



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:39 PM EDT

PDB ID : 3DH7
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

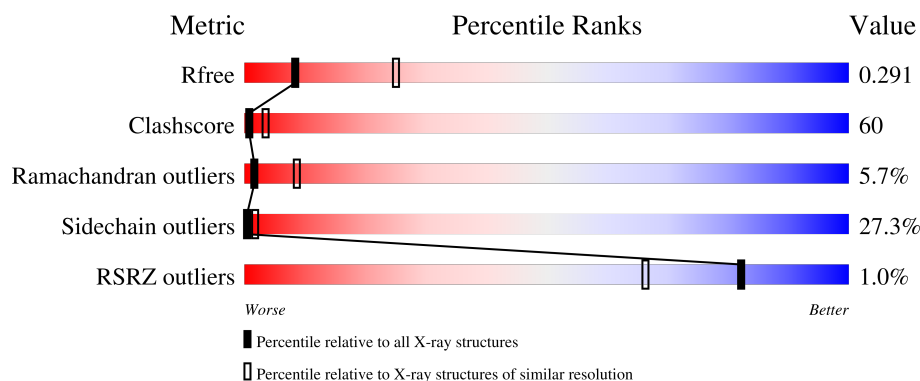
1 Overall quality at a glance

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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (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	<div> <div>27%</div> <div>43%</div> <div>19%</div> <div>7%</div> <div>.</div> </div>
1	B	332	<div> <div>20%</div> <div>51%</div> <div>19%</div> <div>5%</div> <div>.</div> </div>
1	C	332	<div> <div>2%</div> <div>28%</div> <div>42%</div> <div>20%</div> <div>5%</div> <div>5%</div> </div>
1	D	332	<div> <div>25%</div> <div>45%</div> <div>19%</div> <div>5%</div> <div>6%</div> </div>

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](#)

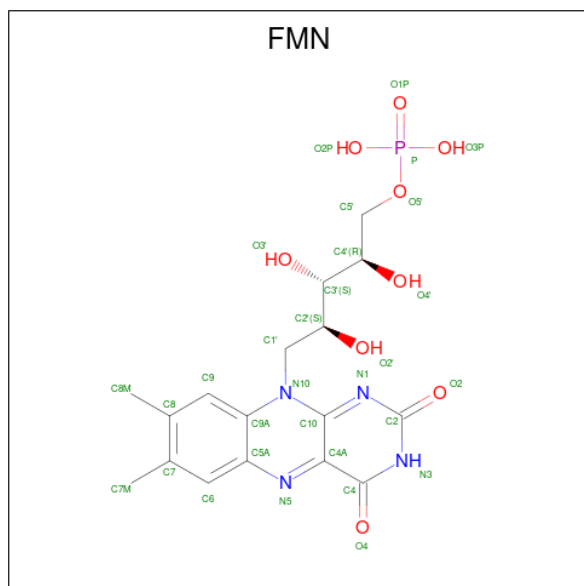
There are 4 unique types of molecules in this entry. The entry contains 9991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



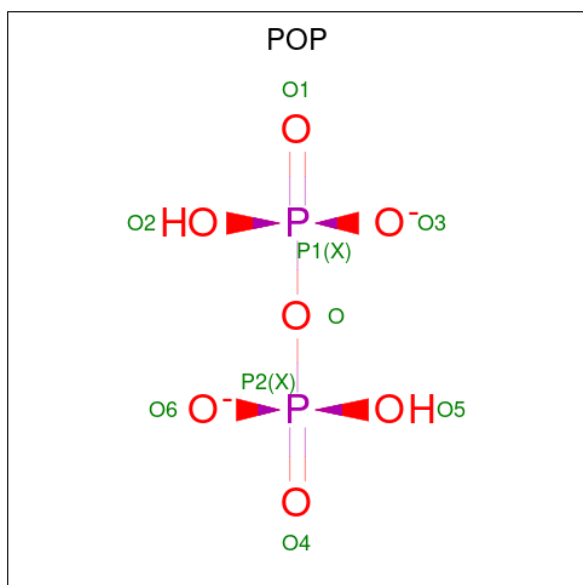
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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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- (three-letter code: 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		

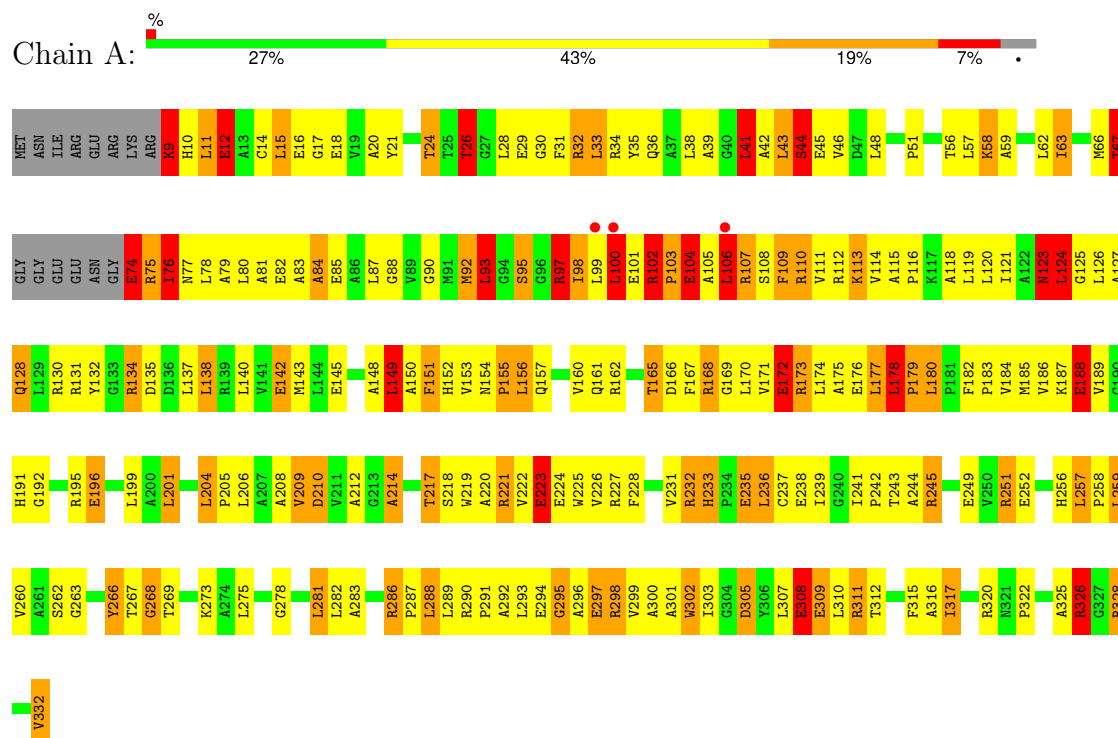
- Molecule 4 is water.

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		

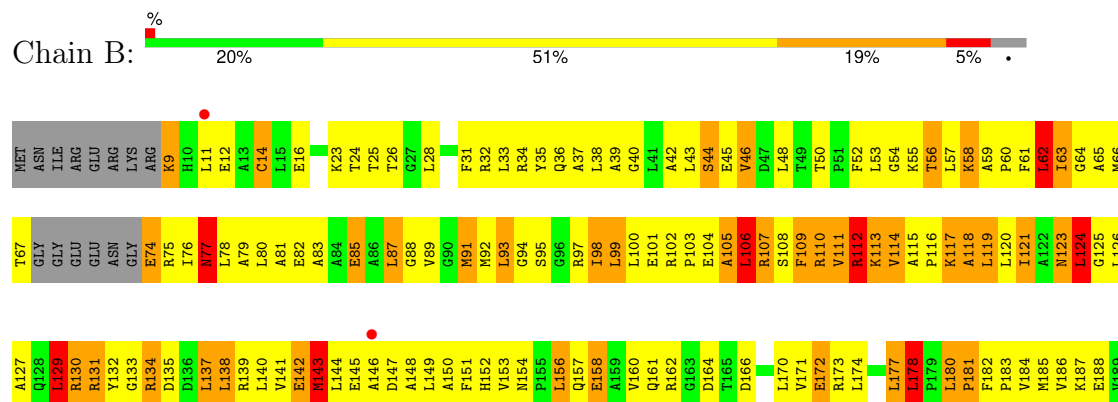
3 Residue-property plots

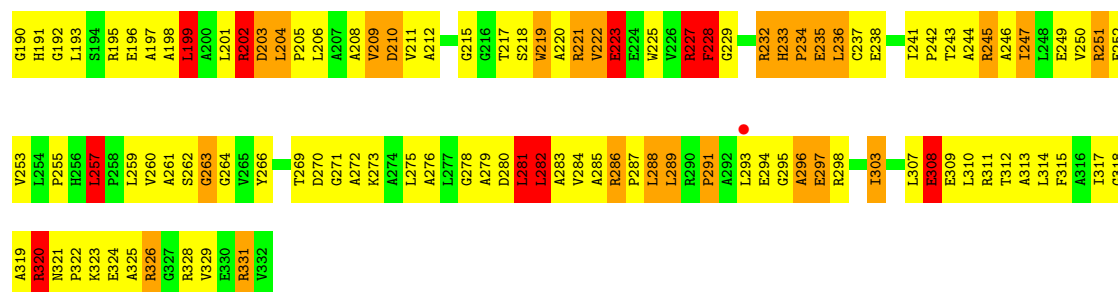
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

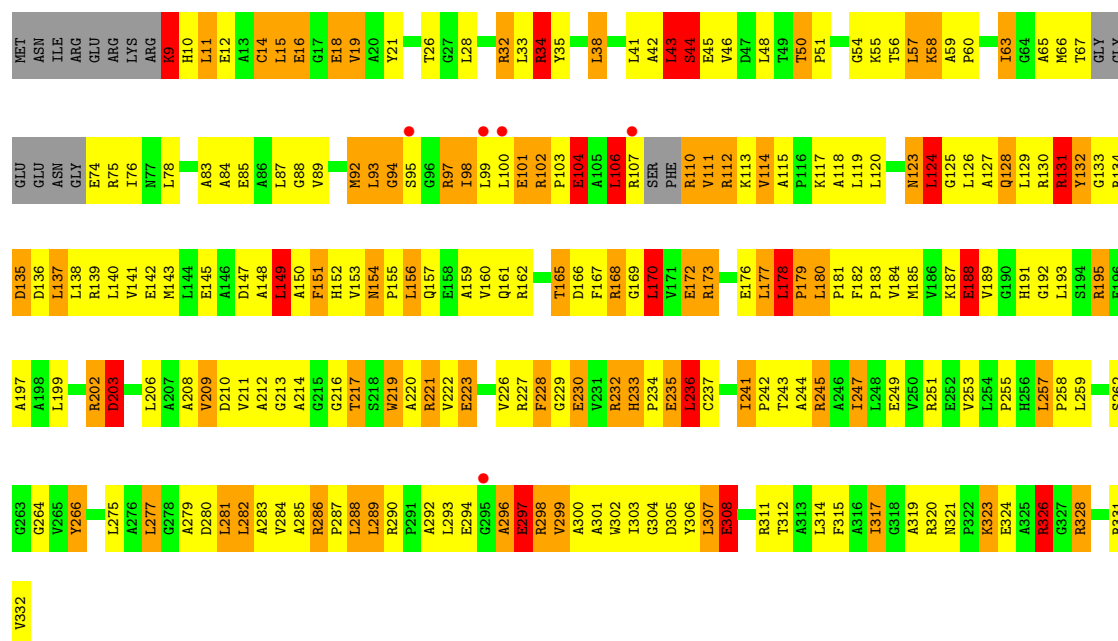


• Molecule 1: Isopentenyl-diphosphate delta-isomerase

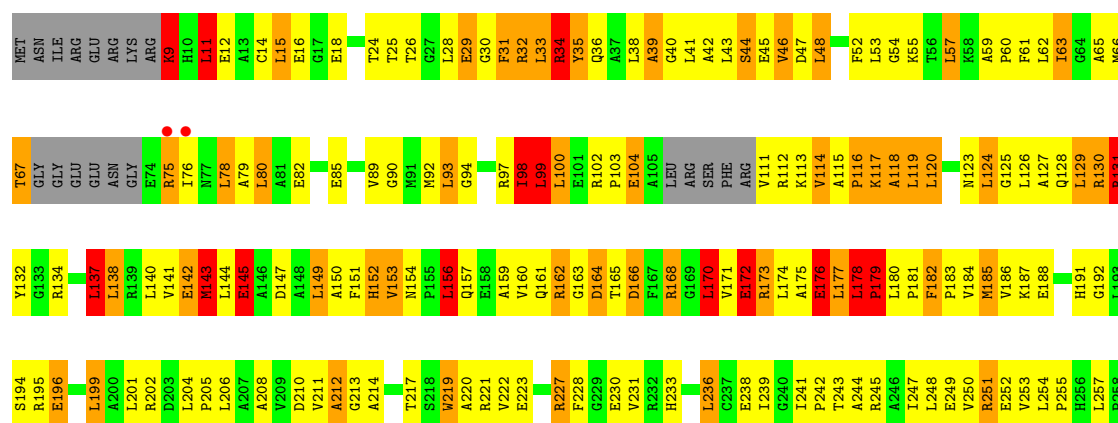




• Molecule 1: Isopentenyl-diphosphate delta-isomerase



• Molecule 1: Isopentenyl-diphosphate delta-isomerase





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 (5.06%)	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)	0.33 , 0.8	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	0.88	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: FMN, POP

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	1.58	32/2457 (1.3%)	1.54	34/3326 (1.0%)
1	B	1.47	22/2462 (0.9%)	1.48	29/3334 (0.9%)
1	C	1.50	17/2443 (0.7%)	1.52	39/3307 (1.2%)
1	D	1.54	26/2408 (1.1%)	1.51	34/3260 (1.0%)
All	All	1.52	97/9770 (1.0%)	1.51	136/13227 (1.0%)

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 (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	35	TYR	C-O	15.71	1.53	1.23
1	A	326	ARG	CG-CD	11.13	1.79	1.51
1	C	326	ARG	CG-CD	10.35	1.77	1.51
1	D	44	SER	CA-CB	8.92	1.66	1.52
1	A	188	GLU	CD-OE2	8.72	1.35	1.25
1	C	44	SER	CB-OG	8.70	1.53	1.42
1	C	308	GLU	CG-CD	8.40	1.64	1.51
1	C	172	GLU	CG-CD	8.33	1.64	1.51
1	C	266	TYR	CD2-CE2	-8.27	1.26	1.39
1	A	58	LYS	CD-CE	8.17	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	GLU	CG-CD	8.06	1.64	1.51
1	D	172	GLU	CB-CG	7.81	1.67	1.52
1	A	209	VAL	CB-CG1	-7.77	1.36	1.52
1	B	297	GLU	CG-CD	7.73	1.63	1.51
1	A	155	PRO	N-CD	7.54	1.58	1.47
1	B	44	SER	CA-CB	7.50	1.64	1.52
1	A	143	MET	CG-SD	7.38	2.00	1.81
1	D	176	GLU	CG-CD	7.35	1.62	1.51
1	D	308	GLU	CG-CD	6.97	1.62	1.51
1	A	326	ARG	CB-CG	6.86	1.71	1.52
1	D	34	ARG	CG-CD	6.86	1.69	1.51
1	A	266	TYR	CD2-CE2	-6.82	1.29	1.39
1	D	164	ASP	CB-CG	6.72	1.65	1.51
1	B	171	VAL	CB-CG2	6.72	1.67	1.52
1	B	308	GLU	CG-CD	6.69	1.61	1.51
1	D	33	LEU	C-N	6.68	1.49	1.34
1	A	74	GLU	CG-CD	6.68	1.61	1.51
1	D	44	SER	CB-OG	6.67	1.50	1.42
1	B	308	GLU	CD-OE1	6.66	1.32	1.25
1	B	172	GLU	CG-CD	6.64	1.61	1.51
1	A	188	GLU	CB-CG	-6.59	1.39	1.52
1	A	143	MET	CB-CG	6.53	1.72	1.51
1	A	214	ALA	CA-CB	-6.52	1.38	1.52
1	D	308	GLU	CD-OE1	6.50	1.32	1.25
1	C	14	CYS	CB-SG	-6.49	1.71	1.82
1	C	323	LYS	CD-CE	6.46	1.67	1.51
1	D	176	GLU	CB-CG	6.39	1.64	1.52
1	A	74	GLU	CB-CG	6.37	1.64	1.52
1	D	39	ALA	CA-CB	6.33	1.65	1.52
1	A	326	ARG	NE-CZ	6.28	1.41	1.33
1	B	172	GLU	CB-CG	6.26	1.64	1.52
1	A	44	SER	CB-OG	6.20	1.50	1.42
1	B	297	GLU	CB-CG	6.20	1.64	1.52
1	D	31	PHE	CE1-CZ	6.08	1.49	1.37
1	B	143	MET	CG-SD	6.07	1.97	1.81
1	D	143	MET	CB-CG	6.06	1.70	1.51
1	C	308	GLU	CD-OE1	6.04	1.32	1.25
1	A	326	ARG	CD-NE	6.00	1.56	1.46
1	A	82	GLU	CD-OE2	5.95	1.32	1.25
1	D	313	ALA	CA-CB	-5.93	1.40	1.52
1	C	151	PHE	CB-CG	-5.85	1.41	1.51
1	A	182	PHE	CE2-CZ	5.83	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	GLU	CG-CD	5.82	1.60	1.51
1	A	286	ARG	CG-CD	5.79	1.66	1.51
1	D	297	GLU	CG-CD	5.79	1.60	1.51
1	A	76	ILE	CA-CB	5.75	1.68	1.54
1	B	235	GLU	CD-OE1	5.75	1.31	1.25
1	C	213	GLY	C-O	5.73	1.32	1.23
1	A	67	THR	CA-CB	5.70	1.68	1.53
1	A	172	GLU	CG-CD	5.65	1.60	1.51
1	B	44	SER	CB-OG	5.64	1.49	1.42
1	A	266	TYR	CG-CD1	-5.62	1.31	1.39
1	A	182	PHE	CD1-CE1	5.61	1.50	1.39
1	C	323	LYS	CE-NZ	5.61	1.63	1.49
1	C	326	ARG	CD-NE	5.60	1.55	1.46
1	A	176	GLU	CG-CD	5.57	1.60	1.51
1	B	85	GLU	CG-CD	5.57	1.60	1.51
1	D	309	GLU	CG-CD	5.57	1.60	1.51
1	D	32	ARG	CZ-NH1	5.54	1.40	1.33
1	B	143	MET	CB-CG	5.52	1.69	1.51
1	A	302	TRP	CB-CG	-5.51	1.40	1.50
1	D	34	ARG	CB-CG	5.50	1.67	1.52
1	D	143	MET	CG-SD	5.47	1.95	1.81
1	D	324	GLU	CD-OE1	5.43	1.31	1.25
1	B	12	GLU	CG-CD	5.41	1.60	1.51
1	A	151	PHE	CE2-CZ	5.40	1.47	1.37
1	B	249	GLU	CG-CD	-5.38	1.43	1.51
1	D	214	ALA	CA-CB	-5.38	1.41	1.52
1	C	16	GLU	CG-CD	5.38	1.60	1.51
1	B	14	CYS	CB-SG	-5.35	1.73	1.81
1	A	29	GLU	CD-OE2	5.33	1.31	1.25
1	A	223	GLU	CG-CD	5.32	1.59	1.51
1	B	58	LYS	CE-NZ	5.25	1.62	1.49
1	B	209	VAL	CB-CG2	-5.25	1.41	1.52
1	D	14	CYS	CB-SG	-5.22	1.73	1.81
1	B	313	ALA	CA-CB	-5.22	1.41	1.52
1	C	331	ARG	CB-CG	5.21	1.66	1.52
1	C	331	ARG	CG-CD	5.18	1.65	1.51
1	B	246	ALA	CA-CB	-5.16	1.41	1.52
1	B	23	LYS	CD-CE	5.14	1.64	1.51
1	B	142	GLU	CG-CD	5.09	1.59	1.51
1	A	58	LYS	CE-NZ	5.08	1.61	1.49
1	D	179	PRO	CB-CG	5.06	1.75	1.50
1	D	104	GLU	CG-CD	5.04	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	SER	CA-CB	5.02	1.60	1.52
1	C	326	ARG	NE-CZ	5.02	1.39	1.33
1	C	266	TYR	CG-CD2	-5.00	1.32	1.39

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	ARG	CG-CD-NE	-10.94	88.83	111.80
1	A	326	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	C	241	ILE	CG1-CB-CG2	-9.74	89.97	111.40
1	A	106	LEU	CA-CB-CG	9.46	137.06	115.30
1	C	326	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	281	LEU	CA-CB-CG	9.17	136.39	115.30
1	D	281	LEU	CA-CB-CG	8.89	135.76	115.30
1	A	257	LEU	CB-CG-CD2	-8.63	96.33	111.00
1	B	129	LEU	CB-CG-CD1	-8.30	96.88	111.00
1	B	106	LEU	CA-CB-CG	8.10	133.94	115.30
1	D	34	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	D	32	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	259	LEU	CB-CG-CD1	-7.91	97.55	111.00
1	D	131	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	289	LEU	CB-CG-CD2	-7.87	97.61	111.00
1	A	177	LEU	CB-CG-CD2	-7.72	97.88	111.00
1	A	32	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	221	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	D	170	LEU	CA-CB-CG	-7.54	97.96	115.30
1	B	199	LEU	CA-CB-CG	-7.49	98.06	115.30
1	C	286	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	280	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	D	282	LEU	CA-CB-CG	7.32	132.14	115.30
1	A	149	LEU	CA-CB-CG	7.25	131.99	115.30
1	D	119	LEU	CB-CG-CD1	-7.04	99.04	111.00
1	C	221	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	75	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	C	57	LEU	CB-CG-CD2	-6.75	99.53	111.00
1	D	311	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	C	177	LEU	CB-CA-C	-6.67	97.53	110.20
1	D	289	LEU	CB-CG-CD2	-6.66	99.67	111.00
1	B	180	LEU	CB-CG-CD1	-6.65	99.69	111.00
1	C	178	LEU	CB-CG-CD2	6.57	122.16	111.00
1	C	188	GLU	CB-CA-C	6.55	123.50	110.40
1	C	178	LEU	N-CA-CB	6.49	123.38	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	143	MET	CB-CG-SD	6.46	131.78	112.40
1	C	170	LEU	CB-CG-CD2	-6.43	100.06	111.00
1	C	236	LEU	CA-CB-CG	6.42	130.08	115.30
1	B	221	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	259	LEU	CB-CA-C	-6.38	98.08	110.20
1	D	166	ASP	CB-CG-OD2	6.37	124.04	118.30
1	C	326	ARG	CG-CD-NE	6.37	125.17	111.80
1	C	170	LEU	CA-CB-CG	-6.36	100.67	115.30
1	D	138	LEU	CB-CG-CD1	6.31	121.73	111.00
1	B	87	LEU	CA-CB-CG	-6.30	100.81	115.30
1	A	282	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	282	LEU	CA-CB-CG	6.27	129.72	115.30
1	A	41	LEU	CB-CG-CD2	-6.24	100.39	111.00
1	C	97	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	119	LEU	CB-CG-CD2	6.23	121.60	111.00
1	C	32	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	326	ARG	NH1-CZ-NH2	-6.22	112.56	119.40
1	A	103	PRO	N-CA-CB	6.17	110.71	103.30
1	C	124	LEU	C-N-CA	-6.16	109.37	122.30
1	A	124	LEU	C-N-CA	-6.13	109.43	122.30
1	A	100	LEU	CA-CB-CG	6.13	129.40	115.30
1	B	280	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	280	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	305	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	155	PRO	N-CD-CG	-6.02	94.16	103.20
1	C	281	LEU	CB-CG-CD1	-5.99	100.82	111.00
1	A	286	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	C	257	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	C	106	LEU	CA-CB-CG	5.94	128.96	115.30
1	C	63	ILE	CG1-CB-CG2	-5.92	98.38	111.40
1	D	326	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	34	ARG	CG-CD-NE	-5.92	99.38	111.80
1	C	177	LEU	CB-CG-CD1	-5.86	101.03	111.00
1	D	280	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	C	137	LEU	CA-CB-CG	5.85	128.75	115.30
1	C	149	LEU	CA-CB-CG	5.84	128.72	115.30
1	C	38	LEU	CB-CG-CD1	-5.83	101.10	111.00
1	A	63	ILE	N-CA-C	-5.80	95.34	111.00
1	A	177	LEU	CA-CB-CG	5.78	128.60	115.30
1	D	119	LEU	CB-CG-CD2	5.76	120.80	111.00
1	C	219	TRP	CA-CB-CG	-5.74	102.79	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	LEU	CB-CG-CD2	5.74	120.75	111.00
1	C	34	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	178	LEU	N-CA-C	5.67	126.32	111.00
1	D	137	LEU	CB-CG-CD1	5.66	120.61	111.00
1	C	54	GLY	N-CA-C	5.65	127.22	113.10
1	B	257	LEU	CA-CB-CG	5.64	128.26	115.30
1	A	298	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	289	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	C	14	CYS	CA-CB-SG	-5.56	103.99	114.00
1	C	328	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	166	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	130	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	295	GLY	N-CA-C	5.39	126.58	113.10
1	A	57	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	D	33	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	B	143	MET	CB-CG-SD	5.36	128.48	112.40
1	B	177	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	143	MET	CG-SD-CE	5.36	108.77	100.20
1	B	124	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	320	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	209	VAL	CB-CA-C	-5.32	101.29	111.40
1	B	219	TRP	CA-CB-CG	-5.31	103.60	113.70
1	C	132	TYR	CA-CB-CG	-5.30	103.32	113.40
1	C	253	VAL	CB-CA-C	-5.30	101.33	111.40
1	D	35	TYR	CB-CG-CD1	5.29	124.17	121.00
1	B	178	LEU	N-CA-CB	5.28	120.97	110.40
1	A	332	VAL	CB-CA-C	-5.28	101.37	111.40
1	B	247	ILE	CG1-CB-CG2	5.28	123.01	111.40
1	D	44	SER	N-CA-CB	5.28	118.42	110.50
1	C	326	ARG	CD-NE-CZ	5.26	130.96	123.60
1	B	143	MET	CA-CB-CG	5.25	122.22	113.30
1	A	33	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	41	LEU	CB-CA-C	5.24	120.15	110.20
1	A	309	GLU	N-CA-CB	5.23	120.02	110.60
1	C	277	LEU	CA-CB-CG	-5.23	103.27	115.30
1	D	48	LEU	CB-CG-CD2	-5.22	102.13	111.00
1	C	209	VAL	CB-CA-C	-5.19	101.53	111.40
1	D	47	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	140	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	A	282	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	D	307	LEU	CA-CB-CG	-5.15	103.45	115.30
1	D	219	TRP	CA-CB-CG	-5.15	103.92	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	LEU	CB-CG-CD1	-5.14	102.25	111.00
1	D	293	LEU	CB-CG-CD2	5.13	119.72	111.00
1	B	204	LEU	CA-CB-CG	-5.12	103.52	115.30
1	B	228	PHE	CB-CA-C	-5.11	100.18	110.40
1	B	263	GLY	N-CA-C	-5.10	100.35	113.10
1	B	131	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	93	LEU	N-CA-C	-5.05	97.36	111.00
1	D	99	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	297	GLU	CB-CA-C	5.04	120.49	110.40
1	A	201	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	D	80	LEU	CB-CG-CD2	5.04	119.57	111.00
1	D	156	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	A	305	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	100	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	A	311	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	85	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	D	248	LEU	CB-CG-CD1	-5.00	102.49	111.00

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
1	B	62	LEU	Peptide
1	C	104	GLU	Peptide
1	C	178	LEU	Peptide
1	C	203	ASP	Peptide

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Mol	Chain	Res	Type	Group
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	314	1
1	B	2423	0	2515	357	1
1	C	2406	0	2500	283	0
1	D	2372	0	2450	292	0
2	A	31	0	19	13	0
2	B	31	0	19	12	0
2	C	31	0	19	14	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	1192	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 60.

All (1192) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:80:LEU:HB3	1:B:91:MET:HE3	1.53	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
1:A:165:THR:CG2	1:D:43:LEU:HB3	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:PHE:HA	1:C:170:LEU:HD12	1.63	0.81
1:A:332:VAL:HG13	1:A:332:VAL:O	1.80	0.80
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: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:41:LEU:HD12	1:A:41:LEU:C	2.01	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:O	1:C:110:ARG:HB2	1.86	0.75
1:B:80:LEU:HB2	1:B:91:MET:HE1	1.69	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:C:41:LEU:C	1:C:41:LEU:HD12	2.07	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:C:296:ALA:O	1:C:297:GLU:C	2.27	0.73
1:D:65:ALA:O	1:D:66:MET:HG3	1.88	0.73
1:D:128:GLN:HA	1:D:128:GLN:NE2	2.02	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:LEU:O	1:A:179:PRO:C	2.26	0.71
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:188:GLU:CD	1:A:189:VAL:H	1.98	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:A:210:ASP:OD1	1:A:210:ASP:C	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:289:LEU:HD22	2:A:502:FMN:HM71	1.78	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:178:LEU:O	1:C:179:PRO:C	2.34	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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:172:GLU:CD	1:D:172:GLU:H	2.00	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:55:LYS:HE3	1:C:147:ASP:CG	2.22	0.60
1:C:59:ALA:CB	1:C:307:LEU:HD22	2.32	0.60
1:A:126:LEU:C	1:A:170:LEU:HD23	2.22	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
1:B:276:ALA:HB1	1:B:329:VAL:HB	1.82	0.60
1:C:95:SER:C	1:C:97:ARG:H	2.05	0.60
1:C:161:GLN:O	1:C:161:GLN:HG3	2.00	0.60
1:C:210:ASP:OD1	1:C:210:ASP:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:188:GLU:CD	1:C:189:VAL:H	2.05	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:A:41:LEU:C	1:A:41:LEU:CD1	2.71	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: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: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:B:162:ARG:HG2	1:B:227:ARG:HH11	1.64	0.58
1:D:161:GLN:O	1:D:162:ARG:C	2.40	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:LYS:HZ3	1:B:9:LYS:N	2.02	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: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:142:GLU:O	1:D:143:MET:C	2.43	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: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
1:C:123:ASN:HB2	1:C:150:ALA:HB3	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:B:28:LEU:HD13	1:B:270:ASP:HB3	1.89	0.55
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:C:133:GLY:O	1:C:134:ARG:C	2.46	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:203:ASP:O	1:B:204:LEU:C	2.45	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:228:PHE:C	1:D:230:GLU:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:14:CYS:SG	2:C:502:FMN:HM82	2.48	0.54
1:C:106:LEU:O	1:C:110:ARG:CB	2.55	0.54
1:A:289:LEU:CD2	2:A:502:FMN:HM71	2.38	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: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:95:SER:C	1:A:97:ARG:H	2.12	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:C:156:LEU:O	1:C:157:GLN:C	2.43	0.53
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: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:60:PRO:C	1:B:281:LEU:HD13	2.30	0.52
1:B:321:ASN:HB2	1:B:322:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:259:LEU:N	1:A:259:LEU:HD23	2.24	0.51
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:A:172:GLU:N	1:A:172:GLU:CD	2.64	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: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: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:285:ALA:C	1:D:287:PRO:HD2	2.30	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:14:CYS:SG	2:B:502:FMN:HM82	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:CD1	1:B:137:LEU:CD1	2.89	0.51
1:B:142:GLU:O	1:B:143:MET:C	2.49	0.51
1:C:176:GLU:C	1:C:178:LEU:H	2.14	0.51
1:D:99:LEU:HD11	1:D:143:MET:SD	2.51	0.51
1:B:75:ARG:HG3	1:B:76:ILE:N	2.26	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:B:232:ARG:C	1:B:234:PRO:HD3	2.31	0.51
1:C:85:GLU:CG	1:C:115:ALA:HA	2.41	0.51
1:D:128:GLN:C	1:D:130:ARG:N	2.63	0.51
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: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:C:157:GLN:OE1	1:C:219:TRP:CE3	2.64	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:106:LEU:N	1:A:107:ARG:CB	2.73	0.50
1:A:293:LEU:C	1:A:295:GLY:H	2.14	0.50
1:B:138:LEU:O	1:B:139:ARG:C	2.46	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:172:GLU:O	1:A:173:ARG:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:190:GLY:HA2	1:B:212:ALA:C	2.32	0.50
1:B:31:PHE:O	1:B:273:LYS:CE	2.60	0.49
1:C:165:THR:CG2	1:C:165:THR:O	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:224:GLU:OE1	1:A:233:HIS:HD2	1.93	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: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:63:ILE:HD11	1:C:303:ILE:CD1	2.42	0.49
1:D:61:PHE:C	1:D:61:PHE:CD2	2.84	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:154:ASN:ND2	1:A:157:GLN:HE21	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:MET:HA	2:A:502:FMN:C5A	2.43	0.49
1:A:249:GLU:CD	1:D:34:ARG:HH22	2.15	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
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:A:108:SER:HA	1:A:109:PHE:C	2.34	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:152:HIS:HA	1:D:187:LYS:O	2.13	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: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:C:176:GLU:C	1:C:178:LEU:N	2.66	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:119:LEU:C	1:B:120:LEU:HD23	2.34	0.48
1:B:233:HIS:ND1	1:B:233:HIS:N	2.60	0.48
1:B:191:HIS:CE1	1:B:219:TRP:N	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:228:PHE:C	1:C:230:GLU:H	2.17	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:B:133:GLY:O	1:B:134:ARG:C	2.53	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:D:266:TYR:OH	2:D:502:FMN:O3P	2.15	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: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:D:176:GLU:C	1:D:178:LEU:N	2.68	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:B:103:PRO:O	1:B:104:GLU:C	2.52	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:A:42:ALA:O	1:A:45:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD13	1:A:80:LEU:HB3	1.97	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: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:142:GLU:C	1:B:144:LEU:N	2.68	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:210:ASP:OD1	1:C:211:VAL:N	2.48	0.47
1:D:100:LEU:HD13	1:D:132:TYR:CE1	2.48	0.47
1:D:303:ILE:O	1:D:304:GLY:C	2.51	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: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:A:156:LEU:O	1:A:157:GLN:C	2.49	0.47
1:B:33:LEU:HB3	1:B:317:ILE:HD13	1.96	0.47
1:C:43:LEU:C	1:C:43:LEU:HD12	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:C	1:B:131:ARG:HG3	2.35	0.46
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.62	0.46
1:D:61:PHE:C	1:D:62:LEU:HD23	2.35	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
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: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: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:D:28:LEU:C	1:D:30:GLY:H	2.18	0.46
1:D:41:LEU:HD12	1:D:41:LEU:C	2.35	0.46
1:A:42:ALA:O	1:A:43:LEU:C	2.54	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:208:ALA:C	1:B:257:LEU:HD11	2.36	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:D:31:PHE:HA	1:D:330:GLU:O	2.15	0.46
1:A:134:ARG:C	1:A:134:ARG:CD	2.84	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:B:110:ARG:O	1:B:111:VAL:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:253:VAL:C	1:B:255:PRO:HD3	2.36	0.46
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:95:SER:C	1:A:97:ARG:N	2.68	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:142:GLU:C	1:B:144:LEU:H	2.19	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:43:LEU:C	1:C:43:LEU:CD1	2.84	0.45
1:C:191:HIS:CE1	1:C:219:TRP:N	2.84	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:B:325:ALA:O	1:B:326:ARG:C	2.55	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:B:108:SER:C	1:B:110:ARG:H	2.20	0.45
1:C:48:LEU:O	1:C:59:ALA:HA	2.17	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: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:172:GLU:CD	1:A:172:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:LEU:O	1:A:81:ALA:C	2.55	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:105:ALA:C	1:B:107:ARG:H	2.20	0.45
1:B:295:GLY:O	1:B:297:GLU:N	2.50	0.45
1:C:41:LEU:CD1	1:C:315:PHE:HD1	2.28	0.45
1:D:285:ALA:O	1:D:286:ARG:C	2.55	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: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:A:134:ARG:C	1:A:134:ARG:HD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:LEU:CD1	1:A:151:PHE:CZ	3.00	0.44
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: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:11:LEU:HD23	1:D:67:THR:C	2.38	0.44
1:D:317:ILE:HG12	1:D:328:ARG:HD3	1.99	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:C:187:LYS:NZ	1:C:188:GLU:O	2.31	0.44
1:D:166:ASP:OD1	1:D:168:ARG:HB2	2.17	0.44
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:A:241:ILE:O	1:A:242:PRO:C	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:CB	1:B:91:MET:HE1	2.35	0.43
1:B:149:LEU:HD11	1:B:151:PHE:CZ	2.53	0.43
1:C:172:GLU:O	1:C:173:ARG:C	2.55	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:A:293:LEU:C	1:A:295:GLY:N	2.71	0.43
1:B:64:GLY:O	1:B:66:MET:HE2	2.18	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
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:38:LEU:C	1:D:40:GLY:N	2.71	0.43
1:D:60:PRO:HG3	1:D:322:PRO:CG	2.48	0.43
1:D:176:GLU:C	1:D:178:LEU:H	2.21	0.43
1:D:247:ILE:HD11	1:D:261:ALA:HB1	2.00	0.43
1:A:267:THR:O	1:A:268:GLY:C	2.57	0.43
1:B:309:GLU:HG3	1:C:236:LEU:HG	1.99	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:A:236:LEU:C	1:A:238:GLU:N	2.69	0.43
1:B:100:LEU:HD13	1:B:132:TYR:CD1	2.54	0.43
1:B:160:VAL:C	1:B:162:ARG:H	2.22	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:B:285:ALA:O	1:B:286:ARG:C	2.56	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:299:VAL:HG12	1:C:300:ALA:N	2.33	0.43
1:C:301:ALA:O	1:C:302:TRP:C	2.57	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
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:D:253:VAL:C	1:D:255:PRO:HD3	2.40	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:A:83:ALA:O	1:A:84:ALA:C	2.57	0.42
1:A:301:ALA:O	1:A:302:TRP:C	2.55	0.42
1:B:106:LEU:CG	1:B:143:MET:CG	2.96	0.42
1:C:214:ALA:HB3	1:C:242:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ALA:C	1:C:298:ARG:N	2.71	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:D:243:THR:O	1:D:244:ALA:C	2.58	0.42
1:A:24:THR:CG2	1:A:238:GLU:HB3	2.48	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:128:GLN:OE1	1:C:128:GLN:HA	2.19	0.42
1:C:147:ASP:O	1:C:183:PRO:HD2	2.20	0.42
1:B:53:LEU:HD11	1:B:121:ILE:HD13	2.01	0.42
1:B:111:VAL:C	1:B:113:LYS:N	2.72	0.42
1:B:202:ARG:C	1:B:203:ASP:OD1	2.58	0.42
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:308:GLU:O	1:B:309:GLU:C	2.58	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:42:ALA:O	1:C:43:LEU:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:148:ALA:HB1	1:A:183:PRO:O	2.21	0.41
1:B:180:LEU:HA	1:B:180:LEU:HD12	1.76	0.41
1:C:217:THR:HG23	2:C:502:FMN:P	2.60	0.41
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:185:MET:HE3	1:D:208:ALA:HB3	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:236:LEU:O	1:A:237:CYS:C	2.58	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: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: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:C:9:LYS:HB2	1:C:9:LYS:HZ3	1.86	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:218:SER:O	1:A:219:TRP:C	2.59	0.41
1:A:291:PRO:HB2	1:A:299:VAL:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:CB	1:B:307:LEU:CD1	2.84	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:D:161:GLN:HB2	1:D:223:GLU:CD	2.41	0.41
1:B:193:LEU:HD22	1:B:197:ALA:HB1	2.02	0.41
1:C:9:LYS:HB2	1:C:9:LYS:HZ2	1.86	0.41
1:C:299:VAL:O	1:C:300:ALA:C	2.59	0.41
1:D:128:GLN:C	1:D:130:ARG:H	2.24	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: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
1:D:112:ARG:O	1:D:112:ARG:CG	2.69	0.40
1:A:41:LEU:CD1	1:A:42:ALA:N	2.85	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:A:165:THR:CG2	1:A:165:THR:O	2.66	0.40
1:C:60:PRO:CA	1:C:281:LEU:HD13	2.52	0.40
1:C:232:ARG:C	1:C:233:HIS:CD2	2.95	0.40
1:D:142:GLU:C	1:D:144:LEU:N	2.73	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: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: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: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	13
1	B	314/332 (95%)	246 (78%)	45 (14%)	23 (7%)	1	4
1	C	310/332 (93%)	243 (78%)	50 (16%)	17 (6%)	2	9
1	D	307/332 (92%)	249 (81%)	41 (13%)	17 (6%)	2	9
All	All	1245/1328 (94%)	995 (80%)	179 (14%)	71 (6%)	1	9

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/252 (95%)	171 (72%)	68 (28%)	0	1
1	B	241/252 (96%)	176 (73%)	65 (27%)	0	2
1	C	239/252 (95%)	173 (72%)	66 (28%)	0	1
1	D	234/252 (93%)	173 (74%)	61 (26%)	0	2
All	All	953/1008 (94%)	693 (73%)	260 (27%)	0	2

All (260) 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

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Mol	Chain	Res	Type
1	A	41	LEU
1	A	44	SER
1	A	67	THR
1	A	74	GLU
1	A	75	ARG
1	A	76	ILE
1	A	77	ASN
1	A	87	LEU
1	A	92	MET
1	A	93	LEU
1	A	95	SER
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	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	188	GLU
1	A	196	GLU
1	A	204	LEU
1	A	210	ASP
1	A	217	THR

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Mol	Chain	Res	Type
1	A	223	GLU
1	A	232	ARG
1	A	233	HIS
1	A	235	GLU
1	A	236	LEU
1	A	245	ARG
1	A	251	ARG
1	A	252	GLU
1	A	281	LEU
1	A	288	LEU
1	A	294	GLU
1	A	297	GLU
1	A	298	ARG
1	A	308	GLU
1	A	309	GLU
1	A	317	ILE
1	A	322	PRO
1	A	326	ARG
1	A	328	ARG
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
1	B	112	ARG
1	B	113	LYS
1	B	114	VAL
1	B	117	LYS

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Mol	Chain	Res	Type
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	153	VAL
1	B	156	LEU
1	B	158	GLU
1	B	172	GLU
1	B	173	ARG
1	B	195	ARG
1	B	199	LEU
1	B	202	ARG
1	B	203	ASP
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	251	ARG
1	B	252	GLU
1	B	257	LEU
1	B	259	LEU
1	B	281	LEU
1	B	282	LEU
1	B	286	ARG
1	B	288	LEU
1	B	291	PRO
1	B	298	ARG
1	B	303	ILE
1	B	308	GLU
1	B	320	ARG
1	B	323	LYS
1	B	326	ARG
1	B	331	ARG

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Mol	Chain	Res	Type
1	C	9	LYS
1	C	11	LEU
1	C	15	LEU
1	C	18	GLU
1	C	19	VAL
1	C	34	ARG
1	C	43	LEU
1	C	44	SER
1	C	50	THR
1	C	58	LYS
1	C	74	GLU
1	C	75	ARG
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	107	ARG
1	C	110	ARG
1	C	111	VAL
1	C	112	ARG
1	C	114	VAL
1	C	123	ASN
1	C	124	LEU
1	C	128	GLN
1	C	131	ARG
1	C	135	ASP
1	C	137	LEU
1	C	149	LEU
1	C	154	ASN
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	195	ARG
1	C	202	ARG

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Mol	Chain	Res	Type
1	C	203	ASP
1	C	217	THR
1	C	223	GLU
1	C	226	VAL
1	C	228	PHE
1	C	230	GLU
1	C	232	ARG
1	C	233	HIS
1	C	235	GLU
1	C	236	LEU
1	C	245	ARG
1	C	247	ILE
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	323	LYS
1	C	326	ARG
1	C	332	VAL
1	D	9	LYS
1	D	11	LEU
1	D	15	LEU
1	D	16	GLU
1	D	18	GLU
1	D	25	THR
1	D	34	ARG
1	D	44	SER
1	D	46	VAL
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

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Mol	Chain	Res	Type
1	D	99	LEU
1	D	104	GLU
1	D	113	LYS
1	D	114	VAL
1	D	117	LYS
1	D	120	LEU
1	D	123	ASN
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	152	HIS
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	182	PHE
1	D	185	MET
1	D	196	GLU
1	D	199	LEU
1	D	227	ARG
1	D	236	LEU
1	D	251	ARG
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	298	ARG
1	D	308	GLU
1	D	314	LEU
1	D	317	ILE
1	D	323	LYS
1	D	326	ARG

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Mol	Chain	Res	Type
1	D	331	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	161	GLN
1	A	191	HIS
1	A	233	HIS
1	B	154	ASN
1	B	191	HIS
1	C	10	HIS
1	C	77	ASN
1	C	154	ASN
1	C	157	GLN
1	C	191	HIS
1	C	233	HIS
1	C	256	HIS
1	D	123	ASN
1	D	157	GLN
1	D	191	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	POP	D	503	-	6,8,8	1.09	1 (16%)	12,13,13	1.61	3 (25%)
2	FMN	C	502	-	33,33,33	3.72	16 (48%)	48,50,50	2.22	18 (37%)
2	FMN	B	502	-	33,33,33	3.34	14 (42%)	48,50,50	2.46	20 (41%)
3	POP	B	503	-	6,8,8	1.04	1 (16%)	12,13,13	1.28	2 (16%)
2	FMN	A	502	-	33,33,33	3.76	13 (39%)	48,50,50	2.22	19 (39%)
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
3	POP	D	503	-	-	5/6/6/6	-
2	FMN	C	502	-	-	13/18/18/18	0/3/3/3
2	FMN	B	502	-	-	8/18/18/18	0/3/3/3
3	POP	B	503	-	-	1/6/6/6	-
2	FMN	A	502	-	-	10/18/18/18	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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'
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'

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Mol	Chain	Res	Type	Atoms
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'

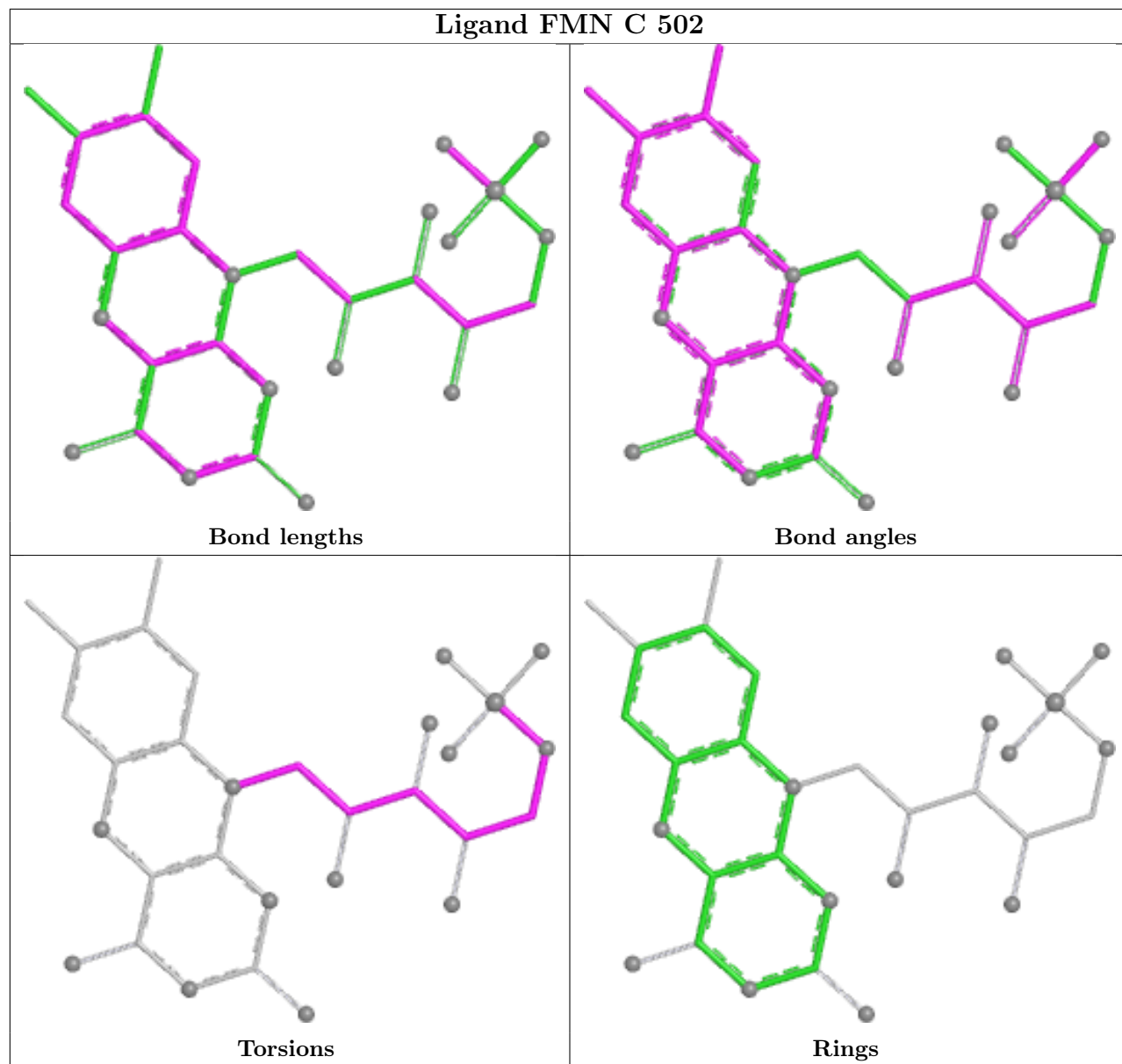
There are no ring outliers.

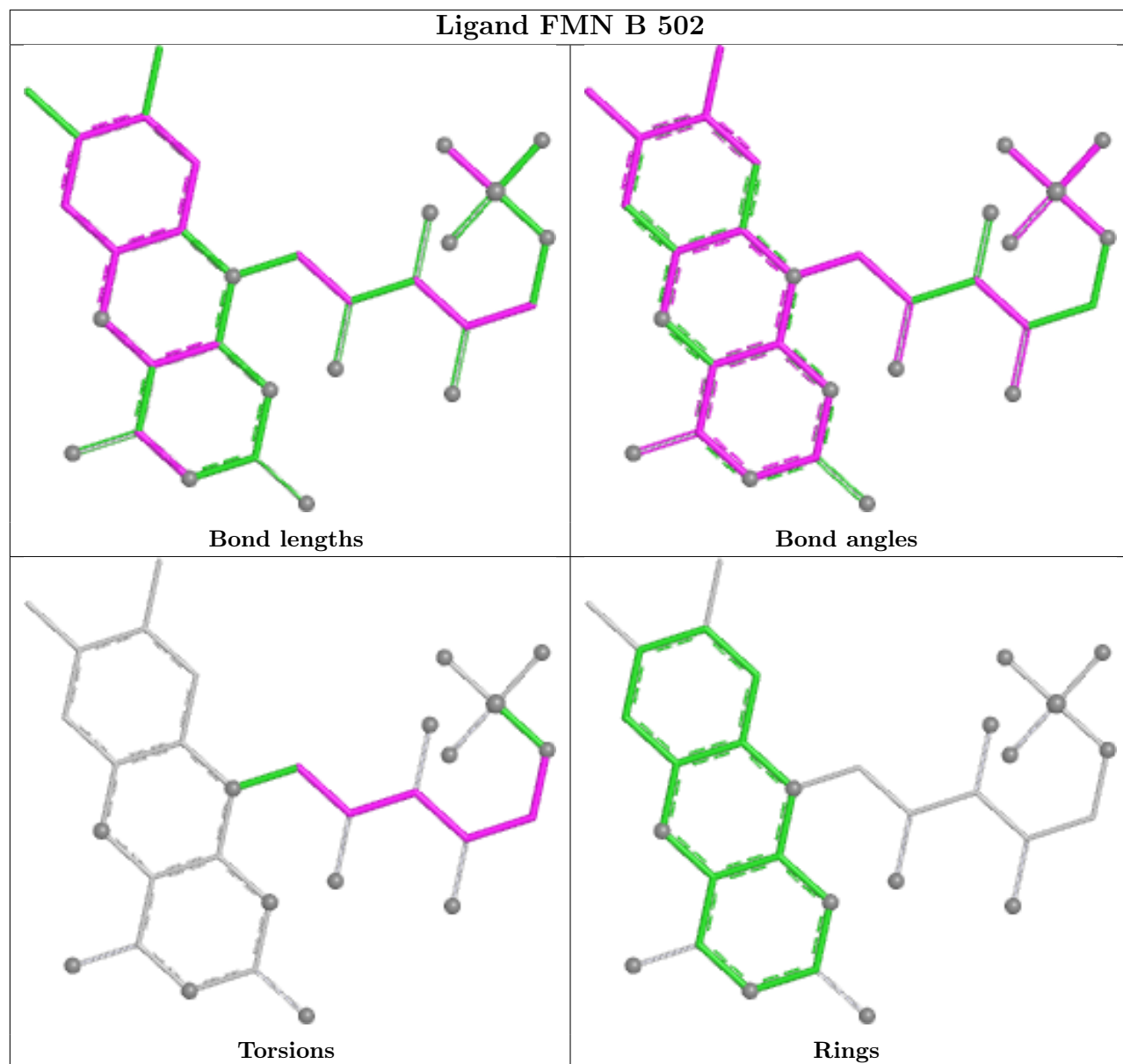
6 monomers are involved in 51 short contacts:

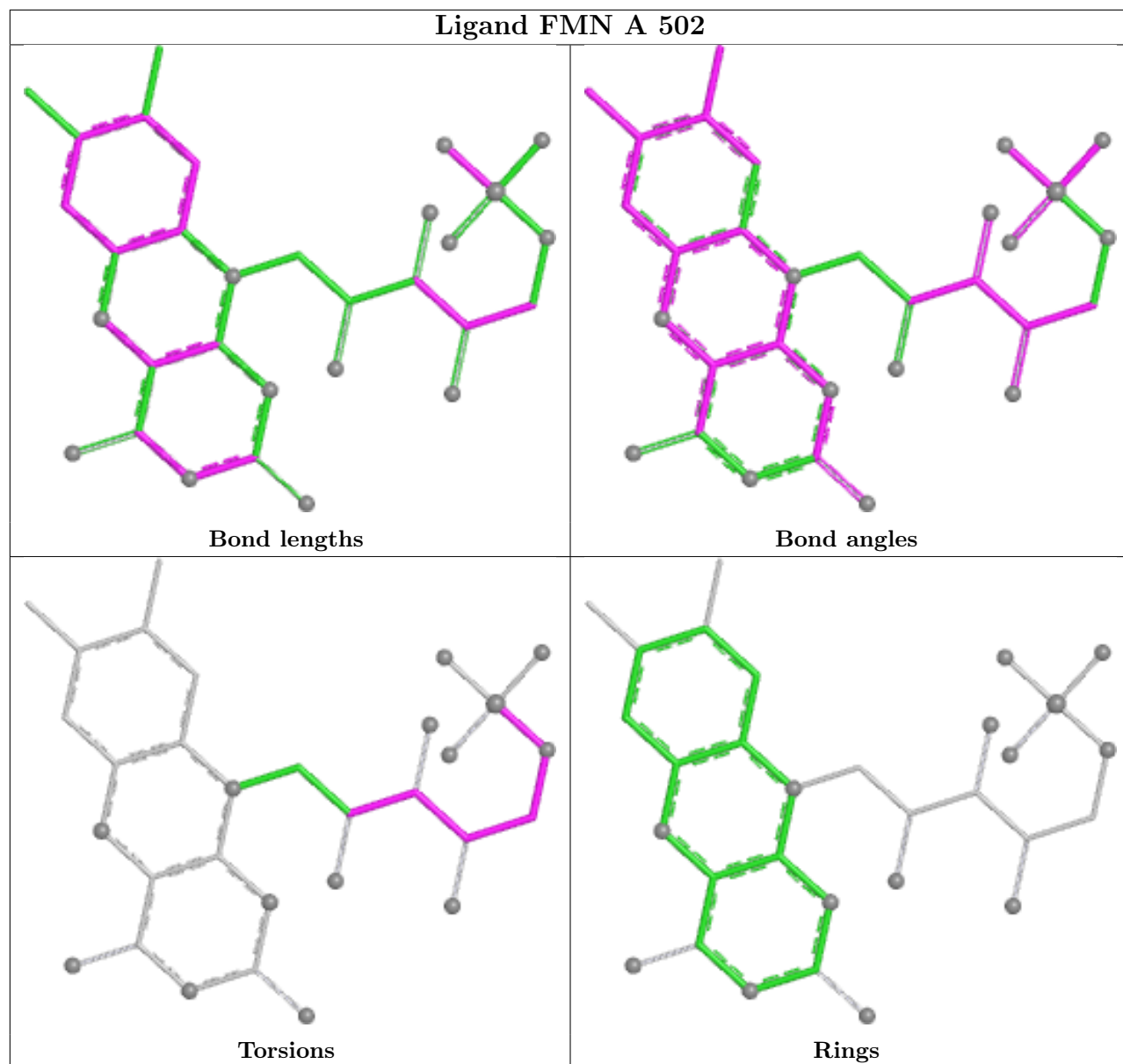
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	POP	1	0
2	C	502	FMN	14	0
2	B	502	FMN	12	0
3	B	503	POP	1	0
2	A	502	FMN	13	0
2	D	502	FMN	10	0

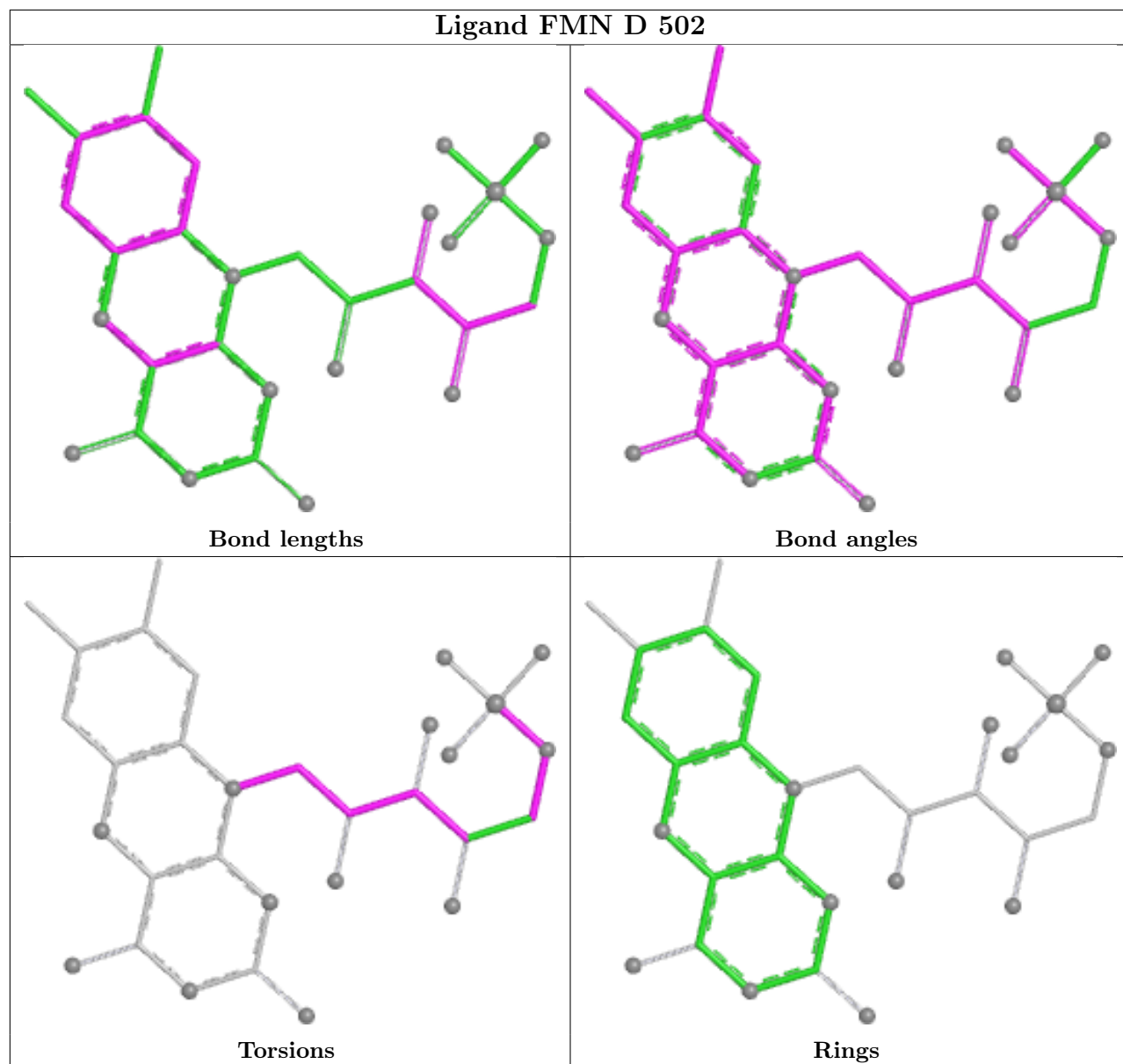
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.17	3 (0%) 84 69	2, 9, 47, 81	0
1	B	318/332 (95%)	0.15	3 (0%) 84 69	2, 16, 44, 68	0
1	C	316/332 (95%)	0.15	5 (1%) 72 52	2, 9, 42, 85	0
1	D	313/332 (94%)	0.16	2 (0%) 89 77	2, 15, 40, 53	0
All	All	1265/1328 (95%)	0.16	13 (1%) 82 66	2, 12, 42, 85	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	LEU	3.8
1	C	99	LEU	3.7
1	A	100	LEU	3.6
1	C	107	ARG	2.9
1	C	100	LEU	2.7
1	C	95	SER	2.6
1	B	11	LEU	2.5
1	C	295	GLY	2.5
1	D	76	ILE	2.4
1	D	75	ARG	2.3
1	A	99	LEU	2.2
1	B	293	LEU	2.2
1	B	146	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

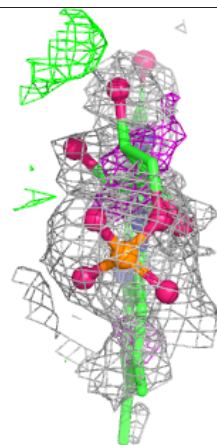
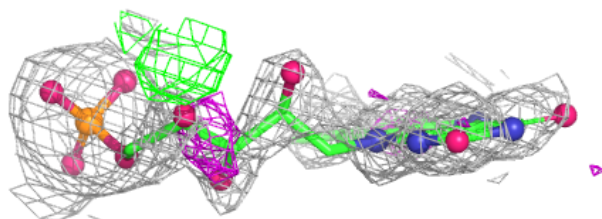
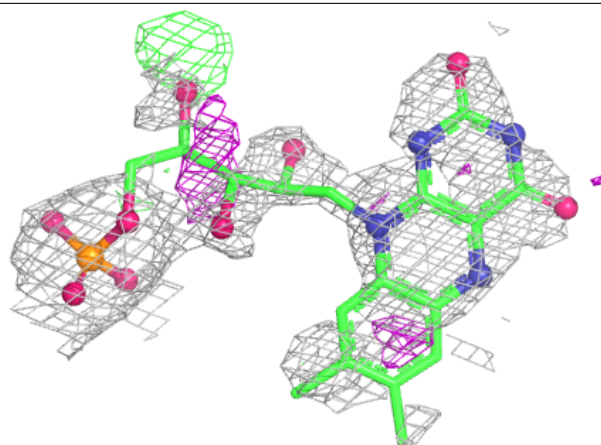
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	POP	B	503	9/9	0.91	0.31	82,84,91,93	0
3	POP	D	503	9/9	0.91	0.31	81,83,93,93	0
2	FMN	D	502	31/31	0.95	0.40	17,70,70,70	0
2	FMN	A	502	31/31	0.96	0.39	8,65,66,66	0
2	FMN	C	502	31/31	0.97	0.36	9,70,71,71	0
2	FMN	B	502	31/31	0.97	0.35	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.

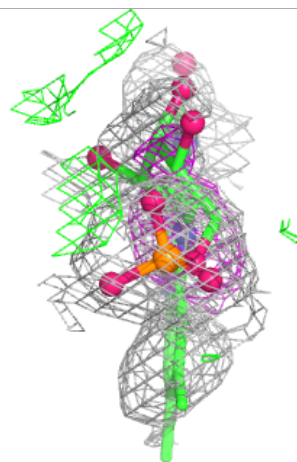
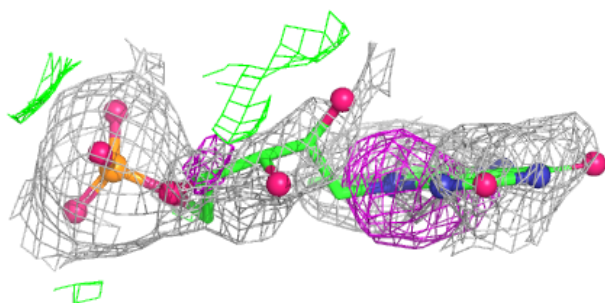
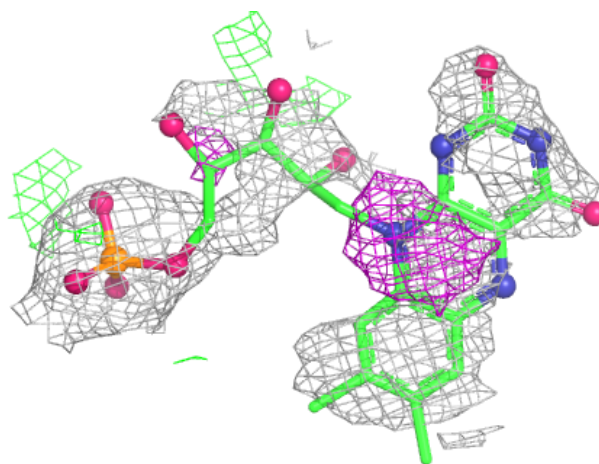
Electron density around FMN D 502:

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



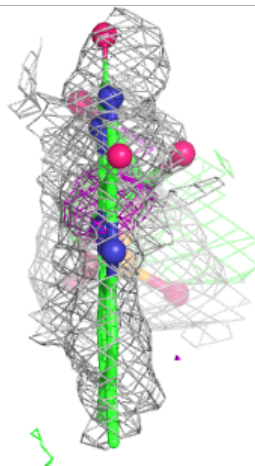
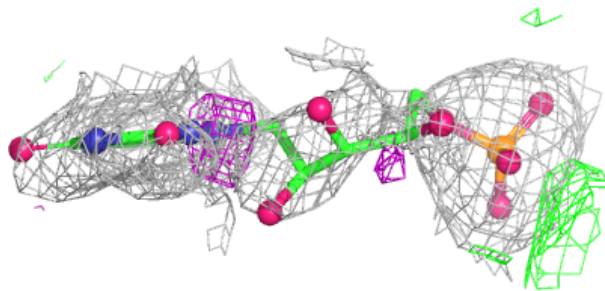
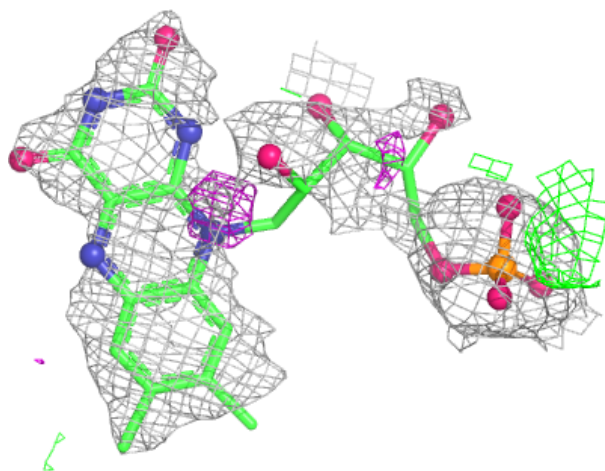
Electron density around FMN A 502:

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



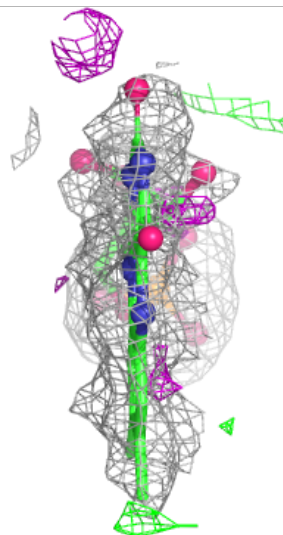
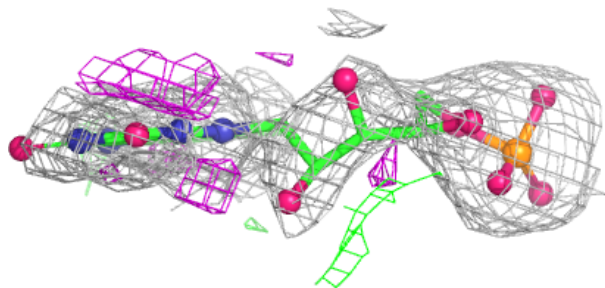
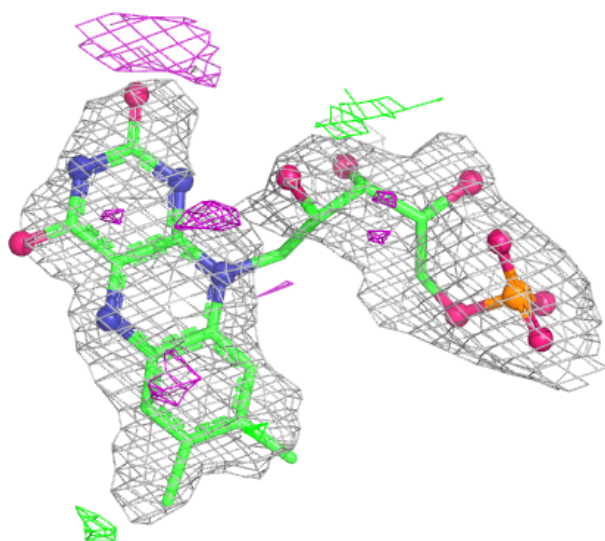
Electron density around FMN C 502:

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



Electron density around FMN 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.