



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:01 PM UTC

PDB ID : 3DH7 / pdb_00003dh7
Title : Structure of T. thermophilus IDI-2 in complex with PPI
Authors : de Ruyck, J.; Wouters, J.
Deposited on : 2008-06-17
Resolution : 2.97 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

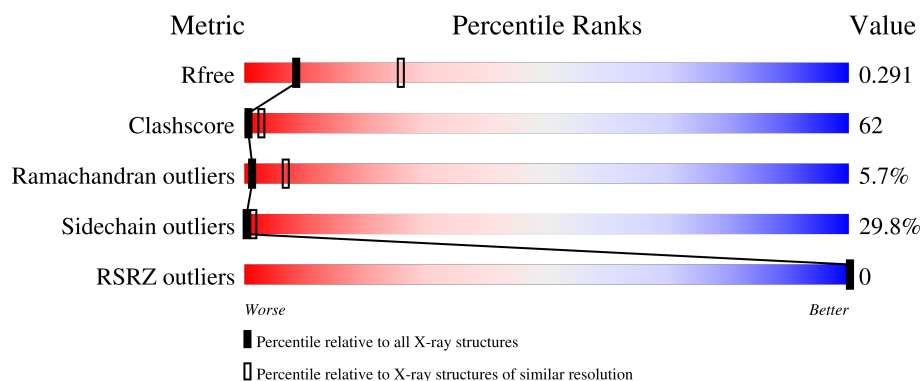
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	332	
1	B	332	
1	C	332	
1	D	332	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	A	502	-	X	X	-
2	FMN	B	502	-	X	X	-
2	FMN	C	502	-	X	X	-
2	FMN	D	502	-	X	X	-

2 Entry composition [i](#)

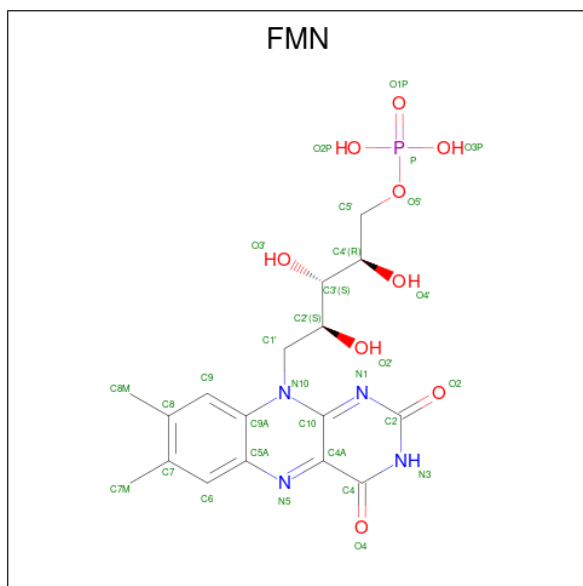
There are 4 unique types of molecules in this entry. The entry contains 9991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2419	1539	439	434	7			
1	B	318	Total	C	N	O	S	0	0	0
			2423	1543	439	434	7			
1	C	316	Total	C	N	O	S	0	0	0
			2406	1531	437	431	7			
1	D	313	Total	C	N	O	S	0	0	0
			2372	1509	428	428	7			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



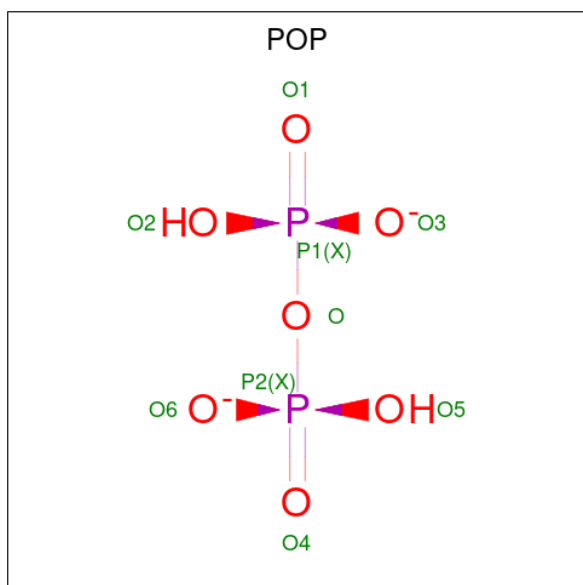
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			9	7	2		
3	D	1	Total	O	P	0	0
			9	7	2		

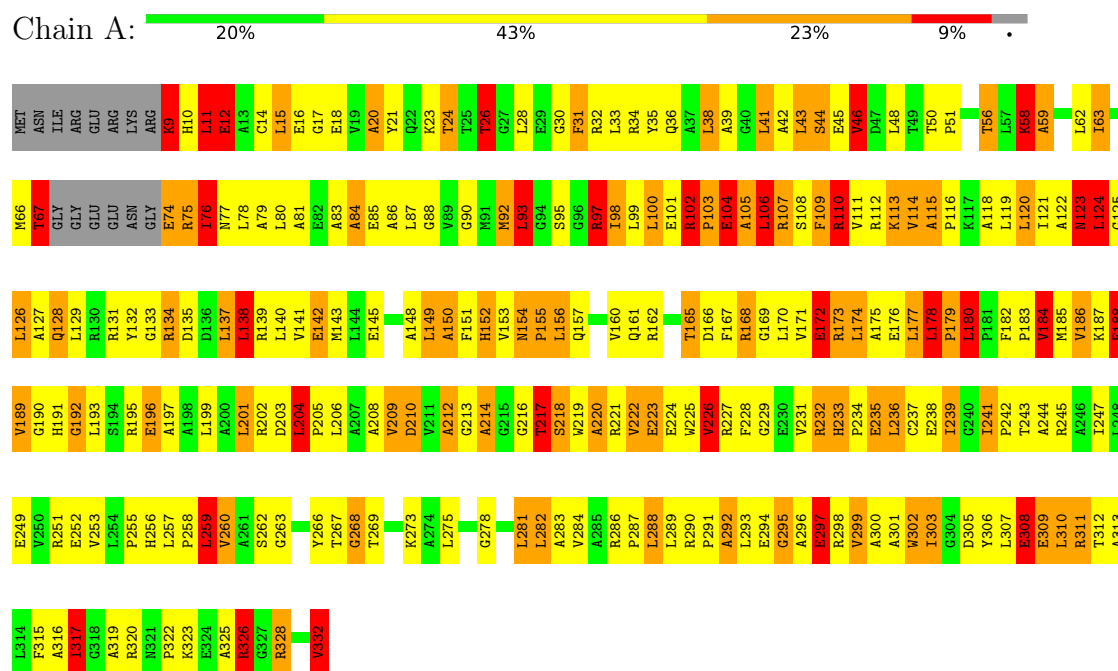
- Molecule 4 is water.

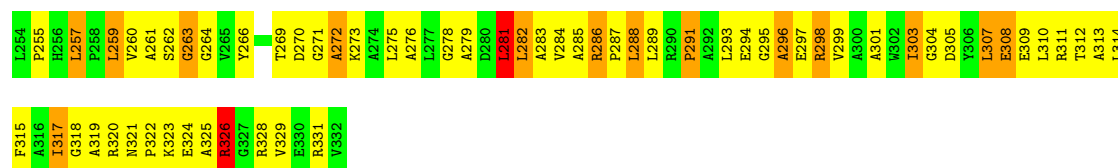
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	48	Total	O	0	0
			48	48		
4	C	59	Total	O	0	0
			59	59		
4	D	68	Total	O	0	0
			68	68		

3 Residue-property plots

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

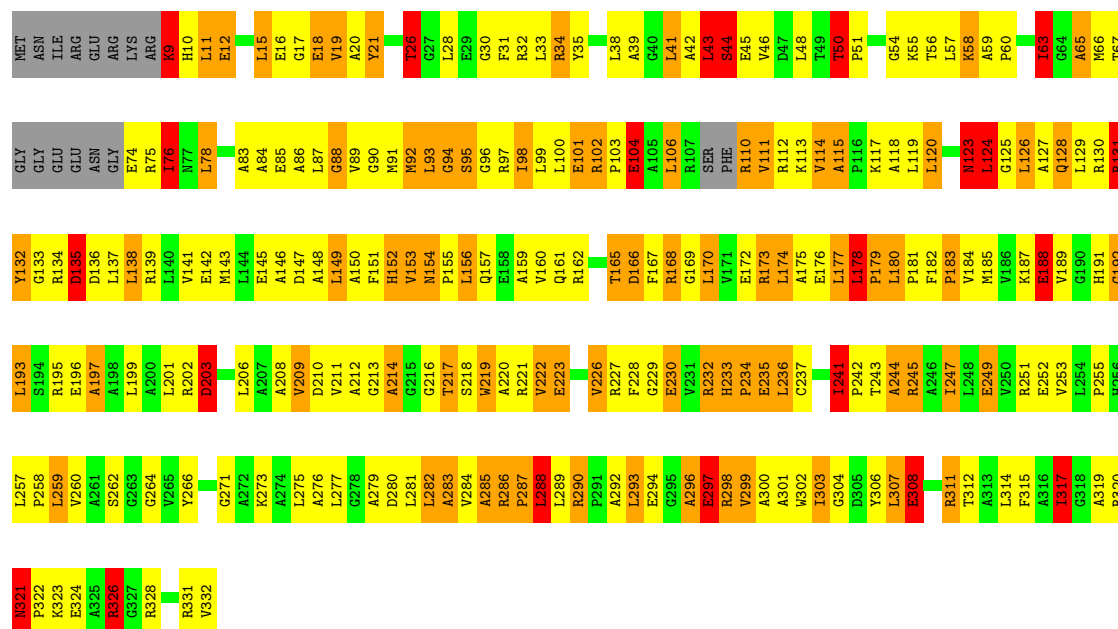
• Molecule 1: Isopentenyl-diphosphate delta-isomerase





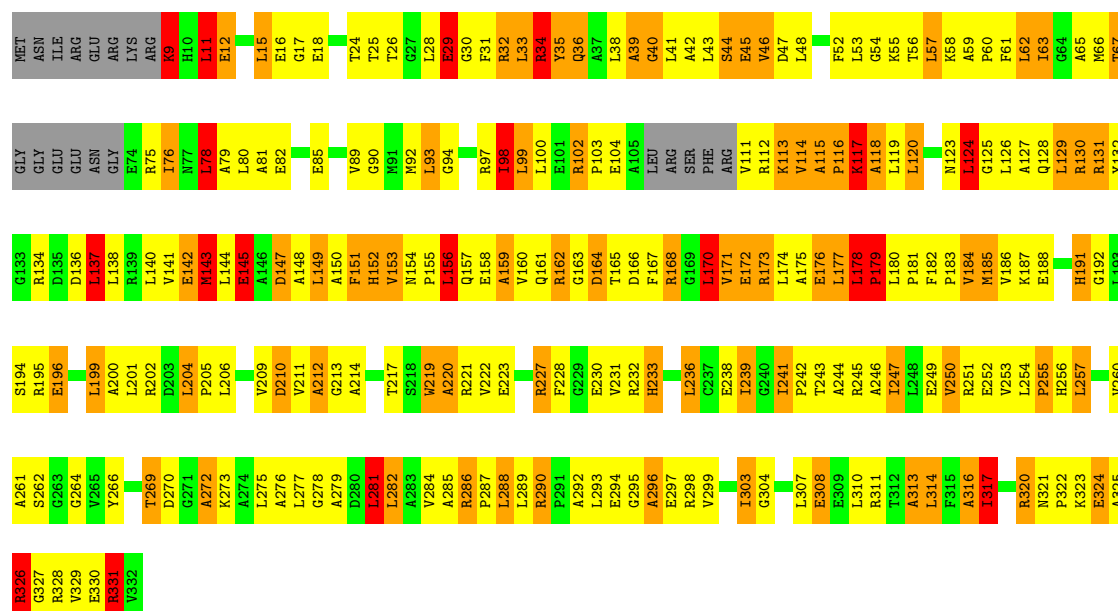
• Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain C: 23% 42% 23% 7% 5%



• Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain D: 23% 43% 23% 6% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	142.53Å 142.53Å 109.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 2.97 19.92 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.92-2.97) 98.0 (19.92-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.293 0.210 , 0.291	Depositor DCC
R_{free} test set	2538 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 1.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l 0.457 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9991	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: POP, FMN

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	1.91	47/2457 (1.9%)	1.99	87/3326 (2.6%)
1	B	1.75	20/2462 (0.8%)	1.80	52/3334 (1.6%)
1	C	1.81	32/2443 (1.3%)	1.87	70/3307 (2.1%)
1	D	1.86	43/2408 (1.8%)	1.81	54/3260 (1.7%)
All	All	1.83	142/9770 (1.5%)	1.87	263/13227 (2.0%)

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	A	0	8
1	B	1	4
1	C	1	5
1	D	0	4
All	All	2	21

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	35	TYR	C-O	21.57	1.53	1.23
1	A	76	ILE	CA-CB	12.99	1.68	1.54
1	D	33	LEU	C-N	11.15	1.49	1.33
1	A	326	ARG	CG-CD	9.11	1.79	1.52
1	A	214	ALA	CA-CB	-8.80	1.38	1.53
1	B	239	ILE	CA-CB	-8.47	1.44	1.54
1	C	326	ARG	CG-CD	8.46	1.77	1.52
1	D	313	ALA	CA-CB	-8.24	1.40	1.53
1	A	38	LEU	N-CA	-8.22	1.36	1.46
1	D	35	TYR	C-N	8.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	GLU	N-CA	8.04	1.56	1.46
1	A	63	ILE	CA-C	-8.01	1.43	1.52
1	C	76	ILE	CA-CB	7.99	1.65	1.54
1	A	114	VAL	CA-CB	7.95	1.64	1.54
1	A	143	MET	CG-SD	7.84	2.00	1.80
1	D	44	SER	CA-CB	7.64	1.66	1.53
1	B	313	ALA	CA-CB	-7.64	1.41	1.53
1	A	155	PRO	N-CD	7.61	1.58	1.47
1	B	50	THR	CA-CB	7.60	1.66	1.53
1	D	214	ALA	CA-CB	-7.57	1.41	1.53
1	D	35	TYR	N-CA	7.46	1.55	1.45
1	A	326	ARG	CD-NE	7.43	1.56	1.46
1	A	326	ARG	NE-CZ	7.42	1.41	1.33
1	B	246	ALA	CA-CB	-7.42	1.41	1.53
1	D	39	ALA	CA-CB	7.30	1.65	1.53
1	C	259	LEU	CA-C	-7.20	1.44	1.52
1	D	115	ALA	CA-CB	-7.02	1.42	1.53
1	C	177	LEU	CA-C	-7.00	1.40	1.52
1	B	59	ALA	C-O	-6.96	1.18	1.24
1	C	326	ARG	CD-NE	6.95	1.55	1.46
1	A	317	ILE	CA-CB	6.95	1.63	1.54
1	A	193	LEU	C-O	-6.88	1.15	1.24
1	C	276	ALA	CA-CB	-6.88	1.42	1.53
1	D	272	ALA	N-CA	-6.84	1.37	1.46
1	D	317	ILE	CA-CB	6.83	1.62	1.54
1	A	186	VAL	CA-C	6.67	1.60	1.52
1	D	272	ALA	CA-CB	-6.65	1.42	1.53
1	D	171	VAL	CA-C	-6.63	1.44	1.52
1	A	143	MET	CB-CG	6.60	1.72	1.52
1	C	222	VAL	N-CA	6.54	1.54	1.46
1	B	143	MET	CG-SD	6.47	1.97	1.80
1	A	50	THR	CA-CB	6.47	1.63	1.53
1	D	34	ARG	N-CA	-6.46	1.38	1.46
1	C	226	VAL	C-O	-6.42	1.17	1.24
1	A	58	LYS	CD-CE	6.41	1.71	1.52
1	B	44	SER	CA-CB	6.35	1.64	1.53
1	C	213	GLY	C-O	6.33	1.32	1.23
1	A	212	ALA	CA-CB	-6.28	1.43	1.53
1	D	179	PRO	N-CA	6.26	1.55	1.47
1	A	326	ARG	CB-CG	6.21	1.71	1.52
1	A	213	GLY	C-O	6.20	1.30	1.23
1	C	126	LEU	N-CA	-6.19	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	GLU	C-O	-6.13	1.16	1.24
1	A	302	TRP	CA-C	-6.13	1.44	1.52
1	D	36	GLN	C-O	-6.12	1.16	1.23
1	D	143	MET	CB-CG	6.09	1.70	1.52
1	C	123	ASN	N-CA	-6.08	1.38	1.46
1	D	313	ALA	CA-C	-6.07	1.45	1.52
1	D	250	VAL	CA-CB	-6.04	1.47	1.54
1	C	135	ASP	CA-C	-5.99	1.45	1.52
1	A	141	VAL	N-CA	-5.98	1.39	1.46
1	B	128	GLN	C-O	-5.98	1.16	1.24
1	D	158	GLU	CA-C	-5.95	1.45	1.52
1	B	165	THR	N-CA	-5.95	1.38	1.46
1	C	166	ASP	CA-C	5.93	1.60	1.53
1	C	326	ARG	NE-CZ	5.93	1.39	1.33
1	C	290	ARG	C-O	-5.91	1.19	1.24
1	C	244	ALA	CA-CB	-5.90	1.44	1.53
1	A	20	ALA	CA-CB	-5.89	1.44	1.53
1	A	59	ALA	CA-CB	-5.89	1.46	1.53
1	C	214	ALA	CA-CB	-5.86	1.44	1.53
1	A	197	ALA	N-CA	5.85	1.53	1.46
1	D	143	MET	CG-SD	5.84	1.95	1.80
1	D	220	ALA	CA-C	5.83	1.60	1.52
1	C	31	PHE	CA-C	-5.81	1.45	1.52
1	D	76	ILE	CA-CB	5.78	1.61	1.54
1	A	150	ALA	CA-C	-5.78	1.45	1.52
1	D	152	HIS	C-O	-5.77	1.16	1.23
1	D	33	LEU	C-O	5.76	1.30	1.24
1	C	297	GLU	CA-C	5.75	1.60	1.52
1	A	217	THR	CA-CB	5.74	1.61	1.53
1	D	62	LEU	CA-C	-5.71	1.45	1.52
1	C	44	SER	CB-OG	5.71	1.53	1.42
1	A	177	LEU	CA-C	-5.67	1.43	1.52
1	C	20	ALA	CA-CB	-5.65	1.43	1.53
1	B	106	LEU	N-CA	5.63	1.53	1.46
1	A	31	PHE	CA-C	-5.62	1.46	1.52
1	D	167	PHE	CA-C	-5.62	1.45	1.52
1	A	126	LEU	N-CA	-5.59	1.39	1.46
1	C	303	ILE	CA-CB	-5.59	1.48	1.54
1	A	150	ALA	CA-CB	-5.58	1.43	1.53
1	C	95	SER	CA-C	5.58	1.60	1.52
1	D	34	ARG	C-N	5.57	1.40	1.33
1	A	186	VAL	CA-CB	5.55	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	34	ARG	CG-CD	5.55	1.69	1.52
1	D	78	LEU	CA-C	-5.53	1.45	1.53
1	B	154	ASN	CA-C	5.53	1.59	1.52
1	D	164	ASP	CB-CG	5.53	1.65	1.52
1	B	143	MET	CB-CG	5.52	1.69	1.52
1	B	115	ALA	CA-CB	-5.51	1.46	1.53
1	A	311	ARG	NE-CZ	5.50	1.39	1.33
1	D	117	LYS	CA-C	5.49	1.60	1.52
1	D	210	ASP	N-CA	-5.47	1.39	1.46
1	D	58	LYS	N-CA	-5.47	1.39	1.46
1	A	319	ALA	CA-CB	-5.46	1.45	1.53
1	C	287	PRO	N-CA	-5.45	1.40	1.47
1	C	271	GLY	C-O	-5.42	1.17	1.23
1	C	178	LEU	C-O	5.41	1.31	1.24
1	C	153	VAL	C-O	-5.36	1.18	1.24
1	D	32	ARG	CZ-NH1	5.36	1.40	1.32
1	D	317	ILE	N-CA	5.35	1.53	1.46
1	B	220	ALA	CA-CB	-5.32	1.45	1.53
1	A	220	ALA	CA-CB	-5.29	1.45	1.53
1	B	272	ALA	N-CA	-5.29	1.39	1.46
1	A	120	LEU	CA-C	-5.29	1.46	1.52
1	A	241	ILE	CA-C	5.28	1.57	1.53
1	B	84	ALA	CA-CB	-5.28	1.45	1.53
1	D	255	PRO	C-O	-5.28	1.17	1.24
1	D	164	ASP	N-CA	5.28	1.52	1.46
1	C	197	ALA	N-CA	5.25	1.52	1.46
1	D	178	LEU	CA-C	-5.22	1.46	1.52
1	A	188	GLU	CD-OE2	5.21	1.35	1.25
1	C	317	ILE	CA-CB	5.20	1.61	1.54
1	B	51	PRO	CA-C	5.18	1.57	1.52
1	A	313	ALA	CA-C	-5.17	1.46	1.52
1	C	311	ARG	NE-CZ	5.17	1.38	1.33
1	B	24	THR	N-CA	5.15	1.52	1.46
1	D	34	ARG	CA-CB	-5.15	1.46	1.52
1	A	124	LEU	N-CA	-5.13	1.39	1.46
1	D	179	PRO	CB-CG	5.12	1.75	1.49
1	A	138	LEU	N-CA	5.09	1.52	1.46
1	A	67	THR	CA-CB	5.08	1.68	1.54
1	A	326	ARG	C-O	-5.08	1.17	1.24
1	C	283	ALA	CA-CB	-5.08	1.43	1.53
1	A	106	LEU	CA-C	5.05	1.59	1.53
1	A	229	GLY	N-CA	5.05	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	ALA	CA-CB	-5.05	1.45	1.53
1	D	269	THR	CA-CB	-5.04	1.45	1.53
1	A	209	VAL	N-CA	5.03	1.51	1.46
1	A	259	LEU	CA-C	-5.03	1.46	1.52
1	A	184	VAL	CA-CB	5.02	1.60	1.54
1	C	308	GLU	CG-CD	5.00	1.64	1.52

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ASN	CA-C-N	12.48	131.95	118.97
1	A	154	ASN	C-N-CA	12.48	131.95	118.97
1	D	34	ARG	CG-CD-NE	-10.53	88.83	112.00
1	A	63	ILE	N-CA-C	-10.20	95.34	109.21
1	A	172	GLU	N-CA-C	-9.86	98.75	112.45
1	A	93	LEU	N-CA-C	-9.77	97.36	110.55
1	A	241	ILE	CA-C-N	-9.64	109.83	119.76
1	A	241	ILE	C-N-CA	-9.64	109.83	119.76
1	B	233	HIS	CA-C-N	9.56	131.78	119.84
1	B	233	HIS	C-N-CA	9.56	131.78	119.84
1	D	115	ALA	CA-C-N	9.38	131.57	119.84
1	D	115	ALA	C-N-CA	9.38	131.57	119.84
1	B	191	HIS	N-CA-C	-9.33	101.90	113.38
1	A	204	LEU	CA-C-N	9.25	131.40	119.84
1	A	204	LEU	C-N-CA	9.25	131.40	119.84
1	A	309	GLU	N-CA-C	9.22	120.94	111.07
1	D	233	HIS	CA-C-N	9.03	131.12	119.84
1	D	233	HIS	C-N-CA	9.03	131.12	119.84
1	C	201	LEU	N-CA-C	-8.98	101.87	112.92
1	B	29	GLU	N-CA-C	-8.94	101.91	113.17
1	C	253	VAL	CB-CA-C	-8.89	101.33	111.55
1	B	27	GLY	N-CA-C	-8.88	101.40	115.08
1	A	114	VAL	N-CA-C	-8.71	102.51	113.22
1	D	326	ARG	N-CA-C	-8.70	97.72	110.42
1	A	123	ASN	N-CA-C	8.61	122.50	109.41
1	D	257	LEU	CA-C-N	-8.55	111.17	119.89
1	D	257	LEU	C-N-CA	-8.55	111.17	119.89
1	C	308	GLU	N-CA-C	-8.47	102.13	111.36
1	B	326	ARG	N-CA-C	-8.29	98.31	110.42
1	C	132	TYR	N-CA-C	8.04	120.90	110.53
1	B	192	GLY	N-CA-C	7.85	122.85	112.65
1	A	50	THR	CA-C-N	7.84	128.45	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	THR	C-N-CA	7.84	128.45	120.14
1	A	176	GLU	CA-C-N	-7.82	109.91	122.66
1	A	176	GLU	C-N-CA	-7.82	109.91	122.66
1	A	295	GLY	N-CA-C	7.78	126.58	112.58
1	A	299	VAL	N-CA-C	-7.74	103.25	110.53
1	B	57	LEU	N-CA-C	7.68	122.17	109.95
1	B	156	LEU	N-CA-C	-7.65	102.28	111.69
1	C	222	VAL	N-CA-CB	7.63	118.64	110.62
1	D	147	ASP	N-CA-C	-7.63	104.10	113.41
1	B	244	ALA	N-CA-C	-7.61	102.98	111.28
1	A	241	ILE	CA-C-O	7.53	123.34	119.12
1	B	28	LEU	N-CA-C	-7.52	104.08	113.18
1	C	178	LEU	N-CA-C	7.47	126.32	109.81
1	C	39	ALA	N-CA-C	-7.40	104.06	113.23
1	C	178	LEU	N-CA-CB	7.31	123.38	110.37
1	D	113	LYS	N-CA-C	-7.29	104.53	113.50
1	B	301	ALA	N-CA-C	-7.28	103.34	111.28
1	A	103	PRO	N-CA-CB	7.11	110.71	103.25
1	A	259	LEU	CB-CA-C	-7.07	98.08	109.75
1	C	86	ALA	N-CA-C	-7.07	103.62	111.82
1	B	41	LEU	N-CA-C	7.06	121.00	109.85
1	A	218	SER	CA-C-N	-7.04	110.14	120.28
1	A	218	SER	C-N-CA	-7.04	110.14	120.28
1	A	182	PHE	N-CA-C	-7.00	101.22	110.40
1	C	174	LEU	N-CA-C	-6.98	103.36	110.97
1	D	33	LEU	N-CA-C	-6.95	99.37	109.59
1	A	297	GLU	N-CA-C	-6.93	104.96	113.41
1	C	241	ILE	CG1-CB-CG2	-6.91	89.97	110.70
1	A	309	GLU	N-CA-CB	6.90	120.02	110.01
1	D	204	LEU	N-CA-C	6.89	117.53	109.60
1	D	35	TYR	CA-C-N	-6.87	112.16	122.47
1	D	35	TYR	C-N-CA	-6.87	112.16	122.47
1	C	209	VAL	CA-C-N	-6.87	113.64	122.77
1	C	209	VAL	C-N-CA	-6.87	113.64	122.77
1	A	105	ALA	N-CA-C	6.85	120.32	109.50
1	A	102	ARG	CA-C-N	6.84	128.40	119.84
1	A	102	ARG	C-N-CA	6.84	128.40	119.84
1	B	19	VAL	CB-CA-C	-6.82	102.74	111.20
1	C	63	ILE	N-CA-C	-6.82	100.16	109.37
1	C	26	THR	N-CA-C	-6.80	103.89	111.71
1	A	122	ALA	CA-C-N	-6.75	111.48	122.82
1	A	122	ALA	C-N-CA	-6.75	111.48	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	TYR	N-CA-C	-6.71	104.04	111.36
1	C	288	LEU	N-CA-C	-6.71	105.06	113.18
1	A	192	GLY	N-CA-C	6.71	120.60	112.48
1	C	115	ALA	N-CA-C	6.68	119.25	109.30
1	B	159	ALA	N-CA-C	-6.67	104.03	111.71
1	D	47	ASP	N-CA-C	6.60	120.74	107.41
1	C	12	GLU	N-CA-C	6.58	118.12	111.07
1	C	188	GLU	CB-CA-C	6.57	123.50	110.42
1	C	177	LEU	CB-CA-C	-6.57	97.53	110.27
1	A	174	LEU	N-CA-C	-6.52	104.09	111.14
1	A	102	ARG	O-C-N	6.51	126.67	121.20
1	A	202	ARG	CA-C-N	-6.50	110.05	122.53
1	A	202	ARG	C-N-CA	-6.50	110.05	122.53
1	D	170	LEU	N-CA-C	6.47	122.05	111.37
1	C	154	ASN	CA-C-N	6.46	125.96	119.24
1	C	154	ASN	C-N-CA	6.46	125.96	119.24
1	D	159	ALA	N-CA-C	-6.44	104.35	111.82
1	C	218	SER	CA-C-N	-6.42	110.54	120.31
1	C	218	SER	C-N-CA	-6.42	110.54	120.31
1	C	326	ARG	N-CA-C	-6.39	100.58	110.10
1	D	286	ARG	CA-C-N	-6.38	113.15	120.04
1	D	286	ARG	C-N-CA	-6.38	113.15	120.04
1	A	150	ALA	N-CA-C	-6.38	98.51	108.90
1	A	143	MET	CB-CG-SD	6.36	131.78	112.70
1	D	40	GLY	N-CA-C	6.34	125.17	113.76
1	C	311	ARG	N-CA-C	-6.33	104.29	111.07
1	D	209	VAL	CA-C-N	-6.33	114.34	122.77
1	D	209	VAL	C-N-CA	-6.33	114.34	122.77
1	A	106	LEU	CA-C-N	6.31	133.06	121.70
1	A	106	LEU	C-N-CA	6.31	133.06	121.70
1	B	209	VAL	N-CA-C	-6.26	99.69	108.27
1	C	273	LYS	N-CA-C	-6.25	103.39	111.02
1	A	115	ALA	N-CA-C	6.21	119.31	108.75
1	C	166	ASP	N-CA-C	6.18	119.56	107.57
1	A	56	THR	CB-CA-C	-6.18	100.62	110.81
1	D	148	ALA	N-CA-C	6.17	118.33	109.14
1	C	209	VAL	CB-CA-C	-6.15	101.53	110.63
1	C	124	LEU	CA-C-N	-6.14	109.37	121.41
1	C	124	LEU	C-N-CA	-6.14	109.37	121.41
1	C	252	GLU	N-CA-C	-6.13	104.66	111.71
1	A	124	LEU	CA-C-N	-6.11	109.43	121.41
1	A	124	LEU	C-N-CA	-6.11	109.43	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ALA	N-CA-C	-6.09	104.72	111.36
1	B	75	ARG	N-CA-C	-6.07	103.99	111.40
1	C	120	LEU	CA-C-N	-6.05	115.25	123.12
1	C	120	LEU	C-N-CA	-6.05	115.25	123.12
1	A	133	GLY	N-CA-C	-6.04	101.04	112.51
1	A	155	PRO	N-CD-CG	-6.02	94.16	103.20
1	D	151	PHE	CB-CA-C	-6.02	100.44	110.19
1	C	326	ARG	CG-CD-NE	5.99	125.17	112.00
1	C	50	THR	CA-C-N	5.98	125.74	119.76
1	C	50	THR	C-N-CA	5.98	125.74	119.76
1	B	178	LEU	N-CA-CB	5.95	120.97	110.37
1	A	106	LEU	CA-CB-CG	5.93	137.06	116.30
1	C	54	GLY	N-CA-C	5.92	127.22	113.18
1	B	191	HIS	CB-CA-C	5.92	119.95	109.65
1	C	317	ILE	CA-CB-CG2	5.92	120.57	110.50
1	D	156	LEU	N-CA-C	-5.90	104.44	111.69
1	B	144	LEU	N-CA-C	-5.89	106.12	113.55
1	D	313	ALA	N-CA-C	-5.88	104.22	111.40
1	C	132	TYR	CA-CB-CG	-5.88	103.32	113.90
1	C	65	ALA	N-CA-C	5.86	118.86	110.24
1	A	203	ASP	N-CA-C	5.82	120.39	113.12
1	D	331	ARG	N-CA-C	-5.79	101.33	109.96
1	D	250	VAL	N-CA-C	-5.78	104.72	110.62
1	D	34	ARG	CB-CG-CD	5.78	124.59	111.30
1	C	222	VAL	CB-CA-C	-5.77	104.31	111.70
1	B	281	LEU	CA-CB-CG	5.74	136.39	116.30
1	A	34	ARG	CG-CD-NE	-5.74	99.38	112.00
1	B	165	THR	N-CA-C	-5.71	98.65	110.80
1	D	137	LEU	N-CA-C	-5.71	104.75	110.97
1	D	34	ARG	N-CA-C	-5.70	99.51	108.63
1	C	219	TRP	CA-CB-CG	-5.69	102.79	113.60
1	A	308	GLU	CB-CA-C	5.68	120.22	110.79
1	A	209	VAL	CA-C-N	-5.68	115.04	123.11
1	A	209	VAL	C-N-CA	-5.68	115.04	123.11
1	C	154	ASN	N-CA-C	5.68	122.36	109.81
1	B	209	VAL	CA-C-N	-5.67	114.70	122.93
1	B	209	VAL	C-N-CA	-5.67	114.70	122.93
1	C	177	LEU	N-CA-C	-5.67	106.44	113.19
1	B	43	LEU	N-CA-C	-5.66	105.01	111.07
1	A	97	ARG	CA-C-N	5.65	128.18	120.77
1	A	97	ARG	C-N-CA	5.65	128.18	120.77
1	C	96	GLY	CA-C-N	5.65	128.16	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	GLY	C-N-CA	5.65	128.16	120.54
1	C	193	LEU	N-CA-C	5.63	117.90	108.73
1	B	252	GLU	N-CA-CB	5.62	119.00	110.28
1	B	162	ARG	N-CA-C	-5.61	103.66	111.52
1	B	115	ALA	CA-C-N	5.61	126.85	119.84
1	B	115	ALA	C-N-CA	5.61	126.85	119.84
1	B	177	LEU	N-CA-C	-5.60	105.10	112.72
1	C	152	HIS	CA-C-N	-5.59	115.88	122.93
1	C	152	HIS	C-N-CA	-5.59	115.88	122.93
1	D	171	VAL	N-CA-C	-5.59	105.28	110.53
1	D	45	GLU	CA-C-N	-5.59	113.98	121.80
1	D	45	GLU	C-N-CA	-5.59	113.98	121.80
1	A	137	LEU	N-CA-C	-5.57	104.71	112.45
1	D	281	LEU	CA-CB-CG	5.56	135.76	116.30
1	B	250	VAL	N-CA-C	-5.54	104.01	111.44
1	B	39	ALA	N-CA-C	-5.53	105.64	112.38
1	D	303	ILE	CB-CA-C	-5.51	104.80	112.02
1	D	81	ALA	N-CA-C	-5.50	105.67	112.38
1	A	201	LEU	N-CA-C	-5.50	106.58	113.28
1	B	9	LYS	CA-C-N	5.49	127.90	120.38
1	B	9	LYS	C-N-CA	5.49	127.90	120.38
1	C	323	LYS	N-CA-CB	5.49	118.28	110.16
1	B	272	ALA	N-CA-C	-5.49	104.94	111.69
1	D	44	SER	CA-CB-OG	5.48	122.06	111.10
1	D	124	LEU	N-CA-C	5.47	119.67	111.96
1	D	164	ASP	N-CA-C	-5.46	101.58	110.20
1	C	331	ARG	CB-CA-C	5.45	119.87	110.77
1	D	191	HIS	N-CA-C	-5.45	106.64	113.72
1	C	17	GLY	N-CA-C	5.43	120.82	112.51
1	D	123	ASN	N-CA-C	5.43	117.53	108.02
1	A	152	HIS	CA-C-N	-5.42	116.47	123.19
1	A	152	HIS	C-N-CA	-5.42	116.47	123.19
1	B	263	GLY	N-CA-C	-5.41	100.35	113.18
1	D	239	ILE	CB-CA-C	-5.40	103.27	111.69
1	A	317	ILE	CA-CB-CG2	5.40	119.67	110.50
1	B	247	ILE	CB-CA-C	-5.38	102.47	111.29
1	D	200	ALA	N-CA-C	-5.38	105.50	111.36
1	D	184	VAL	CB-CA-C	-5.37	102.61	110.62
1	B	188	GLU	N-CA-C	-5.37	101.96	109.69
1	C	286	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	304	GLY	N-CA-C	-5.36	105.91	112.77
1	C	234	PRO	O-C-N	5.35	128.39	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	HIS	N-CA-C	5.33	122.15	110.80
1	D	281	LEU	N-CA-C	5.33	115.57	108.38
1	B	209	VAL	CB-CA-C	-5.32	101.29	110.65
1	C	131	ARG	N-CA-CB	5.32	119.48	110.49
1	B	169	GLY	CA-C-N	5.30	127.70	120.54
1	B	169	GLY	C-N-CA	5.30	127.70	120.54
1	A	332	VAL	CB-CA-C	-5.28	101.37	111.40
1	A	46	VAL	N-CA-CB	5.28	116.86	110.95
1	B	65	ALA	N-CA-C	5.27	117.99	110.24
1	A	86	ALA	N-CA-C	-5.26	105.66	111.71
1	B	143	MET	CB-CG-SD	5.26	128.48	112.70
1	B	219	TRP	CA-CB-CG	-5.26	103.60	113.60
1	C	183	PRO	N-CA-C	5.25	119.45	111.15
1	C	293	LEU	N-CA-C	5.25	118.79	112.38
1	D	170	LEU	CA-CB-CG	-5.24	97.96	116.30
1	D	44	SER	N-CA-CB	5.24	118.42	110.14
1	A	104	GLU	N-CA-C	5.24	121.95	110.80
1	A	284	VAL	N-CA-C	5.23	115.44	108.11
1	C	88	GLY	N-CA-C	-5.23	105.86	114.76
1	C	146	ALA	N-CA-C	-5.23	101.75	109.86
1	A	23	LYS	CA-C-N	-5.23	112.71	121.39
1	A	23	LYS	C-N-CA	-5.23	112.71	121.39
1	A	141	VAL	CB-CA-C	5.23	118.57	111.88
1	A	292	ALA	N-CA-C	-5.22	105.59	111.28
1	A	247	ILE	N-CA-C	-5.21	105.42	110.42
1	B	199	LEU	CA-CB-CG	-5.21	98.06	116.30
1	A	180	LEU	N-CA-C	-5.20	104.15	110.13
1	A	190	GLY	CA-C-N	-5.20	113.97	122.54
1	A	190	GLY	C-N-CA	-5.20	113.97	122.54
1	C	178	LEU	CA-C-N	-5.19	113.35	119.84
1	C	178	LEU	C-N-CA	-5.19	113.35	119.84
1	A	326	ARG	NH1-CZ-NH2	-5.19	112.56	119.30
1	C	285	ALA	N-CA-C	5.18	119.06	111.34
1	D	17	GLY	N-CA-C	5.18	119.62	112.37
1	A	214	ALA	N-CA-C	-5.18	103.56	110.55
1	B	259	LEU	CB-CA-C	-5.15	101.61	110.16
1	B	228	PHE	CB-CA-C	-5.14	100.18	110.42
1	D	158	GLU	CB-CA-C	-5.14	102.11	110.85
1	A	143	MET	N-CA-C	-5.14	104.94	111.11
1	A	178	LEU	CA-C-N	-5.13	113.42	119.84
1	A	178	LEU	C-N-CA	-5.13	113.42	119.84
1	A	282	LEU	CA-C-N	-5.13	113.55	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	LEU	C-N-CA	-5.13	113.55	122.37
1	C	21	TYR	CA-C-N	-5.12	113.40	122.26
1	C	21	TYR	C-N-CA	-5.12	113.40	122.26
1	B	147	ASP	N-CA-CB	-5.11	103.02	110.53
1	D	219	TRP	CA-CB-CG	-5.10	103.92	113.60
1	C	192	GLY	N-CA-C	5.09	118.64	112.48
1	A	172	GLU	N-CA-CB	5.09	117.84	110.26
1	C	321	ASN	N-CA-C	5.08	112.79	108.22
1	C	90	GLY	N-CA-C	-5.07	102.75	111.57
1	C	297	GLU	CB-CA-C	5.06	120.49	110.42
1	C	138	LEU	N-CA-CB	5.05	118.00	110.22
1	A	216	GLY	N-CA-C	-5.04	101.24	113.18
1	B	106	LEU	CA-CB-CG	5.04	133.94	116.30
1	D	136	ASP	N-CA-C	-5.04	106.30	112.90
1	D	308	GLU	CB-CA-C	5.04	119.63	110.11
1	B	164	ASP	N-CA-CB	5.04	118.80	110.69
1	A	328	ARG	CB-CA-C	5.03	117.40	111.22
1	A	234	PRO	CA-C-N	5.02	126.96	120.44
1	A	234	PRO	C-N-CA	5.02	126.96	120.44
1	A	178	LEU	N-CA-C	5.01	120.89	109.81
1	B	235	GLU	N-CA-C	5.01	116.43	110.97

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	178	LEU	CA
1	C	178	LEU	CA

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Peptide
1	A	104	GLU	Peptide
1	A	106	LEU	Peptide
1	A	12	GLU	Peptide
1	A	123	ASN	Peptide
1	A	178	LEU	Peptide
1	A	43	LEU	Peptide
1	A	9	LYS	Peptide
1	B	146	ALA	Peptide
1	B	164	ASP	Peptide
1	B	178	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	62	LEU	Peptide
1	C	104	GLU	Peptide
1	C	178	LEU	Peptide
1	C	203	ASP	Peptide
1	C	43	LEU	Peptide
1	C	9	LYS	Peptide
1	D	163	GLY	Peptide
1	D	178	LEU	Peptide
1	D	327	GLY	Peptide
1	D	9	LYS	Peptide

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	2419	0	2502	320	1
1	B	2423	0	2515	368	1
1	C	2406	0	2500	290	0
1	D	2372	0	2450	296	0
2	A	31	0	19	13	0
2	B	31	0	19	11	0
2	C	31	0	19	13	0
2	D	31	0	19	10	0
3	B	9	0	0	1	0
3	D	9	0	0	1	0
4	A	54	0	0	2	0
4	B	48	0	0	12	0
4	C	59	0	0	9	0
4	D	68	0	0	15	0
All	All	9991	0	10043	1220	1

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 62.

All (1220) 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:A:326:ARG:CG	1:A:326:ARG:CD	1.79	1.56
1:C:326:ARG:CD	1:C:326:ARG:CG	1.77	1.55
1:C:217:THR:HG22	1:C:286:ARG:NH1	1.16	1.41
1:D:179:PRO:CG	1:D:179:PRO:CB	1.75	1.39
1:C:217:THR:CG2	1:C:286:ARG:NH1	1.87	1.33
1:B:217:THR:HG22	1:B:286:ARG:NH1	1.45	1.29
1:D:217:THR:HG22	1:D:286:ARG:NH1	1.45	1.28
1:C:217:THR:CG2	1:C:286:ARG:HH11	1.42	1.28
1:D:125:GLY:HA2	1:D:152:HIS:CD2	1.69	1.27
1:A:308:GLU:HG3	1:B:162:ARG:NH2	1.53	1.24
1:B:85:GLU:HG3	1:B:115:ALA:HA	1.22	1.18
1:A:217:THR:CG2	1:A:286:ARG:HB2	1.73	1.18
1:A:204:LEU:H	1:A:204:LEU:HD12	1.12	1.15
1:B:103:PRO:O	1:B:106:LEU:HB2	1.51	1.11
1:B:158:GLU:OE1	1:B:158:GLU:HA	1.42	1.11
1:A:110:ARG:HB3	1:A:111:VAL:HA	1.19	1.10
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.12	1.09
1:C:102:ARG:HG3	1:C:102:ARG:HH21	1.10	1.08
1:B:66:MET:O	1:B:67:THR:HB	1.54	1.07
1:D:217:THR:CG2	1:D:286:ARG:HH11	1.66	1.07
1:C:110:ARG:HG2	1:C:110:ARG:HH21	1.20	1.06
1:A:154:ASN:HD22	1:A:157:GLN:NE2	1.52	1.06
1:B:245:ARG:HH11	1:B:245:ARG:CG	1.69	1.05
1:D:264:GLY:HA2	1:D:266:TYR:CE1	1.93	1.04
1:D:125:GLY:HA2	1:D:152:HIS:HD2	1.03	1.04
1:B:162:ARG:HG2	1:B:227:ARG:NH1	1.73	1.03
1:A:204:LEU:H	1:A:204:LEU:CD1	1.72	1.03
1:C:161:GLN:HB3	1:C:223:GLU:CG	1.89	1.02
1:D:164:ASP:HB2	4:D:1214:HOH:O	1.55	1.02
1:C:161:GLN:HB3	1:C:223:GLU:HG3	1.37	1.01
1:A:217:THR:HB	1:A:286:ARG:HD3	1.38	1.01
1:D:180:LEU:HG	1:D:181:PRO:HD2	1.39	1.00
1:A:251:ARG:NH2	1:A:257:LEU:O	1.95	1.00
1:A:217:THR:HG21	1:A:286:ARG:HB2	1.01	1.00
1:A:217:THR:HG21	1:A:286:ARG:CB	1.92	0.99
1:C:251:ARG:NH2	1:C:257:LEU:O	1.94	0.99
1:C:296:ALA:O	1:C:298:ARG:N	1.94	0.99
1:B:217:THR:HG22	1:B:286:ARG:HH11	1.02	0.99
1:A:308:GLU:CG	1:B:162:ARG:NH2	2.25	0.99
1:B:217:THR:CG2	1:B:286:ARG:HH11	1.76	0.98
1:B:34:ARG:NH2	1:C:249:GLU:OE1	1.97	0.98
1:B:264:GLY:HA2	1:B:266:TYR:CE1	1.97	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ASP:HA	4:D:1167:HOH:O	1.61	0.98
1:B:174:LEU:HD23	1:B:204:LEU:HD23	1.42	0.98
1:C:161:GLN:CB	1:C:223:GLU:HG3	1.93	0.97
1:A:110:ARG:HB3	1:A:111:VAL:CA	1.91	0.97
1:D:78:LEU:HD22	1:D:114:VAL:HG21	1.45	0.96
1:A:154:ASN:HD22	1:A:157:GLN:HE21	1.12	0.96
1:A:79:ALA:HA	1:A:296:ALA:HB2	1.44	0.96
1:A:308:GLU:CG	1:B:162:ARG:HH22	1.78	0.95
1:D:55:LYS:NZ	1:D:118:ALA:O	1.99	0.95
1:A:241:ILE:HD12	1:D:35:TYR:HB3	1.49	0.95
1:B:63:ILE:HG23	1:B:288:LEU:HD23	1.48	0.95
1:C:217:THR:HG21	1:C:286:ARG:HB2	1.47	0.95
1:B:154:ASN:ND2	1:B:157:GLN:HE21	1.63	0.94
1:B:154:ASN:HD22	1:B:157:GLN:HE21	0.98	0.94
1:C:112:ARG:NH1	1:C:145:GLU:O	2.00	0.94
1:B:138:LEU:HD23	1:B:138:LEU:H	1.33	0.93
1:B:174:LEU:HD23	1:B:204:LEU:CD2	1.98	0.93
1:A:12:GLU:HA	1:A:15:LEU:HB2	1.47	0.93
1:C:217:THR:CB	1:C:286:ARG:NH1	2.32	0.93
1:D:154:ASN:HD22	1:D:157:GLN:HE21	1.14	0.93
1:A:235:GLU:HG2	1:D:269:THR:HB	1.47	0.92
1:B:190:GLY:HA2	1:B:212:ALA:O	1.67	0.92
1:B:106:LEU:HG	1:B:143:MET:HG2	1.50	0.92
1:A:196:GLU:HA	1:A:199:LEU:HD12	1.48	0.92
1:A:33:LEU:HD22	1:A:317:ILE:HG12	1.53	0.91
1:B:109:PHE:CG	1:B:144:LEU:HD21	2.06	0.91
1:A:204:LEU:HD12	1:A:204:LEU:N	1.85	0.90
1:B:312:THR:HG23	1:C:159:ALA:HB1	1.52	0.90
1:C:93:LEU:O	1:C:94:GLY:O	1.89	0.90
1:C:102:ARG:HG3	1:C:102:ARG:NH2	1.84	0.90
1:A:308:GLU:HG3	1:B:162:ARG:HH22	1.17	0.90
1:D:125:GLY:CA	1:D:152:HIS:CD2	2.52	0.90
1:D:127:ALA:HA	1:D:170:LEU:HD21	1.54	0.90
1:A:188:GLU:HG3	1:A:189:VAL:N	1.84	0.89
1:B:266:TYR:HE1	2:B:502:FMN:O3P	1.53	0.89
1:A:138:LEU:HD23	1:A:138:LEU:N	1.86	0.89
1:A:106:LEU:H	1:A:107:ARG:HB2	1.37	0.89
1:C:138:LEU:O	1:C:142:GLU:HG2	1.73	0.88
1:C:160:VAL:HG12	1:C:223:GLU:HB3	1.55	0.88
1:B:55:LYS:NZ	1:B:118:ALA:O	2.07	0.88
1:C:178:LEU:O	1:C:180:LEU:N	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:CG2	1:D:43:LEU:HB3	2.04	0.87
1:B:138:LEU:HD23	1:B:138:LEU:N	1.85	0.87
1:B:43:LEU:HB3	1:C:165:THR:HG21	1.55	0.87
1:B:74:GLU:HA	1:B:77:ASN:HB2	1.57	0.87
1:B:204:LEU:HD12	1:B:204:LEU:H	1.39	0.86
1:A:110:ARG:CB	1:A:111:VAL:HA	2.03	0.86
1:B:80:LEU:HB3	1:B:91:MET:HE3	1.56	0.86
1:B:59:ALA:HB2	1:B:307:LEU:CD1	2.06	0.86
1:B:85:GLU:OE1	1:B:117:LYS:N	2.08	0.86
1:A:303:ILE:O	1:A:307:LEU:HD12	1.76	0.86
1:B:102:ARG:HD3	4:B:1142:HOH:O	1.76	0.86
1:C:209:VAL:HG23	1:C:257:LEU:HD23	1.57	0.86
1:C:235:GLU:OE1	4:C:1175:HOH:O	1.92	0.86
1:D:321:ASN:ND2	1:D:324:GLU:HG3	1.91	0.86
1:C:38:LEU:HD11	1:D:201:LEU:HD21	1.60	0.84
1:B:53:LEU:N	4:B:1091:HOH:O	1.99	0.84
2:B:502:FMN:H4'	2:B:502:FMN:O1P	1.77	0.84
1:A:161:GLN:HB2	1:A:223:GLU:HG3	1.60	0.84
1:B:186:VAL:HG21	1:B:201:LEU:HD22	1.57	0.84
1:B:109:PHE:CD1	1:B:144:LEU:HD21	2.13	0.84
1:A:127:ALA:HA	1:A:170:LEU:HD21	1.58	0.83
1:B:43:LEU:HB3	1:C:165:THR:CG2	2.08	0.83
1:B:127:ALA:HA	1:B:170:LEU:HD21	1.58	0.83
1:A:112:ARG:NH1	1:A:145:GLU:O	2.09	0.83
2:B:502:FMN:O1P	2:B:502:FMN:C4'	2.27	0.83
1:C:245:ARG:NH1	1:C:245:ARG:HG2	1.93	0.83
1:A:241:ILE:CD1	1:D:35:TYR:HB3	2.08	0.82
1:A:41:LEU:HD12	1:A:41:LEU:C	2.01	0.82
1:A:162:ARG:HG3	1:A:227:ARG:NH1	1.93	0.82
1:A:217:THR:CG2	1:A:286:ARG:CB	2.56	0.82
1:A:195:ARG:HB2	1:A:249:GLU:HG2	1.62	0.82
1:B:109:PHE:HB3	1:B:144:LEU:HD23	1.62	0.82
1:C:217:THR:HG22	1:C:286:ARG:HH12	1.03	0.82
1:D:57:LEU:HD23	1:D:90:GLY:H	1.44	0.82
1:D:161:GLN:O	1:D:161:GLN:HG2	1.77	0.82
1:D:29:GLU:O	1:D:29:GLU:HG2	1.80	0.82
1:B:154:ASN:HD22	1:B:157:GLN:NE2	1.76	0.81
1:A:178:LEU:O	1:A:180:LEU:HD13	1.79	0.81
1:B:104:GLU:HG2	1:B:105:ALA:N	1.94	0.81
1:D:112:ARG:HG2	1:D:145:GLU:HG2	1.62	0.81
1:B:80:LEU:CB	1:B:91:MET:HE3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD23	1:A:138:LEU:H	1.44	0.81
1:A:218:SER:O	1:A:222:VAL:HG23	1.81	0.81
1:D:195:ARG:HD2	4:D:1033:HOH:O	1.81	0.81
1:B:109:PHE:HB3	1:B:144:LEU:CD2	2.11	0.81
1:C:167:PHE:HA	1:C:170:LEU:HD12	1.63	0.81
1:B:326:ARG:HA	1:B:326:ARG:HH11	1.46	0.80
1:B:125:GLY:HA2	1:B:152:HIS:O	1.81	0.80
1:A:59:ALA:CB	1:A:307:LEU:CD2	2.60	0.80
1:C:199:LEU:O	1:C:202:ARG:HB2	1.81	0.80
1:D:217:THR:HG21	1:D:286:ARG:HB2	1.64	0.80
1:B:80:LEU:CB	1:B:91:MET:CE	2.59	0.80
1:B:264:GLY:HA2	1:B:266:TYR:CZ	2.17	0.80
1:C:33:LEU:HD22	1:C:317:ILE:HG12	1.63	0.80
1:D:102:ARG:HD2	4:D:1090:HOH:O	1.81	0.80
1:A:332:VAL:HG13	1:A:332:VAL:O	1.80	0.80
1:D:251:ARG:NH1	1:D:278:GLY:O	2.14	0.80
1:B:326:ARG:HB2	1:B:326:ARG:NH1	1.97	0.80
1:D:178:LEU:HD13	1:D:205:PRO:HG2	1.64	0.80
1:C:18:GLU:HG3	4:C:1194:HOH:O	1.80	0.79
1:A:326:ARG:HH11	1:A:326:ARG:HB2	1.46	0.79
1:D:9:LYS:N	1:D:12:GLU:H	1.80	0.79
1:A:166:ASP:OD1	1:A:168:ARG:HB2	1.81	0.79
1:A:105:ALA:HB1	1:A:108:SER:N	1.97	0.79
1:A:219:TRP:HA	1:A:222:VAL:HG23	1.64	0.79
1:A:154:ASN:ND2	1:A:157:GLN:NE2	2.30	0.79
1:B:109:PHE:CB	1:B:144:LEU:CD2	2.60	0.79
1:A:33:LEU:HD22	1:A:317:ILE:CG1	2.11	0.79
1:B:80:LEU:HB2	1:B:91:MET:CE	2.12	0.78
1:C:41:LEU:C	1:C:41:LEU:HD12	2.07	0.78
1:C:296:ALA:O	1:C:297:GLU:C	2.27	0.78
1:A:106:LEU:N	1:A:107:ARG:HB2	1.98	0.78
1:B:98:ILE:HD12	1:B:98:ILE:H	1.49	0.78
1:D:217:THR:HG23	2:D:502:FMN:O3P	1.82	0.78
1:D:186:VAL:HG23	1:D:206:LEU:CD2	2.13	0.78
1:D:134:ARG:HG2	1:D:177:LEU:HD12	1.65	0.77
1:D:264:GLY:HA2	1:D:266:TYR:CZ	2.19	0.77
1:A:85:GLU:OE2	1:A:116:PRO:HD2	1.85	0.77
1:D:321:ASN:HD21	1:D:324:GLU:HG3	1.49	0.77
1:C:33:LEU:HB3	1:C:317:ILE:HD11	1.64	0.77
1:A:217:THR:HG23	2:A:502:FMN:O5'	1.86	0.76
1:B:245:ARG:CG	1:B:245:ARG:NH1	2.38	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:O	1:A:179:PRO:C	2.26	0.76
1:B:85:GLU:CG	1:B:115:ALA:HA	2.10	0.76
1:B:83:ALA:O	1:B:87:LEU:HB2	1.86	0.76
1:A:102:ARG:O	1:A:104:GLU:HB2	1.86	0.75
1:B:210:ASP:HB2	1:B:260:VAL:HB	1.68	0.75
1:D:93:LEU:HD11	1:D:120:LEU:HD13	1.68	0.75
1:C:106:LEU:O	1:C:110:ARG:HB2	1.86	0.75
1:C:102:ARG:HH21	1:C:102:ARG:CG	1.95	0.75
1:A:105:ALA:HB1	1:A:108:SER:H	1.52	0.75
1:A:138:LEU:O	1:A:142:GLU:HG3	1.87	0.75
1:C:209:VAL:CG2	1:C:257:LEU:HD23	2.17	0.75
1:A:123:ASN:HB2	1:A:150:ALA:O	1.87	0.74
1:D:85:GLU:HG2	1:D:118:ALA:HB2	1.70	0.74
1:A:93:LEU:HD21	1:A:120:LEU:HD13	1.69	0.74
1:B:245:ARG:HG3	1:B:245:ARG:NH1	1.95	0.74
1:A:171:VAL:HG12	1:A:171:VAL:O	1.88	0.74
1:C:245:ARG:HG2	1:C:245:ARG:HH11	1.51	0.74
1:D:141:VAL:HG21	1:D:182:PHE:CZ	2.22	0.74
1:A:165:THR:HG21	1:D:43:LEU:HB3	1.69	0.74
1:C:139:ARG:O	1:C:143:MET:HG3	1.87	0.74
1:C:303:ILE:HG22	1:C:307:LEU:HD11	1.70	0.74
1:A:188:GLU:CG	1:A:189:VAL:H	2.00	0.74
1:B:154:ASN:ND2	1:B:157:GLN:NE2	2.36	0.73
1:A:59:ALA:CB	1:A:307:LEU:HD23	2.19	0.73
1:B:59:ALA:HB2	1:B:307:LEU:HD13	1.69	0.73
1:D:125:GLY:HA3	3:D:503:POP:O2	1.88	0.73
1:B:124:LEU:HD12	1:B:137:LEU:CD1	2.18	0.73
1:D:65:ALA:O	1:D:66:MET:HG3	1.88	0.73
1:A:308:GLU:HG3	1:B:162:ARG:HH21	1.49	0.73
1:B:57:LEU:HD23	1:B:89:VAL:HA	1.70	0.73
1:D:284:VAL:CG1	1:D:287:PRO:HG2	2.18	0.73
1:B:85:GLU:HG3	1:B:115:ALA:CA	2.12	0.73
1:D:128:GLN:HA	1:D:128:GLN:NE2	2.02	0.73
1:A:161:GLN:CB	1:A:223:GLU:HG3	2.19	0.73
1:B:232:ARG:HH21	1:B:232:ARG:HB2	1.54	0.73
1:D:85:GLU:OE1	1:D:117:LYS:N	2.22	0.73
1:D:210:ASP:HB2	1:D:260:VAL:HB	1.70	0.72
1:C:217:THR:HB	1:C:286:ARG:NH1	2.04	0.72
1:C:255:PRO:HD3	4:C:1015:HOH:O	1.88	0.72
1:C:298:ARG:HH11	1:C:298:ARG:HG3	1.52	0.72
1:B:275:LEU:HG	1:B:282:LEU:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:CG	1:A:189:VAL:N	2.52	0.72
1:B:80:LEU:HB3	1:B:91:MET:CE	2.19	0.72
1:B:109:PHE:CB	1:B:144:LEU:HD21	2.20	0.72
1:B:180:LEU:HD23	1:B:182:PHE:CZ	2.25	0.72
1:C:110:ARG:HH21	1:C:110:ARG:CG	2.00	0.72
1:D:178:LEU:HD21	1:D:184:VAL:HG21	1.70	0.72
1:A:59:ALA:HB1	1:A:307:LEU:HD23	1.70	0.72
1:C:41:LEU:HD11	1:C:315:PHE:CD1	2.24	0.72
1:A:188:GLU:HG3	1:A:189:VAL:H	1.53	0.72
1:B:36:GLN:HB2	1:B:39:ALA:HB2	1.72	0.72
1:B:180:LEU:HD23	1:B:182:PHE:CE1	2.25	0.72
1:A:178:LEU:HD12	1:A:205:PRO:HG2	1.72	0.72
1:B:266:TYR:CE1	2:B:502:FMN:O3P	2.40	0.72
1:A:235:GLU:HB3	4:A:1185:HOH:O	1.89	0.71
1:B:59:ALA:HB2	1:B:307:LEU:HD11	1.71	0.71
1:B:162:ARG:CG	1:B:227:ARG:NH1	2.53	0.71
1:A:75:ARG:HB2	1:A:75:ARG:HH21	1.56	0.71
1:B:227:ARG:HH21	1:B:228:PHE:HZ	1.37	0.71
1:A:188:GLU:CD	1:A:189:VAL:H	1.98	0.71
2:A:502:FMN:H5'2	2:A:502:FMN:H1'2	1.70	0.71
1:B:127:ALA:CA	1:B:170:LEU:HD21	2.20	0.71
1:B:312:THR:HG23	1:C:159:ALA:CB	2.20	0.71
1:C:11:LEU:HD22	1:C:15:LEU:HD23	1.72	0.71
1:C:191:HIS:CE1	1:C:220:ALA:H	2.08	0.71
1:D:137:LEU:HD21	1:D:177:LEU:HD21	1.72	0.71
1:D:217:THR:HG22	1:D:286:ARG:HH11	0.71	0.71
1:B:112:ARG:NH1	1:B:145:GLU:O	2.24	0.71
1:B:150:ALA:CB	1:B:185:MET:HG3	2.20	0.71
1:B:219:TRP:CZ3	1:B:222:VAL:HG11	2.26	0.71
1:B:26:THR:HG22	1:B:215:GLY:HA3	1.71	0.71
1:A:9:LYS:HG3	1:A:10:HIS:H	1.56	0.71
1:B:63:ILE:HG23	1:B:288:LEU:CD2	2.20	0.71
1:C:233:HIS:N	1:C:233:HIS:CD2	2.59	0.71
1:A:223:GLU:OE2	1:A:223:GLU:HA	1.88	0.71
1:D:9:LYS:HG3	4:D:1075:HOH:O	1.91	0.70
1:B:158:GLU:OE1	1:B:158:GLU:CA	2.28	0.70
1:B:93:LEU:O	1:B:123:ASN:HB2	1.91	0.70
1:B:150:ALA:HB2	1:B:185:MET:HG3	1.71	0.70
1:D:129:LEU:HD21	1:D:151:PHE:CE2	2.25	0.70
1:D:154:ASN:ND2	1:D:157:GLN:HE21	1.89	0.70
1:B:106:LEU:HG	1:B:143:MET:CG	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:HG2	1:B:105:ALA:H	1.54	0.70
1:D:141:VAL:HG21	1:D:182:PHE:CE2	2.26	0.70
1:A:42:ALA:O	1:A:45:GLU:N	2.20	0.70
1:A:58:LYS:HB2	1:A:88:GLY:HA3	1.74	0.70
1:B:134:ARG:HB2	1:B:134:ARG:HH11	1.57	0.70
1:C:178:LEU:O	1:C:179:PRO:C	2.34	0.70
1:A:167:PHE:HA	1:A:170:LEU:CD1	2.21	0.69
1:C:217:THR:HG23	2:C:502:FMN:O5'	1.91	0.69
1:A:210:ASP:OD1	1:A:210:ASP:C	2.34	0.69
1:D:264:GLY:HA2	1:D:266:TYR:CD1	2.27	0.69
1:C:298:ARG:HH11	1:C:298:ARG:CG	2.04	0.69
1:D:79:ALA:HB1	1:D:296:ALA:H	1.57	0.69
1:D:82:GLU:HG3	1:D:114:VAL:CG1	2.23	0.69
1:B:102:ARG:CD	4:B:1142:HOH:O	2.34	0.69
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.58	0.69
1:A:233:HIS:N	1:A:233:HIS:CD2	2.61	0.69
1:B:95:SER:HA	1:B:123:ASN:HB3	1.74	0.69
1:D:57:LEU:HD23	1:D:90:GLY:N	2.08	0.69
1:A:219:TRP:HA	1:A:222:VAL:CG2	2.24	0.68
1:A:85:GLU:HG3	1:A:115:ALA:HA	1.74	0.68
1:B:253:VAL:O	1:B:255:PRO:HD3	1.92	0.68
1:D:172:GLU:CD	1:D:172:GLU:H	2.00	0.68
1:B:109:PHE:CB	1:B:144:LEU:HD23	2.21	0.68
1:A:217:THR:CB	1:A:286:ARG:HD3	2.21	0.68
1:D:85:GLU:HG3	1:D:115:ALA:HB1	1.76	0.68
1:B:264:GLY:HA2	1:B:266:TYR:CD1	2.29	0.67
1:B:251:ARG:NH1	1:B:278:GLY:O	2.27	0.67
1:D:164:ASP:CB	4:D:1214:HOH:O	2.28	0.67
1:A:172:GLU:HA	1:A:175:ALA:HB3	1.76	0.67
1:B:326:ARG:HH11	1:B:326:ARG:CA	2.07	0.67
2:B:502:FMN:O1P	2:B:502:FMN:O4'	2.11	0.67
1:A:221:ARG:HG3	1:A:237:CYS:HB3	1.75	0.67
1:A:269:THR:HG21	1:B:235:GLU:HG2	1.76	0.67
1:C:217:THR:HG21	1:C:286:ARG:HH11	1.52	0.67
1:D:180:LEU:HG	1:D:181:PRO:CD	2.22	0.67
1:C:154:ASN:HD22	1:C:157:GLN:HB3	1.59	0.66
1:C:188:GLU:OE1	1:C:189:VAL:N	2.23	0.66
1:C:166:ASP:OD1	1:C:168:ARG:HB2	1.94	0.66
1:D:186:VAL:HG23	1:D:206:LEU:HD22	1.74	0.66
1:B:65:ALA:O	1:B:66:MET:HG3	1.96	0.66
1:A:74:GLU:OE2	1:A:75:ARG:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:CB	1:B:307:LEU:HD11	2.26	0.66
1:D:186:VAL:HG23	1:D:206:LEU:HD21	1.77	0.66
1:B:46:VAL:HG22	1:B:311:ARG:HG2	1.78	0.66
1:C:67:THR:H	2:C:502:FMN:H6	1.60	0.65
1:D:331:ARG:HB2	4:D:1121:HOH:O	1.95	0.65
1:A:224:GLU:OE2	1:A:231:VAL:HG13	1.96	0.65
1:D:180:LEU:HD23	1:D:182:PHE:CE1	2.31	0.65
1:B:186:VAL:HG23	1:B:206:LEU:HD22	1.78	0.65
1:C:95:SER:O	1:C:98:ILE:CD1	2.44	0.65
1:D:236:LEU:O	1:D:239:ILE:HG13	1.96	0.65
1:D:275:LEU:HD23	1:D:279:ALA:O	1.96	0.65
1:A:35:TYR:HD1	1:A:316:ALA:HB1	1.62	0.65
1:A:326:ARG:HB2	1:A:326:ARG:NH1	2.11	0.65
1:B:61:PHE:O	1:B:62:LEU:HD23	1.95	0.65
1:B:45:GLU:OE2	1:C:168:ARG:HD3	1.96	0.65
1:B:53:LEU:CD1	1:B:121:ILE:HD13	2.27	0.65
1:B:191:HIS:HE1	1:B:219:TRP:N	1.95	0.65
1:C:232:ARG:HB2	1:C:233:HIS:CD2	2.31	0.65
1:D:290:ARG:HG2	1:D:290:ARG:HH11	1.61	0.65
1:A:169:GLY:HA2	1:A:172:GLU:OE2	1.97	0.65
1:D:61:PHE:O	1:D:62:LEU:HD23	1.97	0.65
1:D:156:LEU:HD12	1:D:191:HIS:CD2	2.32	0.65
1:A:126:LEU:C	1:A:170:LEU:HD23	2.22	0.65
1:C:304:GLY:HA2	1:C:307:LEU:HD12	1.79	0.65
1:A:59:ALA:HB3	1:A:307:LEU:CD2	2.25	0.65
1:B:63:ILE:CG2	1:B:288:LEU:HD23	2.26	0.65
1:B:78:LEU:HD22	1:B:114:VAL:CG2	2.27	0.65
1:C:55:LYS:HE3	1:C:147:ASP:CG	2.22	0.65
1:C:217:THR:CG2	1:C:286:ARG:HH12	1.83	0.65
1:C:219:TRP:HZ2	2:C:502:FMN:C9	2.10	0.65
1:D:266:TYR:OH	2:D:502:FMN:O3P	2.15	0.65
1:B:25:THR:O	1:B:242:PRO:HB3	1.97	0.64
1:B:326:ARG:NH1	1:B:326:ARG:CB	2.60	0.64
1:C:95:SER:C	1:C:97:ARG:H	2.05	0.64
1:C:210:ASP:OD1	1:C:210:ASP:C	2.40	0.64
1:A:165:THR:HG23	1:D:43:LEU:HB3	1.76	0.64
1:C:165:THR:HG23	1:C:165:THR:O	1.97	0.64
1:D:176:GLU:HG2	1:D:177:LEU:H	1.61	0.64
1:A:161:GLN:HB2	1:A:223:GLU:CG	2.26	0.64
1:A:217:THR:HG22	1:A:286:ARG:HH11	1.61	0.64
1:A:67:THR:H	2:A:502:FMN:H6	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:GLU:CD	1:C:189:VAL:H	2.05	0.64
1:A:97:ARG:HH11	1:A:97:ARG:CG	2.10	0.64
1:B:232:ARG:NE	4:B:1206:HOH:O	2.30	0.64
1:B:326:ARG:HB2	1:B:326:ARG:CZ	2.27	0.64
1:D:42:ALA:O	1:D:45:GLU:HG2	1.96	0.64
1:C:9:LYS:HB2	1:C:9:LYS:NZ	2.12	0.64
1:C:38:LEU:HD11	1:D:201:LEU:CD2	2.27	0.64
1:D:129:LEU:HD22	1:D:177:LEU:CD2	2.27	0.64
1:B:156:LEU:HD12	1:B:191:HIS:CD2	2.33	0.64
1:D:128:GLN:HA	1:D:128:GLN:HE21	1.62	0.64
1:D:124:LEU:HD12	1:D:137:LEU:HD12	1.80	0.64
1:D:154:ASN:HD22	1:D:157:GLN:NE2	1.90	0.64
1:A:236:LEU:O	1:A:239:ILE:HG13	1.98	0.64
1:B:212:ALA:HA	1:B:262:SER:O	1.98	0.64
1:D:285:ALA:HB3	2:D:502:FMN:O1P	1.98	0.64
1:A:196:GLU:CG	1:D:36:GLN:HE22	2.11	0.63
1:B:232:ARG:HH21	1:B:232:ARG:CG	2.11	0.63
1:D:33:LEU:O	4:D:1148:HOH:O	2.15	0.63
1:A:41:LEU:C	1:A:41:LEU:CD1	2.71	0.63
1:B:46:VAL:HA	1:B:320:ARG:O	1.98	0.63
1:C:289:LEU:O	1:C:292:ALA:HB3	1.98	0.63
1:D:66:MET:HA	2:D:502:FMN:C6	2.28	0.63
1:D:299:VAL:O	1:D:303:ILE:HG13	1.98	0.63
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.64	0.63
1:B:75:ARG:HG2	4:B:1066:HOH:O	1.98	0.63
1:C:46:VAL:HG21	1:C:315:PHE:HB2	1.80	0.63
1:C:195:ARG:HB2	1:C:249:GLU:HG2	1.79	0.63
1:D:127:ALA:CA	1:D:170:LEU:HD21	2.27	0.63
1:A:46:VAL:HG11	1:A:315:PHE:HB2	1.79	0.63
1:B:232:ARG:HH21	1:B:232:ARG:CB	2.12	0.63
1:C:126:LEU:HG	1:C:170:LEU:HD22	1.80	0.63
1:D:52:PHE:HE2	1:D:62:LEU:HD11	1.64	0.63
1:A:105:ALA:HB3	1:A:108:SER:O	1.99	0.63
1:A:178:LEU:O	1:A:180:LEU:N	2.32	0.63
1:D:66:MET:HA	2:D:502:FMN:C5A	2.29	0.63
1:D:161:GLN:O	1:D:162:ARG:C	2.40	0.63
1:A:24:THR:HG23	1:A:238:GLU:HB3	1.81	0.62
1:A:31:PHE:O	1:A:273:LYS:HE2	1.99	0.62
1:B:80:LEU:HB2	1:B:91:MET:HE1	1.80	0.62
1:A:28:LEU:HD23	1:A:244:ALA:HB2	1.81	0.62
1:B:217:THR:HG21	1:B:286:ARG:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ILE:H	1:C:98:ILE:HD12	1.63	0.62
1:C:308:GLU:HA	1:C:311:ARG:NH1	2.13	0.62
1:C:130:ARG:HD2	1:C:131:ARG:HH21	1.64	0.62
1:B:190:GLY:CA	1:B:212:ALA:O	2.44	0.62
1:C:154:ASN:HD22	1:C:157:GLN:HE21	1.48	0.62
1:B:42:ALA:O	1:B:45:GLU:HG2	2.00	0.62
1:B:66:MET:O	1:B:94:GLY:HA3	1.99	0.62
1:B:106:LEU:O	1:B:110:ARG:NH2	2.33	0.62
1:D:82:GLU:HG3	1:D:114:VAL:HG11	1.81	0.62
1:D:253:VAL:O	1:D:255:PRO:HD3	2.00	0.62
1:A:167:PHE:HA	1:A:170:LEU:HD13	1.81	0.62
1:A:171:VAL:O	1:A:171:VAL:CG1	2.47	0.61
1:C:245:ARG:HH11	1:C:245:ARG:CG	2.11	0.61
1:C:298:ARG:HG3	1:C:298:ARG:NH1	2.12	0.61
1:A:126:LEU:O	1:A:170:LEU:HD23	2.00	0.61
1:B:24:THR:OG1	1:B:238:GLU:HB3	2.01	0.61
1:A:110:ARG:HG2	1:A:113:LYS:NZ	2.16	0.61
1:B:204:LEU:H	1:B:204:LEU:CD1	2.12	0.61
1:C:317:ILE:O	1:C:328:ARG:HD3	1.99	0.61
1:B:76:ILE:HG13	1:B:77:ASN:H	1.63	0.61
1:B:219:TRP:O	1:B:223:GLU:HB2	2.01	0.61
1:C:41:LEU:HD11	1:C:315:PHE:HD1	1.66	0.61
1:C:95:SER:O	1:C:98:ILE:HD11	2.00	0.61
1:D:142:GLU:O	1:D:143:MET:C	2.43	0.61
1:D:174:LEU:HD23	1:D:204:LEU:CD2	2.31	0.61
1:B:40:GLY:O	1:C:168:ARG:HA	2.01	0.61
1:A:269:THR:CG2	1:B:235:GLU:HG2	2.31	0.61
1:B:66:MET:O	1:B:67:THR:CB	2.34	0.61
1:D:29:GLU:O	1:D:29:GLU:CG	2.44	0.61
1:D:85:GLU:CG	1:D:118:ALA:HB2	2.31	0.61
1:C:191:HIS:HE1	1:C:220:ALA:H	1.47	0.60
1:C:148:ALA:HB2	1:C:183:PRO:HB2	1.83	0.60
1:D:331:ARG:NH2	4:D:1043:HOH:O	2.33	0.60
1:A:312:THR:CG2	1:B:236:LEU:HD21	2.31	0.60
1:B:111:VAL:O	1:B:114:VAL:N	2.34	0.60
1:B:318:GLY:O	1:B:328:ARG:NH1	2.34	0.60
1:C:160:VAL:CG1	1:C:223:GLU:HB3	2.30	0.60
1:B:111:VAL:HG12	1:B:120:LEU:HD11	1.84	0.60
1:C:59:ALA:CB	1:C:307:LEU:HD22	2.32	0.60
1:A:191:HIS:CE1	1:A:220:ALA:H	2.20	0.60
1:B:126:LEU:HG	1:B:170:LEU:HG	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ALA:HB1	1:B:329:VAL:HB	1.82	0.60
1:C:161:GLN:O	1:C:161:GLN:HG3	2.00	0.60
1:A:138:LEU:N	1:A:138:LEU:CD2	2.62	0.60
1:C:100:LEU:HD11	1:C:124:LEU:HD21	1.83	0.60
1:D:195:ARG:HB3	1:D:249:GLU:HB3	1.84	0.60
1:A:161:GLN:CA	1:A:223:GLU:HG3	2.31	0.59
1:B:148:ALA:HB1	1:B:183:PRO:O	2.01	0.59
1:B:32:ARG:HG3	1:B:32:ARG:NH1	2.17	0.59
1:B:107:ARG:NH2	1:B:107:ARG:HB3	2.17	0.59
1:B:26:THR:CG2	1:B:215:GLY:HA3	2.32	0.59
1:B:95:SER:OG	3:B:503:POP:O5	2.17	0.59
1:C:133:GLY:O	1:C:134:ARG:C	2.46	0.59
1:D:152:HIS:HD2	1:D:152:HIS:O	1.86	0.59
1:B:124:LEU:HD12	1:B:137:LEU:HD11	1.83	0.59
1:B:203:ASP:O	1:B:204:LEU:C	2.45	0.59
1:B:137:LEU:O	1:B:140:LEU:HB3	2.03	0.59
1:C:41:LEU:CD1	1:C:315:PHE:CD1	2.85	0.59
1:D:228:PHE:C	1:D:230:GLU:H	2.09	0.59
1:A:85:GLU:OE2	1:A:116:PRO:CD	2.51	0.59
1:B:79:ALA:HB1	1:B:296:ALA:H	1.67	0.59
1:B:174:LEU:CD2	1:B:204:LEU:HD23	2.25	0.59
1:B:141:VAL:HG11	1:B:182:PHE:CD2	2.38	0.59
1:D:82:GLU:CG	1:D:114:VAL:HG12	2.32	0.59
1:A:148:ALA:HB2	1:A:183:PRO:HG2	1.84	0.58
1:D:152:HIS:CD2	1:D:152:HIS:O	2.56	0.58
1:D:129:LEU:HD21	1:D:151:PHE:CZ	2.39	0.58
1:B:99:LEU:HD13	1:B:143:MET:SD	2.43	0.58
1:B:187:LYS:HE2	1:B:188:GLU:O	2.03	0.58
1:D:52:PHE:HB3	1:D:57:LEU:HD11	1.86	0.58
1:B:310:LEU:HG	1:B:314:LEU:HD12	1.85	0.58
1:B:76:ILE:HG13	1:B:77:ASN:N	2.19	0.58
1:B:275:LEU:HD23	1:B:279:ALA:O	2.03	0.58
1:C:282:LEU:HD23	1:C:306:TYR:HE2	1.68	0.58
1:A:95:SER:C	1:A:97:ARG:H	2.12	0.58
1:B:162:ARG:HG2	1:B:227:ARG:HH11	1.64	0.58
1:B:34:ARG:N	1:B:317:ILE:HD11	2.19	0.58
1:C:262:SER:HB3	1:C:283:ALA:HB3	1.86	0.58
1:A:97:ARG:O	1:A:100:LEU:HD12	2.03	0.58
1:C:156:LEU:O	1:C:157:GLN:C	2.43	0.58
1:B:57:LEU:HD23	1:B:89:VAL:CA	2.34	0.58
1:A:80:LEU:HD21	1:A:292:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:CD2	1:A:170:LEU:HB3	2.34	0.57
1:A:165:THR:HG23	1:A:165:THR:O	2.02	0.57
1:A:196:GLU:CG	1:D:36:GLN:NE2	2.67	0.57
1:A:51:PRO:HA	1:A:56:THR:HA	1.85	0.57
1:A:217:THR:HG23	2:A:502:FMN:P	2.44	0.57
1:A:275:LEU:HD12	1:A:310:LEU:HD11	1.87	0.57
1:C:185:MET:HB3	1:C:208:ALA:HB3	1.85	0.57
1:A:189:VAL:HG23	1:A:189:VAL:O	2.04	0.57
1:C:243:THR:O	1:C:247:ILE:HG13	2.05	0.57
1:C:58:LYS:HB2	1:C:88:GLY:HA3	1.86	0.57
1:D:149:LEU:O	1:D:184:VAL:HA	2.04	0.57
1:A:308:GLU:HA	1:A:311:ARG:NH1	2.20	0.57
1:B:60:PRO:C	1:B:281:LEU:HD13	2.30	0.57
1:C:9:LYS:HB2	1:C:9:LYS:HZ2	1.69	0.57
1:B:108:SER:OG	1:B:109:PHE:N	2.36	0.57
1:C:217:THR:CG2	1:C:286:ARG:HB2	2.29	0.57
1:A:112:ARG:NH2	1:A:118:ALA:O	2.37	0.57
1:B:219:TRP:HZ2	2:B:502:FMN:C9	2.18	0.57
1:C:46:VAL:HA	1:C:320:ARG:O	2.05	0.57
1:C:78:LEU:HD23	1:C:114:VAL:CG2	2.34	0.57
1:C:127:ALA:HA	1:C:170:LEU:HD11	1.87	0.57
1:B:326:ARG:HH11	1:B:326:ARG:CB	2.18	0.57
1:D:35:TYR:CD1	1:D:316:ALA:O	2.58	0.57
1:D:55:LYS:HE3	1:D:147:ASP:OD1	2.05	0.57
1:A:126:LEU:HD23	1:A:170:LEU:HB3	1.87	0.56
1:A:217:THR:CB	1:A:286:ARG:HH11	2.18	0.56
1:B:9:LYS:HZ3	1:B:9:LYS:N	2.02	0.56
1:B:75:ARG:NH1	4:B:1074:HOH:O	2.38	0.56
1:A:196:GLU:HG3	1:D:36:GLN:NE2	2.19	0.56
1:B:107:ARG:HB3	1:B:107:ARG:HH21	1.70	0.56
1:B:245:ARG:NH1	1:B:245:ARG:HG2	2.21	0.56
1:C:21:TYR:OH	1:C:191:HIS:CD2	2.59	0.56
1:C:67:THR:H	2:C:502:FMN:C6	2.18	0.56
1:C:184:VAL:HB	4:C:1110:HOH:O	2.05	0.56
1:D:290:ARG:HH11	1:D:290:ARG:CG	2.17	0.56
1:D:67:THR:N	2:D:502:FMN:H6	2.21	0.56
1:D:243:THR:O	1:D:247:ILE:HG13	2.05	0.56
1:D:284:VAL:HG13	1:D:287:PRO:CG	2.35	0.56
1:A:172:GLU:N	1:A:172:GLU:CD	2.64	0.56
1:D:46:VAL:HG22	1:D:311:ARG:HG3	1.88	0.56
1:D:138:LEU:HD23	1:D:138:LEU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:HB2	1:C:150:ALA:HB3	1.86	0.56
1:C:187:LYS:NZ	1:C:188:GLU:O	2.31	0.56
1:D:142:GLU:O	1:D:144:LEU:N	2.39	0.56
1:B:110:ARG:O	1:B:112:ARG:N	2.38	0.56
1:B:42:ALA:HB3	1:B:45:GLU:HG2	1.88	0.56
1:C:206:LEU:O	1:C:257:LEU:HD11	2.06	0.56
1:C:266:TYR:CD1	1:C:287:PRO:HG2	2.40	0.56
1:D:285:ALA:C	1:D:287:PRO:HD2	2.30	0.56
1:D:111:VAL:O	1:D:114:VAL:HG23	2.06	0.56
1:B:38:LEU:HD21	1:C:153:VAL:HG11	1.88	0.56
1:B:66:MET:SD	1:B:289:LEU:HD13	2.46	0.56
1:C:161:GLN:HB3	1:C:223:GLU:HG2	1.85	0.56
1:D:78:LEU:HD22	1:D:114:VAL:CG2	2.27	0.56
1:A:224:GLU:OE1	1:A:233:HIS:CD2	2.60	0.55
1:B:138:LEU:HD13	1:B:181:PRO:HG3	1.88	0.55
1:B:142:GLU:O	1:B:143:MET:C	2.49	0.55
1:C:138:LEU:HD22	1:C:181:PRO:HG3	1.87	0.55
1:D:35:TYR:HD1	1:D:316:ALA:O	1.89	0.55
1:D:275:LEU:HG	1:D:282:LEU:HD11	1.88	0.55
1:B:130:ARG:CG	1:B:130:ARG:HH11	2.19	0.55
1:C:176:GLU:C	1:C:178:LEU:H	2.14	0.55
1:D:219:TRP:CZ3	1:D:222:VAL:HG11	2.41	0.55
1:A:161:GLN:O	1:A:161:GLN:HG2	2.05	0.55
1:B:129:LEU:HD22	1:B:177:LEU:HD21	1.87	0.55
1:B:150:ALA:HB2	1:B:185:MET:CG	2.36	0.55
1:D:128:GLN:C	1:D:130:ARG:N	2.63	0.55
1:D:180:LEU:CG	1:D:181:PRO:HD2	2.27	0.55
1:D:270:ASP:HA	1:D:273:LYS:HG3	1.88	0.55
1:A:149:LEU:O	1:A:184:VAL:HA	2.05	0.55
1:B:75:ARG:HG3	1:B:76:ILE:H	1.69	0.55
1:B:147:ASP:O	1:B:183:PRO:HD2	2.07	0.55
1:B:232:ARG:C	1:B:234:PRO:HD3	2.31	0.55
1:B:293:LEU:O	1:B:295:GLY:N	2.39	0.55
1:D:53:LEU:HD22	1:D:183:PRO:HB2	1.87	0.55
1:C:138:LEU:HD22	1:C:181:PRO:CG	2.36	0.55
1:B:64:GLY:O	1:B:66:MET:HE2	2.07	0.55
1:B:138:LEU:O	1:B:139:ARG:C	2.46	0.55
1:B:156:LEU:HD13	1:B:220:ALA:HB2	1.89	0.55
1:D:62:LEU:HD22	1:D:90:GLY:HA3	1.88	0.55
1:A:293:LEU:C	1:A:295:GLY:H	2.14	0.55
1:B:28:LEU:HD13	1:B:270:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PHE:O	1:B:273:LYS:HE2	2.07	0.55
1:B:150:ALA:HA	1:B:185:MET:O	2.07	0.55
1:C:28:LEU:HD23	1:C:244:ALA:HB2	1.88	0.55
1:D:31:PHE:CE2	1:D:277:LEU:HD21	2.42	0.55
1:D:144:LEU:O	1:D:145:GLU:CB	2.54	0.55
1:A:12:GLU:CA	1:A:15:LEU:HB2	2.31	0.54
1:B:33:LEU:HB3	1:B:317:ILE:CD1	2.36	0.54
1:C:38:LEU:HD23	1:D:153:VAL:HG21	1.88	0.54
1:A:168:ARG:HD3	1:D:45:GLU:OE2	2.07	0.54
1:A:312:THR:HG22	1:B:236:LEU:HD21	1.89	0.54
1:B:190:GLY:HA2	1:B:212:ALA:C	2.32	0.54
1:C:10:HIS:HE1	1:C:223:GLU:OE2	1.90	0.54
1:D:144:LEU:O	1:D:145:GLU:HB2	2.07	0.54
1:D:242:PRO:HD2	1:D:245:ARG:HD3	1.89	0.54
1:B:221:ARG:HG3	1:B:237:CYS:HB3	1.89	0.54
1:C:66:MET:HA	2:C:502:FMN:C5A	2.38	0.54
1:D:276:ALA:HB1	1:D:329:VAL:HB	1.89	0.54
1:A:262:SER:HB3	1:A:283:ALA:HB3	1.90	0.54
1:B:149:LEU:HB3	1:B:184:VAL:HG22	1.89	0.54
1:B:219:TRP:HZ2	2:B:502:FMN:C8	2.19	0.54
1:A:172:GLU:O	1:A:173:ARG:C	2.47	0.54
1:D:303:ILE:HG22	1:D:307:LEU:CD1	2.37	0.54
1:B:162:ARG:HG2	1:B:227:ARG:HH12	1.64	0.54
1:C:59:ALA:CB	1:C:307:LEU:CD2	2.86	0.54
1:D:61:PHE:C	1:D:61:PHE:CD2	2.84	0.54
1:A:46:VAL:HG22	1:A:311:ARG:HG3	1.89	0.54
1:A:235:GLU:HG2	1:D:269:THR:CB	2.30	0.54
1:B:46:VAL:HG22	1:B:311:ARG:CG	2.37	0.54
1:A:217:THR:CG2	1:A:286:ARG:HH11	2.20	0.54
1:C:106:LEU:O	1:C:110:ARG:CB	2.55	0.54
1:B:79:ALA:HA	1:B:296:ALA:HB2	1.89	0.54
1:D:137:LEU:O	1:D:140:LEU:HB3	2.08	0.54
1:A:249:GLU:CD	1:D:34:ARG:HH22	2.15	0.53
1:B:104:GLU:CG	1:B:105:ALA:N	2.70	0.53
1:A:303:ILE:HG22	1:A:307:LEU:CD1	2.38	0.53
1:A:188:GLU:HG2	1:A:192:GLY:N	2.22	0.53
1:B:130:ARG:HH11	1:B:130:ARG:HG2	1.74	0.53
1:B:191:HIS:CE1	1:B:220:ALA:H	2.25	0.53
1:A:128:GLN:HB3	1:A:132:TYR:HD2	1.72	0.53
1:C:50:THR:O	1:C:57:LEU:HB2	2.07	0.53
1:A:108:SER:HA	1:A:109:PHE:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:N	4:B:1066:HOH:O	2.42	0.53
1:B:106:LEU:CG	1:B:143:MET:HG2	2.33	0.53
1:D:57:LEU:N	1:D:57:LEU:HD12	2.23	0.53
1:D:82:GLU:CG	1:D:114:VAL:CG1	2.87	0.53
1:D:60:PRO:HG3	1:D:322:PRO:HG2	1.90	0.53
1:D:166:ASP:OD2	1:D:168:ARG:HD3	2.09	0.53
1:D:217:THR:CG2	1:D:286:ARG:HB2	2.38	0.53
1:A:188:GLU:HG2	1:A:192:GLY:H	1.74	0.53
1:D:131:ARG:HD2	1:D:132:TYR:CE2	2.44	0.53
1:B:119:LEU:C	1:B:120:LEU:HD23	2.34	0.53
1:C:85:GLU:OE1	1:C:117:LYS:N	2.37	0.53
1:A:98:ILE:HD12	1:A:98:ILE:H	1.74	0.52
1:A:154:ASN:N	1:A:155:PRO:HD3	2.25	0.52
1:C:187:LYS:HB3	1:C:210:ASP:HB3	1.90	0.52
1:C:41:LEU:HD12	1:C:315:PHE:CE1	2.45	0.52
1:A:288:LEU:HD21	1:A:303:ILE:HD11	1.92	0.52
1:B:38:LEU:CD2	1:C:153:VAL:HG11	2.39	0.52
1:B:321:ASN:HB2	1:B:322:PRO:CD	2.39	0.52
1:C:228:PHE:C	1:C:230:GLU:H	2.17	0.52
1:B:133:GLY:O	1:B:134:ARG:C	2.53	0.52
1:C:154:ASN:ND2	1:C:157:GLN:HB3	2.25	0.52
1:A:174:LEU:HD23	1:A:204:LEU:HD23	1.92	0.52
1:B:269:THR:HB	1:C:235:GLU:HG2	1.91	0.52
1:D:221:ARG:CZ	1:D:231:VAL:HG21	2.39	0.52
1:B:222:VAL:O	1:B:225:TRP:N	2.42	0.52
1:C:15:LEU:HD11	1:C:293:LEU:HD12	1.92	0.52
1:C:139:ARG:CB	1:C:139:ARG:HH21	2.23	0.52
1:D:112:ARG:O	1:D:112:ARG:HG3	2.10	0.52
1:B:103:PRO:O	1:B:104:GLU:C	2.52	0.52
1:B:140:LEU:O	1:B:144:LEU:HB2	2.10	0.52
1:B:203:ASP:OD1	1:B:203:ASP:N	2.42	0.52
1:C:41:LEU:HD12	1:C:42:ALA:N	2.25	0.52
1:C:264:GLY:HA2	1:C:266:TYR:CZ	2.45	0.52
1:D:61:PHE:C	1:D:62:LEU:HD23	2.35	0.52
1:D:178:LEU:CD2	1:D:184:VAL:HG21	2.37	0.52
1:A:303:ILE:HG22	1:A:307:LEU:HD11	1.91	0.52
1:C:57:LEU:HD12	1:C:281:LEU:HD11	1.92	0.52
1:A:150:ALA:HA	1:A:185:MET:O	2.09	0.52
1:A:165:THR:HG23	1:D:43:LEU:H	1.74	0.52
1:D:303:ILE:O	1:D:304:GLY:C	2.51	0.52
1:A:259:LEU:N	1:A:259:LEU:HD23	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:O	1:B:247:ILE:HG13	2.09	0.51
1:D:48:LEU:HB3	1:D:59:ALA:HA	1.92	0.51
1:C:112:ARG:NH2	1:C:118:ALA:O	2.43	0.51
1:D:115:ALA:N	1:D:116:PRO:CD	2.74	0.51
1:A:97:ARG:CG	1:A:97:ARG:NH1	2.72	0.51
1:A:156:LEU:O	1:A:157:GLN:C	2.49	0.51
1:A:217:THR:HG22	1:A:286:ARG:NH1	2.26	0.51
1:B:326:ARG:NH1	1:B:326:ARG:CA	2.72	0.51
1:C:43:LEU:C	1:C:43:LEU:HD12	2.35	0.51
1:A:28:LEU:CD2	1:A:244:ALA:HB2	2.41	0.51
1:A:128:GLN:HB3	1:A:132:TYR:CD2	2.45	0.51
1:A:152:HIS:HA	1:A:187:LYS:O	2.11	0.51
1:B:320:ARG:HB2	1:B:324:GLU:OE1	2.10	0.51
1:D:176:GLU:C	1:D:178:LEU:N	2.68	0.51
1:B:208:ALA:C	1:B:257:LEU:HD11	2.36	0.51
1:A:167:PHE:HB3	4:D:1127:HOH:O	2.10	0.51
1:C:35:TYR:CE1	1:D:156:LEU:HB2	2.45	0.51
1:D:326:ARG:HB2	1:D:326:ARG:NH1	2.26	0.51
1:A:308:GLU:HG2	1:B:162:ARG:HH22	1.71	0.51
1:B:55:LYS:HE3	1:B:147:ASP:OD1	2.10	0.51
1:B:177:LEU:HD12	1:B:177:LEU:O	2.11	0.51
1:A:67:THR:H	2:A:502:FMN:C6	2.24	0.51
1:A:105:ALA:CB	1:A:108:SER:H	2.21	0.51
1:A:239:ILE:HD13	1:D:33:LEU:HD12	1.92	0.51
1:B:124:LEU:CD1	1:B:137:LEU:CD1	2.89	0.51
1:D:41:LEU:HD12	1:D:41:LEU:C	2.35	0.51
1:D:99:LEU:HD11	1:D:143:MET:SD	2.51	0.51
1:A:42:ALA:O	1:A:43:LEU:C	2.54	0.51
1:B:75:ARG:HG3	1:B:76:ILE:N	2.26	0.51
1:B:130:ARG:C	1:B:131:ARG:HG3	2.35	0.51
1:B:275:LEU:HA	1:B:279:ALA:O	2.11	0.51
1:C:98:ILE:CD1	1:C:98:ILE:H	2.19	0.51
1:D:134:ARG:O	1:D:137:LEU:HB2	2.11	0.51
1:A:62:LEU:HD23	1:A:90:GLY:HA3	1.92	0.51
1:B:63:ILE:CD1	1:B:303:ILE:HD11	2.41	0.51
1:B:78:LEU:HD22	1:B:114:VAL:HG21	1.93	0.51
1:C:85:GLU:CG	1:C:115:ALA:HA	2.41	0.51
1:A:134:ARG:C	1:A:134:ARG:CD	2.84	0.50
1:A:155:PRO:HD2	1:D:35:TYR:OH	2.11	0.50
1:A:260:VAL:HG13	1:A:281:LEU:HB3	1.93	0.50
1:B:110:ARG:O	1:B:111:VAL:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:CD1	1:B:180:LEU:N	2.71	0.50
1:B:251:ARG:HG3	1:B:251:ARG:O	2.10	0.50
1:A:38:LEU:HD12	1:B:197:ALA:HB1	1.93	0.50
1:B:247:ILE:HD11	1:B:261:ALA:HB1	1.92	0.50
1:B:253:VAL:C	1:B:255:PRO:HD3	2.36	0.50
1:C:157:GLN:OE1	1:C:219:TRP:CE3	2.64	0.50
1:D:28:LEU:C	1:D:30:GLY:H	2.18	0.50
1:D:79:ALA:CB	1:D:296:ALA:H	2.24	0.50
1:D:178:LEU:CD1	1:D:205:PRO:HG2	2.39	0.50
1:A:332:VAL:O	1:A:332:VAL:CG1	2.50	0.50
1:C:26:THR:HG21	4:C:1044:HOH:O	2.11	0.50
1:D:325:ALA:HA	1:D:328:ARG:HD2	1.93	0.50
1:A:214:ALA:HB3	1:A:242:PRO:HA	1.93	0.50
1:B:142:GLU:O	1:B:144:LEU:N	2.44	0.50
1:B:262:SER:HB3	1:B:283:ALA:HB3	1.91	0.50
1:C:217:THR:HG21	1:C:286:ARG:CB	2.31	0.50
1:C:221:ARG:HG3	1:C:237:CYS:HB3	1.93	0.50
1:D:39:ALA:HB3	4:D:1118:HOH:O	2.11	0.50
1:A:95:SER:C	1:A:97:ARG:N	2.68	0.50
1:A:106:LEU:N	1:A:107:ARG:CB	2.73	0.50
1:B:142:GLU:C	1:B:144:LEU:H	2.19	0.50
1:C:43:LEU:C	1:C:43:LEU:CD1	2.84	0.50
1:C:188:GLU:HG3	1:C:189:VAL:N	2.27	0.50
1:A:76:ILE:HG22	1:A:293:LEU:CD2	2.42	0.50
1:A:242:PRO:HG2	1:A:245:ARG:HB2	1.93	0.50
1:A:245:ARG:O	1:A:249:GLU:HB2	2.12	0.50
1:B:139:ARG:O	1:B:143:MET:HB2	2.11	0.50
1:B:325:ALA:O	1:B:326:ARG:C	2.55	0.50
1:A:191:HIS:HD2	1:A:239:ILE:O	1.95	0.50
1:B:217:THR:HG21	1:B:286:ARG:CB	2.41	0.50
1:C:34:ARG:HH12	1:D:194:SER:HB2	1.77	0.50
1:C:162:ARG:HE	1:C:227:ARG:HH22	1.60	0.50
1:D:34:ARG:HB2	1:D:328:ARG:O	2.11	0.50
1:C:139:ARG:HH21	1:C:139:ARG:HB3	1.77	0.50
1:C:161:GLN:O	1:C:161:GLN:CG	2.60	0.50
1:D:52:PHE:CE2	1:D:62:LEU:HD11	2.47	0.50
1:D:129:LEU:HD22	1:D:177:LEU:HD21	1.91	0.50
1:D:186:VAL:CG2	1:D:206:LEU:HD21	2.41	0.50
1:A:98:ILE:H	1:A:98:ILE:CD1	2.25	0.50
1:A:106:LEU:CA	1:A:107:ARG:HB2	2.41	0.50
1:A:220:ALA:HB3	1:A:237:CYS:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:O	1:B:45:GLU:N	2.45	0.50
1:B:103:PRO:O	1:B:106:LEU:CB	2.41	0.50
1:B:108:SER:C	1:B:110:ARG:H	2.20	0.50
1:C:41:LEU:C	1:C:41:LEU:CD1	2.84	0.50
1:A:172:GLU:CD	1:A:172:GLU:H	2.20	0.49
1:B:31:PHE:O	1:B:273:LYS:CE	2.60	0.49
1:D:150:ALA:HA	1:D:185:MET:O	2.12	0.49
1:D:303:ILE:HG22	1:D:307:LEU:HD12	1.93	0.49
1:B:269:THR:O	1:B:272:ALA:HB3	2.11	0.49
1:B:286:ARG:NH2	4:B:1037:HOH:O	2.33	0.49
1:D:326:ARG:HB2	1:D:326:ARG:CZ	2.42	0.49
1:A:80:LEU:O	1:A:81:ALA:C	2.55	0.49
1:A:224:GLU:OE1	1:A:233:HIS:HD2	1.93	0.49
1:B:105:ALA:C	1:B:107:ARG:H	2.20	0.49
1:B:222:VAL:HG12	1:B:223:GLU:N	2.26	0.49
1:B:276:ALA:HA	1:B:325:ALA:O	2.12	0.49
1:D:285:ALA:O	1:D:286:ARG:C	2.55	0.49
1:A:33:LEU:HB3	1:A:317:ILE:HD11	1.95	0.49
1:A:185:MET:HB3	1:A:208:ALA:HB3	1.94	0.49
1:A:266:TYR:CD1	1:A:287:PRO:HG2	2.47	0.49
1:C:176:GLU:C	1:C:178:LEU:N	2.66	0.49
1:C:63:ILE:HD11	1:C:303:ILE:CD1	2.42	0.49
1:B:33:LEU:HD22	1:B:317:ILE:HD13	1.95	0.49
1:B:110:ARG:HA	1:B:110:ARG:CZ	2.42	0.49
1:D:212:ALA:HA	1:D:262:SER:O	2.13	0.49
1:A:228:PHE:CD2	1:A:232:ARG:CZ	2.95	0.49
1:B:99:LEU:CD2	1:B:106:LEU:HA	2.42	0.49
1:C:130:ARG:HD2	1:C:131:ARG:NH2	2.28	0.49
1:D:192:GLY:HA2	1:D:211:VAL:O	2.12	0.49
1:A:134:ARG:C	1:A:134:ARG:HD2	2.38	0.49
1:A:154:ASN:ND2	1:A:157:GLN:HE21	1.94	0.49
1:B:142:GLU:C	1:B:144:LEU:N	2.68	0.49
1:C:298:ARG:CG	1:C:298:ARG:NH1	2.71	0.49
1:D:156:LEU:CD1	1:D:191:HIS:CD2	2.96	0.49
1:A:66:MET:HA	2:A:502:FMN:C5A	2.43	0.49
1:A:302:TRP:O	1:A:305:ASP:HB3	2.12	0.49
1:B:110:ARG:HA	1:B:110:ARG:NE	2.27	0.49
2:B:502:FMN:H1'2	2:B:502:FMN:H5'2	1.94	0.49
1:D:66:MET:O	1:D:94:GLY:HA3	2.13	0.49
1:B:104:GLU:CG	1:B:105:ALA:H	2.22	0.49
1:D:99:LEU:O	1:D:103:PRO:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HA	1:C:170:LEU:HD23	1.41	0.48
1:D:191:HIS:HE1	1:D:219:TRP:N	2.11	0.48
1:B:43:LEU:HB3	1:C:165:THR:HG23	1.90	0.48
1:B:43:LEU:O	1:B:46:VAL:HG13	2.13	0.48
1:D:82:GLU:HG3	1:D:114:VAL:HG12	1.90	0.48
1:B:251:ARG:NH2	1:B:257:LEU:O	2.46	0.48
1:B:261:ALA:HB2	1:B:279:ALA:HB2	1.94	0.48
1:B:284:VAL:HG13	1:B:287:PRO:HG2	1.95	0.48
1:C:59:ALA:HB3	1:C:307:LEU:CD2	2.42	0.48
1:D:11:LEU:HD23	1:D:67:THR:C	2.38	0.48
1:D:152:HIS:HA	1:D:187:LYS:O	2.13	0.48
1:C:172:GLU:O	1:C:173:ARG:C	2.55	0.48
1:D:313:ALA:O	1:D:317:ILE:HG23	2.14	0.48
1:A:195:ARG:HH21	1:A:199:LEU:HD11	1.79	0.48
1:B:325:ALA:HA	1:B:328:ARG:HG3	1.96	0.48
1:C:103:PRO:O	1:C:106:LEU:HG	2.14	0.48
1:C:288:LEU:HD21	1:C:303:ILE:HD11	1.95	0.48
1:C:319:ALA:HA	1:C:324:GLU:HG2	1.96	0.48
1:D:176:GLU:C	1:D:178:LEU:H	2.21	0.48
1:D:177:LEU:HG	1:D:177:LEU:O	2.13	0.48
1:A:102:ARG:O	1:A:102:ARG:HD3	2.14	0.48
1:A:201:LEU:HD13	1:A:206:LEU:HD11	1.95	0.48
1:A:290:ARG:H	1:A:291:PRO:HD2	1.78	0.48
1:B:79:ALA:CB	1:B:296:ALA:H	2.26	0.48
1:B:134:ARG:HD2	1:B:138:LEU:HD11	1.96	0.48
1:C:9:LYS:HG3	1:C:10:HIS:N	2.29	0.48
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.34	0.48
1:A:12:GLU:HG3	1:A:16:GLU:OE2	2.14	0.48
1:B:233:HIS:ND1	1:B:233:HIS:N	2.60	0.48
1:A:236:LEU:C	1:A:238:GLU:N	2.69	0.48
1:A:241:ILE:O	1:A:242:PRO:C	2.52	0.48
1:A:267:THR:O	1:A:268:GLY:C	2.57	0.48
1:B:160:VAL:C	1:B:162:ARG:H	2.22	0.48
1:B:191:HIS:CE1	1:B:219:TRP:N	2.80	0.48
1:B:285:ALA:O	1:B:286:ARG:C	2.56	0.48
1:C:110:ARG:HG2	1:C:110:ARG:NH2	2.01	0.48
1:B:58:LYS:HB2	1:B:88:GLY:HA3	1.95	0.48
1:B:120:LEU:HD23	1:B:120:LEU:N	2.28	0.48
1:B:178:LEU:HD23	1:B:180:LEU:HD13	1.95	0.48
1:D:9:LYS:N	1:D:12:GLU:OE1	2.47	0.48
1:B:138:LEU:N	1:B:138:LEU:CD2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ALA:HB2	1:B:279:ALA:CB	2.44	0.47
1:C:153:VAL:HG22	1:C:155:PRO:HD3	1.96	0.47
1:D:134:ARG:CG	1:D:177:LEU:HD12	2.42	0.47
1:D:210:ASP:CB	1:D:260:VAL:HB	2.39	0.47
1:C:188:GLU:HG2	1:C:192:GLY:N	2.29	0.47
1:C:328:ARG:HG2	4:C:1028:HOH:O	2.14	0.47
1:D:66:MET:HG2	2:D:502:FMN:C7	2.44	0.47
1:D:161:GLN:HB2	1:D:223:GLU:OE2	2.14	0.47
1:D:251:ARG:HG3	1:D:251:ARG:O	2.13	0.47
1:B:124:LEU:HD12	1:B:137:LEU:HD12	1.95	0.47
1:B:127:ALA:N	1:B:170:LEU:HD21	2.28	0.47
1:C:60:PRO:HB2	1:C:281:LEU:HA	1.96	0.47
1:C:301:ALA:O	1:C:302:TRP:C	2.57	0.47
1:D:80:LEU:HD21	1:D:292:ALA:HB2	1.95	0.47
1:D:85:GLU:HG3	1:D:115:ALA:CB	2.43	0.47
1:D:310:LEU:O	1:D:310:LEU:HD12	2.14	0.47
1:A:113:LYS:HE3	1:A:145:GLU:OE2	2.14	0.47
1:A:286:ARG:O	1:A:289:LEU:HB3	2.15	0.47
1:B:64:GLY:O	1:B:66:MET:CE	2.62	0.47
1:B:141:VAL:HG21	1:B:182:PHE:CE2	2.49	0.47
1:C:59:ALA:HB3	1:C:307:LEU:HD22	1.95	0.47
1:A:204:LEU:HA	1:A:205:PRO:HD2	1.47	0.47
1:A:312:THR:HG21	1:B:236:LEU:HD11	1.95	0.47
2:B:502:FMN:H1'2	2:B:502:FMN:H9	1.66	0.47
1:C:139:ARG:CB	1:C:139:ARG:NH2	2.77	0.47
1:C:251:ARG:CZ	1:C:259:LEU:HG	2.45	0.47
1:D:59:ALA:HB1	1:D:307:LEU:CD2	2.45	0.47
1:D:82:GLU:HG2	1:D:114:VAL:HG12	1.94	0.47
1:A:219:TRP:CD2	1:A:222:VAL:HG21	2.50	0.47
1:B:48:LEU:HB3	1:B:59:ALA:HA	1.97	0.47
1:C:10:HIS:CE1	1:C:223:GLU:OE2	2.67	0.47
1:D:98:ILE:HD12	1:D:98:ILE:H	1.79	0.47
1:D:180:LEU:HD23	1:D:182:PHE:HE1	1.79	0.47
1:D:253:VAL:C	1:D:255:PRO:HD3	2.40	0.47
1:A:42:ALA:O	1:A:45:GLU:HG2	2.14	0.47
1:A:63:ILE:HD13	1:A:80:LEU:HB3	1.97	0.47
1:A:83:ALA:O	1:A:84:ALA:C	2.57	0.47
1:A:217:THR:HG23	2:A:502:FMN:O3P	2.14	0.47
1:A:239:ILE:HD13	1:D:33:LEU:CD1	2.44	0.47
1:A:289:LEU:O	1:A:292:ALA:HB3	2.15	0.47
1:A:301:ALA:O	1:A:302:TRP:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:HD13	1:B:303:ILE:HD11	1.97	0.47
1:B:110:ARG:NE	1:B:110:ARG:CA	2.78	0.47
1:B:111:VAL:O	1:B:113:LYS:N	2.48	0.47
1:B:217:THR:HG23	2:B:502:FMN:O2P	2.15	0.47
1:B:312:THR:CG2	1:C:159:ALA:HB1	2.35	0.47
1:C:11:LEU:CD2	1:C:15:LEU:HD23	2.43	0.47
1:C:38:LEU:HD13	1:D:171:VAL:HG21	1.95	0.47
1:C:42:ALA:O	1:C:45:GLU:HG2	2.13	0.47
1:C:188:GLU:CG	1:C:189:VAL:H	2.28	0.47
1:C:188:GLU:CG	1:C:189:VAL:N	2.77	0.47
1:C:296:ALA:C	1:C:298:ARG:N	2.71	0.47
1:D:100:LEU:HD13	1:D:132:TYR:CE1	2.48	0.47
1:C:258:PRO:HA	1:C:280:ASP:OD1	2.15	0.47
1:C:294:GLU:N	1:C:294:GLU:OE1	2.48	0.47
1:C:317:ILE:HG23	1:C:328:ARG:HD2	1.97	0.47
1:D:15:LEU:CD1	1:D:290:ARG:NH2	2.78	0.47
1:D:43:LEU:O	1:D:46:VAL:HG13	2.15	0.47
1:A:98:ILE:HG22	1:A:102:ARG:HB3	1.97	0.47
1:A:293:LEU:C	1:A:295:GLY:N	2.71	0.47
1:C:124:LEU:HD13	1:C:128:GLN:HB2	1.95	0.47
1:D:130:ARG:HA	1:D:173:ARG:HH21	1.80	0.47
1:D:186:VAL:HG21	1:D:201:LEU:HD22	1.96	0.47
1:D:243:THR:O	1:D:244:ALA:C	2.58	0.47
1:B:33:LEU:HB3	1:B:317:ILE:HD13	1.96	0.47
1:C:285:ALA:CB	2:C:502:FMN:H2'	2.45	0.47
1:D:31:PHE:CD2	1:D:277:LEU:HD21	2.50	0.47
1:D:137:LEU:O	1:D:141:VAL:HG23	2.14	0.47
1:A:21:TYR:OH	1:A:191:HIS:CD2	2.69	0.46
1:A:100:LEU:HD13	1:A:101:GLU:OE2	2.14	0.46
1:A:105:ALA:CB	1:A:108:SER:N	2.75	0.46
1:B:134:ARG:O	1:B:137:LEU:HB2	2.15	0.46
1:B:141:VAL:HG21	1:B:182:PHE:CZ	2.50	0.46
1:B:202:ARG:C	1:B:203:ASP:OD1	2.58	0.46
1:B:315:PHE:CE2	1:C:159:ALA:HB2	2.51	0.46
1:C:219:TRP:CZ2	2:C:502:FMN:C9A	2.98	0.46
1:A:281:LEU:HD13	1:A:281:LEU:HA	1.74	0.46
1:B:111:VAL:C	1:B:113:LYS:N	2.72	0.46
1:C:42:ALA:O	1:C:43:LEU:C	2.58	0.46
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.62	0.46
1:D:219:TRP:HZ2	2:D:502:FMN:C8	2.28	0.46
1:A:46:VAL:HA	1:A:320:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:VAL:HG12	1:B:120:LEU:CD1	2.43	0.46
1:B:232:ARG:HH21	1:B:232:ARG:HG3	1.77	0.46
1:B:307:LEU:HD23	1:B:307:LEU:HA	1.56	0.46
1:B:308:GLU:O	1:B:309:GLU:C	2.58	0.46
1:C:149:LEU:O	1:C:184:VAL:HA	2.16	0.46
1:D:124:LEU:HD12	1:D:137:LEU:CD1	2.45	0.46
1:D:191:HIS:CE1	1:D:220:ALA:H	2.33	0.46
1:D:269:THR:O	1:D:272:ALA:HB3	2.15	0.46
1:B:61:PHE:CE2	1:B:303:ILE:HD13	2.49	0.46
1:B:271:GLY:HA2	1:B:282:LEU:HG	1.97	0.46
1:C:210:ASP:OD1	1:C:211:VAL:N	2.48	0.46
1:D:211:VAL:HG12	1:D:250:VAL:HG21	1.97	0.46
1:D:295:GLY:O	1:D:297:GLU:N	2.48	0.46
1:A:217:THR:HG22	1:A:286:ARG:CB	2.40	0.46
1:C:78:LEU:HD23	1:C:114:VAL:HG22	1.97	0.46
1:C:154:ASN:ND2	1:C:157:GLN:HE21	2.12	0.46
1:C:284:VAL:CG1	1:C:287:PRO:HD2	2.45	0.46
1:A:156:LEU:HD12	1:A:191:HIS:CD2	2.51	0.46
1:B:52:PHE:HA	4:B:1137:HOH:O	2.14	0.46
1:B:115:ALA:N	1:B:116:PRO:HD3	2.29	0.46
1:B:227:ARG:O	1:B:228:PHE:CD2	2.69	0.46
1:D:85:GLU:OE1	1:D:118:ALA:N	2.49	0.46
1:A:102:ARG:O	1:A:104:GLU:N	2.48	0.46
1:A:106:LEU:H	1:A:107:ARG:CB	2.16	0.46
1:A:289:LEU:O	1:A:289:LEU:HD12	2.16	0.46
1:B:219:TRP:CZ2	2:B:502:FMN:C9	2.97	0.46
1:B:312:THR:O	1:B:315:PHE:HB3	2.15	0.46
1:C:139:ARG:C	1:C:143:MET:HG3	2.41	0.46
1:D:31:PHE:HA	1:D:330:GLU:O	2.15	0.46
1:B:28:LEU:HD23	1:B:244:ALA:HB2	1.98	0.46
1:B:32:ARG:NH1	1:B:32:ARG:CG	2.79	0.46
1:D:156:LEU:O	1:D:160:VAL:HG23	2.15	0.46
1:A:93:LEU:HD13	1:A:93:LEU:HA	1.59	0.46
1:A:236:LEU:O	1:A:237:CYS:C	2.58	0.46
1:B:36:GLN:CB	1:B:39:ALA:HB2	2.44	0.46
1:C:65:ALA:HB2	1:C:92:MET:HB2	1.98	0.46
1:C:120:LEU:N	1:C:147:ASP:OD2	2.48	0.46
1:D:24:THR:OG1	1:D:238:GLU:HB3	2.16	0.46
1:D:130:ARG:HH22	1:D:168:ARG:NH1	2.14	0.46
1:A:317:ILE:HG23	1:A:328:ARG:CD	2.45	0.46
1:B:185:MET:HB3	1:B:208:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:PHE:CB	1:D:57:LEU:HD11	2.45	0.46
1:D:251:ARG:NH2	1:D:257:LEU:O	2.49	0.46
1:A:67:THR:O	2:A:502:FMN:H6	2.16	0.45
1:A:191:HIS:HE1	1:A:220:ALA:H	1.61	0.45
1:A:317:ILE:HA	1:A:317:ILE:HD12	1.30	0.45
1:B:286:ARG:NH1	4:B:1037:HOH:O	2.41	0.45
1:C:19:VAL:HG12	1:C:222:VAL:HA	1.98	0.45
1:A:127:ALA:HA	1:A:170:LEU:CD2	2.38	0.45
1:B:148:ALA:HA	1:B:182:PHE:HB2	1.98	0.45
1:C:191:HIS:CE1	1:C:219:TRP:N	2.84	0.45
1:D:128:GLN:C	1:D:130:ARG:H	2.24	0.45
1:A:14:CYS:HB3	1:A:286:ARG:HG3	1.99	0.45
1:B:276:ALA:CB	1:B:329:VAL:HB	2.45	0.45
1:B:319:ALA:HB2	1:B:328:ARG:HD2	1.96	0.45
1:C:299:VAL:O	1:C:300:ALA:C	2.59	0.45
1:D:161:GLN:HB2	1:D:223:GLU:CD	2.41	0.45
1:A:67:THR:O	2:A:502:FMN:HM71	2.17	0.45
1:A:153:VAL:HG11	1:D:38:LEU:HD21	1.98	0.45
1:A:221:ARG:CG	1:A:237:CYS:HB3	2.45	0.45
1:C:11:LEU:HD23	1:C:11:LEU:HA	1.71	0.45
1:C:15:LEU:HD11	1:C:293:LEU:CD1	2.46	0.45
1:C:167:PHE:N	1:C:167:PHE:CD2	2.84	0.45
1:C:232:ARG:CB	1:C:233:HIS:CD2	2.99	0.45
1:B:99:LEU:HD22	1:B:106:LEU:HA	1.99	0.45
1:C:48:LEU:O	1:C:59:ALA:HA	2.17	0.45
1:D:142:GLU:C	1:D:144:LEU:N	2.73	0.45
1:D:178:LEU:HB3	1:D:179:PRO:CD	2.46	0.45
1:A:100:LEU:HD22	1:A:132:TYR:CD1	2.52	0.45
1:B:192:GLY:HA2	1:B:211:VAL:O	2.17	0.45
1:C:232:ARG:C	1:C:233:HIS:CD2	2.95	0.45
1:D:26:THR:HG23	4:D:1162:HOH:O	2.16	0.45
1:D:192:GLY:CA	1:D:213:GLY:HA2	2.47	0.45
1:A:38:LEU:HD11	1:B:201:LEU:HD21	1.99	0.45
1:A:297:GLU:O	1:A:300:ALA:HB3	2.16	0.45
1:C:35:TYR:HB3	1:D:241:ILE:HD12	1.99	0.45
1:C:314:LEU:HA	1:C:314:LEU:HD23	1.65	0.45
2:C:502:FMN:O2P	2:C:502:FMN:C4'	2.65	0.45
1:A:167:PHE:HA	1:A:170:LEU:HD11	1.99	0.45
1:A:236:LEU:O	1:A:238:GLU:N	2.50	0.45
1:A:275:LEU:HA	1:A:275:LEU:HD23	1.46	0.45
1:B:295:GLY:O	1:B:297:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LEU:CD1	1:C:315:PHE:HD1	2.28	0.45
1:D:38:LEU:C	1:D:40:GLY:N	2.71	0.45
1:A:105:ALA:HB1	1:A:107:ARG:HB3	1.99	0.45
1:B:208:ALA:HA	1:B:257:LEU:CD1	2.47	0.45
1:C:110:ARG:CG	1:C:110:ARG:NH2	2.69	0.45
2:C:502:FMN:H9	2:C:502:FMN:H1'2	1.59	0.45
1:D:28:LEU:C	1:D:30:GLY:N	2.74	0.45
1:D:150:ALA:CB	1:D:185:MET:HG3	2.46	0.45
1:A:131:ARG:HG3	1:A:132:TYR:CE2	2.52	0.44
1:A:288:LEU:HD12	1:A:288:LEU:HA	1.48	0.44
1:B:37:ALA:HB1	1:C:153:VAL:HG13	1.99	0.44
1:B:218:SER:HB3	1:B:221:ARG:HB2	1.99	0.44
1:C:125:GLY:H	1:C:151:PHE:HA	1.82	0.44
2:C:502:FMN:O2P	2:C:502:FMN:H4'	2.16	0.44
1:D:100:LEU:HD13	1:D:132:TYR:CD1	2.52	0.44
1:D:154:ASN:ND2	1:D:157:GLN:NE2	2.59	0.44
1:A:20:ALA:HB2	1:A:286:ARG:NH2	2.33	0.44
1:B:56:THR:O	1:B:56:THR:HG22	2.16	0.44
1:B:112:ARG:O	1:B:112:ARG:HD3	2.17	0.44
1:B:198:ALA:HB2	1:B:250:VAL:HG13	1.99	0.44
1:D:162:ARG:CZ	1:D:227:ARG:HH22	2.30	0.44
1:A:26:THR:HG21	4:A:1054:HOH:O	2.16	0.44
1:A:167:PHE:CA	1:A:170:LEU:HD13	2.46	0.44
1:A:186:VAL:HB	1:A:201:LEU:CD1	2.48	0.44
1:A:269:THR:CB	1:B:235:GLU:HG2	2.47	0.44
1:B:38:LEU:HD23	1:C:153:VAL:HG21	1.99	0.44
1:B:130:ARG:HG2	1:B:130:ARG:NH1	2.32	0.44
1:C:133:GLY:O	1:C:135:ASP:N	2.51	0.44
1:D:76:ILE:CG2	1:D:293:LEU:HD23	2.47	0.44
1:D:165:THR:HG21	4:D:1116:HOH:O	2.16	0.44
1:D:174:LEU:O	1:D:178:LEU:N	2.50	0.44
1:B:211:VAL:O	1:B:212:ALA:C	2.61	0.44
1:C:43:LEU:HD23	1:D:159:ALA:HB1	2.00	0.44
1:C:161:GLN:CA	1:C:223:GLU:HG3	2.46	0.44
1:C:191:HIS:CE1	1:C:219:TRP:H	2.35	0.44
1:D:154:ASN:HA	1:D:188:GLU:OE2	2.18	0.44
1:C:113:LYS:HD3	4:C:1107:HOH:O	2.18	0.44
1:C:148:ALA:CB	1:C:183:PRO:HB2	2.48	0.44
1:A:92:MET:HA	1:A:121:ILE:O	2.18	0.44
1:A:128:GLN:O	1:A:129:LEU:C	2.60	0.44
1:A:149:LEU:CD1	1:A:151:PHE:CZ	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:HIS:CE1	1:A:219:TRP:N	2.85	0.44
1:C:66:MET:HG2	2:C:502:FMN:C8	2.47	0.44
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.62	0.44
1:D:249:GLU:O	1:D:250:VAL:C	2.61	0.44
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.83	0.44
1:A:153:VAL:HG11	1:D:38:LEU:CD2	2.48	0.44
1:C:95:SER:O	1:C:98:ILE:HD12	2.16	0.44
1:D:137:LEU:CD2	1:D:177:LEU:HD11	2.47	0.44
1:D:150:ALA:HB2	1:D:185:MET:HG3	2.00	0.44
1:D:202:ARG:HA	1:D:254:LEU:HD21	2.00	0.44
1:D:219:TRP:HZ2	2:D:502:FMN:C9	2.31	0.44
1:A:125:GLY:H	1:A:151:PHE:HA	1.83	0.44
1:A:187:LYS:NZ	1:A:188:GLU:O	2.27	0.44
1:B:232:ARG:HB2	1:B:232:ARG:NH2	2.29	0.44
1:C:139:ARG:O	1:C:143:MET:CG	2.62	0.44
1:C:317:ILE:HG23	1:C:328:ARG:CD	2.48	0.44
1:D:317:ILE:HG12	1:D:328:ARG:HD3	1.99	0.44
1:A:253:VAL:C	1:A:255:PRO:HD2	2.43	0.44
1:A:278:GLY:HA2	1:A:326:ARG:NE	2.33	0.44
1:C:19:VAL:HG11	1:C:222:VAL:HG22	2.00	0.44
1:D:166:ASP:OD1	1:D:168:ARG:HB2	2.17	0.44
1:A:139:ARG:O	1:A:140:LEU:C	2.60	0.43
1:A:290:ARG:N	1:A:291:PRO:HD2	2.32	0.43
1:B:35:TYR:OH	1:C:155:PRO:HD2	2.18	0.43
1:C:55:LYS:HB2	1:C:119:LEU:HD13	2.00	0.43
1:C:125:GLY:HA2	1:C:152:HIS:O	2.17	0.43
1:C:188:GLU:CG	1:C:192:GLY:H	2.31	0.43
1:D:60:PRO:O	1:D:281:LEU:HB2	2.18	0.43
1:D:65:ALA:O	1:D:66:MET:CG	2.63	0.43
1:D:98:ILE:H	1:D:98:ILE:CD1	2.30	0.43
1:D:152:HIS:ND1	2:D:502:FMN:O2	2.42	0.43
1:A:134:ARG:O	1:A:138:LEU:CD2	2.66	0.43
1:A:196:GLU:HG2	1:D:36:GLN:HE22	1.83	0.43
1:B:149:LEU:HD11	1:B:151:PHE:CZ	2.53	0.43
1:C:181:PRO:HG2	1:C:182:PHE:CD2	2.54	0.43
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.63	0.43
1:A:251:ARG:NH1	1:A:259:LEU:HG	2.33	0.43
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.74	0.43
1:C:55:LYS:HE3	1:C:147:ASP:OD1	2.18	0.43
1:D:178:LEU:HD23	1:D:178:LEU:HA	1.66	0.43
1:A:124:LEU:HD22	1:A:124:LEU:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLY:HA2	1:A:152:HIS:O	2.19	0.43
1:C:84:ALA:HA	1:C:89:VAL:HG22	2.00	0.43
1:C:124:LEU:HD22	1:C:124:LEU:HA	1.76	0.43
1:D:60:PRO:HG3	1:D:322:PRO:CG	2.48	0.43
1:D:247:ILE:HD11	1:D:261:ALA:HB1	2.00	0.43
1:B:305:ASP:OD2	1:B:305:ASP:C	2.60	0.43
1:B:309:GLU:HG3	1:C:236:LEU:HG	1.99	0.43
1:C:128:GLN:C	1:C:130:ARG:H	2.25	0.43
1:C:149:LEU:HD13	1:C:151:PHE:CZ	2.54	0.43
1:D:79:ALA:HA	1:D:296:ALA:HB2	1.99	0.43
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.79	0.43
1:A:99:LEU:HD23	1:A:140:LEU:CD1	2.48	0.43
1:B:100:LEU:HD13	1:B:132:TYR:CD1	2.54	0.43
1:C:188:GLU:CB	1:C:193:LEU:HD23	2.49	0.43
1:D:90:GLY:HA2	1:D:119:LEU:HB3	2.01	0.43
1:A:78:LEU:HD22	1:A:114:VAL:HG21	2.01	0.43
1:A:162:ARG:HG3	1:A:227:ARG:HH11	1.78	0.43
1:B:58:LYS:HG3	1:B:88:GLY:HA3	2.00	0.43
1:C:43:LEU:HD11	1:C:311:ARG:HG2	2.00	0.43
1:D:32:ARG:N	1:D:330:GLU:O	2.50	0.43
1:A:10:HIS:O	1:A:11:LEU:C	2.62	0.43
2:A:502:FMN:H5'2	2:A:502:FMN:C1'	2.46	0.43
1:B:162:ARG:CG	1:B:227:ARG:HH12	2.26	0.43
1:B:318:GLY:C	1:B:328:ARG:NH1	2.77	0.43
1:C:15:LEU:HD21	1:C:293:LEU:HD11	2.00	0.43
1:C:141:VAL:HG11	1:C:182:PHE:CG	2.54	0.43
1:D:41:LEU:HD22	1:D:320:ARG:HG3	2.01	0.43
1:D:290:ARG:CG	1:D:290:ARG:NH1	2.80	0.43
1:B:81:ALA:CB	1:B:111:VAL:HG13	2.49	0.43
1:B:225:TRP:O	1:B:229:GLY:HA2	2.19	0.43
1:B:331:ARG:HB2	4:B:1052:HOH:O	2.19	0.43
1:C:123:ASN:HA	1:C:150:ALA:O	2.19	0.43
1:C:149:LEU:CD1	1:C:151:PHE:CZ	3.02	0.43
1:C:312:THR:HG21	1:D:236:LEU:HD11	2.01	0.43
1:A:157:GLN:OE1	1:A:219:TRP:CE3	2.72	0.43
1:B:204:LEU:HA	1:B:205:PRO:HD2	1.85	0.43
1:C:28:LEU:C	1:C:30:GLY:N	2.75	0.43
1:C:299:VAL:HG12	1:C:300:ALA:N	2.33	0.43
1:A:17:GLY:HA2	1:A:225:TRP:CZ2	2.54	0.42
1:A:160:VAL:HG12	1:A:223:GLU:HB3	2.01	0.42
1:A:263:GLY:HA2	2:A:502:FMN:O2P	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:O	1:B:44:SER:C	2.62	0.42
1:B:61:PHE:CD2	1:B:62:LEU:N	2.86	0.42
1:C:21:TYR:HD1	1:C:216:GLY:O	2.02	0.42
1:D:126:LEU:HD12	1:D:126:LEU:HA	1.86	0.42
1:B:38:LEU:HD12	1:C:197:ALA:O	2.19	0.42
1:C:51:PRO:HA	1:C:56:THR:HA	2.01	0.42
1:C:247:ILE:HD13	1:C:279:ALA:HB2	2.01	0.42
1:D:162:ARG:HG3	1:D:227:ARG:NH1	2.34	0.42
1:A:32:ARG:HG3	1:A:32:ARG:HH11	1.83	0.42
1:A:104:GLU:OE1	1:A:104:GLU:HA	2.18	0.42
1:A:196:GLU:OE2	1:D:34:ARG:HD3	2.19	0.42
1:A:210:ASP:OD1	1:A:212:ALA:N	2.51	0.42
1:B:241:ILE:HA	1:B:241:ILE:HD13	1.74	0.42
1:C:32:ARG:HH11	1:C:32:ARG:HD3	1.69	0.42
1:C:48:LEU:HB3	1:C:59:ALA:HA	2.00	0.42
1:C:284:VAL:HG12	1:C:285:ALA:N	2.33	0.42
1:D:151:PHE:CE1	1:D:174:LEU:CD1	3.02	0.42
1:D:245:ARG:O	1:D:249:GLU:HG3	2.19	0.42
1:B:210:ASP:CB	1:B:260:VAL:HB	2.44	0.42
1:B:232:ARG:O	1:B:234:PRO:HD3	2.19	0.42
1:C:132:TYR:HB3	1:C:136:ASP:CB	2.50	0.42
1:C:217:THR:CB	1:C:286:ARG:HH11	2.08	0.42
1:A:36:GLN:HB3	1:A:39:ALA:HB2	2.00	0.42
1:B:106:LEU:CG	1:B:143:MET:CG	2.96	0.42
1:B:128:GLN:C	1:B:130:ARG:N	2.76	0.42
1:C:214:ALA:HB3	1:C:242:PRO:HA	2.01	0.42
1:D:264:GLY:CA	1:D:266:TYR:CE1	2.84	0.42
1:D:63:ILE:HG23	1:D:288:LEU:HD23	2.01	0.42
1:D:115:ALA:N	1:D:116:PRO:HD2	2.32	0.42
1:A:59:ALA:CB	1:A:307:LEU:HD22	2.48	0.42
1:A:191:HIS:HE1	1:A:219:TRP:N	2.17	0.42
1:B:227:ARG:NH2	1:B:228:PHE:HZ	2.13	0.42
1:C:177:LEU:O	1:C:180:LEU:HD13	2.19	0.42
1:C:191:HIS:HE1	1:C:220:ALA:N	2.15	0.42
1:A:24:THR:CG2	1:A:238:GLU:HB3	2.48	0.42
1:A:226:VAL:O	1:A:227:ARG:C	2.62	0.42
1:A:303:ILE:CG2	1:A:307:LEU:HD11	2.50	0.42
1:B:58:LYS:N	1:B:88:GLY:O	2.44	0.42
1:C:147:ASP:O	1:C:183:PRO:HD2	2.20	0.42
1:A:218:SER:O	1:A:219:TRP:C	2.59	0.42
1:B:53:LEU:HD11	1:B:121:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:HA	1:C:106:LEU:HD12	2.01	0.42
1:C:134:ARG:N	4:C:1071:HOH:O	2.18	0.42
1:C:308:GLU:HA	1:C:311:ARG:HH12	1.83	0.42
1:D:233:HIS:ND1	1:D:233:HIS:N	2.66	0.42
1:A:48:LEU:HB3	1:A:59:ALA:HA	2.01	0.42
1:A:76:ILE:HG22	1:A:293:LEU:HD23	2.01	0.42
1:B:100:LEU:HB3	1:B:132:TYR:CE1	2.55	0.42
1:B:201:LEU:HB3	1:B:206:LEU:HD11	2.02	0.42
1:C:85:GLU:HG3	1:C:115:ALA:HA	2.02	0.42
1:D:247:ILE:CD1	1:D:261:ALA:HB1	2.50	0.42
1:A:168:ARG:CD	1:D:45:GLU:OE2	2.67	0.41
1:A:251:ARG:O	1:A:251:ARG:HG3	2.19	0.41
1:A:325:ALA:O	1:A:328:ARG:HB2	2.20	0.41
1:B:321:ASN:HB2	1:B:322:PRO:HD3	2.01	0.41
1:C:12:GLU:HB3	1:C:16:GLU:OE1	2.19	0.41
1:C:33:LEU:HD23	1:C:33:LEU:HA	1.52	0.41
1:C:141:VAL:HG11	1:C:182:PHE:CD2	2.54	0.41
1:C:217:THR:CG2	1:C:286:ARG:CB	2.97	0.41
1:D:128:GLN:NE2	1:D:128:GLN:CA	2.77	0.41
1:D:176:GLU:O	1:D:178:LEU:N	2.53	0.41
1:D:199:LEU:HD21	1:D:202:ARG:NH1	2.35	0.41
1:D:261:ALA:HB2	1:D:279:ALA:HB2	2.01	0.41
1:A:30:GLY:O	1:A:332:VAL:HG12	2.20	0.41
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.62	0.41
1:A:220:ALA:CB	1:A:237:CYS:HA	2.49	0.41
1:B:62:LEU:O	1:B:283:ALA:HA	2.21	0.41
1:C:195:ARG:HD2	4:C:1166:HOH:O	2.19	0.41
1:A:219:TRP:CA	1:A:222:VAL:HG23	2.43	0.41
1:B:98:ILE:O	1:B:99:LEU:C	2.61	0.41
1:B:241:ILE:HG23	1:B:241:ILE:HD12	1.85	0.41
1:B:266:TYR:CD1	1:B:287:PRO:HG2	2.56	0.41
1:B:286:ARG:N	1:B:287:PRO:CD	2.83	0.41
1:D:85:GLU:HA	4:D:1149:HOH:O	2.19	0.41
1:A:9:LYS:HG3	1:A:10:HIS:N	2.30	0.41
1:A:15:LEU:HD13	1:A:15:LEU:HA	1.79	0.41
1:A:126:LEU:C	1:A:170:LEU:CD2	2.93	0.41
1:A:148:ALA:HB1	1:A:183:PRO:O	2.21	0.41
1:B:108:SER:C	1:B:110:ARG:N	2.79	0.41
1:B:180:LEU:HA	1:B:180:LEU:HD12	1.76	0.41
1:C:174:LEU:O	1:C:175:ALA:C	2.64	0.41
1:C:217:THR:HG23	2:C:502:FMN:P	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ALA:CB	1:C:237:CYS:HA	2.50	0.41
1:D:36:GLN:HB2	1:D:39:ALA:HB2	2.02	0.41
1:D:195:ARG:CB	1:D:249:GLU:HB3	2.51	0.41
1:B:105:ALA:O	1:B:107:ARG:N	2.48	0.41
1:B:232:ARG:CG	1:B:232:ARG:NH2	2.78	0.41
1:C:228:PHE:HD2	1:C:232:ARG:NH1	2.18	0.41
1:B:331:ARG:HD3	4:B:1223:HOH:O	2.20	0.41
1:C:9:LYS:HG3	1:C:10:HIS:H	1.84	0.41
1:C:219:TRP:CZ2	2:C:502:FMN:C9	2.97	0.41
1:A:109:PHE:O	1:A:110:ARG:HB2	2.21	0.41
1:A:267:THR:O	1:A:269:THR:N	2.53	0.41
1:D:61:PHE:CD2	1:D:62:LEU:N	2.89	0.41
1:D:246:ALA:O	1:D:247:ILE:C	2.61	0.41
1:D:317:ILE:HG13	1:D:328:ARG:HB3	2.03	0.41
1:A:123:ASN:HB3	1:A:150:ALA:HB3	2.02	0.41
1:A:167:PHE:C	1:A:170:LEU:CD1	2.94	0.41
1:A:209:VAL:HG23	1:A:259:LEU:HD22	2.03	0.41
1:B:35:TYR:HB3	1:C:241:ILE:HD12	2.02	0.41
1:B:46:VAL:HG11	1:B:315:PHE:HB2	2.03	0.41
1:B:61:PHE:CD2	1:B:61:PHE:C	2.98	0.41
1:C:11:LEU:HD22	1:C:11:LEU:C	2.46	0.41
1:C:234:PRO:O	1:C:237:CYS:HB2	2.20	0.41
1:D:176:GLU:HG2	1:D:177:LEU:N	2.30	0.41
1:A:156:LEU:CD1	1:A:220:ALA:HB2	2.50	0.41
1:A:291:PRO:HB2	1:A:299:VAL:HA	2.01	0.41
1:B:43:LEU:C	1:B:45:GLU:N	2.79	0.41
1:B:59:ALA:CB	1:B:307:LEU:CD1	2.84	0.41
1:B:125:GLY:O	1:B:126:LEU:C	2.64	0.41
1:B:303:ILE:O	1:B:303:ILE:HG22	2.21	0.41
1:C:78:LEU:HD23	1:C:114:VAL:HG21	2.01	0.41
1:C:128:GLN:N	1:C:128:GLN:CD	2.78	0.41
1:B:193:LEU:HD22	1:B:197:ALA:HB1	2.02	0.41
1:B:235:GLU:C	1:B:237:CYS:N	2.78	0.41
1:C:95:SER:C	1:C:97:ARG:N	2.75	0.41
1:C:128:GLN:OE1	1:C:128:GLN:HA	2.19	0.41
1:D:228:PHE:C	1:D:230:GLU:N	2.75	0.41
1:B:130:ARG:HH11	1:B:130:ARG:CB	2.33	0.40
1:B:180:LEU:N	1:B:180:LEU:HD12	2.31	0.40
1:B:298:ARG:O	1:B:299:VAL:C	2.63	0.40
1:C:83:ALA:CB	1:C:299:VAL:HG12	2.51	0.40
1:C:154:ASN:HD22	1:C:157:GLN:CB	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ARG:O	1:D:112:ARG:CG	2.69	0.40
1:A:217:THR:CG2	1:A:286:ARG:HD3	2.52	0.40
1:A:219:TRP:HZ2	2:A:502:FMN:C9	2.34	0.40
1:B:78:LEU:HD22	1:B:114:VAL:HG22	2.03	0.40
1:C:33:LEU:HD22	1:C:317:ILE:CG1	2.44	0.40
1:C:189:VAL:O	1:C:189:VAL:HG23	2.22	0.40
1:D:15:LEU:HD13	1:D:290:ARG:NH2	2.35	0.40
1:D:80:LEU:CD2	1:D:292:ALA:HB2	2.52	0.40
1:A:100:LEU:CD1	1:A:101:GLU:OE2	2.69	0.40
1:C:60:PRO:CA	1:C:281:LEU:HD13	2.52	0.40
1:C:321:ASN:O	1:C:322:PRO:C	2.63	0.40
1:D:154:ASN:O	1:D:155:PRO:C	2.63	0.40
1:D:217:THR:CG2	1:D:286:ARG:NH1	2.42	0.40
1:A:167:PHE:CB	4:D:1127:HOH:O	2.68	0.40
1:A:220:ALA:O	1:A:221:ARG:C	2.65	0.40
1:B:130:ARG:CG	1:B:130:ARG:NH1	2.84	0.40
1:B:308:GLU:HA	1:B:311:ARG:NH2	2.37	0.40
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.84	0.40
1:C:286:ARG:NH1	1:C:286:ARG:HB3	2.36	0.40
1:D:28:LEU:HD22	1:D:273:LYS:HB2	2.03	0.40
1:D:59:ALA:HB3	1:D:89:VAL:HG12	2.03	0.40
1:D:276:ALA:CB	1:D:329:VAL:HB	2.52	0.40
1:A:35:TYR:CE1	1:B:156:LEU:HB2	2.57	0.40
1:A:167:PHE:N	1:A:167:PHE:CD2	2.89	0.40
1:A:289:LEU:HD22	2:A:502:FMN:HM72	2.03	0.40
1:B:85:GLU:HG2	1:B:118:ALA:HB2	2.03	0.40
1:B:196:GLU:HA	1:B:199:LEU:HB2	2.04	0.40
1:C:91:MET:HE2	1:C:93:LEU:HD13	2.03	0.40
1:D:196:GLU:HA	1:D:199:LEU:HB2	2.02	0.40
1:D:314:LEU:HD23	1:D:314:LEU:HA	1.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:HIS:CD2	1:B:101:GLU:OE2[3_655]	2.03	0.17

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	314/332 (95%)	257 (82%)	43 (14%)	14 (4%)	2	10
1	B	314/332 (95%)	246 (78%)	45 (14%)	23 (7%)	1	3
1	C	310/332 (93%)	243 (78%)	50 (16%)	17 (6%)	1	7
1	D	307/332 (92%)	249 (81%)	41 (13%)	17 (6%)	1	7
All	All	1245/1328 (94%)	995 (80%)	179 (14%)	71 (6%)	1	7

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	44	SER
1	A	97	ARG
1	A	110	ARG
1	A	178	LEU
1	B	44	SER
1	B	106	LEU
1	B	111	VAL
1	B	178	LEU
1	B	202	ARG
1	B	222	VAL
1	B	223	GLU
1	B	227	ARG
1	B	228	PHE
1	B	296	ALA
1	C	44	SER
1	C	94	GLY
1	C	178	LEU
1	C	296	ALA
1	C	297	GLU
1	D	145	GLU
1	D	177	LEU

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Mol	Chain	Res	Type
1	D	178	LEU
1	D	179	PRO
1	D	296	ALA
1	A	11	LEU
1	A	268	GLY
1	B	105	ALA
1	B	112	ARG
1	C	299	VAL
1	D	129	LEU
1	D	175	ALA
1	A	103	PRO
1	A	107	ARG
1	B	54	GLY
1	B	109	PHE
1	B	161	GLN
1	C	179	PRO
1	C	229	GLY
1	C	277	LEU
1	D	29	GLU
1	D	162	ARG
1	D	316	ALA
1	A	179	PRO
1	B	77	ASN
1	B	143	MET
1	B	181	PRO
1	B	294	GLU
1	C	101	GLU
1	C	169	GLY
1	C	203	ASP
1	C	212	ALA
1	D	11	LEU
1	D	118	ALA
1	A	84	ALA
1	A	243	THR
1	B	129	LEU
1	B	263	GLY
1	C	131	ARG
1	D	98	ILE
1	D	116	PRO
1	D	142	GLU
1	B	118	ALA
1	B	291	PRO

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Mol	Chain	Res	Type
1	C	170	LEU
1	D	54	GLY
1	D	212	ALA
1	A	226	VAL
1	C	76	ILE
1	C	111	VAL
1	A	258	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	239/252 (95%)	160 (67%)	79 (33%)	0	1
1	B	241/252 (96%)	170 (70%)	71 (30%)	0	2
1	C	239/252 (95%)	171 (72%)	68 (28%)	0	2
1	D	234/252 (93%)	168 (72%)	66 (28%)	0	2
All	All	953/1008 (94%)	669 (70%)	284 (30%)	0	1

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	11	LEU
1	A	12	GLU
1	A	15	LEU
1	A	18	GLU
1	A	24	THR
1	A	26	THR
1	A	41	LEU
1	A	44	SER
1	A	46	VAL
1	A	58	LYS
1	A	67	THR
1	A	74	GLU
1	A	75	ARG

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Mol	Chain	Res	Type
1	A	76	ILE
1	A	77	ASN
1	A	87	LEU
1	A	92	MET
1	A	93	LEU
1	A	97	ARG
1	A	98	ILE
1	A	100	LEU
1	A	102	ARG
1	A	104	GLU
1	A	106	LEU
1	A	109	PHE
1	A	110	ARG
1	A	113	LYS
1	A	119	LEU
1	A	123	ASN
1	A	124	LEU
1	A	128	GLN
1	A	134	ARG
1	A	135	ASP
1	A	137	LEU
1	A	138	LEU
1	A	142	GLU
1	A	149	LEU
1	A	156	LEU
1	A	165	THR
1	A	168	ARG
1	A	172	GLU
1	A	173	ARG
1	A	177	LEU
1	A	178	LEU
1	A	180	LEU
1	A	184	VAL
1	A	188	GLU
1	A	189	VAL
1	A	196	GLU
1	A	204	LEU
1	A	210	ASP
1	A	217	THR
1	A	222	VAL
1	A	223	GLU
1	A	226	VAL

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Mol	Chain	Res	Type
1	A	232	ARG
1	A	233	HIS
1	A	235	GLU
1	A	236	LEU
1	A	239	ILE
1	A	252	GLU
1	A	259	LEU
1	A	260	VAL
1	A	281	LEU
1	A	282	LEU
1	A	288	LEU
1	A	294	GLU
1	A	297	GLU
1	A	298	ARG
1	A	303	ILE
1	A	308	GLU
1	A	309	GLU
1	A	310	LEU
1	A	317	ILE
1	A	322	PRO
1	A	323	LYS
1	A	326	ARG
1	A	332	VAL
1	B	9	LYS
1	B	11	LEU
1	B	16	GLU
1	B	46	VAL
1	B	50	THR
1	B	56	THR
1	B	62	LEU
1	B	63	ILE
1	B	74	GLU
1	B	77	ASN
1	B	82	GLU
1	B	91	MET
1	B	92	MET
1	B	93	LEU
1	B	97	ARG
1	B	98	ILE
1	B	99	LEU
1	B	107	ARG
1	B	110	ARG

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Mol	Chain	Res	Type
1	B	112	ARG
1	B	113	LYS
1	B	114	VAL
1	B	117	LYS
1	B	121	ILE
1	B	123	ASN
1	B	124	LEU
1	B	130	ARG
1	B	134	ARG
1	B	135	ASP
1	B	137	LEU
1	B	138	LEU
1	B	149	LEU
1	B	153	VAL
1	B	156	LEU
1	B	158	GLU
1	B	168	ARG
1	B	170	LEU
1	B	172	GLU
1	B	173	ARG
1	B	186	VAL
1	B	196	GLU
1	B	199	LEU
1	B	202	ARG
1	B	203	ASP
1	B	206	LEU
1	B	209	VAL
1	B	210	ASP
1	B	223	GLU
1	B	227	ARG
1	B	232	ARG
1	B	233	HIS
1	B	234	PRO
1	B	236	LEU
1	B	245	ARG
1	B	247	ILE
1	B	251	ARG
1	B	252	GLU
1	B	257	LEU
1	B	259	LEU
1	B	281	LEU
1	B	282	LEU

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Mol	Chain	Res	Type
1	B	286	ARG
1	B	288	LEU
1	B	291	PRO
1	B	298	ARG
1	B	303	ILE
1	B	307	LEU
1	B	308	GLU
1	B	317	ILE
1	B	323	LYS
1	B	326	ARG
1	C	9	LYS
1	C	11	LEU
1	C	15	LEU
1	C	18	GLU
1	C	19	VAL
1	C	26	THR
1	C	34	ARG
1	C	41	LEU
1	C	43	LEU
1	C	44	SER
1	C	50	THR
1	C	58	LYS
1	C	63	ILE
1	C	74	GLU
1	C	75	ARG
1	C	76	ILE
1	C	78	LEU
1	C	87	LEU
1	C	92	MET
1	C	93	LEU
1	C	98	ILE
1	C	99	LEU
1	C	101	GLU
1	C	102	ARG
1	C	104	GLU
1	C	106	LEU
1	C	110	ARG
1	C	111	VAL
1	C	114	VAL
1	C	123	ASN
1	C	124	LEU
1	C	128	GLN

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Mol	Chain	Res	Type
1	C	131	ARG
1	C	135	ASP
1	C	137	LEU
1	C	149	LEU
1	C	156	LEU
1	C	165	THR
1	C	168	ARG
1	C	173	ARG
1	C	180	LEU
1	C	188	GLU
1	C	196	GLU
1	C	203	ASP
1	C	217	THR
1	C	223	GLU
1	C	226	VAL
1	C	230	GLU
1	C	232	ARG
1	C	233	HIS
1	C	235	GLU
1	C	236	LEU
1	C	241	ILE
1	C	245	ARG
1	C	247	ILE
1	C	249	GLU
1	C	260	VAL
1	C	282	LEU
1	C	288	LEU
1	C	290	ARG
1	C	297	GLU
1	C	298	ARG
1	C	307	LEU
1	C	308	GLU
1	C	317	ILE
1	C	321	ASN
1	C	326	ARG
1	C	332	VAL
1	D	9	LYS
1	D	11	LEU
1	D	12	GLU
1	D	15	LEU
1	D	16	GLU
1	D	18	GLU

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Mol	Chain	Res	Type
1	D	25	THR
1	D	34	ARG
1	D	44	SER
1	D	46	VAL
1	D	56	THR
1	D	57	LEU
1	D	63	ILE
1	D	67	THR
1	D	75	ARG
1	D	78	LEU
1	D	92	MET
1	D	93	LEU
1	D	97	ARG
1	D	98	ILE
1	D	99	LEU
1	D	102	ARG
1	D	104	GLU
1	D	113	LYS
1	D	114	VAL
1	D	117	LYS
1	D	120	LEU
1	D	124	LEU
1	D	130	ARG
1	D	131	ARG
1	D	137	LEU
1	D	143	MET
1	D	145	GLU
1	D	149	LEU
1	D	153	VAL
1	D	156	LEU
1	D	168	ARG
1	D	170	LEU
1	D	172	GLU
1	D	173	ARG
1	D	176	GLU
1	D	178	LEU
1	D	185	MET
1	D	196	GLU
1	D	199	LEU
1	D	227	ARG
1	D	232	ARG
1	D	236	LEU

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Mol	Chain	Res	Type
1	D	241	ILE
1	D	247	ILE
1	D	252	GLU
1	D	281	LEU
1	D	282	LEU
1	D	288	LEU
1	D	289	LEU
1	D	290	ARG
1	D	294	GLU
1	D	298	ARG
1	D	308	GLU
1	D	314	LEU
1	D	317	ILE
1	D	320	ARG
1	D	323	LYS
1	D	324	GLU
1	D	326	ARG
1	D	331	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	157	GLN
1	A	191	HIS
1	A	233	HIS
1	B	123	ASN
1	B	154	ASN
1	B	191	HIS
1	C	10	HIS
1	C	154	ASN
1	C	157	GLN
1	C	191	HIS
1	C	233	HIS
1	C	256	HIS
1	D	10	HIS
1	D	123	ASN
1	D	157	GLN
1	D	191	HIS

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 ⓘ

6 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	FMN	C	502	-	33,33,33	3.72	16 (48%)	48,50,50	2.22	18 (37%)
2	FMN	A	502	-	33,33,33	3.76	13 (39%)	48,50,50	2.22	19 (39%)
3	POP	D	503	-	6,8,8	1.09	1 (16%)	12,13,13	1.61	3 (25%)
3	POP	B	503	-	6,8,8	1.04	1 (16%)	12,13,13	1.28	2 (16%)
2	FMN	B	502	-	33,33,33	3.34	14 (42%)	48,50,50	2.46	20 (41%)
2	FMN	D	502	-	33,33,33	3.27	12 (36%)	48,50,50	2.18	21 (43%)

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	FMN	C	502	-	-	13/18/18/18	0/3/3/3
2	FMN	A	502	-	-	10/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POP	D	503	-	-	5/6/6/6	-
3	POP	B	503	-	-	1/6/6/6	-
2	FMN	B	502	-	-	8/18/18/18	0/3/3/3
2	FMN	D	502	-	-	10/18/18/18	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	FMN	C6-C7	-10.21	1.25	1.39
2	C	502	FMN	C6-C7	-9.83	1.26	1.39
2	A	502	FMN	C9-C8	-9.56	1.26	1.39
2	C	502	FMN	C6-C5A	-9.34	1.25	1.40
2	B	502	FMN	C6-C7	-9.15	1.27	1.39
2	C	502	FMN	C9-C8	-9.12	1.27	1.39
2	A	502	FMN	C6-C5A	-8.84	1.26	1.40
2	B	502	FMN	C6-C5A	-8.44	1.27	1.40
2	D	502	FMN	C6-C7	-8.31	1.28	1.39
2	D	502	FMN	C6-C5A	-7.94	1.27	1.40
2	D	502	FMN	C9-C8	-7.87	1.28	1.39
2	C	502	FMN	C9-C9A	-7.66	1.27	1.39
2	B	502	FMN	C9-C8	-7.53	1.29	1.39
2	A	502	FMN	C9-C9A	-7.50	1.27	1.39
2	B	502	FMN	C9-C9A	-7.12	1.28	1.39
2	D	502	FMN	C9-C9A	-6.42	1.29	1.39
2	D	502	FMN	C9A-C5A	6.13	1.51	1.41
2	A	502	FMN	C9A-C5A	5.55	1.50	1.41
2	B	502	FMN	C9A-C5A	5.29	1.49	1.41
2	C	502	FMN	C9A-C5A	5.20	1.49	1.41
2	C	502	FMN	C5'-C4'	4.93	1.58	1.51
2	A	502	FMN	C5'-C4'	4.55	1.58	1.51
2	A	502	FMN	C8-C7	-4.35	1.30	1.40
2	D	502	FMN	C4'-C3'	3.89	1.60	1.53
2	D	502	FMN	C8-C7	-3.73	1.31	1.40
2	C	502	FMN	C8-C7	-3.59	1.32	1.40
2	B	502	FMN	C8-C7	-3.47	1.32	1.40
2	A	502	FMN	C4A-N5	3.16	1.37	1.30
2	B	502	FMN	C5'-C4'	3.06	1.56	1.51
2	C	502	FMN	C4A-N5	2.92	1.37	1.30
2	D	502	FMN	C4A-N5	2.85	1.36	1.30
2	A	502	FMN	C4A-C10	2.80	1.52	1.44
2	D	502	FMN	O3'-C3'	2.62	1.49	1.43
2	B	502	FMN	C4A-C10	2.61	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	FMN	C4-N3	-2.56	1.34	1.38
2	D	502	FMN	C4A-C10	2.49	1.51	1.44
2	D	502	FMN	O4'-C4'	2.48	1.48	1.43
2	C	502	FMN	C9A-N10	-2.44	1.36	1.41
2	A	502	FMN	C4-N3	-2.43	1.34	1.38
2	B	502	FMN	C1'-C2'	2.40	1.56	1.52
2	C	502	FMN	P-O2P	-2.39	1.45	1.54
2	A	502	FMN	C4'-C3'	2.38	1.57	1.53
2	C	502	FMN	C4A-C10	2.36	1.51	1.44
2	A	502	FMN	P-O2P	-2.34	1.46	1.54
2	A	502	FMN	C2-N3	-2.28	1.34	1.39
2	B	502	FMN	C4'-C3'	2.28	1.57	1.53
2	B	502	FMN	C4A-N5	2.26	1.35	1.30
2	C	502	FMN	C2-N3	-2.25	1.34	1.39
2	C	502	FMN	C10-N1	2.19	1.37	1.33
2	B	502	FMN	C5A-N5	-2.17	1.35	1.39
2	B	502	FMN	P-O2P	-2.16	1.46	1.54
3	D	503	POP	P1-O3	2.16	1.62	1.54
2	C	502	FMN	C4'-C3'	2.10	1.57	1.53
3	B	503	POP	P1-O3	2.09	1.62	1.54
2	D	502	FMN	C5'-C4'	2.08	1.54	1.51
2	B	502	FMN	C4-N3	-2.02	1.35	1.38
2	C	502	FMN	C1'-C2'	2.02	1.55	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	FMN	O2P-P-O5'	-7.05	88.29	106.67
2	C	502	FMN	C7M-C7-C6	-5.40	110.06	119.57
2	B	502	FMN	C7M-C7-C6	-5.31	110.21	119.57
2	A	502	FMN	C5'-C4'-C3'	5.25	122.11	112.22
2	B	502	FMN	O2P-P-O1P	4.99	130.29	110.83
2	C	502	FMN	C5'-C4'-C3'	4.93	121.51	112.22
2	D	502	FMN	C1'-N10-C9A	4.71	129.79	120.63
2	A	502	FMN	C7M-C7-C6	-4.48	111.68	119.57
2	B	502	FMN	C5A-C9A-N10	4.46	122.00	117.97
2	D	502	FMN	O3P-P-O2P	4.41	124.36	107.80
2	C	502	FMN	C8M-C8-C9	-4.01	112.50	119.57
2	A	502	FMN	C8M-C8-C9	-4.00	112.52	119.57
2	B	502	FMN	C7M-C7-C8	3.94	128.81	120.76
2	B	502	FMN	C8M-C8-C9	-3.94	112.64	119.57
2	D	502	FMN	O3P-P-O5'	-3.92	96.45	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	FMN	O3'-C3'-C4'	3.88	117.76	108.93
2	A	502	FMN	C5A-C9A-N10	3.86	121.46	117.97
2	A	502	FMN	O3'-C3'-C2'	3.86	117.71	108.93
2	B	502	FMN	C4A-C10-N1	-3.83	115.21	124.59
2	D	502	FMN	O4'-C4'-C3'	3.73	117.98	109.25
2	C	502	FMN	C5A-C9A-N10	3.65	121.27	117.97
2	B	502	FMN	C2'-C1'-N10	3.61	127.24	110.20
2	A	502	FMN	C4A-C10-N10	3.57	121.59	116.48
2	D	502	FMN	C4A-C10-N10	3.55	121.56	116.48
2	D	502	FMN	C7M-C7-C6	-3.47	113.46	119.57
2	A	502	FMN	C4A-C10-N1	-3.47	116.09	124.59
2	D	502	FMN	O2-C2-N1	-3.42	116.11	121.80
2	C	502	FMN	C4A-C10-N1	-3.42	116.20	124.59
3	D	503	POP	O3-P1-O2	-3.17	95.93	107.80
2	C	502	FMN	C7M-C7-C8	3.13	127.14	120.76
2	C	502	FMN	O3P-P-O1P	3.10	122.91	110.83
2	D	502	FMN	C4-C4A-N5	3.04	122.41	118.21
2	D	502	FMN	C5A-C9A-N10	3.00	120.68	117.97
2	C	502	FMN	C4A-C10-N10	2.95	120.71	116.48
2	D	502	FMN	O2'-C2'-C3'	2.92	116.08	109.25
3	D	503	POP	O2-P1-O	2.87	114.25	104.64
2	A	502	FMN	C10-C4A-N5	-2.84	119.01	124.81
2	B	502	FMN	C4-N3-C2	-2.82	120.63	125.64
2	A	502	FMN	C4-C4A-N5	2.78	122.05	118.21
2	A	502	FMN	C7M-C7-C8	2.75	126.38	120.76
2	B	502	FMN	C4A-C10-N10	2.74	120.41	116.48
2	C	502	FMN	C4-C4A-N5	2.73	121.97	118.21
2	C	502	FMN	O4'-C4'-C5'	2.72	115.98	109.99
2	A	502	FMN	O3'-C3'-C4'	2.70	115.07	108.93
2	A	502	FMN	C9-C8-C7	2.69	123.63	119.69
2	D	502	FMN	O4-C4-C4A	-2.67	119.49	126.53
3	B	503	POP	O2-P1-O1	2.65	121.18	110.83
2	D	502	FMN	C2'-C1'-N10	2.59	122.46	110.20
2	A	502	FMN	O3P-P-O1P	2.57	120.86	110.83
2	D	502	FMN	C6-C5A-N5	2.51	122.61	118.44
2	D	502	FMN	C8M-C8-C9	-2.50	115.16	119.57
2	D	502	FMN	O3'-C3'-C4'	2.49	114.59	108.93
2	C	502	FMN	C10-C4A-N5	-2.47	119.76	124.81
2	A	502	FMN	O2P-P-O1P	-2.47	101.22	110.83
2	B	502	FMN	C9A-N10-C10	-2.46	117.01	120.75
2	B	502	FMN	C4A-C4-N3	2.39	119.34	113.25
2	A	502	FMN	O2-C2-N1	-2.37	117.87	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	FMN	C9A-N10-C10	-2.33	117.20	120.75
2	A	502	FMN	C6-C5A-N5	2.33	122.31	118.44
2	C	502	FMN	C10-N1-C2	2.33	121.89	116.85
2	B	502	FMN	O5'-P-O1P	-2.31	100.20	106.44
2	D	502	FMN	C10-C4A-N5	-2.28	120.15	124.81
2	C	502	FMN	C9-C8-C7	2.26	123.00	119.69
2	C	502	FMN	O2'-C2'-C3'	-2.24	104.00	109.25
2	B	502	FMN	O3P-P-O5'	2.23	112.49	106.67
2	A	502	FMN	O4'-C4'-C5'	2.23	114.90	109.99
2	D	502	FMN	C1'-C2'-C3'	-2.21	103.68	109.66
2	D	502	FMN	C9A-C5A-N5	-2.19	120.13	122.45
2	C	502	FMN	C4A-C4-N3	2.19	118.82	113.25
2	A	502	FMN	C9A-C5A-N5	-2.17	120.15	122.45
2	D	502	FMN	C4A-C10-N1	-2.15	119.31	124.59
2	D	502	FMN	C4A-C4-N3	2.15	118.72	113.25
2	D	502	FMN	C4'-C3'-C2'	2.15	117.14	113.57
2	B	502	FMN	O2'-C2'-C1'	2.14	118.98	110.20
3	B	503	POP	O6-P2-O	2.12	111.75	104.64
2	B	502	FMN	O4'-C4'-C3'	2.11	114.20	109.25
2	C	502	FMN	C6-C7-C8	2.11	122.78	119.69
2	B	502	FMN	O4-C4-C4A	-2.10	120.99	126.53
2	C	502	FMN	C6-C5A-N5	2.07	121.88	118.44
2	B	502	FMN	N3-C2-N1	2.07	123.90	119.50
3	D	503	POP	O2-P1-O1	2.04	118.78	110.83
2	B	502	FMN	C9-C8-C7	2.04	122.68	119.69
2	B	502	FMN	C9A-C5A-N5	-2.03	120.30	122.45

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	FMN	O3'-C3'-C4'-C5'
2	A	502	FMN	C3'-C4'-C5'-O5'
2	A	502	FMN	O4'-C4'-C5'-O5'
2	A	502	FMN	C4'-C5'-O5'-P
2	A	502	FMN	C5'-O5'-P-O1P
2	A	502	FMN	C5'-O5'-P-O2P
2	A	502	FMN	C5'-O5'-P-O3P
2	B	502	FMN	C1'-C2'-C3'-C4'
2	B	502	FMN	C3'-C4'-C5'-O5'
2	B	502	FMN	C4'-C5'-O5'-P
2	C	502	FMN	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
2	C	502	FMN	N10-C1'-C2'-C3'
2	C	502	FMN	C1'-C2'-C3'-C4'
2	C	502	FMN	C3'-C4'-C5'-O5'
2	C	502	FMN	O4'-C4'-C5'-O5'
2	C	502	FMN	C4'-C5'-O5'-P
2	C	502	FMN	C5'-O5'-P-O1P
2	C	502	FMN	C5'-O5'-P-O2P
2	C	502	FMN	C5'-O5'-P-O3P
2	D	502	FMN	C2'-C1'-N10-C10
2	D	502	FMN	O3'-C3'-C4'-C5'
2	D	502	FMN	C5'-O5'-P-O2P
2	D	502	FMN	C5'-O5'-P-O3P
3	B	503	POP	P1-O-P2-O6
3	D	503	POP	P2-O-P1-O3
3	D	503	POP	P1-O-P2-O6
2	A	502	FMN	C2'-C3'-C4'-C5'
2	B	502	FMN	O2'-C2'-C3'-C4'
2	D	502	FMN	C2'-C3'-C4'-C5'
2	B	502	FMN	O2'-C2'-C3'-O3'
2	D	502	FMN	O3'-C3'-C4'-O4'
2	C	502	FMN	O2'-C2'-C3'-C4'
2	A	502	FMN	O3'-C3'-C4'-O4'
2	A	502	FMN	O2'-C2'-C3'-C4'
2	D	502	FMN	C5'-O5'-P-O1P
2	D	502	FMN	O2'-C2'-C3'-C4'
2	B	502	FMN	C2'-C3'-C4'-O4'
2	B	502	FMN	N10-C1'-C2'-O2'
2	C	502	FMN	C2'-C1'-N10-C10
2	D	502	FMN	C4'-C5'-O5'-P
2	C	502	FMN	O3'-C3'-C4'-C5'
2	B	502	FMN	C1'-C2'-C3'-O3'
3	D	503	POP	P1-O-P2-O4
3	D	503	POP	P2-O-P1-O2
3	D	503	POP	P1-O-P2-O5
2	D	502	FMN	N10-C1'-C2'-O2'
2	C	502	FMN	C2'-C3'-C4'-C5'

There are no ring outliers.

6 monomers are involved in 49 short contacts:

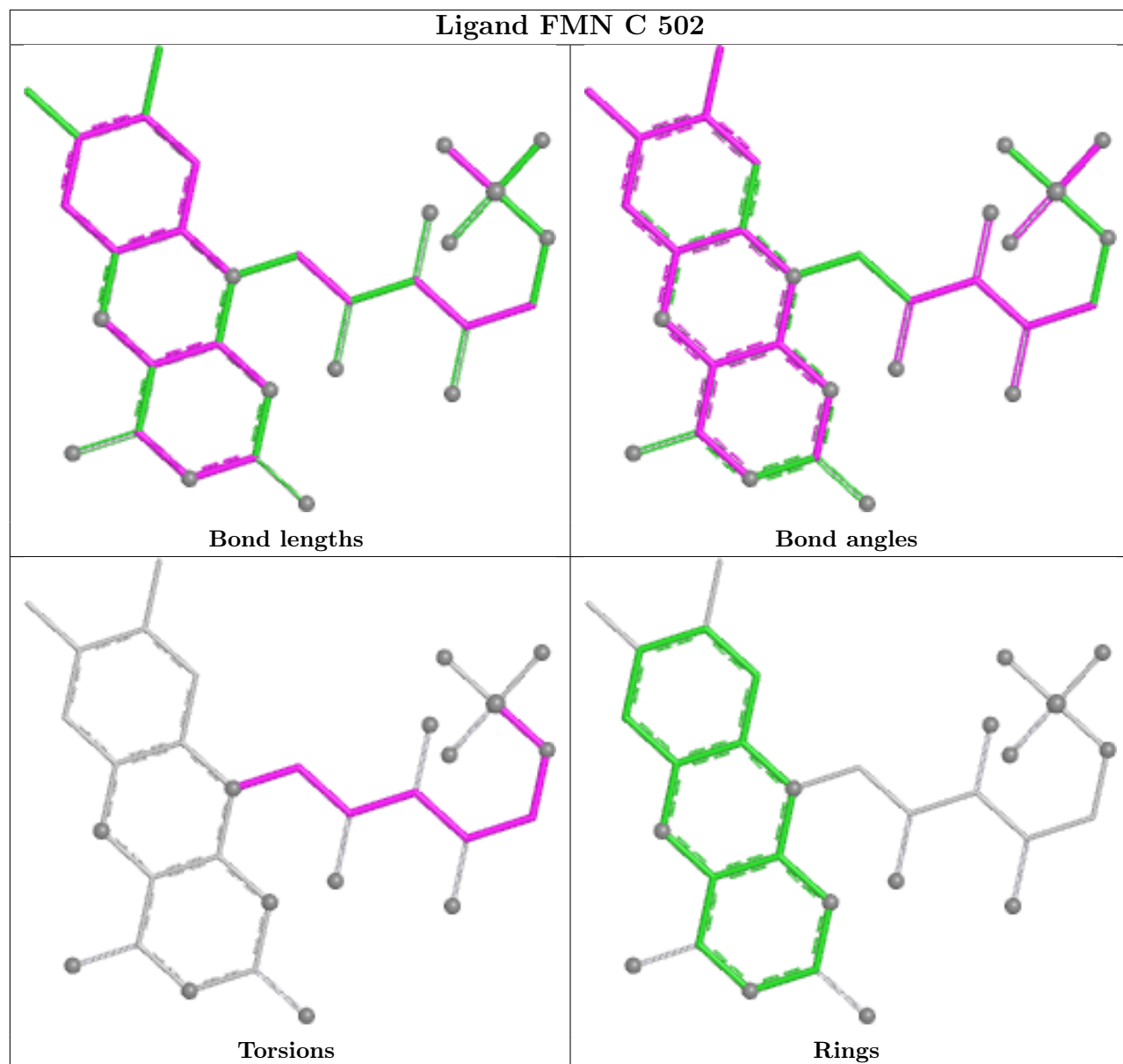
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	FMN	13	0

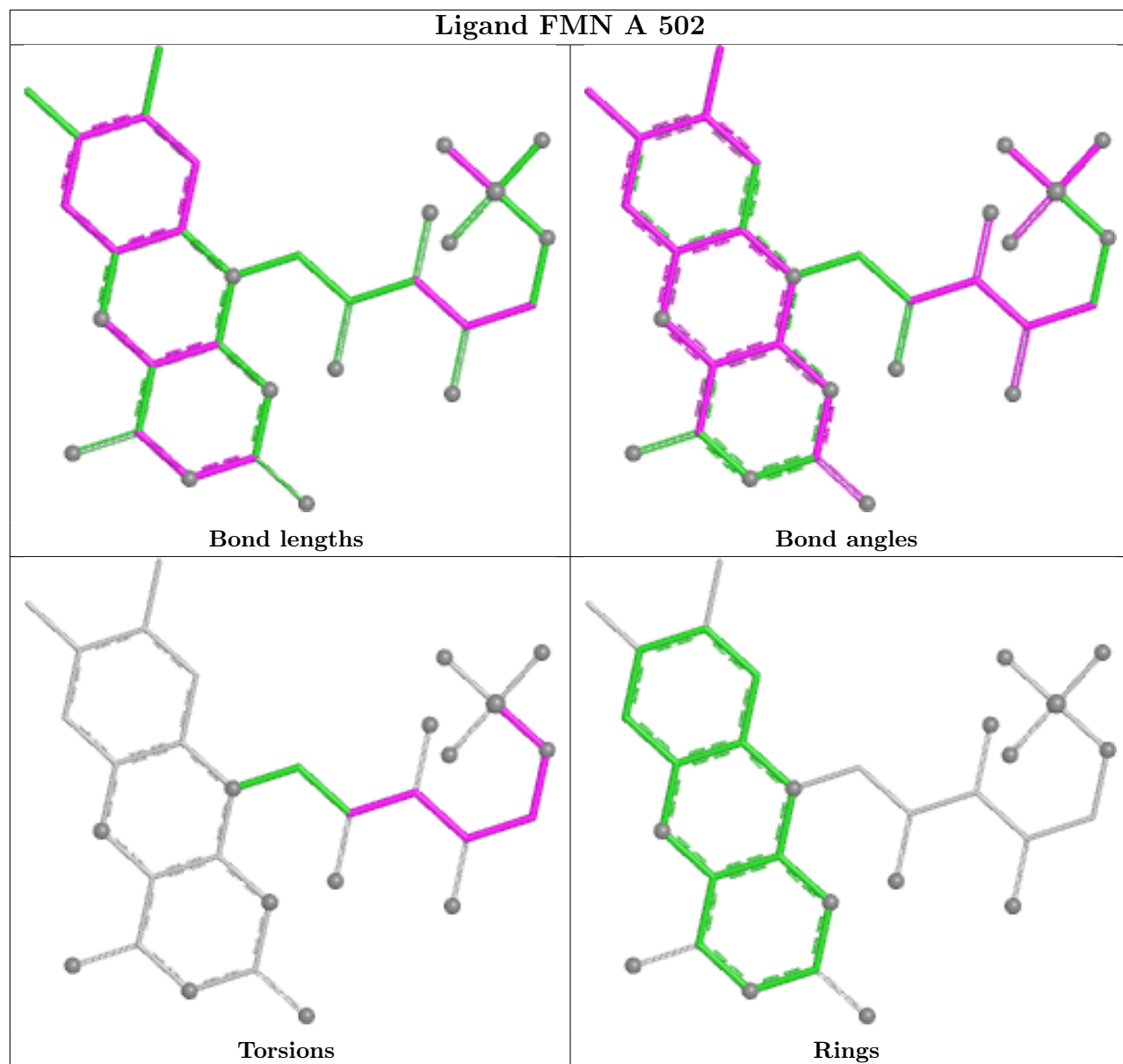
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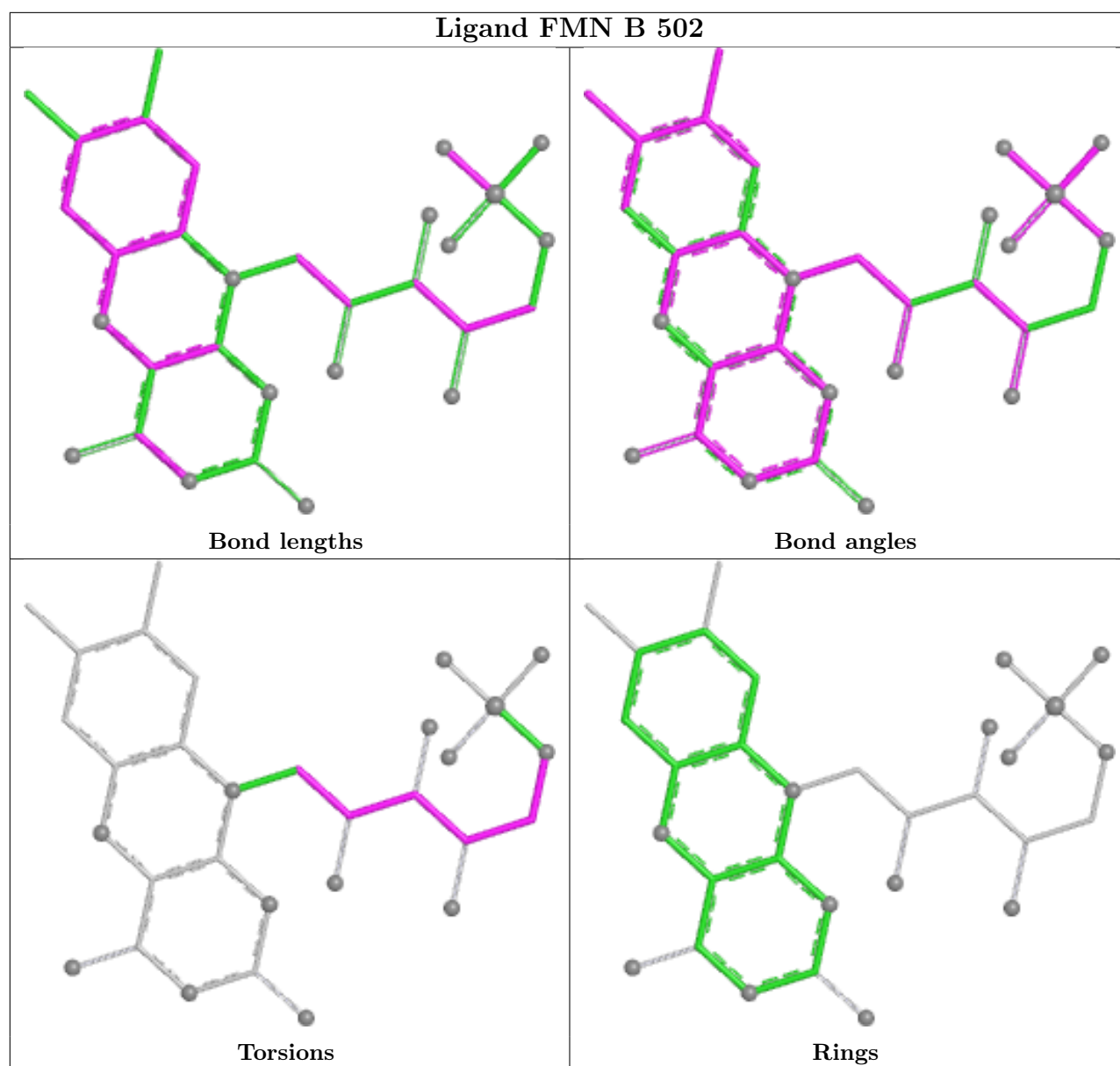
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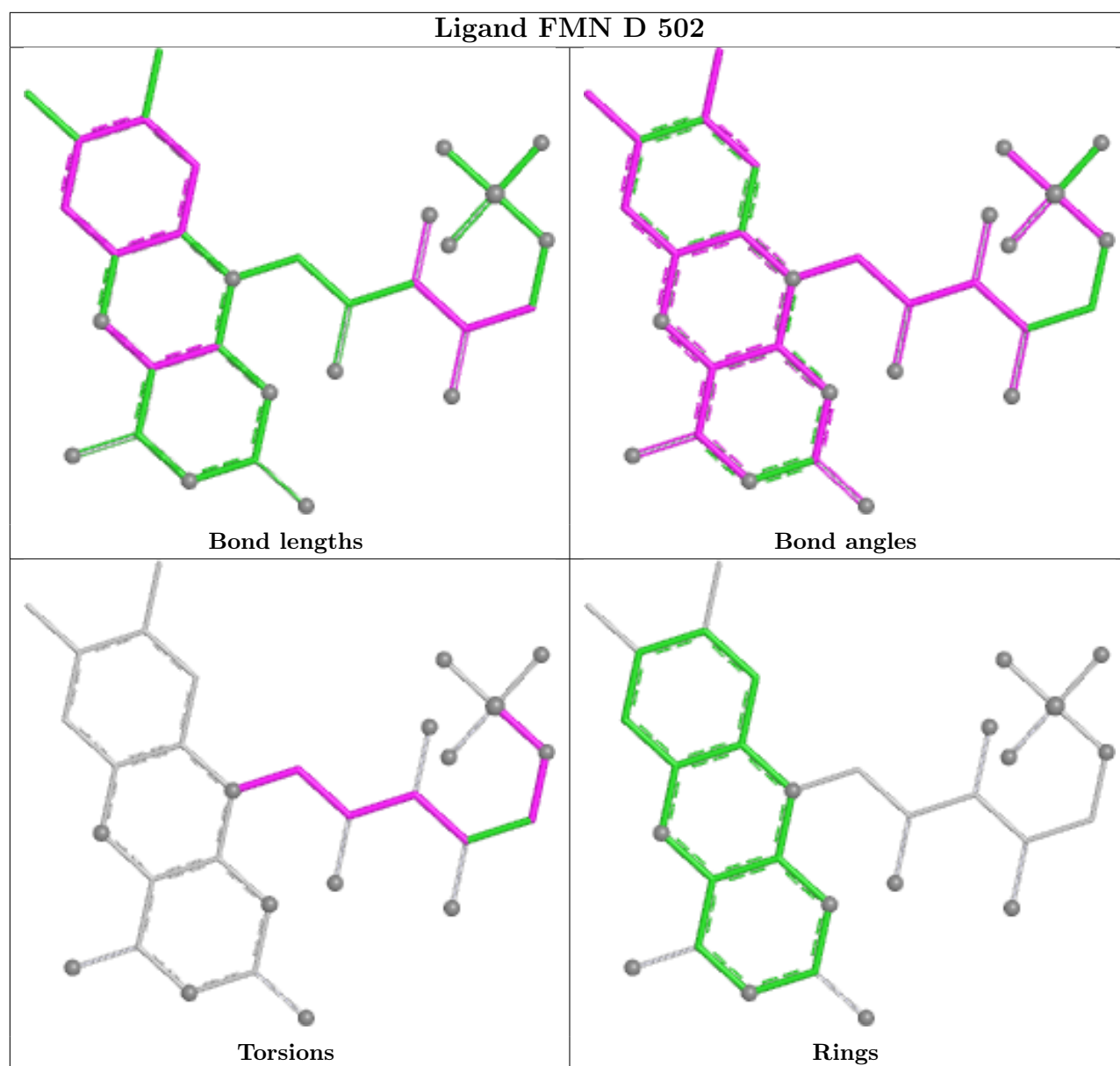
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	FMN	13	0
3	D	503	POP	1	0
3	B	503	POP	1	0
2	B	502	FMN	11	0
2	D	502	FMN	10	0

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	318/332 (95%)	-1.76	0 100 100	2, 9, 47, 81	0
1	B	318/332 (95%)	-1.75	0 100 100	2, 16, 44, 68	0
1	C	316/332 (95%)	-1.78	0 100 100	2, 9, 42, 85	0
1	D	313/332 (94%)	-1.77	0 100 100	2, 15, 40, 53	0
All	All	1265/1328 (95%)	-1.77	0 100 100	2, 12, 42, 85	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	POP	B	503	9/9	0.99	0.09	82,84,91,93	0
3	POP	D	503	9/9	0.99	0.07	81,83,93,93	0
2	FMN	C	502	31/31	1.00	0.03	9,70,71,71	0
2	FMN	D	502	31/31	1.00	0.04	17,70,70,70	0

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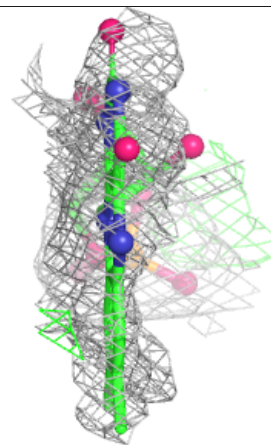
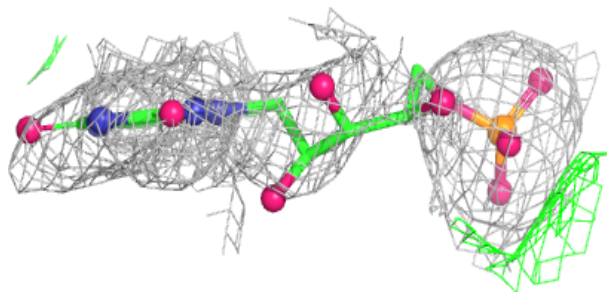
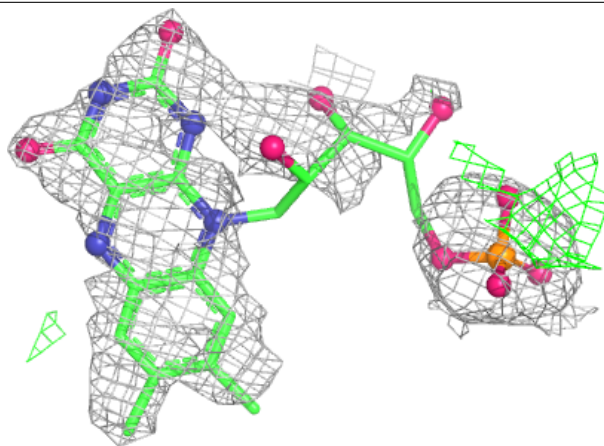
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	A	502	31/31	1.00	0.03	8,65,66,66	0
2	FMN	B	502	31/31	1.00	0.03	2,59,60,60	0

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.

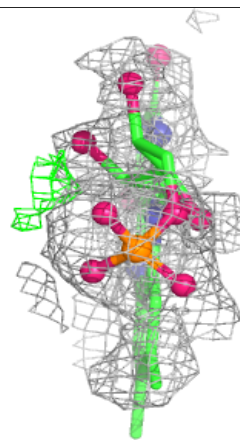
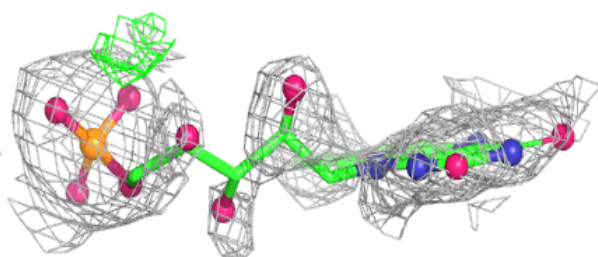
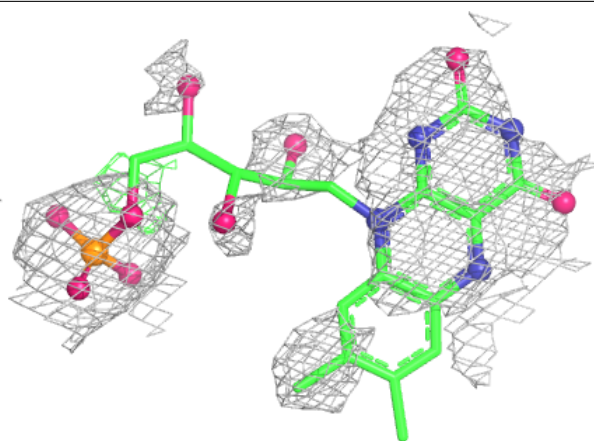
Electron density around FMN C 502:

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



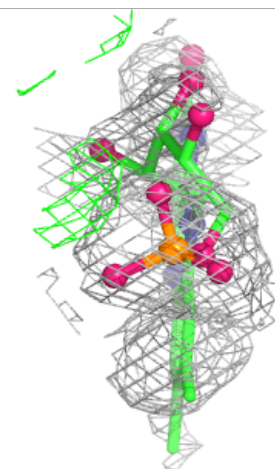
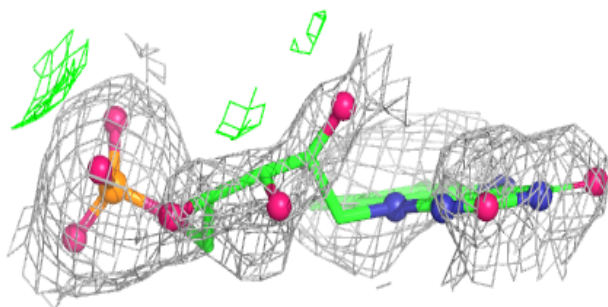
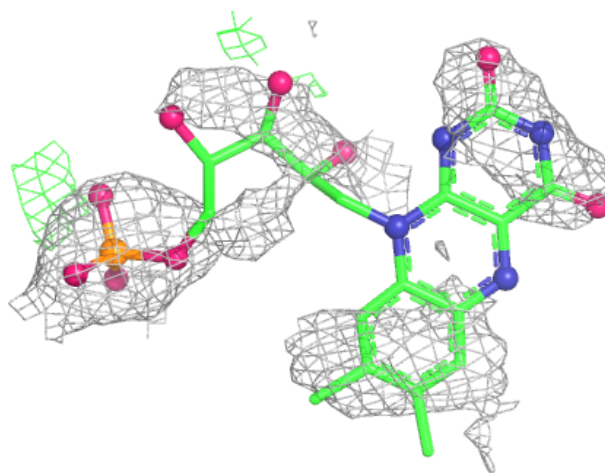
Electron density around FMN D 502:

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



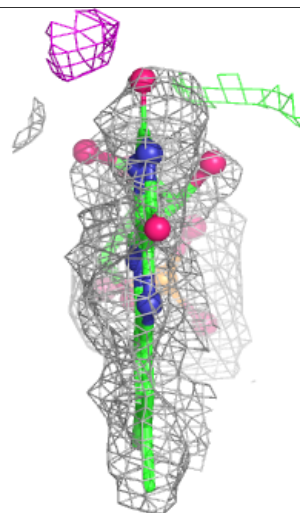
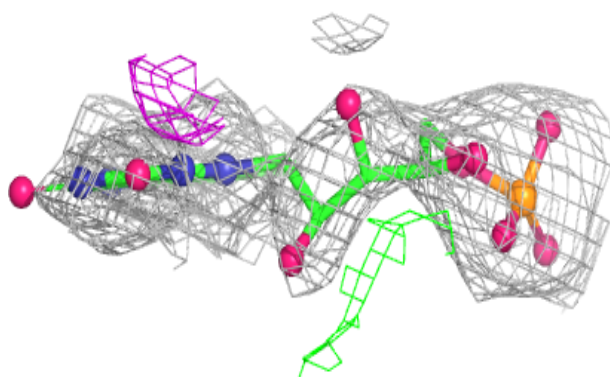
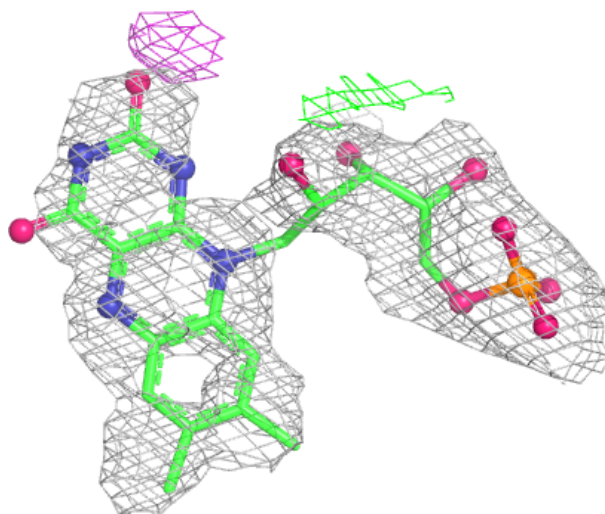
Electron density around FMN A 502:

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



Electron density around FMN B 502:

$2mF_o-DF_c$ (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.