



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:15 AM UTC

PDB ID : 2ZZC / pdb_00002zzc
Title : Crystal structure of NADP(H):human thioredoxin reductase I
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2009-02-09
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

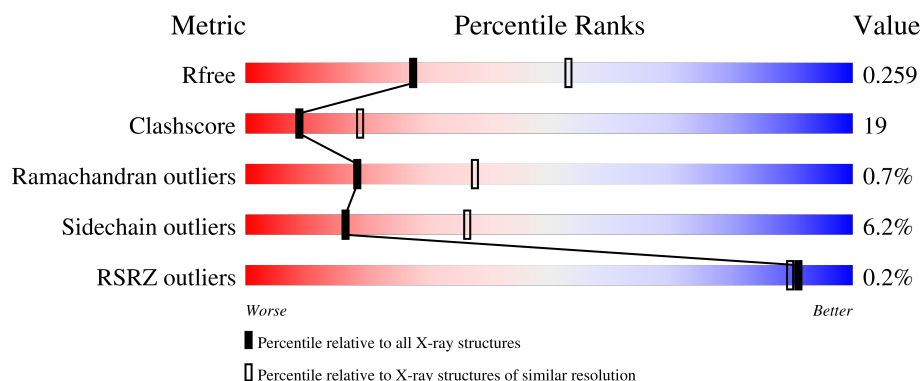
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	513	 54% 33% 8% 5%
1	B	513	 60% 32% 6% 2%
1	C	513	 56% 32% 6% 5%
1	D	513	 57% 31% 6% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16283 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 Thioredoxin reductase 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	19			
1	B	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			
1	C	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	19			
1	D	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q16881
A	-12	ALA	-	expression tag	UNP Q16881
A	-11	HIS	-	expression tag	UNP Q16881
A	-10	HIS	-	expression tag	UNP Q16881
A	-9	HIS	-	expression tag	UNP Q16881
A	-8	HIS	-	expression tag	UNP Q16881
A	-7	HIS	-	expression tag	UNP Q16881
A	-6	HIS	-	expression tag	UNP Q16881
A	-5	VAL	-	expression tag	UNP Q16881
A	-4	ASP	-	expression tag	UNP Q16881
A	-3	ASP	-	expression tag	UNP Q16881
A	-2	ASP	-	expression tag	UNP Q16881
A	-1	ASP	-	expression tag	UNP Q16881
A	498	CYS	U	SEE REMARK 999	UNP Q16881
B	-13	MET	-	expression tag	UNP Q16881
B	-12	ALA	-	expression tag	UNP Q16881
B	-11	HIS	-	expression tag	UNP Q16881
B	-10	HIS	-	expression tag	UNP Q16881
B	-9	HIS	-	expression tag	UNP Q16881
B	-8	HIS	-	expression tag	UNP Q16881
B	-7	HIS	-	expression tag	UNP Q16881

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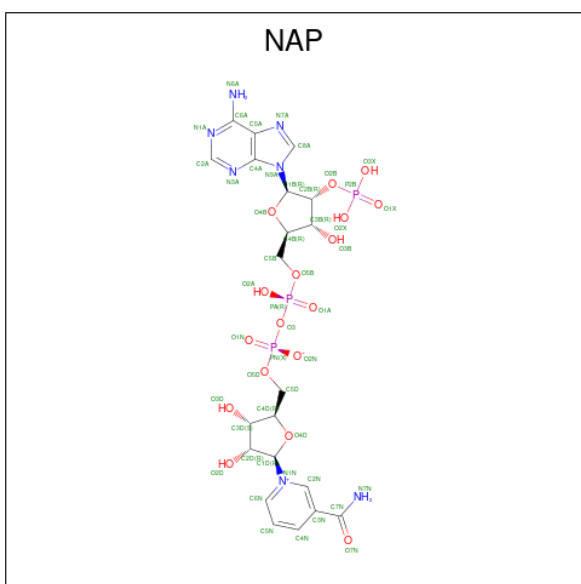
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q16881
B	-5	VAL	-	expression tag	UNP Q16881
B	-4	ASP	-	expression tag	UNP Q16881
B	-3	ASP	-	expression tag	UNP Q16881
B	-2	ASP	-	expression tag	UNP Q16881
B	-1	ASP	-	expression tag	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP Q16881
C	-13	MET	-	expression tag	UNP Q16881
C	-12	ALA	-	expression tag	UNP Q16881
C	-11	HIS	-	expression tag	UNP Q16881
C	-10	HIS	-	expression tag	UNP Q16881
C	-9	HIS	-	expression tag	UNP Q16881
C	-8	HIS	-	expression tag	UNP Q16881
C	-7	HIS	-	expression tag	UNP Q16881
C	-6	HIS	-	expression tag	UNP Q16881
C	-5	VAL	-	expression tag	UNP Q16881
C	-4	ASP	-	expression tag	UNP Q16881
C	-3	ASP	-	expression tag	UNP Q16881
C	-2	ASP	-	expression tag	UNP Q16881
C	-1	ASP	-	expression tag	UNP Q16881
C	498	CYS	U	SEE REMARK 999	UNP Q16881
D	-13	MET	-	expression tag	UNP Q16881
D	-12	ALA	-	expression tag	UNP Q16881
D	-11	HIS	-	expression tag	UNP Q16881
D	-10	HIS	-	expression tag	UNP Q16881
D	-9	HIS	-	expression tag	UNP Q16881
D	-8	HIS	-	expression tag	UNP Q16881
D	-7	HIS	-	expression tag	UNP Q16881
D	-6	HIS	-	expression tag	UNP Q16881
D	-5	VAL	-	expression tag	UNP Q16881
D	-4	ASP	-	expression tag	UNP Q16881
D	-3	ASP	-	expression tag	UNP Q16881
D	-2	ASP	-	expression tag	UNP Q16881
D	-1	ASP	-	expression tag	UNP Q16881
D	498	CYS	U	SEE REMARK 999	UNP Q16881

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

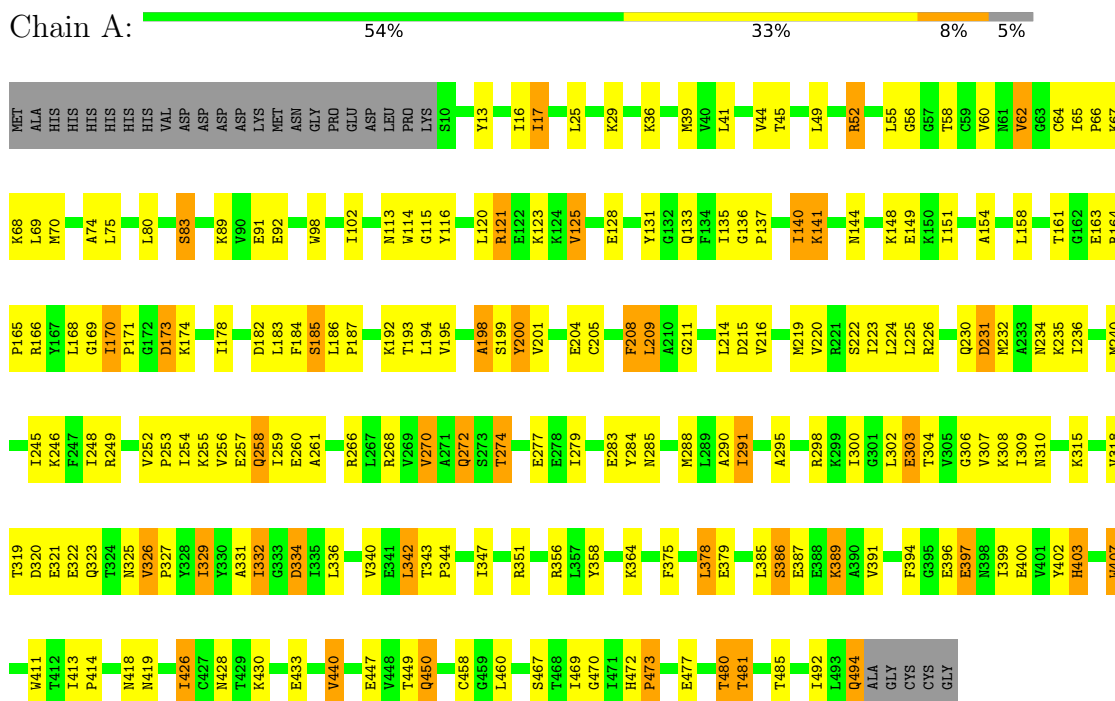
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	260	Total	O	0	0
			260	260		
4	C	184	Total	O	0	0
			184	184		
4	D	207	Total	O	0	0
			207	207		

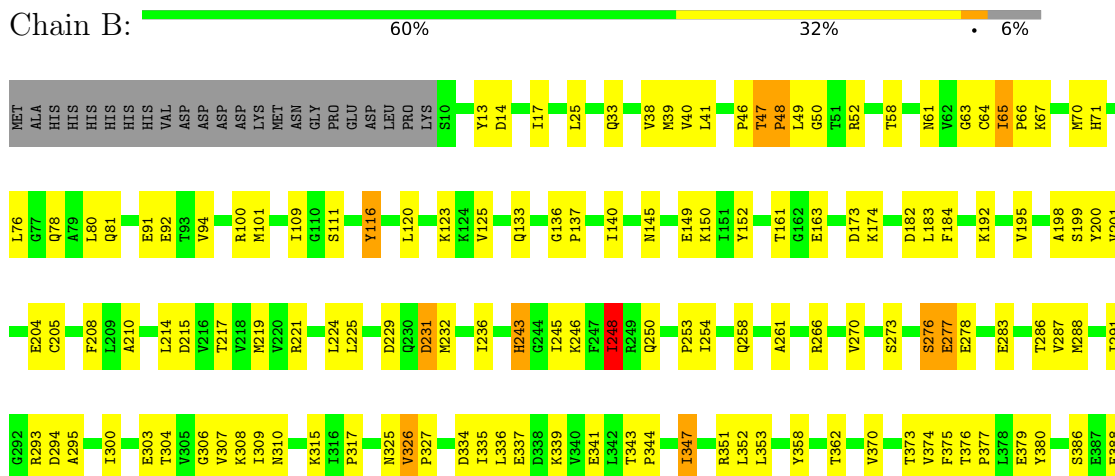
3 Residue-property plots [i](#)

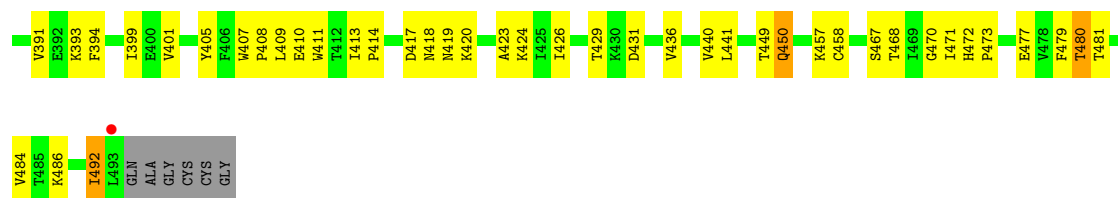
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Thioredoxin reductase 1, cytoplasmic



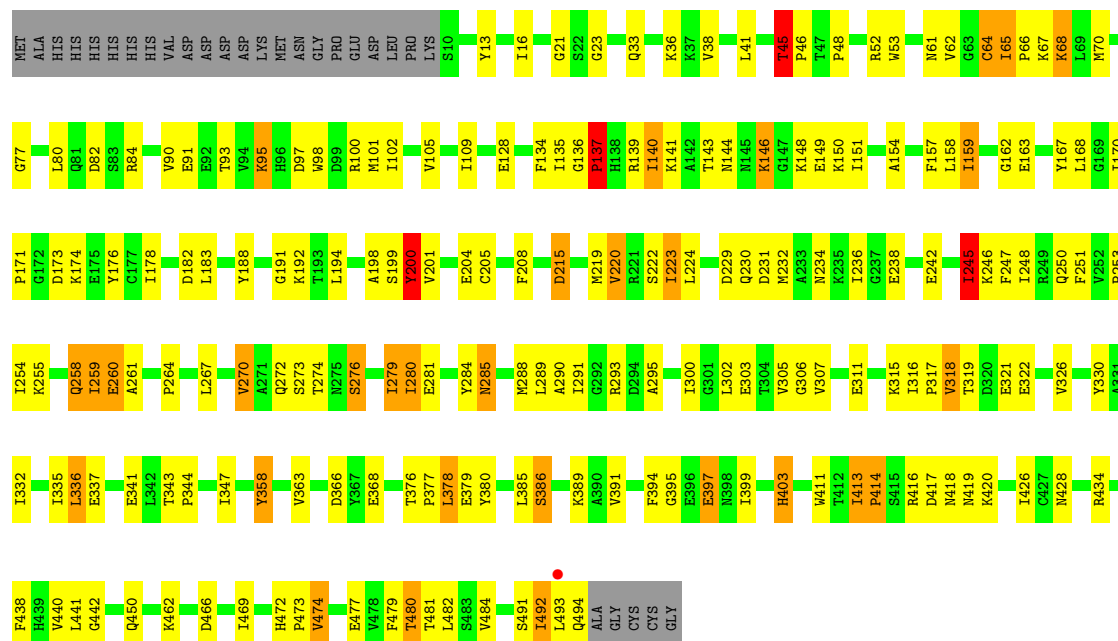
- Molecule 1: Thioredoxin reductase 1, cytoplasmic





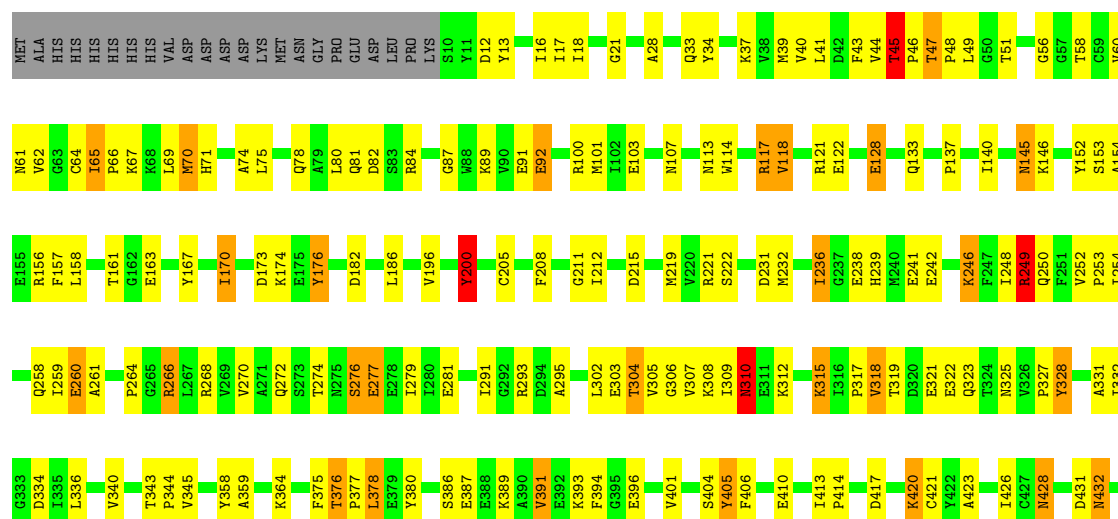
• Molecule 1: Thioredoxin reductase 1, cytoplasmic

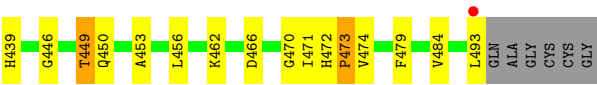
Chain C: 56% 32% 6% • 5%



• Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain D: 57% 31% 6% • 6%





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.86Å 135.17Å 346.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.60) 94.3 (30.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.260 0.210 , 0.259	Depositor DCC
R_{free} test set	4147 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16283	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	13/3824 (0.3%)	1.33	35/5178 (0.7%)
1	B	1.18	9/3815 (0.2%)	1.31	32/5166 (0.6%)
1	C	1.08	8/3824 (0.2%)	1.29	31/5178 (0.6%)
1	D	1.14	8/3815 (0.2%)	1.34	37/5166 (0.7%)
All	All	1.14	38/15278 (0.2%)	1.32	135/20688 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	3
All	All	0	5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	SER	CA-C	8.90	1.56	1.52
1	A	469	ILE	CA-CB	8.64	1.65	1.54
1	B	291	ILE	CA-CB	-7.81	1.46	1.54
1	A	407	TRP	C-O	-7.27	1.19	1.25
1	B	335	ILE	CA-CB	7.11	1.62	1.54
1	A	270	VAL	CA-CB	6.94	1.63	1.54
1	D	118	VAL	CA-CB	6.91	1.63	1.54
1	A	291	ILE	CA-CB	6.88	1.61	1.54
1	A	198	ALA	CA-CB	6.83	1.60	1.53
1	C	290	ALA	CA-C	-6.47	1.46	1.53
1	B	440	VAL	CA-CB	6.40	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	VAL	CA-CB	6.38	1.61	1.53
1	A	44	VAL	CA-CB	6.22	1.61	1.53
1	B	300	ILE	CA-CB	6.15	1.62	1.54
1	D	18	ILE	CA-CB	6.13	1.61	1.53
1	D	219	MET	SD-CE	6.08	1.94	1.79
1	B	436	VAL	CA-CB	6.08	1.62	1.54
1	C	220	VAL	CA-CB	6.03	1.61	1.54
1	C	426	ILE	CA-CB	6.00	1.61	1.54
1	C	170	ILE	CA-CB	5.76	1.64	1.54
1	D	484	VAL	CA-CB	-5.74	1.47	1.54
1	A	426	ILE	CA-CB	5.67	1.60	1.54
1	B	347	ILE	CA-CB	5.60	1.61	1.54
1	D	70	MET	SD-CE	-5.57	1.65	1.79
1	B	407	TRP	CA-C	-5.50	1.46	1.52
1	A	256	VAL	CA-CB	5.46	1.61	1.54
1	C	270	VAL	CA-CB	5.43	1.61	1.54
1	A	440	VAL	CA-C	-5.36	1.46	1.52
1	A	195	VAL	CA-CB	5.26	1.60	1.54
1	A	332	ILE	CA-CB	5.24	1.62	1.54
1	B	17	ILE	CA-CB	5.19	1.60	1.54
1	C	279	ILE	CA-CB	5.17	1.62	1.54
1	B	373	THR	CA-CB	5.15	1.62	1.53
1	C	363	VAL	CA-CB	5.13	1.60	1.54
1	C	62	VAL	CA-CB	5.12	1.61	1.54
1	A	62	VAL	CA-CB	5.12	1.61	1.54
1	D	62	VAL	CA-CB	5.10	1.61	1.54
1	D	170	ILE	CA-C	-5.08	1.48	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ILE	N-CA-C	-11.05	100.13	109.19
1	D	65	ILE	CA-C-N	-9.25	109.39	119.19
1	D	65	ILE	C-N-CA	-9.25	109.39	119.19
1	B	386	SER	N-CA-C	-9.18	98.68	110.53
1	A	170	ILE	N-CA-C	-8.24	102.43	109.19
1	D	327	PRO	N-CA-C	8.12	124.62	113.65
1	C	378	LEU	N-CA-C	-7.82	95.99	108.73
1	B	326	VAL	CA-C-N	7.51	129.23	119.84
1	B	326	VAL	C-N-CA	7.51	129.23	119.84
1	C	38	VAL	N-CA-C	7.50	119.63	108.46
1	D	45	THR	CA-C-N	7.47	127.47	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	45	THR	C-N-CA	7.47	127.47	119.78
1	C	45	THR	CA-C-N	7.30	128.96	119.84
1	C	45	THR	C-N-CA	7.30	128.96	119.84
1	B	370	VAL	N-CA-C	-7.27	102.38	108.63
1	D	310	ASN	N-CA-C	-7.22	95.84	108.20
1	A	326	VAL	CA-C-N	7.17	128.80	119.84
1	A	326	VAL	C-N-CA	7.17	128.80	119.84
1	D	71	HIS	N-CA-C	-7.15	103.42	111.14
1	A	248	ILE	N-CA-C	-7.09	97.40	107.75
1	D	306	GLY	N-CA-C	7.06	125.12	115.30
1	D	161	THR	N-CA-C	7.01	121.66	113.18
1	C	358	TYR	N-CA-C	6.99	122.66	113.30
1	D	248	ILE	N-CA-C	-6.97	97.70	107.80
1	B	420	LYS	N-CA-C	-6.96	105.41	114.04
1	C	484	VAL	N-CA-C	6.94	118.85	108.23
1	B	231	ASP	N-CA-C	-6.81	103.55	110.97
1	C	65	ILE	CA-C-N	-6.75	111.85	119.28
1	C	65	ILE	C-N-CA	-6.75	111.85	119.28
1	B	248	ILE	N-CA-C	-6.74	97.79	107.77
1	C	326	VAL	CA-C-N	6.67	128.18	119.84
1	C	326	VAL	C-N-CA	6.67	128.18	119.84
1	C	230	GLN	N-CA-C	6.66	119.54	111.82
1	A	298	ARG	N-CA-C	6.62	118.57	111.36
1	D	386	SER	N-CA-C	-6.60	102.02	110.53
1	A	481	THR	N-CA-C	6.58	120.65	111.56
1	D	378	LEU	N-CA-C	-6.54	97.86	108.52
1	A	258	GLN	N-CA-C	6.51	120.23	107.98
1	C	386	SER	N-CA-C	-6.51	102.14	110.53
1	C	248	ILE	N-CA-C	-6.50	98.15	107.77
1	A	173	ASP	N-CA-C	6.46	118.01	110.97
1	C	413	ILE	CA-C-N	-6.45	113.16	119.87
1	C	413	ILE	C-N-CA	-6.45	113.16	119.87
1	B	243	HIS	N-CA-C	6.39	119.79	112.57
1	B	310	ASN	N-CA-C	-6.36	96.73	107.99
1	A	449	THR	N-CA-C	6.33	118.27	111.36
1	A	358	TYR	N-CA-C	6.30	121.00	112.88
1	A	231	ASP	N-CA-C	-6.26	104.38	111.14
1	B	161	THR	N-CA-C	6.22	121.01	113.17
1	D	375	PHE	N-CA-C	6.21	120.33	110.70
1	C	403	HIS	N-CA-C	6.18	118.46	109.07
1	C	61	ASN	N-CA-C	6.18	121.03	112.45
1	D	145	ASN	N-CA-C	6.11	117.61	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	GLN	N-CA-C	6.11	118.44	111.11
1	D	236	ILE	N-CA-C	-6.11	104.55	110.72
1	D	231	ASP	N-CA-C	-6.06	104.59	111.14
1	D	81	GLN	N-CA-C	6.05	117.87	111.28
1	B	38	VAL	N-CA-C	6.03	117.17	108.48
1	D	453	ALA	N-CA-C	-6.03	104.71	111.28
1	D	417	ASP	N-CA-C	5.98	119.43	111.30
1	B	65	ILE	CA-C-N	-5.96	112.44	119.05
1	B	65	ILE	C-N-CA	-5.96	112.44	119.05
1	B	61	ASN	N-CA-C	5.94	120.66	113.41
1	B	358	TYR	N-CA-C	5.93	120.53	112.88
1	C	231	ASP	N-CA-C	-5.93	104.90	111.36
1	A	83	SER	N-CA-C	5.91	118.50	111.71
1	A	379	GLU	N-CA-C	5.90	118.82	110.50
1	C	258	GLN	N-CA-C	5.82	118.86	107.57
1	D	471	ILE	N-CA-C	-5.82	100.09	108.53
1	A	209	LEU	N-CA-C	-5.80	105.04	111.36
1	B	306	GLY	N-CA-C	5.80	124.01	115.08
1	A	208	PHE	N-CA-C	5.79	119.53	112.23
1	B	214	LEU	N-CA-C	5.79	119.09	110.52
1	B	450	GLN	N-CA-C	5.78	118.05	111.11
1	A	403	HIS	N-CA-C	5.78	117.86	109.07
1	A	375	PHE	N-CA-C	5.76	119.63	110.70
1	D	315	LYS	CA-C-N	-5.75	118.45	122.59
1	D	315	LYS	C-N-CA	-5.75	118.45	122.59
1	C	385	LEU	N-CA-C	5.71	118.93	110.48
1	D	176	TYR	N-CA-C	5.69	121.12	113.72
1	B	449	THR	N-CA-C	5.69	118.42	111.82
1	A	249	ARG	N-CA-C	5.67	119.06	109.76
1	B	431	ASP	N-CA-C	5.67	117.25	110.44
1	A	270	VAL	N-CA-C	-5.67	100.17	108.11
1	D	113	ASN	N-CA-C	-5.67	105.00	111.07
1	D	60	VAL	N-CA-C	5.65	116.38	110.62
1	B	375	PHE	N-CA-C	5.62	118.49	110.68
1	C	53	TRP	N-CA-C	5.62	117.33	108.96
1	C	413	ILE	CA-C-O	5.60	122.44	118.69
1	D	420	LYS	N-CA-C	-5.58	106.52	113.55
1	D	37	LYS	N-CA-C	-5.56	100.75	109.25
1	A	386	SER	N-CA-C	-5.55	103.37	110.53
1	A	378	LEU	N-CA-C	-5.53	99.72	108.73
1	B	14	ASP	N-CA-C	-5.52	105.27	112.23
1	C	414	PRO	N-CA-C	-5.52	107.24	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ASP	N-CA-C	-5.51	101.69	109.96
1	A	193	THR	N-CA-C	5.49	118.18	109.50
1	B	471	ILE	N-CA-C	-5.49	100.51	108.36
1	D	404	SER	N-CA-C	5.49	117.43	108.76
1	B	277	GLU	N-CA-C	-5.47	105.98	113.30
1	A	306	GLY	N-CA-C	5.45	122.88	115.30
1	A	342	LEU	N-CA-C	5.40	118.26	109.24
1	D	249	ARG	N-CA-C	5.40	118.04	109.24
1	C	347	ILE	N-CA-C	5.37	116.10	110.62
1	D	87	GLY	N-CA-C	5.35	122.14	114.64
1	B	413	ILE	CB-CA-C	-5.35	108.68	114.35
1	B	201	VAL	N-CA-C	5.35	115.55	110.42
1	A	334	ASP	N-CA-C	5.33	118.57	111.75
1	A	60	VAL	N-CA-C	5.32	115.53	110.42
1	C	492	ILE	CA-C-N	5.29	128.86	121.02
1	C	492	ILE	C-N-CA	5.29	128.86	121.02
1	B	195	VAL	CB-CA-C	-5.29	102.81	110.63
1	A	17	ILE	CA-C-N	-5.25	116.05	122.93
1	A	17	ILE	C-N-CA	-5.25	116.05	122.93
1	A	385	LEU	N-CA-C	5.24	118.65	110.32
1	C	201	VAL	N-CA-C	5.24	115.96	110.62
1	A	327	PRO	N-CA-C	5.22	123.22	112.47
1	A	222	SER	O-C-N	5.21	124.68	120.83
1	D	61	ASN	N-CA-C	5.19	119.61	113.12
1	D	405	TYR	N-CA-C	-5.18	103.84	110.53
1	A	161	THR	N-CA-C	5.18	119.60	113.28
1	D	82	ASP	N-CA-C	-5.18	105.81	111.82
1	B	71	HIS	N-CA-C	-5.16	105.55	111.07
1	A	75	LEU	N-CA-C	-5.15	105.74	111.36
1	B	484	VAL	N-CA-C	5.14	115.73	109.30
1	B	327	PRO	N-CA-C	5.13	123.03	112.47
1	C	245	ILE	N-CA-C	5.13	115.85	108.93
1	B	468	THR	N-CA-C	-5.12	101.36	109.76
1	C	306	GLY	N-CA-C	5.11	122.63	115.43
1	C	215	ASP	N-CA-C	-5.10	102.32	109.96
1	D	449	THR	N-CA-C	5.06	117.69	111.82
1	B	294	ASP	N-CA-C	5.05	117.20	109.07
1	D	43	PHE	CA-C-N	-5.04	116.25	123.10
1	D	43	PHE	C-N-CA	-5.04	116.25	123.10
1	D	358	TYR	N-CA-C	5.02	121.09	114.12

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	TYR	Sidechain
1	C	200	TYR	Sidechain
1	D	200	TYR	Sidechain
1	D	328	TYR	Sidechain
1	D	405	TYR	Sidechain

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	3750	0	3759	166	0
1	B	3741	0	3751	122	0
1	C	3750	0	3759	173	0
1	D	3741	0	3751	138	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	48	0	25	3	0
3	B	48	0	25	4	0
3	C	48	0	25	3	0
3	D	48	0	25	3	0
4	A	246	0	0	5	0
4	B	260	0	0	8	0
4	C	184	0	0	5	0
4	D	207	0	0	1	0
All	All	16283	0	15244	571	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 19.

All (571) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LYS:N	1:B:325:ASN:HD21	1.43	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ASN:ND2	1:C:494:GLN:HB2	1.62	1.13
1:D:302:LEU:HD22	1:D:307:VAL:HG21	1.27	1.12
1:B:308:LYS:H	1:B:325:ASN:ND2	1.48	1.09
1:D:39:MET:HE2	1:D:128:GLU:HG3	1.37	1.07
1:C:258:GLN:HE22	1:C:261:ALA:HB2	1.18	1.05
1:C:419:ASN:HD21	1:C:494:GLN:CB	1.69	1.05
1:C:183:LEU:HD22	1:C:288:MET:HE1	1.40	1.02
1:C:311:GLU:OE2	4:C:702:HOH:O	1.77	1.01
1:A:49:LEU:HD11	4:A:559:HOH:O	1.61	0.99
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.44	0.99
1:B:66:PRO:HG3	1:B:109:ILE:HD11	1.41	0.97
1:C:254:ILE:HD11	1:C:270:VAL:HG12	1.47	0.96
1:B:480:THR:HG22	1:B:481:THR:HG23	1.48	0.95
1:D:302:LEU:HD22	1:D:307:VAL:CG2	1.97	0.94
1:D:303:GLU:HG2	1:D:304:THR:N	1.84	0.93
1:C:493:LEU:O	1:C:493:LEU:HD12	1.70	0.92
1:D:39:MET:CE	1:D:128:GLU:HG3	1.99	0.92
1:A:36:LYS:HE2	1:A:36:LYS:HA	1.52	0.92
1:C:285:ASN:N	1:C:285:ASN:HD22	1.68	0.92
1:C:258:GLN:NE2	1:C:261:ALA:HB2	1.86	0.91
1:C:70:MET:HG2	1:C:101:MET:HE3	1.54	0.89
1:D:303:GLU:HG2	1:D:304:THR:H	1.38	0.89
1:D:84:ARG:NH1	1:D:92:GLU:HA	1.86	0.88
1:C:419:ASN:HD21	1:C:494:GLN:HB2	0.77	0.88
1:C:302:LEU:HD22	1:C:307:VAL:HB	1.56	0.88
1:C:318:VAL:HG11	1:C:322:GLU:HA	1.55	0.87
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.56	0.85
1:D:47:THR:HG22	1:D:49:LEU:H	1.38	0.85
1:C:173:ASP:OD1	1:C:174:LYS:N	2.09	0.85
1:C:397:GLU:CD	1:C:397:GLU:H	1.84	0.83
1:C:68:LYS:HE3	1:D:410:GLU:OE2	1.83	0.79
1:C:199:SER:OG	1:C:200:TYR:N	2.11	0.79
1:C:183:LEU:HD22	1:C:288:MET:CE	2.12	0.79
1:D:70:MET:HG2	1:D:101:MET:HE3	1.65	0.78
1:C:258:GLN:HE21	1:C:261:ALA:N	1.81	0.78
1:C:254:ILE:CD1	1:C:270:VAL:HG12	2.14	0.77
1:C:254:ILE:HD11	1:C:270:VAL:CG1	2.14	0.77
1:A:121:ARG:HH11	1:A:121:ARG:CG	1.98	0.77
1:A:70:MET:HE1	1:A:184:PHE:HD1	1.49	0.77
1:A:67:LYS:C	1:A:67:LYS:HD2	2.09	0.77
1:C:67:LYS:C	1:C:67:LYS:HD2	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:THR:HG22	1:A:481:THR:HG23	1.66	0.77
1:D:238:GLU:O	1:D:242:GLU:HG3	1.84	0.77
1:B:39:MET:HE1	1:B:152:TYR:CD1	2.20	0.76
1:C:158:LEU:HD11	1:C:332:ILE:HG12	1.68	0.75
1:D:47:THR:HG22	1:D:49:LEU:N	2.00	0.75
1:C:168:LEU:HD23	1:C:291:ILE:HD13	1.69	0.74
1:B:100:ARG:HG2	1:B:100:ARG:HH21	1.51	0.74
1:D:117:ARG:HG2	1:D:117:ARG:HH21	1.52	0.73
1:D:259:ILE:HD11	1:D:268:ARG:HB2	1.70	0.73
1:D:200:TYR:HB3	3:D:901:NAP:C5N	2.19	0.73
1:D:17:ILE:HG12	1:D:158:LEU:HD23	1.69	0.72
1:D:84:ARG:HH11	1:D:92:GLU:HA	1.52	0.72
1:B:215:ASP:OD1	1:B:246:LYS:NZ	2.23	0.72
1:B:258:GLN:OE1	1:B:261:ALA:HB2	1.90	0.72
1:A:200:TYR:HB3	3:A:901:NAP:C5N	2.20	0.71
1:B:200:TYR:HB3	3:B:901:NAP:C5N	2.20	0.71
1:C:394:PHE:HB2	1:C:399:ILE:HD11	1.73	0.71
1:B:405:TYR:CD1	1:B:492:ILE:HD13	2.25	0.70
1:C:41:LEU:HD23	1:C:128:GLU:HB2	1.73	0.70
1:A:173:ASP:OD1	1:A:174:LYS:N	2.25	0.70
1:C:16:ILE:HB	1:C:157:PHE:CE2	2.25	0.70
1:A:254:ILE:HD11	1:A:270:VAL:HG12	1.73	0.70
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.57	0.70
1:C:36:LYS:HE2	1:C:358:TYR:CD1	2.27	0.69
1:D:47:THR:CG2	1:D:49:LEU:H	2.05	0.69
1:A:266:ARG:NH1	1:A:283:GLU:OE1	2.22	0.69
1:B:250:GLN:HE22	1:D:222:SER:HB2	1.56	0.69
1:C:378:LEU:HD11	1:C:442:GLY:HA2	1.75	0.68
1:A:120:LEU:HD22	1:A:125:VAL:HG11	1.74	0.68
1:C:200:TYR:HB3	3:C:901:NAP:C5N	2.24	0.68
1:D:205:CYS:HA	1:D:208:PHE:CE2	2.28	0.68
1:A:36:LYS:HE2	1:A:36:LYS:CA	2.22	0.68
1:C:80:LEU:HD23	1:D:80:LEU:HD23	1.76	0.68
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.08	0.68
1:D:315:LYS:HE3	1:D:336:LEU:O	1.92	0.67
1:C:146:LYS:HE3	1:C:148:LYS:HE2	1.76	0.67
1:C:259:ILE:HG22	1:C:259:ILE:O	1.94	0.67
1:D:47:THR:HG21	1:D:182:ASP:OD1	1.94	0.67
1:D:302:LEU:HB3	1:D:307:VAL:HG23	1.75	0.67
1:A:70:MET:CE	1:A:184:PHE:HD1	2.07	0.67
1:C:474:VAL:O	1:C:477:GLU:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD23	1:B:80:LEU:CD2	2.23	0.66
1:A:194:LEU:HD22	1:A:284:TYR:CE1	2.29	0.66
1:C:254:ILE:CG1	1:C:270:VAL:HG12	2.24	0.66
1:B:315:LYS:HB2	1:B:337:GLU:HB2	1.76	0.66
1:C:168:LEU:CD2	1:C:291:ILE:HD13	2.25	0.66
1:B:205:CYS:HA	1:B:208:PHE:CE2	2.30	0.66
1:A:318:VAL:HG23	1:A:323:GLN:C	2.21	0.66
1:C:258:GLN:NE2	1:C:261:ALA:CB	2.56	0.66
1:C:238:GLU:O	1:C:242:GLU:HG3	1.94	0.66
1:A:121:ARG:HG3	1:A:121:ARG:NH1	2.09	0.66
1:A:319:THR:HG23	1:A:323:GLN:O	1.96	0.66
1:C:198:ALA:HB2	1:C:220:VAL:HG13	1.78	0.66
1:C:379:GLU:O	1:C:441:LEU:HD12	1.96	0.66
1:B:393:LYS:HD3	1:B:394:PHE:CE1	2.30	0.65
1:D:428:ASN:ND2	1:D:431:ASP:HB3	2.10	0.65
1:C:480:THR:HG22	1:C:481:THR:HG23	1.79	0.65
1:D:176:TYR:CE1	1:D:258:GLN:HB2	2.31	0.65
1:A:205:CYS:HA	1:A:208:PHE:CE2	2.32	0.65
1:C:258:GLN:NE2	1:C:261:ALA:CA	2.60	0.64
1:B:219:MET:SD	1:B:253:PRO:HD3	2.37	0.64
1:D:117:ARG:HG2	1:D:117:ARG:NH2	2.13	0.64
1:A:315:LYS:HD2	1:A:336:LEU:O	1.98	0.64
1:A:480:THR:CG2	1:A:481:THR:HG23	2.28	0.64
1:A:340:VAL:CG1	1:A:342:LEU:HD12	2.28	0.64
1:C:105:VAL:O	1:C:109:ILE:HG13	1.98	0.64
1:A:192:LYS:H	1:A:285:ASN:HD22	1.43	0.64
1:D:272:GLN:HB2	1:D:279:ILE:HD13	1.80	0.63
1:A:400:GLU:OE2	1:A:400:GLU:HA	1.97	0.63
1:D:258:GLN:NE2	1:D:261:ALA:HA	2.14	0.63
1:D:462:LYS:HD2	1:D:466:ASP:OD1	1.99	0.63
1:A:223:ILE:HD11	1:A:226:ARG:HB2	1.81	0.63
1:A:477:GLU:O	1:A:480:THR:HB	1.99	0.63
1:B:47:THR:HG23	1:B:48:PRO:HD2	1.81	0.62
1:B:47:THR:HG21	1:B:182:ASP:OD1	1.99	0.62
1:A:308:LYS:N	1:A:325:ASN:OD1	2.27	0.62
1:A:39:MET:HE2	1:A:41:LEU:HG	1.79	0.62
1:D:242:GLU:OE2	1:D:420:LYS:NZ	2.23	0.62
1:C:318:VAL:CG1	1:C:322:GLU:HA	2.27	0.62
1:A:472:HIS:ND1	1:A:473:PRO:HA	2.14	0.62
1:B:325:ASN:OD1	1:B:326:VAL:HG23	1.99	0.62
1:B:374:VAL:HG12	1:B:376:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LYS:HD3	1:C:149:GLU:OE2	1.99	0.62
1:A:318:VAL:CG2	1:A:322:GLU:C	2.73	0.62
1:C:171:PRO:CG	1:C:255:LYS:HD2	2.30	0.61
1:D:100:ARG:HG2	1:D:100:ARG:NH2	2.14	0.61
1:B:91:GLU:OE2	4:B:660:HOH:O	2.16	0.61
1:C:254:ILE:HG12	1:C:270:VAL:O	2.00	0.61
1:C:322:GLU:HG2	1:C:332:ILE:HG22	1.83	0.61
1:A:186:LEU:HD12	1:A:187:PRO:HD2	1.80	0.61
1:A:387:GLU:O	1:A:391:VAL:HG23	2.01	0.60
1:C:315:LYS:HD2	1:C:336:LEU:O	2.01	0.60
1:A:17:ILE:HG12	1:A:158:LEU:HD23	1.83	0.60
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.67	0.60
1:D:413:ILE:HB	1:D:414:PRO:HD3	1.83	0.60
1:A:209:LEU:HB3	1:A:214:LEU:HD12	1.84	0.59
1:A:80:LEU:CD2	1:B:80:LEU:HD23	2.26	0.59
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.83	0.59
1:A:303:GLU:OE1	1:A:304:THR:HG23	2.02	0.59
1:A:319:THR:C	1:A:321:GLU:H	2.10	0.58
1:D:305:VAL:CG2	1:D:328:TYR:OH	2.51	0.58
1:D:258:GLN:NE2	1:D:261:ALA:CA	2.66	0.58
1:A:318:VAL:HG21	1:A:322:GLU:C	2.29	0.58
1:D:254:ILE:HD11	1:D:270:VAL:HG12	1.83	0.58
1:D:387:GLU:O	1:D:391:VAL:HG12	2.03	0.58
1:C:178:ILE:HB	1:C:182:ASP:HB2	1.86	0.58
1:C:293:ARG:HG2	1:C:293:ARG:NH1	2.17	0.58
1:A:325:ASN:ND2	1:A:326:VAL:HG23	2.18	0.58
1:A:419:ASN:OD1	1:A:494:GLN:HB2	2.03	0.58
1:A:168:LEU:HD21	3:A:901:NAP:N6A	2.19	0.58
1:B:100:ARG:HG2	1:B:100:ARG:NH2	2.19	0.57
1:B:245:ILE:H	1:B:245:ILE:HD12	1.68	0.57
1:C:319:THR:C	1:C:321:GLU:H	2.11	0.57
1:B:401:VAL:HG11	1:B:486:LYS:HD2	1.86	0.57
1:A:183:LEU:O	1:A:183:LEU:HD12	2.04	0.57
1:B:405:TYR:CE1	1:B:492:ILE:HD13	2.39	0.57
1:C:98:TRP:NE1	1:C:102:ILE:HG13	2.20	0.57
1:C:366:ASP:OD1	1:C:366:ASP:C	2.48	0.57
1:C:378:LEU:CD2	1:C:441:LEU:HG	2.35	0.57
1:D:270:VAL:HG22	1:D:281:GLU:HG2	1.87	0.57
1:D:272:GLN:OE1	1:D:279:ILE:HD11	2.04	0.57
1:C:36:LYS:HE2	1:C:358:TYR:HD1	1.70	0.57
1:A:394:PHE:HD2	1:A:430:LYS:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ARG:HG3	1:D:156:ARG:HH11	1.70	0.57
1:A:351:ARG:HD3	4:A:723:HOH:O	2.05	0.57
1:B:92:GLU:O	1:B:92:GLU:HG2	2.05	0.57
1:C:234:ASN:O	1:C:238:GLU:HG3	2.05	0.57
1:D:241:GLU:CD	1:D:249:ARG:HH22	2.13	0.57
1:C:137:PRO:O	1:C:139:ARG:HG3	2.04	0.56
1:C:250:GLN:HB3	1:C:274:THR:HG22	1.87	0.56
1:D:334:ASP:OD2	2:D:900:FAD:H5'1	2.05	0.56
1:A:234:ASN:ND2	4:A:699:HOH:O	2.37	0.56
1:D:41:LEU:HD23	1:D:128:GLU:HB2	1.88	0.56
1:A:288:MET:HE2	1:A:290:ALA:HB2	1.87	0.56
1:A:343:THR:HB	1:A:344:PRO:HD3	1.87	0.56
1:C:417:ASP:HB3	1:C:420:LYS:HG3	1.87	0.56
1:B:424:LYS:HE3	1:B:426:ILE:HD11	1.87	0.56
1:D:309:ILE:HG13	1:D:310:ASN:N	2.20	0.56
1:D:91:GLU:HG2	1:D:92:GLU:N	2.21	0.56
1:A:472:HIS:HD1	1:A:473:PRO:HA	1.71	0.56
1:A:259:ILE:HG21	1:A:266:ARG:NH2	2.21	0.56
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.87	0.56
1:D:16:ILE:HD12	1:D:157:PHE:CZ	2.41	0.56
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.87	0.56
1:D:140:ILE:HG21	1:D:157:PHE:HE2	1.69	0.56
1:A:140:ILE:HG12	1:A:141:LYS:N	2.21	0.55
1:B:343:THR:HB	1:B:344:PRO:HD3	1.88	0.55
1:A:391:VAL:HG13	1:A:396:GLU:HA	1.86	0.55
1:C:173:ASP:HB2	1:C:289:LEU:HD11	1.88	0.55
1:A:240:MET:HE2	1:A:245:ILE:CD1	2.36	0.55
1:B:173:ASP:OD1	1:B:174:LYS:N	2.37	0.55
1:D:39:MET:HE1	1:D:152:TYR:CZ	2.41	0.55
1:B:405:TYR:HD1	1:B:492:ILE:HD13	1.72	0.55
1:C:245:ILE:HG22	1:C:247:PHE:CE2	2.42	0.55
1:B:410:GLU:H	1:B:410:GLU:CD	2.15	0.55
1:C:477:GLU:O	1:C:480:THR:HB	2.07	0.55
1:D:319:THR:HG23	1:D:323:GLN:O	2.07	0.55
1:D:428:ASN:ND2	1:D:431:ASP:CB	2.70	0.55
1:A:331:ALA:C	1:A:336:LEU:HD21	2.31	0.54
1:D:133:GLN:O	1:D:140:ILE:HG13	2.08	0.54
1:A:258:GLN:OE1	1:A:261:ALA:HB2	2.07	0.54
1:A:67:LYS:NZ	1:A:204:GLU:OE1	2.33	0.54
1:D:259:ILE:CD1	1:D:268:ARG:HB2	2.36	0.54
1:B:308:LYS:HB2	1:B:325:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLN:O	1:B:140:ILE:HG13	2.08	0.54
1:D:423:ALA:HB1	1:D:479:PHE:CZ	2.43	0.54
1:B:308:LYS:HE2	1:B:325:ASN:HD22	1.72	0.53
1:C:259:ILE:O	1:C:260:GLU:CB	2.56	0.53
1:B:47:THR:HG22	1:B:49:LEU:H	1.72	0.53
1:C:258:GLN:HE21	1:C:261:ALA:CA	2.21	0.53
1:A:428:ASN:OD1	1:A:430:LYS:HG2	2.08	0.53
1:B:273:SER:OG	1:B:278:GLU:HG2	2.08	0.53
1:A:340:VAL:HG12	1:A:342:LEU:HD12	1.89	0.53
1:A:240:MET:HE2	1:A:245:ILE:HD13	1.91	0.53
1:C:258:GLN:HE21	1:C:260:GLU:C	2.16	0.53
1:A:236:ILE:O	1:A:240:MET:HG3	2.09	0.53
1:A:391:VAL:HG13	1:A:396:GLU:CA	2.39	0.53
1:D:17:ILE:HB	1:D:40:VAL:HG22	1.89	0.53
1:A:325:ASN:HD21	1:A:326:VAL:HG23	1.74	0.53
1:A:178:ILE:HB	1:A:182:ASP:HB2	1.89	0.53
1:A:255:LYS:HE3	1:A:257:GLU:HB3	1.91	0.53
1:A:13:TYR:O	1:A:154:ALA:HA	2.08	0.53
1:B:293:ARG:HD3	3:B:901:NAP:H51N	1.90	0.53
1:B:379:GLU:O	1:B:441:LEU:HD12	2.09	0.53
1:C:302:LEU:HD22	1:C:307:VAL:CB	2.35	0.53
1:C:95:LYS:CB	1:D:89:LYS:HE3	2.39	0.52
1:D:34:TYR:CE2	1:D:359:ALA:HB2	2.45	0.52
1:D:293:ARG:HD3	3:D:901:NAP:H51N	1.90	0.52
1:B:308:LYS:HB2	1:B:325:ASN:ND2	2.24	0.52
1:D:272:GLN:HB2	1:D:279:ILE:CD1	2.39	0.52
1:B:217:THR:HG21	1:B:248:ILE:HD12	1.92	0.52
1:C:322:GLU:O	1:C:330:TYR:HB3	2.10	0.52
1:C:450:GLN:OE1	1:D:470:GLY:HA2	2.09	0.52
1:D:258:GLN:HE21	1:D:261:ALA:HA	1.73	0.52
1:C:84:ARG:HG2	1:C:90:VAL:HG23	1.91	0.52
1:C:90:VAL:HG11	1:D:80:LEU:CD2	2.40	0.52
1:C:134:PHE:CD1	1:C:305:VAL:HG11	2.45	0.52
1:C:343:THR:HB	1:C:344:PRO:HD3	1.92	0.52
1:B:33:GLN:HE21	1:B:123:LYS:NZ	2.09	0.51
1:C:480:THR:CG2	1:C:481:THR:HG23	2.40	0.51
1:A:223:ILE:HD11	1:A:226:ARG:CB	2.39	0.51
1:D:100:ARG:HG2	1:D:100:ARG:HH21	1.74	0.51
1:C:258:GLN:HG2	1:C:260:GLU:H	1.75	0.50
1:C:462:LYS:HD2	1:C:462:LYS:O	2.11	0.50
1:D:309:ILE:HA	1:D:317:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LYS:HD3	1:D:389:LYS:N	2.25	0.50
1:A:29:LYS:HG2	1:A:123:LYS:HG3	1.93	0.50
1:C:135:ILE:HD13	1:C:151:ILE:HD12	1.94	0.50
1:B:315:LYS:HE3	1:B:336:LEU:O	2.10	0.50
1:D:114:TRP:HZ3	1:D:117:ARG:HH11	1.58	0.50
1:D:276:SER:OG	1:D:277:GLU:N	2.44	0.50
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.94	0.50
1:C:140:ILE:HG21	1:C:157:PHE:CE2	2.47	0.50
1:C:198:ALA:CB	1:C:220:VAL:HG13	2.41	0.50
1:C:259:ILE:O	1:C:259:ILE:CG2	2.60	0.50
1:A:318:VAL:HG22	1:A:319:THR:N	2.27	0.50
1:D:322:GLU:HG2	1:D:332:ILE:HG22	1.94	0.50
1:A:394:PHE:CD2	1:A:430:LYS:HE2	2.46	0.50
1:C:23:GLY:HA3	1:C:332:ILE:HD12	1.94	0.50
1:C:285:ASN:N	1:C:285:ASN:ND2	2.43	0.49
1:A:274:THR:CG2	1:A:274:THR:O	2.60	0.49
1:A:447:GLU:OE1	1:A:447:GLU:HA	2.13	0.49
1:B:307:VAL:HA	1:B:325:ASN:OD1	2.12	0.49
1:C:215:ASP:OD1	1:C:246:LYS:NZ	2.41	0.49
1:A:309:ILE:HG13	1:A:310:ASN:N	2.27	0.49
1:B:198:ALA:HB1	1:B:224:LEU:HD22	1.93	0.49
1:A:303:GLU:CD	1:A:303:GLU:H	2.19	0.49
1:B:245:ILE:HD12	1:B:245:ILE:N	2.27	0.49
1:C:440:VAL:HG13	1:C:440:VAL:O	2.13	0.49
1:D:236:ILE:HD11	1:D:380:TYR:HB2	1.95	0.49
1:C:251:PHE:CE1	1:C:280:ILE:HD12	2.48	0.49
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.48	0.49
1:B:47:THR:O	1:B:50:GLY:N	2.37	0.49
1:D:343:THR:HB	1:D:344:PRO:HD3	1.95	0.49
1:A:318:VAL:HG23	1:A:323:GLN:O	2.13	0.49
1:B:200:TYR:CD2	3:B:901:NAP:H3D	2.47	0.49
1:D:376:THR:O	1:D:377:PRO:C	2.56	0.49
1:A:356:ARG:NH1	1:A:364:LYS:HA	2.28	0.48
1:B:339:LYS:CE	4:B:783:HOH:O	2.60	0.48
1:C:143:THR:HG23	1:C:149:GLU:HG2	1.94	0.48
1:D:260:GLU:OE1	1:D:266:ARG:NH2	2.46	0.48
1:A:214:LEU:O	1:A:216:VAL:HG23	2.13	0.48
1:B:405:TYR:CE1	1:B:492:ILE:CD1	2.96	0.48
1:B:46:PRO:HB3	1:B:52:ARG:NH1	2.28	0.48
1:B:339:LYS:NZ	4:B:783:HOH:O	2.45	0.48
1:D:75:LEU:O	1:D:78:GLN:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:SER:O	1:C:200:TYR:C	2.57	0.48
1:D:12:ASP:HB2	1:D:153:SER:O	2.13	0.48
1:A:135:ILE:CD1	1:A:151:ILE:HD13	2.42	0.48
1:A:198:ALA:HB1	1:A:224:LEU:HD23	1.95	0.48
1:B:418:ASN:OD1	1:B:419:ASN:ND2	2.47	0.48
1:C:90:VAL:HG11	1:D:80:LEU:HD21	1.95	0.48
1:C:97:ASP:OD1	4:C:561:HOH:O	2.20	0.48
1:A:55:LEU:O	1:A:113:ASN:OD1	2.32	0.48
1:A:194:LEU:HD21	1:A:219:MET:HE3	1.96	0.48
1:C:95:LYS:HB3	1:D:89:LYS:HE3	1.96	0.48
1:A:450:GLN:OE1	1:B:470:GLY:HA2	2.14	0.48
1:C:13:TYR:O	1:C:154:ALA:HA	2.14	0.48
1:C:67:LYS:HD2	1:C:68:LYS:N	2.29	0.48
1:A:272:GLN:HB2	1:A:279:ILE:HG12	1.95	0.48
1:C:70:MET:HG2	1:C:101:MET:CE	2.36	0.48
1:C:198:ALA:HB1	1:C:224:LEU:CD2	2.43	0.48
1:B:308:LYS:CB	1:B:325:ASN:ND2	2.76	0.48
1:C:149:GLU:O	1:C:150:LYS:HG3	2.14	0.48
1:C:188:TYR:CD1	1:C:188:TYR:C	2.92	0.48
1:C:272:GLN:HB2	1:C:279:ILE:HD13	1.94	0.48
1:D:173:ASP:OD1	1:D:174:LYS:N	2.40	0.47
1:C:91:GLU:HG3	1:C:93:THR:H	1.78	0.47
1:C:171:PRO:HG3	1:C:255:LYS:HD2	1.94	0.47
1:C:397:GLU:OE2	1:C:397:GLU:N	2.43	0.47
1:C:493:LEU:O	1:C:493:LEU:CD1	2.52	0.47
1:D:74:ALA:HB1	1:D:211:GLY:HA3	1.97	0.47
1:D:258:GLN:HE22	1:D:261:ALA:HB2	1.79	0.47
1:B:47:THR:HG22	1:B:49:LEU:N	2.30	0.47
1:C:474:VAL:HG11	1:D:446:GLY:HA3	1.96	0.47
1:A:25:LEU:HD13	1:A:116:TYR:CD1	2.49	0.47
1:B:47:THR:O	1:B:48:PRO:C	2.58	0.47
1:D:302:LEU:HB3	1:D:307:VAL:CG2	2.42	0.47
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.49	0.47
1:A:232:MET:O	1:A:236:ILE:HG13	2.14	0.47
1:A:343:THR:O	1:A:347:ILE:HG13	2.14	0.47
1:C:167:TYR:CE2	1:C:174:LYS:HA	2.50	0.47
1:C:222:SER:OG	1:C:223:ILE:N	2.44	0.47
1:D:21:GLY:HA2	1:D:56:GLY:O	2.13	0.47
1:D:167:TYR:CE2	1:D:174:LYS:HA	2.50	0.47
1:D:118:VAL:O	1:D:122:GLU:HG3	2.14	0.47
1:A:55:LEU:HD12	1:A:56:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:CD	1:A:91:GLU:H	2.23	0.47
1:A:302:LEU:HD13	1:A:307:VAL:HG12	1.97	0.47
1:B:215:ASP:CG	1:B:246:LYS:HZ1	2.19	0.47
1:A:192:LYS:N	1:A:285:ASN:HD22	2.12	0.47
1:A:411:TRP:C	1:A:414:PRO:HD2	2.39	0.47
1:C:135:ILE:HD11	1:C:139:ARG:NH1	2.29	0.47
1:C:229:ASP:OD1	1:C:232:MET:HG2	2.15	0.47
1:D:340:VAL:HB	1:D:345:VAL:HG21	1.97	0.47
1:A:397:GLU:CD	1:A:397:GLU:H	2.23	0.46
1:C:171:PRO:HG2	1:C:255:LYS:HD2	1.97	0.46
1:C:419:ASN:ND2	1:C:494:GLN:HE21	2.12	0.46
1:D:258:GLN:NE2	1:D:261:ALA:HB2	2.30	0.46
1:D:65:ILE:HG22	1:D:66:PRO:N	2.30	0.46
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.30	0.46
1:C:318:VAL:CG1	1:C:319:THR:N	2.76	0.46
1:D:232:MET:HE2	1:D:439:HIS:HB3	1.96	0.46
1:B:200:TYR:HD2	3:B:901:NAP:H3D	1.81	0.46
1:C:200:TYR:HB3	3:C:901:NAP:C4N	2.45	0.46
1:D:70:MET:HG2	1:D:101:MET:CE	2.41	0.46
1:A:131:TYR:C	1:A:131:TYR:CD2	2.94	0.46
1:A:246:LYS:HE2	4:A:738:HOH:O	2.15	0.46
1:A:403:HIS:CE1	1:A:492:ILE:HD13	2.51	0.46
1:B:477:GLU:O	1:B:480:THR:HB	2.15	0.46
1:C:46:PRO:HG3	1:C:52:ARG:HG2	1.96	0.46
1:A:121:ARG:HH11	1:A:121:ARG:HG2	1.79	0.46
1:B:145:ASN:HB2	4:B:746:HOH:O	2.16	0.46
1:B:266:ARG:NH1	1:B:283:GLU:OE1	2.47	0.46
1:D:196:VAL:HG21	1:D:253:PRO:HG2	1.97	0.46
1:A:230:GLN:O	1:A:234:ASN:ND2	2.48	0.46
1:C:418:ASN:OD1	1:C:419:ASN:N	2.49	0.46
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.60	0.46
1:C:302:LEU:CD2	1:C:307:VAL:HB	2.35	0.46
1:B:308:LYS:H	1:B:325:ASN:HD21	0.66	0.45
1:C:259:ILE:O	1:C:260:GLU:HB2	2.15	0.45
1:D:215:ASP:OD1	1:D:246:LYS:HE2	2.16	0.45
1:D:318:VAL:HG22	1:D:322:GLU:C	2.41	0.45
1:A:120:LEU:HD22	1:A:125:VAL:CG1	2.44	0.45
1:A:133:GLN:CD	1:A:141:LYS:HZ2	2.24	0.45
1:A:386:SER:OG	1:A:389:LYS:HB2	2.17	0.45
1:A:407:TRP:CD1	1:A:418:ASN:HA	2.52	0.45
1:B:236:ILE:HD11	1:B:380:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:VAL:HG12	1:D:291:ILE:CG2	2.46	0.45
1:A:458:CYS:CB	1:B:458:CYS:HB3	2.46	0.45
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.98	0.45
1:B:303:GLU:HG2	1:B:304:THR:N	2.30	0.45
1:D:308:LYS:N	1:D:325:ASN:OD1	2.41	0.45
1:D:319:THR:C	1:D:321:GLU:H	2.23	0.45
1:A:307:VAL:HA	1:A:325:ASN:OD1	2.15	0.45
1:D:13:TYR:O	1:D:154:ALA:HA	2.15	0.45
1:D:221:ARG:O	1:D:250:GLN:HA	2.16	0.45
1:A:268:ARG:NH2	4:A:619:HOH:O	2.49	0.45
1:B:347:ILE:O	1:B:351:ARG:HG3	2.16	0.45
1:A:166:ARG:HB3	1:A:291:ILE:HD12	1.97	0.45
1:A:186:LEU:HA	1:A:187:PRO:HD2	1.80	0.45
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.81	0.45
1:C:21:GLY:HA3	2:C:900:FAD:O5B	2.17	0.45
1:C:462:LYS:HE2	1:C:466:ASP:OD2	2.17	0.45
1:A:407:TRP:CG	1:A:418:ASN:HD22	2.35	0.45
1:A:440:VAL:HG13	1:A:440:VAL:O	2.17	0.45
1:B:120:LEU:HD22	1:B:125:VAL:HG11	1.99	0.45
1:C:258:GLN:C	1:C:260:GLU:H	2.24	0.45
1:B:13:TYR:CE2	1:B:39:MET:HB2	2.52	0.45
1:D:114:TRP:HZ3	1:D:117:ARG:NH1	2.13	0.45
1:D:140:ILE:HG21	1:D:157:PHE:CE2	2.49	0.45
1:D:266:ARG:HH11	1:D:266:ARG:HG2	1.81	0.45
1:D:303:GLU:CG	1:D:304:THR:N	2.68	0.45
1:C:67:LYS:HB3	1:C:67:LYS:HE2	1.73	0.45
1:C:251:PHE:CZ	1:C:280:ILE:HD12	2.52	0.45
1:C:440:VAL:HB	1:C:479:PHE:HZ	1.82	0.45
1:A:168:LEU:CD2	3:A:901:NAP:N6A	2.79	0.44
1:B:65:ILE:HG22	1:B:66:PRO:N	2.28	0.44
1:B:351:ARG:HD2	4:B:539:HOH:O	2.17	0.44
1:A:67:LYS:HD2	1:A:68:LYS:N	2.33	0.44
1:A:185:SER:O	1:A:186:LEU:C	2.59	0.44
1:A:467:SER:OG	1:B:457:LYS:HD2	2.17	0.44
1:C:219:MET:SD	1:C:253:PRO:HG3	2.58	0.44
1:C:411:TRP:O	1:C:414:PRO:HD2	2.17	0.44
1:C:494:GLN:O	1:C:494:GLN:HG3	2.17	0.44
1:C:67:LYS:C	1:C:67:LYS:CD	2.82	0.44
1:C:191:GLY:O	1:C:192:LYS:C	2.60	0.44
1:A:300:ILE:HD11	1:A:302:LEU:HD21	1.99	0.44
1:C:82:ASP:OD2	1:C:416:ARG:NH1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.99	0.44
1:C:391:VAL:O	1:C:395:GLY:N	2.41	0.44
1:A:163:GLU:HG2	1:A:295:ALA:CA	2.39	0.44
1:B:325:ASN:OD1	1:B:326:VAL:N	2.50	0.44
1:A:351:ARG:HE	1:A:351:ARG:HB3	1.36	0.44
1:B:411:TRP:O	1:B:414:PRO:HG2	2.18	0.44
1:C:97:ASP:OD2	1:C:100:ARG:HB2	2.18	0.44
1:C:188:TYR:CE1	1:C:264:PRO:HB3	2.53	0.44
1:A:141:LYS:HB3	1:A:141:LYS:HE3	1.69	0.44
1:A:318:VAL:CG2	1:A:323:GLN:N	2.80	0.44
1:A:470:GLY:HA2	1:B:450:GLN:OE1	2.18	0.44
1:C:417:ASP:HB3	1:C:420:LYS:CG	2.46	0.44
1:D:117:ARG:HH21	1:D:117:ARG:CG	2.28	0.44
1:D:322:GLU:HB3	1:D:331:ALA:O	2.18	0.44
1:A:321:GLU:O	1:A:322:GLU:HB2	2.17	0.43
1:C:95:LYS:HB2	1:D:89:LYS:HE3	2.00	0.43
1:C:162:GLY:O	1:C:335:ILE:HG22	2.18	0.43
1:C:194:LEU:HA	1:C:194:LEU:HD12	1.67	0.43
1:C:318:VAL:HG12	1:C:319:THR:O	2.18	0.43
1:D:156:ARG:HG3	1:D:156:ARG:NH1	2.33	0.43
1:A:83:SER:HA	1:B:76:LEU:HD13	2.01	0.43
1:A:300:ILE:HG13	1:A:302:LEU:HG	2.00	0.43
1:A:402:TYR:CE2	1:A:485:THR:HG22	2.53	0.43
1:C:65:ILE:HB	1:C:66:PRO:CD	2.48	0.43
1:A:49:LEU:HD12	1:A:49:LEU:H	1.83	0.43
1:A:114:TRP:O	1:A:115:GLY:C	2.59	0.43
1:A:303:GLU:OE1	1:A:304:THR:CG2	2.67	0.43
1:B:254:ILE:CG1	1:B:270:VAL:HG12	2.47	0.43
1:A:136:GLY:O	1:A:137:PRO:C	2.60	0.43
1:B:199:SER:HA	1:B:225:LEU:HD23	1.99	0.43
1:B:205:CYS:SG	1:B:288:MET:HE1	2.59	0.43
1:C:236:ILE:HD11	1:C:380:TYR:CD2	2.53	0.43
1:D:428:ASN:HD21	1:D:431:ASP:HB2	1.83	0.43
1:A:133:GLN:NE2	1:A:141:LYS:NZ	2.67	0.43
1:A:319:THR:C	1:A:321:GLU:N	2.76	0.43
1:B:67:LYS:HD3	1:B:204:GLU:OE1	2.18	0.43
1:B:163:GLU:CD	1:B:334:ASP:HB3	2.42	0.43
1:C:428:ASN:OD1	1:C:428:ASN:C	2.61	0.43
1:C:273:SER:OG	1:C:276:SER:N	2.46	0.43
1:C:394:PHE:HB2	1:C:399:ILE:CD1	2.46	0.43
1:C:163:GLU:HG2	1:C:295:ALA:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLN:NE2	1:C:261:ALA:N	2.57	0.43
1:C:378:LEU:HD12	1:C:378:LEU:HA	1.72	0.43
1:D:176:TYR:CD1	1:D:258:GLN:HB2	2.53	0.43
1:A:231:ASP:O	1:A:235:LYS:HG3	2.19	0.43
1:A:472:HIS:CE1	1:A:473:PRO:HB3	2.54	0.43
1:B:47:THR:HG23	1:B:48:PRO:CD	2.49	0.43
1:B:423:ALA:HB1	1:B:479:PHE:CE1	2.53	0.43
1:C:319:THR:C	1:C:321:GLU:N	2.76	0.43
1:C:472:HIS:HB2	1:D:344:PRO:HG3	2.00	0.43
1:D:254:ILE:HD11	1:D:270:VAL:CG1	2.49	0.43
1:B:70:MET:HG2	1:B:101:MET:HE3	2.01	0.42
1:A:164:ARG:O	1:A:165:PRO:C	2.62	0.42
1:B:470:GLY:H	1:B:480:THR:HG21	1.85	0.42
1:C:411:TRP:C	1:C:414:PRO:HD2	2.44	0.42
1:A:58:THR:HG23	1:A:62:VAL:HG23	2.01	0.42
1:C:176:TYR:HB3	1:C:267:LEU:HD21	2.00	0.42
1:D:252:VAL:HG13	3:D:901:NAP:N1A	2.34	0.42
1:D:393:LYS:HE2	1:D:394:PHE:CZ	2.54	0.42
1:D:472:HIS:HA	1:D:473:PRO:HA	1.81	0.42
1:A:144:ASN:HD21	1:A:148:LYS:HB2	1.83	0.42
1:B:70:MET:HE1	1:B:184:PHE:HA	2.00	0.42
1:B:210:ALA:CB	1:B:245:ILE:HD11	2.50	0.42
1:A:98:TRP:HE1	1:A:102:ILE:HG13	1.84	0.42
1:B:25:LEU:HD13	1:B:116:TYR:CD1	2.54	0.42
1:B:192:LYS:NZ	4:B:754:HOH:O	2.52	0.42
1:B:229:ASP:OD1	1:B:232:MET:HG2	2.20	0.42
1:B:376:THR:O	1:B:377:PRO:C	2.62	0.42
1:B:411:TRP:CE3	1:B:417:ASP:HB2	2.55	0.42
1:A:418:ASN:ND2	1:A:419:ASN:H	2.17	0.42
1:C:68:LYS:HE2	1:D:473:PRO:O	2.20	0.42
1:C:198:ALA:HB1	1:C:224:LEU:HD23	2.00	0.42
1:D:65:ILE:O	1:D:69:LEU:HG	2.19	0.42
1:A:219:MET:SD	1:A:253:PRO:HD3	2.59	0.42
1:B:100:ARG:NH2	1:B:100:ARG:CG	2.83	0.42
1:C:366:ASP:OD1	1:C:368:GLU:N	2.45	0.42
1:D:302:LEU:CD2	1:D:307:VAL:CG2	2.85	0.42
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.85	0.42
1:B:100:ARG:NH2	4:B:602:HOH:O	2.53	0.42
1:B:405:TYR:HE1	1:B:492:ILE:CD1	2.32	0.42
1:A:458:CYS:HB3	1:B:458:CYS:HB3	2.02	0.42
1:B:136:GLY:O	1:B:137:PRO:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LYS:HE2	1:D:146:LYS:O	2.20	0.42
1:D:163:GLU:HG2	1:D:295:ALA:HA	2.02	0.42
1:A:307:VAL:HG21	1:A:329:ILE:HG21	2.01	0.41
1:C:45:THR:HG23	4:C:813:HOH:O	2.19	0.41
1:D:170:ILE:O	1:D:170:ILE:HG13	2.19	0.41
1:B:243:HIS:CD2	4:B:625:HOH:O	2.72	0.41
1:C:386:SER:H	1:C:389:LYS:HE2	1.85	0.41
1:C:438:PHE:CE2	1:C:479:PHE:CE1	3.08	0.41
1:D:318:VAL:HG22	1:D:323:GLN:N	2.35	0.41
1:B:286:THR:HG22	1:B:287:VAL:N	2.36	0.41
1:C:91:GLU:CD	1:C:93:THR:H	2.28	0.41
1:C:284:TYR:C	1:C:285:ASN:HD22	2.26	0.41
1:C:377:PRO:HD2	4:C:569:HOH:O	2.19	0.41
1:D:47:THR:HB	1:D:51:THR:H	1.85	0.41
1:D:137:PRO:HA	1:D:305:VAL:HG23	2.01	0.41
1:B:221:ARG:O	1:B:250:GLN:HA	2.21	0.41
1:C:67:LYS:HD3	1:C:204:GLU:OE1	2.21	0.41
1:C:134:PHE:N	1:C:300:ILE:O	2.52	0.41
1:A:288:MET:CE	1:A:290:ALA:HB2	2.49	0.41
1:B:58:THR:O	1:B:63:GLY:N	2.53	0.41
1:C:77:GLY:HA2	1:C:80:LEU:HD12	2.03	0.41
1:C:341:GLU:HB2	3:C:901:NAP:O2D	2.19	0.41
1:D:449:THR:O	1:D:450:GLN:C	2.63	0.41
1:B:309:ILE:HA	1:B:317:PRO:HD2	2.02	0.41
1:D:67:LYS:HE2	1:D:67:LYS:HB3	1.81	0.41
1:C:205:CYS:HA	1:C:208:PHE:CE2	2.56	0.41
1:C:482:LEU:HB2	4:C:878:HOH:O	2.21	0.41
1:D:310:ASN:OD1	1:D:312:LYS:HB3	2.20	0.41
1:A:169:GLY:N	1:A:173:ASP:OD2	2.50	0.41
1:D:239:HIS:CE1	1:D:378:LEU:HB2	2.56	0.41
1:A:89:LYS:O	1:B:94:VAL:HG13	2.20	0.41
1:B:229:ASP:OD1	1:B:231:ASP:HB3	2.20	0.41
1:C:251:PHE:CD2	1:C:273:SER:HA	2.56	0.41
1:C:403:HIS:CE1	1:C:492:ILE:HD13	2.55	0.41
1:D:401:VAL:HG22	1:D:426:ILE:HG13	2.02	0.41
1:D:446:GLY:N	4:D:551:HOH:O	2.36	0.41
1:A:70:MET:SD	1:A:208:PHE:CE1	3.14	0.41
1:A:315:LYS:HE3	1:A:334:ASP:O	2.21	0.41
1:B:199:SER:O	1:B:200:TYR:C	2.63	0.41
1:B:276:SER:OG	1:B:277:GLU:N	2.53	0.41
1:C:315:LYS:O	1:C:317:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:THR:HA	1:D:46:PRO:HD3	1.71	0.41
1:A:69:LEU:HD21	1:B:409:LEU:HG	2.03	0.40
1:A:201:VAL:HG12	1:A:288:MET:HE1	2.03	0.40
1:A:224:LEU:O	1:A:225:LEU:C	2.64	0.40
1:A:318:VAL:HG21	1:A:322:GLU:HA	2.02	0.40
1:A:460:LEU:HD12	1:B:458:CYS:SG	2.62	0.40
1:B:149:GLU:C	1:B:150:LYS:HG2	2.45	0.40
1:B:183:LEU:HD22	1:B:288:MET:SD	2.61	0.40
1:B:352:LEU:O	1:B:353:LEU:C	2.64	0.40
1:C:159:ILE:HD12	1:C:316:ILE:HD13	2.03	0.40
1:C:469:ILE:HG22	1:D:344:PRO:HB2	2.02	0.40
1:D:493:LEU:HD12	1:D:493:LEU:H	1.87	0.40
1:A:170:ILE:O	1:A:171:PRO:C	2.62	0.40
1:A:198:ALA:CB	1:A:220:VAL:HG13	2.51	0.40
1:A:199:SER:O	1:A:200:TYR:C	2.64	0.40
1:B:198:ALA:HB1	1:B:224:LEU:CD2	2.51	0.40
1:C:136:GLY:O	1:C:137:PRO:C	2.64	0.40
1:D:16:ILE:HG13	1:D:154:ALA:HB2	2.02	0.40
1:D:332:ILE:HA	1:D:336:LEU:HD11	2.03	0.40
1:A:74:ALA:HB1	1:A:211:GLY:HA3	2.03	0.40
1:A:378:LEU:HD12	1:A:378:LEU:HA	1.80	0.40
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.86	0.40
1:B:217:THR:CG2	1:B:248:ILE:HD12	2.51	0.40
1:B:229:ASP:HA	1:B:388:GLU:OE1	2.21	0.40
1:B:258:GLN:OE1	1:B:261:ALA:CB	2.67	0.40
1:B:408:PRO:O	1:B:409:LEU:C	2.64	0.40
1:C:315:LYS:HB3	1:C:337:GLU:HB2	2.03	0.40
1:A:39:MET:HE3	1:A:128:GLU:HB2	2.03	0.40
1:A:65:ILE:HB	1:A:66:PRO:CD	2.52	0.40
1:A:67:LYS:HE2	1:A:67:LYS:HB3	1.84	0.40
1:A:399:ILE:HG23	1:A:426:ILE:HG23	2.04	0.40
1:D:58:THR:OG1	2:D:900:FAD:O2A	2.18	0.40
1:D:133:GLN:C	1:D:140:ILE:HG13	2.46	0.40
1:C:321:GLU:O	1:C:322:GLU:HB2	2.20	0.40
1:D:28:ALA:HB2	1:D:40:VAL:HG21	2.04	0.40
1:D:100:ARG:HH21	1:D:100:ARG:CG	2.33	0.40
1:D:431:ASP:C	1:D:432:ASN:OD1	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	483/513 (94%)	446 (92%)	33 (7%)	4 (1%)	16	34
1	B	482/513 (94%)	455 (94%)	26 (5%)	1 (0%)	43	66
1	C	483/513 (94%)	443 (92%)	34 (7%)	6 (1%)	10	23
1	D	482/513 (94%)	443 (92%)	36 (8%)	3 (1%)	21	42
All	All	1930/2052 (94%)	1787 (93%)	129 (7%)	14 (1%)	18	38

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	260	GLU
1	A	200	TYR
1	C	200	TYR
1	D	260	GLU
1	A	260	GLU
1	A	320	ASP
1	D	200	TYR
1	B	473	PRO
1	C	64	CYS
1	C	137	PRO
1	C	259	ILE
1	A	473	PRO
1	C	473	PRO
1	D	473	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/422 (94%)	376 (94%)	23 (6%)	18	39
1	B	398/422 (94%)	381 (96%)	17 (4%)	26	51
1	C	399/422 (94%)	372 (93%)	27 (7%)	14	32
1	D	398/422 (94%)	366 (92%)	32 (8%)	11	25
All	All	1594/1688 (94%)	1495 (94%)	99 (6%)	16	36

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	45	THR
1	A	52	ARG
1	A	64	CYS
1	A	92	GLU
1	A	121	ARG
1	A	125	VAL
1	A	140	ILE
1	A	141	LYS
1	A	149	GLU
1	A	185	SER
1	A	252	VAL
1	A	272	GLN
1	A	274	THR
1	A	277	GLU
1	A	303	GLU
1	A	329	ILE
1	A	389	LYS
1	A	397	GLU
1	A	413	ILE
1	A	433	GLU
1	A	480	THR
1	A	494	GLN
1	B	40	VAL
1	B	47	THR
1	B	48	PRO
1	B	64	CYS
1	B	78	GLN
1	B	81	GLN
1	B	111	SER
1	B	248	ILE
1	B	276	SER
1	B	341	GLU

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Mol	Chain	Res	Type
1	B	362	THR
1	B	391	VAL
1	B	399	ILE
1	B	429	THR
1	B	467	SER
1	B	480	THR
1	B	492	ILE
1	C	33	GLN
1	C	45	THR
1	C	48	PRO
1	C	64	CYS
1	C	68	LYS
1	C	95	LYS
1	C	137	PRO
1	C	140	ILE
1	C	144	ASN
1	C	146	LYS
1	C	159	ILE
1	C	223	ILE
1	C	245	ILE
1	C	276	SER
1	C	280	ILE
1	C	281	GLU
1	C	285	ASN
1	C	303	GLU
1	C	318	VAL
1	C	336	LEU
1	C	376	THR
1	C	397	GLU
1	C	413	ILE
1	C	434	ARG
1	C	474	VAL
1	C	480	THR
1	C	491	SER
1	D	33	GLN
1	D	45	THR
1	D	47	THR
1	D	48	PRO
1	D	64	CYS
1	D	92	GLU
1	D	103	GLU
1	D	107	ASN

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Mol	Chain	Res	Type
1	D	117	ARG
1	D	121	ARG
1	D	128	GLU
1	D	145	ASN
1	D	186	LEU
1	D	212	ILE
1	D	246	LYS
1	D	249	ARG
1	D	264	PRO
1	D	266	ARG
1	D	274	THR
1	D	276	SER
1	D	277	GLU
1	D	304	THR
1	D	310	ASN
1	D	318	VAL
1	D	364	LYS
1	D	376	THR
1	D	391	VAL
1	D	396	GLU
1	D	428	ASN
1	D	432	ASN
1	D	456	LEU
1	D	474	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	108	HIS
1	A	113	ASN
1	A	129	ASN
1	A	133	GLN
1	A	234	ASN
1	A	285	ASN
1	A	418	ASN
1	A	494	GLN
1	B	33	GLN
1	B	107	ASN
1	B	113	ASN
1	B	129	ASN
1	B	145	ASN

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	272	GLN
1	B	325	ASN
1	B	355	GLN
1	B	419	ASN
1	B	432	ASN
1	C	85	ASN
1	C	113	ASN
1	C	129	ASN
1	C	145	ASN
1	C	258	GLN
1	C	285	ASN
1	C	419	ASN
1	C	494	GLN
1	D	81	GLN
1	D	106	GLN
1	D	107	ASN
1	D	129	ASN
1	D	145	ASN
1	D	234	ASN
1	D	250	GLN
1	D	258	GLN
1	D	355	GLN
1	D	428	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAP	A	901	-	50,52,52	1.59	8 (16%)	71,80,80	0.99	4 (5%)
2	FAD	D	900	-	58,58,58	1.62	7 (12%)	85,89,89	1.65	18 (21%)
2	FAD	A	900	-	58,58,58	1.40	10 (17%)	85,89,89	1.64	15 (17%)
3	NAP	C	901	-	50,52,52	1.77	9 (18%)	71,80,80	1.05	3 (4%)
2	FAD	C	900	-	58,58,58	1.51	10 (17%)	85,89,89	1.67	16 (18%)
2	FAD	B	900	-	58,58,58	1.37	9 (15%)	85,89,89	1.68	16 (18%)
3	NAP	B	901	-	50,52,52	1.58	8 (16%)	71,80,80	1.19	4 (5%)
3	NAP	D	901	-	50,52,52	1.42	6 (12%)	71,80,80	1.06	4 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	901	-	-	5/35/67/67	0/5/5/5
2	FAD	D	900	-	-	3/34/50/50	0/6/6/6
2	FAD	A	900	-	-	4/34/50/50	0/6/6/6
3	NAP	C	901	-	-	9/35/67/67	0/5/5/5
2	FAD	C	900	-	-	3/34/50/50	0/6/6/6
2	FAD	B	900	-	-	2/34/50/50	0/6/6/6
3	NAP	B	901	-	-	6/35/67/67	0/5/5/5
3	NAP	D	901	-	-	7/35/67/67	0/5/5/5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	FAD	PA-O3P	7.37	1.67	1.59
3	B	901	NAP	C2N-N1N	6.36	1.42	1.35
3	C	901	NAP	C2N-N1N	5.23	1.40	1.35
3	A	901	NAP	C2N-N1N	4.93	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAP	C4N-C3N	4.51	1.46	1.39
2	C	900	FAD	PA-O3P	4.27	1.64	1.59
3	C	901	NAP	PA-O3	4.21	1.64	1.59
3	C	901	NAP	P2B-O2B	4.19	1.66	1.59
3	A	901	NAP	C6N-N1N	4.09	1.44	1.35
3	C	901	NAP	C4N-C3N	4.03	1.45	1.39
3	D	901	NAP	C2N-N1N	3.97	1.39	1.35
3	C	901	NAP	C4A-N3A	3.80	1.41	1.34
2	B	900	FAD	C6-C5X	3.75	1.45	1.40
3	C	901	NAP	C6N-N1N	3.73	1.43	1.35
3	B	901	NAP	C6N-N1N	3.72	1.43	1.35
2	D	900	FAD	P-O3P	3.68	1.63	1.59
3	D	901	NAP	C4N-C3N	3.45	1.44	1.39
3	B	901	NAP	C4N-C3N	3.41	1.44	1.39
2	A	900	FAD	O4-C4	-3.36	1.17	1.23
2	C	900	FAD	C9A-C5X	3.25	1.46	1.41
3	D	901	NAP	C6N-N1N	3.24	1.42	1.35
3	B	901	NAP	C3N-C7N	3.14	1.55	1.50
2	B	900	FAD	C2-N3	-3.13	1.32	1.39
3	A	901	NAP	PA-O3	3.08	1.62	1.59
3	D	901	NAP	C4A-N3A	3.05	1.40	1.34
2	A	900	FAD	P-O3P	2.90	1.62	1.59
2	D	900	FAD	C9A-N10	2.90	1.46	1.41
2	A	900	FAD	PA-O3P	2.80	1.62	1.59
2	A	900	FAD	C6A-N6A	2.72	1.41	1.34
2	A	900	FAD	C9A-C5X	2.72	1.45	1.41
3	C	901	NAP	C3N-C7N	2.70	1.54	1.50
2	B	900	FAD	O4B-C1B	2.68	1.48	1.42
2	A	900	FAD	C5A-N7A	-2.58	1.34	1.39
3	A	901	NAP	O4B-C1B	2.54	1.47	1.42
2	A	900	FAD	C4X-C10	2.54	1.51	1.44
2	C	900	FAD	P-O3P	2.52	1.62	1.59
2	C	900	FAD	C9A-N10	2.50	1.45	1.41
3	A	901	NAP	P2B-O2B	2.50	1.63	1.59
2	B	900	FAD	P-O1P	-2.46	1.42	1.50
2	C	900	FAD	O4B-C1B	2.45	1.47	1.42
3	A	901	NAP	C5A-N7A	-2.41	1.34	1.39
2	D	900	FAD	C6-C5X	2.34	1.43	1.40
2	C	900	FAD	C1'-C2'	2.33	1.55	1.52
2	C	900	FAD	C10-N1	2.29	1.37	1.33
2	B	900	FAD	C10-N10	2.28	1.42	1.37
2	C	900	FAD	O2-C2	-2.28	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	NAP	O3B-C3B	2.28	1.48	1.43
3	D	901	NAP	C3N-C7N	2.22	1.53	1.50
2	D	900	FAD	O4B-C1B	2.22	1.47	1.42
3	C	901	NAP	PN-O3	2.22	1.61	1.59
3	C	901	NAP	O4B-C1B	2.20	1.47	1.42
3	D	901	NAP	O3B-C3B	2.20	1.48	1.43
2	A	900	FAD	C9A-N10	2.19	1.45	1.41
3	B	901	NAP	O4B-C1B	2.18	1.47	1.42
3	A	901	NAP	C3N-C7N	2.16	1.53	1.50
2	C	900	FAD	C2'-C3'	-2.15	1.49	1.53
2	B	900	FAD	C5X-N5	-2.14	1.35	1.39
2	D	900	FAD	C4X-N5	2.12	1.35	1.30
2	A	900	FAD	O4B-C1B	2.12	1.46	1.42
2	C	900	FAD	C6A-N6A	2.10	1.39	1.34
2	B	900	FAD	P-O3P	-2.09	1.57	1.59
2	B	900	FAD	C6A-N6A	2.08	1.39	1.34
2	A	900	FAD	C1'-C2'	-2.08	1.49	1.52
2	B	900	FAD	C5A-C4A	2.05	1.42	1.39
3	B	901	NAP	C2A-N3A	2.04	1.37	1.33
3	B	901	NAP	PA-O3	2.03	1.61	1.59
2	D	900	FAD	C9A-C5X	2.00	1.44	1.41

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	C5A-C4A-N3A	-4.96	119.89	126.72
2	C	900	FAD	N3A-C2A-N1A	-4.85	121.25	128.58
2	A	900	FAD	N3A-C2A-N1A	-4.83	121.27	128.58
2	D	900	FAD	C5A-C4A-N3A	-4.80	120.11	126.72
2	A	900	FAD	C5A-C4A-N3A	-4.67	120.28	126.72
2	C	900	FAD	N3A-C4A-N9A	4.61	135.00	127.17
2	B	900	FAD	N3A-C2A-N1A	-4.58	121.65	128.58
2	B	900	FAD	C5A-C4A-N3A	-4.48	120.55	126.72
2	A	900	FAD	N3A-C4A-N9A	4.27	134.43	127.17
2	A	900	FAD	C5A-N7A-C8A	4.25	110.13	103.45
3	B	901	NAP	C6N-N1N-C2N	-4.25	118.26	121.88
2	B	900	FAD	N3A-C4A-N9A	4.20	134.32	127.17
2	D	900	FAD	C5A-N7A-C8A	4.13	109.94	103.45
2	C	900	FAD	C5A-N7A-C8A	4.09	109.87	103.45
2	D	900	FAD	N3A-C4A-N9A	4.06	134.07	127.17
2	B	900	FAD	C5A-N7A-C8A	3.88	109.55	103.45
2	C	900	FAD	C2A-N3A-C4A	3.86	121.27	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	FAD	C2A-N3A-C4A	3.73	120.93	111.83
2	D	900	FAD	N3A-C2A-N1A	-3.71	122.97	128.58
3	C	901	NAP	C6N-N1N-C2N	-3.61	118.81	121.88
3	D	901	NAP	C6N-N1N-C2N	-3.60	118.82	121.88
2	D	900	FAD	C4-C4X-N5	3.55	123.11	118.21
2	B	900	FAD	C5X-N5-C4X	3.52	123.79	118.09
2	B	900	FAD	C2A-N3A-C4A	3.47	120.30	111.83
2	C	900	FAD	C4-C4X-N5	3.40	122.90	118.21
2	D	900	FAD	C2A-N3A-C4A	3.37	120.07	111.83
3	A	901	NAP	C6N-N1N-C2N	-3.26	119.10	121.88
2	A	900	FAD	C4A-C5A-N7A	-3.24	106.88	110.58
2	D	900	FAD	C4A-C5A-N7A	-3.18	106.95	110.58
2	A	900	FAD	N9A-C8A-N7A	-3.10	109.54	113.94
2	D	900	FAD	N9A-C8A-N7A	-3.06	109.59	113.94
2	C	900	FAD	N9A-C8A-N7A	-2.98	109.71	113.94
2	B	900	FAD	C9A-C5X-N5	-2.91	119.36	122.45
2	C	900	FAD	C4A-C5A-N7A	-2.91	107.25	110.58
2	B	900	FAD	C4X-C10-N1	-2.90	117.47	124.59
2	A	900	FAD	C4-C4X-N5	2.89	122.20	118.21
2	B	900	FAD	N9A-C8A-N7A	-2.87	109.86	113.94
3	C	901	NAP	N3A-C2A-N1A	-2.80	124.35	128.58
2	D	900	FAD	C5X-N5-C4X	2.79	122.60	118.09
2	B	900	FAD	C4-C4X-N5	2.65	121.88	118.21
2	D	900	FAD	C4'-C3'-C2'	-2.64	109.18	113.57
2	D	900	FAD	C9A-C5X-N5	-2.62	119.67	122.45
3	B	901	NAP	N3A-C2A-N1A	-2.60	124.64	128.58
3	B	901	NAP	O3B-C3B-C4B	-2.59	103.65	111.08
3	D	901	NAP	N3A-C2A-N1A	-2.57	124.69	128.58
2	B	900	FAD	C4-N3-C2	-2.55	121.12	125.64
3	D	901	NAP	C2A-N1A-C6A	2.52	122.88	118.73
3	A	901	NAP	N3A-C2A-N1A	-2.52	124.77	128.58
2	B	900	FAD	C10-N1-C2	2.49	122.25	116.85
3	A	901	NAP	C2A-N1A-C6A	2.49	122.81	118.73
2	B	900	FAD	C4A-C5A-N7A	-2.48	107.74	110.58
2	A	900	FAD	C5X-N5-C4X	2.47	122.09	118.09
3	B	901	NAP	C2B-C1B-N9A	2.43	117.75	113.75
3	C	901	NAP	C2A-N1A-C6A	2.43	122.72	118.73
2	C	900	FAD	C5X-N5-C4X	2.37	121.92	118.09
2	C	900	FAD	C4X-C10-N1	-2.37	118.78	124.59
2	A	900	FAD	C4A-N9A-C8A	2.31	108.17	105.74
2	A	900	FAD	O4-C4-C4X	-2.31	120.44	126.53
2	C	900	FAD	C10-N1-C2	2.30	121.83	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	O2-C2-N1	-2.29	118.00	121.80
2	B	900	FAD	C10-C4X-N5	-2.28	120.15	124.81
2	D	900	FAD	O2-C2-N1	-2.26	118.05	121.80
2	B	900	FAD	O4B-C1B-C2B	-2.24	101.83	106.62
2	B	900	FAD	O4-C4-C4X	-2.24	120.63	126.53
2	A	900	FAD	C4X-C10-N1	-2.23	119.12	124.59
2	D	900	FAD	C10-C4X-N5	-2.21	120.29	124.81
2	C	900	FAD	C4A-N9A-C8A	2.21	108.06	105.74
2	D	900	FAD	C4-N3-C2	-2.20	121.73	125.64
2	D	900	FAD	C10-N1-C2	2.20	121.61	116.85
2	C	900	FAD	O4-C4-C4X	-2.20	120.73	126.53
2	D	900	FAD	O4B-C1B-C2B	-2.20	101.92	106.62
2	D	900	FAD	C4X-C10-N1	-2.14	119.35	124.59
2	D	900	FAD	O2A-PA-O3P	2.12	113.01	107.27
2	A	900	FAD	C9A-C5X-N5	-2.12	120.20	122.45
2	C	900	FAD	C9A-C5X-N5	-2.12	120.21	122.45
2	C	900	FAD	O4B-C1B-C2B	-2.09	102.14	106.62
3	A	901	NAP	O3D-C3D-C4D	2.07	117.02	111.08
2	A	900	FAD	C2A-N1A-C6A	2.06	122.12	118.73
2	A	900	FAD	C4'-C3'-C2'	-2.02	110.22	113.57
3	D	901	NAP	O4D-C4D-C3D	-2.00	101.17	105.15

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	NAP	C5D-O5D-PN-O1N
3	B	901	NAP	O4D-C1D-N1N-C2N
3	C	901	NAP	C5B-O5B-PA-O1A
3	C	901	NAP	PA-O3-PN-O5D
3	C	901	NAP	O4D-C1D-N1N-C2N
3	C	901	NAP	O4D-C1D-N1N-C6N
2	B	900	FAD	O4B-C4B-C5B-O5B
2	B	900	FAD	C3B-C4B-C5B-O5B
2	D	900	FAD	C3B-C4B-C5B-O5B
2	A	900	FAD	O4B-C4B-C5B-O5B
2	A	900	FAD	C3B-C4B-C5B-O5B
2	C	900	FAD	O4B-C4B-C5B-O5B
2	D	900	FAD	O4B-C4B-C5B-O5B
2	C	900	FAD	C3B-C4B-C5B-O5B
3	B	901	NAP	C2B-O2B-P2B-O1X
3	D	901	NAP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
2	A	900	FAD	PA-O3P-P-O5'
2	C	900	FAD	PA-O3P-P-O5'
3	B	901	NAP	PA-O3-PN-O5D
3	C	901	NAP	PN-O3-PA-O2A
3	D	901	NAP	PN-O3-PA-O1A
3	A	901	NAP	C2B-O2B-P2B-O1X
3	C	901	NAP	C2B-O2B-P2B-O1X
3	C	901	NAP	C5B-O5B-PA-O3
3	D	901	NAP	C5B-O5B-PA-O1A
3	D	901	NAP	C5D-O5D-PN-O1N
3	B	901	NAP	PN-O3-PA-O1A
3	C	901	NAP	PN-O3-PA-O1A
3	A	901	NAP	O4D-C1D-N1N-C2N
3	B	901	NAP	O4D-C1D-N1N-C6N
3	D	901	NAP	O4D-C1D-N1N-C2N
3	A	901	NAP	PN-O3-PA-O1A
3	D	901	NAP	PN-O3-PA-O2A
3	D	901	NAP	O4B-C4B-C5B-O5B
3	B	901	NAP	PN-O3-PA-O2A
3	C	901	NAP	O4B-C4B-C5B-O5B
2	D	900	FAD	C2B-C1B-N9A-C8A
2	A	900	FAD	P-O3P-PA-O2A
3	A	901	NAP	PN-O3-PA-O2A

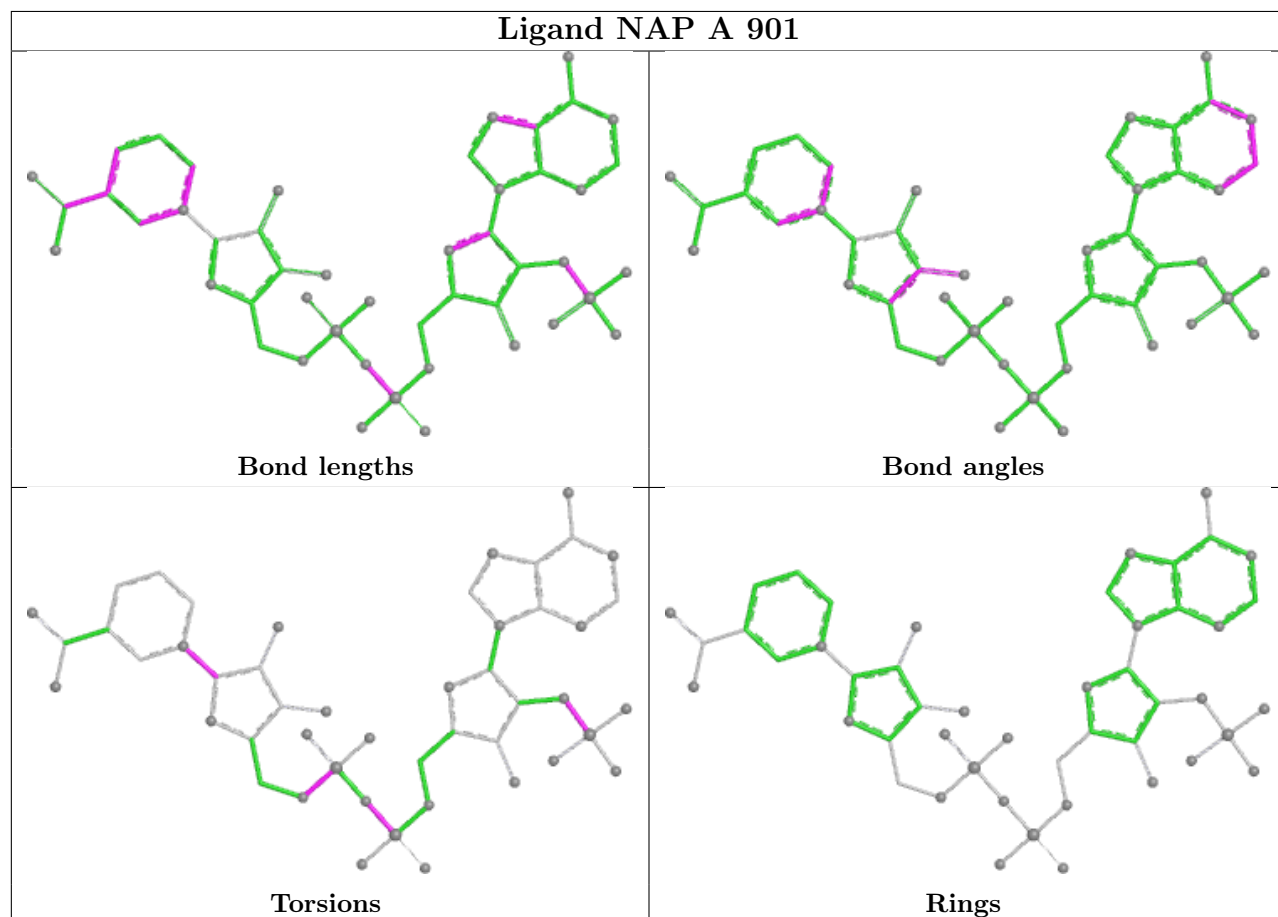
There are no ring outliers.

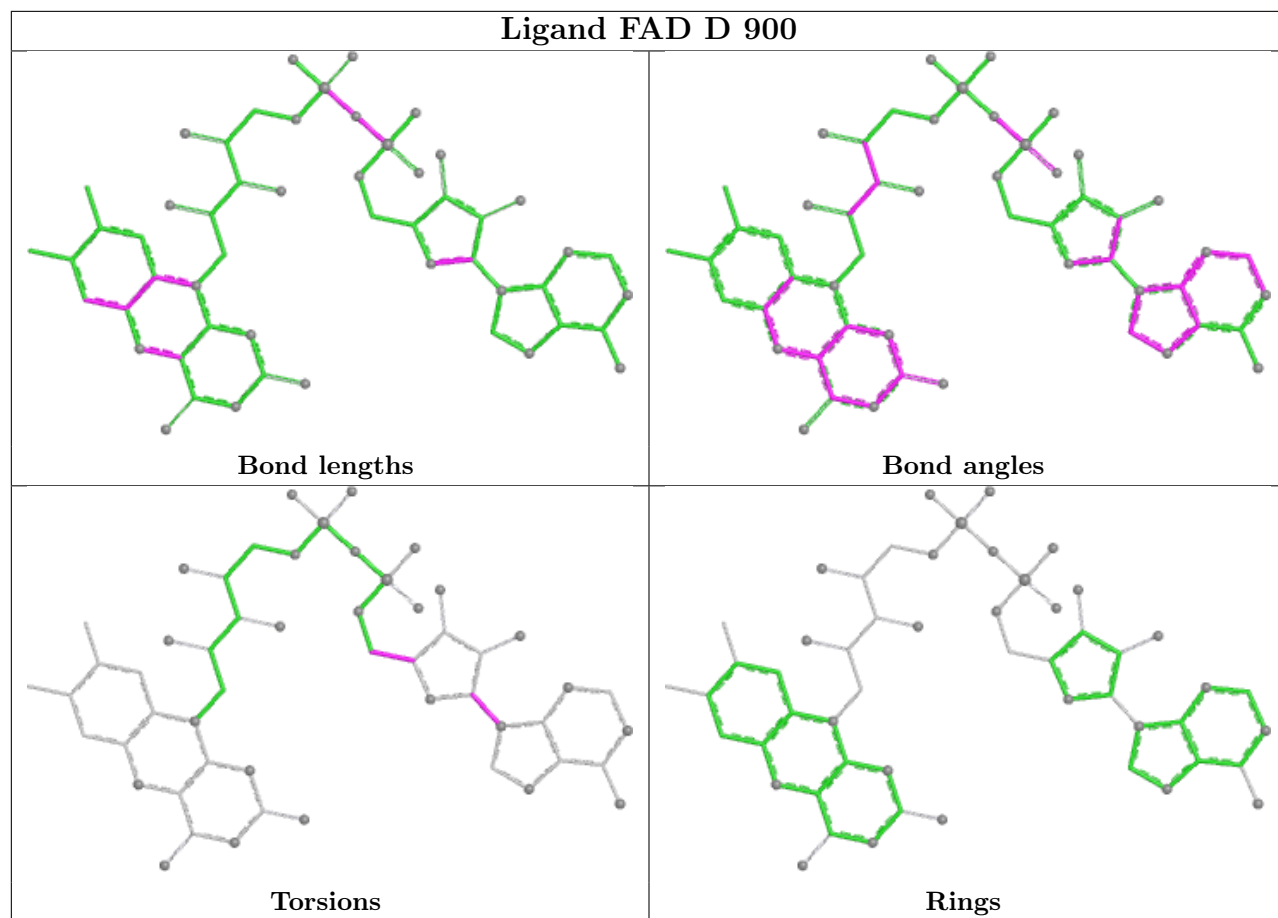
6 monomers are involved in 16 short contacts:

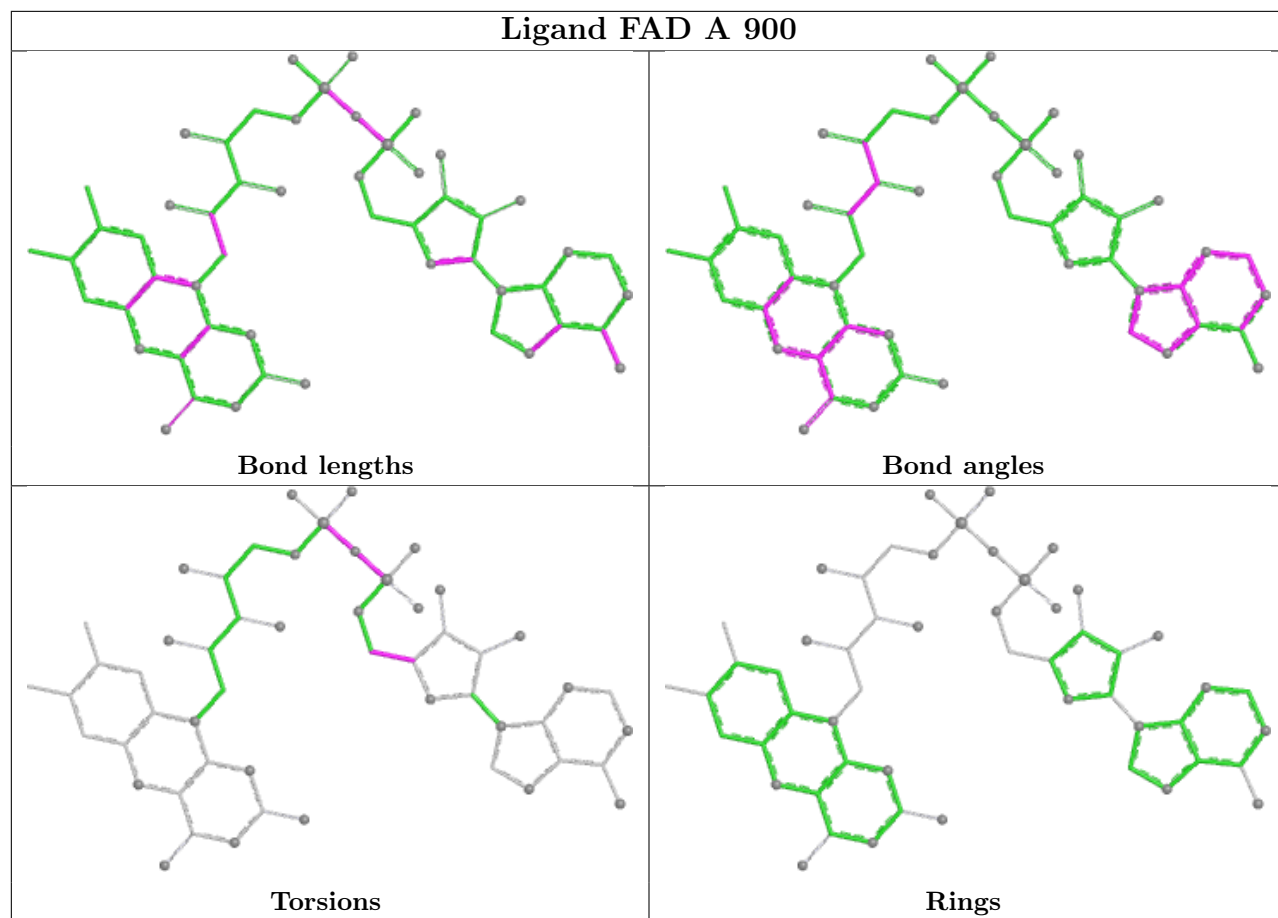
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	NAP	3	0
2	D	900	FAD	2	0
3	C	901	NAP	3	0
2	C	900	FAD	1	0
3	B	901	NAP	4	0
3	D	901	NAP	3	0

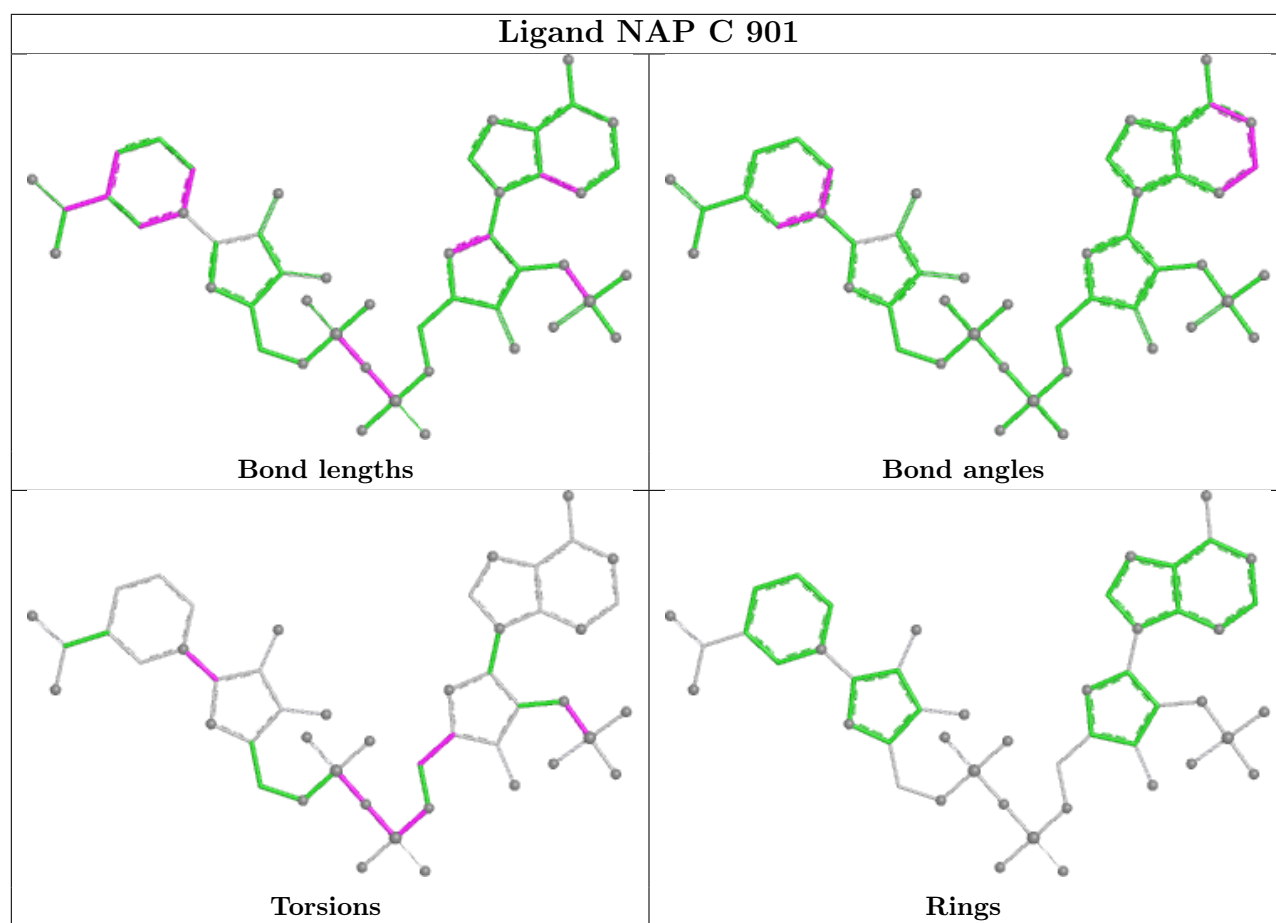
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

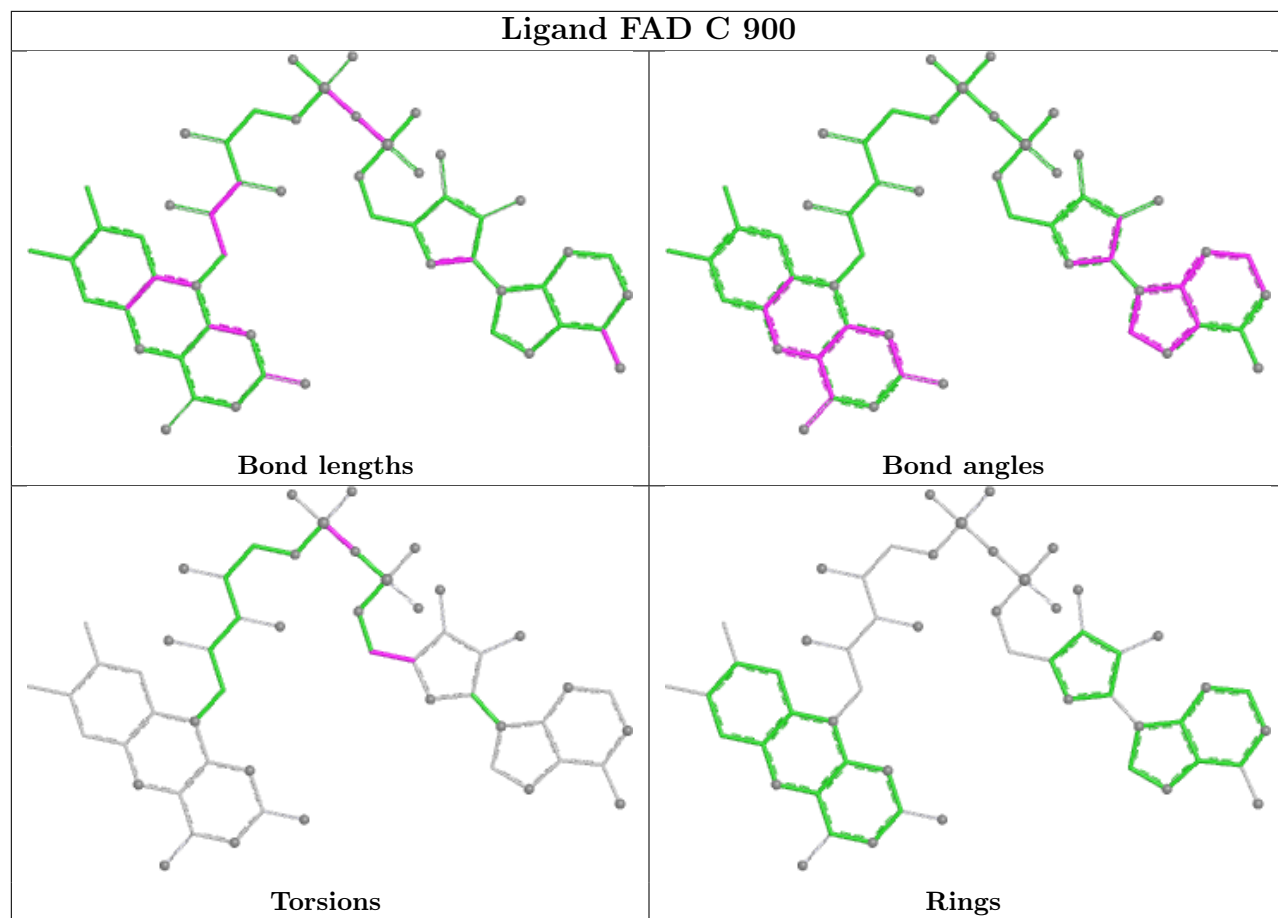
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

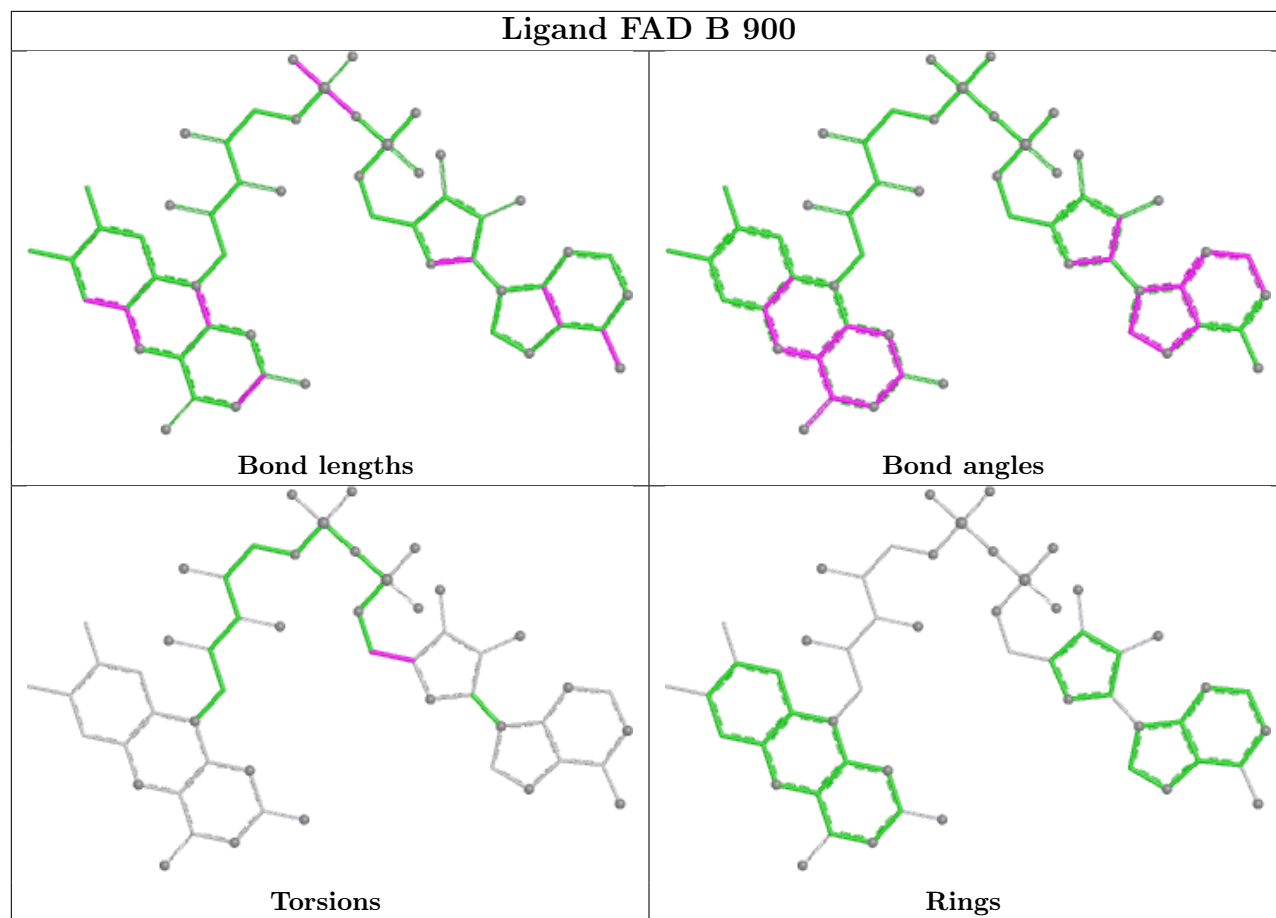


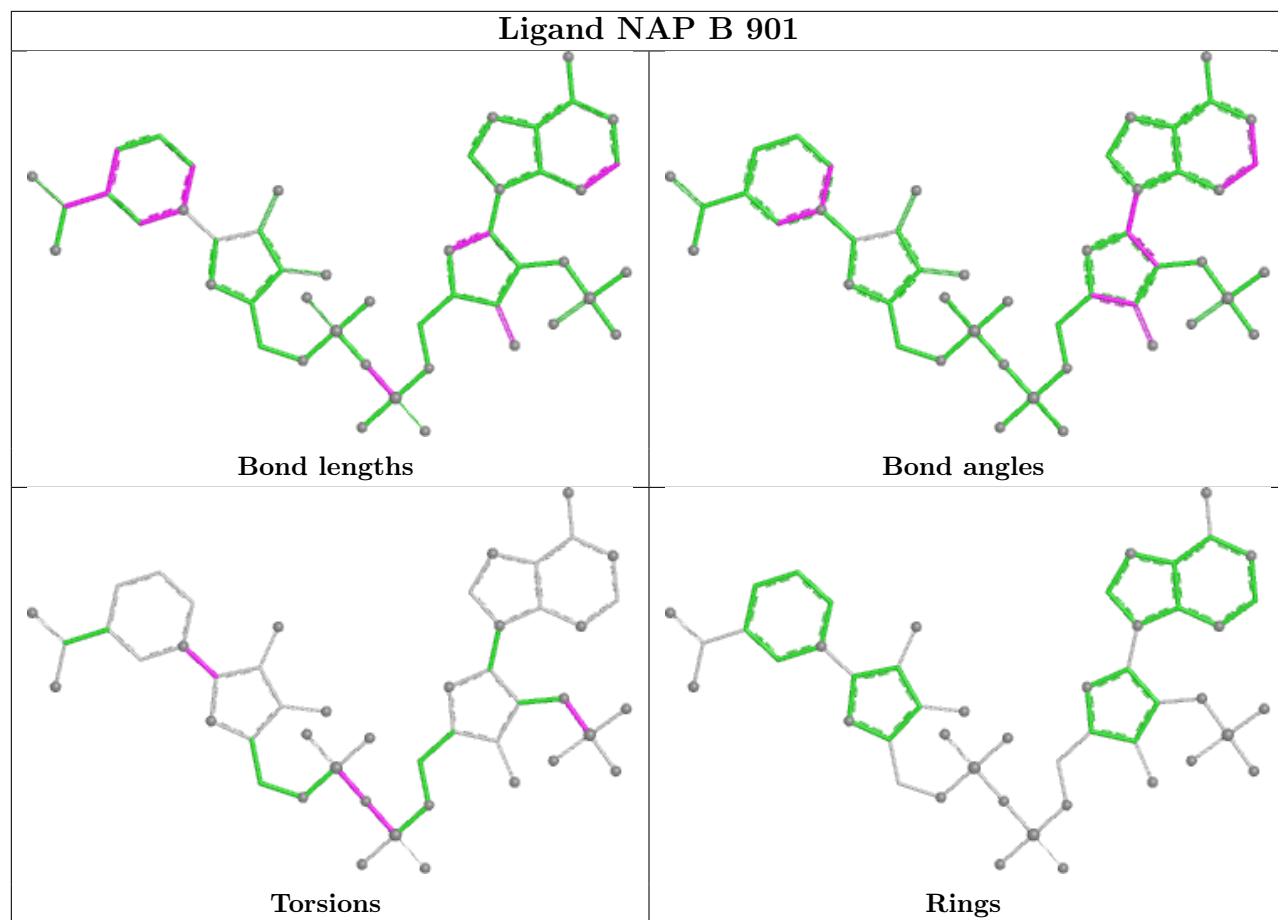


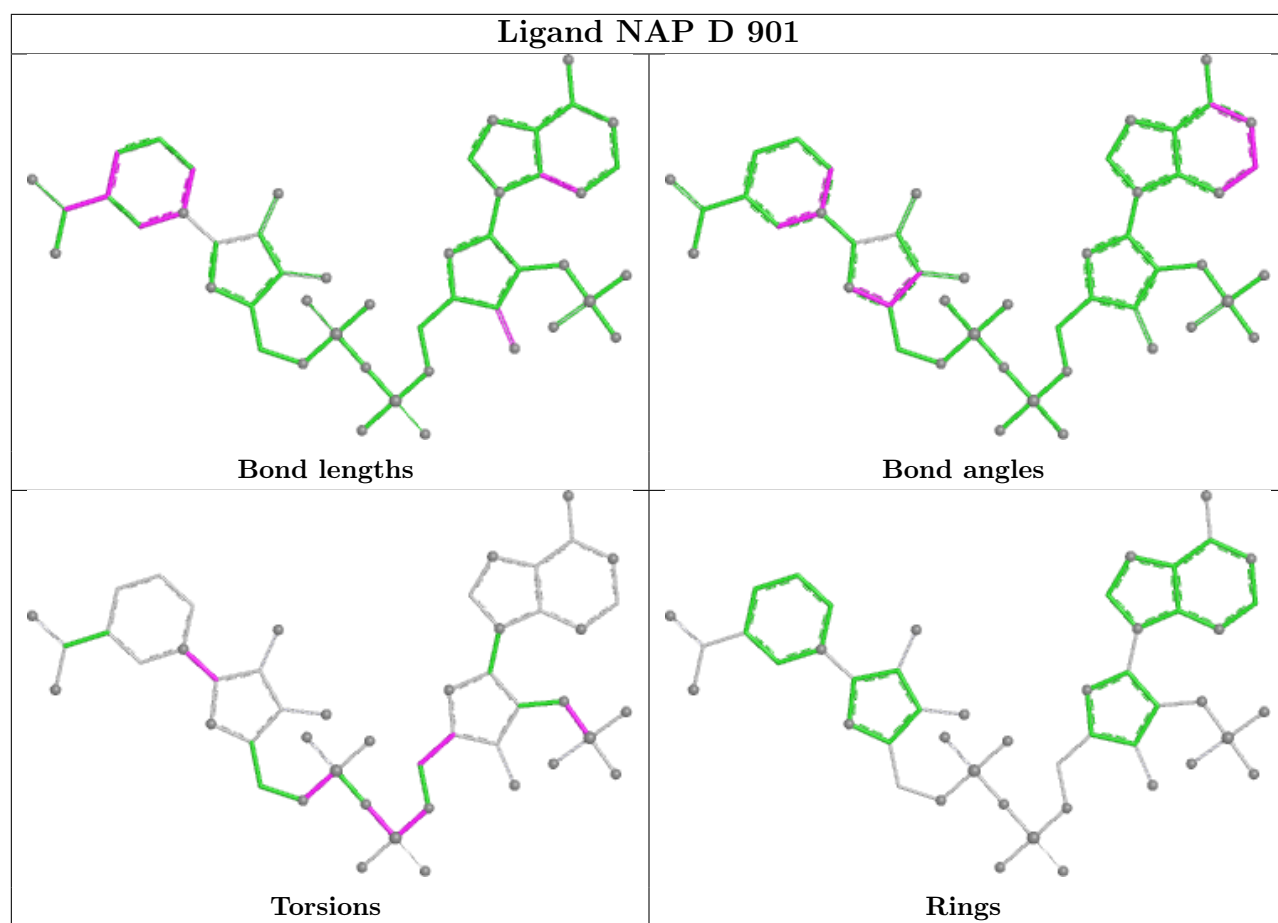












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	485/513 (94%)	-0.30	0	100 100	26, 50, 70, 84	0
1	B	484/513 (94%)	-0.47	1 (0%)	91 90	28, 44, 63, 87	0
1	C	485/513 (94%)	-0.15	1 (0%)	91 90	34, 53, 74, 94	0
1	D	484/513 (94%)	-0.33	1 (0%)	91 90	28, 49, 70, 89	0
All	All	1938/2052 (94%)	-0.31	3 (0%)	91 90	26, 49, 71, 94	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	493	LEU	3.7
1	C	493	LEU	2.9
1	D	493	LEU	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

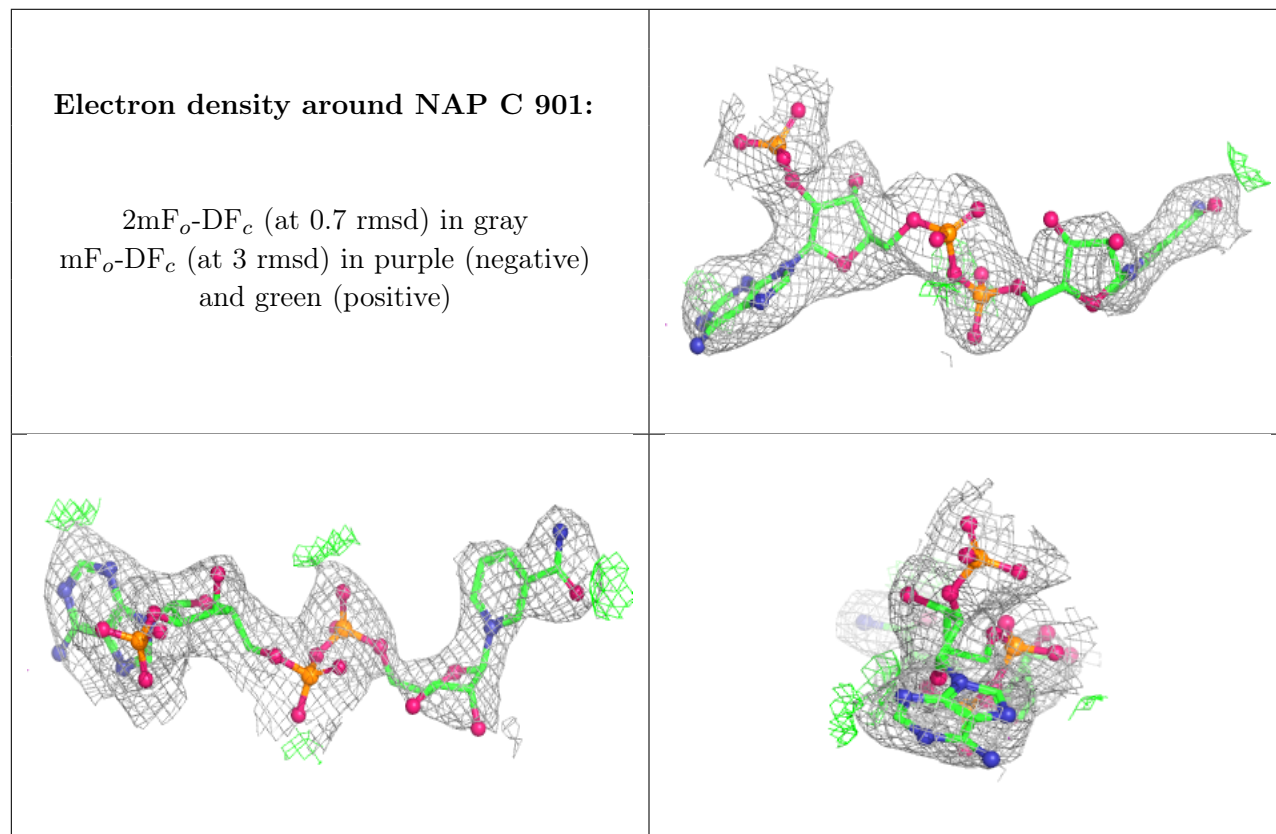
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

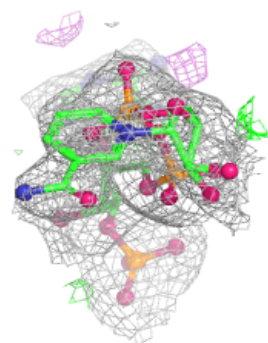
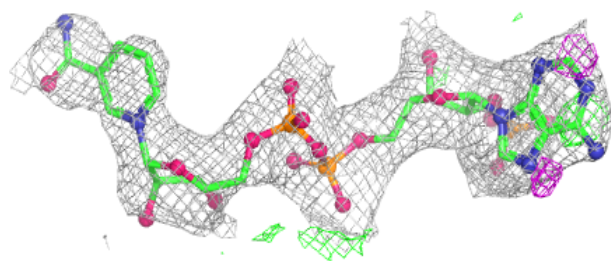
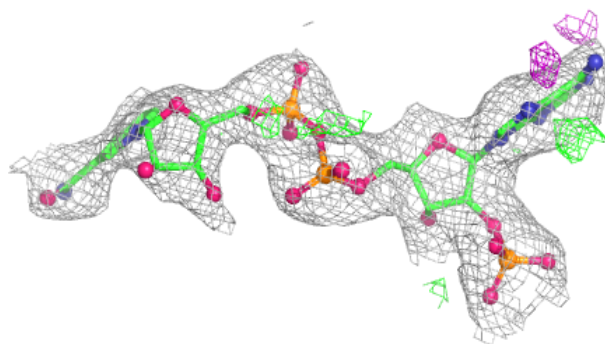
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	C	901	48/48	0.92	0.10	61,72,86,87	0
3	NAP	A	901	48/48	0.94	0.10	49,64,87,87	0
2	FAD	C	900	53/53	0.94	0.09	38,48,65,66	0
2	FAD	A	900	53/53	0.95	0.09	42,50,68,68	0
3	NAP	D	901	48/48	0.95	0.09	51,60,83,85	0
3	NAP	B	901	48/48	0.96	0.08	45,53,63,64	0
2	FAD	B	900	53/53	0.97	0.06	30,37,43,43	0
2	FAD	D	900	53/53	0.97	0.06	30,42,49,51	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.

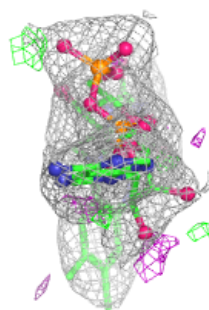
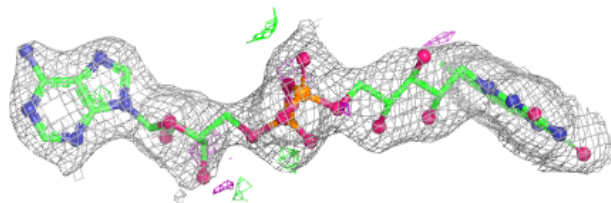
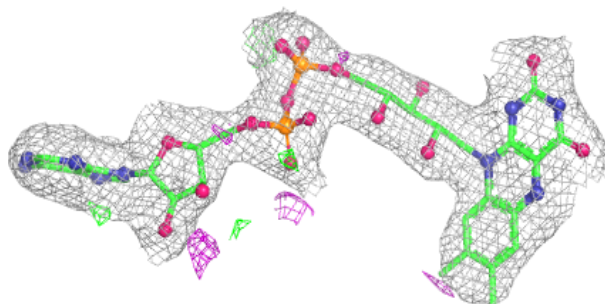


Electron density around NAP A 901:

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

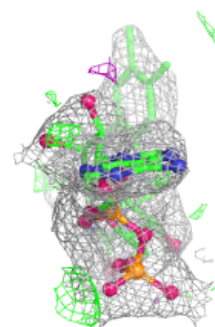
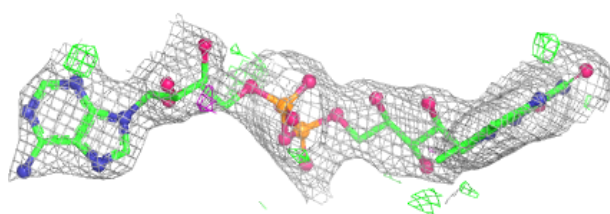
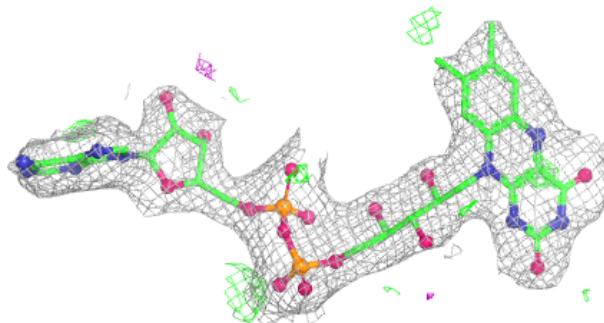
**Electron density around FAD C 900:**

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

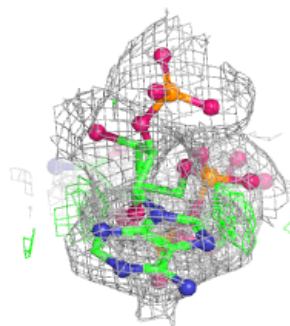
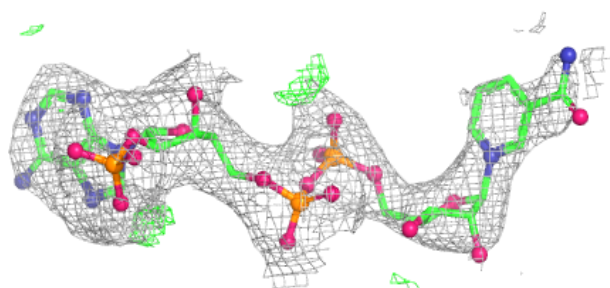
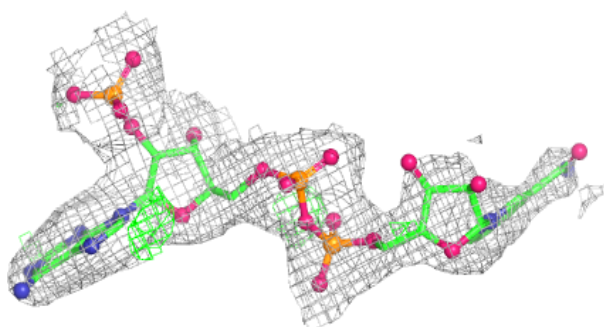


Electron density around FAD A 900:

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

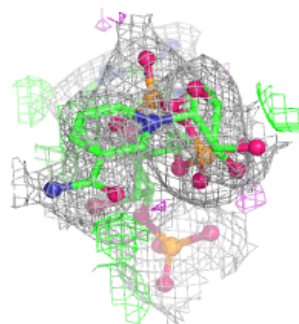
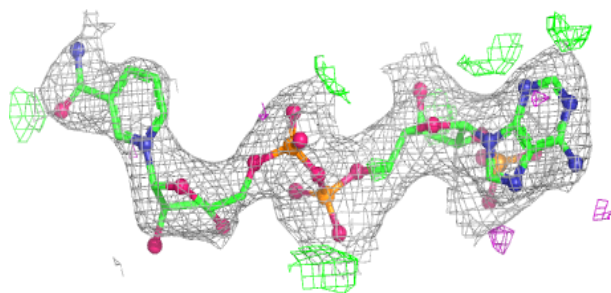
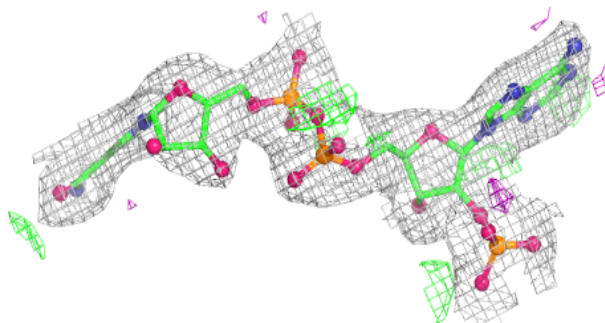
**Electron density around NAP D 901:**

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

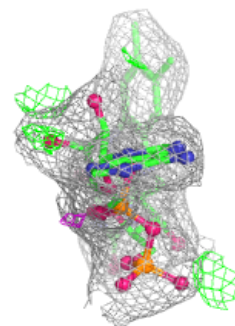
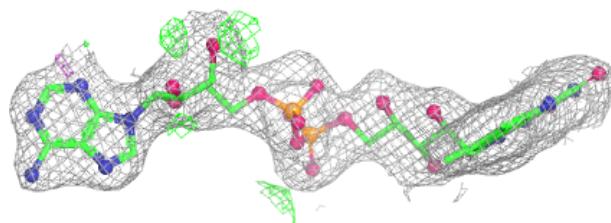
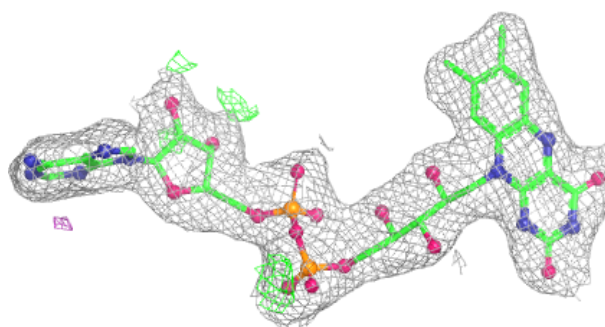


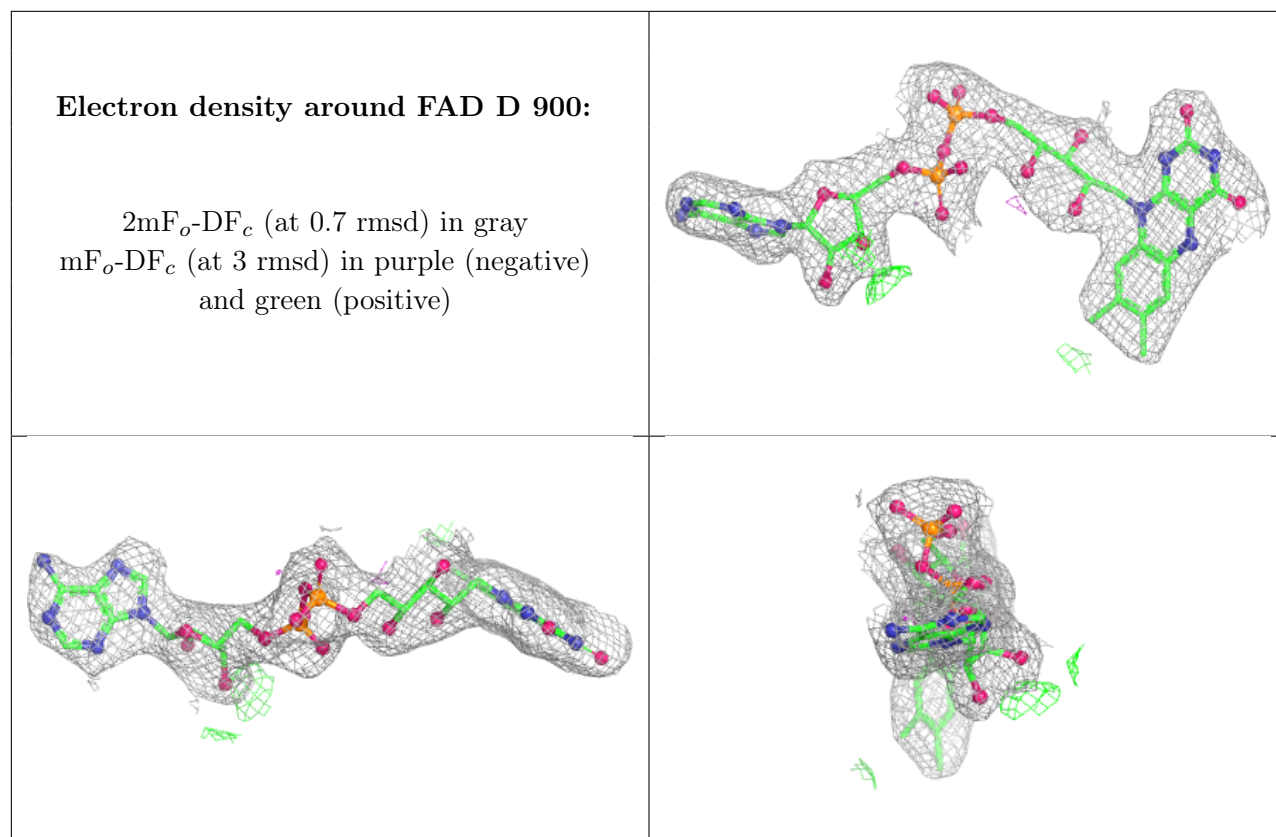
Electron density around NAP B 901:

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

**Electron density around FAD B 900:**

$2mF_o-DF_c$ (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.