLY:HA3	2.10	0.51
1:D:252:ARG:NH1	1:D:252:ARG:HG2	2.23	0.51
1:D:105:GLN:HE21	1:D:109:LEU:HD22	1.76	0.50
1:B:178:PRO:C	1:B:179:MET:HG3	2.31	0.50
1:C:37:VAL:HG21	1:C:54:LEU:HD22	1.93	0.50
1:C:203:VAL:CG2	1:C:204:SER:N	2.75	0.50
1:C:77:HIS:CD2	1:C:81:LEU:HD11	2.46	0.50
1:A:77:HIS:O	1:A:81:LEU:HG	2.10	0.50
3:B:1:T30:C15	3:B:1:T30:C16	2.88	0.50
1:D:41:GLY:O	1:D:47:GLY:HA3	2.12	0.50
1:D:55:ALA:C	1:D:57:MET:H	2.14	0.50
1:A:178:PRO:O	1:A:179:MET:HB2	2.12	0.50
1:B:52:TYR:O	1:B:55:ALA:HB3	2.11	0.50
1:D:50:MET:HE1	1:D:117:ILE:CG2	2.40	0.50
1:D:275:ILE:C	1:D:279:LEU:HG	2.32	0.50
1:A:133:ILE:HD11	1:B:152:VAL:HG21	1.94	0.50
1:D:177:TYR:CG	3:D:1:T30:H23	2.47	0.50
1:B:50:MET:O	1:B:54:LEU:HG	2.12	0.49
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.27	0.49
1:C:37:VAL:HG11	1:C:54:LEU:CD1	2.42	0.49
1:D:234:GLN:HE21	1:D:235:ALA:N	2.10	0.49
1:B:46:ILE:CG2	1:B:50:MET:HE1	2.41	0.49
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.48	0.49
1:C:270:ASN:OD1	1:C:273:ARG:CB	2.61	0.49
1:D:155:LEU:O	1:D:159:LYS:HG3	2.12	0.49
1:A:277:GLU:HG3	1:B:175:VAL:HB	1.94	0.49
1:B:201:TYR:CE2	1:B:210:ILE:HD11	2.47	0.49
1:C:198:ARG:NE	1:C:254:GLU:HG2	2.28	0.49
1:A:46:ILE:HG22	1:A:50:MET:CE	2.42	0.49
1:B:154:ALA:O	1:B:155:LEU:C	2.50	0.49
1:C:48:ARG:O	1:C:49:GLU:C	2.50	0.49
1:C:197:ILE:HD11	1:C:200:GLU:OE2	2.13	0.49
1:A:191:ASP:OD1	1:A:195:SER:OG	2.27	0.49
1:D:270:ASN:HD21	1:D:272:SER:HB2	1.77	0.49
1:D:206:VAL:HG12	1:D:208:VAL:HG23	1.94	0.48
1:A:139:SER:O	1:A:143:ASN:HB2	2.13	0.48
1:C:197:ILE:HD11	1:D:129:PHE:HB3	1.94	0.48
3:D:1:T30:C15	3:D:1:T30:C16	2.91	0.48
1:B:44:LYS:HG3	2:B:2:NAP:H3B	1.95	0.48
1:C:145:LEU:O	1:C:149:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:MET:SD	1:D:233:MET:N	2.86	0.48
1:D:275:ILE:HB	1:D:276:LEU:H	1.52	0.48
1:C:175:VAL:HG12	1:D:273:ARG:HG3	1.95	0.48
1:D:218:ILE:HD13	1:D:236:ALA:HB3	1.96	0.48
1:C:118:LEU:N	1:C:118:LEU:HD23	2.29	0.48
1:D:23:LEU:HG	1:D:252:ARG:HD2	1.96	0.48
1:D:209:SER:HB2	1:D:252:ARG:HG2	1.96	0.47
1:A:275:ILE:O	1:A:279:LEU:HG	2.15	0.47
1:D:178:PRO:O	1:D:179:MET:CG	2.61	0.47
1:C:123:ASN:ND2	1:C:124:THR:N	2.61	0.47
1:C:203:VAL:HG23	1:C:204:SER:N	2.30	0.47
1:A:88:TYR:C	1:A:89:ILE:HG13	2.34	0.47
1:C:164:SER:OG	1:C:209:SER:OG	2.24	0.47
1:D:53:HIS:HE1	1:D:243:LEU:HB2	1.79	0.47
1:A:171:LEU:CD2	1:A:268:ILE:HD11	2.45	0.47
1:B:94:GLU:OE2	1:B:138:LYS:NZ	2.46	0.47
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.48	0.47
1:C:133:ILE:HD12	1:C:133:ILE:H	1.80	0.47
1:C:207:ASN:OD1	1:C:252:ARG:NH2	2.47	0.47
1:A:237:PRO:HD2	1:A:258:TYR:OH	2.14	0.47
3:A:293:T30:C15	3:A:293:T30:C16	2.92	0.47
1:A:55:ALA:HB1	1:A:83:ALA:HB2	1.97	0.47
1:A:260:SER:O	1:A:260:SER:OG	2.30	0.47
1:B:278:PHE:O	1:B:281:SER:HB3	2.14	0.47
1:D:37:VAL:HG11	1:D:54:LEU:CD1	2.44	0.47
1:D:46:ILE:HG13	1:D:220:THR:CG2	2.43	0.47
1:D:178:PRO:O	1:D:179:MET:HG2	2.15	0.47
1:A:238:LYS:HE2	1:A:239:GLU:OE2	2.15	0.46
1:B:75:VAL:HG21	1:B:88:TYR:HD2	1.80	0.46
1:C:224:MET:CE	1:C:224:MET:CA	2.92	0.46
1:D:136:VAL:O	1:D:140[A]:MET:HG2	2.15	0.46
1:D:37:VAL:O	1:D:61:VAL:HA	2.14	0.46
1:D:275:ILE:HG22	1:D:279:LEU:CD1	2.44	0.46
1:B:271:PRO:O	1:B:275:ILE:HG12	2.15	0.46
1:C:171:LEU:HD12	1:C:216:GLY:HA2	1.98	0.46
1:B:22:PRO:CA	1:B:251:LEU:O	2.62	0.46
1:B:224:MET:CE	1:B:235:ALA:HB2	2.46	0.46
1:D:115:MET:HG2	1:D:117:ILE:HG13	1.97	0.46
1:A:234:GLN:O	1:A:260:SER:OG	2.24	0.46
1:B:268:ILE:HG23	1:B:269:ARG:N	2.31	0.46
1:A:116:LEU:CD1	1:A:118:LEU:HD21	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:PRO:O	1:D:272:SER:C	2.53	0.46
1:A:186:SER:O	1:A:189:ALA:HB3	2.16	0.46
1:A:287:ASP:C	1:A:289:PHE:N	2.66	0.46
1:C:115:MET:HA	1:C:164:SER:O	2.16	0.46
1:D:51:ALA:O	1:D:52:TYR:C	2.54	0.46
3:D:1:T30:H20	3:D:1:T30:H17A	1.96	0.46
1:A:276:LEU:HD23	1:A:276:LEU:N	2.24	0.46
1:D:92:THR:HG23	1:D:94:GLU:N	2.17	0.46
1:D:139:SER:O	1:D:143:ASN:HB2	2.15	0.45
1:B:68:LYS:O	1:B:72[A]:GLN:HG3	2.16	0.45
1:C:105:GLN:O	1:C:108:LYS:HB2	2.16	0.45
1:A:38:ILE:HG13	1:A:113:LEU:HD13	1.97	0.45
1:C:186:SER:O	1:C:189:ALA:HB3	2.17	0.45
1:A:244:GLU:O	1:A:245:ILE:C	2.55	0.45
1:A:268:ILE:CG2	1:A:269:ARG:N	2.80	0.45
1:A:278:PHE:HA	1:A:281:SER:CB	2.47	0.45
1:D:36:LYS:HB3	1:D:110:MET:CE	2.44	0.45
1:A:36:LYS:HD3	1:A:110:MET:O	2.16	0.45
1:D:127:ASN:O	1:D:179:MET:HA	2.16	0.45
1:B:171:LEU:HD21	1:B:268:ILE:HG12	1.99	0.45
1:B:201:TYR:HE2	1:B:210:ILE:HD11	1.82	0.45
1:B:270:ASN:HA	1:B:271:PRO:HD3	1.79	0.45
1:C:149:VAL:HG22	1:D:133:ILE:HD13	1.99	0.45
1:C:195:SER:HB3	1:D:176:ALA:HB2	1.98	0.45
1:D:52:TYR:N	1:D:52:TYR:HD1	2.14	0.45
1:C:163:GLY:O	1:C:208:VAL:HA	2.17	0.45
1:D:63:VAL:HG23	1:D:71:LEU:HD22	1.98	0.45
1:B:227:VAL:HB	1:B:231:VAL:HB	1.99	0.44
1:D:95:ASP:HB3	1:D:98:PHE:CB	2.40	0.44
1:B:98:PHE:O	1:B:99:ALA:C	2.54	0.44
1:C:88:TYR:CD1	1:C:88:TYR:C	2.89	0.44
1:C:92:THR:OG1	1:C:94:GLU:HG3	2.17	0.44
1:B:64:THR:HB	1:B:102:PHE:CE1	2.52	0.44
1:C:35:LYS:O	1:C:59:ALA:HB1	2.18	0.44
1:C:105:GLN:OE1	1:C:105:GLN:HA	2.17	0.44
1:D:187:LYS:NZ	2:D:4:NAP:O2D	2.41	0.44
1:D:240:GLU:HB2	1:D:258:TYR:OH	2.16	0.44
1:C:119:ASN:HD21	2:C:3:NAP:H4D	1.82	0.44
1:D:155:LEU:HD12	1:D:155:LEU:HA	1.86	0.44
1:B:52:TYR:O	1:B:53:HIS:C	2.54	0.44
1:D:273:ARG:O	1:D:276:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:HG23	1:A:165:ILE:HD13	1.99	0.44
1:D:40:THR:O	1:D:41:GLY:C	2.54	0.44
1:D:133:ILE:O	1:D:134:HIS:C	2.55	0.44
1:B:203:VAL:C	1:B:205:ARG:H	2.21	0.44
1:C:75:VAL:O	1:C:76:SER:C	2.56	0.44
1:B:225:LYS:O	1:B:228:SER:OG	2.36	0.43
1:C:140:MET:HE2	1:C:186:SER:HB3	2.00	0.43
1:B:221:GLU:CD	1:B:221:GLU:H	2.22	0.43
1:C:36:LYS:HG2	1:C:110:MET:HB3	2.00	0.43
1:C:270:ASN:HA	1:C:271:PRO:HD2	1.78	0.43
1:D:250:ALA:C	1:D:252:ARG:H	2.22	0.43
1:C:44:LYS:HE3	1:C:44:LYS:HB2	1.74	0.43
1:D:276:LEU:HA	1:D:279:LEU:HD12	2.00	0.43
1:A:170:SER:O	1:A:173:GLY:N	2.37	0.43
1:D:174:LYS:NZ	1:D:191:ASP:OD2	2.43	0.43
1:A:40:THR:OG1	1:A:120:HIS:CD2	2.53	0.43
1:D:75:VAL:O	1:D:78:CYS:HB2	2.17	0.43
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.82	0.43
1:C:133:ILE:HD11	1:D:152:VAL:HG11	2.00	0.43
1:D:171:LEU:HD12	3:D:1:T30:H22	1.98	0.43
1:C:35:LYS:O	1:C:60:HIS:N	2.47	0.43
1:C:259:ASP:CG	1:C:264:THR:HG21	2.39	0.43
1:A:93:MET:HG3	1:A:120:HIS:CE1	2.54	0.43
1:A:114:ASP:O	1:A:163:GLY:CA	2.66	0.43
1:A:145:LEU:HD12	1:A:145:LEU:HA	1.90	0.42
1:A:140:MET:CE	1:A:144:PHE:CD2	3.02	0.42
1:B:212:LEU:O	1:B:255:GLU:HA	2.19	0.42
1:C:216:GLY:O	1:C:217:LEU:C	2.57	0.42
1:D:273:ARG:HA	1:D:276:LEU:HD12	1.87	0.42
1:A:215:LEU:HD11	1:A:245:ILE:HD11	2.00	0.42
1:C:50:MET:CG	1:C:242:ALA:HB1	2.49	0.42
1:C:161:SER:O	1:C:162:ASN:C	2.58	0.42
1:B:95:ASP:C	1:B:95:ASP:OD1	2.58	0.42
1:C:144:PHE:CD2	1:C:145:LEU:HD12	2.54	0.42
1:D:58:GLY:HA2	1:D:82:GLY:O	2.19	0.42
1:D:168:VAL:HG13	1:D:215:LEU:HD11	2.01	0.42
1:B:270:ASN:ND2	1:B:272:SER:H	2.17	0.42
1:B:155:LEU:N	1:B:156:PRO:CD	2.83	0.42
1:B:158:LEU:O	1:B:159:LYS:C	2.55	0.42
1:B:222:THR:O	1:B:225:LYS:HB2	2.19	0.42
1:C:219:ASP:O	1:C:219:ASP:OD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PRO:O	1:B:160:GLN:HG3	2.20	0.42
1:B:197[B]:ILE:HG23	1:B:201:TYR:CZ	2.55	0.42
1:B:214:VAL:O	1:B:214:VAL:HG12	2.19	0.42
1:C:219:ASP:OD2	1:C:238:LYS:HG2	2.19	0.42
1:C:248:GLY:HA3	1:C:256:VAL:HG21	2.00	0.42
1:D:38:ILE:HG13	1:D:113:LEU:HD11	2.02	0.42
1:A:75:VAL:O	1:A:78:CYS:HB2	2.20	0.42
1:C:64:THR:HB	1:C:102:PHE:CE1	2.54	0.42
1:D:126:LEU:HD23	1:D:126:LEU:HA	1.88	0.42
1:B:157:MET:O	1:B:160:GLN:N	2.52	0.42
1:D:40:THR:HG1	1:D:120:HIS:HD2	1.64	0.42
3:B:1:T30:H16B	3:B:1:T30:C20	2.50	0.42
1:D:124:THR:HG21	1:D:135:HIS:HE1	1.79	0.42
1:A:46:ILE:HG22	1:A:50:MET:HE1	2.02	0.41
1:A:287:ASP:O	1:A:289:PHE:N	2.53	0.41
1:D:147:TYR:HA	1:D:150:LEU:HD12	2.02	0.41
1:D:276:LEU:H	1:D:276:LEU:HD23	1.85	0.41
1:A:243:LEU:HG	1:A:247:LYS:HE3	2.02	0.41
1:B:63:VAL:O	1:B:88:TYR:HA	2.21	0.41
1:B:118:LEU:O	1:B:168:VAL:HG23	2.19	0.41
1:C:93:MET:HG3	1:C:120:HIS:NE2	2.35	0.41
1:D:169:SER:O	2:D:4:NAP:H6N	2.20	0.41
1:D:272:SER:O	1:D:276:LEU:CD2	2.53	0.41
1:A:53:HIS:O	1:A:57:MET:HG3	2.20	0.41
1:D:238:LYS:H	1:D:238:LYS:HG2	1.64	0.41
1:A:43:SER:HB3	1:A:65:ALA:CB	2.51	0.41
1:B:38:ILE:HG13	1:B:113:LEU:HD13	2.01	0.41
1:A:55:ALA:CB	1:A:83:ALA:HB2	2.51	0.41
1:B:88:TYR:CD1	1:B:88:TYR:C	2.94	0.41
1:B:120:HIS:HE1	1:B:146:SER:OG	2.02	0.41
1:B:224:MET:HE1	1:B:235:ALA:CB	2.50	0.41
1:A:220:THR:O	1:A:221:GLU:C	2.59	0.41
1:B:38:ILE:HD13	1:B:102:PHE:CE2	2.55	0.41
1:C:69:GLU:O	1:C:73:LYS:CG	2.67	0.41
1:D:105:GLN:HE21	1:D:109:LEU:CD2	2.33	0.41
1:A:116:LEU:CG	1:A:118:LEU:HD21	2.51	0.41
1:C:140:MET:HG2	1:D:140[B]:MET:CG	2.49	0.41
1:C:172:ALA:HB2	3:C:1:T30:H20	2.02	0.41
1:D:105:GLN:HE21	1:D:109:LEU:CD1	2.33	0.41
1:D:244:GLU:HG3	1:D:258:TYR:CD2	2.56	0.41
1:D:276:LEU:H	1:D:276:LEU:CD2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:OD1	1:A:97:THR:N	2.54	0.41
1:C:259:ASP:HB3	1:C:265:THR:HG22	2.01	0.41
1:D:259:ASP:C	1:D:261:SER:H	2.23	0.41
1:A:144:PHE:O	1:A:148:VAL:HG23	2.21	0.41
1:D:50:MET:HE3	1:D:117:ILE:CG2	2.47	0.41
1:D:170:SER:OG	1:D:171:LEU:N	2.53	0.41
1:A:64:THR:O	1:A:65:ALA:HB2	2.21	0.40
1:A:215:LEU:HD23	1:A:215:LEU:N	2.36	0.40
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.21	0.40
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.56	0.40
1:C:197:ILE:HG22	1:C:210:ILE:CD1	2.51	0.40
1:D:64:THR:OG1	1:D:65:ALA:N	2.54	0.40
1:B:140:MET:HE2	1:B:140:MET:HB3	1.80	0.40
1:C:36:LYS:O	1:C:113:LEU:HD12	2.22	0.40
1:D:69:GLU:H	1:D:69:GLU:HG2	1.63	0.40
1:D:170:SER:HB2	2:D:4:NAP:H5N	2.03	0.40
1:A:268:ILE:HG22	1:A:269:ARG:N	2.37	0.40
1:D:88:TYR:CD1	1:D:88:TYR:C	2.93	0.40
1:A:140:MET:HE3	1:A:144:PHE:CD2	2.56	0.40
1:A:195:SER:HB3	1:B:176:ALA:HB2	2.03	0.40
1:B:224:MET:HE2	1:B:235:ALA:HB1	2.02	0.40
1:C:75:VAL:O	1:C:78:CYS:N	2.54	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	261/272 (96%)	229 (88%)	29 (11%)	3 (1%)	14 19
1	B	267/272 (98%)	230 (86%)	31 (12%)	6 (2%)	6 7
1	C	250/272 (92%)	217 (87%)	28 (11%)	5 (2%)	7 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	254/272 (93%)	201 (79%)	44 (17%)	9 (4%)	3 2
All	All	1032/1088 (95%)	877 (85%)	132 (13%)	23 (2%)	6 7

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLU
1	D	205	ARG
1	A	234	GLN
1	A	288	ARG
1	B	45	GLY
1	B	263	TRP
1	D	65	ALA
1	D	67	SER
1	D	275	ILE
1	B	65	ALA
1	B	264	THR
1	B	281	SER
1	C	65	ALA
1	C	204	SER
1	D	130	HIS
1	D	276	LEU
1	C	85	SER
1	C	202	SER
1	D	56	LYS
1	A	22	PRO
1	C	203	VAL
1	D	22	PRO
1	D	23	LEU

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	223/229 (97%)	206 (92%)	17 (8%)	13 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	226/229 (99%)	214 (95%)	12 (5%)	22 30
1	C	212/229 (93%)	199 (94%)	13 (6%)	18 24
1	D	216/229 (94%)	190 (88%)	26 (12%)	5 5
All	All	877/916 (96%)	809 (92%)	68 (8%)	12 16

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	GLU
1	A	44	LYS
1	A	70	THR
1	A	121	ILE
1	A	125	SER
1	A	130	HIS
1	A	131	ASP
1	A	202	SER
1	A	234	GLN
1	A	262	LEU
1	A	268	ILE
1	A	272	SER
1	A	275	ILE
1	A	276	LEU
1	A	281	SER
1	A	287	ASP
1	B	26	GLU
1	B	69	GLU
1	B	184	SER
1	B	203	VAL
1	B	228	SER
1	B	234	GLN
1	B	261	SER
1	B	265	THR
1	B	268	ILE
1	B	269	ARG
1	B	270	ASN
1	B	272	SER
1	C	43	SER
1	C	44	LYS
1	C	56	LYS
1	C	88	TYR

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Mol	Chain	Res	Type
1	C	123	ASN
1	C	145	LEU
1	C	160	GLN
1	C	162	ASN
1	C	197	ILE
1	C	205	ARG
1	C	221	GLU
1	C	262	LEU
1	C	269	ARG
1	D	21	GLN
1	D	43	SER
1	D	69	GLU
1	D	76	SER
1	D	80	GLU
1	D	88	TYR
1	D	92	THR
1	D	109	LEU
1	D	145	LEU
1	D	146	SER
1	D	161	SER
1	D	179	MET
1	D	205	ARG
1	D	209	SER
1	D	222	THR
1	D	225	LYS
1	D	252	ARG
1	D	261	SER
1	D	263	TRP
1	D	266	LEU
1	D	267	LEU
1	D	268	ILE
1	D	270	ASN
1	D	272	SER
1	D	275	ILE
1	D	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	87	HIS
1	A	119	ASN

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Mol	Chain	Res	Type
1	A	120	HIS
1	A	127	ASN
1	A	207	ASN
1	A	270	ASN
1	B	77	HIS
1	B	119	ASN
1	B	120	HIS
1	B	160	GLN
1	B	234	GLN
1	B	253	GLN
1	B	270	ASN
1	C	72	GLN
1	C	77	HIS
1	C	119	ASN
1	C	123	ASN
1	C	160	GLN
1	D	53	HIS
1	D	87	HIS
1	D	105	GLN
1	D	119	ASN
1	D	120	HIS
1	D	160	GLN
1	D	234	GLN
1	D	270	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

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	C	3	-	45,52,52	1.62	2 (4%)	56,80,80	1.40	7 (12%)
2	NAP	A	1	-	45,52,52	1.66	3 (6%)	56,80,80	1.15	4 (7%)
2	NAP	D	4	-	45,52,52	1.69	3 (6%)	56,80,80	1.36	3 (5%)
2	NAP	B	2	-	45,52,52	1.70	2 (4%)	56,80,80	1.21	3 (5%)
3	T30	A	293	-	29,32,32	0.92	2 (6%)	37,49,49	1.12	4 (10%)
3	T30	B	1	-	29,32,32	1.02	2 (6%)	37,49,49	1.18	3 (8%)
3	T30	D	1	-	29,32,32	0.99	2 (6%)	37,49,49	1.30	6 (16%)
3	T30	C	1	-	29,32,32	1.03	2 (6%)	37,49,49	1.16	2 (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	C	3	-	-	5/31/67/67	0/5/5/5
2	NAP	A	1	-	-	4/31/67/67	0/5/5/5
2	NAP	D	4	-	-	5/31/67/67	0/5/5/5
2	NAP	B	2	-	-	10/31/67/67	0/5/5/5
3	T30	A	293	-	-	5/19/29/29	0/4/4/4
3	T30	B	1	-	-	10/19/29/29	0/4/4/4
3	T30	D	1	-	-	7/19/29/29	0/4/4/4
3	T30	C	1	-	-	7/19/29/29	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAP	O7N-C7N	8.94	1.41	1.24
2	C	3	NAP	O7N-C7N	8.67	1.40	1.24
2	D	4	NAP	O7N-C7N	8.63	1.40	1.24
2	A	1	NAP	O7N-C7N	8.62	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAP	C2A-N3A	4.00	1.38	1.32
2	D	4	NAP	C2A-N3A	3.90	1.38	1.32
2	A	1	NAP	C2A-N3A	3.82	1.38	1.32
3	C	1	T30	C1-C3	-3.61	1.49	1.54
3	B	1	T30	C1-C3	-3.57	1.49	1.54
3	D	1	T30	C1-C3	-3.43	1.49	1.54
2	C	3	NAP	C2A-N3A	3.38	1.37	1.32
3	A	293	T30	C1-C3	-2.75	1.50	1.54
2	A	1	NAP	C2D-C1D	-2.30	1.50	1.53
3	A	293	T30	O25-C26	2.28	1.44	1.31
2	D	4	NAP	C2A-N1A	2.28	1.38	1.33
3	C	1	T30	O25-C26	2.20	1.44	1.31
3	B	1	T30	O25-C26	2.15	1.43	1.31
3	D	1	T30	O25-C26	2.05	1.43	1.31

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAP	N3A-C2A-N1A	-5.56	119.99	128.68
2	C	3	NAP	N3A-C2A-N1A	-5.38	120.27	128.68
2	A	1	NAP	N3A-C2A-N1A	-5.26	120.46	128.68
2	D	4	NAP	N3A-C2A-N1A	-5.09	120.73	128.68
2	C	3	NAP	C3N-C7N-N7N	3.98	122.53	117.75
2	D	4	NAP	C3N-C7N-N7N	3.94	122.48	117.75
3	C	1	T30	C5-C1-C4	3.06	60.59	58.70
3	D	1	T30	C5-C1-C4	2.99	60.55	58.70
2	C	3	NAP	O4D-C1D-C2D	-2.97	102.59	106.93
2	D	4	NAP	O7N-C7N-C3N	-2.88	116.19	119.63
3	B	1	T30	C5-C1-C4	2.88	60.48	58.70
3	B	1	T30	C16-C11-N6	-2.85	108.18	111.52
3	D	1	T30	C4-C1-C2	-2.84	112.17	117.43
2	B	2	NAP	O7N-C7N-N7N	-2.79	118.61	122.58
2	C	3	NAP	O7N-C7N-N7N	-2.77	118.64	122.58
2	B	2	NAP	O2N-PN-O1N	2.46	124.38	112.24
3	A	293	T30	C13-C18-C14	-2.45	119.57	122.83
3	C	1	T30	C8-C3-C9	2.43	121.59	117.97
2	A	1	NAP	C5B-C4B-C3B	-2.35	106.37	115.18
2	C	3	NAP	O5D-C5D-C4D	-2.29	101.11	108.99
3	A	293	T30	C5-C1-C4	2.28	60.11	58.70
3	D	1	T30	C17-C11-N6	-2.18	108.97	111.52
3	D	1	T30	C8-C3-C9	2.11	121.12	117.97
2	A	1	NAP	O7N-C7N-N7N	-2.11	119.58	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	NAP	C4A-C5A-N7A	-2.07	107.24	109.40
3	D	1	T30	C20-C15-C10	-2.06	116.25	120.72
3	B	1	T30	C13-C18-C14	-2.05	120.10	122.83
2	C	3	NAP	O4B-C1B-C2B	-2.04	103.05	106.59
2	A	1	NAP	C4A-C5A-N7A	-2.03	107.28	109.40
3	A	293	T30	C22-C19-C15	-2.03	118.21	121.13
3	D	1	T30	C22-C19-C15	-2.03	118.22	121.13
3	A	293	T30	C4-C1-C2	-2.01	113.72	117.43

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C2B-O2B-P2B-O1X
2	B	2	NAP	C5B-O5B-PA-O2A
2	B	2	NAP	C2B-O2B-P2B-O2X
2	B	2	NAP	C5D-O5D-PN-O1N
2	C	3	NAP	O4D-C4D-C5D-O5D
2	D	4	NAP	C2B-O2B-P2B-O1X
2	D	4	NAP	C5D-O5D-PN-O1N
3	B	1	T30	N6-C10-C15-C19
3	B	1	T30	N6-C10-C15-C20
3	C	1	T30	N6-C10-C15-C19
3	C	1	T30	N6-C10-C15-C20
3	D	1	T30	N6-C10-C15-C19
3	D	1	T30	N6-C10-C15-C20
3	D	1	T30	N12-C10-C15-C20
3	D	1	T30	F27-C26-O25-C24
2	B	2	NAP	O4B-C4B-C5B-O5B
2	C	3	NAP	C3D-C4D-C5D-O5D
3	A	293	T30	F27-C26-O25-C24
3	B	1	T30	F28-C26-O25-C24
3	B	1	T30	N12-C10-C15-C20
3	C	1	T30	N12-C10-C15-C19
3	C	1	T30	N12-C10-C15-C20
3	D	1	T30	N12-C10-C15-C19
2	B	2	NAP	C3B-C4B-C5B-O5B
2	C	3	NAP	O4B-C4B-C5B-O5B
3	A	293	T30	F28-C26-O25-C24
3	A	293	T30	F29-C26-O25-C24
3	D	1	T30	F28-C26-O25-C24
3	D	1	T30	F29-C26-O25-C24

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	B	1	T30	F29-C26-O25-C24
3	A	293	T30	C16-C11-N6-C2
3	B	1	T30	F27-C26-O25-C24
3	B	1	T30	N12-C10-C15-C19
2	B	2	NAP	C3B-C2B-O2B-P2B
2	B	2	NAP	C1B-C2B-O2B-P2B
2	B	2	NAP	C5B-O5B-PA-O3
2	B	2	NAP	C5D-O5D-PN-O3
2	C	3	NAP	PN-O3-PA-O1A
2	B	2	NAP	C5B-O5B-PA-O1A
3	B	1	T30	C5-C1-C3-C9
3	A	293	T30	C16-C11-N6-C10
3	C	1	T30	C23-C24-O25-C26
2	D	4	NAP	PN-O3-PA-O1A
3	C	1	T30	C22-C24-O25-C26
2	D	4	NAP	O4B-C4B-C5B-O5B
2	A	1	NAP	C5D-O5D-PN-O3
2	D	4	NAP	C5D-O5D-PN-O3
2	A	1	NAP	PN-O3-PA-O2A
2	C	3	NAP	C5D-O5D-PN-O1N
2	A	1	NAP	O4B-C4B-C5B-O5B
3	B	1	T30	C23-C24-O25-C26
3	C	1	T30	C2-C1-C3-C9
3	B	1	T30	C22-C24-O25-C26

There are no ring outliers.

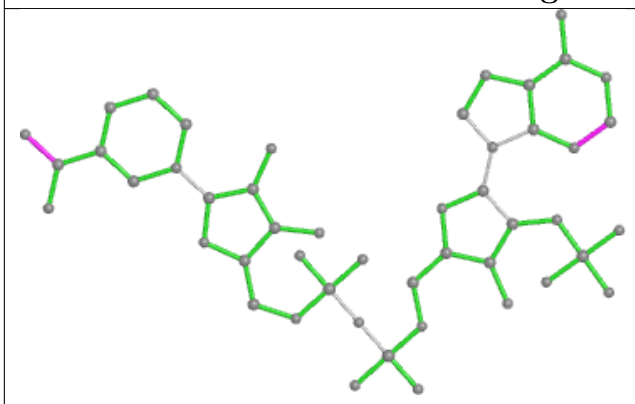
8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	NAP	4	0
2	A	1	NAP	1	0
2	D	4	NAP	3	0
2	B	2	NAP	1	0
3	A	293	T30	5	0
3	B	1	T30	5	0
3	D	1	T30	6	0
3	C	1	T30	2	0

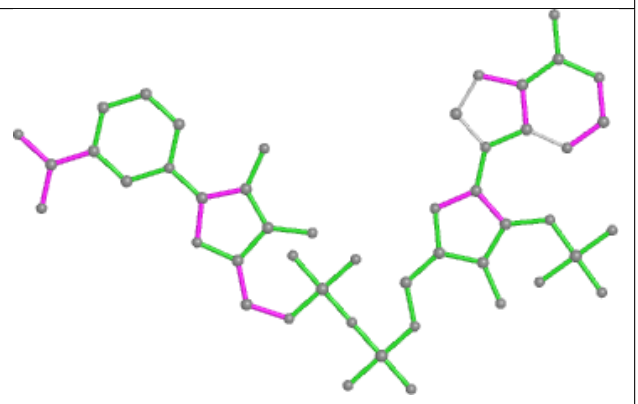
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

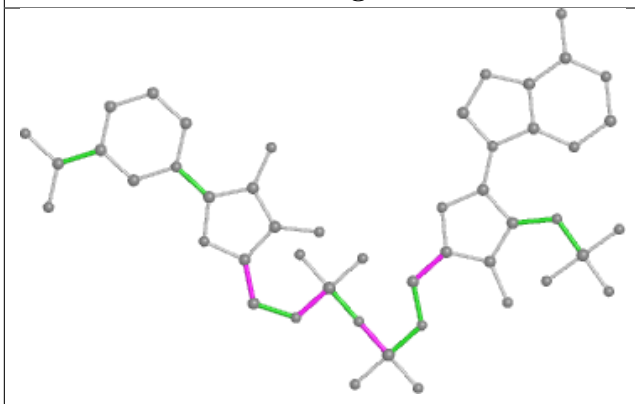
Ligand NAP C 3



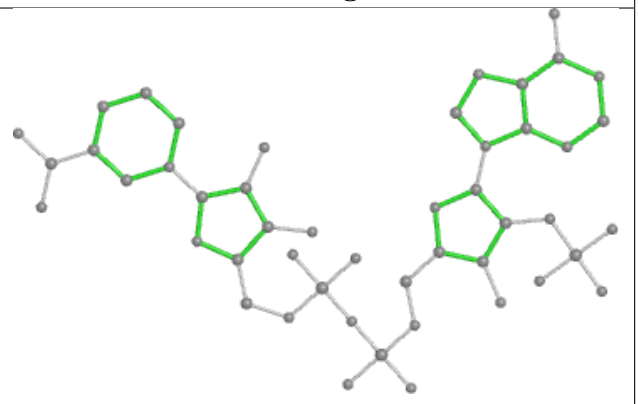
Bond lengths



Bond angles

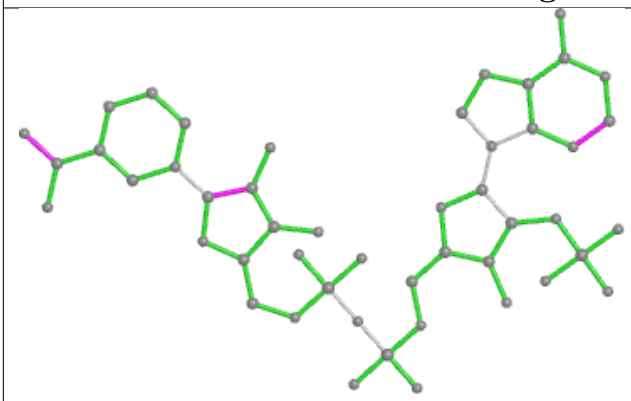


Torsions

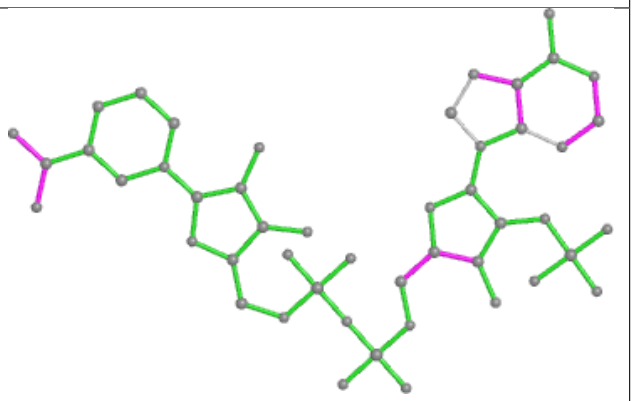


Rings

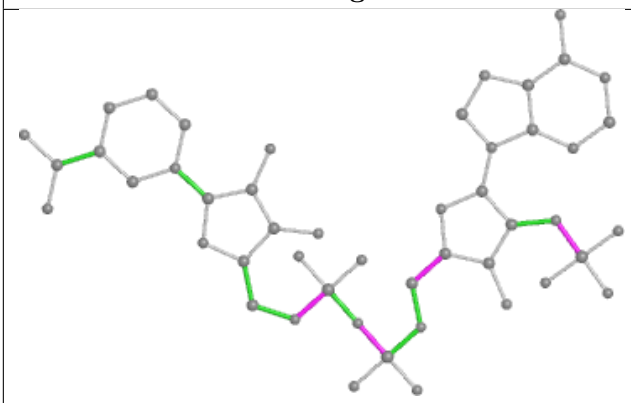
Ligand NAP A 1



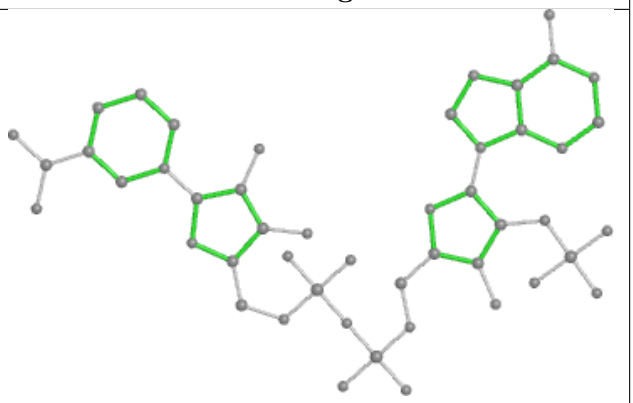
Bond lengths



Bond angles

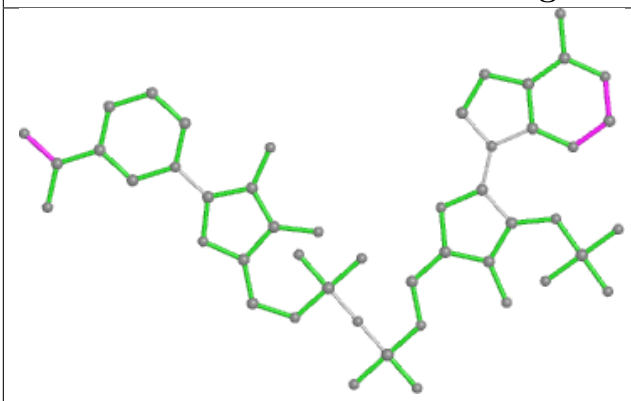


Torsions

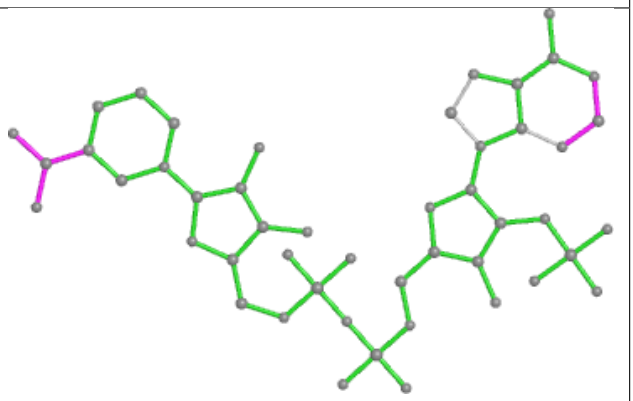


Rings

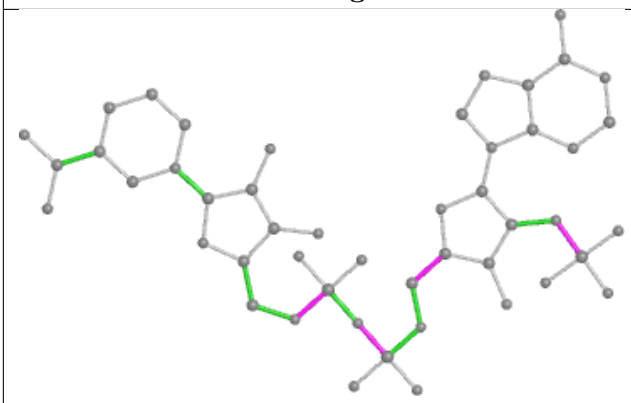
Ligand NAP D 4



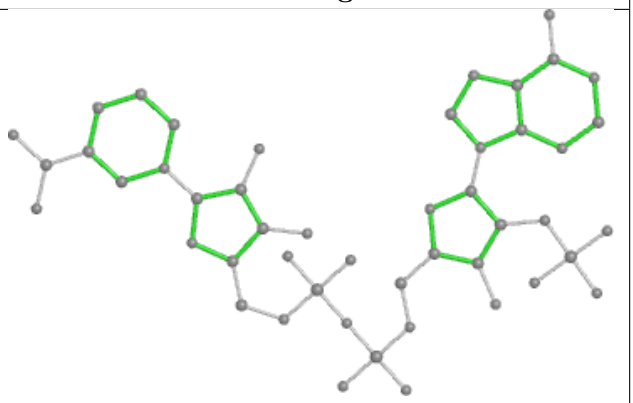
Bond lengths



Bond angles

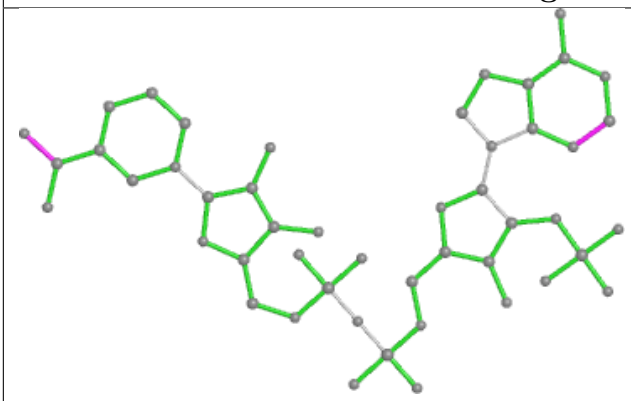


Torsions

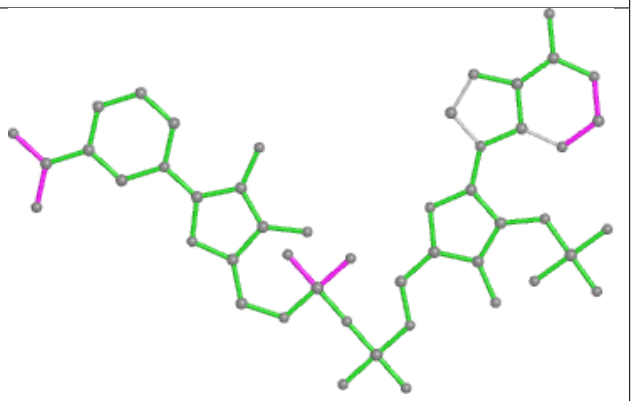


Rings

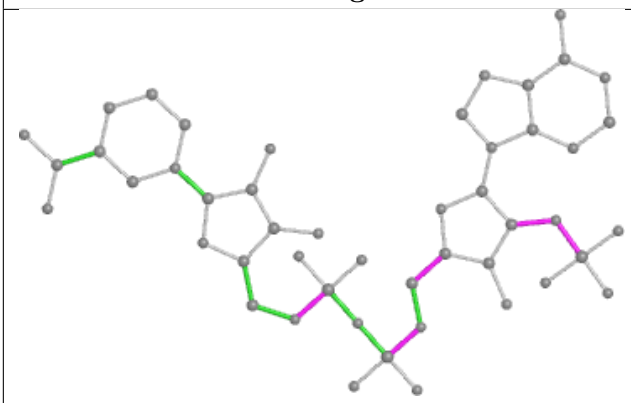
Ligand NAP B 2



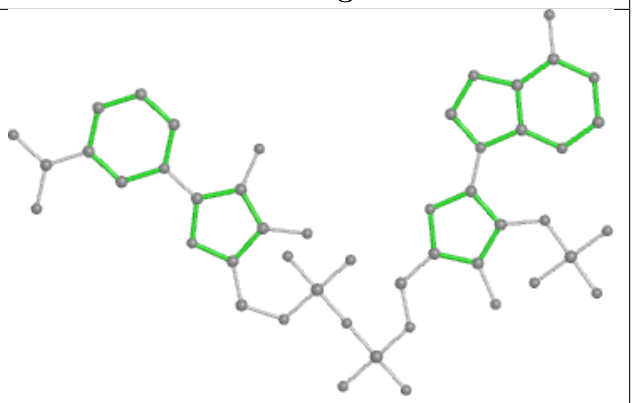
Bond lengths



Bond angles

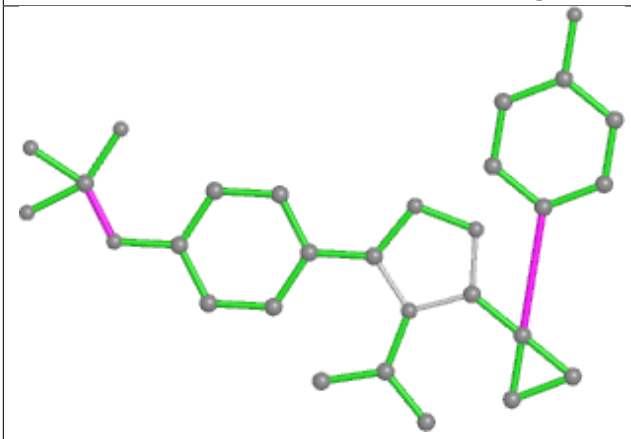


Torsions

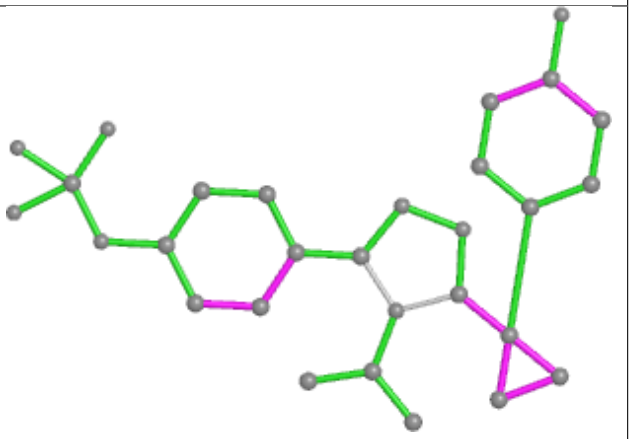


Rings

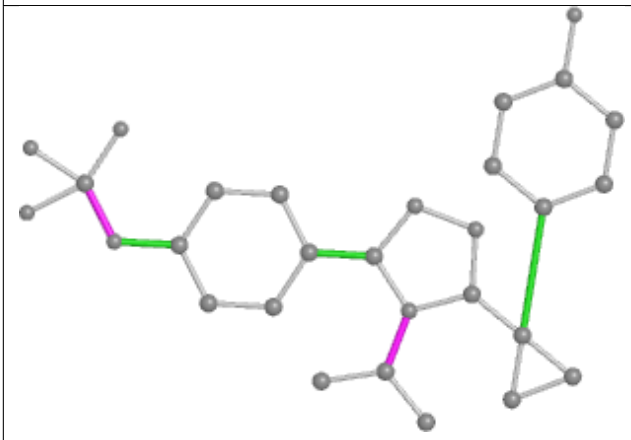
Ligand T30 A 293



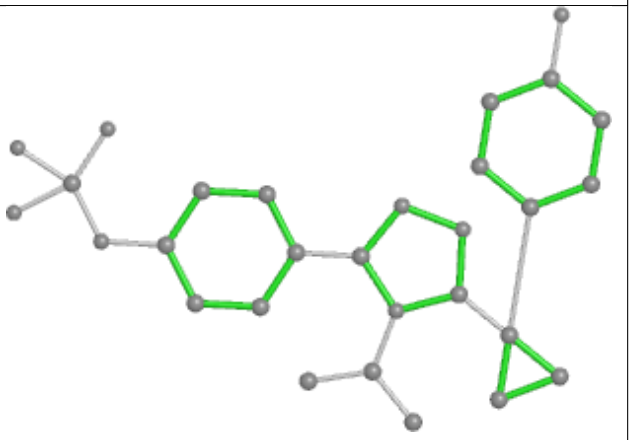
Bond lengths



Bond angles

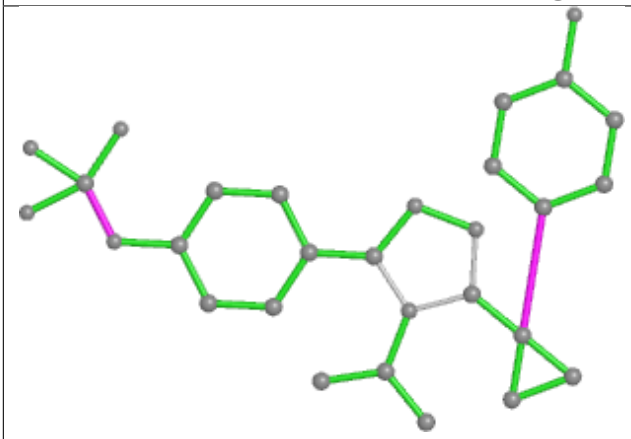


Torsions

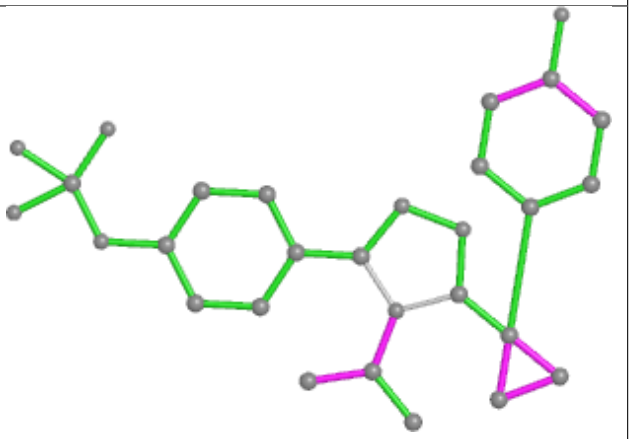


Rings

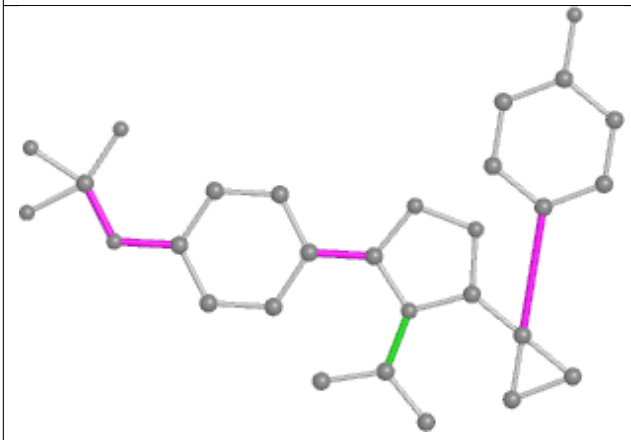
Ligand T30 B 1



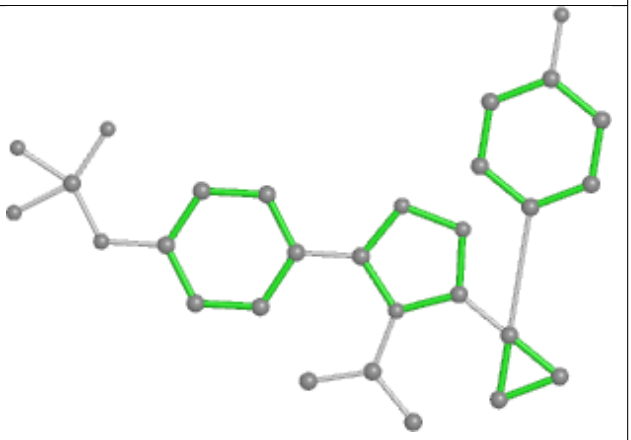
Bond lengths



Bond angles

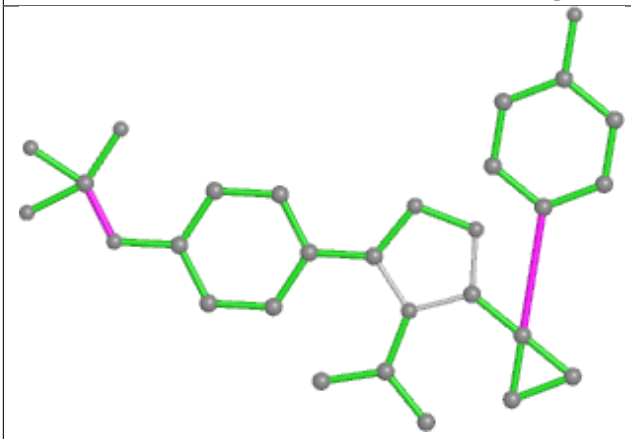


Torsions

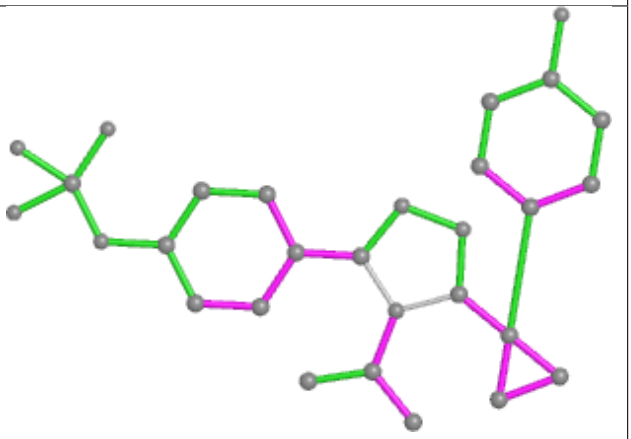


Rings

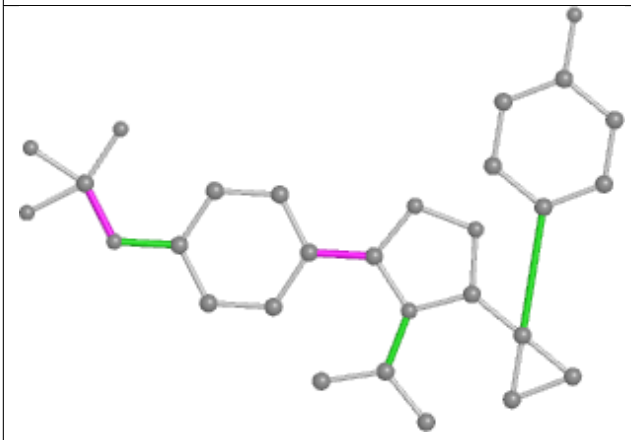
Ligand T30 D 1



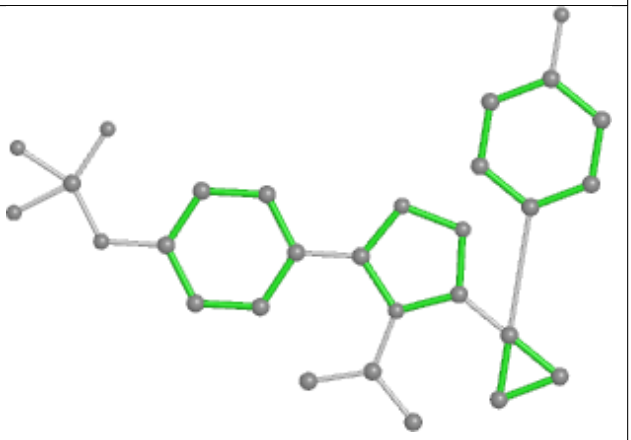
Bond lengths



Bond angles

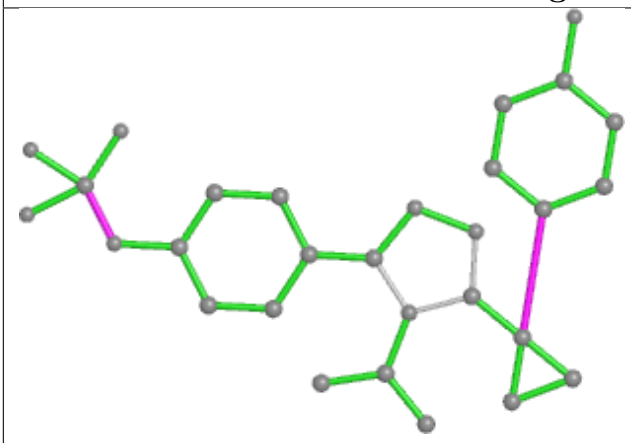


Torsions

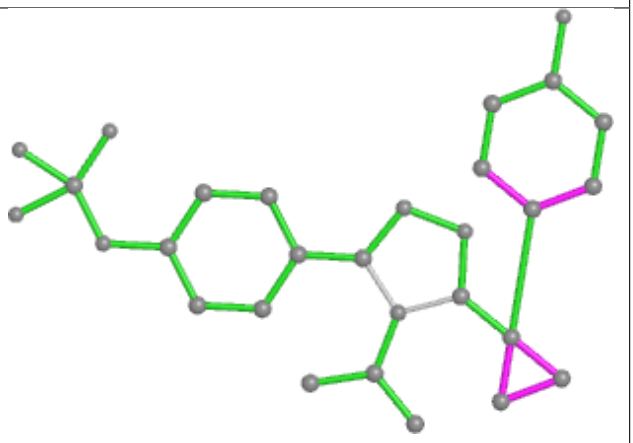


Rings

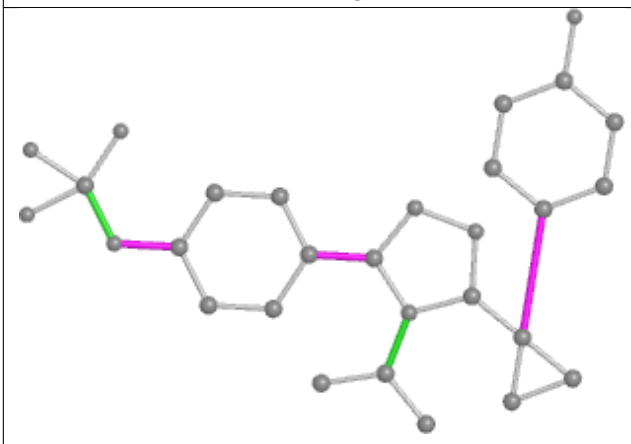
Ligand T30 C 1



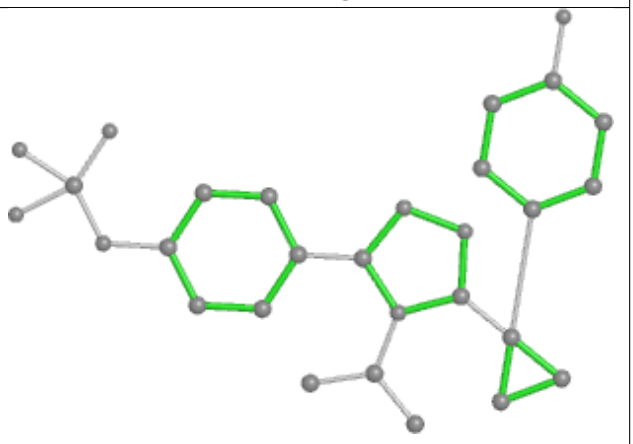
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	264/272 (97%)	0.28	8 (3%) 50 57	39, 62, 94, 108	0
1	B	264/272 (97%)	0.38	12 (4%) 33 40	39, 58, 86, 101	0
1	C	253/272 (93%)	0.35	10 (3%) 38 45	37, 58, 79, 90	0
1	D	257/272 (94%)	0.79	34 (13%) 3 4	40, 77, 99, 115	0
All	All	1038/1088 (95%)	0.45	64 (6%) 20 24	37, 62, 96, 115	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	LEU	8.7
1	B	231	VAL	6.8
1	A	23	LEU	5.6
1	D	22	PRO	5.2
1	D	263	TRP	4.7
1	D	226	ALA	4.2
1	C	23	LEU	4.2
1	D	74	VAL	4.2
1	D	24	ASN	4.1
1	B	177	TYR	4.1
1	D	62	VAL	4.0
1	D	60	HIS	3.6
1	D	38	ILE	3.5
1	A	263	TRP	3.4
1	D	32	LEU	3.4
1	A	249	GLY	3.3
1	D	79	LEU	3.2
1	D	212	LEU	3.2
1	A	25	GLU	3.0
1	D	50	MET	2.9
1	C	267	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	145	LEU	2.9
1	B	23	LEU	2.8
1	D	116	LEU	2.8
1	D	87	HIS	2.7
1	C	27	PHE	2.7
1	D	63	VAL	2.7
1	D	51	ALA	2.7
1	D	215	LEU	2.6
1	D	113	LEU	2.6
1	C	263	TRP	2.6
1	A	284	TYR	2.6
1	C	175	VAL	2.5
1	D	54	LEU	2.5
1	D	81	LEU	2.5
1	B	278	PHE	2.5
1	D	223	ALA	2.5
1	B	230	ILE	2.5
1	D	278	PHE	2.5
1	B	268	ILE	2.4
1	D	280	TYR	2.4
1	D	251	LEU	2.4
1	A	286	MET	2.3
1	B	197[A]	ILE	2.3
1	B	263	TRP	2.3
1	B	21	GLN	2.3
1	B	72[A]	GLN	2.3
1	C	268	ILE	2.3
1	D	210	ILE	2.3
1	A	63	VAL	2.3
1	C	266	LEU	2.3
1	D	103	VAL	2.2
1	D	218	ILE	2.2
1	A	264	THR	2.2
1	C	279	LEU	2.2
1	B	22	PRO	2.2
1	C	212	LEU	2.2
1	D	64	THR	2.1
1	B	266	LEU	2.1
1	D	266	LEU	2.1
1	D	37	VAL	2.1
1	D	279	LEU	2.0
1	C	103	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	155	LEU	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)

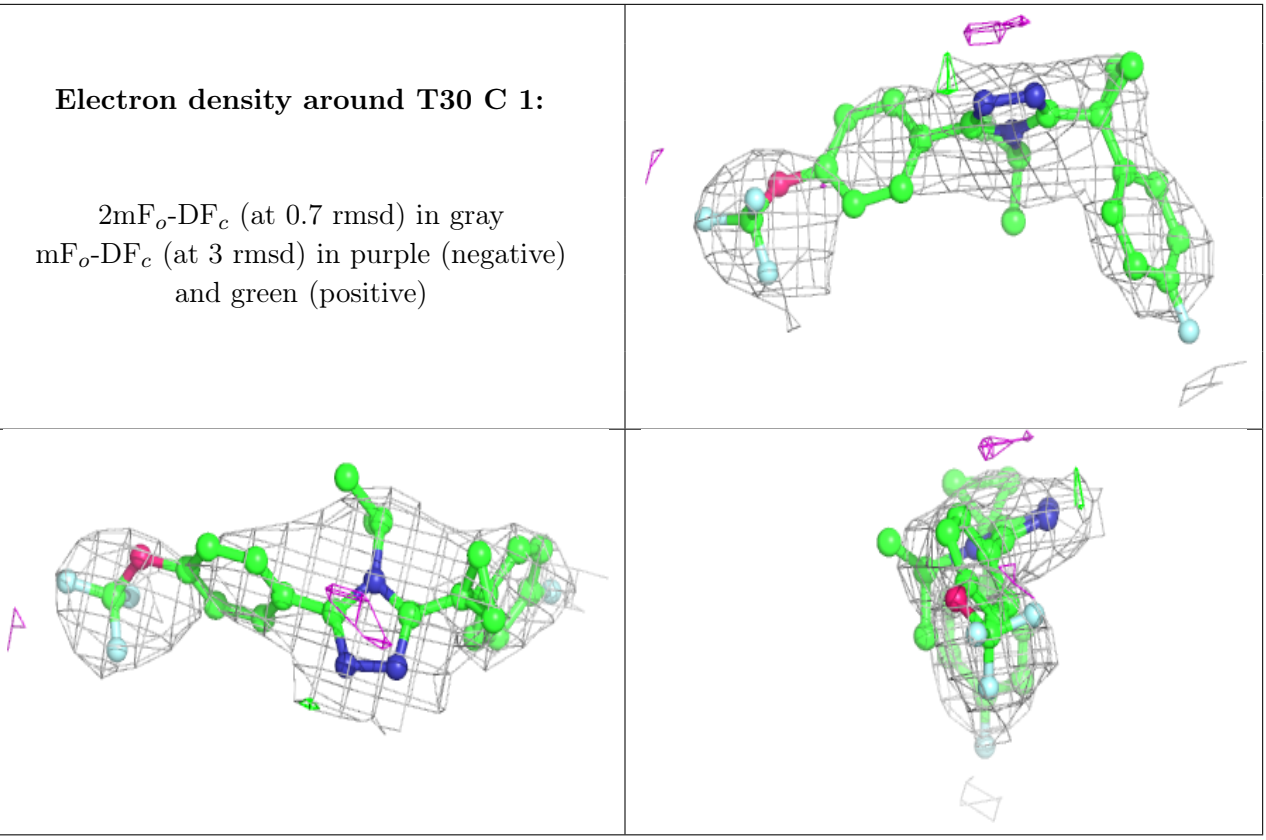
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	T30	C	1	29/29	0.90	0.31	90,92,98,99	0
3	T30	B	1	29/29	0.94	0.17	62,66,68,68	0
3	T30	A	293	29/29	0.94	0.17	63,65,66,68	0
3	T30	D	1	29/29	0.94	0.30	82,83,84,84	0
2	NAP	B	2	48/48	0.96	0.16	41,49,54,57	0
2	NAP	D	4	48/48	0.96	0.14	60,62,70,72	0
2	NAP	C	3	48/48	0.97	0.15	42,47,52,54	0
2	NAP	A	1	48/48	0.97	0.15	42,48,54,57	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.

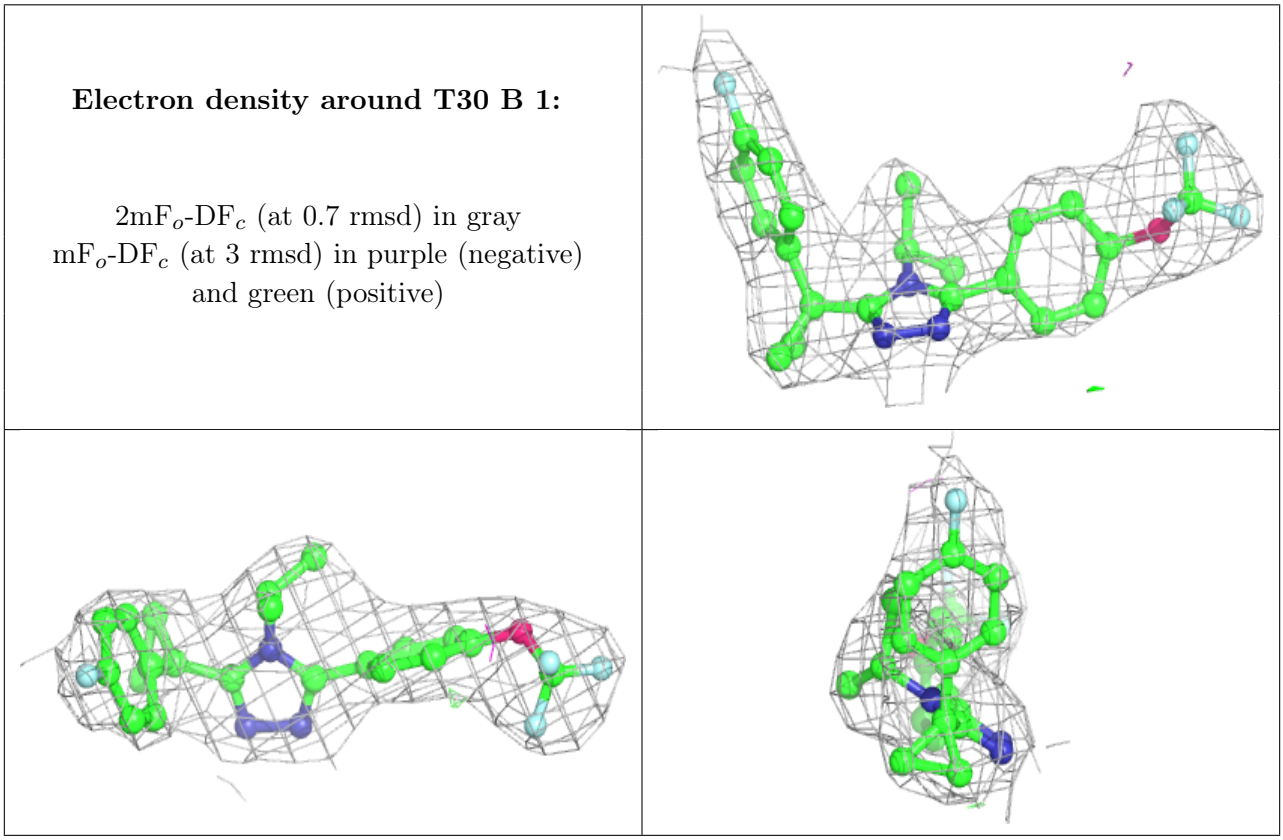
Electron density around T30 C 1:

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



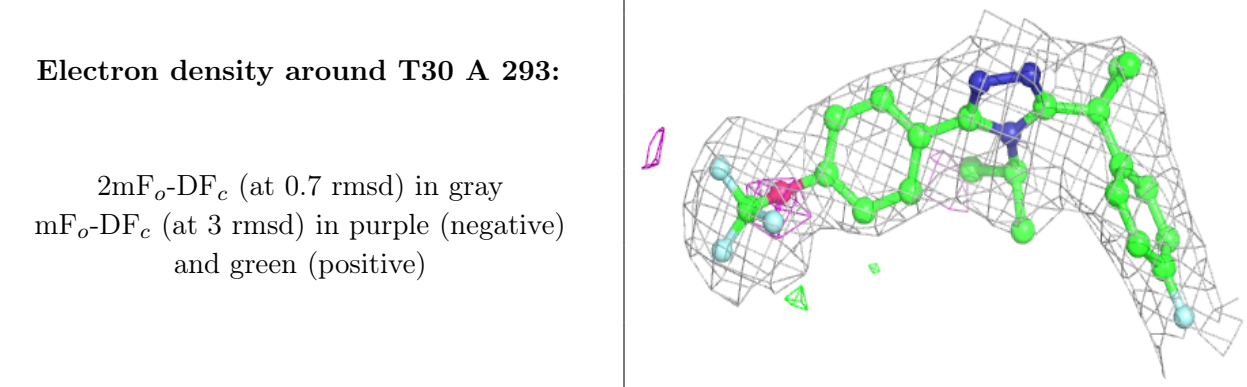
Electron density around T30 B 1:

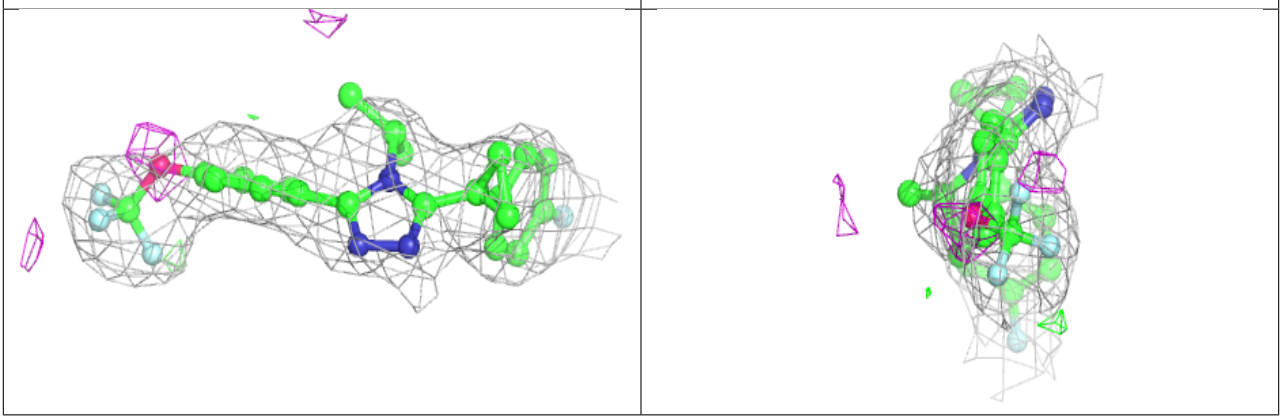
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around T30 A 293:

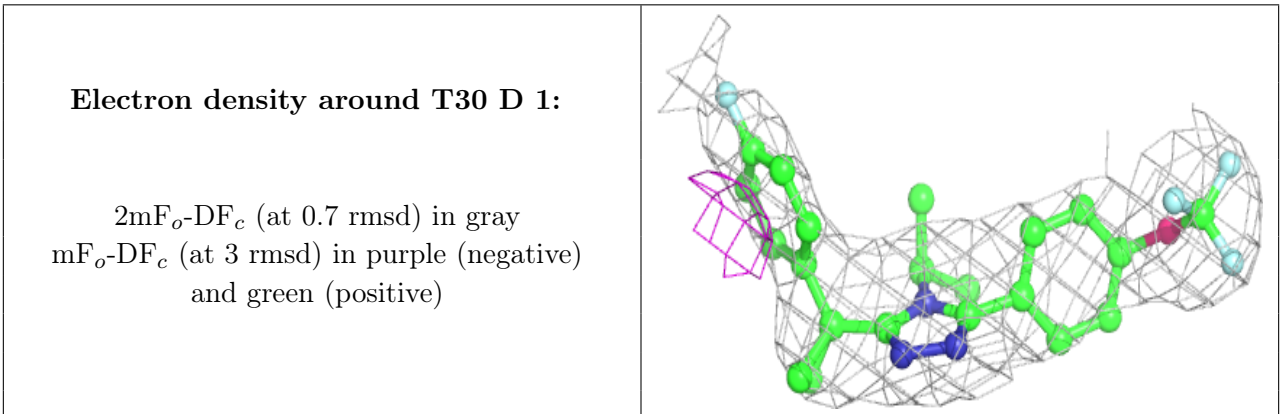
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

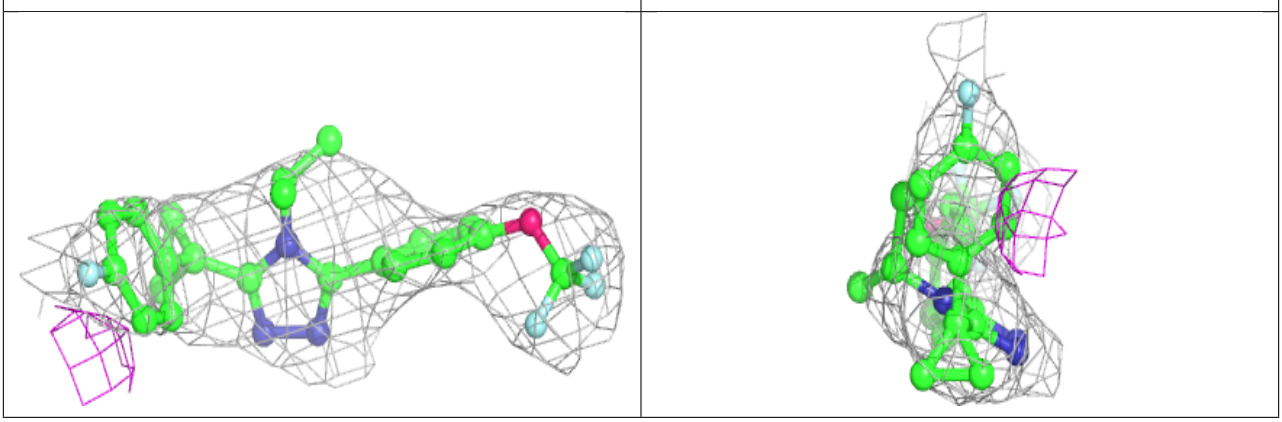




Electron density around T30 D 1:

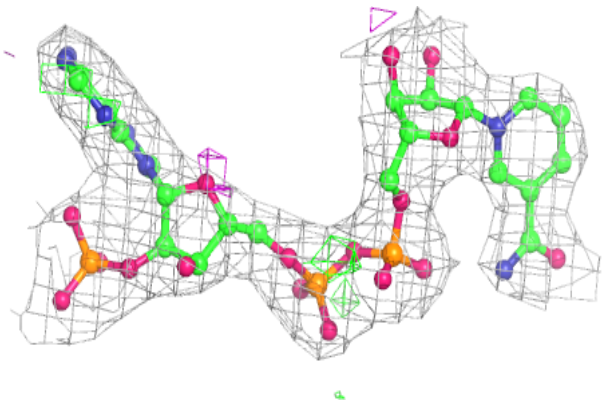
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

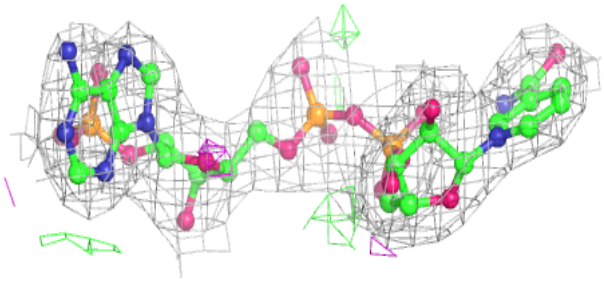


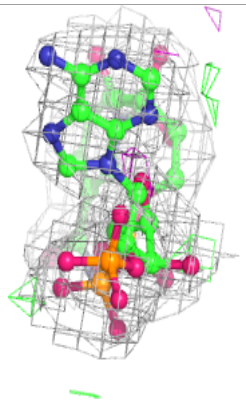


Electron density around NAP B 2:

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

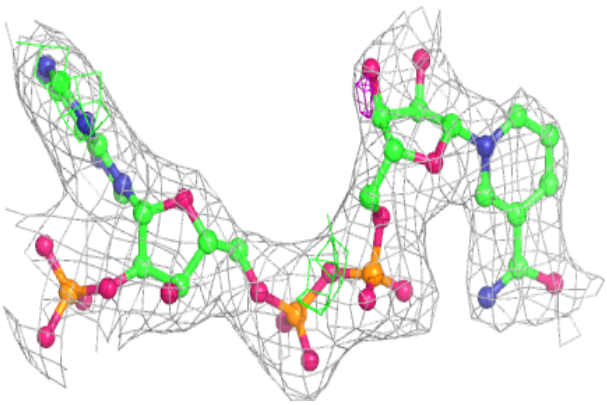


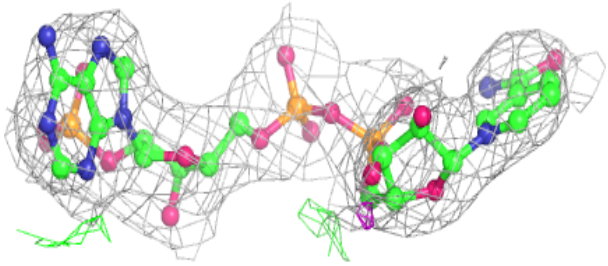


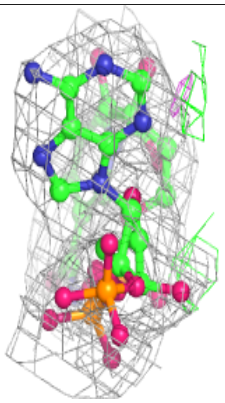


Electron density around NAP D 4:

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

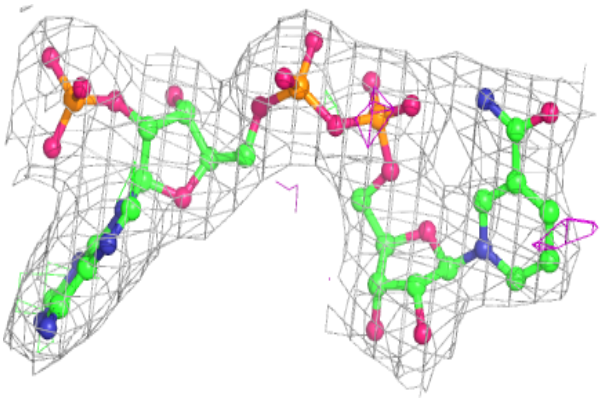


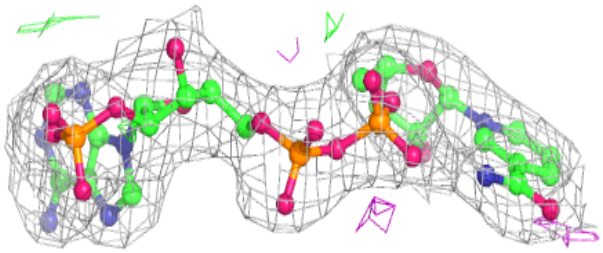


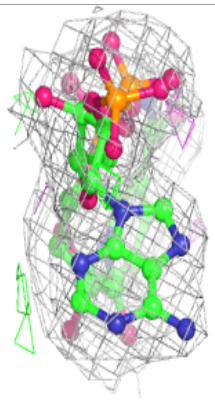


Electron density around NAP C 3:

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

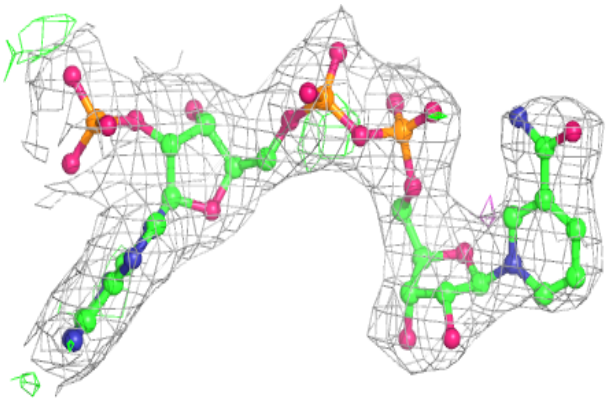


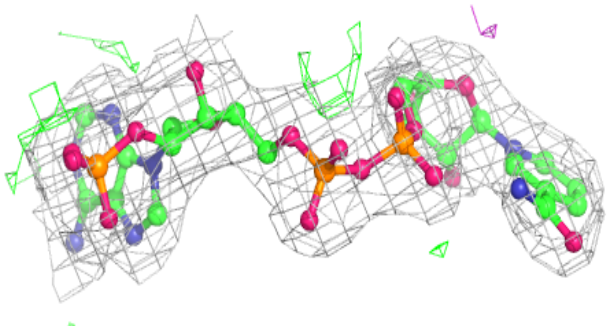


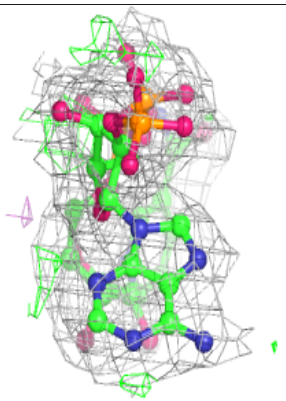


Electron density around NAP A 1:

$2mF_o$-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.