Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:54 am BST

PDB ID	:	1GT8
Title	:	DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG, TERNARY COMPLEX WITH NADPH AND URACIL-4-ACETIC ACID
Authors	:	Dobritzsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on	:	2002-01-14
Resolution	:	3.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

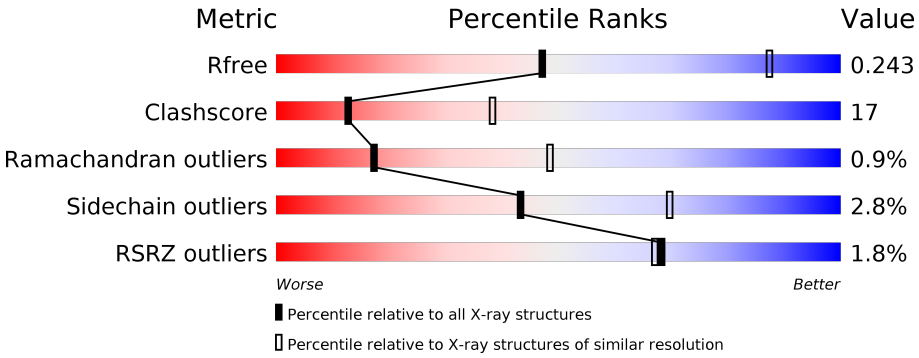
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	1025	70% 28%
1	B	1025	68% 29%
1	C	1025	66% 31%
1	D	1025	64% 34%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	1027	-	-	X	-
2	SF4	A	1028	-	-	X	-
2	SF4	B	1026	-	-	X	-
2	SF4	B	1027	-	-	X	-
2	SF4	B	1028	-	-	X	-
2	SF4	B	1029	-	-	X	-
2	SF4	C	1027	-	-	X	-
2	SF4	C	1028	-	-	X	-
2	SF4	D	1027	-	-	X	-
2	SF4	D	1028	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31588 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.

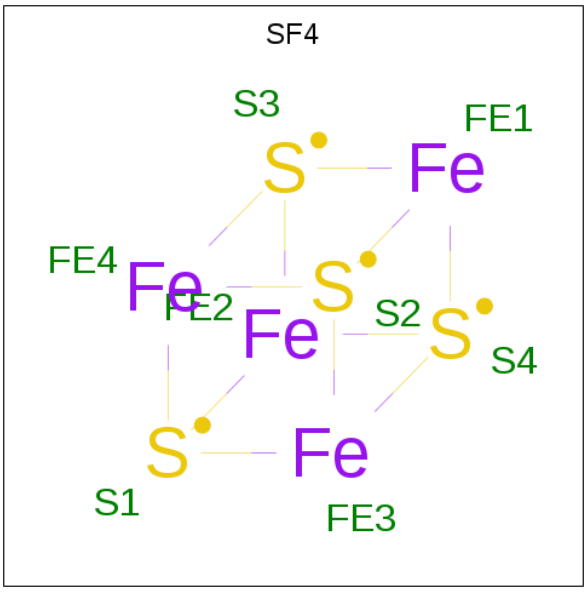
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			7755	4919	1312	1468	56			
1	B	1010	Total	C	N	O	S	0	0	0
			7703	4885	1304	1458	56			
1	C	1010	Total	C	N	O	S	0	0	0
			7708	4892	1303	1459	54			
1	D	1012	Total	C	N	O	S	0	0	0
			7718	4894	1307	1461	56			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

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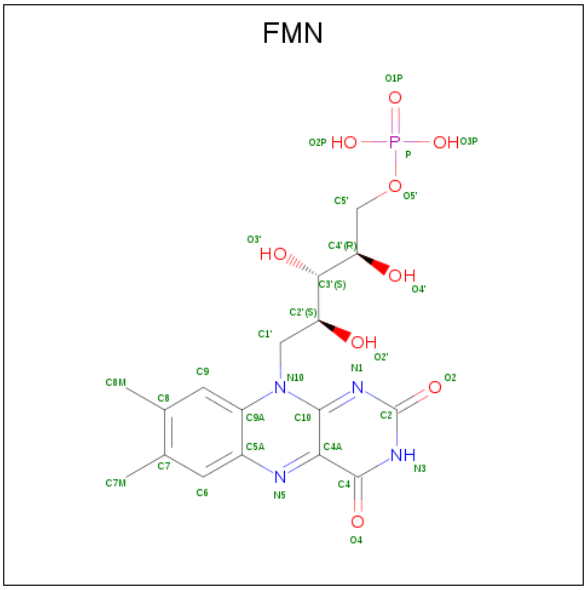
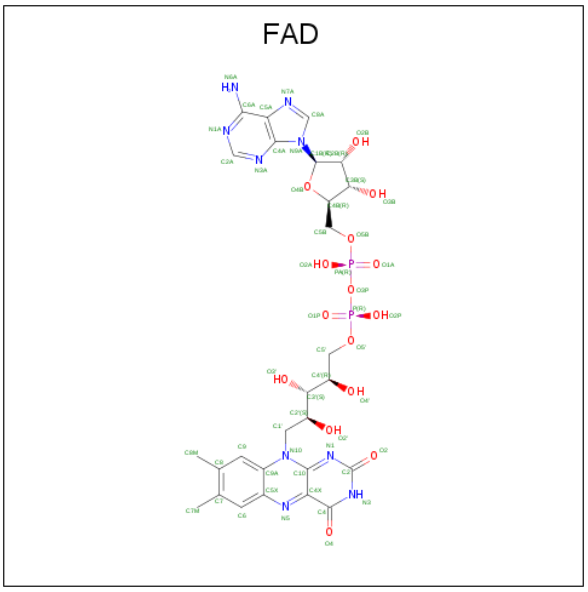
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



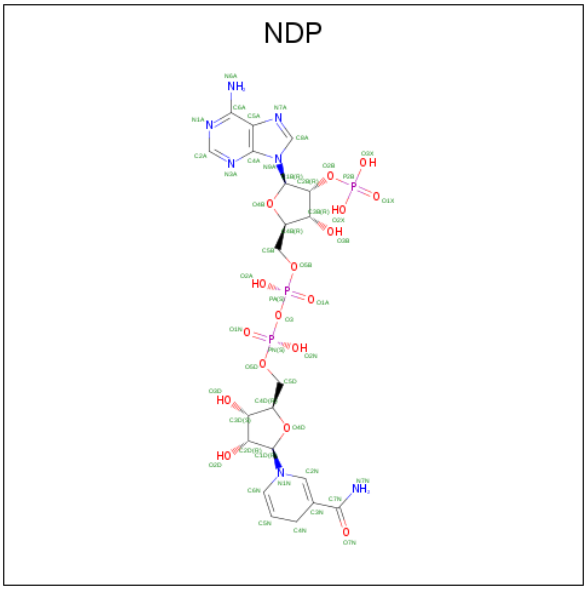
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 17 4 9 1	0	0
3	B	1	Total C N O P 31 17 4 9 1	0	0
3	C	1	Total C N O P 31 17 4 9 1	0	0
3	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



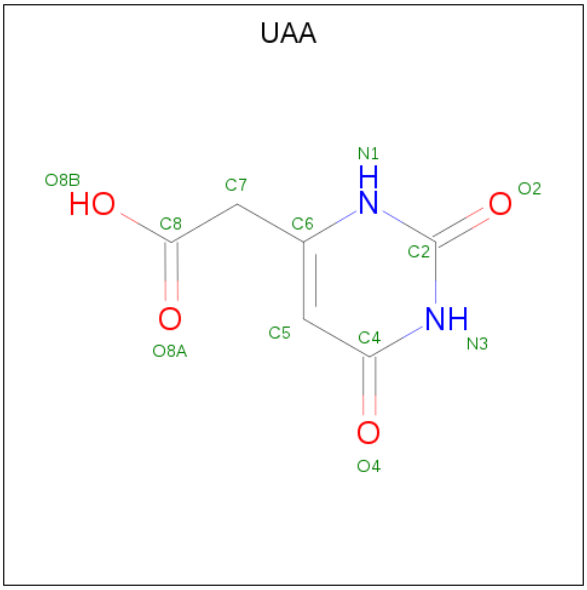
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 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
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is URACIL-6-ACETIC ACID (three-letter code: UAA) (formula: $C_6H_6N_2O_4$).



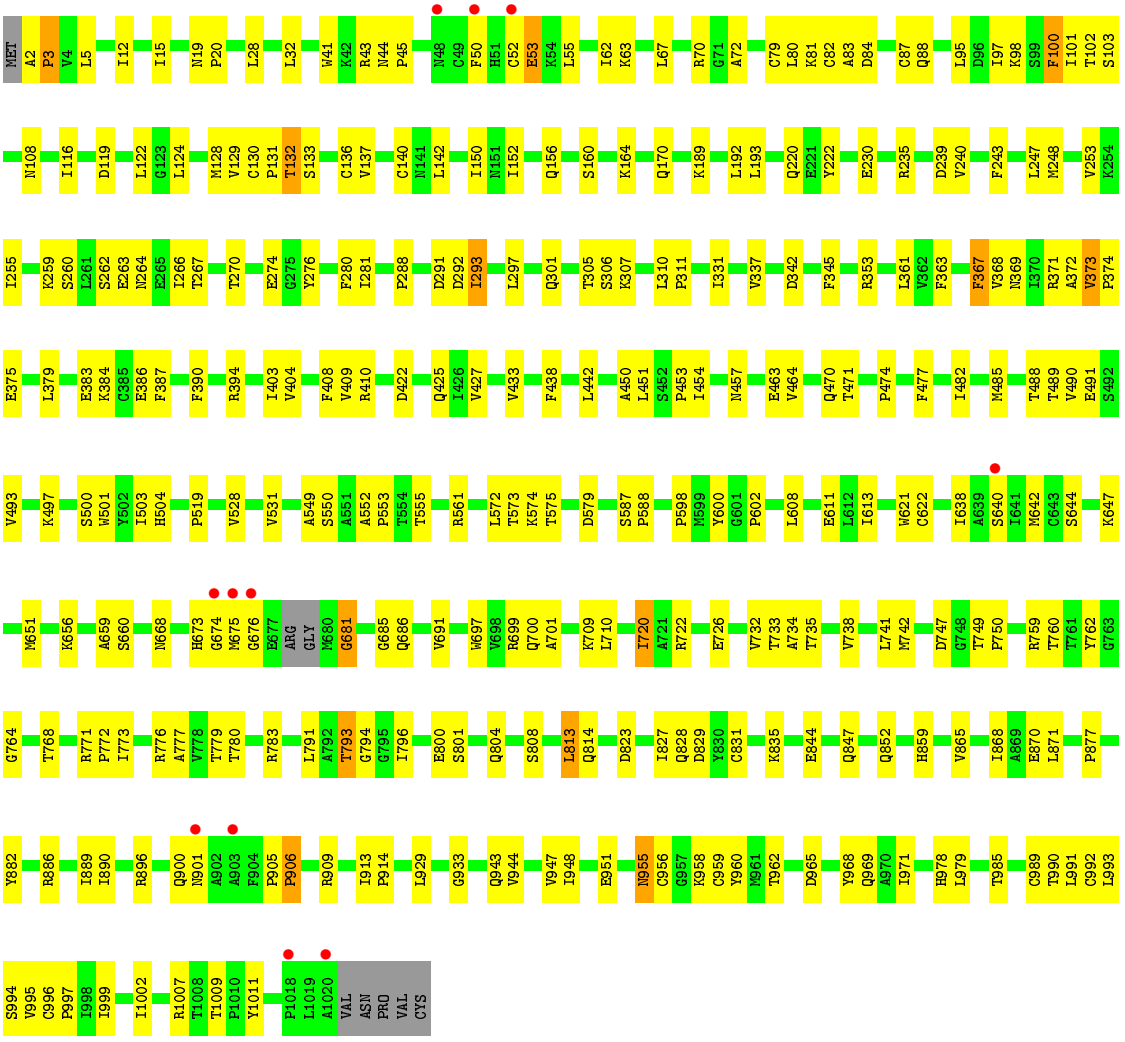
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	2	4		
6	B	1	Total	C	N	O	0	0
			12	6	2	4		
6	C	1	Total	C	N	O	0	0
			12	6	2	4		
6	D	1	Total	C	N	O	0	0
			12	6	2	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

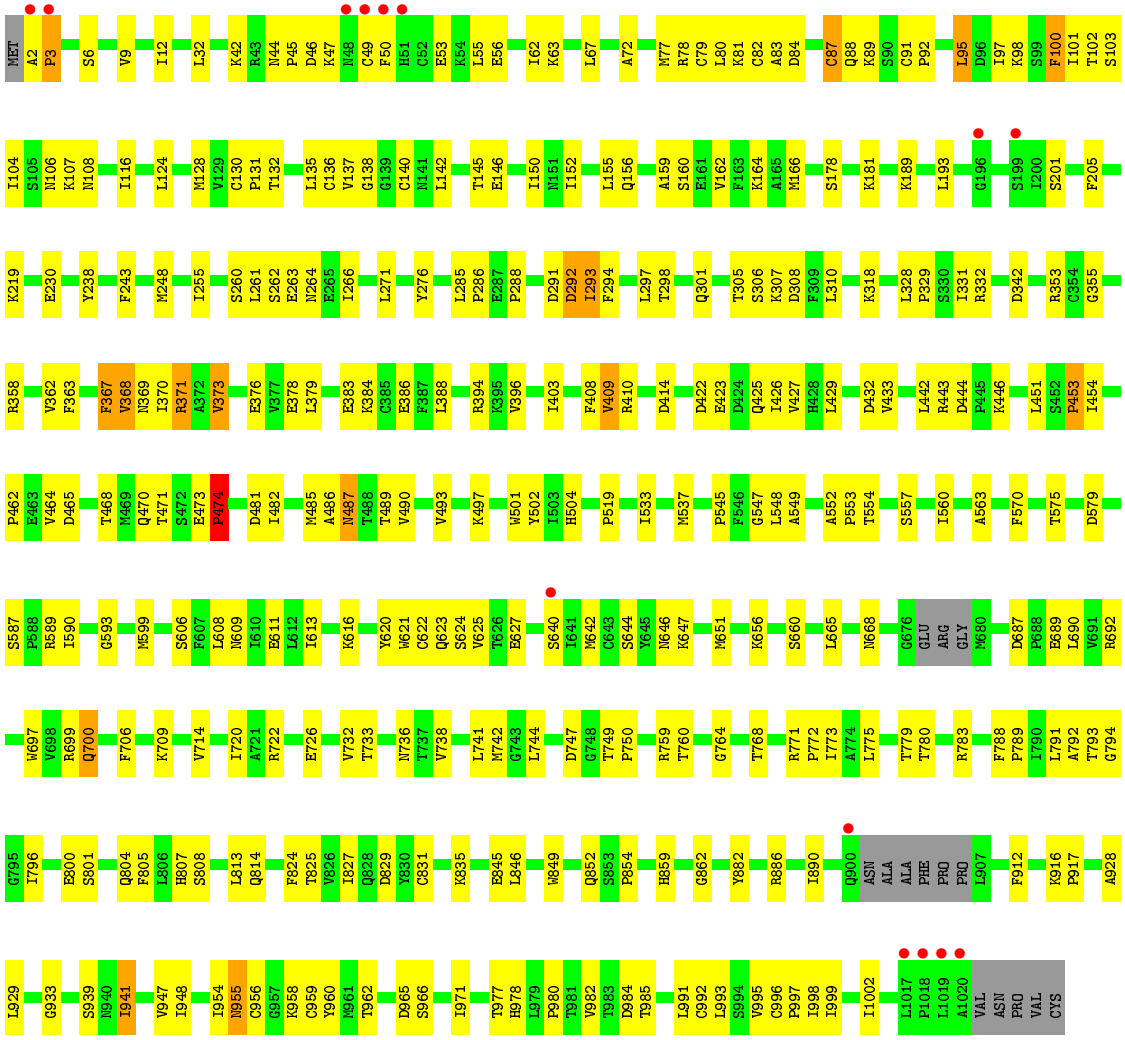
- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain A:



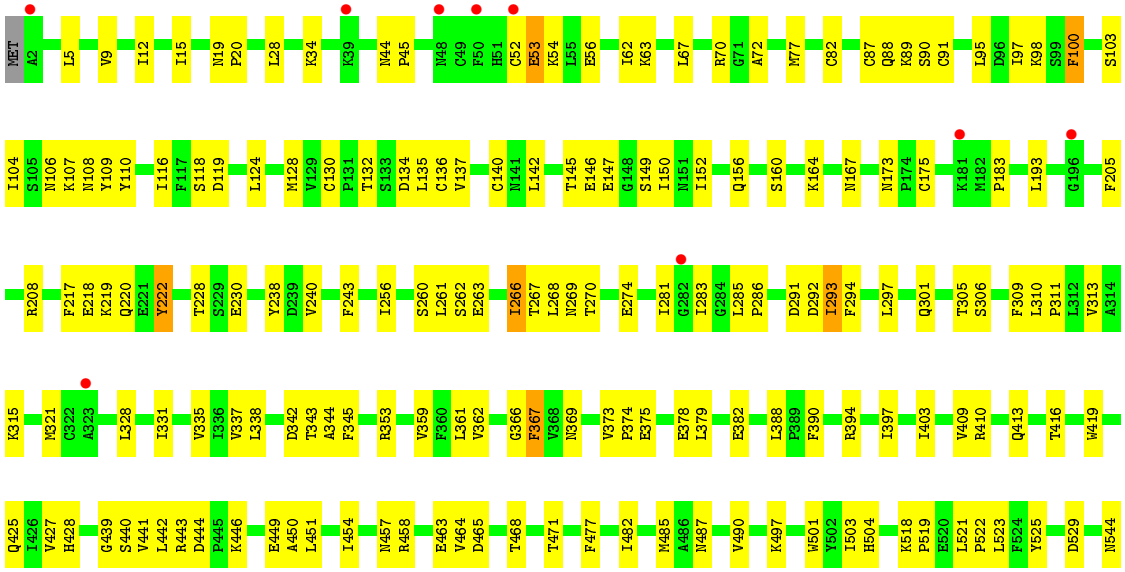
- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

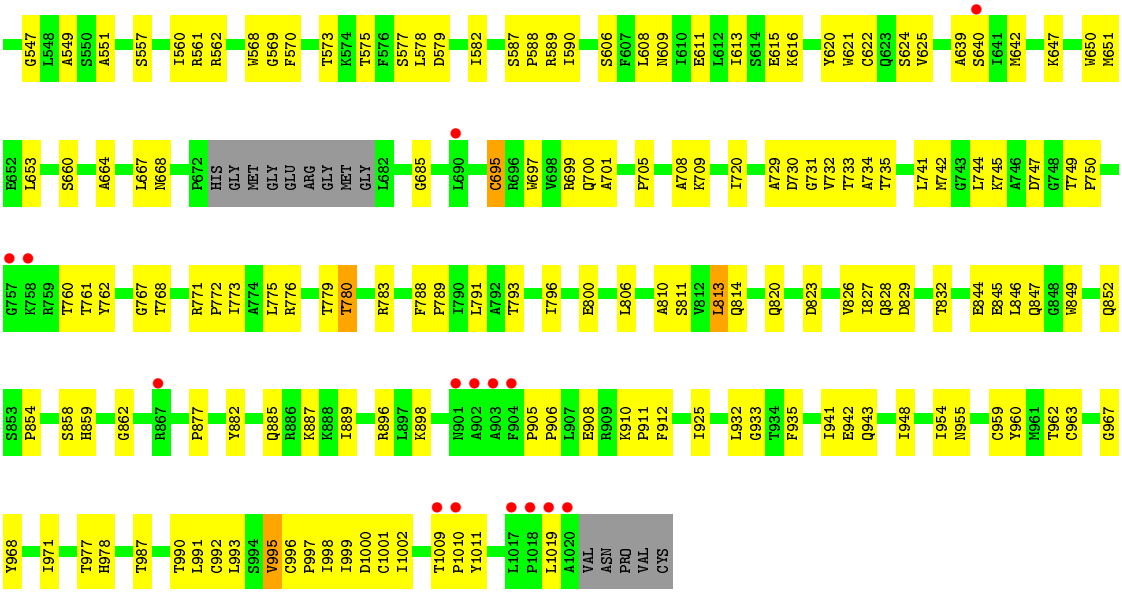
Chain B:



• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

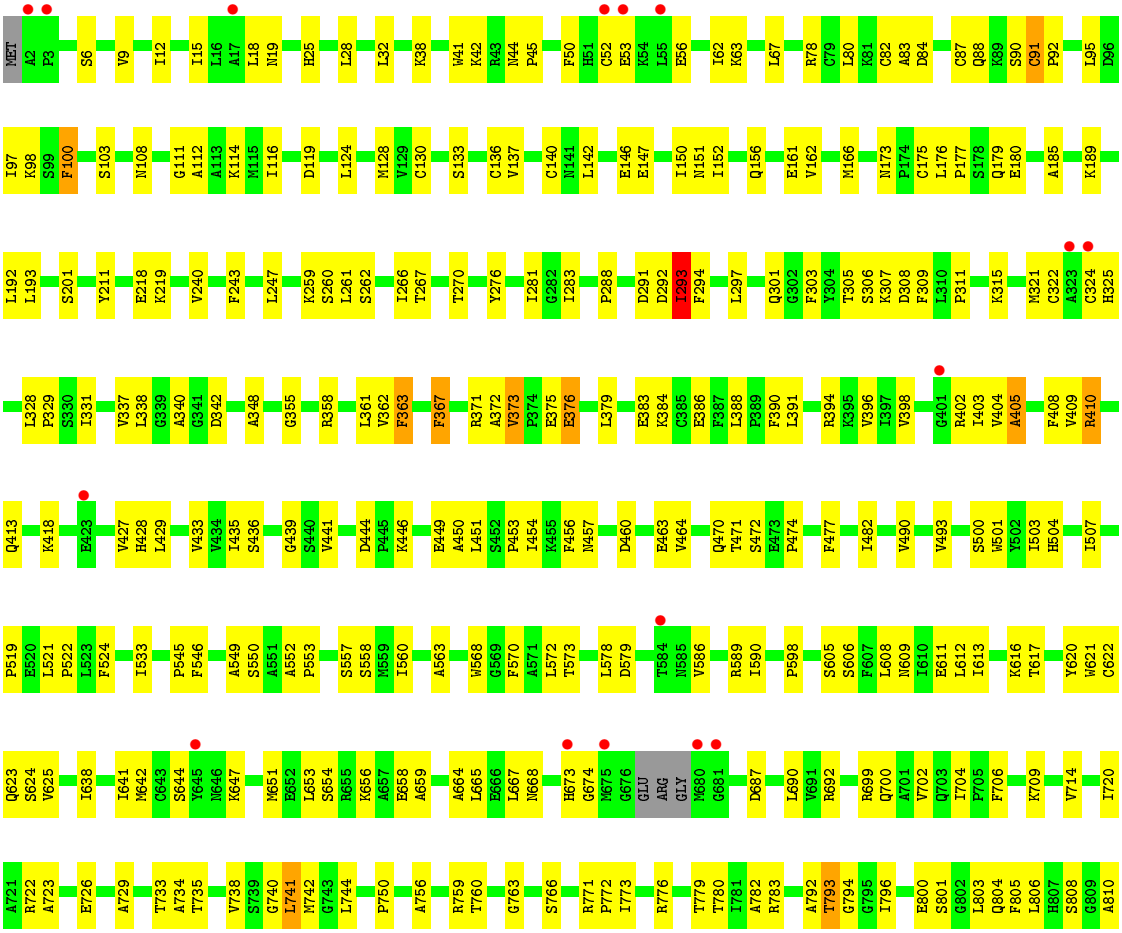
Chain C:

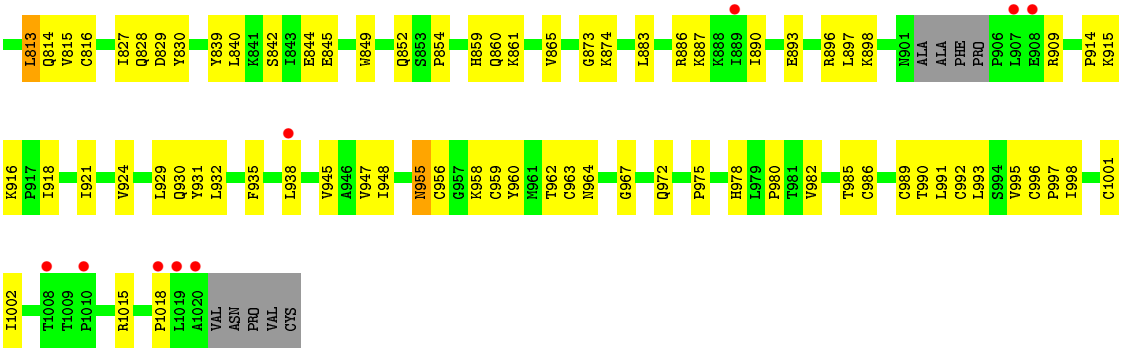




• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain D:




L813 Q814 V815 C816 I827 Q828 D829 Y830 Y839 L840 K841 S842 I843 E844 E845 W849 Q852 S853 P854 H859 Q860 K861 V865 G873 K874 L883 R886 K887 K888 I889 I890 E893 R896 L897 K898 N901 ALA ALA PHE PRO P906 L907 E908 R909 P914 K915
K916 P917 I918 I921 V924 L929 Q930 Y931 L932 F935 L938 V945 A946 V947 I948 N955 C956 G957 K958 C959 Y960 M961 T962 C963 N964 G967 Q972 P975 H978 L979 P980 I981 V982 T985 C986 C989 T990 L991 C992 L993 S994 V995 C996 P997 I998 C1001
I1002 T1008 T1009 P1010 R1015 P1018 L1019 A1020 VAL ASN PRO VAL CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.03Å 159.53Å 166.02Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	29.75 – 3.30 29.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.75-3.30) 98.5 (29.75-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.269 0.195 , 0.243	Depositor DCC
R_{free} test set	1247 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	71.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31588	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: FMN, NDP, SF4, FAD, UAA

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	0/7916	0.65	0/10729
1	B	0.45	1/7860 (0.0%)	0.65	0/10649
1	C	0.44	0/7868	0.64	0/10667
1	D	0.43	0/7876	0.64	0/10671
All	All	0.44	1/31520 (0.0%)	0.65	0/42716

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	CYS	CB-SG	-5.12	1.73	1.81

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	7755	0	7781	262	0
1	B	7703	0	7735	274	0
1	C	7708	0	7743	307	0
1	D	7718	0	7750	313	0
2	A	32	0	0	6	0
2	B	32	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	32	0	0	6	0
2	D	32	0	0	8	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	C	31	0	19	0	0
3	D	31	0	19	1	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	C	53	0	31	2	0
4	D	53	0	31	3	0
5	A	48	0	26	6	0
5	B	48	0	26	5	0
5	C	48	0	26	6	0
5	D	48	0	26	6	0
6	A	12	0	5	1	0
6	B	12	0	5	1	0
6	C	12	0	5	1	0
6	D	12	0	5	0	0
All	All	31588	0	31333	1044	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 17.

All (1044) 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:136:CYS:SG	1:C:137:VAL:HG23	2.02	1.00
1:C:116:ILE:HD13	1:C:156:GLN:HG3	1.43	0.99
1:C:410:ARG:NH1	1:D:427:VAL:HG13	1.84	0.92
1:C:776:ARG:O	1:C:780:THR:HG22	1.71	0.90
1:C:173:ASN:HD21	1:C:175:CYS:HB2	1.36	0.90
1:C:136:CYS:SG	1:C:137:VAL:N	2.44	0.88
1:A:608:LEU:HD13	1:A:742:MET:HB2	1.55	0.88
1:D:673:HIS:HD2	1:D:690:LEU:HD11	1.39	0.87
1:A:501:TRP:O	1:A:504:HIS:HB3	1.75	0.86
1:C:608:LEU:HD13	1:C:742:MET:HB2	1.58	0.86
1:D:116:ILE:HD13	1:D:156:GLN:HG3	1.57	0.85
1:D:608:LEU:HD13	1:D:742:MET:HB2	1.59	0.85
1:B:95:LEU:HD21	1:B:116:ILE:HG23	1.59	0.84
1:B:549:ALA:HB2	1:B:814:GLN:HB3	1.59	0.84
1:A:63:LYS:HE3	1:A:128:MET:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:HIS:CD2	1:D:690:LEU:HD11	2.13	0.84
1:C:410:ARG:NH2	1:D:427:VAL:HG22	1.93	0.83
1:A:896:ARG:HH21	1:A:900:GLN:HE22	1.22	0.83
1:C:410:ARG:HH22	1:D:427:VAL:HG22	1.42	0.83
1:C:362:VAL:HG22	1:C:388:LEU:HB2	1.61	0.83
1:A:549:ALA:HB2	1:A:814:GLN:HB3	1.61	0.82
1:D:651:MET:HE3	1:D:700:GLN:HG3	1.60	0.82
1:C:291:ASP:OD1	1:C:293:ILE:HG12	1.79	0.82
1:D:572:LEU:HD13	1:D:638:ILE:HB	1.60	0.81
1:D:839:TYR:HA	1:D:918:ILE:HD12	1.62	0.81
1:B:342:ASP:HB3	5:B:1032:NDP:H42N	1.63	0.81
1:A:427:VAL:HG22	1:B:410:ARG:HH21	1.47	0.80
1:C:410:ARG:HE	1:D:410:ARG:NH2	1.79	0.80
1:D:124:LEU:HD23	1:D:240:VAL:HG13	1.63	0.80
1:D:842:SER:HB3	1:D:918:ILE:HD13	1.65	0.79
1:D:410:ARG:HG3	1:D:410:ARG:HH11	1.46	0.79
1:D:342:ASP:HB3	5:D:1032:NDP:H42N	1.65	0.78
1:C:501:TRP:O	1:C:504:HIS:HB3	1.83	0.78
1:B:193:LEU:HG	1:B:261:LEU:HD22	1.67	0.77
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.64	0.77
1:D:673:HIS:HD2	1:D:690:LEU:CD1	1.97	0.77
1:C:173:ASN:ND2	1:C:175:CYS:HB2	2.00	0.77
1:C:549:ALA:HB2	1:C:814:GLN:HB3	1.64	0.77
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.66	0.77
1:B:608:LEU:HD13	1:B:742:MET:HB2	1.67	0.76
1:C:369:ASN:HA	1:D:50:PHE:HE2	1.50	0.76
1:A:962:THR:HG21	1:A:991:LEU:HB3	1.68	0.75
1:C:820:GLN:O	1:D:962:THR:HG22	1.86	0.75
1:A:611:GLU:O	6:A:1035:UAA:H5	1.85	0.75
1:B:193:LEU:HD12	1:B:261:LEU:HB2	1.67	0.75
1:B:687:ASP:HB3	1:B:690:LEU:HD12	1.69	0.75
1:A:747:ASP:OD2	1:A:749:THR:HG23	1.86	0.74
1:B:487:ASN:N	1:B:487:ASN:HD22	1.85	0.74
1:C:369:ASN:HA	1:D:50:PHE:CE2	2.24	0.73
1:B:768:THR:HG22	1:B:771:ARG:HH21	1.53	0.73
1:D:87:CYS:SG	1:D:97:ILE:HD12	2.28	0.73
1:A:451:LEU:O	1:A:454:ILE:HG12	1.88	0.73
1:B:422:ASP:OD2	1:B:425:GLN:HG3	1.88	0.73
1:A:342:ASP:HB3	5:A:1032:NDP:H42N	1.69	0.73
1:A:451:LEU:HB3	1:A:454:ILE:HD11	1.71	0.73
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:HD12	1:B:379:LEU:HD22	1.70	0.73
1:C:647:LYS:HA	1:C:697:TRP:CE3	2.24	0.73
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.70	0.72
1:D:331:ILE:HG23	1:D:433:VAL:HG21	1.70	0.72
1:C:477:PHE:CD1	1:C:503:ILE:HG12	2.24	0.72
1:A:133:SER:HB3	1:A:375:GLU:OE1	1.90	0.72
1:A:427:VAL:HG22	1:B:410:ARG:NH2	2.05	0.72
1:A:410:ARG:NH2	1:B:427:VAL:CG2	2.53	0.72
1:C:146:GLU:HG2	1:D:67:LEU:HD23	1.70	0.72
1:D:78:ARG:NH2	1:D:150:ILE:HD13	2.05	0.71
1:A:410:ARG:HH21	1:B:427:VAL:HG22	1.55	0.71
1:C:573:THR:OG1	1:C:639:ALA:HA	1.89	0.71
1:C:962:THR:OG1	1:C:995:VAL:HG21	1.90	0.71
1:C:394:ARG:HG3	1:C:409:VAL:HG13	1.71	0.71
1:C:762:TYR:CZ	1:D:780:THR:HG22	2.26	0.71
1:B:294:PHE:HA	1:B:297:LEU:HD12	1.73	0.71
1:C:779:THR:O	1:C:783:ARG:HG3	1.90	0.71
1:A:87:CYS:SG	1:A:97:ILE:HD12	2.30	0.71
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.72	0.71
1:D:337:VAL:HB	1:D:361:LEU:HD23	1.72	0.70
1:D:451:LEU:HD13	1:D:454:ILE:HD11	1.73	0.70
1:A:267:THR:OG1	1:A:270:THR:HG23	1.91	0.70
1:D:410:ARG:HH11	1:D:410:ARG:CG	2.04	0.70
1:A:367:PHE:HB2	1:B:386:GLU:OE1	1.91	0.70
1:D:549:ALA:HB2	1:D:814:GLN:HB3	1.74	0.70
1:D:259:LYS:HB3	1:D:266:ILE:HD11	1.73	0.70
1:D:201:SER:HB2	1:D:493:VAL:HG13	1.73	0.70
1:C:150:ILE:HB	2:C:1027:SF4:S4	2.31	0.69
1:D:793:THR:HB	1:D:814:GLN:HB2	1.72	0.69
1:A:62:ILE:HD12	1:A:379:LEU:HD22	1.74	0.69
1:B:470:GLN:NE2	1:B:474:PRO:HA	2.07	0.69
1:A:95:LEU:HD23	1:A:119:ASP:HB2	1.72	0.69
1:A:779:THR:HG22	1:A:808:SER:HB3	1.73	0.69
1:B:608:LEU:HD23	1:B:609:ASN:N	2.07	0.69
1:C:9:VAL:HG22	1:C:12:ILE:HG12	1.74	0.69
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.73	0.69
1:C:959:CYS:HB2	1:C:992:CYS:HB2	1.73	0.69
1:D:52:CYS:HB3	1:D:384:LYS:HG2	1.75	0.69
1:D:108:ASN:HA	1:D:852:GLN:NE2	2.08	0.69
1:D:776:ARG:O	1:D:780:THR:HG23	1.93	0.69
1:B:116:ILE:HD13	1:B:156:GLN:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:VAL:HG21	1:D:410:ARG:HH21	1.57	0.68
1:A:52:CYS:HB2	1:A:384:LYS:HG2	1.74	0.68
1:B:992:CYS:SG	1:B:993:LEU:N	2.66	0.68
1:D:722:ARG:O	1:D:726:GLU:HG3	1.94	0.68
1:B:779:THR:HG23	1:B:808:SER:HB3	1.75	0.68
1:C:342:ASP:HB3	5:C:1032:NDP:H42N	1.76	0.68
1:B:297:LEU:HA	1:B:301:GLN:OE1	1.94	0.68
1:A:896:ARG:HH21	1:A:900:GLN:NE2	1.93	0.67
1:A:422:ASP:OD2	1:A:425:GLN:HG3	1.95	0.67
1:D:996:CYS:HA	2:D:1028:SF4:S3	2.35	0.67
1:D:992:CYS:SG	1:D:993:LEU:N	2.68	0.67
1:D:699:ARG:HE	1:D:699:ARG:HA	1.60	0.67
1:B:747:ASP:OD2	1:B:749:THR:HG23	1.95	0.67
1:C:457:ASN:HB3	1:C:463:GLU:OE1	1.94	0.67
1:D:616:LYS:HD3	1:D:620:TYR:CE2	2.30	0.67
1:C:283:ILE:HG13	1:C:482:ILE:HD13	1.78	0.66
1:A:410:ARG:CZ	1:B:410:ARG:NH2	2.58	0.66
1:B:87:CYS:SG	1:B:97:ILE:HD12	2.35	0.66
1:C:811:SER:HA	1:C:925:ILE:HD13	1.77	0.66
1:B:219:LYS:HG3	1:B:260:SER:OG	1.93	0.66
1:C:193:LEU:HD23	1:C:281:ILE:HD13	1.76	0.66
1:A:342:ASP:HB2	5:A:1032:NDP:C5N	2.25	0.66
1:C:611:GLU:O	6:C:1035:UAA:H5	1.95	0.66
1:D:328:LEU:HD12	1:D:329:PRO:HD2	1.76	0.66
1:C:261:LEU:HD12	1:C:266:ILE:O	1.96	0.66
1:B:996:CYS:HA	2:B:1028:SF4:S3	2.35	0.66
1:A:80:LEU:HD11	1:B:954:ILE:HD11	1.78	0.66
1:C:578:LEU:HD23	1:C:653:LEU:HD13	1.78	0.66
1:D:291:ASP:OD1	1:D:293:ILE:HG13	1.96	0.66
1:C:557:SER:HA	1:C:560:ILE:HD12	1.77	0.66
1:C:954:ILE:HD11	1:D:80:LEU:HD11	1.77	0.65
1:C:427:VAL:HG13	1:D:410:ARG:HE	1.60	0.65
1:D:568:TRP:NE1	1:D:827:ILE:HB	2.12	0.65
1:B:150:ILE:HB	2:B:1027:SF4:S4	2.36	0.65
1:D:699:ARG:NE	1:D:699:ARG:HA	2.11	0.65
1:A:369:ASN:HD22	1:B:50:PHE:HE2	1.43	0.65
1:C:709:LYS:HA	1:C:733:THR:HB	1.79	0.65
1:C:294:PHE:HA	1:C:297:LEU:HD12	1.78	0.65
1:C:335:VAL:HB	1:C:359:VAL:HG22	1.79	0.65
1:D:873:GLY:O	1:D:874:LYS:HD3	1.97	0.65
1:A:32:LEU:HB2	1:B:485:MET:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:MET:HE1	1:B:32:LEU:HD13	1.77	0.65
1:B:859:HIS:HD2	1:B:862:GLY:H	1.45	0.65
1:C:378:GLU:O	1:C:382:GLU:HG2	1.97	0.65
1:A:342:ASP:CB	5:A:1032:NDP:H42N	2.27	0.64
1:A:342:ASP:OD1	1:A:372:ALA:HB1	1.96	0.64
1:D:860:GLN:O	1:D:861:LYS:HB2	1.95	0.64
1:C:130:CYS:SG	1:C:490:VAL:HB	2.38	0.64
1:D:82:CYS:O	1:D:98:LYS:HD2	1.97	0.64
1:B:408:PHE:CE1	1:B:429:LEU:HD12	2.32	0.64
1:C:410:ARG:CZ	1:D:427:VAL:HG22	2.28	0.64
1:D:150:ILE:HB	2:D:1027:SF4:S4	2.37	0.64
1:D:959:CYS:HB2	1:D:992:CYS:HB2	1.78	0.64
1:C:310:LEU:HB2	1:C:311:PRO:HD3	1.79	0.64
1:C:342:ASP:HB2	5:C:1032:NDP:C5N	2.27	0.64
1:C:615:GLU:O	1:D:1015:ARG:HD3	1.98	0.64
1:B:621:TRP:O	1:B:625:VAL:HG23	1.97	0.64
1:D:180:GLU:H	1:D:180:GLU:CD	2.01	0.64
1:D:301:GLN:O	1:D:403:ILE:HG22	1.96	0.64
1:A:297:LEU:HA	1:A:301:GLN:OE1	1.98	0.64
1:B:470:GLN:HE21	1:B:474:PRO:HA	1.60	0.63
1:B:709:LYS:HE2	1:B:736:ASN:ND2	2.12	0.63
1:D:311:PRO:O	1:D:315:LYS:HG3	1.99	0.63
1:A:647:LYS:HA	1:A:697:TRP:CE3	2.32	0.63
1:B:993:LEU:HD23	1:B:993:LEU:C	2.19	0.63
1:A:410:ARG:NH2	1:B:427:VAL:HG22	2.13	0.63
1:C:768:THR:HG22	1:C:771:ARG:HH21	1.63	0.63
1:C:761:THR:HG22	1:D:938:LEU:HD11	1.81	0.63
1:B:501:TRP:O	1:B:504:HIS:HB3	1.97	0.63
1:D:464:VAL:HG12	1:D:471:THR:HG22	1.80	0.63
1:C:297:LEU:HA	1:C:301:GLN:OE1	1.99	0.63
1:D:651:MET:CE	1:D:700:GLN:HG3	2.29	0.63
1:B:79:CYS:SG	1:B:101:ILE:HG21	2.39	0.62
1:D:62:ILE:HD12	1:D:379:LEU:HD22	1.81	0.62
1:D:501:TRP:O	1:D:504:HIS:HB3	1.99	0.62
1:B:959:CYS:HB2	1:B:992:CYS:HB2	1.81	0.62
1:C:108:ASN:HA	1:C:852:GLN:NE2	2.15	0.62
1:C:859:HIS:HD2	1:C:862:GLY:H	1.46	0.62
1:C:451:LEU:HB3	1:C:454:ILE:CD1	2.30	0.62
1:C:410:ARG:NH1	1:D:427:VAL:HG22	2.15	0.62
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.82	0.62
1:C:747:ASP:OD2	1:C:749:THR:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASP:HB2	5:D:1032:NDP:C5N	2.29	0.62
1:A:796:ILE:CD1	1:A:813:LEU:HB3	2.29	0.61
1:B:95:LEU:HD13	2:B:1026:SF4:S2	2.40	0.61
1:C:87:CYS:SG	1:C:97:ILE:HD12	2.39	0.61
1:A:691:VAL:HG21	1:A:720:ILE:CG2	2.30	0.61
1:A:959:CYS:SG	1:A:960:TYR:N	2.73	0.61
1:B:92:PRO:HB2	1:B:490:VAL:HG22	1.82	0.61
1:C:124:LEU:HD23	1:C:240:VAL:HG13	1.80	0.61
1:C:451:LEU:HB3	1:C:454:ILE:HD11	1.82	0.61
1:A:996:CYS:HA	2:A:1028:SF4:S3	2.40	0.61
1:B:62:ILE:HD11	1:B:379:LEU:HD13	1.81	0.61
1:A:561:ARG:NE	1:B:6:SER:O	2.27	0.61
1:A:116:ILE:HD13	1:A:156:GLN:HG3	1.83	0.61
1:B:142:LEU:HD12	1:B:150:ILE:HD11	1.82	0.61
1:C:95:LEU:HD23	1:C:119:ASP:HB2	1.81	0.61
1:D:261:LEU:HD21	1:D:451:LEU:HD21	1.81	0.61
1:B:291:ASP:OD1	1:B:293:ILE:HG12	2.01	0.61
1:A:427:VAL:CG2	1:B:410:ARG:NH2	2.64	0.61
1:D:560:ILE:O	1:D:563:ALA:HB3	2.01	0.61
1:D:9:VAL:HG22	1:D:12:ILE:HG12	1.81	0.61
1:A:768:THR:HG22	1:A:771:ARG:HH21	1.64	0.60
1:D:883:LEU:HG	1:D:887:LYS:HE3	1.83	0.60
1:A:150:ILE:HB	2:A:1027:SF4:S4	2.41	0.60
1:B:589:ARG:HD2	1:B:611:GLU:HB2	1.83	0.60
1:C:908:GLU:OE1	1:C:910:LYS:HE3	2.00	0.60
1:A:164:LYS:HD2	1:A:243:PHE:CD2	2.36	0.60
1:A:470:GLN:HE21	1:A:474:PRO:HA	1.66	0.60
1:C:261:LEU:HD21	1:C:451:LEU:HD21	1.83	0.60
1:B:709:LYS:HA	1:B:733:THR:HB	1.84	0.60
1:C:651:MET:CE	1:C:700:GLN:HG3	2.30	0.60
1:D:283:ILE:HG13	1:D:482:ILE:HD13	1.84	0.60
1:D:706:PHE:CZ	1:D:729:ALA:HA	2.37	0.60
1:D:108:ASN:HA	1:D:852:GLN:HE22	1.67	0.60
1:A:741:LEU:O	1:B:772:PRO:HA	2.02	0.60
1:B:362:VAL:HG22	1:B:388:LEU:HB2	1.84	0.60
1:D:998:ILE:CG2	1:D:1001:CYS:HB2	2.32	0.60
1:A:673:HIS:O	1:A:675:MET:N	2.34	0.59
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.85	0.59
1:A:651:MET:CE	1:A:700:GLN:HG3	2.32	0.59
1:D:261:LEU:HD21	1:D:451:LEU:CD2	2.33	0.59
1:B:608:LEU:CD1	1:B:742:MET:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:HD23	1:D:119:ASP:HB2	1.84	0.59
1:C:410:ARG:HH12	1:D:427:VAL:HA	1.66	0.59
1:D:621:TRP:O	1:D:625:VAL:HG23	2.02	0.59
1:D:641:ILE:HB	1:D:653:LEU:CD2	2.32	0.59
1:A:301:GLN:O	1:A:403:ILE:HG13	2.03	0.59
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.38	0.59
1:C:477:PHE:CE1	1:C:503:ILE:HG12	2.37	0.59
1:D:373:VAL:HG22	1:D:376:GLU:HB2	1.85	0.59
1:A:192:LEU:HG	1:A:280:PHE:HB3	1.84	0.58
1:A:50:PHE:CE2	1:B:369:ASN:HA	2.38	0.58
1:A:368:VAL:HG13	1:B:384:LYS:HD2	1.84	0.58
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.85	0.58
1:A:193:LEU:HD22	1:A:193:LEU:N	2.18	0.58
1:C:846:LEU:HD22	1:C:849:TRP:CE2	2.37	0.58
1:B:342:ASP:CB	5:B:1032:NDP:H42N	2.33	0.58
1:B:42:LYS:HE3	1:B:44:ASN:OD1	2.03	0.58
1:C:410:ARG:HE	1:D:410:ARG:CZ	2.16	0.58
1:A:489:THR:O	1:A:493:VAL:HG23	2.04	0.58
1:B:136:CYS:SG	1:B:137:VAL:N	2.77	0.58
1:B:916:LYS:HG3	1:B:917:PRO:HD2	1.84	0.58
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.39	0.58
1:A:248:MET:HE1	1:A:255:ILE:HD11	1.86	0.58
1:A:189:LYS:HB3	1:A:276:TYR:CD2	2.39	0.58
1:A:962:THR:CG2	1:A:991:LEU:HB3	2.33	0.58
1:B:80:LEU:HD11	1:B:142:LEU:HD21	1.85	0.58
1:C:732:VAL:HG22	1:C:788:PHE:CE2	2.38	0.58
1:C:82:CYS:O	1:C:98:LYS:HD2	2.03	0.58
1:A:394:ARG:HG3	1:A:409:VAL:HG13	1.86	0.57
1:B:687:ASP:HB3	1:B:690:LEU:CD1	2.33	0.57
1:B:744:LEU:HD23	1:B:750:PRO:HA	1.85	0.57
1:C:394:ARG:HG3	1:C:409:VAL:CG1	2.34	0.57
1:C:458:ARG:HG2	1:C:458:ARG:HH11	1.68	0.57
1:D:342:ASP:CB	5:D:1032:NDP:H42N	2.33	0.57
1:A:451:LEU:HB3	1:A:454:ILE:CD1	2.34	0.57
1:C:451:LEU:O	1:C:454:ILE:HG12	2.05	0.57
1:C:561:ARG:NE	1:D:6:SER:O	2.34	0.57
1:D:806:LEU:HD23	1:D:810:ALA:O	2.04	0.57
1:D:87:CYS:SG	1:D:88:GLN:N	2.76	0.57
1:B:982:VAL:HG13	2:B:1029:SF4:S2	2.44	0.57
1:D:997:PRO:HD2	2:D:1028:SF4:S3	2.45	0.57
1:B:722:ARG:O	1:B:726:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLU:OE2	1:C:887:LYS:O	2.23	0.57
1:D:294:PHE:HB3	1:D:303:PHE:CZ	2.40	0.57
1:A:947:VAL:O	1:A:947:VAL:HG13	2.05	0.57
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.35	0.57
1:D:962:THR:HG21	1:D:995:VAL:HG21	1.87	0.57
1:C:745:LYS:HG3	1:C:749:THR:OG1	2.05	0.57
1:D:124:LEU:HD11	1:D:161:GLU:HG2	1.86	0.57
1:D:262:SER:OG	1:D:446:LYS:HB3	2.04	0.57
1:C:772:PRO:HA	1:D:741:LEU:O	2.05	0.57
1:D:738:VAL:HG21	1:D:773:ILE:HD12	1.85	0.57
1:A:12:ILE:O	1:A:15:ILE:HG22	2.05	0.57
1:C:270:THR:O	1:C:274:GLU:HG3	2.05	0.57
1:C:410:ARG:NH2	1:D:410:ARG:NH1	2.52	0.57
1:D:956:CYS:SG	1:D:958:LYS:HG3	2.44	0.57
1:B:738:VAL:HG21	1:B:773:ILE:HD12	1.87	0.57
1:C:337:VAL:HB	1:C:361:LEU:HD23	1.86	0.57
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.87	0.57
1:C:108:ASN:HA	1:C:852:GLN:HE22	1.67	0.57
1:A:337:VAL:HB	1:A:361:LEU:HD23	1.87	0.56
1:C:844:GLU:O	1:C:847:GLN:HG3	2.05	0.56
1:A:259:LYS:HB3	1:A:266:ILE:HD11	1.87	0.56
1:A:2:ALA:O	1:A:3:PRO:O	2.23	0.56
1:B:608:LEU:C	1:B:608:LEU:HD23	2.25	0.56
1:C:501:TRP:CZ2	1:C:519:PRO:HA	2.39	0.56
1:D:100:PHE:C	1:D:100:PHE:CD1	2.78	0.56
1:B:305:THR:O	1:B:306:SER:C	2.44	0.56
1:D:130:CYS:SG	1:D:490:VAL:HB	2.46	0.56
1:C:642:MET:HB2	1:C:668:ASN:HB3	1.88	0.56
1:A:19:ASN:OD1	1:A:20:PRO:HD2	2.05	0.56
1:B:124:LEU:HD13	1:B:160:SER:HB2	1.85	0.56
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	1.88	0.56
1:C:410:ARG:HH21	1:D:410:ARG:CZ	2.18	0.56
1:D:709:LYS:HG3	1:D:733:THR:CG2	2.36	0.56
1:B:410:ARG:HD2	1:B:425:GLN:OE1	2.05	0.56
1:C:823:ASP:O	1:C:826:VAL:HG22	2.06	0.56
1:C:9:VAL:CG2	1:C:12:ILE:HG12	2.36	0.56
1:D:283:ILE:CG1	1:D:482:ILE:HD13	2.35	0.56
1:A:368:VAL:CG1	1:B:384:LYS:HD2	2.36	0.56
1:B:342:ASP:HB2	5:B:1032:NDP:C5N	2.36	0.56
1:B:993:LEU:HD23	1:B:993:LEU:O	2.05	0.56
1:A:734:ALA:HB1	1:A:735:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LEU:HG	1:D:623:GLN:HE22	1.71	0.56
1:C:741:LEU:O	1:D:772:PRO:HA	2.05	0.56
1:C:5:LEU:HG	1:D:623:GLN:NE2	2.20	0.56
1:A:464:VAL:HG12	1:A:471:THR:HG22	1.87	0.56
1:B:997:PRO:HD2	2:B:1028:SF4:S3	2.46	0.56
1:B:238:TYR:HB2	1:B:318:LYS:HD3	1.87	0.56
1:C:193:LEU:N	1:C:193:LEU:HD22	2.21	0.56
1:A:97:ILE:HA	1:A:100:PHE:CD2	2.41	0.55
1:C:410:ARG:HH12	1:D:427:VAL:HG22	1.71	0.55
1:A:779:THR:CG2	1:A:808:SER:HB3	2.37	0.55
1:C:519:PRO:HB3	1:D:28:LEU:HD22	1.87	0.55
1:D:451:LEU:HB3	1:D:454:ILE:CD1	2.36	0.55
1:D:709:LYS:HA	1:D:733:THR:HB	1.89	0.55
1:C:616:LYS:HB2	1:C:621:TRP:HE1	1.72	0.55
1:D:408:PHE:HB2	1:D:427:VAL:HB	1.89	0.55
1:C:427:VAL:CG1	1:D:410:ARG:HE	2.19	0.55
1:D:792:ALA:HB1	1:D:805:PHE:CD2	2.41	0.55
1:B:261:LEU:HD12	1:B:266:ILE:O	2.06	0.55
1:D:573:THR:HB	1:D:621:TRP:CE3	2.42	0.55
1:D:714:VAL:HG21	1:D:720:ILE:HD11	1.88	0.55
1:B:189:LYS:HB3	1:B:276:TYR:CD2	2.42	0.55
1:B:651:MET:CE	1:B:700:GLN:HG2	2.37	0.55
1:B:948:ILE:HD13	1:B:980:PRO:HG2	1.89	0.55
1:C:147:GLU:OE1	1:C:147:GLU:N	2.36	0.55
1:C:97:ILE:HD13	1:C:152:ILE:HD13	1.88	0.55
1:B:44:ASN:HB2	1:B:45:PRO:HD2	1.89	0.55
1:C:996:CYS:HA	2:C:1028:SF4:S3	2.47	0.55
1:D:315:LYS:HA	1:D:321:MET:SD	2.47	0.55
1:D:444:ASP:OD1	1:D:446:LYS:HB2	2.07	0.55
1:C:62:ILE:HD11	1:C:379:LEU:HD13	1.89	0.54
1:D:451:LEU:HD12	1:D:456:PHE:HZ	1.70	0.54
1:B:104:ILE:HD11	1:B:159:ALA:HB2	1.89	0.54
1:C:1009:THR:CG2	1:C:1010:PRO:HD2	2.37	0.54
1:D:606:SER:HB2	1:D:766:SER:O	2.07	0.54
1:A:759:ARG:HH21	1:B:933:GLY:HA3	1.72	0.54
1:B:623:GLN:O	1:B:627:GLU:HG3	2.06	0.54
1:B:699:ARG:HA	1:B:699:ARG:NE	2.22	0.54
1:B:164:LYS:HD2	1:B:243:PHE:CG	2.43	0.54
1:C:19:ASN:OD1	1:C:20:PRO:HD2	2.08	0.54
1:C:228:THR:HG23	1:C:238:TYR:CD1	2.42	0.54
1:C:933:GLY:HA3	1:D:759:ARG:NH2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD13	1:A:160:SER:HB2	1.88	0.54
1:A:394:ARG:HG3	1:A:409:VAL:CG1	2.38	0.54
1:A:709:LYS:HG3	1:A:733:THR:CG2	2.38	0.54
1:A:997:PRO:HD2	2:A:1028:SF4:S3	2.47	0.54
1:B:62:ILE:CD1	1:B:379:LEU:HD13	2.36	0.54
1:C:164:LYS:HD2	1:C:243:PHE:CG	2.43	0.54
1:D:656:LYS:O	1:D:659:ALA:HB3	2.08	0.54
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.88	0.54
1:D:886:ARG:O	1:D:890:ILE:HG13	2.08	0.54
1:C:97:ILE:HA	1:C:100:PHE:CD2	2.42	0.54
1:A:193:LEU:HD23	1:A:281:ILE:HD13	1.89	0.54
1:B:947:VAL:O	1:B:947:VAL:HG13	2.08	0.54
1:B:956:CYS:SG	1:B:958:LYS:HG3	2.48	0.54
1:C:651:MET:HE3	1:C:700:GLN:HG3	1.88	0.54
1:A:699:ARG:NE	1:A:699:ARG:HA	2.23	0.54
1:C:67:LEU:HD13	1:C:72:ALA:HA	1.90	0.54
1:D:136:CYS:SG	1:D:137:VAL:N	2.81	0.54
1:B:465:ASP:HB3	1:B:468:THR:OG1	2.08	0.53
1:C:145:THR:OG1	1:C:147:GLU:HG2	2.07	0.53
1:D:211:TYR:HE2	1:D:507:ILE:HG21	1.73	0.53
1:D:709:LYS:HG3	1:D:733:THR:HG22	1.90	0.53
1:C:219:LYS:HG3	1:C:260:SER:OG	2.08	0.53
1:C:708:ALA:HB3	1:C:732:VAL:HG12	1.90	0.53
1:A:709:LYS:HG3	1:A:733:THR:HG22	1.89	0.53
1:B:80:LEU:HD11	1:B:142:LEU:CD2	2.39	0.53
1:B:575:THR:HA	1:B:640:SER:O	2.08	0.53
1:B:962:THR:OG1	1:B:995:VAL:HG21	2.07	0.53
1:C:827:ILE:HG23	1:C:828:GLN:N	2.24	0.53
1:A:470:GLN:NE2	1:A:474:PRO:HA	2.24	0.53
1:B:468:THR:HA	1:B:502:TYR:CD1	2.44	0.53
1:C:311:PRO:O	1:C:315:LYS:HG3	2.08	0.53
1:D:162:VAL:O	1:D:166:MET:HG3	2.08	0.53
1:C:589:ARG:HD2	1:C:611:GLU:HB2	1.91	0.53
1:A:651:MET:HE3	1:A:700:GLN:HG3	1.90	0.53
1:A:32:LEU:HB2	1:B:485:MET:CE	2.39	0.53
1:B:647:LYS:O	1:B:651:MET:HG3	2.09	0.53
1:D:608:LEU:CD1	1:D:742:MET:HB2	2.36	0.53
1:C:136:CYS:SG	1:C:152:ILE:HD12	2.48	0.53
1:D:404:VAL:O	1:D:405:ALA:HB2	2.08	0.53
1:D:990:THR:HG22	1:D:990:THR:O	2.07	0.53
1:D:267:THR:OG1	1:D:270:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:PHE:O	1:D:391:LEU:HD23	2.09	0.53
1:B:78:ARG:NH2	1:B:150:ILE:HD13	2.24	0.53
1:A:410:ARG:NH2	1:B:427:VAL:HG21	2.23	0.52
1:D:218:GLU:OE1	4:D:1031:FAD:H1B	2.09	0.52
1:C:999:ILE:O	1:C:1000:ASP:HB2	2.09	0.52
1:A:956:CYS:SG	1:A:958:LYS:HG3	2.49	0.52
1:C:642:MET:HA	1:C:650:TRP:CH2	2.45	0.52
1:D:470:GLN:NE2	1:D:474:PRO:HA	2.24	0.52
1:B:230:GLU:HG2	1:B:310:LEU:HB2	1.92	0.52
1:A:410:ARG:NE	1:B:410:ARG:NH2	2.56	0.52
1:D:78:ARG:CZ	1:D:150:ILE:HD13	2.39	0.52
1:D:379:LEU:O	1:D:383:GLU:HG3	2.10	0.52
1:B:489:THR:O	1:B:493:VAL:HG23	2.10	0.52
1:C:53:GLU:HG2	1:C:54:LYS:N	2.25	0.52
1:C:942:GLU:OE2	1:D:756:ALA:N	2.39	0.52
1:D:451:LEU:O	1:D:454:ILE:HG12	2.10	0.52
1:D:842:SER:CB	1:D:918:ILE:HD13	2.37	0.52
1:A:944:VAL:HG22	1:B:587:SER:OG	2.09	0.52
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.92	0.52
1:B:831:CYS:O	1:B:835:LYS:HG3	2.09	0.52
1:A:136:CYS:SG	1:A:137:VAL:N	2.83	0.52
1:A:990:THR:O	1:A:990:THR:HG22	2.09	0.52
1:C:465:ASP:HB3	1:C:468:THR:OG1	2.10	0.52
1:C:89:LYS:HD2	1:D:41:TRP:CE2	2.45	0.52
1:D:783:ARG:HG3	1:D:929:LEU:HD22	1.91	0.52
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.91	0.52
1:B:971:ILE:HG13	2:B:1029:SF4:S2	2.50	0.52
1:D:451:LEU:HB3	1:D:454:ILE:HD11	1.91	0.52
1:A:831:CYS:O	1:A:835:LYS:HG3	2.10	0.51
1:A:772:PRO:HA	1:B:741:LEU:O	2.09	0.51
1:C:1009:THR:HG22	1:C:1010:PRO:HD2	1.92	0.51
1:C:410:ARG:NH1	1:D:427:VAL:CG1	2.66	0.51
1:C:622:CYS:O	1:C:660:SER:HB2	2.09	0.51
1:A:136:CYS:SG	1:A:152:ILE:HD12	2.50	0.51
1:A:575:THR:HA	1:A:640:SER:O	2.10	0.51
1:B:9:VAL:HG22	1:B:12:ILE:HG12	1.91	0.51
1:B:779:THR:CG2	1:B:808:SER:HB3	2.39	0.51
1:B:82:CYS:O	1:B:98:LYS:HD2	2.10	0.51
1:D:398:VAL:HG13	1:D:402:ARG:O	2.09	0.51
1:B:331:ILE:HG23	1:B:433:VAL:HG21	1.91	0.51
1:B:948:ILE:HD13	1:B:980:PRO:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:THR:HA	1:C:640:SER:HB3	1.92	0.51
1:A:485:MET:HE1	1:B:32:LEU:HB2	1.92	0.51
1:B:647:LYS:HA	1:B:697:TRP:CE3	2.46	0.51
1:B:647:LYS:HG3	1:B:697:TRP:CG	2.45	0.51
1:C:100:PHE:O	1:C:104:ILE:HG13	2.10	0.51
1:C:342:ASP:CB	5:C:1032:NDP:H42N	2.39	0.51
1:C:664:ALA:HB1	1:C:705:PRO:O	2.11	0.51
1:D:394:ARG:HG3	1:D:409:VAL:CG1	2.39	0.51
1:D:477:PHE:CD1	1:D:503:ILE:HG12	2.45	0.51
1:D:945:VAL:HB	1:D:986:CYS:SG	2.50	0.51
1:A:673:HIS:CE1	1:A:675:MET:CB	2.94	0.51
1:A:992:CYS:SG	1:A:993:LEU:N	2.84	0.51
1:C:959:CYS:SG	1:C:960:TYR:N	2.84	0.51
1:A:776:ARG:HH11	1:A:776:ARG:HG2	1.74	0.51
1:B:846:LEU:HD22	1:B:849:TRP:CE2	2.45	0.51
1:D:243:PHE:CZ	1:D:247:LEU:HD11	2.46	0.51
1:A:288:PRO:HB3	1:A:307:LYS:HB2	1.92	0.51
1:A:573:THR:HB	1:A:621:TRP:CE3	2.46	0.51
1:A:80:LEU:CD1	1:B:954:ILE:HD11	2.40	0.51
1:C:616:LYS:HD3	1:C:620:TYR:CE2	2.46	0.51
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.92	0.51
1:A:933:GLY:HA3	1:B:759:ARG:NH2	2.25	0.50
1:C:577:SER:HA	1:C:653:LEU:HD21	1.92	0.50
1:D:19:ASN:OD1	1:D:964:ASN:ND2	2.38	0.50
1:B:486:ALA:C	1:B:487:ASN:HD22	2.13	0.50
1:D:219:LYS:HG3	1:D:260:SER:OG	2.10	0.50
1:D:578:LEU:HD23	1:D:653:LEU:HD13	1.93	0.50
1:A:909:ARG:HH11	1:A:909:ARG:HG3	1.76	0.50
1:B:271:LEU:HD22	1:B:276:TYR:CD1	2.47	0.50
1:C:90:SER:HB3	1:C:135:LEU:O	2.11	0.50
1:C:342:ASP:CB	5:C:1032:NDP:C5N	2.88	0.50
1:D:124:LEU:CD2	1:D:240:VAL:HG13	2.34	0.50
1:A:108:ASN:HA	1:A:852:GLN:NE2	2.26	0.50
1:A:699:ARG:HE	1:A:699:ARG:HA	1.76	0.50
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.94	0.50
1:C:997:PRO:HD2	2:C:1028:SF4:S3	2.52	0.50
1:D:658:GLU:HB2	1:D:704:ILE:HD11	1.94	0.50
1:D:962:THR:HG21	1:D:995:VAL:HG11	1.94	0.50
1:A:485:MET:CE	1:B:32:LEU:HB2	2.41	0.50
1:B:886:ARG:O	1:B:890:ILE:HG13	2.12	0.50
1:C:991:LEU:O	1:C:995:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:THR:O	1:D:306:SER:C	2.50	0.50
1:C:132:THR:HB	1:C:137:VAL:HG23	1.94	0.50
1:C:294:PHE:HZ	1:C:338:LEU:HD12	1.77	0.50
1:D:470:GLN:HB2	1:D:477:PHE:CE2	2.46	0.50
1:D:578:LEU:HD21	1:D:653:LEU:HB2	1.92	0.50
1:B:201:SER:HB2	1:B:493:VAL:HG13	1.93	0.50
1:B:622:CYS:O	1:B:660:SER:HB2	2.11	0.50
1:C:768:THR:HG22	1:C:771:ARG:NH2	2.27	0.50
1:B:140:CYS:HA	2:B:1027:SF4:S3	2.52	0.49
1:B:487:ASN:N	1:B:487:ASN:ND2	2.56	0.49
1:C:53:GLU:CG	1:C:54:LYS:N	2.75	0.49
1:C:547:GLY:HA3	1:C:570:PHE:CZ	2.47	0.49
1:A:342:ASP:CB	5:A:1032:NDP:C5N	2.90	0.49
1:A:933:GLY:HA3	1:B:759:ARG:HH21	1.77	0.49
1:D:801:SER:O	1:D:804:GLN:HB2	2.11	0.49
1:D:947:VAL:O	1:D:947:VAL:HG13	2.12	0.49
1:A:81:LYS:HD3	1:A:102:THR:OG1	2.12	0.49
1:B:699:ARG:HE	1:B:699:ARG:HA	1.77	0.49
1:D:827:ILE:HG23	1:D:828:GLN:N	2.26	0.49
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.42	0.49
1:A:759:ARG:NH2	1:B:933:GLY:HA3	2.28	0.49
1:C:315:LYS:HA	1:C:321:MET:SD	2.51	0.49
1:C:845:GLU:H	1:C:845:GLU:CD	2.15	0.49
1:D:457:ASN:HB3	1:D:463:GLU:OE1	2.12	0.49
1:A:673:HIS:CE1	1:A:675:MET:HB3	2.48	0.49
1:B:285:LEU:HG	1:B:481:ASP:HB3	1.94	0.49
1:B:87:CYS:SG	1:B:88:GLN:N	2.85	0.49
1:D:362:VAL:HG22	1:D:388:LEU:HB2	1.94	0.49
1:D:396:VAL:HG13	1:D:403:ILE:CD1	2.42	0.49
1:D:557:SER:HB3	1:D:624:SER:HB3	1.94	0.49
1:D:815:VAL:HG12	1:D:816:CYS:N	2.27	0.49
1:D:103:SER:HA	1:D:829:ASP:OD1	2.12	0.49
1:D:842:SER:OG	1:D:914:PRO:HB3	2.12	0.49
1:A:67:LEU:HD13	1:A:72:ALA:HA	1.95	0.49
1:A:1007:ARG:HG2	1:A:1009:THR:O	2.12	0.49
1:B:130:CYS:SG	1:B:490:VAL:HB	2.52	0.49
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.95	0.49
1:C:699:ARG:NE	1:C:699:ARG:HA	2.28	0.49
1:C:990:THR:O	1:C:990:THR:HG22	2.13	0.49
1:D:56:GLU:OE2	1:D:898:LYS:NZ	2.43	0.49
1:A:97:ILE:HG22	1:A:101:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:ILE:HB	1:A:871:LEU:HD12	1.94	0.49
1:A:962:THR:OG1	1:A:995:VAL:HG21	2.12	0.49
1:C:621:TRP:O	1:C:625:VAL:HG23	2.12	0.49
1:D:909:ARG:HG2	1:D:909:ARG:HH11	1.78	0.49
1:A:793:THR:HB	1:A:814:GLN:HB2	1.94	0.49
1:C:582:ILE:HD11	1:D:1015:ARG:HH11	1.78	0.49
1:A:971:ILE:HG13	2:A:1029:SF4:S4	2.53	0.48
1:D:189:LYS:HB3	1:D:276:TYR:CD2	2.47	0.48
1:A:122:LEU:HD22	1:A:493:VAL:HG22	1.96	0.48
1:C:77:MET:SD	1:D:598:PRO:HG2	2.53	0.48
1:C:954:ILE:HD11	1:D:80:LEU:CD1	2.42	0.48
1:D:193:LEU:HD22	1:D:193:LEU:N	2.28	0.48
1:D:545:PRO:O	1:D:570:PHE:HE2	1.95	0.48
1:B:732:VAL:HG13	1:B:788:PHE:CE2	2.48	0.48
1:C:367:PHE:HB2	1:D:386:GLU:OE1	2.13	0.48
1:A:776:ARG:O	1:A:780:THR:HG22	2.13	0.48
1:C:932:LEU:HD21	1:D:741:LEU:HD11	1.96	0.48
1:C:992:CYS:SG	1:C:993:LEU:N	2.86	0.48
1:D:97:ILE:HD13	1:D:152:ILE:HD13	1.95	0.48
1:A:220:GLN:HG3	1:A:222:TYR:CZ	2.48	0.48
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.13	0.48
1:A:573:THR:O	1:A:574:LYS:C	2.52	0.48
1:A:779:THR:HG22	1:A:808:SER:CB	2.42	0.48
1:A:410:ARG:CZ	1:B:410:ARG:CZ	2.92	0.48
1:C:1019:LEU:HD21	1:D:617:THR:HG22	1.96	0.48
1:C:933:GLY:HA3	1:D:759:ARG:HH21	1.78	0.48
1:D:42:LYS:HE3	1:D:44:ASN:OD1	2.14	0.48
1:A:270:THR:O	1:A:274:GLU:HG3	2.13	0.48
1:A:608:LEU:CD1	1:A:742:MET:HB2	2.36	0.48
1:B:453:PRO:HG2	1:B:473:GLU:OE1	2.14	0.48
1:B:642:MET:HB2	1:B:668:ASN:HB3	1.96	0.48
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.43	0.48
1:D:410:ARG:NH1	1:D:410:ARG:CG	2.70	0.48
1:D:647:LYS:O	1:D:651:MET:HG3	2.14	0.48
1:B:408:PHE:HB2	1:B:427:VAL:HB	1.95	0.48
1:B:485:MET:O	1:B:487:ASN:ND2	2.46	0.48
1:D:288:PRO:HB3	1:D:307:LYS:HB2	1.96	0.48
1:D:750:PRO:HG3	1:D:760:THR:HG22	1.95	0.48
1:D:546:PHE:CE1	1:D:830:TYR:HB3	2.49	0.48
1:C:343:THR:HG23	4:C:1031:FAD:HM73	1.95	0.48
1:C:487:ASN:O	5:C:1032:NDP:H1D	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:LYS:O	1:C:651:MET:HG3	2.13	0.48
1:C:608:LEU:CD1	1:C:742:MET:HB2	2.37	0.48
1:D:699:ARG:HE	1:D:699:ARG:CA	2.25	0.48
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.95	0.48
1:A:768:THR:HG22	1:A:771:ARG:NH2	2.28	0.48
1:B:108:ASN:HA	1:B:852:GLN:HE22	1.79	0.48
1:B:371:ARG:HE	1:B:371:ARG:HB2	1.32	0.48
1:B:801:SER:O	1:B:804:GLN:HB2	2.14	0.48
1:C:828:GLN:O	1:C:832:THR:HG23	2.14	0.48
1:C:845:GLU:HG3	1:C:912:PHE:CE2	2.49	0.48
1:D:142:LEU:HD12	1:D:150:ILE:HD11	1.95	0.48
1:A:230:GLU:HG2	1:A:310:LEU:HB2	1.96	0.48
1:A:989:CYS:O	1:A:990:THR:HB	2.14	0.48
1:D:664:ALA:O	1:D:665:LEU:HD23	2.14	0.48
1:A:291:ASP:OD1	1:A:292:ASP:N	2.47	0.47
1:A:305:THR:O	1:A:306:SER:C	2.52	0.47
1:C:963:CYS:HA	1:C:967:GLY:HA3	1.96	0.47
1:D:608:LEU:HD21	1:D:763:GLY:HA3	1.96	0.47
1:D:771:ARG:N	1:D:772:PRO:CD	2.77	0.47
1:B:288:PRO:HB3	1:B:307:LYS:HB2	1.95	0.47
1:B:81:LYS:HD3	1:B:102:THR:OG1	2.14	0.47
1:A:685:GLY:O	1:A:720:ILE:HD12	2.13	0.47
1:C:776:ARG:HB2	1:D:740:GLY:HA2	1.96	0.47
1:B:263:GLU:O	1:B:264:ASN:HB2	2.14	0.47
1:B:807:HIS:HB3	1:B:928:ALA:HB2	1.95	0.47
1:C:557:SER:HB3	1:C:624:SER:HB3	1.97	0.47
1:A:651:MET:HE1	1:A:700:GLN:HG3	1.96	0.47
1:B:332:ARG:HG2	1:B:332:ARG:HH11	1.79	0.47
1:B:747:ASP:CG	1:B:749:THR:HG23	2.35	0.47
1:B:845:GLU:H	1:B:845:GLU:CD	2.15	0.47
1:C:124:LEU:CD2	1:C:240:VAL:HG13	2.43	0.47
1:C:261:LEU:HD21	1:C:451:LEU:CD2	2.44	0.47
1:C:810:ALA:O	1:C:925:ILE:HG23	2.14	0.47
1:D:449:GLU:C	1:D:451:LEU:H	2.17	0.47
1:D:642:MET:HB2	1:D:668:ASN:HB3	1.96	0.47
1:B:261:LEU:HD21	1:B:451:LEU:HD21	1.96	0.47
1:C:87:CYS:SG	1:C:88:GLN:N	2.88	0.47
1:A:371:ARG:HB2	1:A:371:ARG:NH1	2.30	0.47
1:B:533:ILE:O	1:B:545:PRO:HD3	2.14	0.47
1:C:651:MET:HE1	1:C:700:GLN:HG3	1.96	0.47
1:A:97:ILE:HA	1:A:100:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LYS:HA	1:A:733:THR:HB	1.97	0.47
1:A:989:CYS:O	1:A:990:THR:CB	2.61	0.47
1:B:83:ALA:O	1:B:84:ASP:C	2.53	0.47
1:C:521:LEU:HA	1:C:522:PRO:HD3	1.79	0.47
1:C:62:ILE:CD1	1:C:379:LEU:HD13	2.44	0.47
1:D:307:LYS:O	1:D:311:PRO:HG2	2.14	0.47
1:D:744:LEU:HD23	1:D:750:PRO:HA	1.95	0.47
1:A:408:PHE:HB2	1:A:427:VAL:HB	1.97	0.47
1:A:738:VAL:HG21	1:A:773:ILE:HD12	1.97	0.47
1:A:909:ARG:NH1	1:A:909:ARG:HG3	2.29	0.47
1:B:622:CYS:HB3	1:B:660:SER:HB3	1.96	0.47
1:D:108:ASN:ND2	1:D:111:GLY:HA3	2.29	0.47
1:C:410:ARG:HH12	1:D:427:VAL:CA	2.27	0.47
1:D:454:ILE:HA	1:D:472:SER:OG	2.15	0.47
1:D:568:TRP:CE2	1:D:827:ILE:HB	2.49	0.47
1:C:292:ASP:O	1:C:294:PHE:N	2.48	0.47
1:A:386:GLU:OE2	1:B:368:VAL:HG23	2.15	0.47
1:A:699:ARG:HE	1:A:699:ARG:CA	2.29	0.47
1:B:46:ASP:HB3	1:B:49:CYS:HB2	1.96	0.47
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.15	0.47
1:A:827:ILE:HG23	1:A:828:GLN:N	2.29	0.46
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.50	0.46
1:C:267:THR:HG23	1:C:450:ALA:HA	1.96	0.46
1:C:301:GLN:O	1:C:403:ILE:HG13	2.15	0.46
1:C:806:LEU:CD2	1:C:813:LEU:HD21	2.45	0.46
1:D:687:ASP:HB3	1:D:690:LEU:HD12	1.96	0.46
1:B:451:LEU:O	1:B:454:ILE:HG23	2.15	0.46
1:B:193:LEU:N	1:B:193:LEU:HD22	2.30	0.46
1:B:63:LYS:HE3	1:B:128:MET:HG2	1.97	0.46
1:B:103:SER:HA	1:B:829:ASP:OD1	2.15	0.46
1:A:477:PHE:CD1	1:A:503:ILE:HG12	2.51	0.46
1:C:943:GLN:HG3	1:C:1011:TYR:CD2	2.51	0.46
1:D:557:SER:CB	1:D:624:SER:HB3	2.46	0.46
1:D:921:ILE:O	1:D:924:VAL:HG22	2.15	0.46
1:C:345:PHE:CE2	1:C:361:LEU:HD13	2.51	0.46
1:C:443:ARG:O	1:C:444:ASP:C	2.54	0.46
1:C:971:ILE:HG13	2:C:1029:SF4:S4	2.56	0.46
1:A:100:PHE:C	1:A:100:PHE:CD1	2.88	0.46
1:B:824:PHE:O	1:B:827:ILE:HG22	2.16	0.46
1:C:124:LEU:HD13	1:C:160:SER:HB2	1.97	0.46
1:C:70:ARG:HH22	1:D:147:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:CYS:SG	1:B:152:ILE:HD12	2.55	0.46
1:C:262:SER:OG	1:C:263:GLU:N	2.49	0.46
1:C:410:ARG:HH11	1:D:427:VAL:HG13	1.76	0.46
1:D:959:CYS:SG	1:D:960:TYR:N	2.88	0.46
1:A:823:ASP:HB2	1:B:965:ASP:OD2	2.16	0.46
1:A:896:ARG:NH2	1:A:900:GLN:HE22	2.02	0.46
1:C:97:ILE:HD11	2:C:1026:SF4:S4	2.56	0.46
1:D:388:LEU:HD12	1:D:429:LEU:HD21	1.97	0.46
1:D:641:ILE:HB	1:D:653:LEU:HD21	1.98	0.46
1:A:457:ASN:HB3	1:A:463:GLU:OE1	2.16	0.46
1:A:103:SER:HA	1:A:829:ASP:OD1	2.16	0.46
1:C:132:THR:HB	1:C:137:VAL:CG2	2.45	0.46
1:C:575:THR:HA	1:C:640:SER:O	2.16	0.46
1:D:291:ASP:OD1	1:D:292:ASP:N	2.49	0.46
1:B:142:LEU:HD22	1:B:145:THR:HG21	1.98	0.46
1:B:699:ARG:HE	1:B:699:ARG:CA	2.29	0.46
1:C:218:GLU:OE1	4:C:1031:FAD:H1B	2.16	0.46
1:C:410:ARG:HH21	1:D:410:ARG:NH1	2.13	0.46
1:D:166:MET:HE1	1:D:840:LEU:HD11	1.97	0.46
1:A:193:LEU:N	1:A:193:LEU:CD2	2.80	0.45
1:A:70:ARG:HG3	1:A:999:ILE:HG13	1.97	0.45
1:B:548:LEU:HD11	1:B:563:ALA:CB	2.46	0.45
1:B:783:ARG:HG3	1:B:929:LEU:HD22	1.98	0.45
1:C:294:PHE:CZ	1:C:338:LEU:HD12	2.51	0.45
1:D:294:PHE:HA	1:D:297:LEU:HD12	1.97	0.45
1:D:297:LEU:HA	1:D:301:GLN:OE1	2.16	0.45
1:D:608:LEU:HD23	1:D:609:ASN:N	2.31	0.45
1:D:962:THR:CG2	1:D:995:VAL:HG21	2.45	0.45
1:C:578:LEU:HD21	1:C:653:LEU:HB2	1.98	0.45
1:C:695:CYS:SG	1:C:729:ALA:HB2	2.56	0.45
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.51	0.45
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.96	0.45
1:A:651:MET:CE	1:A:701:ALA:HB2	2.46	0.45
1:A:734:ALA:HA	1:A:735:THR:HA	1.57	0.45
1:A:750:PRO:HG3	1:A:760:THR:HG22	1.98	0.45
1:B:100:PHE:C	1:B:100:PHE:CD1	2.89	0.45
1:B:379:LEU:O	1:B:383:GLU:HG3	2.15	0.45
1:D:449:GLU:C	1:D:451:LEU:N	2.69	0.45
1:A:248:MET:HE3	1:A:253:VAL:HG11	1.98	0.45
1:A:310:LEU:HB2	1:A:311:PRO:HD3	1.98	0.45
1:B:205:PHE:CZ	1:B:497:LYS:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:VAL:HG12	1:B:471:THR:HG22	1.98	0.45
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.51	0.45
1:C:208:ARG:HB3	1:C:522:PRO:HB2	1.98	0.45
1:A:587:SER:HA	1:A:588:PRO:C	2.36	0.45
1:B:373:VAL:HG22	1:B:376:GLU:HB3	1.98	0.45
1:C:544:ASN:HD21	1:C:569:GLY:N	2.14	0.45
1:D:958:LYS:HB2	2:D:1028:SF4:S3	2.57	0.45
1:C:34:LYS:HG3	1:D:92:PRO:HA	1.99	0.45
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.57	0.45
1:A:488:THR:OG1	1:A:491:GLU:HG3	2.17	0.45
1:A:710:LEU:HD11	1:A:732:VAL:HG11	1.98	0.45
1:A:608:LEU:HA	1:A:764:GLY:O	2.17	0.45
1:C:791:LEU:HB3	1:C:814:GLN:HE21	1.81	0.45
1:C:877:PRO:CG	1:C:977:THR:HB	2.46	0.45
1:C:962:THR:HG21	1:C:991:LEU:HB3	1.97	0.45
1:D:982:VAL:HG13	2:D:1029:SF4:S4	2.56	0.45
1:A:129:VAL:O	1:A:130:CYS:C	2.54	0.45
1:A:130:CYS:SG	1:A:490:VAL:HB	2.56	0.45
1:C:485:MET:HE3	1:D:32:LEU:HB2	1.99	0.45
1:C:734:ALA:HA	1:C:735:THR:HA	1.64	0.45
1:D:859:HIS:HA	1:D:865:VAL:HG23	1.98	0.45
1:A:28:LEU:HD22	1:B:519:PRO:HB3	1.97	0.45
1:A:791:LEU:HD12	1:A:791:LEU:N	2.32	0.45
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.69	0.45
1:A:773:ILE:HD11	1:B:738:VAL:HG11	1.98	0.45
1:D:375:GLU:CD	1:D:375:GLU:H	2.21	0.45
1:A:622:CYS:O	1:A:660:SER:HB2	2.17	0.45
1:A:877:PRO:HD2	1:A:882:TYR:CD2	2.51	0.45
1:A:87:CYS:SG	1:A:88:GLN:N	2.89	0.45
1:C:744:LEU:HD23	1:C:750:PRO:HA	1.98	0.45
1:C:568:TRP:NE1	1:C:827:ILE:HB	2.31	0.45
1:C:845:GLU:HG3	1:C:912:PHE:CD2	2.52	0.45
1:D:193:LEU:HD23	1:D:281:ILE:HD13	1.99	0.45
1:C:935:PHE:CZ	1:D:612:LEU:HD21	2.51	0.45
1:B:108:ASN:HA	1:B:852:GLN:NE2	2.32	0.44
1:B:328:LEU:O	1:B:329:PRO:C	2.55	0.44
1:B:788:PHE:HA	1:B:789:PRO:HD3	1.84	0.44
1:D:44:ASN:HB2	1:D:45:PRO:CD	2.47	0.44
1:D:267:THR:HG22	1:D:450:ALA:CB	2.47	0.44
1:D:521:LEU:HA	1:D:522:PRO:HD3	1.77	0.44
1:D:929:LEU:HD23	1:D:932:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.98	0.44
1:A:771:ARG:N	1:A:772:PRO:CD	2.80	0.44
1:A:886:ARG:O	1:A:890:ILE:HG13	2.16	0.44
1:B:342:ASP:CB	5:B:1032:NDP:C5N	2.96	0.44
1:C:458:ARG:NH1	1:C:458:ARG:HG2	2.32	0.44
1:C:367:PHE:CE1	1:D:367:PHE:CE1	3.06	0.44
1:D:893:GLU:OE1	1:D:896:ARG:NH1	2.50	0.44
1:A:871:LEU:HG	1:A:889:ILE:HG21	2.00	0.44
1:B:162:VAL:O	1:B:166:MET:HG3	2.18	0.44
1:A:97:ILE:HD11	2:A:1026:SF4:S4	2.58	0.44
1:A:267:THR:HG22	1:A:450:ALA:CB	2.47	0.44
1:A:991:LEU:O	1:A:994:SER:HB2	2.17	0.44
1:B:294:PHE:HA	1:B:297:LEU:CD1	2.46	0.44
1:B:292:ASP:O	1:B:294:PHE:N	2.51	0.44
1:B:298:THR:N	1:B:301:GLN:OE1	2.48	0.44
1:C:140:CYS:SG	1:C:149:SER:HA	2.57	0.44
1:C:375:GLU:CD	1:C:375:GLU:H	2.19	0.44
1:C:410:ARG:HD2	1:C:425:GLN:OE1	2.18	0.44
1:C:959:CYS:SG	1:C:971:ILE:HD13	2.57	0.44
1:D:342:ASP:CB	5:D:1032:NDP:C5N	2.94	0.44
1:D:201:SER:CB	1:D:493:VAL:HG13	2.44	0.44
1:C:773:ILE:HD11	1:D:738:VAL:HG11	1.99	0.44
1:A:734:ALA:HB1	1:A:735:THR:CG2	2.47	0.44
1:A:905:PRO:O	1:A:906:PRO:O	2.35	0.44
1:C:305:THR:O	1:C:306:SER:C	2.56	0.44
1:C:110:TYR:OH	1:C:529:ASP:OD2	2.26	0.44
1:C:56:GLU:OE2	1:C:898:LYS:NZ	2.51	0.44
1:D:192:LEU:N	1:D:192:LEU:HD12	2.32	0.44
1:A:97:ILE:HG22	1:A:101:ILE:HD12	2.00	0.44
1:B:560:ILE:O	1:B:563:ALA:HB3	2.17	0.44
1:B:651:MET:HE1	1:B:700:GLN:HG2	1.98	0.44
1:D:816:CYS:HB3	3:D:1030:FMN:O1P	2.18	0.44
1:A:870:GLU:O	1:A:889:ILE:HD13	2.17	0.44
1:A:968:TYR:O	1:A:969:GLN:C	2.55	0.44
1:B:131:PRO:HB3	1:B:373:VAL:HG11	2.00	0.44
1:A:390:PHE:CE1	1:B:388:LEU:HD21	2.53	0.44
1:C:140:CYS:HA	2:C:1027:SF4:S3	2.58	0.44
1:C:954:ILE:HG23	1:C:998:ILE:HG13	2.00	0.44
1:D:90:SER:CB	1:D:136:CYS:HA	2.48	0.44
1:D:963:CYS:HA	1:D:967:GLY:HA3	1.99	0.44
1:A:142:LEU:HA	1:A:142:LEU:HD23	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:LEU:CD2	1:C:653:LEU:HD13	2.47	0.44
1:D:533:ILE:O	1:D:545:PRO:HD3	2.18	0.44
1:D:779:THR:HG22	1:D:808:SER:HB3	1.99	0.44
1:C:313:VAL:HG13	1:C:328:LEU:HD11	1.99	0.44
1:C:309:PHE:HE1	1:C:331:ILE:HD11	1.81	0.44
1:C:547:GLY:HA3	1:C:570:PHE:CE1	2.52	0.44
1:D:589:ARG:HG3	1:D:590:ILE:HG13	1.99	0.44
1:D:734:ALA:HA	1:D:735:THR:HA	1.62	0.44
1:A:345:PHE:CE2	1:A:361:LEU:HD13	2.52	0.43
1:A:656:LYS:O	1:A:659:ALA:HB3	2.18	0.43
1:B:294:PHE:CA	1:B:297:LEU:HD12	2.45	0.43
1:B:792:ALA:HB1	1:B:805:PHE:CD2	2.53	0.43
1:C:106:ASN:O	1:C:107:LYS:HB2	2.17	0.43
1:C:568:TRP:CE2	1:C:827:ILE:HB	2.53	0.43
1:D:998:ILE:HB	1:D:1001:CYS:HB2	1.99	0.43
1:D:796:ILE:CD1	1:D:813:LEU:HB3	2.48	0.43
1:B:262:SER:O	1:B:263:GLU:C	2.57	0.43
1:B:373:VAL:HG22	1:B:376:GLU:CB	2.47	0.43
1:B:593:GLY:HA3	1:B:606:SER:OG	2.18	0.43
1:C:291:ASP:OD1	1:C:292:ASP:N	2.51	0.43
1:C:521:LEU:O	1:D:25:HIS:HB3	2.18	0.43
1:A:331:ILE:HG23	1:A:433:VAL:HG21	2.00	0.43
1:A:55:LEU:HD13	1:A:353:ARG:NH1	2.34	0.43
1:A:865:VAL:HG11	1:A:951:GLU:OE1	2.18	0.43
1:B:363:PHE:CZ	1:B:370:ILE:HD11	2.53	0.43
1:C:589:ARG:O	1:C:609:ASN:HA	2.18	0.43
1:C:62:ILE:HG21	1:C:353:ARG:HH22	1.83	0.43
1:D:173:ASN:ND2	1:D:175:CYS:HB2	2.32	0.43
1:C:590:ILE:HG21	1:D:991:LEU:HG	1.99	0.43
1:A:131:PRO:CB	1:A:373:VAL:HG11	2.49	0.43
1:A:342:ASP:CB	5:A:1032:NDP:C4N	2.95	0.43
1:A:600:TYR:CE1	1:B:999:ILE:HD11	2.53	0.43
1:B:611:GLU:O	6:B:1035:UAA:H5	2.19	0.43
1:B:146:GLU:N	1:B:146:GLU:OE1	2.45	0.43
1:B:699:ARG:CA	1:B:699:ARG:NE	2.81	0.43
1:B:67:LEU:HD13	1:B:72:ALA:HA	1.98	0.43
1:A:598:PRO:HG2	1:B:77:MET:SD	2.57	0.43
1:B:537:MET:CE	1:B:791:LEU:HD11	2.48	0.43
1:C:439:GLY:HA2	5:C:1032:NDP:O2N	2.19	0.43
1:D:309:PHE:CD2	1:D:435:ILE:HD13	2.53	0.43
1:C:485:MET:CE	1:D:32:LEU:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.78	0.43
1:B:750:PRO:HG3	1:B:760:THR:HG22	2.00	0.43
1:B:954:ILE:HG23	1:B:998:ILE:HG13	1.99	0.43
1:D:108:ASN:HD21	1:D:111:GLY:HA3	1.81	0.43
1:D:454:ILE:HG13	1:D:456:PHE:HE1	1.83	0.43
1:A:500:SER:OG	1:A:501:TRP:N	2.52	0.43
1:A:528:VAL:O	1:A:531:VAL:HG23	2.18	0.43
1:C:788:PHE:HA	1:C:789:PRO:HD3	1.84	0.43
1:D:324:CYS:SG	1:D:325:HIS:N	2.91	0.43
1:D:845:GLU:OE2	1:D:845:GLU:N	2.47	0.43
1:A:379:LEU:O	1:A:383:GLU:HG3	2.18	0.43
1:D:348:ALA:HB2	1:D:361:LEU:HD21	1.99	0.43
1:D:782:ALA:HB1	1:D:929:LEU:HD11	1.99	0.43
1:A:79:CYS:SG	1:A:101:ILE:HG21	2.58	0.43
1:A:63:LYS:HD3	1:A:235:ARG:O	2.19	0.43
1:A:262:SER:O	1:A:264:ASN:N	2.51	0.43
1:A:410:ARG:HH22	1:B:427:VAL:HG21	1.82	0.43
1:A:63:LYS:HE3	1:A:128:MET:CG	2.39	0.43
1:B:353:ARG:HH12	1:B:383:GLU:CD	2.22	0.43
1:B:409:VAL:HG21	1:B:423:GLU:HA	2.00	0.43
1:B:46:ASP:HB3	1:B:49:CYS:CB	2.48	0.43
1:B:557:SER:CB	1:B:624:SER:HB3	2.49	0.43
1:B:771:ARG:N	1:B:772:PRO:CD	2.82	0.43
1:C:217:PHE:CE2	1:C:256:ILE:HD12	2.54	0.43
1:D:935:PHE:CD1	1:D:938:LEU:HD12	2.53	0.43
1:D:997:PRO:CD	2:D:1028:SF4:S3	3.07	0.43
1:A:108:ASN:HA	1:A:852:GLN:HE22	1.84	0.43
1:B:454:ILE:HD12	1:B:462:PRO:HB3	2.01	0.43
1:A:369:ASN:ND2	1:B:50:PHE:CE2	2.82	0.43
1:C:230:GLU:HG2	1:C:310:LEU:HB2	2.00	0.43
1:C:267:THR:HG22	1:C:269:ASN:H	1.83	0.43
1:C:449:GLU:C	1:C:451:LEU:N	2.72	0.43
1:D:622:CYS:SG	1:D:656:LYS:HG2	2.59	0.43
1:A:83:ALA:O	1:A:84:ASP:C	2.55	0.42
1:A:992:CYS:O	1:A:993:LEU:C	2.56	0.42
1:B:106:ASN:O	1:B:107:LYS:HB2	2.19	0.42
1:B:807:HIS:O	1:B:928:ALA:HB3	2.19	0.42
1:C:294:PHE:HZ	1:C:338:LEU:CD1	2.31	0.42
1:C:379:LEU:HA	1:C:379:LEU:HD23	1.91	0.42
1:C:440:SER:O	1:C:441:VAL:HG13	2.19	0.42
1:D:150:ILE:O	1:D:152:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:PHE:CZ	1:D:830:TYR:HB3	2.54	0.42
1:A:572:LEU:HD13	1:A:638:ILE:HB	2.01	0.42
1:B:131:PRO:HG2	1:B:135:LEU:HD11	2.00	0.42
1:A:390:PHE:CD1	1:B:388:LEU:HD21	2.54	0.42
1:B:665:LEU:HB2	1:B:706:PHE:HB2	2.01	0.42
1:C:103:SER:HA	1:C:829:ASP:OD1	2.19	0.42
1:D:305:THR:H	1:D:308:ASP:HB2	1.84	0.42
1:D:779:THR:HG22	1:D:808:SER:CB	2.49	0.42
1:B:622:CYS:SG	1:B:656:LYS:HG2	2.59	0.42
1:B:714:VAL:HG21	1:B:720:ILE:HD11	2.00	0.42
1:B:845:GLU:HG3	1:B:912:PHE:CE1	2.55	0.42
1:C:309:PHE:CE1	1:C:331:ILE:CD1	3.02	0.42
1:A:41:TRP:CZ2	1:B:89:LYS:HD2	2.55	0.42
1:A:647:LYS:O	1:A:651:MET:HG3	2.20	0.42
1:B:646:ASN:C	1:B:646:ASN:OD1	2.58	0.42
1:B:991:LEU:HD23	1:B:991:LEU:HA	1.90	0.42
1:C:905:PRO:HA	1:C:906:PRO:HD3	1.86	0.42
1:D:893:GLU:O	1:D:897:LEU:HG	2.19	0.42
1:A:801:SER:O	1:A:804:GLN:HB2	2.20	0.42
1:B:193:LEU:CD2	1:B:193:LEU:N	2.82	0.42
1:B:2:ALA:O	1:B:3:PRO:O	2.38	0.42
1:C:771:ARG:N	1:C:772:PRO:CD	2.83	0.42
1:C:731:GLY:HA2	1:C:788:PHE:CZ	2.54	0.42
1:D:844:GLU:OE1	1:D:915:LYS:HD2	2.18	0.42
1:A:608:LEU:HB2	1:A:742:MET:CE	2.48	0.42
1:A:965:ASP:O	1:B:553:PRO:HA	2.19	0.42
1:B:248:MET:HE1	1:B:255:ILE:HD11	2.00	0.42
1:C:464:VAL:HG12	1:C:471:THR:HG22	2.02	0.42
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.53	0.42
1:B:554:THR:HG22	1:B:560:ILE:HG12	2.02	0.42
1:B:616:LYS:HD3	1:B:620:TYR:CE2	2.55	0.42
1:C:885:GLN:O	1:C:889:ILE:HG13	2.19	0.42
1:C:910:LYS:HA	1:C:911:PRO:HD3	1.85	0.42
1:D:930:GLN:HG3	1:D:931:TYR:N	2.34	0.42
1:A:260:SER:O	1:A:266:ILE:HB	2.19	0.42
1:A:43:ARG:HB2	1:B:138:GLY:O	2.19	0.42
1:A:651:MET:HE3	1:A:701:ALA:HB2	2.02	0.42
1:A:859:HIS:ND1	1:A:859:HIS:C	2.73	0.42
1:B:589:ARG:HG3	1:B:590:ILE:HG13	2.02	0.42
1:B:692:ARG:HH11	1:B:692:ARG:HB3	1.85	0.42
1:B:939:SER:OG	1:B:941:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:GLU:C	1:C:451:LEU:H	2.23	0.42
1:C:968:TYR:N	1:C:968:TYR:CD1	2.87	0.42
1:A:80:LEU:HD23	1:A:602:PRO:HD3	2.00	0.42
1:C:140:CYS:SG	1:C:149:SER:HB3	2.60	0.42
1:C:560:ILE:HG13	1:C:560:ILE:H	1.73	0.42
1:C:606:SER:HA	1:C:767:GLY:HA3	2.02	0.42
1:D:305:THR:O	1:D:308:ASP:N	2.39	0.42
1:D:413:GLN:HA	1:D:418:LYS:O	2.20	0.42
1:D:972:GLN:O	1:D:980:PRO:HA	2.19	0.42
1:A:132:THR:HB	1:A:137:VAL:HG23	2.02	0.42
1:A:699:ARG:NE	1:A:699:ARG:CA	2.83	0.42
1:A:722:ARG:O	1:A:726:GLU:HG3	2.20	0.42
1:A:82:CYS:O	1:A:98:LYS:HD2	2.19	0.42
1:B:414:ASP:OD1	1:B:414:ASP:C	2.59	0.42
1:A:369:ASN:ND2	1:B:50:PHE:CD2	2.88	0.42
1:C:220:GLN:HG3	1:C:222:TYR:CZ	2.55	0.42
1:C:477:PHE:CE1	1:C:503:ILE:HA	2.55	0.42
1:C:806:LEU:O	1:C:925:ILE:HA	2.20	0.42
1:C:943:GLN:HE22	1:D:586:VAL:HA	1.84	0.42
1:D:699:ARG:NE	1:D:699:ARG:CA	2.81	0.42
1:A:192:LEU:N	1:A:192:LEU:HD12	2.35	0.41
1:B:55:LEU:HD13	1:B:353:ARG:NH1	2.35	0.41
1:B:608:LEU:HA	1:B:764:GLY:O	2.20	0.41
1:C:608:LEU:HB2	1:C:742:MET:HE2	2.02	0.41
1:C:608:LEU:HD13	1:C:742:MET:CB	2.41	0.41
1:D:112:ALA:O	1:D:116:ILE:HG13	2.20	0.41
1:D:342:ASP:CB	5:D:1032:NDP:C4N	2.98	0.41
1:A:152:ILE:H	1:A:152:ILE:HG13	1.65	0.41
1:A:905:PRO:HA	1:A:906:PRO:HD3	1.79	0.41
1:A:947:VAL:O	1:A:947:VAL:CG1	2.68	0.41
1:A:95:LEU:O	1:A:97:ILE:HG13	2.20	0.41
1:A:5:LEU:HG	1:B:623:GLN:NE2	2.36	0.41
1:B:689:GLU:HA	1:B:692:ARG:HH12	1.86	0.41
1:B:959:CYS:SG	1:B:960:TYR:N	2.93	0.41
1:C:587:SER:HA	1:C:588:PRO:C	2.39	0.41
1:C:651:MET:CE	1:C:701:ALA:HB2	2.50	0.41
1:C:709:LYS:HG3	1:C:733:THR:CG2	2.49	0.41
1:B:50:PHE:CD1	1:B:50:PHE:N	2.89	0.41
1:C:750:PRO:HG3	1:C:760:THR:HG22	2.02	0.41
1:D:173:ASN:HD21	1:D:175:CYS:HB2	1.85	0.41
1:D:315:LYS:HG2	1:D:321:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASP:OD1	1:D:372:ALA:HA	2.19	0.41
1:B:958:LYS:HE3	1:B:958:LYS:HB3	1.88	0.41
1:C:142:LEU:HA	1:C:142:LEU:HD23	1.78	0.41
1:C:140:CYS:HB3	1:C:149:SER:HB3	2.02	0.41
1:C:962:THR:CG2	1:C:991:LEU:HB3	2.50	0.41
1:D:589:ARG:O	1:D:609:ASN:HA	2.20	0.41
1:D:714:VAL:HG11	1:D:720:ILE:HD13	2.03	0.41
1:D:839:TYR:C	1:D:839:TYR:CD2	2.93	0.41
1:D:859:HIS:CA	1:D:865:VAL:HG23	2.50	0.41
1:A:170:GLN:NE2	1:A:247:LEU:O	2.53	0.41
1:A:373:VAL:HA	1:A:374:PRO:HD3	1.94	0.41
1:A:497:LYS:O	1:A:500:SER:OG	2.30	0.41
1:A:844:GLU:O	1:A:847:GLN:HG3	2.20	0.41
1:C:998:ILE:CG2	1:C:1001:CYS:HB2	2.51	0.41
1:D:90:SER:HB2	1:D:136:CYS:HA	2.03	0.41
1:D:991:LEU:HA	1:D:991:LEU:HD23	1.85	0.41
1:A:783:ARG:CG	1:A:929:LEU:HD22	2.50	0.41
1:B:342:ASP:CB	5:B:1032:NDP:C4N	2.98	0.41
1:B:775:LEU:HA	1:B:775:LEU:HD23	1.91	0.41
1:A:762:TYR:CZ	1:B:780:THR:HG23	2.56	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.01	0.41
1:C:343:THR:O	1:C:344:ALA:C	2.58	0.41
1:C:205:PHE:CE1	1:C:497:LYS:HG3	2.55	0.41
1:C:589:ARG:NH2	1:D:989:CYS:HB3	2.36	0.41
1:C:685:GLY:O	1:C:720:ILE:HD13	2.20	0.41
1:C:849:TRP:CG	1:C:854:PRO:HA	2.55	0.41
1:D:56:GLU:HG3	1:D:355:GLY:HA2	2.03	0.41
1:D:611:GLU:HG2	1:D:612:LEU:O	2.21	0.41
1:D:803:LEU:O	1:D:803:LEU:HD12	2.21	0.41
1:D:83:ALA:O	1:D:84:ASP:C	2.57	0.41
1:A:259:LYS:HB3	1:A:266:ILE:CD1	2.49	0.41
1:A:95:LEU:HD22	1:A:116:ILE:HA	2.01	0.41
1:A:386:GLU:OE1	1:B:367:PHE:HB2	2.21	0.41
1:C:167:ASN:HB2	1:C:912:PHE:CD1	2.56	0.41
1:C:34:LYS:HD3	1:C:34:LYS:HA	1.77	0.41
1:D:114:LYS:NZ	1:D:524:PHE:O	2.50	0.41
1:D:91:CYS:HA	1:D:92:PRO:HD3	1.92	0.41
1:D:18:LEU:HD21	1:D:975:PRO:HA	2.03	0.41
1:A:681:GLY:HA3	1:A:686:GLN:NE2	2.35	0.41
1:A:747:ASP:C	1:A:747:ASP:OD2	2.59	0.41
1:A:943:GLN:HG3	1:A:1011:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:SER:OG	1:B:181:LYS:HG3	2.21	0.41
1:B:56:GLU:HG3	1:B:355:GLY:HA2	2.01	0.41
1:A:28:LEU:HD23	1:B:519:PRO:HG2	2.03	0.41
1:B:692:ARG:CB	1:B:692:ARG:NH1	2.84	0.41
1:C:762:TYR:OH	1:D:780:THR:HG22	2.19	0.41
1:C:87:CYS:SG	1:C:97:ILE:CD1	3.08	0.41
1:D:439:GLY:HA2	5:D:1032:NDP:O2N	2.21	0.41
1:D:815:VAL:CG1	1:D:816:CYS:N	2.83	0.41
1:A:642:MET:HB2	1:A:668:ASN:HB3	2.03	0.41
1:C:109:TYR:CD2	1:C:109:TYR:N	2.86	0.41
1:C:217:PHE:HE2	1:C:256:ILE:HD12	1.84	0.41
1:C:283:ILE:CG1	1:C:482:ILE:HD13	2.49	0.41
1:C:523:LEU:HB2	1:C:525:TYR:CE1	2.55	0.41
1:C:63:LYS:HE3	1:C:128:MET:HG2	2.03	0.41
1:C:968:TYR:CD2	1:C:987:THR:HG21	2.55	0.41
1:D:375:GLU:CD	1:D:375:GLU:N	2.74	0.41
1:B:608:LEU:HD13	1:B:742:MET:CB	2.45	0.41
1:B:738:VAL:HG21	1:B:773:ILE:CD1	2.50	0.41
1:B:796:ILE:CD1	1:B:813:LEU:HB3	2.46	0.41
1:B:962:THR:HG21	1:B:991:LEU:HB3	2.02	0.41
1:C:62:ILE:HG21	1:C:353:ARG:NH2	2.36	0.41
1:C:954:ILE:HG21	1:C:998:ILE:HD11	2.02	0.41
1:D:218:GLU:OE2	4:D:1031:FAD:H1B	2.20	0.41
1:D:654:SER:O	1:D:702:VAL:HG11	2.21	0.41
1:D:97:ILE:HD11	2:D:1026:SF4:S4	2.61	0.41
1:A:131:PRO:HB2	1:A:373:VAL:HG11	2.03	0.41
1:A:410:ARG:NH2	1:B:410:ARG:CZ	2.84	0.41
1:A:438:PHE:HA	5:A:1032:NDP:O4B	2.21	0.41
1:A:673:HIS:C	1:A:675:MET:H	2.21	0.41
1:A:979:LEU:HD23	1:A:979:LEU:HA	1.91	0.41
1:B:443:ARG:O	1:B:444:ASP:C	2.60	0.41
1:B:825:THR:C	1:B:827:ILE:N	2.75	0.41
1:C:263:GLU:HB2	1:C:446:LYS:HB3	2.03	0.41
1:C:267:THR:HG22	1:C:268:LEU:N	2.36	0.41
1:D:108:ASN:O	1:D:108:ASN:CG	2.60	0.41
1:D:124:LEU:CD1	1:D:161:GLU:HG2	2.49	0.41
1:C:410:ARG:NE	1:D:410:ARG:NH2	2.59	0.41
1:D:605:SER:O	1:D:606:SER:HB3	2.20	0.41
1:D:692:ARG:HA	1:D:723:ALA:O	2.21	0.41
1:A:124:LEU:HG	1:A:240:VAL:HG13	2.03	0.40
1:A:771:ARG:HB3	1:A:772:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LEU:HA	1:B:286:PRO:HD2	1.83	0.40
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.85	0.40
1:B:444:ASP:OD1	1:B:446:LYS:HB2	2.21	0.40
1:B:547:GLY:HA3	1:B:570:PHE:CE2	2.56	0.40
1:B:732:VAL:HG13	1:B:788:PHE:HE2	1.86	0.40
1:B:882:TYR:CZ	1:B:977:THR:HG22	2.56	0.40
1:C:482:ILE:O	1:C:482:ILE:HG13	2.21	0.40
1:C:557:SER:CB	1:C:624:SER:HB3	2.50	0.40
1:D:176:LEU:HA	1:D:177:PRO:HD3	1.93	0.40
1:D:294:PHE:CZ	1:D:338:LEU:HD12	2.56	0.40
1:D:340:ALA:HB2	1:D:363:PHE:HB3	2.03	0.40
1:D:63:LYS:HE3	1:D:128:MET:HG2	2.03	0.40
1:A:913:ILE:HA	1:A:914:PRO:HD3	1.99	0.40
1:B:92:PRO:HD2	2:B:1026:SF4:S3	2.61	0.40
1:C:366:GLY:HA2	1:C:390:PHE:CE1	2.56	0.40
1:C:397:ILE:HD11	1:C:428:HIS:NE2	2.36	0.40
1:C:134:ASP:O	1:D:38:LYS:HD2	2.21	0.40
1:D:396:VAL:CG1	1:D:403:ILE:HD12	2.51	0.40
1:B:305:THR:H	1:B:308:ASP:HB2	1.86	0.40
1:A:373:VAL:HA	1:B:47:LYS:HD3	2.03	0.40
1:B:962:THR:O	1:B:966:SER:N	2.54	0.40
1:B:97:ILE:HD13	1:B:152:ILE:HD13	2.03	0.40
1:C:373:VAL:HA	1:C:374:PRO:HD3	1.90	0.40
1:D:552:ALA:HB3	1:D:553:PRO:HD3	2.03	0.40
1:D:806:LEU:HA	1:D:810:ALA:O	2.21	0.40
1:C:820:GLN:NE2	1:D:991:LEU:HD11	2.37	0.40
1:A:777:ALA:O	1:A:780:THR:HG22	2.21	0.40
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.87	0.40
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.22	0.40
1:B:396:VAL:HG11	1:B:403:ILE:HD13	2.02	0.40
1:B:993:LEU:CD2	1:B:993:LEU:C	2.88	0.40
1:C:775:LEU:HA	1:C:775:LEU:HD23	1.77	0.40
1:C:896:ARG:HG2	1:C:896:ARG:NH1	2.35	0.40
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.60	0.40
4:D:1031:FAD:H1'1	4:D:1031:FAD:H9	1.96	0.40
1:D:142:LEU:HD23	1:D:142:LEU:HA	1.77	0.40
1:C:410:ARG:NE	1:D:410:ARG:CZ	2.85	0.40
1:D:842:SER:HA	1:D:916:LYS:HG2	2.03	0.40
1:A:164:LYS:HD2	1:A:243:PHE:CG	2.57	0.40
1:A:248:MET:CE	1:A:255:ILE:HD11	2.51	0.40
1:A:673:HIS:CE1	1:A:675:MET:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LEU:HA	1:C:286:PRO:HD2	1.87	0.40
1:C:413:GLN:HG3	1:C:419:TRP:CE2	2.57	0.40
1:C:518:LYS:HA	1:C:519:PRO:HD3	1.90	0.40
1:C:577:SER:HA	1:C:653:LEU:CD2	2.51	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	1013/1025 (99%)	927 (92%)	72 (7%)	14 (1%)	11	38
1	B	1004/1025 (98%)	920 (92%)	77 (8%)	7 (1%)	22	54
1	C	1006/1025 (98%)	926 (92%)	74 (7%)	6 (1%)	25	57
1	D	1006/1025 (98%)	924 (92%)	73 (7%)	9 (1%)	17	48
All	All	4029/4100 (98%)	3697 (92%)	296 (7%)	36 (1%)	17	48

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	GLY
1	A	676	GLY
1	A	906	PRO
1	C	613	ILE
1	A	3	PRO
1	A	550	SER
1	A	613	ILE
1	A	681	GLY
1	B	293	ILE
1	B	613	ILE
1	C	293	ILE

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Mol	Chain	Res	Type
1	D	613	ILE
1	A	53	GLU
1	A	263	GLU
1	A	901	ASN
1	B	3	PRO
1	B	53	GLU
1	C	53	GLU
1	D	405	ALA
1	A	132	THR
1	D	151	ASN
1	D	293	ILE
1	D	550	SER
1	A	794	GLY
1	B	132	THR
1	C	266	ILE
1	C	551	ALA
1	D	185	ALA
1	D	1018	PRO
1	B	474	PRO
1	C	183	PRO
1	D	674	GLY
1	D	794	GLY
1	A	293	ILE
1	B	794	GLY
1	A	404	VAL

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	847/854 (99%)	829 (98%)	18 (2%)	53	75
1	B	842/854 (99%)	815 (97%)	27 (3%)	39	67
1	C	843/854 (99%)	824 (98%)	19 (2%)	50	73
1	D	844/854 (99%)	813 (96%)	31 (4%)	34	63
All	All	3376/3416 (99%)	3281 (97%)	95 (3%)	43	70

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	100	PHE
1	A	239	ASP
1	A	363	PHE
1	A	367	PHE
1	A	373	VAL
1	A	387	PHE
1	A	453	PRO
1	A	519	PRO
1	A	555	THR
1	A	579	ASP
1	A	644	SER
1	A	720	ILE
1	A	793	THR
1	A	800	GLU
1	A	813	LEU
1	A	955	ASN
1	A	985	THR
1	B	91	CYS
1	B	95	LEU
1	B	100	PHE
1	B	292	ASP
1	B	358	ARG
1	B	367	PHE
1	B	368	VAL
1	B	371	ARG
1	B	373	VAL
1	B	378	GLU
1	B	394	ARG
1	B	409	VAL
1	B	426	ILE
1	B	432	ASP
1	B	453	PRO
1	B	474	PRO
1	B	487	ASN
1	B	579	ASP
1	B	599	MET
1	B	644	SER
1	B	700	GLN
1	B	793	THR
1	B	800	GLU
1	B	941	ILE

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Mol	Chain	Res	Type
1	B	955	ASN
1	B	984	ASP
1	B	985	THR
1	C	15	ILE
1	C	52	CYS
1	C	91	CYS
1	C	100	PHE
1	C	118	SER
1	C	222	TYR
1	C	367	PHE
1	C	416	THR
1	C	562	ARG
1	C	579	ASP
1	C	667	LEU
1	C	695	CYS
1	C	780	THR
1	C	793	THR
1	C	800	GLU
1	C	813	LEU
1	C	858	SER
1	C	941	ILE
1	C	995	VAL
1	D	15	ILE
1	D	53	GLU
1	D	91	CYS
1	D	100	PHE
1	D	133	SER
1	D	179	GLN
1	D	293	ILE
1	D	322	CYS
1	D	358	ARG
1	D	363	PHE
1	D	367	PHE
1	D	371	ARG
1	D	373	VAL
1	D	376	GLU
1	D	410	ARG
1	D	428	HIS
1	D	436	SER
1	D	441	VAL
1	D	453	PRO
1	D	460	ASP

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Mol	Chain	Res	Type
1	D	500	SER
1	D	558	SER
1	D	579	ASP
1	D	644	SER
1	D	667	LEU
1	D	741	LEU
1	D	793	THR
1	D	800	GLU
1	D	813	LEU
1	D	955	ASN
1	D	985	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	470	GLN
1	A	487	ASN
1	A	673	HIS
1	A	686	GLN
1	A	900	GLN
1	A	978	HIS
1	B	51	HIS
1	B	170	GLN
1	B	407	GLN
1	B	470	GLN
1	B	487	ASN
1	B	498	GLN
1	B	623	GLN
1	B	807	HIS
1	B	859	HIS
1	C	64	HIS
1	C	170	GLN
1	C	173	ASN
1	C	487	ASN
1	C	544	ASN
1	C	814	GLN
1	C	859	HIS
1	D	170	GLN
1	D	220	GLN
1	D	487	ASN
1	D	673	HIS

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Mol	Chain	Res	Type
1	D	693	ASN
1	D	828	GLN
1	D	943	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

32 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	SF4	A	1026	-	0,12,12	0.00	-	-		
2	SF4	D	1029	1	0,12,12	0.00	-	-		
5	NDP	D	1032	-	45,52,52	1.72	9 (20%)	53,80,80	1.59	12 (22%)
3	FMN	C	1030	-	31,33,33	3.27	10 (32%)	40,50,50	3.30	14 (35%)
2	SF4	A	1029	1	0,12,12	0.00	-	-		
2	SF4	A	1027	-	0,12,12	0.00	-	-		
2	SF4	C	1029	1	0,12,12	0.00	-	-		
2	SF4	D	1027	1	0,12,12	0.00	-	-		
6	UAA	B	1035	-	7,12,12	1.48	2 (28%)	5,16,16	3.67	1 (20%)
6	UAA	A	1035	-	7,12,12	1.48	2 (28%)	5,16,16	3.91	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FAD	A	1031	-	51,58,58	2.48	18 (35%)	60,89,89	1.78	10 (16%)
5	NDP	B	1032	-	45,52,52	1.71	6 (13%)	53,80,80	1.60	7 (13%)
5	NDP	A	1032	-	45,52,52	1.67	8 (17%)	53,80,80	1.74	9 (16%)
3	FMN	A	1030	-	31,33,33	3.05	10 (32%)	40,50,50	3.34	14 (35%)
6	UAA	C	1035	-	7,12,12	1.62	2 (28%)	5,16,16	3.79	1 (20%)
2	SF4	D	1026	1	0,12,12	0.00	-	-		
2	SF4	A	1028	1	0,12,12	0.00	-	-		
2	SF4	C	1027	1	0,12,12	0.00	-	-		
6	UAA	D	1035	-	7,12,12	1.86	2 (28%)	5,16,16	3.99	2 (40%)
2	SF4	B	1029	1	0,12,12	0.00	-	-		
4	FAD	B	1031	-	51,58,58	2.61	19 (37%)	60,89,89	1.77	11 (18%)
4	FAD	D	1031	-	51,58,58	2.64	20 (39%)	60,89,89	1.83	11 (18%)
3	FMN	D	1030	-	31,33,33	3.00	10 (32%)	40,50,50	3.32	14 (35%)
2	SF4	D	1028	1	0,12,12	0.00	-	-		
2	SF4	B	1028	1	0,12,12	0.00	-	-		
4	FAD	C	1031	-	51,58,58	2.55	19 (37%)	60,89,89	1.72	12 (20%)
5	NDP	C	1032	-	45,52,52	1.65	7 (15%)	53,80,80	1.59	7 (13%)
2	SF4	C	1026	1	0,12,12	0.00	-	-		
3	FMN	B	1030	-	31,33,33	3.00	10 (32%)	40,50,50	3.31	14 (35%)
2	SF4	B	1026	1	0,12,12	0.00	-	-		
2	SF4	B	1027	1	0,12,12	0.00	-	-		
2	SF4	C	1028	1	0,12,12	0.00	-	-		

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	SF4	A	1026	-	-	-	0/6/5/5
2	SF4	D	1029	1	-	-	0/6/5/5
5	NDP	D	1032	-	-	5/30/77/77	0/5/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1029	1	-	-	0/6/5/5
2	SF4	A	1027	-	-	-	0/6/5/5
2	SF4	C	1029	1	-	-	0/6/5/5
2	SF4	D	1027	1	-	-	0/6/5/5
6	UAA	B	1035	-	-	0/2/4/4	0/1/1/1
6	UAA	A	1035	-	-	0/2/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	1031	-	-	4/30/50/50	0/6/6/6
5	NDP	B	1032	-	-	5/30/77/77	0/5/5/5
5	NDP	A	1032	-	-	5/30/77/77	0/5/5/5
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
6	UAA	C	1035	-	-	0/2/4/4	0/1/1/1
2	SF4	D	1026	1	-	-	0/6/5/5
2	SF4	A	1028	1	-	-	0/6/5/5
2	SF4	C	1027	1	-	-	0/6/5/5
6	UAA	D	1035	-	-	0/2/4/4	0/1/1/1
2	SF4	B	1029	1	-	-	0/6/5/5
4	FAD	B	1031	-	-	6/30/50/50	0/6/6/6
4	FAD	D	1031	-	-	3/30/50/50	0/6/6/6
4	FAD	C	1031	-	-	3/30/50/50	0/6/6/6
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	B	1028	1	-	-	0/6/5/5
5	NDP	C	1032	-	-	6/30/77/77	0/5/5/5
2	SF4	C	1026	1	-	-	0/6/5/5
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	B	1026	1	-	-	0/6/5/5
2	SF4	B	1027	1	-	-	0/6/5/5
2	SF4	C	1028	1	-	-	0/6/5/5

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1031	FAD	C4X-C10	10.42	1.49	1.38
4	D	1031	FAD	C4X-C10	10.29	1.49	1.38
3	A	1030	FMN	C1'-N10	-10.24	1.37	1.48
3	C	1030	FMN	C1'-N10	-9.94	1.38	1.48
3	B	1030	FMN	C1'-N10	-9.69	1.38	1.48
3	D	1030	FMN	C1'-N10	-9.69	1.38	1.48
4	A	1031	FAD	C4X-C10	9.59	1.48	1.38
4	C	1031	FAD	C4X-C10	8.73	1.47	1.38
3	C	1030	FMN	C9A-N10	6.88	1.47	1.38
3	C	1030	FMN	C4A-C10	6.71	1.45	1.38
4	D	1031	FAD	C9A-N10	6.27	1.47	1.38
3	B	1030	FMN	C9A-N10	6.15	1.46	1.38
3	A	1030	FMN	C4A-C10	6.10	1.44	1.38
3	D	1030	FMN	C4A-C10	6.04	1.44	1.38
4	B	1031	FAD	C9A-N10	5.92	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1030	FMN	C9A-N10	5.83	1.46	1.38
3	A	1030	FMN	C9A-N10	5.78	1.46	1.38
4	C	1031	FAD	C9A-N10	5.71	1.46	1.38
3	C	1030	FMN	C4A-N5	5.62	1.41	1.33
3	B	1030	FMN	C4A-C10	5.44	1.44	1.38
4	A	1031	FAD	C9A-N10	5.31	1.45	1.38
5	A	1032	NDP	C4N-C3N	-5.24	1.39	1.49
4	C	1031	FAD	O4B-C1B	5.13	1.48	1.41
5	B	1032	NDP	C4N-C3N	-5.11	1.39	1.49
5	C	1032	NDP	C4N-C3N	-4.84	1.40	1.49
3	B	1030	FMN	C4A-N5	4.84	1.40	1.33
4	B	1031	FAD	O4B-C1B	4.81	1.47	1.41
5	D	1032	NDP	C4N-C3N	-4.77	1.40	1.49
5	B	1032	NDP	C4N-C5N	-4.55	1.37	1.48
3	D	1030	FMN	C4A-N5	4.54	1.39	1.33
5	A	1032	NDP	C4N-C5N	-4.46	1.37	1.48
3	D	1030	FMN	C7M-C7	4.45	1.59	1.51
5	D	1032	NDP	C4N-C5N	-4.42	1.37	1.48
5	C	1032	NDP	C4N-C5N	-4.39	1.37	1.48
4	C	1031	FAD	C4-C4X	4.37	1.48	1.41
3	C	1030	FMN	C4-N3	4.32	1.40	1.33
3	A	1030	FMN	C4A-N5	4.31	1.39	1.33
3	B	1030	FMN	C7M-C7	4.26	1.59	1.51
4	C	1031	FAD	C10-N1	4.23	1.38	1.33
5	D	1032	NDP	C2N-C3N	4.16	1.46	1.34
4	C	1031	FAD	C4-N3	4.16	1.40	1.33
4	B	1031	FAD	PA-O2A	-4.15	1.35	1.55
4	A	1031	FAD	C4-N3	4.10	1.40	1.33
4	D	1031	FAD	PA-O2A	-4.10	1.36	1.55
3	A	1030	FMN	C4-N3	4.09	1.40	1.33
4	A	1031	FAD	PA-O2A	-4.07	1.36	1.55
4	D	1031	FAD	C4-C4X	4.04	1.48	1.41
4	A	1031	FAD	C10-N1	3.99	1.38	1.33
3	C	1030	FMN	C7M-C7	3.99	1.59	1.51
4	D	1031	FAD	C4-N3	3.97	1.40	1.33
3	A	1030	FMN	C7M-C7	3.95	1.58	1.51
6	D	1035	UAA	C6-N1	3.91	1.41	1.34
4	C	1031	FAD	PA-O2A	-3.88	1.37	1.55
5	B	1032	NDP	C2N-C3N	3.87	1.45	1.34
5	C	1032	NDP	C2N-C3N	3.87	1.45	1.34
4	B	1031	FAD	C10-N1	3.86	1.38	1.33
3	D	1030	FMN	C4-N3	3.86	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C10-N1	3.85	1.38	1.33
3	B	1030	FMN	C4-C4A	3.83	1.48	1.41
4	A	1031	FAD	O4B-C1B	3.82	1.46	1.41
4	B	1031	FAD	C4-N3	3.80	1.39	1.33
4	D	1031	FAD	O4B-C1B	3.78	1.46	1.41
3	C	1030	FMN	C4-C4A	3.78	1.47	1.41
4	D	1031	FAD	C10-N1	3.67	1.38	1.33
4	A	1031	FAD	C4-C4X	3.58	1.47	1.41
5	A	1032	NDP	C2N-C3N	3.56	1.44	1.34
4	D	1031	FAD	C4X-N5	3.53	1.38	1.33
3	D	1030	FMN	C10-N1	3.43	1.37	1.33
4	B	1031	FAD	P-O2P	-3.42	1.39	1.55
4	C	1031	FAD	P-O2P	-3.42	1.39	1.55
4	B	1031	FAD	C4-C4X	3.38	1.47	1.41
4	C	1031	FAD	C4X-N5	3.36	1.38	1.33
4	B	1031	FAD	C4X-N5	3.36	1.38	1.33
4	A	1031	FAD	P-O2P	-3.30	1.39	1.55
4	A	1031	FAD	C2B-C1B	-3.30	1.48	1.53
3	D	1030	FMN	C4-C4A	3.21	1.46	1.41
3	A	1030	FMN	C10-N1	3.20	1.37	1.33
4	B	1031	FAD	C2B-C1B	-3.18	1.48	1.53
4	B	1031	FAD	O5'-C5'	3.17	1.57	1.44
3	B	1030	FMN	C5A-N5	3.14	1.40	1.35
5	B	1032	NDP	C3B-C2B	-3.13	1.46	1.52
4	C	1031	FAD	O5'-C5'	3.12	1.56	1.44
4	A	1031	FAD	O5'-C5'	3.12	1.56	1.44
3	B	1030	FMN	C4-N3	3.09	1.38	1.33
3	B	1030	FMN	C10-N1	3.05	1.37	1.33
3	A	1030	FMN	C4-C4A	3.04	1.46	1.41
4	D	1031	FAD	O5'-C5'	2.99	1.56	1.44
4	C	1031	FAD	C4A-N3A	2.98	1.39	1.35
6	A	1035	UAA	C6-N1	2.94	1.39	1.34
4	A	1031	FAD	C8-C7	2.94	1.48	1.40
3	C	1030	FMN	C4'-C3'	2.92	1.59	1.53
4	C	1031	FAD	C2A-N3A	2.91	1.36	1.32
4	B	1031	FAD	C2-N3	2.91	1.43	1.38
4	A	1031	FAD	C4A-N3A	2.89	1.39	1.35
4	C	1031	FAD	C2-N3	2.89	1.43	1.38
3	C	1030	FMN	C5A-N5	2.88	1.40	1.35
4	D	1031	FAD	P-O2P	-2.85	1.41	1.55
3	D	1030	FMN	C4'-C3'	2.83	1.58	1.53
6	C	1035	UAA	C6-N1	2.82	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1031	FAD	C2-N3	2.80	1.43	1.38
6	B	1035	UAA	C6-N1	2.79	1.39	1.34
4	D	1031	FAD	C4A-N3A	2.78	1.39	1.35
5	D	1032	NDP	C6N-C5N	2.74	1.38	1.33
5	A	1032	NDP	P2B-O2B	-2.73	1.54	1.59
3	A	1030	FMN	C4'-C3'	2.71	1.58	1.53
4	D	1031	FAD	O4B-C4B	2.70	1.51	1.45
6	D	1035	UAA	C4-N3	2.70	1.37	1.33
4	D	1031	FAD	C5X-N5	2.69	1.39	1.35
4	B	1031	FAD	C4A-N3A	2.68	1.39	1.35
4	D	1031	FAD	C2B-C1B	-2.68	1.49	1.53
4	D	1031	FAD	C2-N3	2.66	1.43	1.38
6	C	1035	UAA	C4-N3	2.63	1.37	1.33
4	B	1031	FAD	O4B-C4B	2.62	1.50	1.45
4	D	1031	FAD	C5B-C4B	2.61	1.59	1.51
4	D	1031	FAD	C2A-N1A	2.61	1.38	1.33
3	B	1030	FMN	C4'-C3'	2.61	1.58	1.53
4	A	1031	FAD	C4X-N5	2.58	1.37	1.33
5	C	1032	NDP	C5D-C4D	2.58	1.59	1.51
3	A	1030	FMN	C5A-N5	2.56	1.39	1.35
4	C	1031	FAD	O4B-C4B	2.55	1.50	1.45
4	A	1031	FAD	O4B-C4B	2.54	1.50	1.45
5	C	1032	NDP	C6N-C5N	2.48	1.37	1.33
3	D	1030	FMN	C5A-N5	2.47	1.39	1.35
4	D	1031	FAD	C2A-N3A	2.46	1.36	1.32
4	D	1031	FAD	C8-C7	2.46	1.47	1.40
5	C	1032	NDP	O4B-C1B	2.44	1.44	1.41
5	B	1032	NDP	C6N-C5N	2.44	1.37	1.33
4	A	1031	FAD	C2A-N3A	2.42	1.36	1.32
4	C	1031	FAD	C8-C7	2.41	1.46	1.40
4	B	1031	FAD	C5X-N5	2.40	1.39	1.35
4	B	1031	FAD	C5B-C4B	2.40	1.59	1.51
5	A	1032	NDP	C6N-C5N	2.38	1.37	1.33
5	D	1032	NDP	C5D-C4D	2.37	1.59	1.51
5	A	1032	NDP	C5D-C4D	2.36	1.59	1.51
4	C	1031	FAD	C2A-N1A	2.35	1.38	1.33
4	C	1031	FAD	C5B-C4B	2.34	1.58	1.51
5	D	1032	NDP	P2B-O2B	-2.34	1.54	1.59
5	D	1032	NDP	C4A-N3A	2.29	1.38	1.35
4	D	1031	FAD	C2-N1	-2.28	1.33	1.38
5	B	1032	NDP	C5D-C4D	2.28	1.58	1.51
5	D	1032	NDP	C3B-C2B	-2.27	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1032	NDP	C3B-C2B	-2.19	1.48	1.52
4	B	1031	FAD	C2-N1	-2.17	1.33	1.38
4	A	1031	FAD	C2A-N1A	2.16	1.37	1.33
4	C	1031	FAD	PA-O5B	-2.13	1.50	1.59
4	C	1031	FAD	C2B-C1B	-2.12	1.50	1.53
6	A	1035	UAA	C4-N3	2.10	1.36	1.33
4	A	1031	FAD	C2-N1	-2.08	1.34	1.38
5	D	1032	NDP	PA-O1A	-2.04	1.43	1.50
4	B	1031	FAD	C8-C7	2.04	1.46	1.40
5	C	1032	NDP	PA-O1A	-2.04	1.43	1.50
5	A	1032	NDP	PA-O1A	-2.04	1.43	1.50
4	B	1031	FAD	C2A-N1A	2.03	1.37	1.33
6	B	1035	UAA	C4-N3	2.00	1.36	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1030	FMN	C4-N3-C2	14.15	127.09	115.14
3	B	1030	FMN	C4-N3-C2	13.99	126.95	115.14
3	C	1030	FMN	C4-N3-C2	13.96	126.93	115.14
3	D	1030	FMN	C4-N3-C2	13.80	126.79	115.14
6	A	1035	UAA	C5-C4-N3	-8.40	114.27	124.08
6	D	1035	UAA	C5-C4-N3	-8.28	114.41	124.08
6	C	1035	UAA	C5-C4-N3	-8.26	114.44	124.08
4	A	1031	FAD	C4-N3-C2	8.25	122.10	115.14
4	D	1031	FAD	C4-N3-C2	8.24	122.10	115.14
3	A	1030	FMN	C4A-C4-N3	-8.13	112.31	123.43
4	B	1031	FAD	C4-N3-C2	8.11	121.99	115.14
3	D	1030	FMN	C4A-C4-N3	-7.98	112.51	123.43
6	B	1035	UAA	C5-C4-N3	-7.97	114.77	124.08
3	C	1030	FMN	C4A-C4-N3	-7.91	112.62	123.43
4	C	1031	FAD	C4-N3-C2	7.79	121.72	115.14
3	B	1030	FMN	C4A-C4-N3	-7.75	112.84	123.43
3	A	1030	FMN	C1'-N10-C9A	6.33	123.28	118.29
3	D	1030	FMN	C4-C4A-C10	6.20	124.05	119.95
3	B	1030	FMN	C1'-N10-C9A	6.07	123.07	118.29
3	C	1030	FMN	C1'-N10-C9A	5.87	122.91	118.29
5	C	1032	NDP	PN-O3-PA	5.80	152.72	132.83
5	B	1032	NDP	PN-O3-PA	5.73	152.49	132.83
3	A	1030	FMN	C4-C4A-C10	5.50	123.59	119.95
3	D	1030	FMN	C1'-N10-C9A	5.49	122.61	118.29
3	C	1030	FMN	C4-C4A-C10	5.33	123.48	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1030	FMN	C4-C4A-C10	5.28	123.45	119.95
5	A	1032	NDP	PN-O3-PA	5.24	150.81	132.83
5	B	1032	NDP	C3N-C2N-N1N	-4.90	116.10	123.10
5	C	1032	NDP	C3N-C2N-N1N	-4.90	116.10	123.10
5	D	1032	NDP	C3N-C2N-N1N	-4.79	116.26	123.10
5	A	1032	NDP	C3N-C2N-N1N	-4.74	116.34	123.10
4	D	1031	FAD	C4X-C4-N3	-4.62	117.11	123.43
4	A	1031	FAD	C4X-C4-N3	-4.59	117.15	123.43
4	B	1031	FAD	C4X-C4-N3	-4.47	117.31	123.43
4	C	1031	FAD	C4X-C4-N3	-4.45	117.34	123.43
5	A	1032	NDP	O5D-PN-O1N	4.25	125.67	109.07
4	D	1031	FAD	C4-C4X-C10	-4.23	117.15	119.95
5	A	1032	NDP	O2A-PA-O1A	4.07	132.34	112.24
3	D	1030	FMN	C4A-N5-C5A	3.90	120.67	116.77
5	D	1032	NDP	PN-O3-PA	3.84	146.00	132.83
4	B	1031	FAD	C4-C4X-C10	-3.82	117.42	119.95
4	A	1031	FAD	C4-C4X-C10	-3.78	117.45	119.95
3	B	1030	FMN	C4A-N5-C5A	3.76	120.53	116.77
3	C	1030	FMN	O4'-C4'-C3'	3.75	118.23	109.10
3	B	1030	FMN	O4'-C4'-C3'	3.75	118.21	109.10
3	D	1030	FMN	O2'-C2'-C1'	3.72	118.55	109.59
3	C	1030	FMN	C4A-N5-C5A	3.71	120.48	116.77
3	A	1030	FMN	P-O5'-C5'	3.66	128.37	118.30
3	A	1030	FMN	O4'-C4'-C3'	3.65	117.97	109.10
3	D	1030	FMN	O4'-C4'-C3'	3.63	117.92	109.10
3	B	1030	FMN	O2'-C2'-C1'	3.62	118.31	109.59
3	C	1030	FMN	P-O5'-C5'	3.60	128.22	118.30
4	C	1031	FAD	C4-C4X-C10	-3.55	117.60	119.95
3	B	1030	FMN	P-O5'-C5'	3.54	128.05	118.30
3	A	1030	FMN	O2'-C2'-C1'	3.51	118.03	109.59
3	D	1030	FMN	P-O5'-C5'	3.45	127.80	118.30
4	A	1031	FAD	O2A-PA-O1A	3.42	129.15	112.24
3	A	1030	FMN	C4A-N5-C5A	3.42	120.19	116.77
5	A	1032	NDP	C1D-N1N-C2N	-3.40	115.45	121.11
3	A	1030	FMN	O3'-C3'-C2'	-3.39	100.63	108.81
4	D	1031	FAD	O2A-PA-O1A	3.36	128.87	112.24
5	B	1032	NDP	O2A-PA-O1A	3.32	128.65	112.24
4	B	1031	FAD	O2A-PA-O1A	3.29	128.50	112.24
4	C	1031	FAD	O2A-PA-O1A	3.27	128.40	112.24
3	C	1030	FMN	O2'-C2'-C1'	3.25	117.42	109.59
5	C	1032	NDP	O5D-PN-O1N	3.14	121.34	109.07
3	C	1030	FMN	O3'-C3'-C2'	-3.11	101.31	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1030	FMN	O3'-C3'-C2'	-3.10	101.33	108.81
5	D	1032	NDP	O5D-PN-O1N	3.09	121.16	109.07
5	C	1032	NDP	C1D-N1N-C2N	-3.09	115.97	121.11
3	D	1030	FMN	C4-C4A-N5	-3.03	115.13	118.60
3	C	1030	FMN	C5'-C4'-C3'	-2.99	106.42	112.20
3	D	1030	FMN	O3'-C3'-C2'	-2.99	101.60	108.81
5	B	1032	NDP	C1D-N1N-C2N	-2.95	116.20	121.11
3	A	1030	FMN	C4-C4A-N5	-2.91	115.27	118.60
5	D	1032	NDP	O2A-PA-O1A	2.84	126.28	112.24
3	B	1030	FMN	C5'-C4'-C3'	-2.81	106.77	112.20
5	D	1032	NDP	C1D-N1N-C2N	-2.78	116.48	121.11
3	B	1030	FMN	O3'-C3'-C4'	2.75	115.46	108.81
5	A	1032	NDP	O5B-PA-O1A	-2.72	98.43	109.07
3	D	1030	FMN	C5'-C4'-C3'	-2.72	106.95	112.20
5	D	1032	NDP	O7N-C7N-N7N	-2.71	116.54	122.88
5	C	1032	NDP	O7N-C7N-N7N	-2.68	116.62	122.88
4	D	1031	FAD	C5'-C4'-C3'	-2.67	107.04	112.20
4	B	1031	FAD	P-O3P-PA	2.66	141.94	132.83
3	C	1030	FMN	C4-C4A-N5	-2.65	115.56	118.60
5	A	1032	NDP	O2B-C2B-C3B	2.60	121.09	111.68
4	B	1031	FAD	C2A-N1A-C6A	2.59	123.18	118.75
3	C	1030	FMN	O3'-C3'-C4'	2.57	115.03	108.81
3	A	1030	FMN	C5'-C4'-C3'	-2.57	107.24	112.20
3	D	1030	FMN	O3'-C3'-C4'	2.53	114.93	108.81
4	D	1031	FAD	C5A-C6A-N1A	-2.53	114.62	120.35
4	D	1031	FAD	C2A-N1A-C6A	2.51	123.05	118.75
6	D	1035	UAA	C7-C6-N1	2.51	120.53	116.61
5	B	1032	NDP	O7N-C7N-N7N	-2.50	117.02	122.88
4	A	1031	FAD	P-O3P-PA	2.50	141.40	132.83
4	C	1031	FAD	C5X-C9A-N10	-2.50	115.91	117.72
3	B	1030	FMN	C4-C4A-N5	-2.48	115.76	118.60
4	D	1031	FAD	C5X-C9A-N10	-2.48	115.92	117.72
5	A	1032	NDP	O7N-C7N-N7N	-2.48	117.09	122.88
4	C	1031	FAD	C5'-C4'-C3'	-2.42	107.52	112.20
5	D	1032	NDP	O2B-C2B-C3B	2.40	120.37	111.68
4	A	1031	FAD	C2A-N1A-C6A	2.36	122.79	118.75
3	B	1030	FMN	C6-C5A-C9A	2.35	122.13	119.05
3	B	1030	FMN	C7-C6-C5A	-2.33	117.92	121.22
3	A	1030	FMN	O3'-C3'-C4'	2.31	114.40	108.81
4	A	1031	FAD	C5X-C9A-N10	-2.31	116.04	117.72
4	B	1031	FAD	C5A-C6A-N1A	-2.30	115.14	120.35
5	C	1032	NDP	O2B-C2B-C3B	2.30	120.00	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1031	FAD	C5'-C4'-C3'	-2.29	107.78	112.20
4	D	1031	FAD	C4-C4X-N5	2.27	121.19	118.60
5	A	1032	NDP	N3A-C2A-N1A	-2.25	125.16	128.68
4	A	1031	FAD	C5A-C6A-N1A	-2.24	115.27	120.35
3	D	1030	FMN	C6-C5A-C9A	2.23	121.97	119.05
4	D	1031	FAD	C5A-C6A-N6A	2.23	123.73	120.35
4	D	1031	FAD	P-O3P-PA	2.21	140.41	132.83
5	C	1032	NDP	N3A-C2A-N1A	-2.20	125.24	128.68
5	D	1032	NDP	N3A-C2A-N1A	-2.18	125.27	128.68
4	C	1031	FAD	C5A-C6A-N1A	-2.16	115.44	120.35
5	D	1032	NDP	O4B-C1B-C2B	2.16	110.34	106.59
4	C	1031	FAD	C2A-N1A-C6A	2.16	122.45	118.75
3	C	1030	FMN	C6-C5A-C9A	2.16	121.88	119.05
4	A	1031	FAD	C5'-C4'-C3'	-2.16	108.04	112.20
3	D	1030	FMN	C7-C6-C5A	-2.15	118.18	121.22
4	B	1031	FAD	C4A-C5A-N7A	2.14	111.63	109.40
4	B	1031	FAD	C5A-C6A-N6A	2.13	123.59	120.35
5	B	1032	NDP	O5B-C5B-C4B	-2.13	101.67	108.99
3	A	1030	FMN	C7-C6-C5A	-2.13	118.21	121.22
3	C	1030	FMN	C7-C6-C5A	-2.12	118.22	121.22
4	C	1031	FAD	C5A-C6A-N6A	2.11	123.56	120.35
5	D	1032	NDP	O5B-PA-O1A	-2.10	100.86	109.07
5	D	1032	NDP	O2N-PN-O1N	2.10	122.62	112.24
5	B	1032	NDP	N3A-C2A-N1A	-2.08	125.43	128.68
4	C	1031	FAD	C4-C4X-N5	2.06	120.95	118.60
4	C	1031	FAD	P-O3P-PA	2.04	139.84	132.83
4	C	1031	FAD	C4X-N5-C5X	2.03	118.81	116.77
3	A	1030	FMN	C6-C5A-C9A	2.03	121.72	119.05
5	D	1032	NDP	O5B-C5B-C4B	-2.03	102.01	108.99
4	B	1031	FAD	C1'-N10-C10	2.02	120.22	118.41
4	A	1031	FAD	C5A-C6A-N6A	2.00	123.40	120.35

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1032	NDP	C3B-C2B-O2B-P2B
5	D	1032	NDP	O4D-C1D-N1N-C2N
5	B	1032	NDP	O4D-C1D-N1N-C2N
5	A	1032	NDP	O4D-C1D-N1N-C2N
4	C	1031	FAD	O4B-C4B-C5B-O5B
5	C	1032	NDP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	O4B-C4B-C5B-O5B
4	B	1031	FAD	O4B-C4B-C5B-O5B
4	D	1031	FAD	O4B-C4B-C5B-O5B
5	B	1032	NDP	C3B-C2B-O2B-P2B
5	A	1032	NDP	C3B-C2B-O2B-P2B
5	C	1032	NDP	C3B-C2B-O2B-P2B
4	A	1031	FAD	C3B-C4B-C5B-O5B
4	B	1031	FAD	C3B-C4B-C5B-O5B
4	D	1031	FAD	C3B-C4B-C5B-O5B
4	C	1031	FAD	C3B-C4B-C5B-O5B
5	D	1032	NDP	C1B-C2B-O2B-P2B
5	B	1032	NDP	C1B-C2B-O2B-P2B
5	A	1032	NDP	C1B-C2B-O2B-P2B
5	C	1032	NDP	C1B-C2B-O2B-P2B
3	C	1030	FMN	C4'-C5'-O5'-P
3	A	1030	FMN	C4'-C5'-O5'-P
3	D	1030	FMN	C4'-C5'-O5'-P
3	B	1030	FMN	C4'-C5'-O5'-P
5	D	1032	NDP	PN-O3-PA-O5B
5	B	1032	NDP	PN-O3-PA-O5B
5	A	1032	NDP	PN-O3-PA-O5B
4	B	1031	FAD	PA-O3P-P-O5'
5	C	1032	NDP	PN-O3-PA-O5B
4	A	1031	FAD	C5B-O5B-PA-O3P
4	B	1031	FAD	C5B-O5B-PA-O3P
4	D	1031	FAD	C5B-O5B-PA-O3P
4	C	1031	FAD	C5B-O5B-PA-O3P
4	B	1031	FAD	P-O3P-PA-O1A
4	B	1031	FAD	P-O3P-PA-O2A
4	A	1031	FAD	PA-O3P-P-O5'
5	D	1032	NDP	O4B-C4B-C5B-O5B
5	B	1032	NDP	O4B-C4B-C5B-O5B
5	A	1032	NDP	O4B-C4B-C5B-O5B
5	C	1032	NDP	O4B-C4B-C5B-O5B
5	C	1032	NDP	PN-O3-PA-O1A

There are no ring outliers.

26 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1026	SF4	1	0
2	D	1029	SF4	1	0

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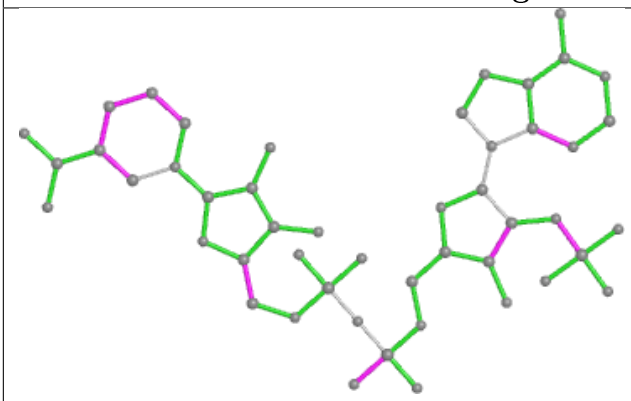
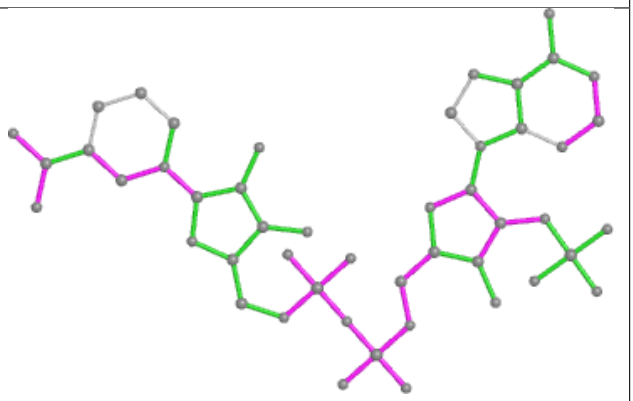
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1032	NDP	6	0
2	A	1029	SF4	1	0
2	A	1027	SF4	2	0
2	C	1029	SF4	1	0
2	D	1027	SF4	2	0
6	B	1035	UAA	1	0
6	A	1035	UAA	1	0
5	B	1032	NDP	5	0
5	A	1032	NDP	6	0
6	C	1035	UAA	1	0
2	D	1026	SF4	1	0
2	A	1028	SF4	2	0
2	C	1027	SF4	2	0
2	B	1029	SF4	2	0
4	D	1031	FAD	3	0
3	D	1030	FMN	1	0
2	D	1028	SF4	4	0
2	B	1028	SF4	2	0
4	C	1031	FAD	2	0
5	C	1032	NDP	6	0
2	C	1026	SF4	1	0
2	B	1026	SF4	2	0
2	B	1027	SF4	2	0
2	C	1028	SF4	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.

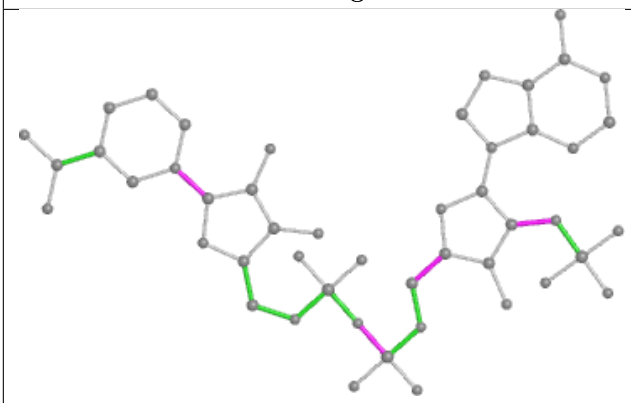
Ligand NDP D 1032



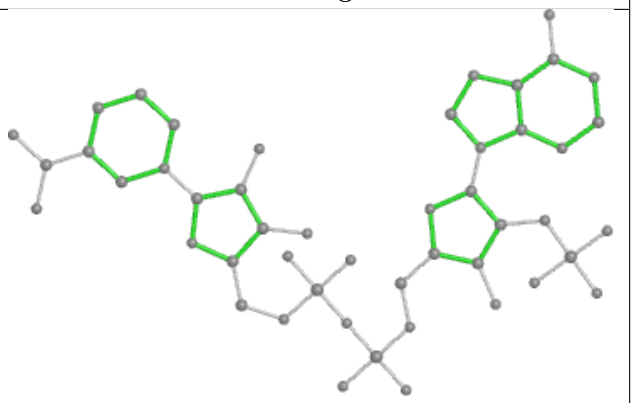
Bond lengths



Bond angles

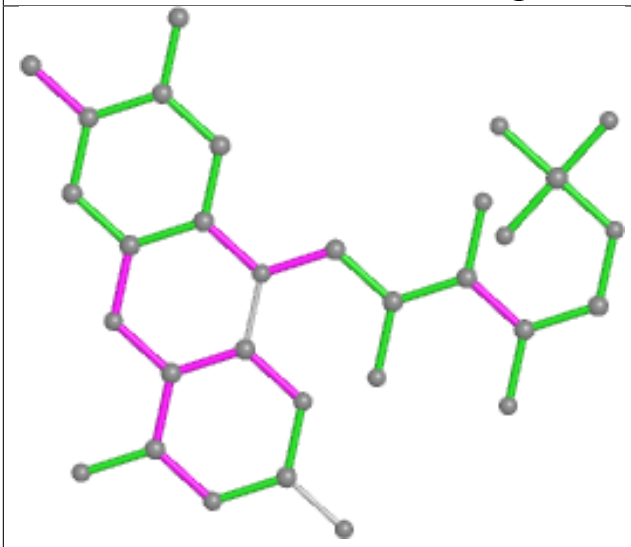


Torsions

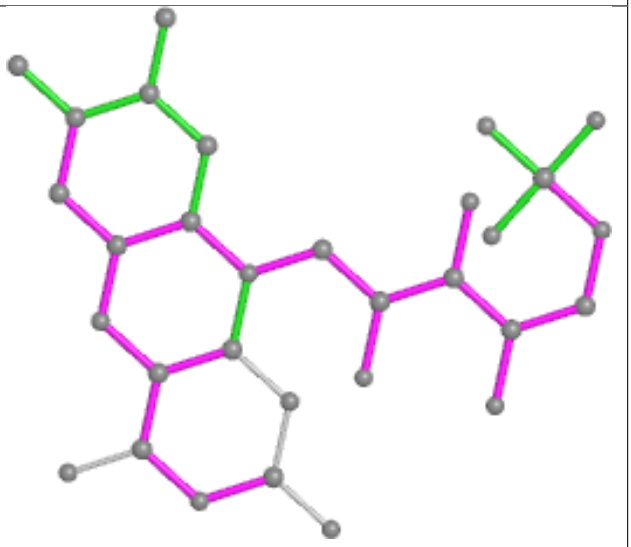


Rings

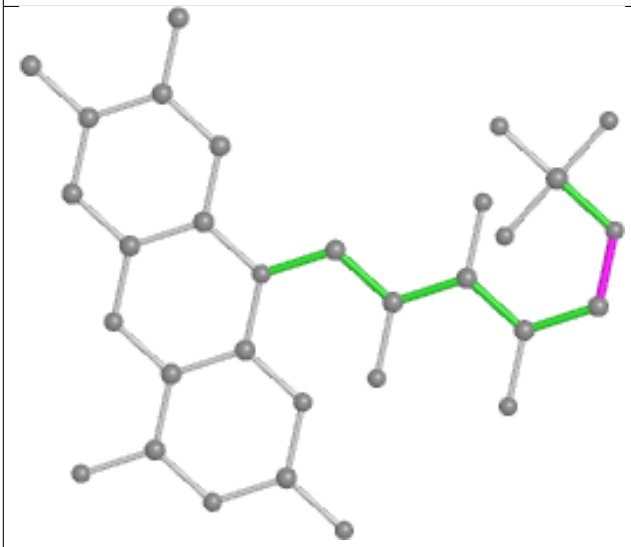
Ligand FMN C 1030



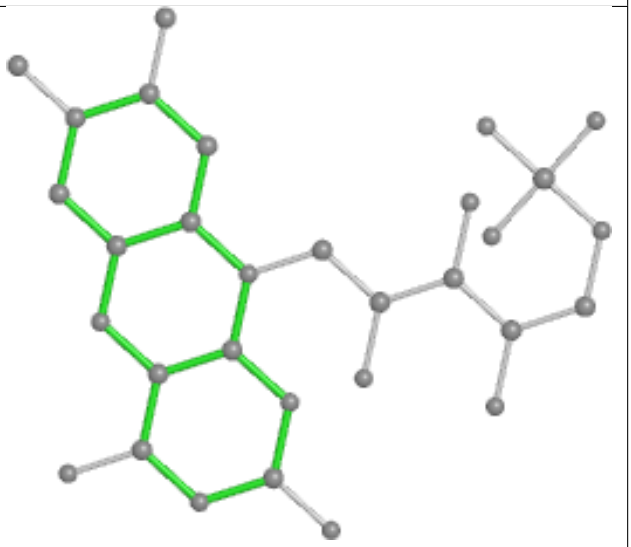
Bond lengths



Bond angles

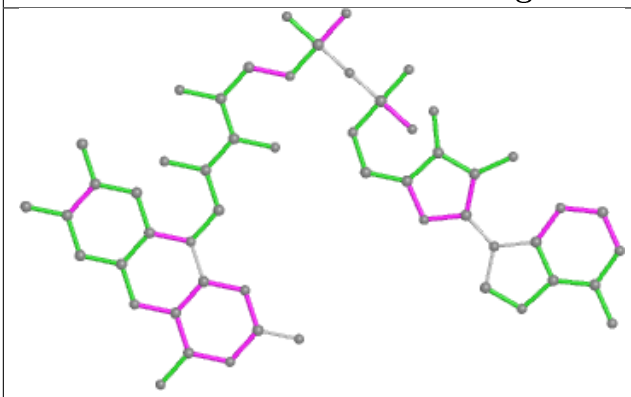


Torsions

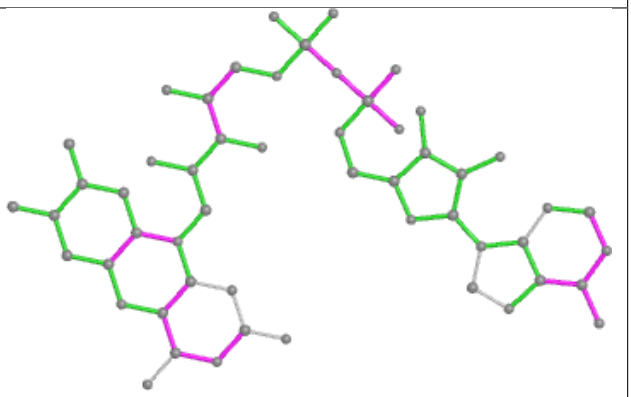


Rings

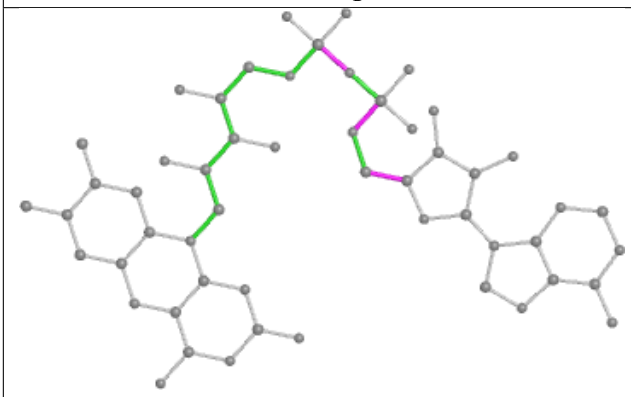
Ligand FAD A 1031



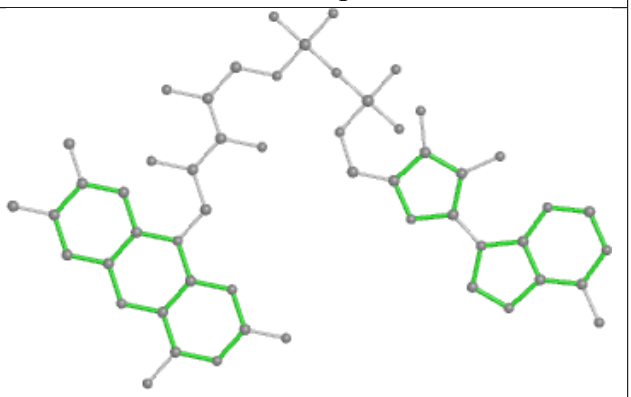
Bond lengths



Bond angles

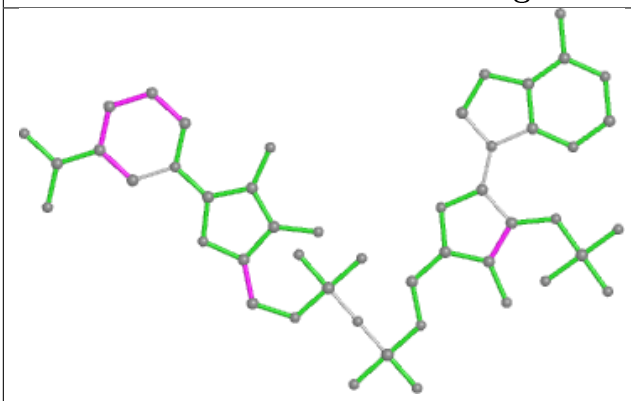


Torsions

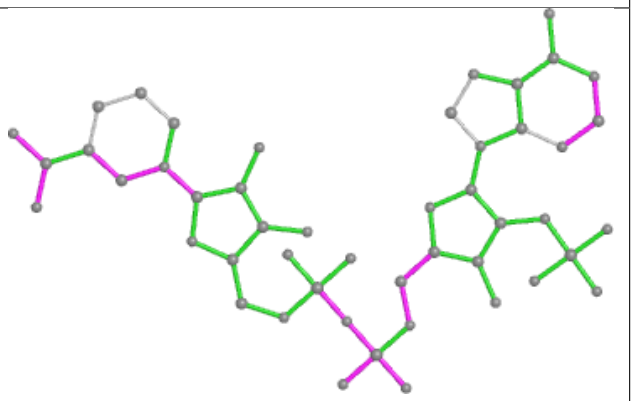


Rings

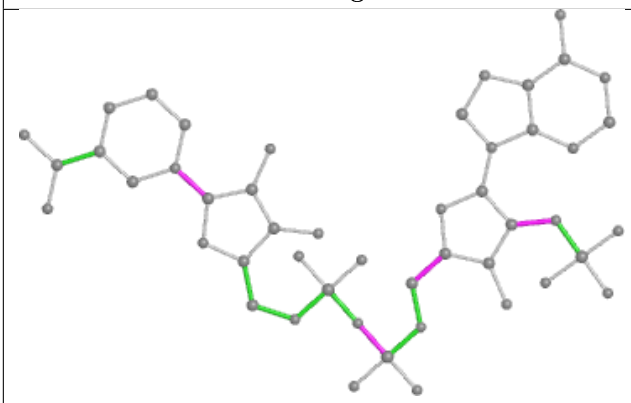
Ligand NDP B 1032



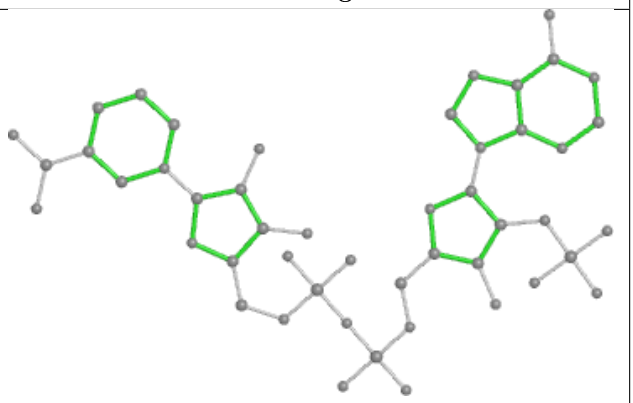
Bond lengths



Bond angles

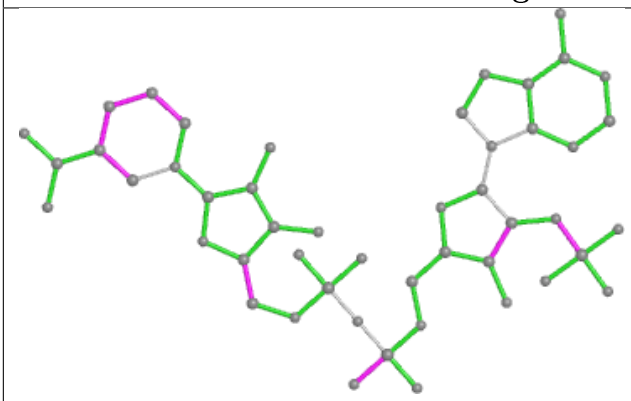


Torsions

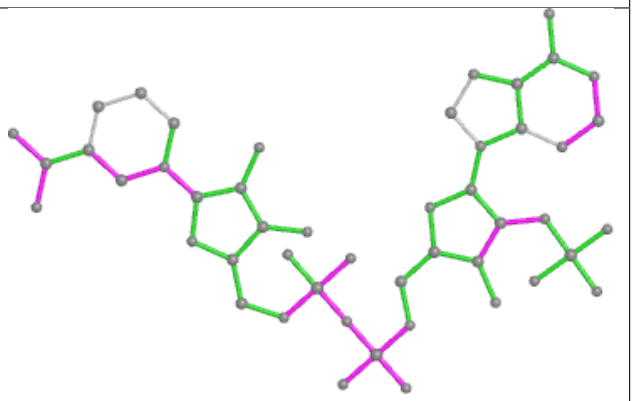


Rings

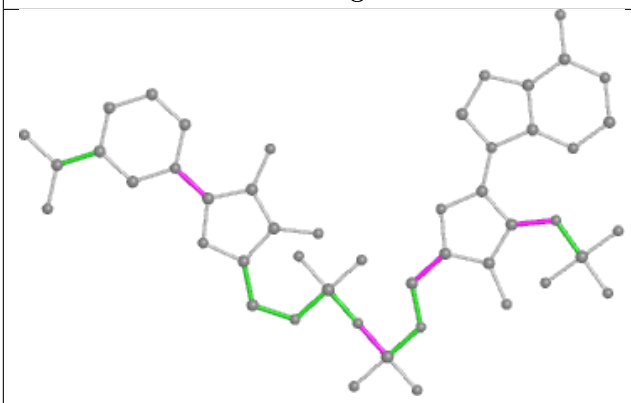
Ligand NDP A 1032



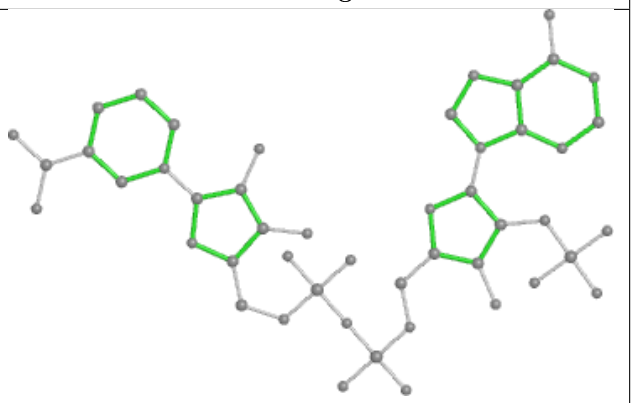
Bond lengths



Bond angles

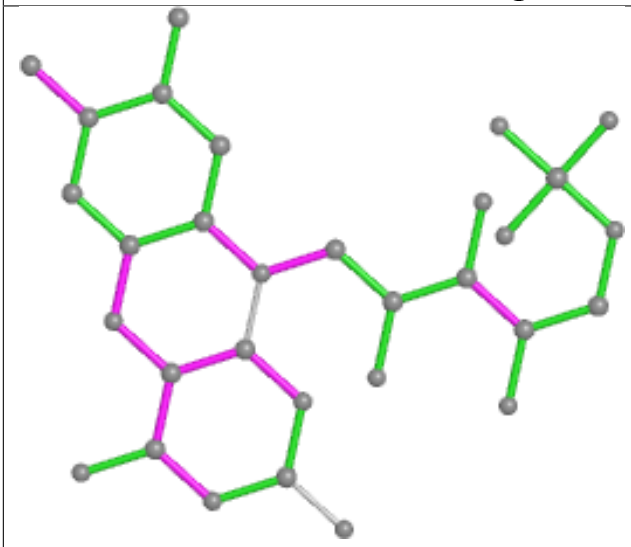


Torsions

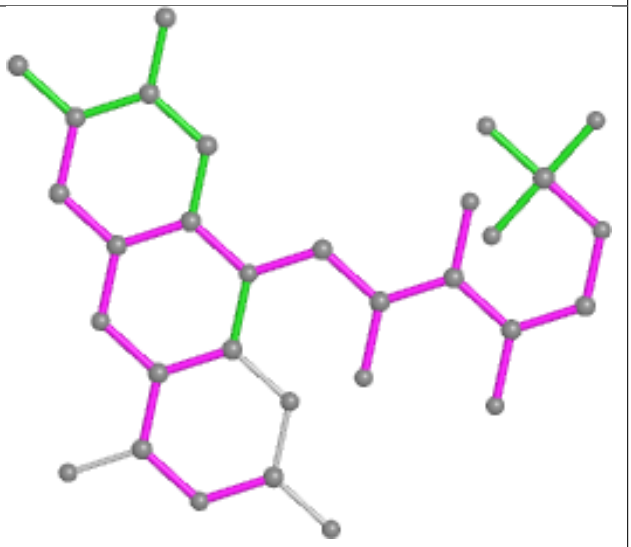


Rings

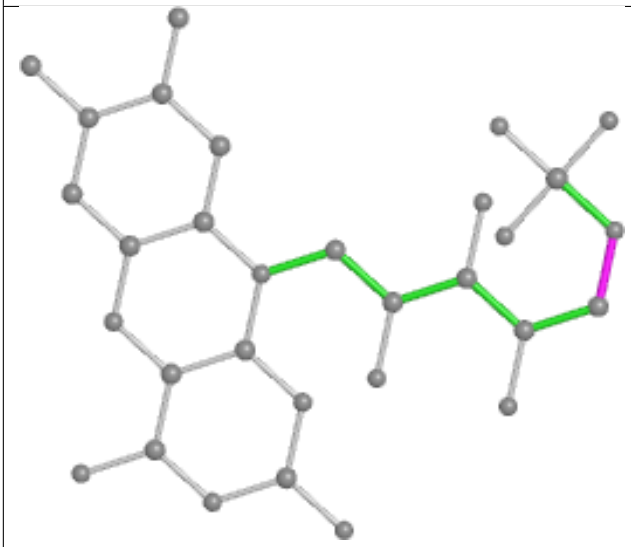
Ligand FMN A 1030



Bond lengths



Bond angles



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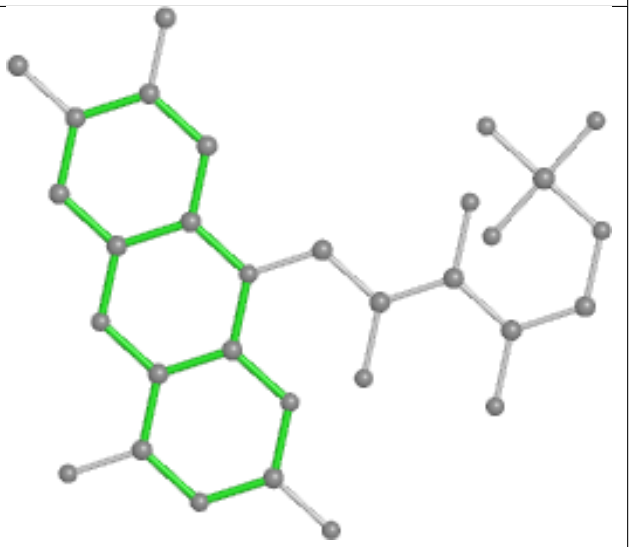
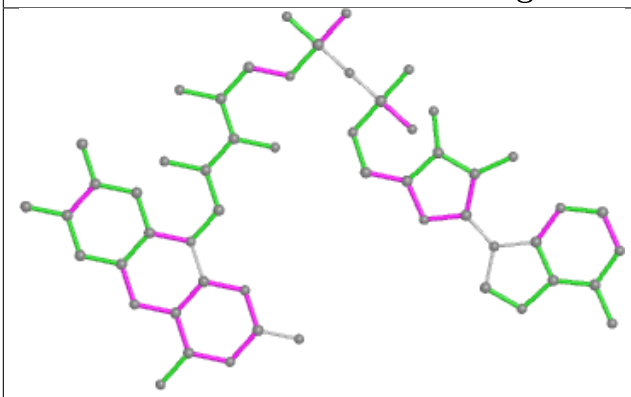
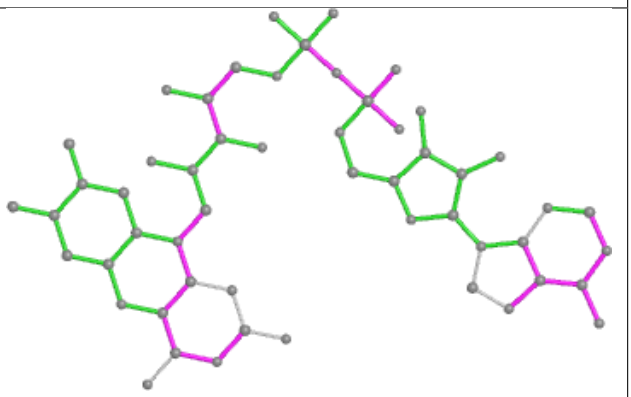


Rings

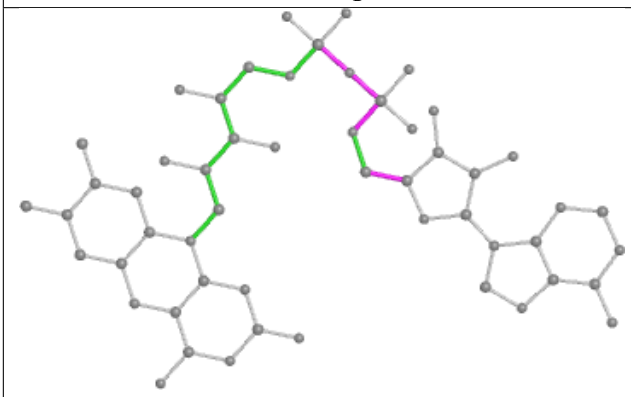
Ligand FAD B 1031



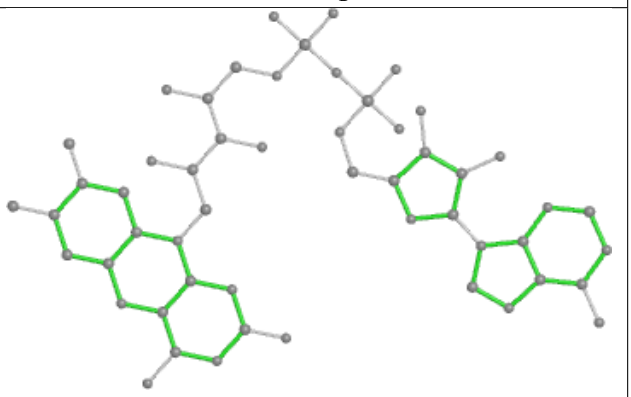
Bond lengths



Bond angles

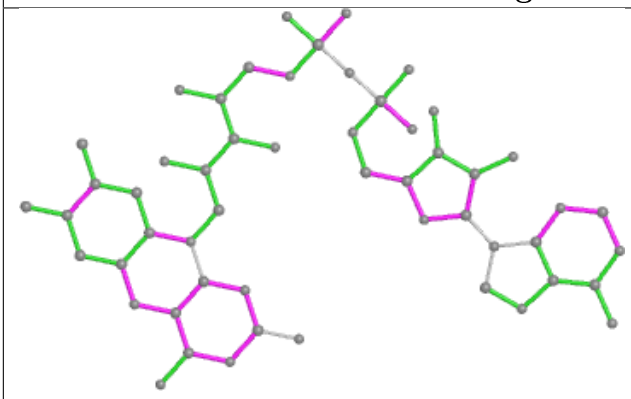


Torsions



Rings

Ligand FAD D 1031



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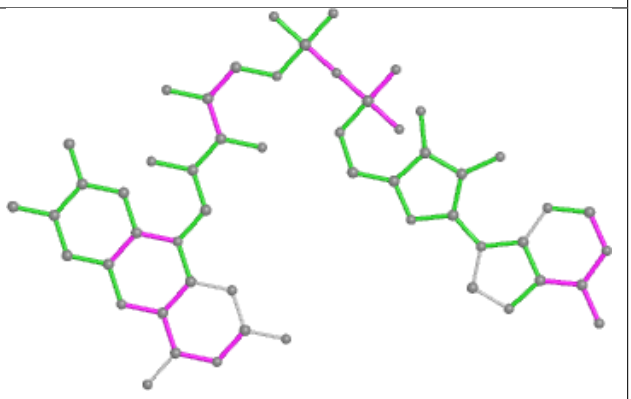
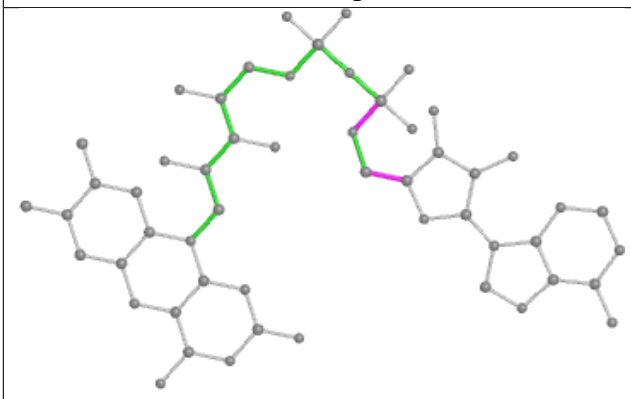
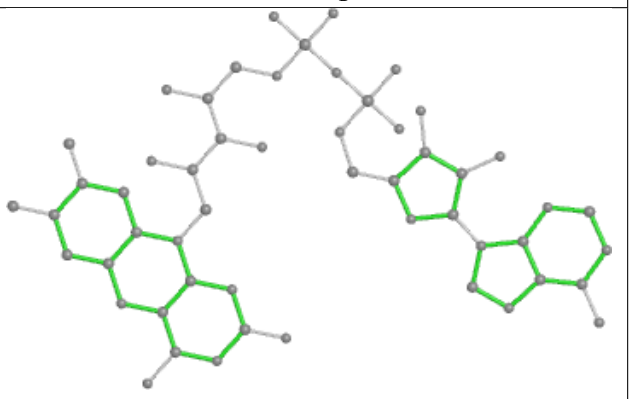


Bond angles

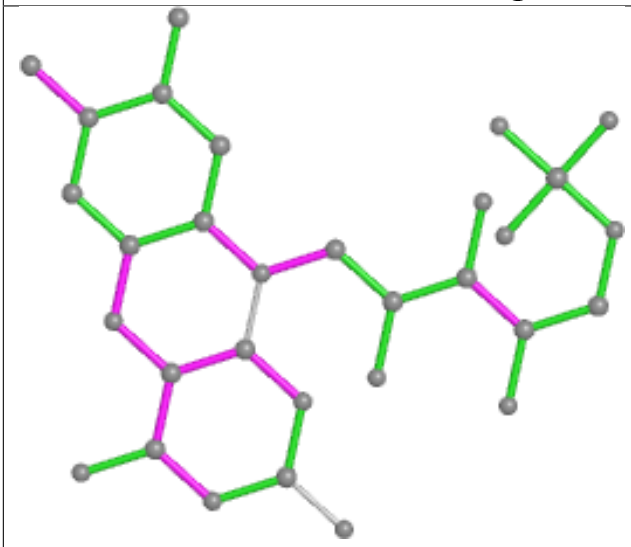


Torsions

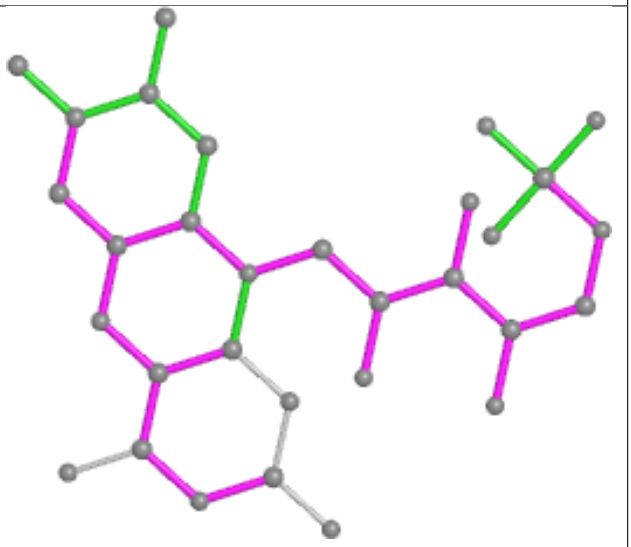


Rings

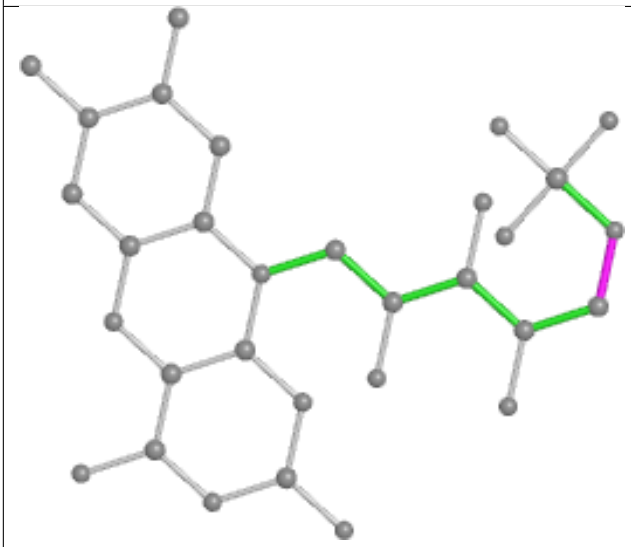
Ligand FMN D 1030



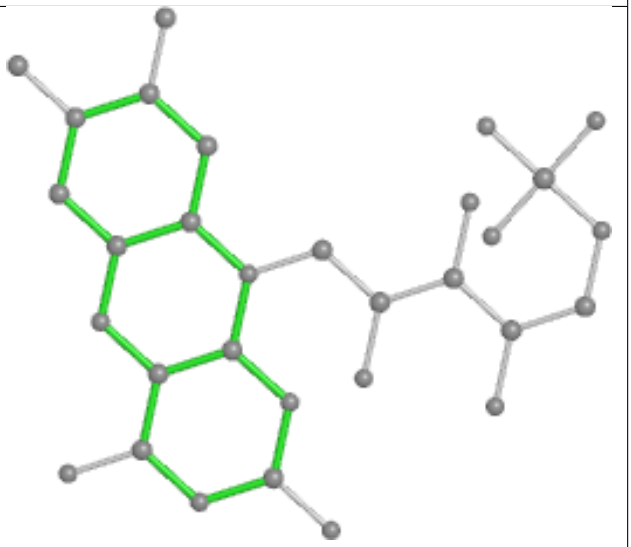
Bond lengths



Bond angles

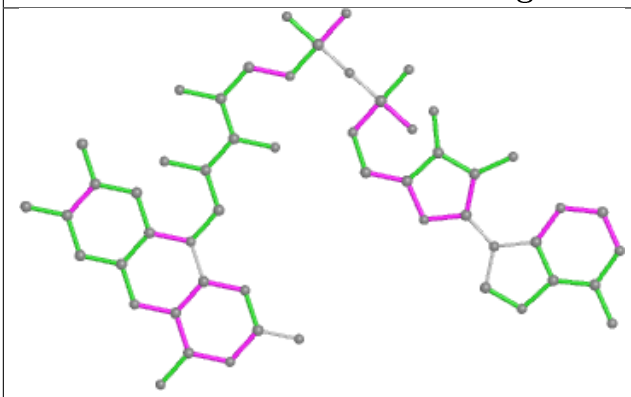


Torsions

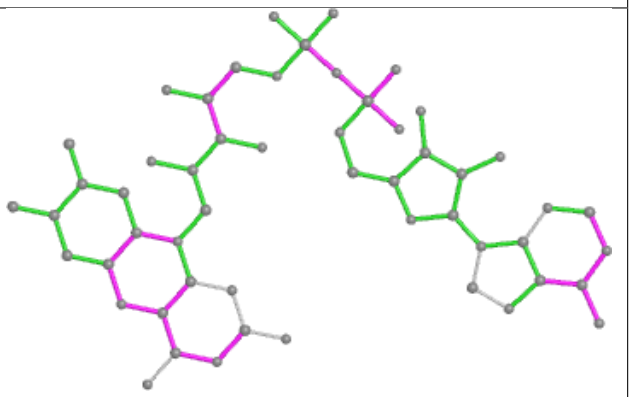


Rings

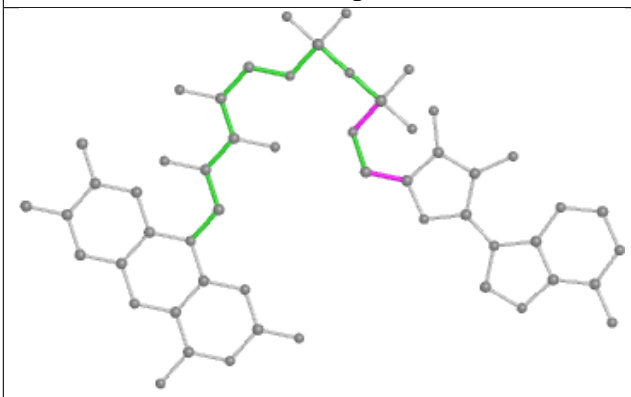
Ligand FAD C 1031



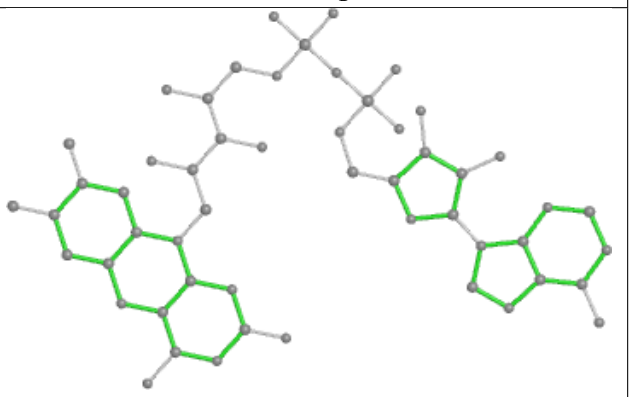
Bond lengths



Bond angles

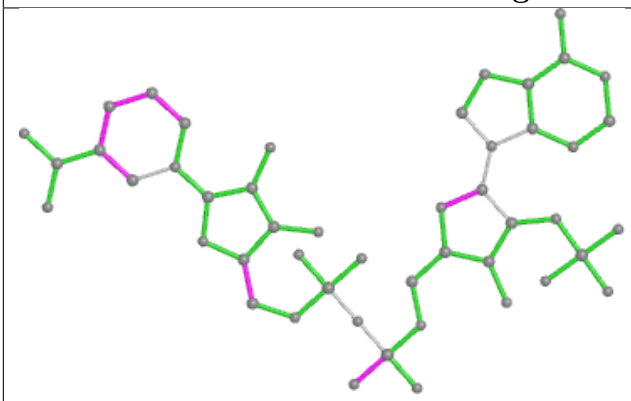


Torsions

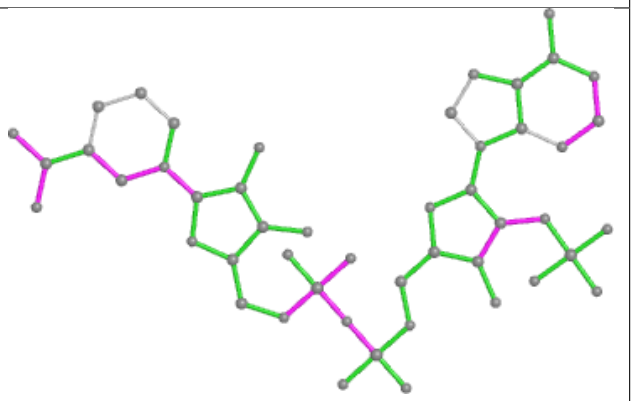


Rings

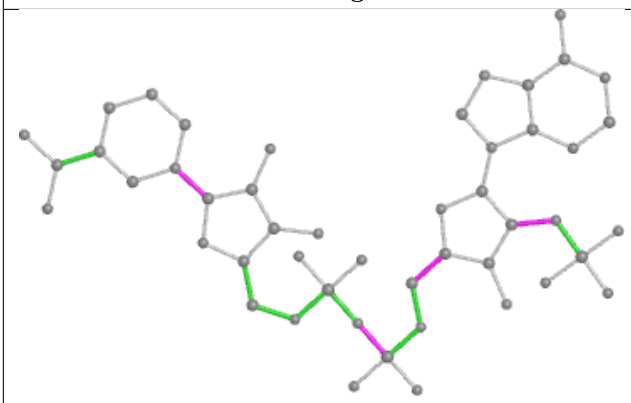
Ligand NDP C 1032



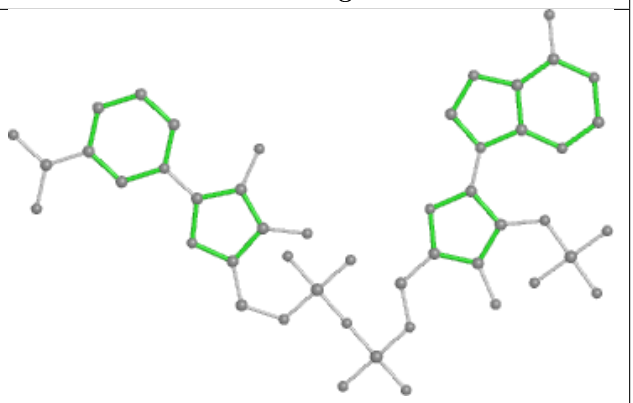
Bond lengths



Bond angles

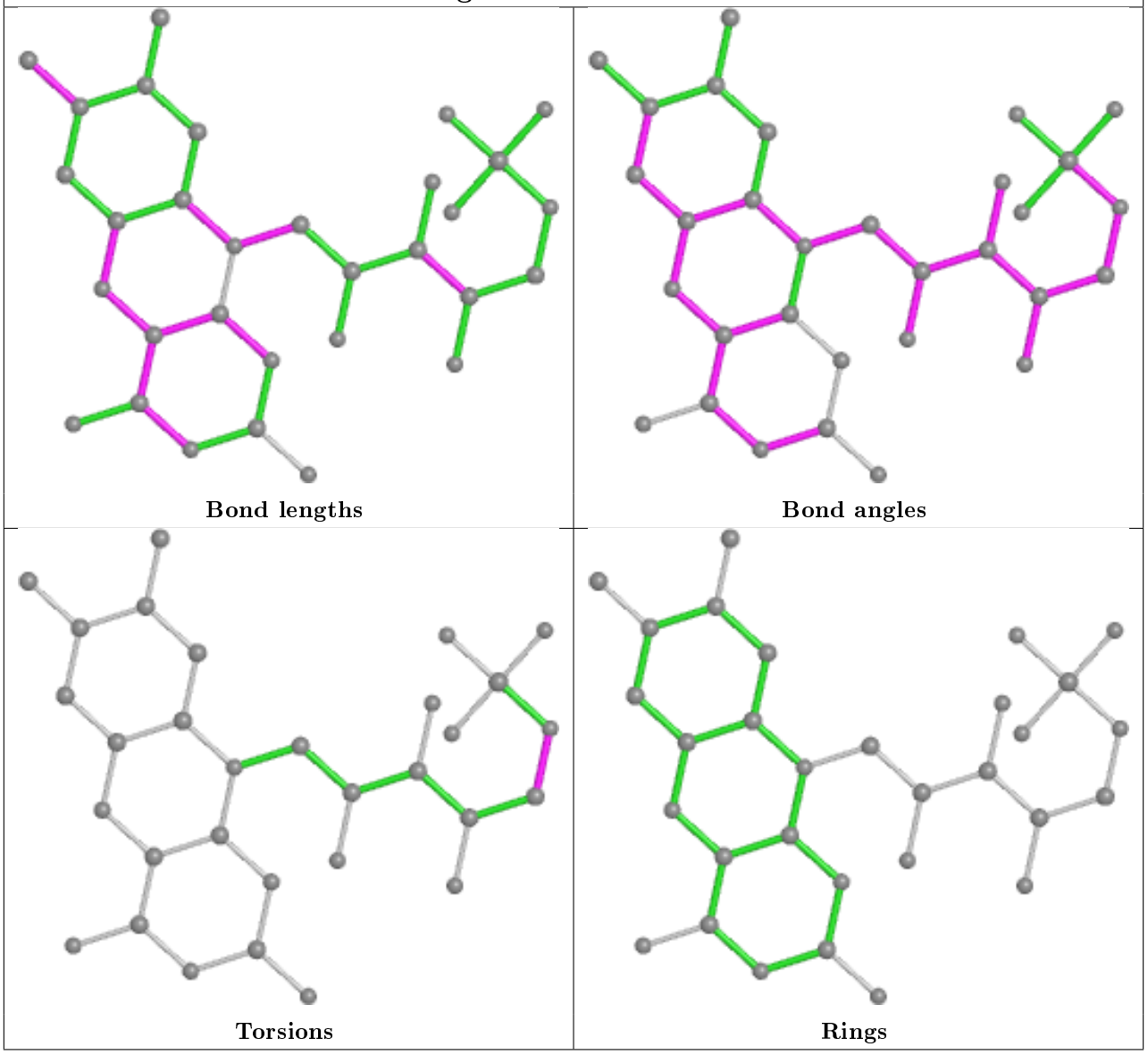


Torsions



Rings

Ligand FMN B 1030



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	1017/1025 (99%)	-0.42	11 (1%)	80	81	7, 39, 93, 147	0
1	B	1010/1025 (98%)	-0.37	14 (1%)	75	75	7, 40, 96, 141	0
1	C	1010/1025 (98%)	-0.19	24 (2%)	59	56	14, 54, 106, 140	0
1	D	1012/1025 (98%)	-0.12	25 (2%)	57	54	14, 57, 107, 162	0
All	All	4049/4100 (98%)	-0.28	74 (1%)	68	67	7, 47, 102, 162	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1019	LEU	7.4
1	D	2	ALA	7.1
1	C	1020	ALA	5.9
1	C	1018	PRO	5.8
1	B	2	ALA	5.6
1	B	1020	ALA	5.3
1	C	1010	PRO	5.1
1	D	1020	ALA	4.6
1	A	48	ASN	4.3
1	C	1017	LEU	4.3
1	C	2	ALA	4.3
1	D	1019	LEU	4.1
1	D	1010	PRO	4.0
1	B	1018	PRO	4.0
1	D	1018	PRO	3.9
1	A	903	ALA	3.8
1	D	52	CYS	3.7
1	A	676	GLY	3.6
1	D	680	MET	3.5
1	C	50	PHE	3.4
1	A	52	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	901	ASN	3.3
1	D	17	ALA	3.2
1	B	1019	LEU	3.2
1	D	673	HIS	3.1
1	D	3	PRO	3.1
1	B	49	CYS	3.1
1	A	675	MET	3.1
1	C	902	ALA	3.0
1	B	1017	LEU	3.0
1	B	48	ASN	3.0
1	D	324	CYS	2.9
1	C	758	LYS	2.8
1	D	645	TYR	2.8
1	C	48	ASN	2.8
1	D	401	GLY	2.8
1	B	50	PHE	2.8
1	A	50	PHE	2.7
1	B	196	GLY	2.7
1	D	1008	THR	2.6
1	B	900	GLN	2.6
1	C	52	CYS	2.6
1	C	640	SER	2.6
1	C	867	ARG	2.6
1	C	181	LYS	2.5
1	C	323	ALA	2.5
1	C	904	PHE	2.5
1	C	903	ALA	2.5
1	D	323	ALA	2.4
1	A	640	SER	2.4
1	C	1009	THR	2.4
1	D	675	MET	2.4
1	A	1018	PRO	2.3
1	D	907	LEU	2.3
1	D	681	GLY	2.3
1	B	51	HIS	2.3
1	A	901	ASN	2.3
1	C	196	GLY	2.2
1	C	757	GLY	2.2
1	D	889	ILE	2.2
1	C	282	GLY	2.2
1	D	55	LEU	2.2
1	D	938	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	584	THR	2.2
1	B	3	PRO	2.2
1	D	53	GLU	2.2
1	D	908	GLU	2.1
1	B	640	SER	2.1
1	A	674	GLY	2.1
1	B	199	SER	2.1
1	D	423	GLU	2.0
1	A	1020	ALA	2.0
1	C	39	LYS	2.0
1	C	690	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 carbohydrates 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
6	UAA	C	1035	12/12	0.78	0.38	138,140,144,144	0
6	UAA	D	1035	12/12	0.82	0.36	107,108,108,109	0
6	UAA	A	1035	12/12	0.86	0.26	111,112,113,113	0
6	UAA	B	1035	12/12	0.88	0.27	146,147,148,148	0
4	FAD	D	1031	53/53	0.91	0.24	40,46,60,60	0
5	NDP	C	1032	48/48	0.93	0.18	53,57,86,88	0
5	NDP	D	1032	48/48	0.94	0.19	57,60,89,92	0
3	FMN	C	1030	31/31	0.94	0.21	45,48,52,55	0
4	FAD	B	1031	53/53	0.94	0.20	19,25,35,37	0
4	FAD	A	1031	53/53	0.94	0.20	20,23,37,38	0
4	FAD	C	1031	53/53	0.94	0.19	29,36,49,50	0
3	FMN	A	1030	31/31	0.94	0.20	31,37,42,45	0

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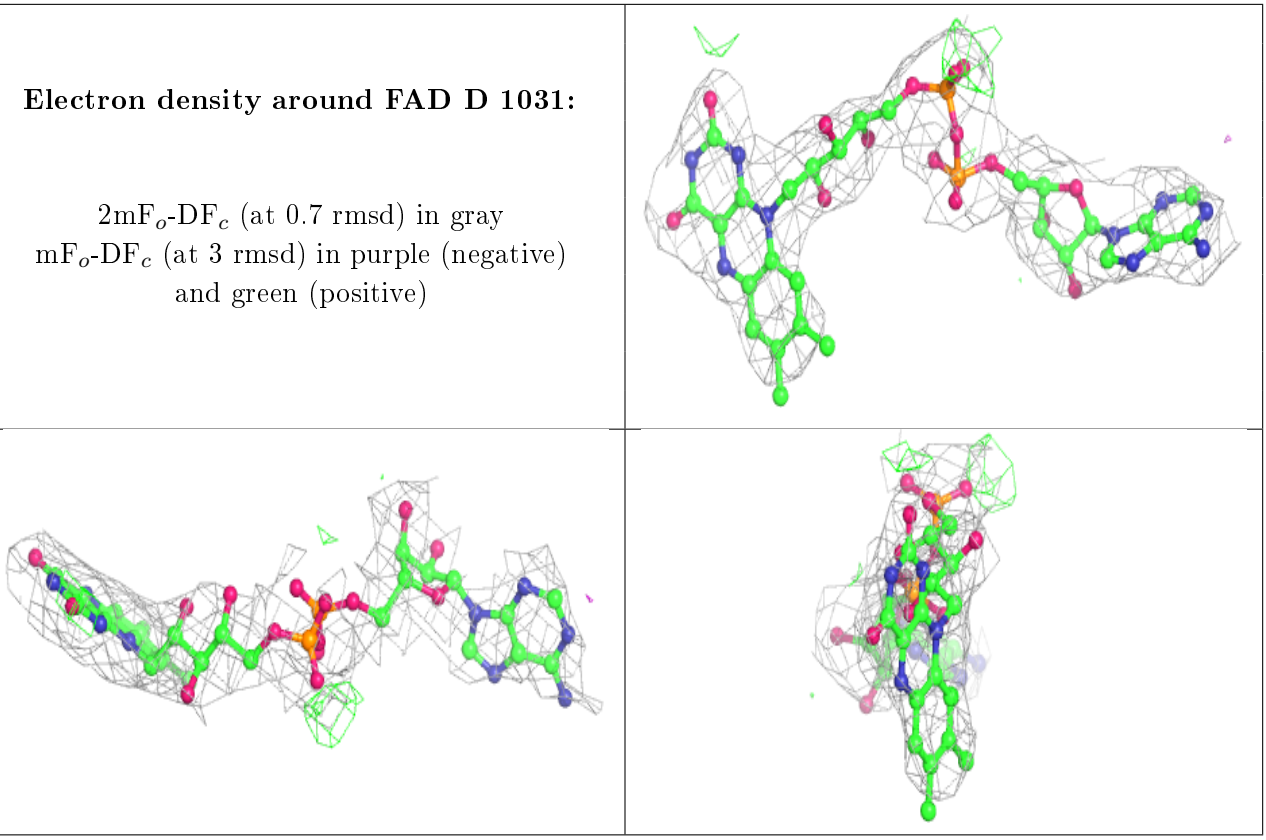
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMN	D	1030	31/31	0.95	0.20	48,52,56,59	0
5	NDP	A	1032	48/48	0.95	0.15	42,47,76,78	0
5	NDP	B	1032	48/48	0.95	0.15	42,46,77,81	0
3	FMN	B	1030	31/31	0.95	0.22	28,33,34,38	0
2	SF4	A	1028	8/8	0.99	0.12	9,11,13,14	0
2	SF4	C	1027	8/8	0.99	0.09	25,26,27,28	0
2	SF4	B	1027	8/8	0.99	0.12	4,4,4,4	0
2	SF4	B	1029	8/8	0.99	0.09	13,15,16,18	0
2	SF4	D	1029	8/8	0.99	0.08	39,40,41,42	0
2	SF4	A	1029	8/8	0.99	0.15	18,21,23,24	0
2	SF4	A	1027	8/8	0.99	0.10	6,10,11,12	0
2	SF4	C	1029	8/8	0.99	0.07	34,35,37,37	0
2	SF4	D	1028	8/8	0.99	0.10	34,35,37,38	0
2	SF4	B	1028	8/8	0.99	0.13	21,23,24,25	0
2	SF4	D	1027	8/8	0.99	0.09	28,30,32,32	0
2	SF4	A	1026	8/8	0.99	0.13	18,21,24,24	0
2	SF4	C	1026	8/8	0.99	0.10	22,24,26,27	0
2	SF4	D	1026	8/8	0.99	0.13	26,27,28,28	0
2	SF4	B	1026	8/8	0.99	0.14	7,10,10,12	0
2	SF4	C	1028	8/8	0.99	0.08	29,31,33,33	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.

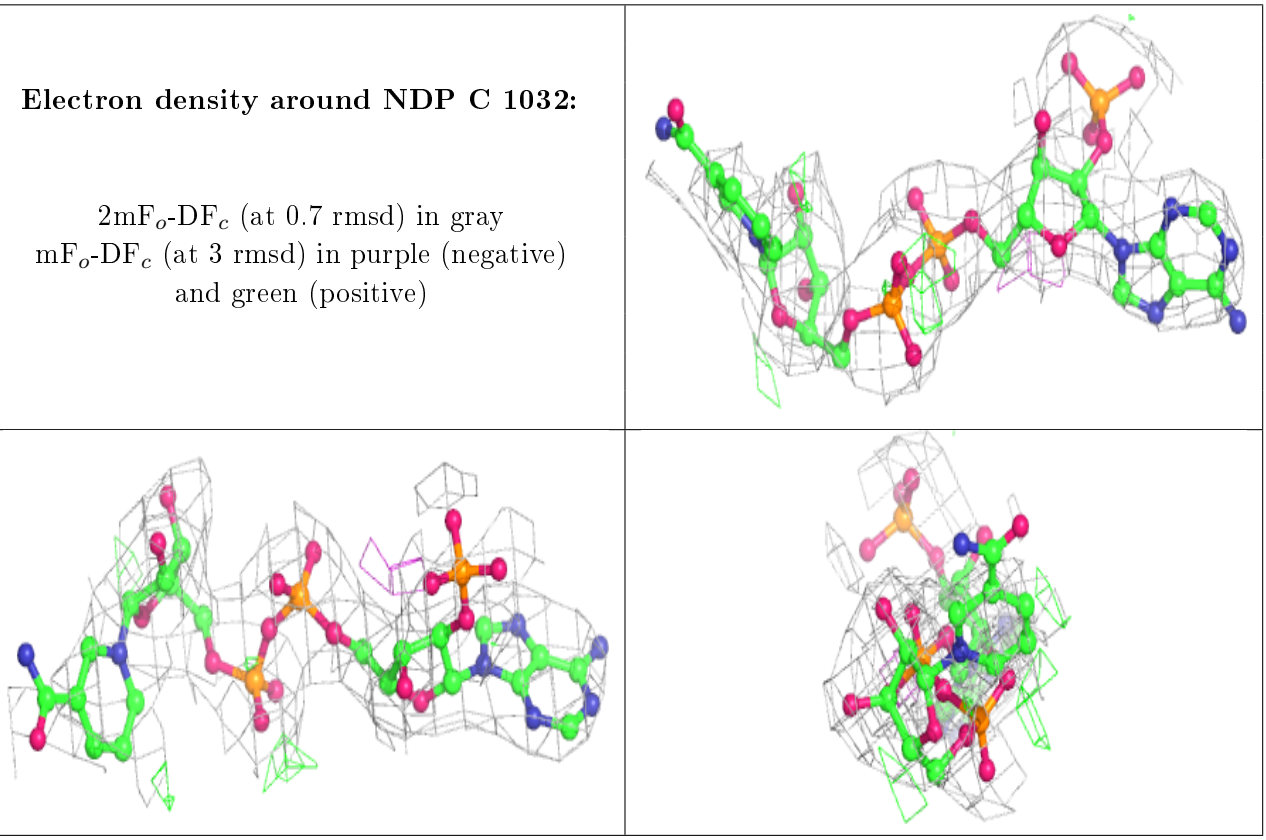
Electron density around FAD D 1031:

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



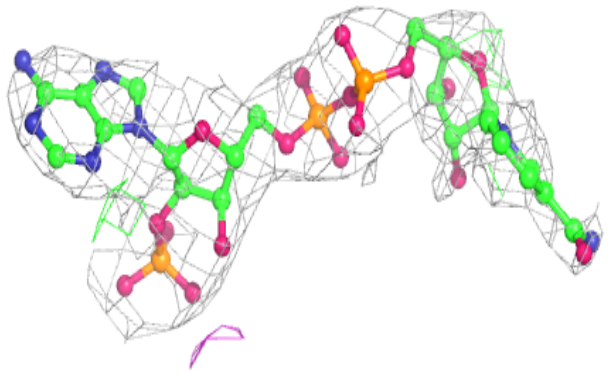
Electron density around NDP C 1032:

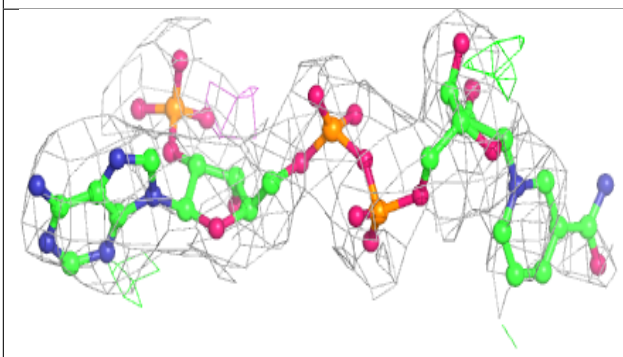
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

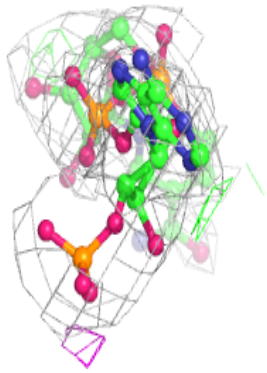


Electron density around NDP D 1032:

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

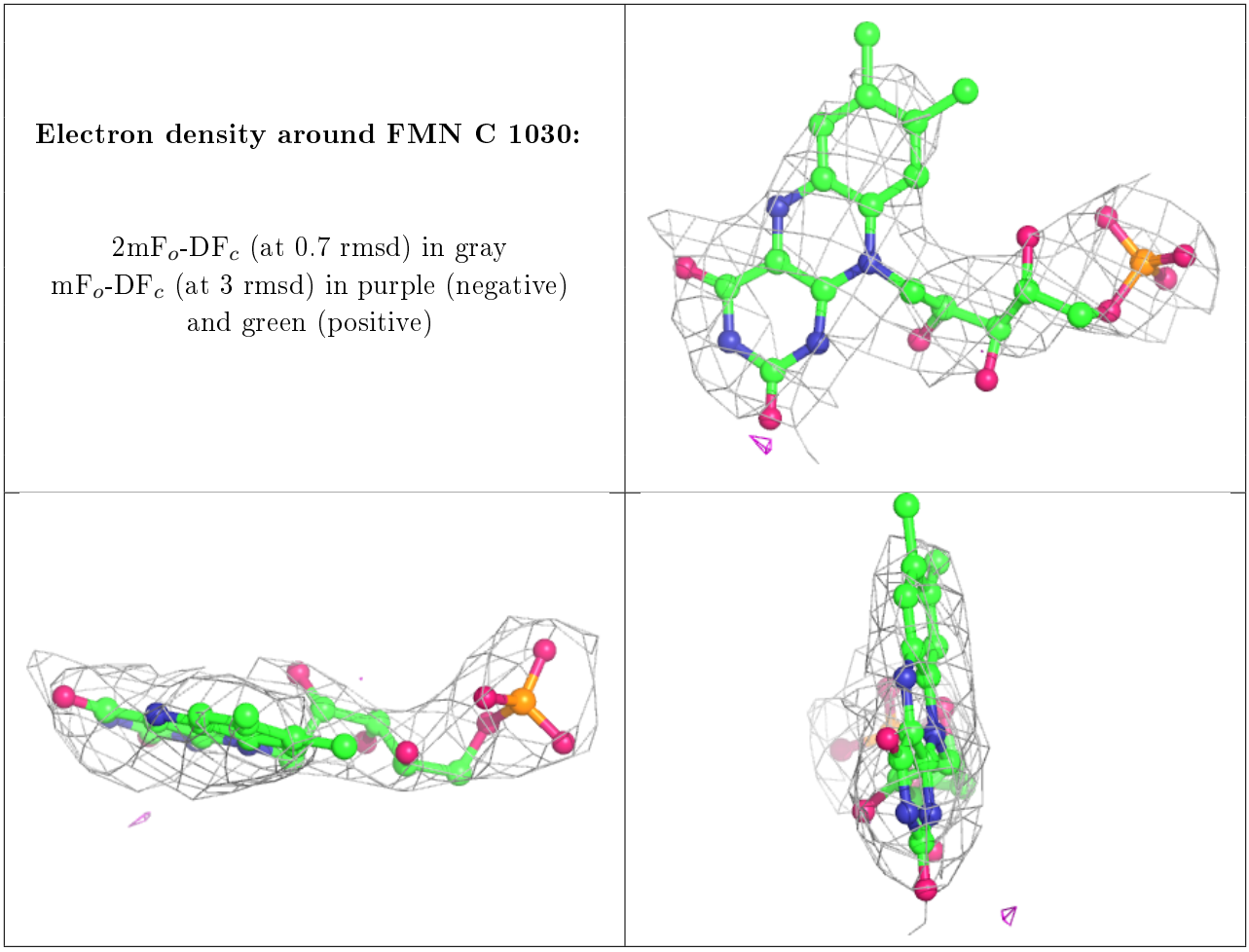






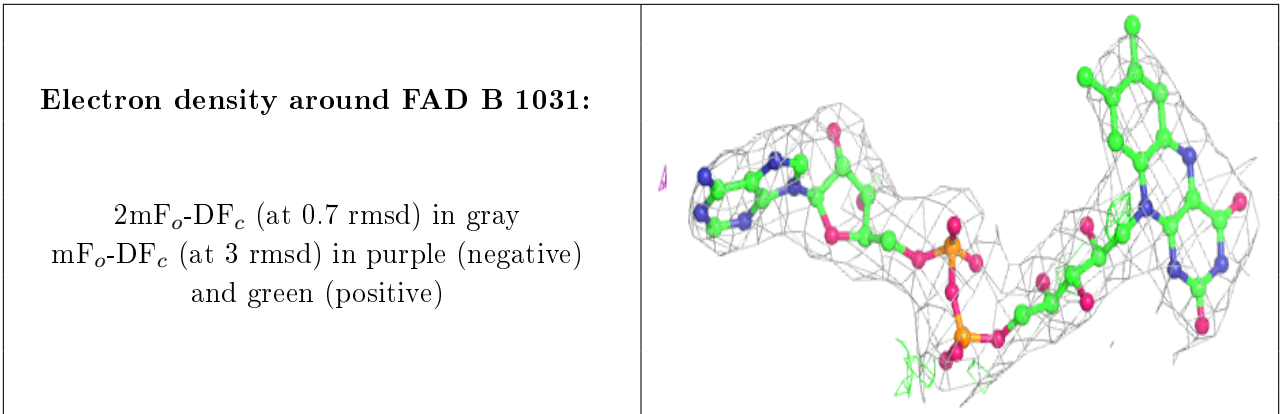
Electron density around FMN C 1030:

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



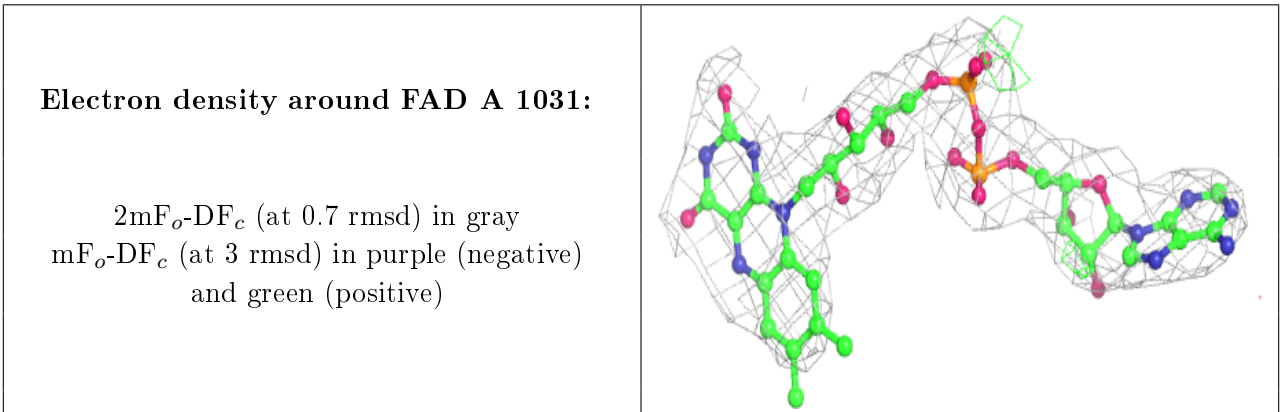
Electron density around FAD B 1031:

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



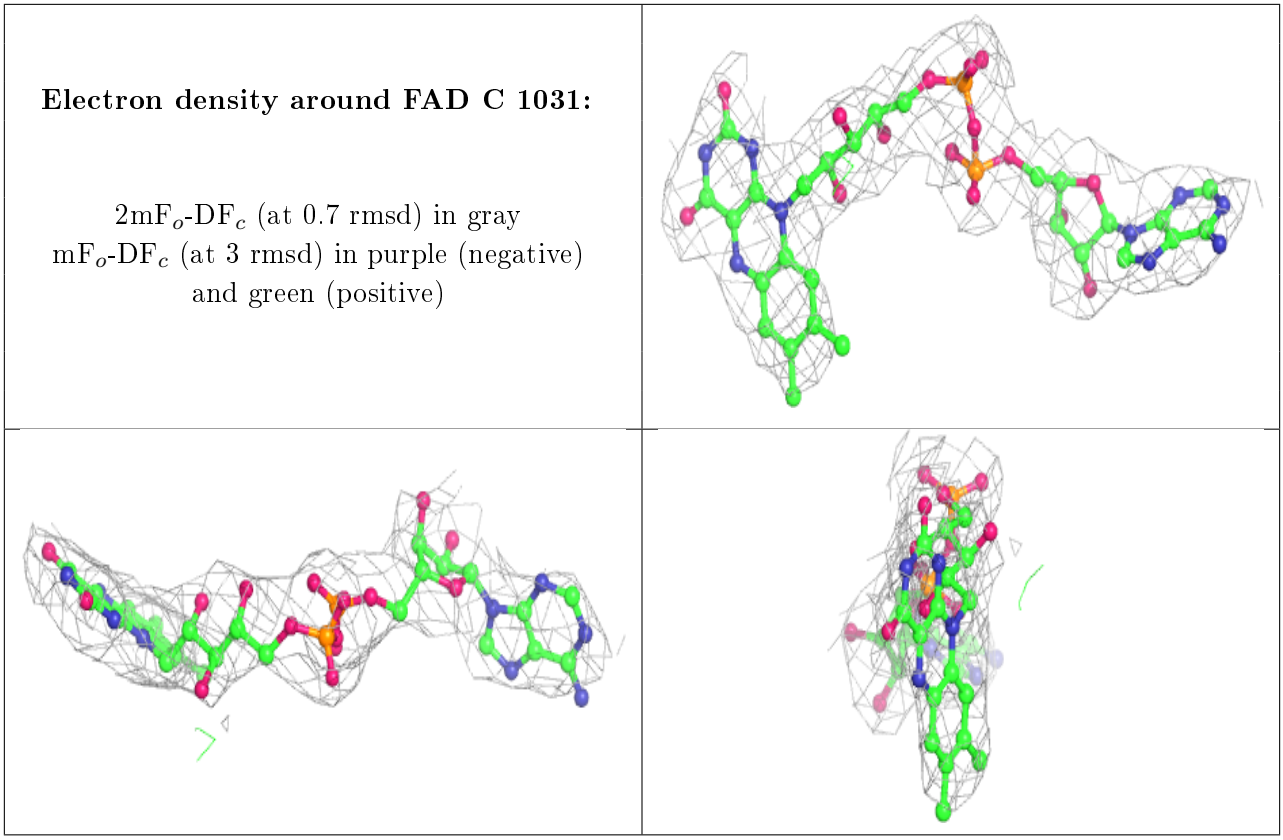
Electron density around FAD A 1031:

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



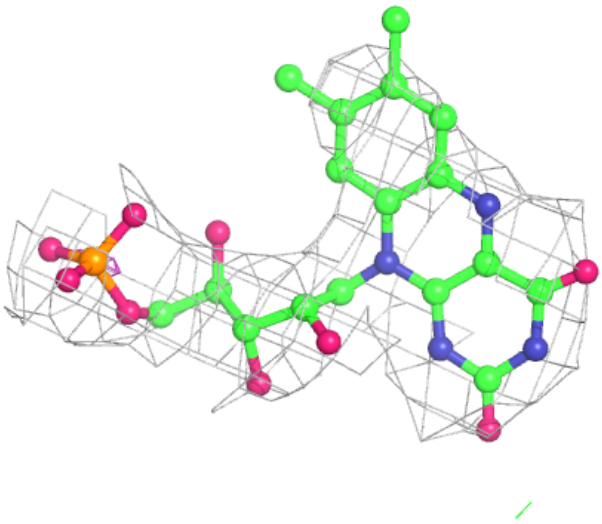
Electron density around FAD C 1031:

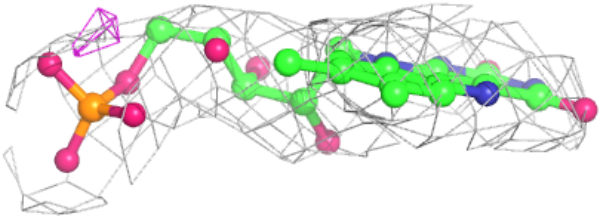
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

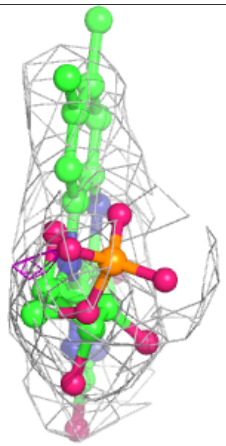


Electron density around FMN A 1030:

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

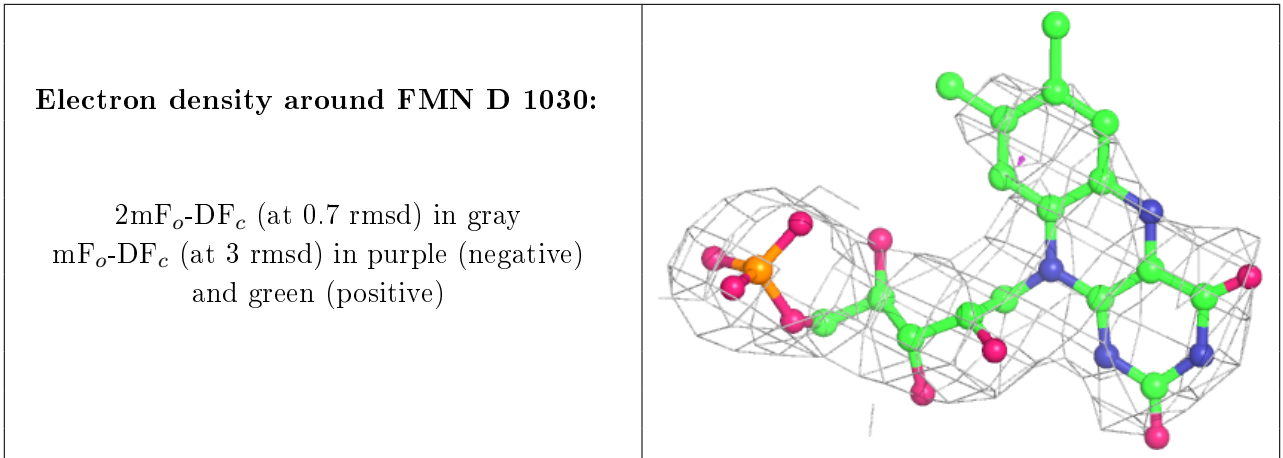






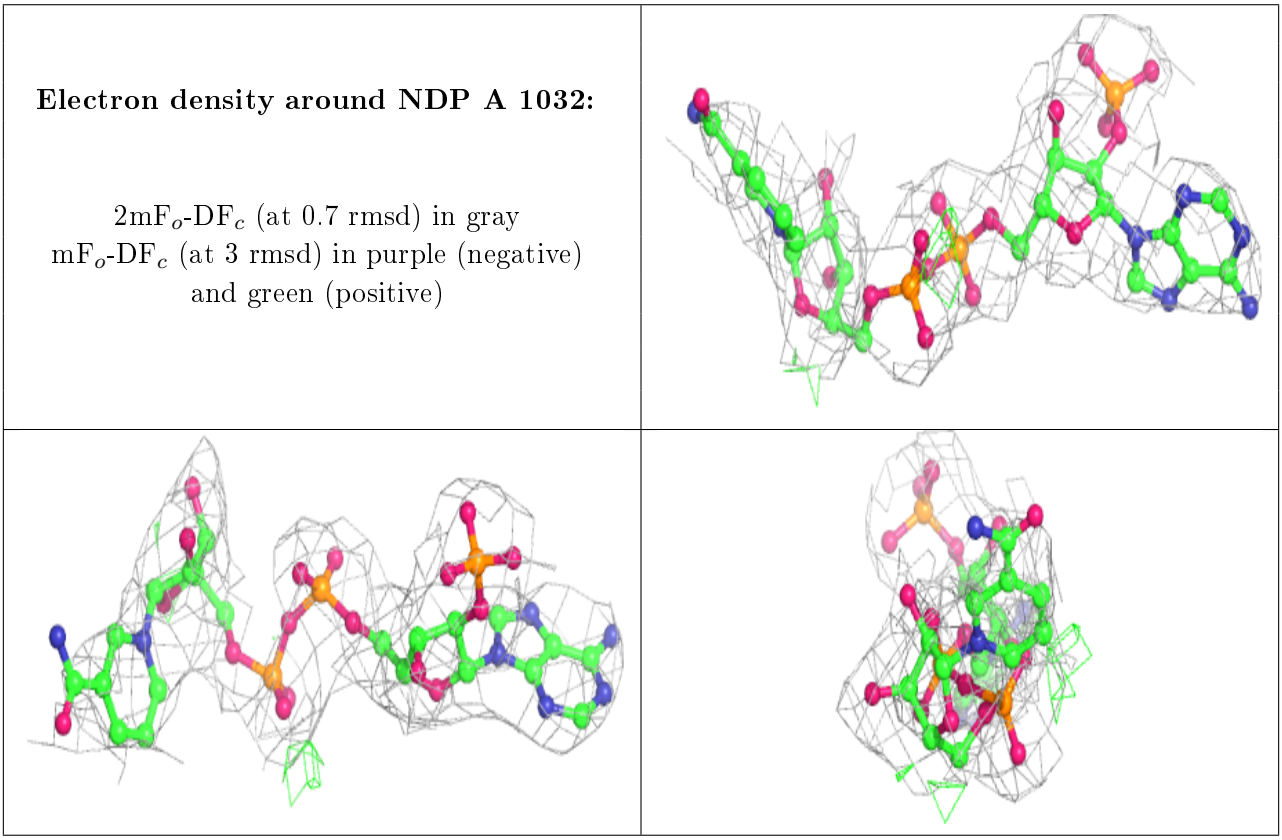
Electron density around FMN D 1030:

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



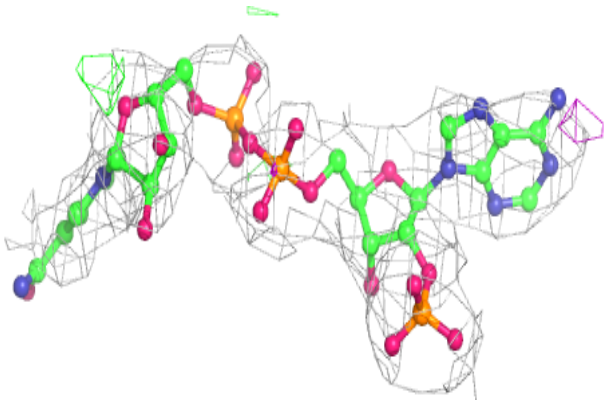
Electron density around NDP A 1032:

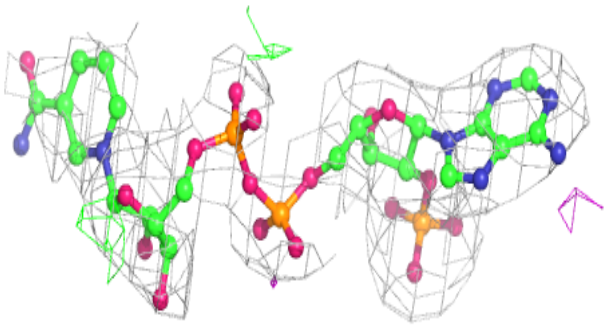
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

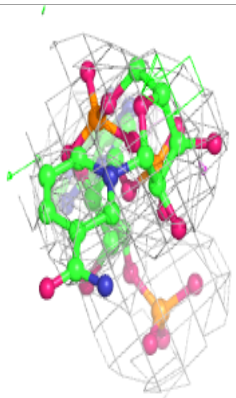


Electron density around NDP B 1032:

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

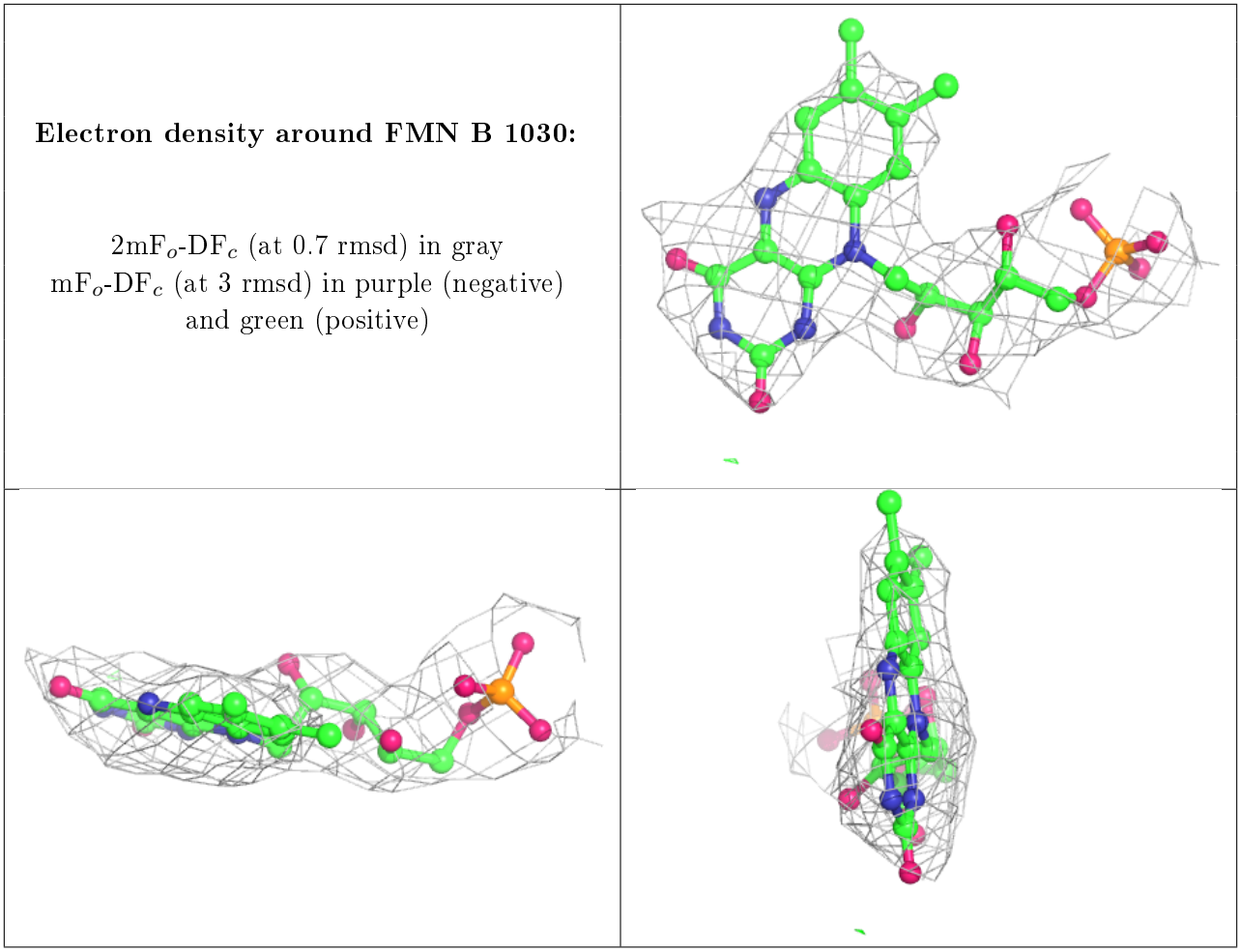






Electron density around FMN B 1030:

$2mF_o$-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.