



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 AM UTC

PDB ID : 1O95 / pdb_00001o95
Title : Ternary complex between trimethylamine dehydrogenase and electron transferring flavoprotein
Authors : Leys, D.; Basran, J.; Talfournier, F.; Sutcliffe, M.J.; Scrutton, N.S.
Deposited on : 2002-12-11
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

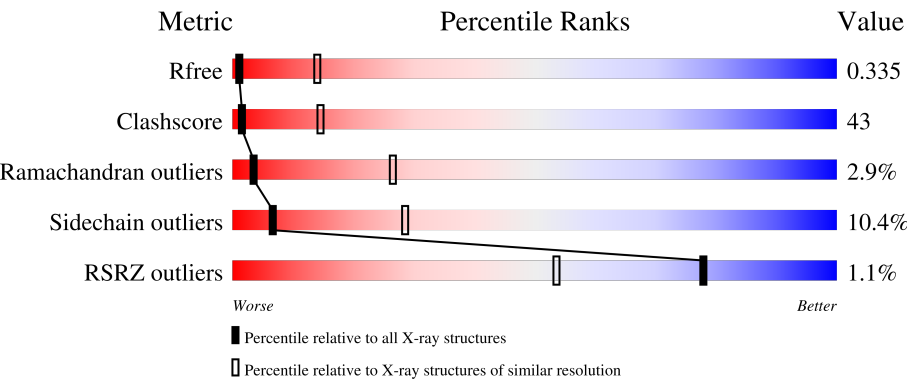
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	729	% 28%48%22%.
1	B	729	% 24%49%24%.
2	C	264	2% 34%38%14%.12%
2	E	264	30%38%18%.11%
3	D	320	% 21%24%11%.41%

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Mol	Chain	Length	Quality of chain
3	F	320	2%15%24%18%.41%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17776 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 TRIMETHYLAMINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5692	3589	996	1079	28			
1	B	729	Total	C	N	O	S	0	0	0
			5676	3583	994	1071	28			

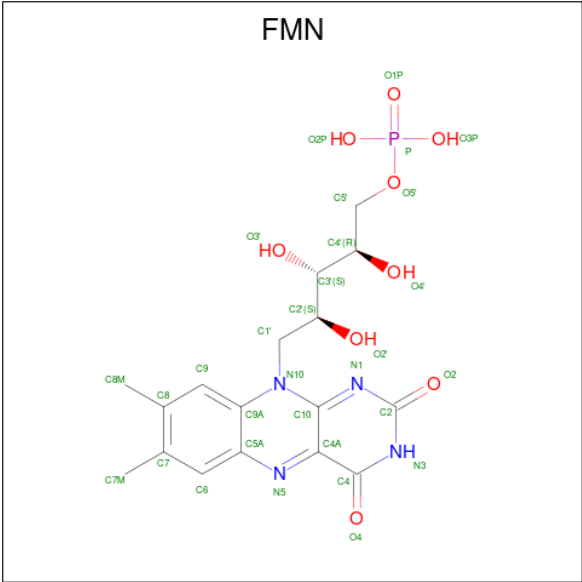
- Molecule 2 is a protein called ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	233	Total	C	N	O	S	0	0	0
			1749	1097	301	341	10			
2	E	236	Total	C	N	O	S	0	0	0
			1751	1102	299	340	10			

- Molecule 3 is a protein called ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT.

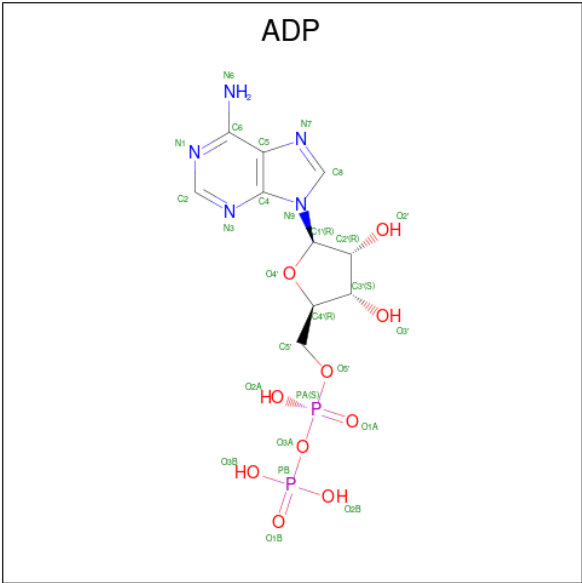
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O	0	0	0
			1354	857	230	267			
3	F	189	Total	C	N	O	0	0	0
			1376	870	232	274			

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



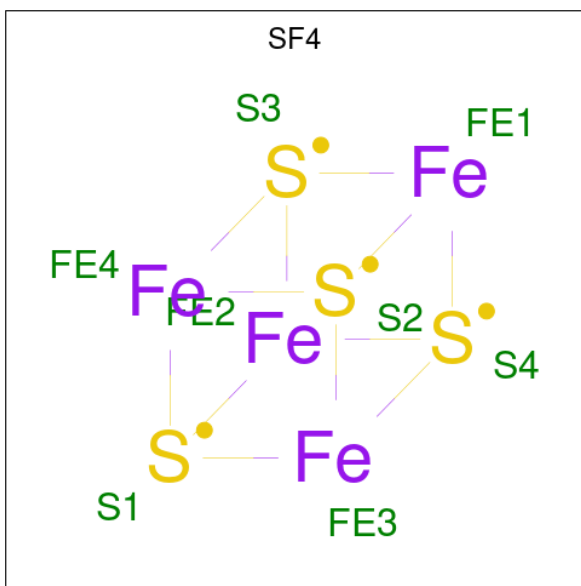
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



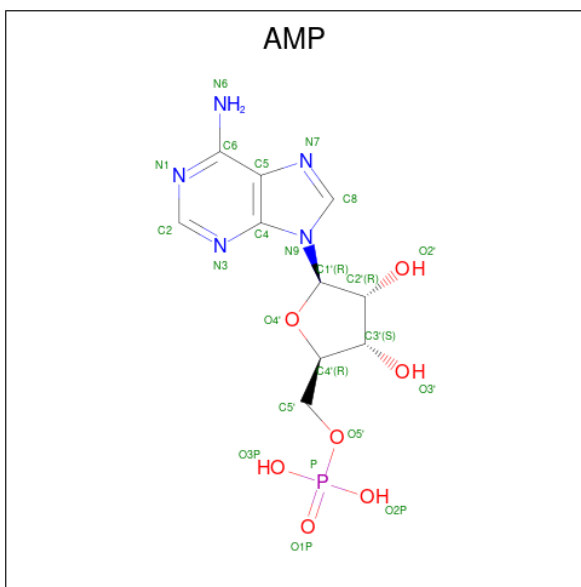
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			23	10	5	7		

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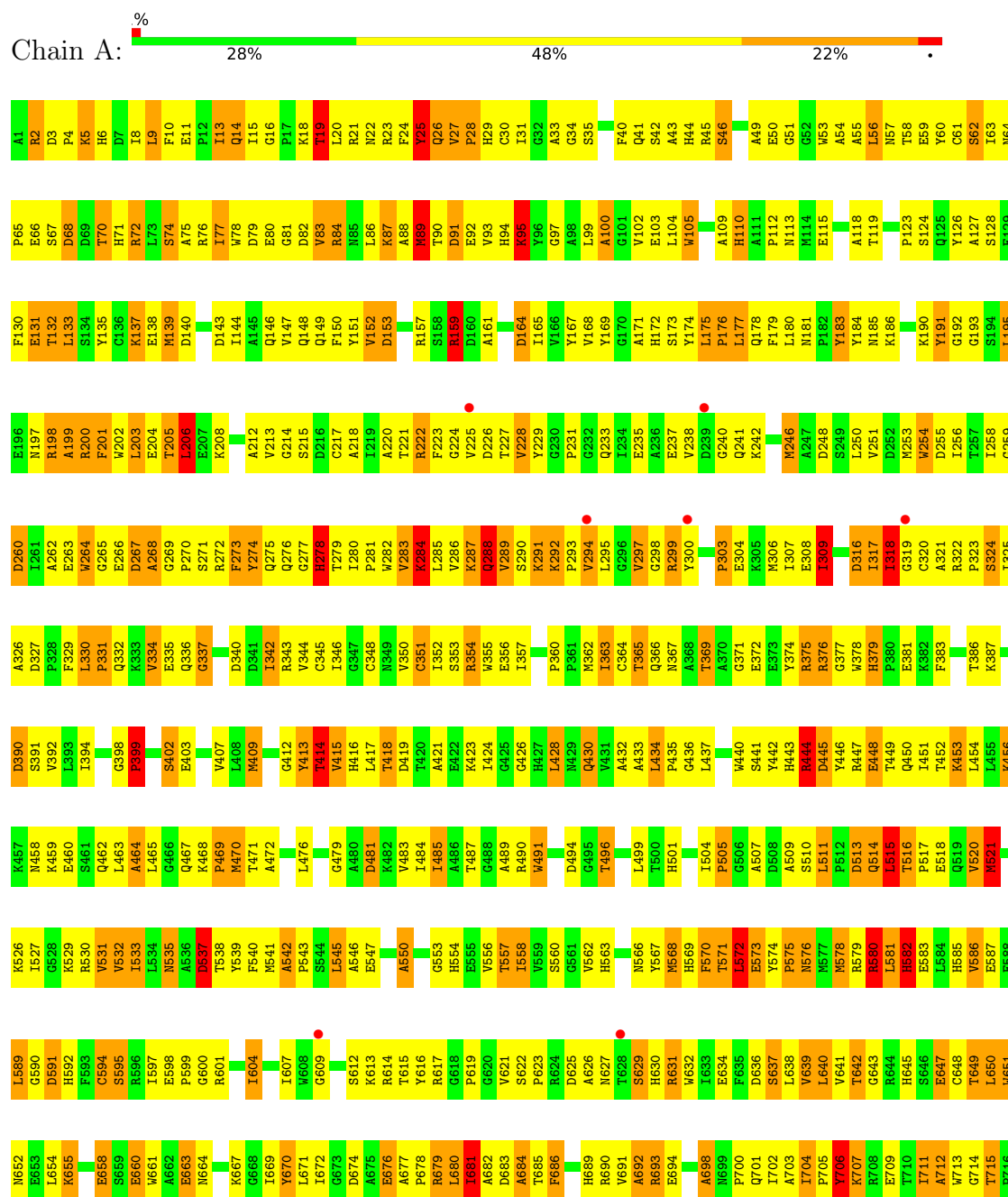
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

3 Residue-property plots

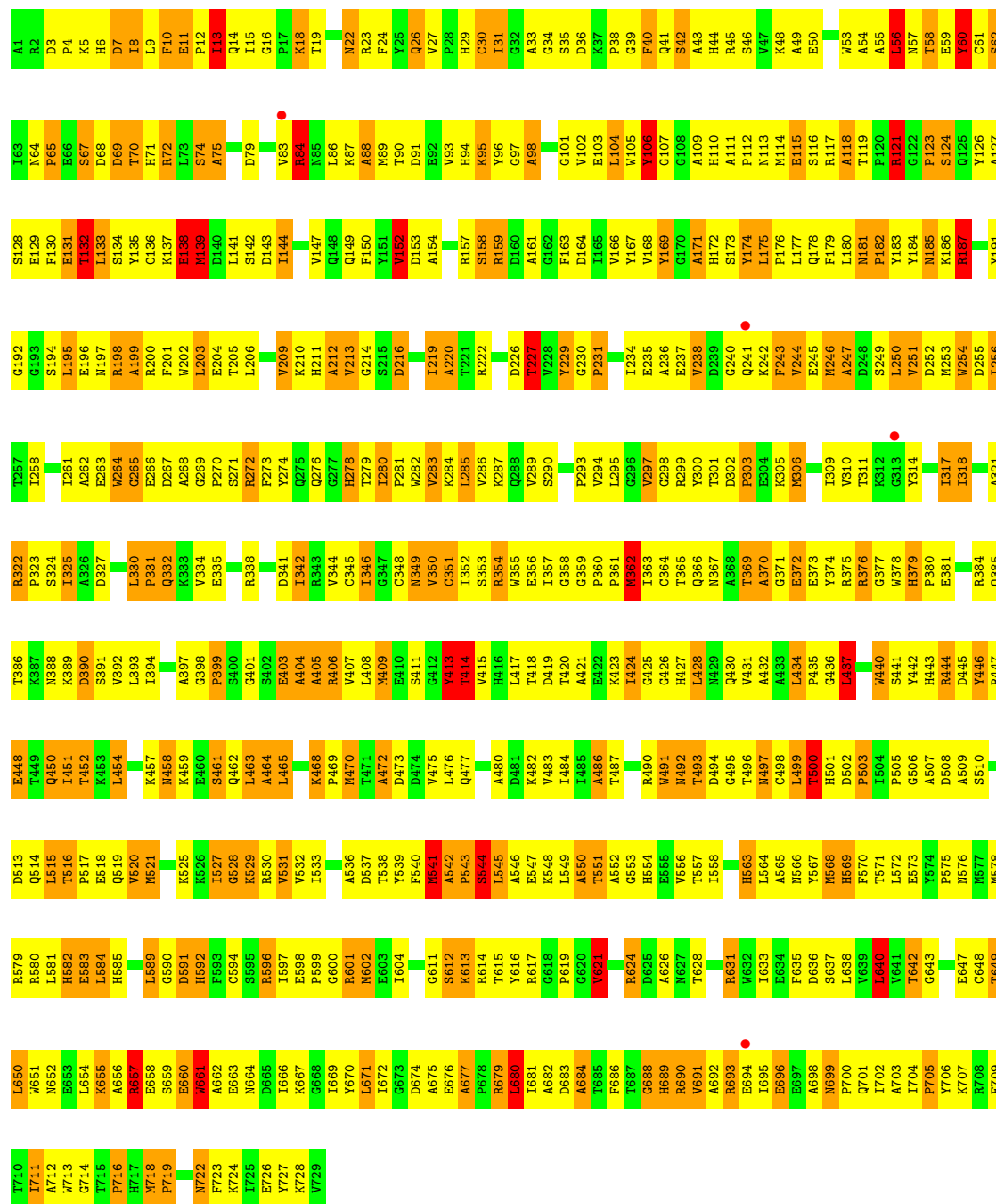
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



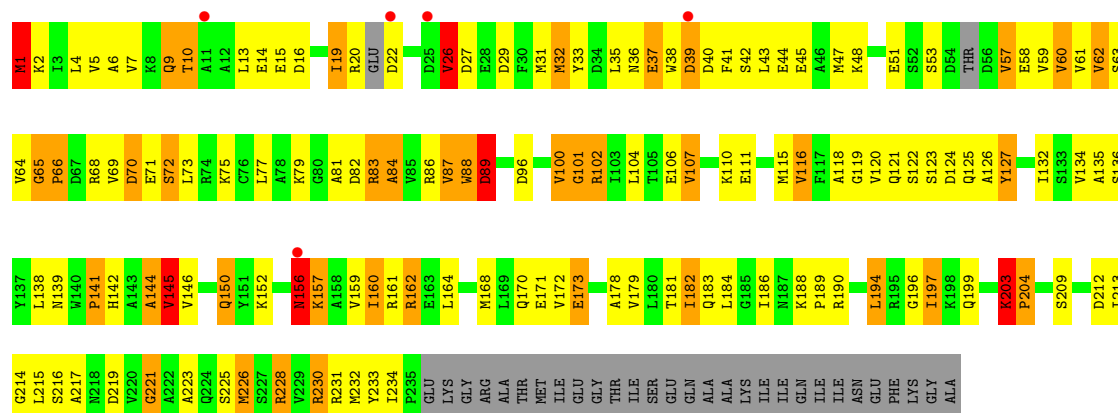


● Molecule 1: TRIMETHYLAMINE DEHYDROGENASE

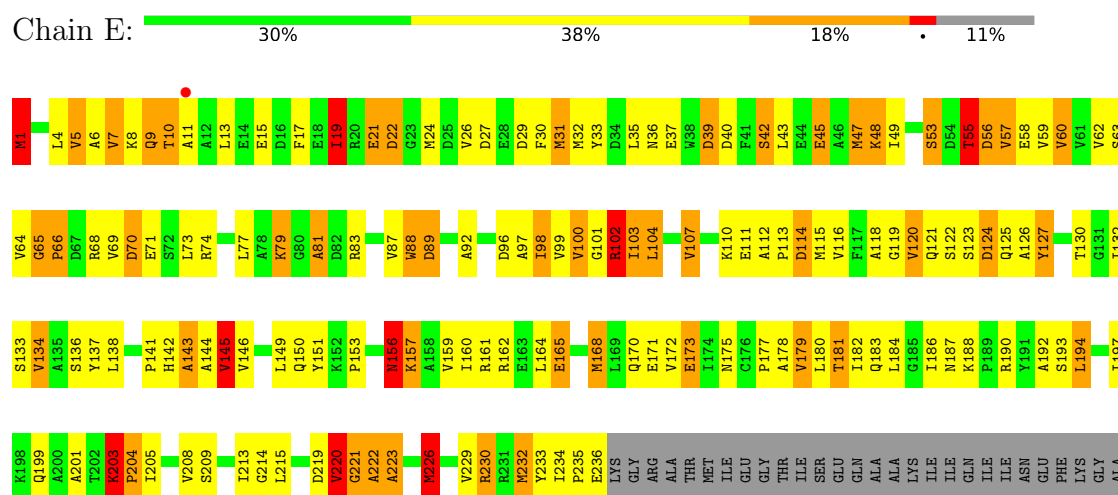


● Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT

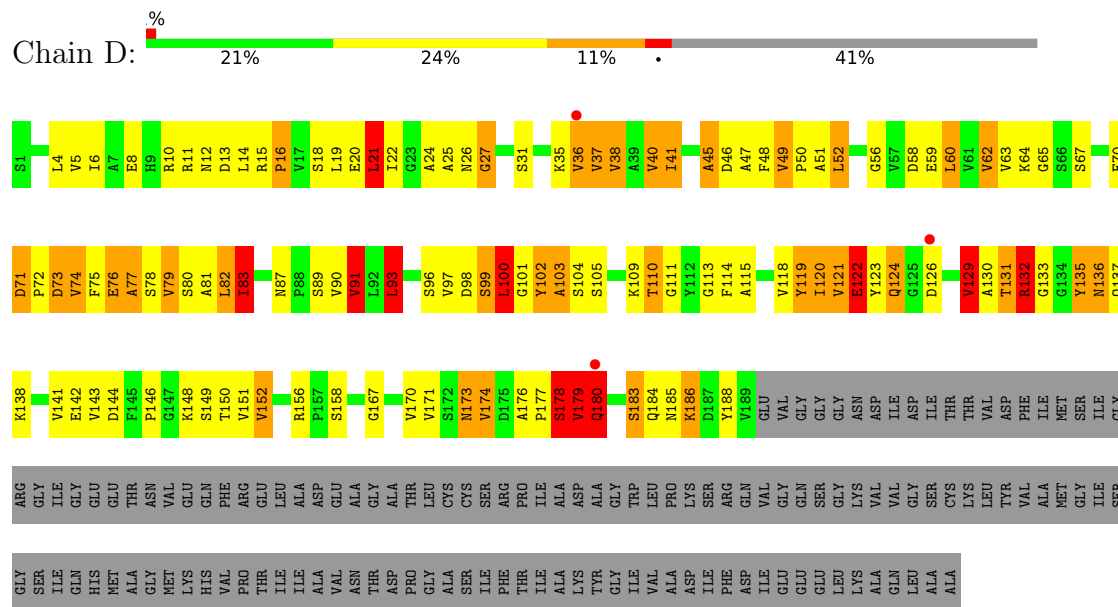




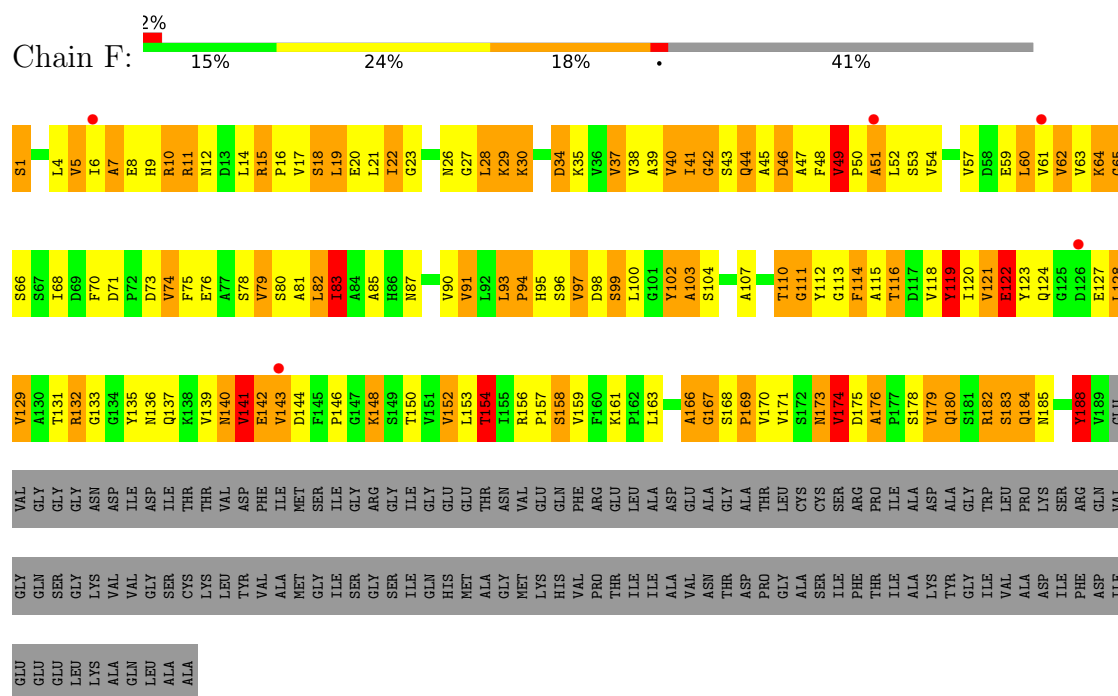
• Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT



• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT



• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.50Å 116.51Å 138.71Å 90.00° 95.35° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.70) 96.3 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.71Å)	Xtrriage
Refinement program	REFMAC 5.1.08	Depositor
R, R_{free}	0.252 , 0.353 0.237 , 0.335	Depositor DCC
R_{free} test set	1679 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtrriage
Anisotropy	0.862	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17776	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2278e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: AMP, FMN, ADP, SF4

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	2.00	143/5834 (2.5%)	2.04	202/7918 (2.6%)
1	B	2.08	150/5818 (2.6%)	2.06	228/7902 (2.9%)
2	C	2.01	40/1771 (2.3%)	1.92	50/2399 (2.1%)
2	E	2.19	47/1775 (2.6%)	1.98	44/2408 (1.8%)
3	D	2.02	37/1378 (2.7%)	2.00	55/1884 (2.9%)
3	F	2.53	77/1400 (5.5%)	2.16	58/1913 (3.0%)
All	All	2.09	494/17976 (2.7%)	2.04	637/24424 (2.6%)

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	4
1	B	0	3
2	E	0	1
3	D	0	3
3	F	0	3
All	All	0	14

All (494) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	718	MET	SD-CE	27.20	2.47	1.79
3	F	49	VAL	CA-CB	18.74	1.63	1.54
2	E	168	MET	SD-CE	17.31	2.22	1.79
1	B	500	THR	CA-CB	14.79	1.75	1.53
2	C	1	MET	SD-CE	13.48	2.13	1.79
2	E	232	MET	C-O	12.84	1.40	1.24
1	A	89	MET	SD-CE	12.06	2.09	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	22	ASP	CA-C	11.68	1.68	1.52
1	A	704	ILE	CA-CB	11.46	1.69	1.54
2	E	100	VAL	CA-CB	11.36	1.67	1.54
1	B	13	ILE	CA-CB	11.35	1.70	1.54
3	F	129	VAL	CA-CB	10.98	1.68	1.53
2	C	6	ALA	CA-CB	-10.91	1.39	1.53
1	B	350	VAL	CA-CB	-10.68	1.39	1.54
1	B	515	LEU	CA-C	10.62	1.65	1.52
1	B	541	MET	SD-CE	10.44	2.05	1.79
2	E	226	MET	SD-CE	10.41	2.05	1.79
3	F	41	ILE	CA-CB	10.32	1.67	1.54
1	A	711	ILE	CA-CB	-10.30	1.41	1.54
1	B	537	ASP	CA-C	-10.18	1.40	1.52
2	E	1	MET	SD-CE	10.17	2.04	1.79
1	B	331	PRO	CA-C	10.15	1.66	1.52
1	B	656	ALA	CA-C	9.93	1.66	1.52
1	B	621	VAL	CA-CB	9.86	1.67	1.54
1	A	718	MET	SD-CE	9.84	2.04	1.79
3	F	87	ASN	CA-C	9.70	1.63	1.53
3	D	152	VAL	CA-CB	-9.64	1.42	1.54
2	E	103	ILE	CA-CB	-9.59	1.43	1.54
2	C	10	THR	CA-C	-9.54	1.41	1.52
1	A	599	PRO	CA-C	9.14	1.63	1.52
1	B	509	ALA	CA-CB	9.13	1.65	1.53
1	A	331	PRO	CA-C	9.05	1.65	1.52
2	E	6	ALA	CA-CB	-9.02	1.41	1.53
1	B	621	VAL	CA-C	8.91	1.64	1.52
2	C	135	ALA	CA-CB	-8.88	1.38	1.53
3	D	62	VAL	CA-CB	8.79	1.64	1.54
3	D	179	VAL	CA-C	8.62	1.63	1.52
3	D	123	TYR	CA-C	8.53	1.63	1.52
3	F	154	THR	CA-CB	8.51	1.66	1.53
3	D	71	ASP	CA-C	8.50	1.59	1.52
1	A	621	VAL	CA-C	8.49	1.62	1.52
3	F	34	ASP	CA-C	8.46	1.63	1.52
1	B	169	TYR	CA-C	-8.43	1.42	1.52
1	A	318	ILE	CA-C	8.39	1.62	1.52
3	F	87	ASN	C-O	8.34	1.28	1.23
2	C	115	MET	SD-CE	-8.30	1.58	1.79
1	B	684	ALA	CA-CB	-8.28	1.40	1.53
1	B	649	THR	CA-CB	8.28	1.66	1.53
1	A	206	LEU	CA-C	-8.25	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	90	VAL	CA-CB	8.24	1.64	1.55
1	A	496	THR	CA-CB	8.24	1.66	1.53
1	B	121	ARG	CA-C	-8.22	1.43	1.52
2	C	5	VAL	CA-CB	-8.20	1.43	1.54
1	B	486	ALA	CA-CB	-8.17	1.47	1.53
2	C	168	MET	SD-CE	8.17	2.00	1.79
1	A	13	ILE	CA-CB	8.14	1.66	1.54
3	D	180	GLN	CB-CG	8.08	1.76	1.52
2	C	57	VAL	CA-CB	8.07	1.64	1.54
1	A	532	VAL	C-O	8.06	1.33	1.24
1	B	370	ALA	CA-CB	-8.05	1.40	1.53
3	F	128	LEU	CA-C	8.05	1.63	1.52
1	A	706	TYR	CA-C	-8.04	1.42	1.52
1	A	83	VAL	CA-CB	-7.94	1.45	1.54
1	B	344	VAL	CA-CB	-7.92	1.44	1.54
1	B	551	THR	CA-CB	7.90	1.67	1.53
3	F	159	VAL	CA-CB	7.86	1.65	1.54
2	E	19	ILE	CA-C	7.84	1.62	1.52
2	C	142	HIS	CA-C	7.82	1.62	1.52
2	C	26	VAL	CA-CB	7.79	1.65	1.54
1	A	578	MET	CA-C	7.79	1.62	1.52
3	F	139	VAL	CA-CB	-7.79	1.44	1.55
1	A	131	GLU	CA-C	-7.71	1.44	1.53
1	B	351	CYS	CA-C	-7.71	1.42	1.52
2	E	98	ILE	CA-CB	-7.69	1.45	1.54
3	F	66	SER	N-CA	7.67	1.55	1.46
3	F	68	ILE	CA-CB	7.67	1.64	1.54
2	C	118	ALA	CA-C	-7.66	1.43	1.52
1	A	538	THR	CA-CB	-7.63	1.40	1.53
1	A	68	ASP	CA-C	7.61	1.62	1.52
3	D	118	VAL	CA-CB	-7.59	1.44	1.54
1	A	520	VAL	CA-CB	-7.57	1.46	1.54
1	A	262	ALA	CA-CB	-7.56	1.40	1.53
1	A	351	CYS	CA-C	-7.56	1.43	1.52
2	C	19	ILE	CA-C	7.54	1.62	1.52
1	B	213	VAL	CA-CB	7.53	1.62	1.54
1	B	659	SER	CA-C	7.51	1.62	1.52
3	F	97	VAL	CA-CB	7.51	1.64	1.54
1	A	621	VAL	CA-CB	7.50	1.64	1.54
2	E	24	MET	CA-C	7.47	1.62	1.52
3	F	174	VAL	C-O	7.46	1.32	1.23
1	B	689	HIS	CA-C	-7.39	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	VAL	CA-C	-7.38	1.43	1.52
1	A	685	THR	CA-CB	-7.37	1.40	1.53
1	A	639	VAL	CA-CB	7.37	1.62	1.53
1	A	231	PRO	C-O	7.35	1.32	1.23
1	A	226	ASP	CA-C	-7.31	1.43	1.52
1	B	525	LYS	CA-C	7.30	1.61	1.52
1	B	499	LEU	N-CA	7.28	1.55	1.46
3	F	171	VAL	CA-CB	-7.28	1.45	1.54
1	A	369	THR	CA-CB	-7.27	1.43	1.54
1	B	468	LYS	CB-CG	7.25	1.74	1.52
1	A	364	CYS	CA-C	-7.25	1.43	1.52
1	A	5	LYS	CA-C	7.23	1.62	1.52
1	A	698	ALA	CA-C	-7.21	1.43	1.52
2	C	53	SER	CA-C	7.20	1.63	1.53
1	B	133	LEU	CA-C	-7.18	1.43	1.52
1	A	228	VAL	CA-CB	7.17	1.64	1.54
1	A	292	LYS	CA-C	7.16	1.61	1.52
3	F	174	VAL	CA-C	7.16	1.61	1.52
2	C	60	VAL	CA-CB	-7.14	1.45	1.54
1	A	576	ASN	C-O	-7.11	1.15	1.24
2	E	31	MET	SD-CE	7.08	1.97	1.79
1	A	537	ASP	CA-C	-7.07	1.44	1.52
1	A	604	ILE	CA-CB	-7.06	1.43	1.55
3	D	124	GLN	N-CA	7.06	1.55	1.46
2	E	5	VAL	CA-CB	-7.03	1.45	1.54
2	C	100	VAL	CA-CB	7.03	1.64	1.54
1	A	18	LYS	CA-C	7.01	1.61	1.52
3	F	137	GLN	CA-C	7.00	1.63	1.52
1	B	520	VAL	CA-CB	-7.00	1.45	1.54
3	D	171	VAL	CA-CB	-6.99	1.45	1.54
1	B	486	ALA	CA-C	-6.98	1.45	1.53
1	A	287	LYS	CA-C	6.97	1.62	1.52
3	F	168	SER	CA-CB	6.97	1.61	1.53
1	B	272	ARG	N-CA	6.96	1.55	1.46
1	A	651	TRP	CA-C	-6.96	1.42	1.52
1	A	292	LYS	N-CA	6.94	1.54	1.45
2	E	192	ALA	CA-C	-6.94	1.44	1.52
1	A	658	GLU	CA-C	-6.94	1.43	1.52
2	E	181	THR	CA-CB	6.94	1.61	1.53
1	B	716	PRO	CA-C	-6.93	1.46	1.52
1	B	470	MET	SD-CE	6.93	1.96	1.79
1	B	311	THR	CA-CB	6.92	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	64	LYS	CA-C	6.90	1.61	1.52
2	C	146	VAL	CA-CB	-6.89	1.46	1.54
1	B	583	GLU	CA-C	-6.88	1.43	1.52
3	D	20	GLU	N-CA	6.88	1.55	1.46
3	F	93	LEU	N-CA	-6.86	1.40	1.45
2	E	26	VAL	CA-CB	6.80	1.61	1.54
3	F	28	LEU	CA-C	6.78	1.62	1.52
1	A	513	ASP	CA-C	6.76	1.62	1.52
2	E	165	GLU	CA-C	6.76	1.61	1.52
1	A	46	SER	CA-CB	6.75	1.64	1.53
2	C	156	ASN	CB-CG	6.74	1.69	1.52
1	B	26	GLN	CA-C	-6.74	1.44	1.52
2	E	49	ILE	CA-CB	-6.73	1.46	1.54
2	C	197	ILE	CA-C	-6.72	1.42	1.52
1	B	75	ALA	CA-CB	-6.70	1.43	1.53
1	A	715	THR	C-O	-6.70	1.18	1.25
3	F	68	ILE	C-O	6.69	1.32	1.24
1	B	463	LEU	N-CA	6.69	1.54	1.46
3	F	180	GLN	CB-CG	6.64	1.72	1.52
1	A	246	MET	SD-CE	6.63	1.96	1.79
1	B	499	LEU	CA-C	6.62	1.61	1.52
3	F	141	VAL	CA-CB	-6.62	1.45	1.54
3	F	114	PHE	CA-C	-6.61	1.44	1.52
1	B	290	SER	CA-C	-6.60	1.44	1.52
3	F	121	VAL	CA-CB	6.59	1.63	1.54
1	B	195	LEU	CA-C	6.58	1.61	1.52
1	A	693	ARG	NE-CZ	-6.58	1.25	1.33
2	C	10	THR	CA-CB	6.57	1.63	1.53
1	B	364	CYS	CA-C	-6.57	1.44	1.52
2	E	188	LYS	CA-C	6.54	1.61	1.52
1	A	647	GLU	CA-C	-6.51	1.45	1.53
2	C	182	ILE	CA-C	-6.51	1.45	1.52
1	A	308	GLU	CA-C	6.49	1.61	1.52
2	E	47	MET	SD-CE	6.48	1.95	1.79
3	F	139	VAL	CA-C	-6.47	1.46	1.52
1	B	451	ILE	CA-CB	-6.45	1.46	1.54
1	B	289	VAL	CA-CB	6.44	1.63	1.54
1	A	317	ILE	CA-CB	6.44	1.65	1.54
2	E	60	VAL	N-CA	-6.43	1.38	1.46
2	C	62	VAL	CA-CB	-6.43	1.45	1.54
1	A	250	LEU	CG-CD1	6.42	1.73	1.52
1	B	462	GLN	N-CA	6.41	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	656	ALA	CA-CB	6.41	1.64	1.53
1	A	672	ILE	CA-C	6.40	1.59	1.52
2	E	173	GLU	CA-C	-6.40	1.45	1.52
3	D	141	VAL	C-O	-6.40	1.16	1.24
1	B	531	VAL	CA-CB	-6.39	1.46	1.54
3	D	120	ILE	CA-CB	-6.39	1.45	1.54
2	C	225	SER	CA-C	-6.39	1.44	1.53
1	B	266	GLU	C-O	-6.37	1.15	1.24
1	A	572	LEU	CA-C	6.37	1.61	1.52
1	A	578	MET	SD-CE	6.37	1.95	1.79
1	B	88	ALA	CA-CB	-6.36	1.43	1.53
2	E	56	ASP	CA-C	-6.36	1.45	1.52
1	B	580	ARG	NE-CZ	6.35	1.40	1.33
1	B	397	ALA	CA-C	-6.35	1.44	1.53
3	D	93	LEU	C-O	-6.34	1.18	1.24
1	B	677	ALA	CA-C	6.34	1.58	1.52
1	A	471	THR	CA-C	-6.33	1.44	1.53
1	B	602	MET	SD-CE	6.33	1.95	1.79
1	B	628	THR	CA-CB	6.33	1.61	1.53
1	B	131	GLU	CA-C	-6.31	1.45	1.53
3	D	35	LYS	CA-C	6.31	1.60	1.52
3	F	184	GLN	CA-C	6.30	1.59	1.53
1	A	649	THR	CA-CB	6.30	1.63	1.53
1	B	626	ALA	CA-CB	6.29	1.63	1.53
1	A	203	LEU	C-O	6.28	1.31	1.24
2	C	139	ASN	CA-C	-6.28	1.45	1.53
1	B	626	ALA	CA-C	6.26	1.61	1.53
3	F	182	ARG	NE-CZ	6.24	1.40	1.33
3	F	35	LYS	CA-C	6.23	1.60	1.52
1	A	568	MET	CA-C	-6.22	1.44	1.52
2	E	133	SER	CA-C	-6.20	1.45	1.52
1	B	537	ASP	C-O	-6.20	1.16	1.24
1	B	346	ILE	CG1-CD1	6.19	1.75	1.51
3	D	64	LYS	CA-C	6.19	1.60	1.52
2	E	229	VAL	CA-CB	6.19	1.61	1.54
1	B	243	PHE	C-O	6.18	1.31	1.24
2	C	150	GLN	CA-C	6.18	1.60	1.52
1	B	424	ILE	CA-CB	6.17	1.61	1.54
1	B	246	MET	SD-CE	-6.16	1.64	1.79
1	A	432	ALA	CA-C	6.15	1.61	1.52
1	B	332	GLN	CA-C	-6.13	1.44	1.52
1	B	515	LEU	C-O	6.13	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	82	LEU	C-O	-6.11	1.16	1.24
1	B	663	GLU	CA-C	6.11	1.61	1.52
2	E	235	PRO	CA-C	6.09	1.59	1.52
3	D	83	ILE	CB-CG2	-6.09	1.32	1.52
3	F	40	VAL	CA-CB	6.09	1.63	1.54
1	A	294	VAL	CA-C	6.08	1.60	1.52
3	F	15	ARG	CB-CG	6.07	1.70	1.52
3	F	159	VAL	CA-C	6.07	1.60	1.52
1	A	573	GLU	C-O	-6.06	1.16	1.24
2	C	150	GLN	CG-CD	6.04	1.67	1.52
1	B	372	GLU	N-CA	-6.04	1.38	1.46
3	F	124	GLN	C-O	6.03	1.30	1.23
1	A	670	TYR	CA-C	-6.03	1.45	1.52
2	C	107	VAL	CA-CB	-6.03	1.46	1.54
3	F	140	ASN	C-O	6.02	1.30	1.23
1	A	357	ILE	CA-CB	-6.01	1.45	1.54
1	A	450	GLN	C-O	-5.99	1.17	1.24
3	F	15	ARG	CA-C	5.98	1.60	1.52
3	F	140	ASN	CB-CG	5.96	1.67	1.52
1	A	218	ALA	CA-C	-5.96	1.45	1.52
1	B	568	MET	SD-CE	5.96	1.94	1.79
1	A	309	ILE	CA-C	5.96	1.59	1.52
3	D	122	GLU	C-O	5.95	1.31	1.24
1	B	144	ILE	CA-C	5.95	1.60	1.52
3	F	5	VAL	CA-C	-5.95	1.45	1.52
3	F	176	ALA	C-O	5.95	1.31	1.23
1	B	345	CYS	CA-C	-5.94	1.45	1.52
3	F	129	VAL	CA-C	5.93	1.60	1.52
1	A	70	THR	CA-CB	5.93	1.63	1.53
3	F	132	ARG	NE-CZ	5.93	1.39	1.33
1	B	428	LEU	CA-C	-5.93	1.44	1.52
1	B	505	PRO	C-O	5.93	1.30	1.23
3	F	167	GLY	CA-C	5.93	1.57	1.51
1	B	61	CYS	CA-C	5.92	1.59	1.52
3	F	161	LYS	C-O	5.92	1.32	1.24
1	A	557	THR	C-O	5.91	1.30	1.24
1	A	727	TYR	CA-C	-5.91	1.45	1.52
3	F	37	VAL	CA-CB	5.91	1.61	1.54
3	D	179	VAL	N-CA	5.89	1.53	1.46
1	A	712	ALA	CA-CB	-5.88	1.44	1.53
1	A	526	LYS	CA-C	5.88	1.60	1.52
2	C	60	VAL	N-CA	-5.88	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	21	GLU	CA-CB	5.88	1.63	1.53
1	B	533	ILE	CA-C	5.88	1.59	1.53
1	B	652	ASN	CA-C	5.87	1.60	1.52
1	B	22	ASN	CA-C	-5.87	1.45	1.52
1	A	268	ALA	CA-C	5.86	1.60	1.53
2	C	84	ALA	CA-C	-5.86	1.45	1.52
1	A	316	ASP	CA-C	-5.85	1.45	1.52
1	A	414	THR	CA-C	-5.85	1.45	1.52
3	F	119	TYR	CA-C	5.84	1.59	1.52
1	A	105	TRP	CA-C	-5.84	1.45	1.52
1	A	27	VAL	CA-C	5.84	1.59	1.52
1	A	432	ALA	C-O	5.84	1.31	1.24
1	B	477	GLN	CA-CB	5.84	1.62	1.53
3	F	168	SER	N-CA	5.84	1.53	1.46
3	F	180	GLN	CG-CD	5.84	1.66	1.52
3	F	183	SER	CA-C	5.83	1.61	1.53
1	B	250	LEU	N-CA	-5.83	1.39	1.46
1	B	696	GLU	CA-C	5.83	1.60	1.52
1	B	468	LYS	CG-CD	5.82	1.70	1.52
1	B	446	TYR	CA-C	-5.82	1.45	1.52
1	A	409	MET	SD-CE	-5.82	1.65	1.79
2	E	124	ASP	CA-C	5.82	1.58	1.53
1	B	354	ARG	CA-CB	-5.81	1.44	1.53
1	A	448	GLU	CA-C	-5.81	1.45	1.52
1	A	709	GLU	N-CA	5.81	1.54	1.46
2	E	136	SER	C-O	5.80	1.30	1.24
1	B	111	ALA	CA-CB	-5.79	1.43	1.53
1	A	2	ARG	NE-CZ	5.79	1.39	1.33
2	C	6	ALA	CA-C	-5.79	1.45	1.52
1	B	357	ILE	CA-CB	-5.79	1.46	1.54
1	B	601	ARG	CG-CD	5.79	1.69	1.52
2	E	97	ALA	N-CA	5.78	1.53	1.46
3	F	44	GLN	CA-CB	5.78	1.61	1.53
1	B	499	LEU	C-O	5.77	1.30	1.24
2	C	231	ARG	C-O	-5.77	1.16	1.23
3	F	174	VAL	CA-CB	5.75	1.62	1.54
1	A	510	SER	CA-C	5.74	1.60	1.52
1	B	601	ARG	CA-C	5.73	1.59	1.52
1	B	18	LYS	CA-C	5.73	1.59	1.52
3	F	10	ARG	NE-CZ	5.73	1.39	1.33
1	A	275	GLN	CB-CG	5.73	1.69	1.52
1	A	289	VAL	CA-CB	5.73	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	VAL	CA-CB	-5.72	1.46	1.54
1	B	7	ASP	C-O	5.72	1.31	1.24
1	B	115	GLU	CA-C	5.72	1.60	1.52
2	C	32	MET	CG-SD	-5.72	1.66	1.80
1	B	690	ARG	CA-C	5.71	1.60	1.52
3	F	74	VAL	CA-CB	5.70	1.60	1.54
1	A	481	ASP	CA-C	-5.70	1.45	1.52
1	A	206	LEU	CA-CB	-5.69	1.44	1.53
1	A	275	GLN	CG-CD	5.68	1.66	1.52
1	A	481	ASP	N-CA	-5.68	1.39	1.46
3	D	51	ALA	CA-C	5.66	1.60	1.52
3	D	41	ILE	CA-CB	-5.66	1.47	1.54
2	E	10	THR	CA-C	-5.66	1.45	1.52
3	F	167	GLY	C-O	5.66	1.30	1.24
1	B	516	THR	CA-C	5.66	1.59	1.52
2	E	156	ASN	CB-CG	5.65	1.66	1.52
1	B	484	ILE	CA-CB	-5.65	1.47	1.53
1	B	662	ALA	CA-C	5.65	1.60	1.52
3	D	45	ALA	CA-CB	-5.65	1.43	1.53
1	A	586	VAL	CA-CB	-5.65	1.47	1.54
1	B	318	ILE	CA-C	5.65	1.59	1.52
3	F	51	ALA	CA-CB	5.65	1.62	1.53
1	A	248	ASP	CB-CG	5.64	1.66	1.52
2	E	143	ALA	CA-C	5.63	1.59	1.52
2	C	144	ALA	C-O	-5.63	1.17	1.23
2	E	118	ALA	C-O	-5.62	1.17	1.23
1	B	722	ASN	CA-C	5.62	1.59	1.52
3	F	35	LYS	C-O	5.62	1.30	1.24
1	B	270	PRO	CA-C	-5.62	1.46	1.52
3	F	175	ASP	C-O	5.61	1.30	1.23
2	C	142	HIS	C-O	5.61	1.31	1.23
1	A	74	SER	CA-C	-5.61	1.45	1.53
3	D	76	GLU	C-O	-5.61	1.17	1.24
3	D	167	GLY	CA-C	5.61	1.57	1.51
1	B	168	VAL	CA-CB	5.60	1.60	1.53
1	B	106	TYR	CA-C	-5.60	1.45	1.52
1	B	492	ASN	C-O	5.58	1.30	1.23
1	B	405	ALA	CA-CB	-5.58	1.44	1.53
2	C	116	VAL	CA-CB	-5.58	1.47	1.54
1	A	18	LYS	C-O	5.57	1.30	1.24
2	E	88	TRP	CA-C	5.57	1.59	1.52
2	C	186	ILE	CA-CB	-5.57	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	THR	CA-C	-5.57	1.45	1.52
1	B	583	GLU	CA-CB	-5.57	1.44	1.53
1	A	533	ILE	CA-CB	-5.57	1.47	1.54
1	A	5	LYS	N-CA	5.56	1.53	1.46
2	C	118	ALA	C-O	-5.56	1.16	1.23
1	A	19	THR	N-CA	5.55	1.52	1.46
1	A	363	ILE	CA-C	-5.55	1.45	1.52
3	F	176	ALA	CA-C	5.55	1.59	1.53
1	B	14	GLN	CA-C	5.55	1.60	1.52
1	A	343	ARG	NE-CZ	5.52	1.39	1.33
1	A	451	ILE	CA-CB	-5.52	1.47	1.54
1	A	287	LYS	C-O	5.52	1.30	1.24
3	D	178	SER	CA-CB	5.52	1.62	1.53
1	B	529	LYS	CA-C	5.52	1.60	1.52
1	A	343	ARG	CA-C	-5.51	1.46	1.52
1	A	402	SER	CA-C	-5.51	1.45	1.52
1	A	119	THR	CA-CB	-5.50	1.44	1.53
1	B	563	HIS	CA-CB	5.50	1.61	1.53
1	A	283	VAL	CA-CB	5.50	1.60	1.54
1	A	625	ASP	CA-C	-5.50	1.45	1.52
1	B	216	ASP	CA-C	5.48	1.59	1.52
1	A	278	HIS	N-CA	5.48	1.53	1.46
1	A	449	THR	CA-CB	-5.47	1.44	1.53
3	D	74	VAL	CA-CB	5.46	1.60	1.54
1	B	626	ALA	C-O	5.45	1.31	1.23
3	F	11	ARG	CA-C	5.45	1.60	1.52
1	A	195	LEU	CA-C	5.45	1.60	1.52
1	A	418	THR	CA-C	-5.45	1.46	1.52
1	A	273	PHE	CA-C	-5.43	1.45	1.52
3	F	161	LYS	N-CA	5.43	1.54	1.46
1	B	543	PRO	CB-CG	-5.43	1.22	1.49
1	B	519	GLN	N-CA	5.43	1.53	1.46
1	B	56	LEU	CA-C	-5.43	1.46	1.52
1	A	483	VAL	CA-CB	-5.42	1.47	1.54
1	A	212	ALA	CA-C	5.42	1.59	1.52
1	B	139	MET	N-CA	-5.42	1.39	1.46
1	B	209	VAL	C-O	5.41	1.30	1.24
3	D	180	GLN	CG-CD	5.40	1.65	1.52
2	E	232	MET	CG-SD	5.39	1.94	1.80
1	A	294	VAL	CA-CB	5.39	1.61	1.54
1	B	294	VAL	CA-C	5.38	1.59	1.52
1	A	470	MET	SD-CE	5.38	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	82	LEU	CA-C	-5.38	1.45	1.52
3	D	93	LEU	CA-C	-5.38	1.47	1.52
2	C	29	ASP	CB-CG	5.37	1.65	1.52
1	A	591	ASP	CA-C	-5.36	1.45	1.53
3	F	79	VAL	CA-CB	5.36	1.60	1.54
1	A	464	ALA	CA-C	-5.36	1.46	1.52
1	B	414	THR	CA-C	-5.36	1.46	1.52
1	B	480	ALA	CA-C	-5.36	1.45	1.52
1	A	283	VAL	C-O	5.35	1.30	1.24
1	A	582	HIS	CA-CB	5.35	1.62	1.53
3	F	175	ASP	CA-C	5.35	1.59	1.52
1	B	325	ILE	CA-CB	-5.34	1.47	1.54
2	E	6	ALA	CA-C	-5.33	1.46	1.52
1	B	505	PRO	CA-C	5.33	1.58	1.52
3	F	10	ARG	CZ-NH1	5.33	1.40	1.32
3	D	6	ILE	CA-C	-5.33	1.45	1.52
1	A	274	TYR	N-CA	5.33	1.52	1.46
3	F	116	THR	CA-CB	-5.32	1.45	1.53
1	B	95	LYS	CA-C	5.32	1.59	1.52
3	F	7	ALA	N-CA	5.32	1.52	1.45
1	A	199	ALA	N-CA	5.31	1.53	1.46
1	B	360	PRO	CA-C	-5.31	1.47	1.52
1	A	560	SER	N-CA	-5.30	1.39	1.46
1	B	464	ALA	CA-C	-5.29	1.46	1.52
1	B	538	THR	N-CA	-5.29	1.39	1.46
1	A	558	ILE	CA-CB	-5.29	1.47	1.54
3	D	27	GLY	CA-C	5.29	1.59	1.51
1	A	248	ASP	CA-C	5.29	1.59	1.52
1	A	374	TYR	C-O	-5.29	1.18	1.23
1	B	171	ALA	CA-CB	-5.28	1.46	1.53
1	A	681	ILE	CA-CB	-5.27	1.47	1.54
2	E	57	VAL	CA-CB	5.27	1.61	1.54
1	B	350	VAL	N-CA	-5.26	1.39	1.46
1	B	98	ALA	CA-CB	-5.26	1.45	1.53
1	A	550	ALA	CA-C	-5.26	1.46	1.52
1	A	607	ILE	CA-CB	-5.24	1.48	1.54
2	E	236	GLU	N-CA	5.24	1.56	1.46
3	F	85	ALA	CA-C	5.24	1.59	1.52
1	A	100	ALA	CA-C	-5.24	1.46	1.52
3	D	171	VAL	CA-C	-5.23	1.46	1.52
3	F	62	VAL	CA-C	5.23	1.59	1.52
1	B	596	ARG	C-O	5.23	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	40	ASP	CA-C	-5.23	1.45	1.52
2	E	223	ALA	CA-CB	5.23	1.61	1.53
1	B	254	TRP	CB-CG	-5.22	1.34	1.50
3	D	93	LEU	N-CA	-5.22	1.41	1.45
1	A	235	GLU	CA-C	-5.22	1.46	1.52
3	D	93	LEU	C-N	-5.21	1.26	1.33
1	B	268	ALA	CA-CB	-5.21	1.45	1.52
1	A	387	LYS	CA-CB	5.21	1.60	1.53
1	B	60	TYR	N-CA	-5.20	1.39	1.46
3	F	152	VAL	CA-CB	5.19	1.60	1.54
3	F	169	PRO	C-O	5.19	1.30	1.23
2	E	149	LEU	N-CA	-5.18	1.40	1.46
3	F	9	HIS	CA-C	5.18	1.59	1.52
1	A	713	TRP	CA-C	-5.18	1.46	1.52
3	F	121	VAL	CB-CG2	-5.17	1.35	1.52
3	D	180	GLN	CA-CB	5.17	1.60	1.53
1	A	623	PRO	CA-C	-5.16	1.47	1.52
1	B	118	ALA	CA-CB	-5.15	1.45	1.53
1	A	153	ASP	CA-C	5.15	1.60	1.52
1	A	693	ARG	N-CA	-5.14	1.40	1.46
1	A	447	ARG	CA-CB	-5.14	1.44	1.53
1	B	219	ILE	CG1-CD1	5.13	1.71	1.51
3	D	131	THR	CA-CB	-5.13	1.44	1.53
1	B	205	THR	N-CA	-5.13	1.40	1.46
1	B	363	ILE	CA-C	-5.13	1.48	1.52
3	D	91	VAL	N-CA	-5.12	1.40	1.46
1	B	510	SER	CA-C	5.11	1.59	1.52
1	B	647	GLU	CA-C	-5.10	1.48	1.53
3	F	143	VAL	C-O	5.10	1.29	1.24
1	A	459	LYS	CA-C	5.10	1.59	1.52
2	E	220	VAL	C-O	5.10	1.30	1.24
1	B	465	LEU	CA-C	-5.09	1.46	1.52
2	E	118	ALA	CA-C	-5.09	1.46	1.52
3	F	94	PRO	CA-C	5.09	1.57	1.52
2	C	107	VAL	N-CA	-5.08	1.40	1.46
1	A	521	MET	SD-CE	5.08	1.92	1.79
1	B	464	ALA	CA-CB	-5.08	1.45	1.53
2	E	159	VAL	CA-CB	5.08	1.60	1.54
1	B	689	HIS	N-CA	-5.07	1.40	1.46
1	A	266	GLU	CA-C	-5.07	1.45	1.52
1	B	569	HIS	CA-C	-5.07	1.46	1.52
3	D	79	VAL	C-O	-5.07	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	9	GLN	C-O	5.06	1.30	1.24
1	A	692	ALA	CA-C	-5.06	1.46	1.52
2	E	223	ALA	CA-C	5.05	1.59	1.52
1	B	249	SER	CA-C	5.05	1.59	1.52
1	A	118	ALA	CA-CB	-5.05	1.45	1.53
1	B	437	LEU	CG-CD1	-5.05	1.35	1.52
1	A	95	LYS	CG-CD	5.04	1.67	1.52
1	B	699	ASN	N-CA	-5.04	1.41	1.46
1	B	89	MET	SD-CE	5.04	1.92	1.79
1	B	507	ALA	CA-CB	5.03	1.60	1.53
1	B	583	GLU	C-O	-5.03	1.17	1.24
1	A	87	LYS	CA-C	5.03	1.59	1.52
1	A	684	ALA	CA-CB	-5.03	1.45	1.53
1	B	124	SER	CA-C	5.03	1.58	1.52
1	B	601	ARG	CB-CG	5.02	1.67	1.52
2	E	89	ASP	C-O	5.02	1.30	1.23
1	B	271	SER	N-CA	-5.02	1.39	1.46
2	C	81	ALA	CA-C	-5.02	1.46	1.52
1	A	291	LYS	CD-CE	5.02	1.67	1.52
1	A	607	ILE	C-O	5.02	1.30	1.24
1	A	153	ASP	CB-CG	5.01	1.64	1.52
1	B	236	ALA	C-O	5.01	1.29	1.24
3	F	188	TYR	CE1-CZ	5.01	1.50	1.38
3	F	44	GLN	CB-CG	5.00	1.67	1.52
3	F	128	LEU	C-O	5.00	1.30	1.24

All (637) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	621	VAL	CB-CA-C	11.91	123.99	110.41
1	A	556	VAL	N-CA-C	11.17	123.99	107.80
1	B	53	TRP	N-CA-C	-11.02	95.68	110.55
1	A	318	ILE	N-CA-C	10.95	123.53	106.88
1	B	556	VAL	N-CA-C	10.49	123.07	107.75
3	F	80	SER	N-CA-C	-10.36	99.98	111.07
1	B	169	TYR	N-CA-C	-10.31	92.35	109.46
2	E	15	GLU	N-CA-C	-10.07	95.62	110.52
1	B	8	ILE	N-CA-C	-9.97	100.45	110.62
1	A	434	LEU	N-CA-C	9.88	122.19	109.64
1	A	469	PRO	N-CD-CG	-9.71	88.64	103.20
3	D	91	VAL	CB-CA-C	9.40	124.62	110.62
1	B	463	LEU	N-CA-C	9.38	125.02	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	461	SER	N-CA-C	-9.31	97.36	110.50
1	B	462	GLN	N-CA-C	9.08	123.34	108.26
2	E	89	ASP	N-CA-C	-8.96	94.90	108.52
2	C	101	GLY	N-CA-C	-8.93	101.69	112.49
1	A	686	PHE	N-CA-C	-8.87	100.78	111.69
3	F	22	ILE	N-CA-C	-8.83	101.94	110.42
1	A	448	GLU	N-CA-C	-8.83	100.83	111.69
1	A	672	ILE	N-CA-C	8.76	121.34	108.65
3	D	179	VAL	N-CA-C	8.70	120.30	108.11
1	B	106	TYR	N-CA-C	-8.61	94.03	108.75
1	B	363	ILE	N-CA-C	-8.57	98.08	108.53
1	A	647	GLU	CA-C-N	-8.53	109.11	122.67
1	A	647	GLU	C-N-CA	-8.53	109.11	122.67
1	B	569	HIS	N-CA-C	-8.51	101.03	111.33
1	B	716	PRO	CB-CA-C	-8.50	103.67	111.40
3	F	179	VAL	N-CA-C	8.49	120.34	107.77
1	A	292	LYS	N-CA-C	8.46	121.70	110.36
2	C	197	ILE	N-CA-C	-8.46	100.10	111.44
1	B	500	THR	CB-CA-C	8.43	122.68	109.03
2	C	182	ILE	CB-CA-C	-8.40	100.23	111.15
2	E	146	VAL	N-CA-C	8.39	119.36	108.12
1	A	53	TRP	N-CA-C	-8.36	98.71	110.50
1	A	215	SER	N-CA-C	8.34	122.42	111.75
1	B	515	LEU	N-CA-C	8.28	123.34	109.76
1	B	318	ILE	N-CA-C	8.27	119.45	106.88
1	B	505	PRO	CB-CA-C	8.25	121.44	111.46
1	B	212	ALA	N-CA-C	8.22	119.93	110.97
1	B	403	GLU	N-CA-C	-8.14	101.47	111.40
1	A	205	THR	N-CA-C	-8.12	102.51	111.36
1	A	168	VAL	N-CA-C	-8.11	94.39	107.28
3	F	35	LYS	N-CA-C	8.11	121.73	108.52
1	A	445	ASP	N-CA-C	-8.04	102.47	111.07
3	F	111	GLY	CA-C-O	8.03	126.96	120.30
1	B	527	ILE	CA-C-N	8.00	127.60	119.92
1	B	527	ILE	C-N-CA	8.00	127.60	119.92
3	F	143	VAL	CB-CA-C	-7.94	97.98	110.69
1	B	689	HIS	N-CA-C	-7.94	102.57	111.14
2	E	7	VAL	N-CA-C	7.89	120.88	108.89
1	B	591	ASP	N-CA-C	-7.88	101.82	113.40
1	A	226	ASP	N-CA-C	-7.85	97.06	109.23
1	B	409	MET	N-CA-C	-7.85	102.71	111.82
3	D	35	LYS	N-CA-C	7.81	122.56	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ASP	O-C-N	7.79	126.68	121.23
1	B	661	TRP	N-CA-CB	7.79	121.81	110.20
1	A	516	THR	N-CA-CB	7.79	118.78	109.74
1	B	262	ALA	CA-C-N	-7.79	109.32	123.34
1	B	262	ALA	C-N-CA	-7.79	109.32	123.34
3	F	15	ARG	NE-CZ-NH2	7.78	126.20	119.20
1	A	299	ARG	CA-C-N	-7.73	111.29	122.19
1	A	299	ARG	C-N-CA	-7.73	111.29	122.19
2	C	189	PRO	CB-CA-C	-7.72	101.83	111.64
1	B	448	GLU	N-CA-C	-7.72	102.95	111.36
1	B	366	GLN	N-CA-C	-7.71	104.40	113.88
1	A	289	VAL	CB-CA-C	7.70	118.19	110.65
1	B	205	THR	N-CA-C	-7.70	102.97	111.36
3	D	120	ILE	N-CA-C	7.68	119.90	108.46
1	B	545	LEU	N-CA-C	-7.65	102.89	111.07
3	D	186	LYS	N-CA-C	-7.62	101.43	108.75
3	F	129	VAL	CB-CA-C	7.61	120.89	110.99
1	B	612	SER	CA-C-N	-7.59	112.24	122.72
1	B	612	SER	C-N-CA	-7.59	112.24	122.72
2	E	203	LYS	N-CA-C	7.57	119.31	109.93
1	A	334	VAL	CB-CA-C	-7.56	101.96	111.94
1	B	647	GLU	CA-C-N	-7.53	111.33	122.86
1	B	647	GLU	C-N-CA	-7.53	111.33	122.86
3	F	49	VAL	N-CA-CB	7.53	115.57	110.52
1	B	133	LEU	CA-C-N	-7.52	112.18	122.86
1	B	133	LEU	C-N-CA	-7.52	112.18	122.86
1	B	548	LYS	N-CA-C	-7.51	102.70	111.03
1	B	272	ARG	NE-CZ-NH2	7.48	125.93	119.20
1	B	72	ARG	CA-C-N	-7.48	112.68	123.00
1	B	72	ARG	C-N-CA	-7.48	112.68	123.00
1	B	133	LEU	N-CA-C	-7.45	102.72	112.41
2	C	234	ILE	CB-CA-C	-7.44	102.86	110.89
1	B	613	LYS	N-CA-C	7.42	121.34	109.24
3	F	148	LYS	N-CA-C	7.40	120.48	108.63
1	A	709	GLU	N-CA-C	7.38	119.94	110.65
2	E	37	GLU	N-CA-C	7.35	118.93	111.07
1	B	569	HIS	CA-C-O	-7.34	112.70	120.63
1	A	711	ILE	CB-CA-C	-7.33	100.93	111.34
3	F	184	GLN	N-CA-C	7.30	119.42	107.23
2	E	88	TRP	N-CA-C	7.29	119.95	108.79
1	A	344	VAL	CB-CA-C	-7.29	102.14	110.96
1	B	272	ARG	NE-CZ-NH1	-7.28	114.22	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	THR	N-CA-C	-7.26	104.45	113.38
1	A	511	LEU	N-CA-C	7.26	117.94	109.60
1	B	459	LYS	N-CA-C	7.24	120.21	111.82
1	A	640	LEU	N-CA-C	7.21	119.53	109.15
3	D	6	ILE	N-CA-C	-7.20	97.23	107.75
1	B	648	CYS	CA-C-N	7.20	129.79	120.44
1	B	648	CYS	C-N-CA	7.20	129.79	120.44
1	B	458	ASN	CA-C-N	-7.17	109.41	120.31
1	B	458	ASN	C-N-CA	-7.17	109.41	120.31
1	B	152	VAL	N-CA-C	-7.17	103.35	110.30
1	A	363	ILE	N-CA-C	-7.17	94.43	109.34
1	B	79	ASP	N-CA-C	7.16	118.96	108.86
1	B	406	ARG	N-CA-C	-7.16	103.41	111.07
1	A	379	HIS	N-CA-C	-7.16	99.52	110.32
3	F	46	ASP	CB-CA-C	-7.15	98.97	110.84
1	B	711	ILE	N-CA-C	7.15	118.80	109.58
1	A	706	TYR	N-CA-C	-7.15	98.88	109.81
3	F	83	ILE	CG1-CB-CG2	-7.14	89.27	110.70
1	B	520	VAL	CB-CA-C	-7.13	102.51	112.14
1	A	220	ALA	CA-C-N	-7.13	111.39	122.87
1	A	220	ALA	C-N-CA	-7.13	111.39	122.87
1	B	186	LYS	CA-C-N	-7.13	112.03	122.65
1	B	186	LYS	C-N-CA	-7.13	112.03	122.65
2	E	173	GLU	N-CA-C	-7.13	97.28	108.90
1	A	221	THR	CA-C-N	-7.09	112.65	122.93
1	A	221	THR	C-N-CA	-7.09	112.65	122.93
1	B	450	GLN	N-CA-C	7.05	119.05	111.36
1	A	399	PRO	N-CA-C	-7.04	102.38	113.78
3	F	133	GLY	N-CA-C	-7.04	101.83	113.02
1	B	349	ASN	CA-C-N	-7.03	109.36	120.47
1	B	349	ASN	C-N-CA	-7.03	109.36	120.47
2	C	39	ASP	N-CA-C	-7.02	103.39	112.23
1	A	469	PRO	CA-C-O	-7.01	113.44	121.36
3	F	180	GLN	N-CA-CB	6.98	121.05	109.60
1	A	428	LEU	N-CA-C	-6.98	104.24	112.89
1	B	500	THR	N-CA-C	-6.98	105.30	113.88
1	A	456	LYS	N-CA-C	-6.96	103.69	111.28
1	A	133	LEU	CA-C-N	-6.96	112.91	123.07
1	A	133	LEU	C-N-CA	-6.96	112.91	123.07
1	B	726	GLU	N-CA-C	6.95	122.34	107.67
2	C	5	VAL	CB-CA-C	-6.95	100.90	110.77
1	A	4	PRO	CA-C-O	-6.95	108.67	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	SER	CB-CA-C	-6.95	101.21	111.77
3	D	83	ILE	CG1-CB-CG2	-6.94	89.87	110.70
1	B	141	LEU	N-CA-C	6.94	120.63	111.75
1	B	454	LEU	CA-CB-CG	-6.93	92.03	116.30
1	B	379	HIS	N-CA-C	-6.91	100.77	110.31
2	C	219	ASP	N-CA-C	-6.89	105.41	113.88
3	F	122	GLU	N-CA-C	6.88	120.74	109.72
1	A	465	LEU	N-CA-C	-6.85	99.03	109.85
1	B	164	ASP	N-CA-C	-6.85	105.06	113.41
1	B	132	THR	CA-C-N	-6.84	111.74	122.49
1	B	132	THR	C-N-CA	-6.84	111.74	122.49
3	D	89	SER	N-CA-C	6.84	118.81	111.36
1	B	414	THR	N-CA-C	-6.82	97.78	108.90
2	C	10	THR	N-CA-C	-6.82	100.11	110.14
1	A	25	TYR	CA-CB-CG	6.80	126.14	113.90
1	A	409	MET	N-CA-C	-6.79	103.94	111.82
1	B	124	SER	CA-C-N	-6.79	111.47	121.24
1	B	124	SER	C-N-CA	-6.79	111.47	121.24
3	D	158	SER	N-CA-C	-6.79	102.83	111.92
3	D	93	LEU	CD1-CG-CD2	-6.78	95.88	110.80
1	A	275	GLN	CA-CB-CG	6.78	127.66	114.10
2	C	15	GLU	N-CA-C	-6.77	100.46	110.48
1	B	344	VAL	N-CA-C	6.77	118.58	108.23
3	D	150	THR	N-CA-C	-6.77	96.71	108.69
1	A	563	HIS	N-CA-C	-6.76	98.22	109.24
1	B	621	VAL	N-CA-CB	-6.75	103.56	112.34
3	F	18	SER	N-CA-C	-6.75	103.73	112.23
1	B	552	ALA	N-CA-C	-6.74	104.80	113.16
1	B	254	TRP	CA-CB-CG	-6.73	100.81	113.60
2	C	53	SER	N-CA-C	6.71	120.12	109.65
2	C	72	SER	CA-CB-OG	-6.71	97.67	111.10
1	A	444	ARG	N-CA-C	-6.70	104.12	112.90
1	A	271	SER	N-CA-C	-6.70	105.08	113.18
1	A	222	ARG	CB-CA-C	6.70	121.43	109.38
1	A	110	HIS	N-CA-C	-6.69	104.99	113.02
2	C	194	LEU	CA-C-N	6.69	129.25	120.28
2	C	194	LEU	C-N-CA	6.69	129.25	120.28
1	B	628	THR	CA-C-N	-6.68	111.86	122.29
1	B	628	THR	C-N-CA	-6.68	111.86	122.29
3	F	135	TYR	N-CA-C	6.68	120.61	111.39
1	B	434	LEU	N-CA-C	6.67	117.27	109.60
1	A	402	SER	N-CA-C	-6.66	103.50	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	TRP	N-CA-C	6.66	120.66	112.54
1	A	529	LYS	N-CA-C	6.65	118.22	110.97
1	A	617	ARG	CG-CD-NE	6.65	126.62	112.00
3	D	73	ASP	N-CA-C	-6.64	103.97	111.07
1	A	693	ARG	CG-CD-NE	-6.63	97.41	112.00
1	A	621	VAL	CB-CA-C	6.62	120.49	110.62
3	D	123	TYR	N-CA-C	6.62	119.82	110.23
2	C	156	ASN	N-CA-C	-6.61	104.97	113.16
1	B	348	CYS	N-CA-C	-6.61	105.38	113.50
1	A	599	PRO	CB-CA-C	6.60	119.84	111.39
3	D	133	GLY	N-CA-C	-6.59	98.66	111.12
3	F	179	VAL	CB-CA-C	-6.59	101.53	110.42
1	A	622	SER	N-CA-C	6.58	117.17	109.60
1	B	19	THR	N-CA-C	6.58	119.14	108.41
1	A	126	TYR	N-CA-C	6.57	119.40	109.41
1	A	91	ASP	N-CA-C	-6.57	104.04	111.07
2	E	123	SER	N-CA-C	-6.57	104.75	112.89
1	A	413	TYR	CA-C-N	-6.56	113.87	123.05
1	A	413	TYR	C-N-CA	-6.56	113.87	123.05
2	C	146	VAL	N-CA-C	6.54	118.24	108.23
1	A	70	THR	OG1-CB-CG2	-6.54	96.22	109.30
1	B	9	LEU	CA-C-N	-6.52	112.24	122.73
1	B	9	LEU	C-N-CA	-6.52	112.24	122.73
2	E	214	GLY	N-CA-C	-6.51	103.67	114.48
1	A	74	SER	CB-CA-C	-6.50	98.08	111.22
1	A	456	LYS	CB-CA-C	6.50	121.58	110.79
1	B	423	LYS	N-CA-C	6.48	119.57	109.52
1	B	496	THR	OG1-CB-CG2	-6.48	96.34	109.30
2	E	230	ARG	CG-CD-NE	6.47	126.24	112.00
1	A	652	ASN	N-CA-CB	6.47	120.31	110.28
3	F	12	ASN	CA-C-N	-6.47	112.25	122.73
3	F	12	ASN	C-N-CA	-6.47	112.25	122.73
2	C	16	ASP	N-CA-C	-6.46	92.92	111.00
1	A	164	ASP	CA-C-O	6.45	125.87	118.97
1	B	436	GLY	CA-C-O	6.44	125.58	119.20
1	A	366	GLN	CA-C-N	-6.44	113.97	123.11
1	A	366	GLN	C-N-CA	-6.44	113.97	123.11
3	F	161	LYS	O-C-N	6.43	126.91	121.31
1	A	19	THR	N-CA-C	6.43	119.01	108.52
1	B	360	PRO	CB-CA-C	-6.39	103.12	110.92
2	C	14	GLU	N-CA-C	6.38	118.76	110.53
1	B	361	PRO	CA-C-O	-6.36	114.17	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	204	PRO	N-CD-CG	-6.33	93.70	103.20
3	F	103	ALA	N-CA-C	-6.33	100.99	111.37
1	B	10	PHE	N-CA-C	6.33	119.93	112.72
1	B	61	CYS	N-CA-C	6.32	119.08	108.02
1	B	655	LYS	N-CA-C	-6.30	103.71	111.40
2	E	204	PRO	CB-CA-C	-6.30	101.17	111.56
2	C	234	ILE	N-CA-C	-6.26	102.81	108.95
1	A	183	TYR	N-CA-C	-6.24	104.53	111.71
1	A	253	MET	N-CA-C	6.24	118.22	107.93
1	A	366	GLN	N-CA-C	-6.24	106.21	113.88
1	A	513	ASP	N-CA-C	6.22	120.88	113.16
1	A	459	LYS	N-CA-C	6.22	120.12	112.54
1	B	369	THR	N-CA-C	-6.22	105.64	113.72
1	B	131	GLU	N-CA-C	-6.19	96.59	107.73
1	B	256	ILE	CA-C-O	-6.18	113.62	121.48
1	B	202	TRP	N-CA-C	-6.18	104.09	111.69
1	A	365	THR	OG1-CB-CG2	-6.18	96.94	109.30
1	B	187	ARG	CG-CD-NE	-6.17	98.42	112.00
3	D	143	VAL	CB-CA-C	-6.17	100.81	110.69
1	B	152	VAL	CB-CA-C	-6.17	104.09	111.81
3	F	183	SER	N-CA-C	6.17	118.58	109.69
1	B	267	ASP	N-CA-C	-6.17	103.28	111.24
2	C	173	GLU	N-CA-C	-6.17	98.35	108.41
1	B	270	PRO	CB-CA-C	-6.16	103.74	111.56
1	B	399	PRO	N-CA-C	-6.16	103.80	113.78
3	D	183	SER	N-CA-C	6.16	117.92	109.18
1	A	28	PRO	CB-CA-C	-6.15	103.03	111.21
1	A	637	SER	CB-CA-C	6.14	120.82	109.70
1	A	449	THR	N-CA-C	6.14	117.77	111.14
3	D	90	VAL	CA-C-N	-6.14	114.59	123.06
3	D	90	VAL	C-N-CA	-6.14	114.59	123.06
1	B	716	PRO	CA-C-O	-6.13	113.25	120.85
3	D	115	ALA	CA-C-N	-6.12	111.82	123.32
3	D	115	ALA	C-N-CA	-6.12	111.82	123.32
1	A	360	PRO	CA-C-O	-6.11	111.70	120.56
1	B	404	ALA	CA-C-N	-6.11	112.10	120.28
1	B	404	ALA	C-N-CA	-6.11	112.10	120.28
2	E	146	VAL	CB-CA-C	-6.11	104.69	111.35
1	A	46	SER	CA-CB-OG	6.10	123.31	111.10
1	B	196	GLU	N-CA-CB	6.10	120.66	110.41
2	E	8	LYS	N-CA-C	6.10	118.35	108.34
1	A	450	GLN	N-CA-C	6.09	118.00	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	82	LEU	CA-C-N	-6.09	111.38	120.82
3	F	82	LEU	C-N-CA	-6.09	111.38	120.82
1	A	291	LYS	N-CA-C	-6.08	105.90	113.38
1	B	592	HIS	N-CA-C	6.08	119.91	107.69
1	B	544	SER	CB-CA-C	6.08	121.19	110.85
2	C	14	GLU	CA-CB-CG	-6.08	101.94	114.10
3	D	136	ASN	N-CA-C	-6.08	103.00	111.39
3	F	136	ASN	N-CA-C	-6.07	103.08	111.28
1	A	446	TYR	CA-C-N	-6.07	110.52	121.14
1	A	446	TYR	C-N-CA	-6.07	110.52	121.14
1	B	472	ALA	N-CA-C	-6.07	105.37	112.89
1	A	369	THR	N-CA-C	-6.04	105.86	113.72
1	A	504	ILE	CB-CA-C	-6.04	104.36	110.89
1	A	109	ALA	CA-C-N	-6.04	112.18	122.56
1	A	109	ALA	C-N-CA	-6.04	112.18	122.56
1	B	428	LEU	N-CA-C	-6.04	105.18	112.54
1	B	83	VAL	N-CA-C	6.03	117.50	110.62
1	A	61	CYS	CA-C-N	6.02	129.31	120.82
1	A	61	CYS	C-N-CA	6.02	129.31	120.82
1	B	601	ARG	CA-CB-CG	6.00	126.09	114.10
2	E	127	TYR	N-CA-C	5.99	117.89	111.36
2	C	194	LEU	O-C-N	5.99	128.47	122.12
1	B	357	ILE	CA-C-O	5.99	126.20	119.92
2	C	66	PRO	N-CA-C	5.98	124.79	112.47
1	A	483	VAL	N-CA-C	5.98	116.48	108.11
1	A	505	PRO	CB-CA-C	-5.97	101.71	111.56
2	C	141	PRO	CB-CA-C	-5.97	103.95	111.71
1	B	14	GLN	N-CA-C	5.96	118.85	109.96
3	F	153	LEU	N-CA-C	5.96	119.12	109.40
3	F	15	ARG	NE-CZ-NH1	-5.96	115.54	121.50
3	D	87	ASN	N-CA-C	5.96	122.97	109.81
1	B	702	ILE	N-CA-C	5.95	116.69	108.12
3	F	93	LEU	CD1-CG-CD2	-5.95	97.70	110.80
1	A	437	LEU	N-CA-C	-5.95	106.66	112.97
1	A	208	LYS	N-CA-C	-5.95	104.80	111.28
1	A	62	SER	N-CA-C	5.94	118.96	110.10
1	A	82	ASP	N-CA-C	5.94	117.43	111.07
3	F	7	ALA	CA-C-N	-5.94	113.10	122.73
3	F	7	ALA	C-N-CA	-5.94	113.10	122.73
1	B	138	GLU	CA-C-N	-5.92	113.14	121.72
1	B	138	GLU	C-N-CA	-5.92	113.14	121.72
1	B	457	LYS	CA-C-N	-5.92	114.31	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	457	LYS	C-N-CA	-5.92	114.31	122.30
2	E	70	ASP	N-CA-C	-5.90	104.19	111.33
3	F	182	ARG	N-CA-C	-5.89	105.95	113.02
1	A	711	ILE	N-CA-C	5.89	117.22	109.21
2	E	22	ASP	N-CA-C	5.89	123.35	110.80
1	A	535	ASN	N-CA-C	5.88	118.54	109.07
1	A	413	TYR	N-CA-C	5.88	118.14	110.43
1	B	558	ILE	N-CA-C	5.87	117.22	108.23
2	C	127	TYR	N-CA-C	5.87	117.48	111.14
2	C	88	TRP	N-CA-C	5.87	117.70	108.96
1	B	306	MET	N-CA-C	5.86	118.17	111.02
1	A	28	PRO	CA-C-O	-5.86	114.28	121.31
1	B	70	THR	OG1-CB-CG2	-5.85	97.59	109.30
1	B	569	HIS	O-C-N	5.85	128.32	122.12
1	A	222	ARG	N-CA-C	-5.85	100.18	109.59
3	D	35	LYS	CA-C-N	-5.84	115.06	122.37
3	D	35	LYS	C-N-CA	-5.84	115.06	122.37
2	C	37	GLU	N-CA-C	5.84	117.32	111.07
1	A	704	ILE	N-CA-CB	5.83	119.38	111.21
1	B	626	ALA	N-CA-C	5.83	118.07	110.43
2	E	199	GLN	N-CA-C	5.83	120.01	113.01
1	B	376	ARG	N-CA-C	-5.82	104.88	113.61
1	A	327	ASP	O-C-N	5.82	125.92	121.27
1	B	272	ARG	N-CA-C	5.81	119.84	112.87
1	B	680	LEU	CB-CG-CD2	-5.81	93.28	110.70
1	B	563	HIS	N-CA-C	-5.80	99.82	109.46
1	A	550	ALA	N-CA-C	-5.80	104.86	111.07
2	E	179	VAL	CB-CA-C	-5.80	103.94	110.96
1	B	366	GLN	CA-C-N	-5.79	114.13	123.23
1	B	366	GLN	C-N-CA	-5.79	114.13	123.23
1	B	338	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	A	647	GLU	CB-CA-C	-5.79	103.00	112.03
1	A	469	PRO	CB-CA-C	-5.78	104.22	111.56
3	F	30	LYS	CA-CB-CG	5.78	125.66	114.10
1	B	371	GLY	CA-C-O	5.78	125.40	119.10
1	B	380	PRO	N-CD-CG	-5.78	94.54	103.20
2	E	104	LEU	CB-CA-C	-5.78	101.15	110.74
3	D	141	VAL	CB-CA-C	-5.77	104.68	111.09
1	A	689	HIS	N-CA-C	-5.77	104.90	111.07
1	B	58	THR	N-CA-C	-5.77	102.92	110.53
1	B	251	VAL	N-CA-C	5.77	117.02	109.58
3	D	103	ALA	N-CA-C	-5.76	101.92	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	698	ALA	CA-C-N	5.76	130.90	122.66
1	A	698	ALA	C-N-CA	5.76	130.90	122.66
2	E	102	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	B	6	HIS	N-CA-C	5.75	119.91	113.01
3	D	21	LEU	N-CA-C	-5.75	104.61	111.69
1	B	359	GLY	N-CA-C	5.74	124.05	112.34
1	A	591	ASP	N-CA-C	-5.73	105.59	112.58
1	A	452	THR	OG1-CB-CG2	-5.73	97.84	109.30
3	D	142	GLU	N-CA-C	5.73	118.97	109.46
1	B	342	ILE	N-CA-C	5.72	117.00	108.54
1	A	721	GLY	CA-C-N	-5.71	115.17	122.77
1	A	721	GLY	C-N-CA	-5.71	115.17	122.77
1	B	123	PRO	N-CD-CG	-5.71	94.64	103.20
3	F	139	VAL	CB-CA-C	-5.71	100.51	110.38
1	A	643	GLY	O-C-N	-5.70	118.25	123.78
1	A	515	LEU	N-CA-C	5.70	119.01	109.95
1	B	458	ASN	N-CA-CB	5.69	119.73	110.17
1	B	311	THR	CA-CB-CG2	5.68	120.16	110.50
3	F	42	GLY	N-CA-C	-5.68	101.32	110.18
1	A	198	ARG	CB-CA-C	5.68	120.21	110.79
1	A	671	LEU	CA-C-N	5.68	130.75	123.03
1	A	671	LEU	C-N-CA	5.68	130.75	123.03
1	B	219	ILE	CA-C-N	-5.67	113.28	122.81
1	B	219	ILE	C-N-CA	-5.67	113.28	122.81
3	F	142	GLU	N-CA-C	5.67	117.77	108.52
1	B	305	LYS	CA-C-N	5.67	128.67	120.79
1	B	305	LYS	C-N-CA	5.67	128.67	120.79
1	A	173	SER	N-CA-C	5.67	119.50	112.24
1	A	212	ALA	N-CA-C	5.67	117.26	111.14
3	D	135	TYR	N-CA-C	5.67	119.16	111.17
1	B	363	ILE	CA-C-O	-5.66	115.49	121.44
2	C	51	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	132	THR	CA-C-N	-5.64	112.72	122.14
1	A	132	THR	C-N-CA	-5.64	112.72	122.14
1	B	297	VAL	CB-CA-C	-5.64	102.04	111.29
1	B	544	SER	N-CA-C	-5.64	105.21	111.36
3	D	83	ILE	N-CA-C	-5.64	104.86	111.00
1	B	177	LEU	CA-CB-CG	5.63	136.01	116.30
2	C	162	ARG	CG-CD-NE	5.63	124.38	112.00
3	F	19	LEU	CA-C-N	5.62	128.07	120.65
3	F	19	LEU	C-N-CA	5.62	128.07	120.65
1	B	584	LEU	CB-CA-C	-5.62	102.57	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	40	VAL	CB-CA-C	5.62	118.99	110.62
1	A	190	LYS	CD-CE-NZ	-5.59	94.00	111.90
1	A	692	ALA	CA-C-N	-5.59	112.43	120.82
1	A	692	ALA	C-N-CA	-5.59	112.43	120.82
1	B	705	PRO	CA-C-O	-5.59	114.26	122.31
1	A	436	GLY	N-CA-C	5.59	122.55	114.67
1	B	50	GLU	CA-CB-CG	-5.59	102.92	114.10
2	E	65	GLY	CA-C-N	5.59	126.82	119.84
2	E	65	GLY	C-N-CA	5.59	126.82	119.84
2	C	7	VAL	N-CA-C	5.58	117.38	108.89
3	F	119	TYR	CB-CA-C	5.57	118.77	109.80
1	B	688	GLY	N-CA-C	-5.57	99.99	113.18
1	A	191	TYR	CA-CB-CG	-5.56	103.89	113.90
1	A	334	VAL	N-CA-CB	5.56	117.31	110.64
1	A	580	ARG	CA-C-N	-5.56	112.28	120.28
1	A	580	ARG	C-N-CA	-5.56	112.28	120.28
2	C	188	LYS	CA-C-N	5.55	125.87	119.93
2	C	188	LYS	C-N-CA	5.55	125.87	119.93
3	F	83	ILE	CB-CA-C	5.55	119.48	111.65
3	D	13	ASP	N-CA-C	5.55	117.95	108.90
3	F	113	GLY	N-CA-C	-5.55	105.55	111.93
1	A	303	PRO	N-CA-C	-5.54	105.82	113.53
1	B	40	PHE	CB-CA-C	5.54	119.57	110.88
1	A	218	ALA	CA-C-N	-5.54	115.81	122.90
1	A	218	ALA	C-N-CA	-5.54	115.81	122.90
1	B	498	CYS	N-CA-C	5.53	119.53	112.34
3	D	80	SER	N-CA-C	-5.53	104.68	111.75
1	B	220	ALA	CA-C-N	-5.52	113.54	122.81
1	B	220	ALA	C-N-CA	-5.52	113.54	122.81
1	B	338	ARG	NE-CZ-NH1	-5.52	115.98	121.50
2	C	19	ILE	N-CA-C	5.52	120.81	109.34
1	B	62	SER	N-CA-C	5.51	118.35	110.24
1	B	499	LEU	N-CA-C	5.50	118.11	111.40
3	F	65	GLY	CA-C-N	5.50	128.11	120.63
3	F	65	GLY	C-N-CA	5.50	128.11	120.63
3	D	113	GLY	CA-C-N	-5.50	112.92	122.37
3	D	113	GLY	C-N-CA	-5.50	112.92	122.37
1	B	462	GLN	CB-CA-C	-5.49	101.68	110.14
3	F	110	THR	N-CA-C	5.48	120.62	113.88
1	A	254	TRP	CA-CB-CG	-5.48	103.19	113.60
1	A	623	PRO	N-CA-C	-5.47	107.67	114.68
1	B	198	ARG	CB-CA-C	5.47	119.39	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	214	GLY	N-CA-C	-5.47	105.39	114.48
2	E	114	ASP	N-CA-C	-5.47	107.25	114.31
2	E	134	VAL	CB-CA-C	-5.47	104.87	112.04
1	B	413	TYR	CA-C-N	-5.47	115.28	122.99
1	B	413	TYR	C-N-CA	-5.47	115.28	122.99
1	B	303	PRO	N-CA-C	-5.46	106.41	113.57
1	A	491	TRP	CB-CA-C	5.46	119.39	109.62
1	B	311	THR	N-CA-CB	5.46	119.59	110.41
1	B	525	LYS	CB-CA-C	5.46	118.24	109.61
1	A	119	THR	N-CA-C	5.46	117.53	109.62
1	A	203	LEU	CA-CB-CG	-5.46	97.20	116.30
1	A	434	LEU	CA-CB-CG	-5.46	97.20	116.30
1	B	181	ASN	CB-CA-C	5.44	116.00	109.31
1	A	626	ALA	N-CA-C	5.44	117.71	110.53
3	F	158	SER	N-CA-C	-5.44	106.22	112.86
1	B	437	LEU	N-CA-C	-5.44	106.43	112.57
3	D	36	VAL	CA-C-N	-5.43	115.14	122.91
3	D	36	VAL	C-N-CA	-5.43	115.14	122.91
1	A	467	GLN	CB-CG-CD	-5.43	103.37	112.60
1	A	284	LYS	N-CA-C	5.43	117.20	111.28
1	B	265	GLY	N-CA-C	-5.43	106.13	113.24
3	D	38	VAL	CB-CA-C	5.43	119.69	110.95
1	B	640	LEU	N-CA-C	5.43	118.39	109.76
2	C	87	VAL	CB-CA-C	-5.42	103.04	110.96
3	F	166	ALA	CA-C-N	5.42	129.00	121.09
3	F	166	ALA	C-N-CA	5.42	129.00	121.09
1	A	9	LEU	CA-C-N	-5.41	114.15	122.60
1	A	9	LEU	C-N-CA	-5.41	114.15	122.60
3	D	184	GLN	CA-C-N	-5.41	113.19	120.87
3	D	184	GLN	C-N-CA	-5.41	113.19	120.87
1	B	461	SER	CB-CA-C	5.40	119.48	109.54
2	E	208	VAL	N-CA-C	-5.40	100.29	108.17
1	A	273	PHE	CB-CA-C	-5.39	99.70	110.42
1	B	727	TYR	N-CA-C	5.38	118.09	110.50
2	E	39	ASP	N-CA-C	-5.38	105.45	112.23
1	B	662	ALA	N-CA-C	5.38	117.56	111.11
1	A	531	VAL	N-CA-C	5.38	115.64	108.11
1	A	538	THR	N-CA-CB	-5.38	102.53	110.49
3	D	64	LYS	N-CA-C	5.37	117.47	109.25
1	B	705	PRO	N-CA-C	-5.37	103.65	111.33
3	D	173	ASN	CB-CA-C	5.36	119.36	109.71
3	D	51	ALA	N-CA-C	5.36	119.44	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	106	GLU	CA-C-N	-5.36	111.98	120.55
2	C	106	GLU	C-N-CA	-5.36	111.98	120.55
1	B	121	ARG	N-CA-C	-5.35	100.97	109.59
2	E	29	ASP	CB-CA-C	5.35	120.42	109.55
2	E	45	GLU	N-CA-C	-5.35	105.61	111.82
2	E	230	ARG	NH1-CZ-NH2	-5.35	112.35	119.30
2	E	235	PRO	CA-C-O	-5.35	115.49	122.12
2	E	66	PRO	N-CA-C	5.34	123.48	112.47
1	A	613	LYS	N-CA-C	5.34	117.33	108.20
3	F	133	GLY	CA-C-N	5.34	126.85	121.35
3	F	133	GLY	C-N-CA	5.34	126.85	121.35
1	B	722	ASN	N-CA-C	5.33	116.94	108.67
2	C	152	LYS	N-CA-C	-5.33	102.40	110.50
1	B	693	ARG	N-CA-C	-5.32	104.94	111.75
1	A	259	GLY	N-CA-C	5.32	117.46	112.04
3	D	52	LEU	N-CA-C	-5.31	106.48	113.17
1	A	342	ILE	N-CA-C	5.31	115.90	108.89
1	A	376	ARG	N-CA-C	-5.30	106.31	114.16
1	A	479	GLY	N-CA-C	-5.30	107.90	115.64
1	B	174	TYR	N-CA-C	5.30	117.67	110.35
3	D	126	ASP	N-CA-C	-5.30	105.52	112.41
3	F	115	ALA	CA-C-N	-5.30	113.55	123.03
3	F	115	ALA	C-N-CA	-5.30	113.55	123.03
1	B	718	MET	N-CA-C	-5.29	103.37	109.93
2	C	9	GLN	CA-C-N	-5.29	113.58	123.05
2	C	9	GLN	C-N-CA	-5.29	113.58	123.05
1	A	651	TRP	N-CA-C	-5.29	105.97	112.90
1	A	214	GLY	CA-C-N	5.29	128.10	120.38
1	A	214	GLY	C-N-CA	5.29	128.10	120.38
1	B	728	LYS	CB-CG-CD	5.29	123.46	111.30
3	D	180	GLN	N-CA-CB	5.28	117.83	109.71
1	A	324	SER	CA-C-N	5.27	127.15	120.72
1	A	324	SER	C-N-CA	5.27	127.15	120.72
1	A	460	GLU	N-CA-C	-5.27	106.53	113.17
1	B	206	LEU	CA-C-N	5.27	128.11	120.79
1	B	206	LEU	C-N-CA	5.27	128.11	120.79
2	C	102	ARG	NE-CZ-NH2	5.27	123.94	119.20
3	D	63	VAL	CB-CA-C	-5.26	103.88	111.19
1	A	343	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	676	GLU	N-CA-C	-5.25	105.61	112.23
1	B	671	LEU	CA-C-N	5.25	129.39	122.51
1	B	671	LEU	C-N-CA	5.25	129.39	122.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	59	VAL	CA-C-N	-5.24	115.15	122.75
2	E	59	VAL	C-N-CA	-5.24	115.15	122.75
1	A	54	ALA	N-CA-C	5.24	119.58	112.04
1	A	421	ALA	CA-C-N	5.24	127.72	120.29
1	A	421	ALA	C-N-CA	5.24	127.72	120.29
1	A	641	VAL	CA-C-N	-5.24	114.01	122.23
1	A	641	VAL	C-N-CA	-5.24	114.01	122.23
3	D	132	ARG	CA-CB-CG	5.24	124.57	114.10
1	A	334	VAL	O-C-N	5.23	128.32	121.94
3	F	119	TYR	N-CA-C	-5.23	105.99	114.09
1	B	231	PRO	N-CA-C	-5.22	102.99	111.19
1	B	250	LEU	CA-CB-CG	-5.22	98.02	116.30
3	D	70	PHE	N-CA-C	5.22	121.93	110.80
1	A	159	ARG	CB-CG-CD	5.21	123.30	111.30
1	B	11	GLU	N-CA-C	5.21	117.13	109.42
1	B	582	HIS	N-CA-C	-5.21	99.70	110.80
3	D	6	ILE	N-CA-CB	-5.21	104.86	111.64
1	A	499	LEU	N-CA-C	5.21	119.72	112.90
3	F	107	ALA	N-CA-C	-5.21	106.08	112.90
2	E	32	MET	CB-CG-SD	5.21	128.31	112.70
1	A	72	ARG	CA-C-N	-5.20	115.83	123.00
1	A	72	ARG	C-N-CA	-5.20	115.83	123.00
2	E	201	ALA	N-CA-C	-5.20	105.69	111.36
1	B	468	LYS	CB-CG-CD	5.20	123.25	111.30
1	B	624	ARG	CB-CG-CD	5.19	123.24	111.30
1	B	414	THR	OG1-CB-CG2	-5.19	98.92	109.30
1	A	445	ASP	N-CA-CB	5.19	117.53	110.01
2	E	236	GLU	N-CA-C	5.19	125.52	111.00
1	A	412	GLY	N-CA-C	5.19	122.44	115.59
3	F	35	LYS	CA-C-O	5.19	126.02	120.32
1	A	514	GLN	N-CA-C	5.18	117.09	108.02
1	A	334	VAL	N-CA-C	-5.18	106.02	110.74
1	B	42	SER	CA-C-N	-5.18	113.71	120.44
1	B	42	SER	C-N-CA	-5.18	113.71	120.44
1	B	74	SER	CA-C-N	-5.18	113.71	122.67
1	B	74	SER	C-N-CA	-5.18	113.71	122.67
2	C	65	GLY	CA-C-N	5.18	126.31	119.84
2	C	65	GLY	C-N-CA	5.18	126.31	119.84
3	F	64	LYS	N-CA-C	5.17	116.69	108.67
1	B	182	PRO	CA-C-N	5.17	127.20	120.28
1	B	182	PRO	C-N-CA	5.17	127.20	120.28
1	A	152	VAL	N-CA-C	5.16	115.27	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	196	GLY	N-CA-C	5.16	118.92	112.73
1	A	496	THR	OG1-CB-CG2	-5.15	98.99	109.30
1	A	430	GLN	N-CA-C	5.15	117.56	111.33
1	A	453	LYS	N-CA-C	5.15	117.79	111.82
3	D	178	SER	CA-CB-OG	5.15	121.40	111.10
1	A	612	SER	CA-C-N	-5.14	116.15	122.84
1	A	612	SER	C-N-CA	-5.14	116.15	122.84
1	B	719	PRO	CA-C-O	5.14	126.94	120.92
2	E	230	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	B	199	ALA	N-CA-C	5.14	119.30	113.19
2	E	65	GLY	N-CA-C	5.14	122.82	112.34
1	A	423	LYS	N-CA-C	5.14	117.94	109.72
1	A	511	LEU	CA-C-N	5.13	124.74	119.56
1	A	511	LEU	C-N-CA	5.13	124.74	119.56
1	A	266	GLU	N-CA-C	-5.13	106.53	112.89
1	A	469	PRO	N-CA-C	-5.13	103.05	111.15
1	B	290	SER	N-CA-C	-5.13	101.92	110.17
1	B	314	TYR	N-CA-C	5.12	119.61	112.90
1	B	144	ILE	CB-CA-C	5.12	118.75	112.04
2	C	181	THR	N-CA-C	5.12	117.10	108.96
2	E	219	ASP	N-CA-C	-5.12	107.16	113.41
1	B	503	PRO	CA-C-O	-5.11	115.17	121.31
1	B	551	THR	N-CA-CB	5.11	118.87	110.39
3	D	67	SER	N-CA-C	-5.11	102.92	110.48
1	B	230	GLY	O-C-N	5.11	126.88	121.77
3	D	129	VAL	CB-CA-C	5.11	118.02	110.77
2	C	203	LYS	CA-C-N	5.10	125.34	119.83
2	C	203	LYS	C-N-CA	5.10	125.34	119.83
1	A	434	LEU	CA-C-O	5.09	125.47	120.17
1	B	185	ASN	N-CA-C	5.09	116.99	108.23
1	B	30	CYS	CA-CB-SG	-5.09	102.69	114.40
2	C	75	LYS	N-CA-C	-5.09	105.92	111.82
1	B	491	TRP	CB-CA-C	5.09	118.73	109.62
1	A	642	THR	CB-CA-C	-5.09	100.83	109.38
1	A	599	PRO	CA-C-O	-5.08	115.73	121.43
1	A	570	PHE	CB-CA-C	-5.08	100.86	110.01
1	A	371	GLY	CA-C-O	5.08	124.76	119.07
1	A	655	LYS	N-CA-C	-5.08	107.47	113.97
1	B	283	VAL	N-CA-C	-5.08	105.38	110.30
1	B	528	GLY	CA-C-N	5.07	128.43	120.82
1	B	528	GLY	C-N-CA	5.07	128.43	120.82
1	A	658	GLU	N-CA-C	-5.07	105.75	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PHE	N-CA-CB	5.07	117.66	110.16
1	B	18	LYS	CB-CA-C	5.07	119.31	109.33
1	B	285	LEU	CA-C-N	-5.07	112.45	120.55
1	B	285	LEU	C-N-CA	-5.07	112.45	120.55
1	B	657	ARG	N-CA-C	-5.07	105.82	112.41
1	B	229	TYR	O-C-N	5.06	129.32	122.59
1	A	649	THR	N-CA-C	-5.06	105.65	111.07
1	A	715	THR	OG1-CB-CG2	-5.06	99.18	109.30
1	B	69	ASP	CB-CG-OD2	5.06	130.03	118.40
1	B	432	ALA	N-CA-C	-5.06	107.06	113.18
1	B	484	ILE	N-CA-C	5.06	114.86	107.37
1	B	362	MET	CG-SD-CE	5.05	112.02	100.90
3	F	173	ASN	CB-CA-C	5.05	119.28	109.33
1	B	549	LEU	N-CA-C	-5.05	105.86	111.36
1	A	376	ARG	CA-CB-CG	5.04	124.19	114.10
3	D	77	ALA	N-CA-C	-5.04	105.91	111.71
2	E	194	LEU	CA-C-N	5.04	127.54	120.28
2	E	194	LEU	C-N-CA	5.04	127.54	120.28
1	A	343	ARG	N-CA-C	-5.04	100.30	108.41
1	A	334	VAL	CA-C-N	5.04	128.38	120.82
1	A	334	VAL	C-N-CA	5.04	128.38	120.82
1	B	642	THR	N-CA-C	-5.04	107.68	113.88
1	B	159	ARG	N-CA-C	5.04	116.46	111.07
1	B	698	ALA	CA-C-N	-5.04	115.46	122.66
1	B	698	ALA	C-N-CA	-5.04	115.46	122.66
2	C	204	PRO	CA-C-N	-5.04	115.87	122.37
2	C	204	PRO	C-N-CA	-5.04	115.87	122.37
1	B	280	ILE	O-C-N	5.03	123.64	120.42
1	A	707	LYS	CA-C-N	-5.03	114.78	122.87
1	A	707	LYS	C-N-CA	-5.03	114.78	122.87
3	D	151	VAL	N-CA-C	5.02	115.14	108.11
1	A	331	PRO	CB-CA-C	5.01	119.83	111.56
1	A	198	ARG	N-CA-C	-5.01	105.82	111.28
1	B	550	ALA	N-CA-C	-5.01	105.71	111.07
3	F	135	TYR	N-CA-CB	-5.01	104.29	111.70
2	E	142	HIS	N-CA-C	5.00	117.72	109.72

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	MET	Peptide

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Mol	Chain	Res	Type	Group
1	A	320	CYS	Peptide
1	A	539	TYR	Peptide
1	A	66	GLU	Peptide
1	B	139	MET	Peptide
1	B	247	ALA	Peptide
1	B	493	THR	Peptide
3	D	110	THR	Peptide
3	D	119	TYR	Peptide
3	D	121	VAL	Peptide
2	E	55	THR	Peptide
3	F	110	THR	Peptide
3	F	119	TYR	Peptide
3	F	122	GLU	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	5692	0	5445	532	0
1	B	5676	0	5424	552	0
2	C	1749	0	1722	124	0
2	E	1751	0	1716	136	0
3	D	1354	0	1311	89	0
3	F	1376	0	1358	136	0
4	A	31	0	18	6	0
4	B	31	0	18	6	0
5	A	27	0	12	7	0
5	B	27	0	12	2	0
6	A	8	0	0	1	0
6	B	8	0	0	0	0
7	C	23	0	11	6	0
7	E	23	0	12	4	0
All	All	17776	0	17059	1484	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (1484) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ILE:CD1	1:B:346:ILE:CG1	1.75	1.63
1:B:500:THR:CA	1:B:500:THR:CB	1.75	1.57
3:D:180:GLN:CG	3:D:180:GLN:CB	1.76	1.56
3:D:16:PRO:CB	3:D:16:PRO:CG	1.74	1.48
1:A:718:MET:SD	1:A:718:MET:CE	2.04	1.46
2:E:226:MET:SD	2:E:226:MET:CE	2.05	1.45
1:B:541:MET:SD	1:B:541:MET:CE	2.05	1.44
2:E:1:MET:SD	2:E:1:MET:CE	2.05	1.42
1:A:89:MET:SD	1:A:89:MET:CE	2.09	1.40
2:C:1:MET:SD	2:C:1:MET:CE	2.13	1.35
1:B:251:VAL:HG21	1:B:254:TRP:NE1	1.39	1.33
2:E:168:MET:SD	2:E:168:MET:CE	2.22	1.27
1:B:54:ALA:O	1:B:98:ALA:HB1	1.23	1.25
1:A:24:PHE:CD1	1:A:331:PRO:HB3	1.72	1.24
1:A:148:GLN:NE2	1:A:201:PHE:CE1	2.06	1.21
3:F:26:ASN:O	3:F:29:LYS:HG3	1.38	1.18
2:E:162:ARG:HH22	3:F:98:ASP:HA	1.06	1.14
1:A:237:GLU:HB2	1:B:619:PRO:HG3	1.17	1.12
2:E:162:ARG:NH2	3:F:98:ASP:HA	1.63	1.12
1:B:72:ARG:NH1	1:B:131:GLU:OE1	1.83	1.12
1:B:276:GLN:HE21	1:B:300:TYR:HA	1.12	1.10
2:E:226:MET:HE3	3:F:148:LYS:NZ	1.68	1.09
1:B:147:VAL:O	1:B:150:PHE:HB2	1.54	1.08
1:A:254:TRP:HB3	1:A:256:ILE:HD11	1.36	1.08
1:A:24:PHE:HE2	1:A:306:MET:SD	1.76	1.07
1:A:354:ARG:HH21	1:A:354:ARG:HG3	1.17	1.06
1:B:251:VAL:CG2	1:B:254:TRP:HE1	1.67	1.06
1:A:195:LEU:HD23	1:A:246:MET:CE	1.87	1.05
1:A:355:TRP:CZ3	1:A:356:GLU:HG2	1.92	1.05
1:B:517:PRO:HB3	1:B:545:LEU:HD11	1.38	1.04
1:B:129:GLU:OE2	1:B:184:TYR:OH	1.75	1.03
1:B:660:GLU:O	1:B:664:ASN:ND2	1.91	1.03
1:A:139:MET:HE3	1:A:147:VAL:HG21	1.36	1.03
1:B:718:MET:SD	1:B:718:MET:CE	2.47	1.02
1:B:631:ARG:HH21	1:B:631:ARG:HG3	1.18	1.01
1:B:126:TYR:CE1	1:B:136:CYS:SG	2.53	1.00
2:C:230:ARG:HH22	3:D:124:GLN:NE2	1.58	0.99
1:B:72:ARG:NH1	1:B:130:PHE:HE1	1.60	0.98
1:B:26:GLN:HE21	1:B:48:LYS:NZ	1.60	0.98
1:B:185:ASN:OD1	1:B:187:ARG:HG3	1.64	0.98
1:B:175:LEU:HB3	1:B:176:PRO:HD3	1.45	0.97
1:B:716:PRO:HB2	1:B:718:MET:O	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:CD1	1:B:136:CYS:SG	2.59	0.96
1:B:251:VAL:HG21	1:B:254:TRP:HE1	0.79	0.96
1:A:619:PRO:HG3	1:B:237:GLU:CB	1.95	0.96
2:E:1:MET:CE	2:E:1:MET:HB2	1.95	0.95
1:A:619:PRO:HG3	1:B:237:GLU:HB2	1.47	0.95
1:A:647:GLU:OE2	1:A:649:THR:OG1	1.82	0.95
1:A:251:VAL:HG21	1:A:254:TRP:NE1	1.82	0.95
1:A:354:ARG:HG3	1:A:354:ARG:NH2	1.78	0.95
3:F:42:GLY:O	3:F:64:LYS:HA	1.67	0.94
2:E:183:GLN:HE21	2:E:184:LEU:N	1.63	0.94
1:A:24:PHE:CE1	1:A:331:PRO:HB3	2.03	0.93
1:A:272:ARG:O	1:A:272:ARG:HG2	1.68	0.93
1:B:127:ALA:HB2	1:B:135:TYR:CE1	2.03	0.93
1:B:589:LEU:HD23	1:B:592:HIS:ND1	1.82	0.93
1:A:237:GLU:CB	1:B:619:PRO:HG3	1.99	0.93
3:F:26:ASN:O	3:F:29:LYS:CG	2.16	0.93
1:B:240:GLY:O	1:B:244:VAL:HG23	1.70	0.92
3:F:71:ASP:OD1	3:F:74:VAL:HG23	1.68	0.92
1:B:532:VAL:O	1:B:638:LEU:HD12	1.69	0.92
1:A:195:LEU:HD23	1:A:246:MET:HE1	1.52	0.92
1:A:24:PHE:CE2	1:A:306:MET:SD	2.63	0.92
1:A:568:MET:HE3	1:A:573:GLU:OE1	1.70	0.92
2:E:183:GLN:NE2	2:E:184:LEU:H	1.68	0.91
1:A:251:VAL:HG21	1:A:254:TRP:CE2	2.04	0.91
1:B:15:ILE:HG22	1:B:293:PRO:HG2	1.51	0.91
2:E:64:VAL:HG22	2:E:87:VAL:HB	1.50	0.91
1:A:175:LEU:O	1:A:178:GLN:N	2.04	0.90
1:A:692:ALA:O	1:A:693:ARG:C	2.13	0.90
1:A:139:MET:CE	1:A:147:VAL:HG21	2.01	0.90
2:C:1:MET:CE	2:C:1:MET:HB2	2.01	0.90
3:D:19:LEU:HA	3:D:22:ILE:HD12	1.53	0.90
1:A:399:PRO:HD2	5:A:1731:ADP:O3B	1.71	0.89
3:F:49:VAL:HG23	3:F:50:PRO:HD3	1.53	0.89
2:C:31:MET:HE2	2:C:33:TYR:OH	1.71	0.89
2:C:63:SER:HB2	2:C:73:LEU:HD21	1.52	0.89
1:A:729:VAL:OXT	1:B:384:ARG:HA	1.73	0.88
1:A:515:LEU:HD12	1:A:515:LEU:N	1.86	0.88
1:B:139:MET:HB3	1:B:143:ASP:HB2	1.52	0.88
2:C:183:GLN:HE21	2:C:184:LEU:H	0.95	0.88
1:A:650:LEU:HD22	1:A:654:LEU:HD11	1.55	0.88
1:B:57:ASN:OD1	1:B:101:GLY:HA3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:46:ASP:O	3:D:49:VAL:HG23	1.73	0.88
1:B:349:ASN:ND2	1:B:571:THR:O	2.07	0.88
2:E:162:ARG:HH22	3:F:98:ASP:CA	1.85	0.88
1:A:175:LEU:HB3	1:A:176:PRO:HD3	1.54	0.87
1:A:355:TRP:CE3	1:A:356:GLU:HG2	2.10	0.87
1:A:441:SER:O	1:A:444:ARG:HG3	1.74	0.87
1:A:589:LEU:CD2	1:A:592:HIS:ND1	2.38	0.87
1:A:195:LEU:HD23	1:A:246:MET:HE3	1.54	0.86
1:A:352:ILE:HG22	1:A:352:ILE:O	1.76	0.86
1:A:35:SER:OG	1:A:76:ARG:N	2.07	0.86
1:A:254:TRP:HB2	1:A:294:VAL:HG22	1.56	0.86
2:C:230:ARG:HH22	3:D:124:GLN:HE22	1.20	0.86
1:A:515:LEU:HD22	1:A:527:ILE:HD11	1.58	0.86
2:E:226:MET:HE3	3:F:148:LYS:HZ1	1.37	0.86
1:A:375:ARG:O	1:A:706:TYR:HB2	1.76	0.85
1:A:137:LYS:HB2	1:B:676:GLU:O	1.74	0.85
1:A:148:GLN:NE2	1:A:201:PHE:CD1	2.45	0.85
1:A:589:LEU:HD22	1:A:592:HIS:ND1	1.91	0.85
1:B:589:LEU:HD23	1:B:592:HIS:CG	2.10	0.85
2:C:226:MET:HE2	3:D:111:GLY:HA2	1.58	0.85
1:A:469:PRO:HG2	1:A:469:PRO:O	1.76	0.85
1:A:127:ALA:HB2	1:A:135:TYR:CE1	2.12	0.84
1:B:352:ILE:HG21	1:B:572:LEU:HD11	1.58	0.84
2:E:226:MET:HE2	3:F:111:GLY:HA3	1.57	0.84
1:B:26:GLN:HE21	1:B:48:LYS:HZ3	1.22	0.83
1:B:631:ARG:HG3	1:B:631:ARG:NH2	1.82	0.83
1:A:11:GLU:O	1:A:23:ARG:NE	2.11	0.83
1:A:650:LEU:CD2	1:A:654:LEU:HD11	2.09	0.82
1:B:276:GLN:NE2	1:B:301:THR:H	1.77	0.82
1:B:30:CYS:HA	1:B:59:GLU:HB3	1.62	0.82
1:A:679:ARG:O	1:A:680:LEU:O	1.97	0.82
1:B:458:ASN:HB3	1:B:461:SER:HB2	1.59	0.82
3:D:137:GLN:HE22	3:D:156:ARG:HH22	1.26	0.82
1:A:714:GLY:HA2	1:A:723:PHE:CD2	2.15	0.81
1:B:695:ILE:HG23	1:B:696:GLU:HG2	1.60	0.81
2:E:165:GLU:OE2	3:F:96:SER:HB2	1.80	0.81
2:E:183:GLN:HE21	2:E:184:LEU:H	0.84	0.81
2:E:103:ILE:HD11	2:E:220:VAL:CG1	2.11	0.81
1:A:14:GLN:OE1	1:A:14:GLN:HA	1.79	0.80
1:A:627:ASN:OD1	1:A:629:SER:OG	1.98	0.80
1:B:302:ASP:OD2	1:B:303:PRO:HD2	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:O	1:B:158:SER:OG	1.99	0.80
2:C:4:LEU:HD11	2:C:62:VAL:HG21	1.64	0.80
2:E:172:VAL:CG1	3:F:183:SER:HB2	2.12	0.80
1:A:417:LEU:HB3	1:A:463:LEU:HD12	1.62	0.80
1:A:690:ARG:HD2	1:A:703:ALA:HB2	1.64	0.80
2:E:134:VAL:HG12	2:E:138:LEU:HD12	1.62	0.79
1:B:276:GLN:NE2	1:B:300:TYR:HA	1.95	0.79
2:C:183:GLN:HE21	2:C:184:LEU:N	1.77	0.79
1:A:369:THR:O	1:A:372:GLU:N	2.17	0.79
1:A:690:ARG:HD2	1:A:703:ALA:CB	2.13	0.79
2:E:1:MET:HB2	2:E:1:MET:HE2	1.64	0.79
3:F:83:ILE:HD11	3:F:112:TYR:CE2	2.18	0.79
1:B:589:LEU:CD2	1:B:592:HIS:CG	2.65	0.78
3:F:46:ASP:O	3:F:49:VAL:HG22	1.82	0.78
1:A:660:GLU:HB3	1:A:663:GLU:CD	2.08	0.78
1:A:711:ILE:HG12	1:A:712:ALA:N	1.98	0.78
1:B:26:GLN:NE2	1:B:48:LYS:NZ	2.31	0.78
1:B:72:ARG:NH1	1:B:130:PHE:CE1	2.49	0.78
1:B:56:LEU:HD23	1:B:93:VAL:CG1	2.12	0.78
1:B:272:ARG:O	1:B:272:ARG:CG	2.31	0.78
3:D:120:ILE:O	3:D:130:ALA:HA	1.83	0.78
2:E:132:ILE:HB	3:F:104:SER:OG	1.83	0.78
1:A:164:ASP:C	1:A:165:ILE:HG13	2.09	0.77
1:A:711:ILE:CG1	1:A:712:ALA:N	2.47	0.77
2:E:103:ILE:HD11	2:E:220:VAL:HG11	1.66	0.77
1:B:87:LYS:HG3	1:B:161:ALA:O	1.84	0.77
1:B:424:ILE:HD12	1:B:448:GLU:HA	1.65	0.77
1:A:515:LEU:HD12	1:A:515:LEU:H	1.47	0.77
1:B:127:ALA:HB2	1:B:135:TYR:CD1	2.18	0.77
2:C:1:MET:HB2	2:C:1:MET:HE2	1.65	0.77
2:E:164:LEU:HD11	2:E:170:GLN:HB2	1.66	0.77
1:A:195:LEU:CD2	1:A:246:MET:CE	2.63	0.77
1:B:147:VAL:HA	1:B:150:PHE:CD1	2.20	0.77
2:C:31:MET:CE	2:C:33:TYR:OH	2.32	0.77
1:B:661:TRP:HB3	1:B:666:ILE:HB	1.67	0.77
1:A:303:PRO:O	1:A:306:MET:HB2	1.84	0.76
2:E:226:MET:HE3	3:F:148:LYS:HZ3	1.47	0.76
1:A:227:THR:HG21	1:A:233:GLN:OE1	1.85	0.76
1:B:582:HIS:O	1:B:585:HIS:N	2.19	0.76
1:B:55:ALA:C	1:B:56:LEU:HD13	2.10	0.76
1:A:419:ASP:OD1	5:A:1731:ADP:O2'	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ARG:CD	1:A:703:ALA:HB2	2.16	0.76
1:A:722:ASN:O	1:B:707:LYS:HE2	1.86	0.76
3:D:132:ARG:HG3	3:D:132:ARG:HH11	1.50	0.76
1:A:110:HIS:HD1	1:A:128:SER:HG	0.76	0.75
1:B:112:PRO:O	1:B:113:ASN:HB2	1.86	0.75
2:C:102:ARG:HG3	2:C:102:ARG:HH11	1.50	0.75
1:A:195:LEU:CD2	1:A:246:MET:HE3	2.16	0.75
2:C:136:SER:OG	3:D:109:LYS:HG3	1.86	0.75
1:B:280:ILE:HA	1:B:283:VAL:HB	1.67	0.75
2:C:125:GLN:HB2	2:C:127:TYR:CE1	2.22	0.74
2:C:183:GLN:NE2	2:C:184:LEU:H	1.80	0.74
1:A:489:ALA:HB1	1:A:645:HIS:O	1.87	0.74
2:C:226:MET:HE2	3:D:111:GLY:CA	2.17	0.74
3:D:177:PRO:O	3:D:179:VAL:N	2.20	0.74
1:A:409:MET:HG2	1:A:415:VAL:HG13	1.69	0.74
1:B:55:ALA:O	1:B:56:LEU:HD13	1.88	0.74
1:B:102:VAL:HB	1:B:163:PHE:CZ	2.23	0.74
1:A:444:ARG:HD3	1:A:445:ASP:OD1	1.88	0.74
1:A:472:ALA:O	1:A:476:LEU:HG	1.87	0.74
3:D:78:SER:O	3:D:81:ALA:HB3	1.86	0.74
3:F:19:LEU:HA	3:F:22:ILE:HD12	1.69	0.74
1:B:68:ASP:OD2	1:B:68:ASP:C	2.30	0.74
1:A:660:GLU:HB3	1:A:663:GLU:OE1	1.87	0.73
1:B:500:THR:CA	1:B:500:THR:HB	2.12	0.73
1:A:89:MET:O	1:A:93:VAL:HG23	1.89	0.73
1:A:355:TRP:HZ3	1:A:356:GLU:HG2	1.53	0.73
1:B:272:ARG:HG2	1:B:273:PHE:CE2	2.23	0.73
2:E:156:ASN:OD1	2:E:157:LYS:HD2	1.89	0.73
1:A:8:ILE:HG23	1:A:9:LEU:HD23	1.70	0.73
1:A:277:GLY:O	1:A:280:ILE:HG13	1.89	0.72
2:C:125:GLN:O	2:C:126:ALA:C	2.30	0.72
1:A:251:VAL:CG2	1:A:254:TRP:NE1	2.52	0.72
1:A:485:ILE:HG22	1:A:487:THR:HG23	1.71	0.72
1:B:175:LEU:HB3	1:B:176:PRO:CD	2.19	0.72
1:B:589:LEU:CD2	1:B:592:HIS:ND1	2.52	0.72
1:A:251:VAL:HG21	1:A:254:TRP:CZ2	2.25	0.72
1:A:276:GLN:HG3	1:A:299:ARG:O	1.89	0.72
1:B:350:VAL:O	1:B:353:SER:OG	2.02	0.72
1:A:416:HIS:CD2	1:A:462:GLN:HB3	2.24	0.72
1:A:340:ASP:OD2	1:A:453:LYS:NZ	2.18	0.72
1:B:26:GLN:NE2	1:B:48:LYS:HZ2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:C	1:B:330:LEU:HD23	2.15	0.72
2:E:7:VAL:O	7:E:1237:AMP:C2	2.43	0.72
1:A:568:MET:HE2	1:A:573:GLU:HB3	1.72	0.72
1:A:287:LYS:O	1:A:289:VAL:N	2.23	0.72
2:C:88:TRP:CG	2:C:89:ASP:H	2.08	0.72
1:A:352:ILE:O	1:A:352:ILE:CG2	2.38	0.71
1:B:183:TYR:HD1	1:B:184:TYR:CE2	2.07	0.71
1:A:650:LEU:HD22	1:A:654:LEU:CD1	2.20	0.71
1:A:670:TYR:CZ	1:A:700:PRO:HG2	2.25	0.71
1:B:527:ILE:HG22	1:B:554:HIS:CE1	2.26	0.71
3:F:119:TYR:OH	3:F:140:ASN:OD1	2.08	0.71
1:A:140:ASP:O	1:A:143:ASP:HB2	1.90	0.71
1:A:354:ARG:HH21	1:A:354:ARG:CG	2.01	0.71
1:A:33:ALA:HB2	1:A:40:PHE:CD1	2.26	0.71
1:A:589:LEU:HD22	1:A:592:HIS:CG	2.24	0.71
1:B:56:LEU:HD23	1:B:93:VAL:HG11	1.73	0.70
1:B:181:ASN:OD1	1:B:182:PRO:HD2	1.90	0.70
1:A:712:ALA:HB1	1:B:84:ARG:CZ	2.21	0.70
1:B:500:THR:CB	1:B:500:THR:HA	2.09	0.70
1:A:148:GLN:NE2	1:A:201:PHE:HE1	1.87	0.70
1:A:542:ALA:HB3	1:A:543:PRO:CD	2.21	0.70
1:A:21:ARG:HG3	1:A:22:ASN:ND2	2.06	0.70
1:A:31:ILE:HG21	1:A:44:HIS:CD2	2.27	0.70
1:B:579:ARG:O	1:B:583:GLU:HG3	1.90	0.70
2:C:19:ILE:HD11	2:C:233:TYR:HA	1.73	0.70
1:A:346:ILE:HG22	1:A:442:TYR:HB2	1.73	0.70
1:A:647:GLU:O	1:A:647:GLU:HG3	1.92	0.70
1:B:44:HIS:CE1	1:B:362:MET:HE1	2.26	0.70
1:A:272:ARG:O	1:A:272:ARG:CG	2.40	0.70
3:F:54:VAL:HA	3:F:166:ALA:HA	1.74	0.70
1:A:557:THR:HG23	1:A:587:GLU:HG2	1.73	0.70
3:F:8:GLU:OE1	3:F:96:SER:OG	2.08	0.70
3:F:102:TYR:O	3:F:103:ALA:C	2.35	0.70
1:B:276:GLN:HE22	1:B:301:THR:H	1.40	0.70
1:A:350:VAL:O	1:A:353:SER:OG	2.10	0.70
1:A:516:THR:HB	1:A:517:PRO:CD	2.22	0.70
1:A:83:VAL:HG13	1:A:161:ALA:HB2	1.75	0.69
1:A:68:ASP:OD1	1:A:115:GLU:HB3	1.92	0.69
1:A:63:ILE:HG23	1:A:105:TRP:O	1.92	0.69
1:A:81:GLY:HA3	1:A:717:HIS:CE1	2.28	0.69
1:A:515:LEU:CD2	1:A:527:ILE:HD11	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ARG:NH2	1:B:518:GLU:HG2	2.08	0.69
1:A:372:GLU:OE1	1:A:376:ARG:NE	2.22	0.69
1:B:107:GLY:HA3	1:B:174:TYR:HD1	1.58	0.69
3:F:43:SER:O	3:F:64:LYS:HD3	1.93	0.69
1:B:107:GLY:CA	1:B:174:TYR:HD1	2.05	0.69
1:B:331:PRO:O	1:B:334:VAL:N	2.24	0.69
1:B:302:ASP:OD2	1:B:303:PRO:CD	2.41	0.68
1:B:367:ASN:OD1	1:B:367:ASN:C	2.34	0.68
1:A:21:ARG:HG3	1:A:22:ASN:HD22	1.58	0.68
1:B:517:PRO:O	1:B:521:MET:HB2	1.93	0.68
3:D:5:VAL:HB	3:D:38:VAL:HG22	1.75	0.68
1:B:517:PRO:O	1:B:521:MET:HE2	1.93	0.68
2:C:63:SER:CB	2:C:73:LEU:HD21	2.21	0.68
1:A:139:MET:HB3	1:A:143:ASP:CB	2.23	0.68
1:A:35:SER:HG	1:A:76:ARG:H	1.37	0.68
2:C:230:ARG:HH22	3:D:124:GLN:CD	2.01	0.68
1:B:379:HIS:ND1	1:B:381:GLU:N	2.39	0.68
3:D:4:LEU:HB3	3:D:91:VAL:HB	1.76	0.68
1:B:515:LEU:N	1:B:515:LEU:HD12	2.08	0.67
2:C:145:VAL:HG21	3:D:97:VAL:HG13	1.76	0.67
1:A:326:ALA:HB2	1:A:345:CYS:HB2	1.76	0.67
1:A:22:ASN:OD1	1:A:22:ASN:C	2.36	0.67
1:A:167:TYR:CD1	1:A:222:ARG:HB2	2.29	0.67
1:A:268:ALA:O	1:A:270:PRO:HD3	1.94	0.67
1:A:674:ASP:OD1	5:A:1731:ADP:O1B	2.12	0.67
1:B:46:SER:O	1:B:49:ALA:HB3	1.95	0.67
2:E:31:MET:HE3	2:E:33:TYR:OH	1.95	0.67
3:F:46:ASP:C	3:F:48:PHE:H	2.00	0.67
1:B:515:LEU:HD12	1:B:515:LEU:H	1.58	0.67
1:B:102:VAL:HB	1:B:163:PHE:CE1	2.30	0.67
1:B:107:GLY:HA3	1:B:174:TYR:CD1	2.28	0.67
1:B:393:LEU:HD23	1:B:483:VAL:HG13	1.77	0.67
1:A:375:ARG:O	1:A:706:TYR:CB	2.42	0.67
1:B:102:VAL:HG11	1:B:163:PHE:CD2	2.29	0.67
1:B:152:VAL:HG12	1:B:153:ASP:N	2.10	0.67
1:B:346:ILE:HG22	1:B:442:TYR:HB2	1.77	0.67
1:B:281:PRO:O	1:B:284:LYS:HG2	1.94	0.67
3:F:173:ASN:O	3:F:174:VAL:HG12	1.95	0.67
1:B:401:GLY:O	1:B:404:ALA:HB3	1.95	0.67
1:B:540:PHE:O	1:B:543:PRO:HD2	1.95	0.67
1:A:352:ILE:HG21	1:A:572:LEU:HD11	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLY:O	1:B:399:PRO:C	2.39	0.66
1:B:272:ARG:HG2	1:B:273:PHE:CD2	2.30	0.66
1:B:276:GLN:HE21	1:B:300:TYR:CA	1.99	0.66
1:B:159:ARG:NH2	1:B:213:VAL:HG12	2.11	0.66
1:B:254:TRP:CD1	1:B:254:TRP:N	2.60	0.66
2:E:1:MET:CE	2:E:1:MET:CB	2.71	0.66
1:A:175:LEU:HB3	1:A:176:PRO:CD	2.26	0.66
1:B:295:LEU:C	1:B:295:LEU:HD12	2.21	0.66
1:A:330:LEU:HD23	1:A:342:ILE:HG21	1.77	0.66
3:D:40:VAL:HG13	3:D:45:ALA:HB1	1.77	0.66
1:B:321:ALA:HB3	4:B:1730:FMN:O1P	1.96	0.65
3:F:45:ALA:HB3	3:F:62:VAL:HG13	1.78	0.65
3:F:120:ILE:HB	3:F:131:THR:HB	1.76	0.65
1:A:322:ARG:NH1	4:A:1730:FMN:O2P	2.24	0.65
1:A:711:ILE:HG23	1:A:711:ILE:O	1.97	0.65
3:F:45:ALA:CB	3:F:62:VAL:HG13	2.27	0.65
1:A:222:ARG:HG3	1:A:255:ASP:CG	2.22	0.65
1:A:443:HIS:O	1:A:443:HIS:ND1	2.29	0.65
1:A:535:ASN:ND2	1:A:537:ASP:H	1.94	0.65
1:A:542:ALA:HB3	1:A:543:PRO:HD3	1.77	0.65
1:A:139:MET:HB3	1:A:143:ASP:HB2	1.78	0.65
1:B:56:LEU:HD23	1:B:93:VAL:HG13	1.77	0.65
1:A:329:PHE:O	1:A:330:LEU:C	2.40	0.65
1:B:106:TYR:OH	1:B:121:ARG:HB2	1.97	0.65
2:C:230:ARG:NH2	3:D:124:GLN:HE22	1.92	0.65
3:D:137:GLN:NE2	3:D:156:ARG:HH22	1.94	0.65
1:B:31:ILE:CD1	1:B:33:ALA:HB2	2.27	0.65
2:C:1:MET:HG3	2:C:57:VAL:HG13	1.79	0.65
2:C:136:SER:CB	3:D:109:LYS:HZ2	2.10	0.65
1:A:153:ASP:HB3	1:A:157:ARG:NH1	2.13	0.64
1:A:202:TRP:CD1	1:A:206:LEU:HD11	2.33	0.64
1:A:295:LEU:HD13	1:A:319:GLY:HA3	1.79	0.64
1:B:263:GLU:O	1:B:265:GLY:N	2.30	0.64
1:A:287:LYS:O	1:A:288:GLN:C	2.39	0.64
1:A:598:GLU:HG3	1:A:632:TRP:HZ3	1.62	0.64
1:B:355:TRP:CZ3	1:B:356:GLU:HG2	2.32	0.64
2:C:134:VAL:HG12	2:C:138:LEU:HD12	1.79	0.64
1:A:485:ILE:CG2	1:A:487:THR:HG23	2.28	0.64
1:A:614:ARG:O	1:A:614:ARG:HG2	1.98	0.64
1:A:679:ARG:C	1:A:680:LEU:O	2.37	0.64
1:B:374:TYR:CE1	1:B:707:LYS:HD2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:GLU:O	2:E:48:LYS:HB2	1.97	0.64
1:A:367:ASN:OD1	1:A:367:ASN:C	2.39	0.64
3:F:45:ALA:HB3	3:F:62:VAL:CG1	2.27	0.64
1:A:485:ILE:N	1:A:485:ILE:HD13	2.13	0.64
1:A:183:TYR:O	1:A:186:LYS:NZ	2.30	0.64
2:C:58:GLU:OE2	2:C:83:ARG:NH1	2.30	0.64
1:B:159:ARG:CZ	1:B:213:VAL:HG12	2.27	0.64
1:A:280:ILE:O	1:A:283:VAL:N	2.31	0.64
2:C:172:VAL:CG1	3:D:183:SER:HB2	2.28	0.64
2:E:164:LEU:HB3	3:F:10:ARG:NH1	2.12	0.64
1:B:11:GLU:O	1:B:12:PRO:O	2.16	0.64
2:C:61:VAL:HG23	2:C:84:ALA:HA	1.78	0.64
3:D:119:TYR:CD2	3:D:156:ARG:NH1	2.66	0.64
1:A:444:ARG:HH21	1:A:445:ASP:HA	1.61	0.64
1:B:352:ILE:HG21	1:B:572:LEU:CD1	2.28	0.64
2:E:213:ILE:HG13	2:E:215:LEU:HD12	1.80	0.64
1:A:87:LYS:O	1:A:88:ALA:C	2.42	0.63
2:E:36:ASN:HB3	2:E:39:ASP:OD2	1.97	0.63
1:B:264:TRP:CH2	1:B:352:ILE:HD13	2.33	0.63
2:E:13:LEU:HA	2:E:30:PHE:O	1.97	0.63
1:A:167:TYR:CE1	1:A:222:ARG:HB2	2.33	0.63
1:A:430:GLN:O	1:A:433:ALA:HB3	1.97	0.63
1:B:492:ASN:ND2	1:B:643:GLY:C	2.56	0.63
3:F:40:VAL:HG13	3:F:45:ALA:HB1	1.78	0.63
1:A:30:CYS:HA	1:A:59:GLU:HB3	1.81	0.63
1:A:241:GLN:HE21	1:A:289:VAL:CG1	2.11	0.63
1:B:54:ALA:O	1:B:98:ALA:CB	2.20	0.63
2:C:100:VAL:HG12	2:C:104:LEU:HD11	1.81	0.63
1:A:417:LEU:HD23	1:A:463:LEU:CD1	2.28	0.63
1:A:428:LEU:HD21	1:A:440:TRP:O	1.99	0.63
1:A:678:PRO:HB2	1:B:135:TYR:CD2	2.34	0.63
3:F:65:GLY:HA2	3:F:176:ALA:HB3	1.81	0.63
1:B:59:GLU:O	1:B:60:TYR:C	2.39	0.62
1:B:102:VAL:CG1	1:B:163:PHE:CD2	2.82	0.62
1:B:272:ARG:O	1:B:272:ARG:HG3	1.99	0.62
3:F:46:ASP:C	3:F:48:PHE:N	2.57	0.62
3:F:79:VAL:O	3:F:82:LEU:N	2.32	0.62
1:A:71:HIS:CD2	1:A:71:HIS:H	2.16	0.62
1:B:379:HIS:CE1	1:B:381:GLU:H	2.16	0.62
1:A:330:LEU:CD2	1:A:342:ILE:HG21	2.28	0.62
1:B:31:ILE:HD11	1:B:33:ALA:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ASN:OD1	1:B:701:GLN:HB3	1.99	0.62
2:C:69:VAL:O	2:C:70:ASP:C	2.41	0.62
1:A:46:SER:O	1:A:49:ALA:HB3	1.99	0.62
1:A:648:CYS:O	1:A:651:TRP:HB3	1.98	0.62
1:A:353:SER:HA	1:A:570:PHE:O	1.99	0.62
1:A:532:VAL:O	1:A:638:LEU:HD12	1.99	0.62
1:A:571:THR:C	1:A:572:LEU:HG	2.23	0.62
1:B:264:TRP:CH2	1:B:352:ILE:CD1	2.83	0.62
1:A:443:HIS:ND1	1:A:443:HIS:C	2.57	0.62
1:A:616:TYR:OH	1:B:237:GLU:HG3	1.99	0.62
1:B:604:ILE:HD13	1:B:633:ILE:HD13	1.81	0.62
1:A:568:MET:O	1:A:569:HIS:C	2.43	0.62
1:A:598:GLU:HB2	1:A:601:ARG:HG3	1.81	0.62
1:A:681:ILE:O	1:A:682:ALA:C	2.41	0.62
1:B:3:ASP:OD1	1:B:4:PRO:CD	2.48	0.62
2:E:19:ILE:HD11	2:E:234:ILE:H	1.64	0.62
2:E:96:ASP:OD1	2:E:96:ASP:C	2.42	0.62
2:E:162:ARG:NH2	3:F:98:ASP:CA	2.52	0.62
2:E:232:MET:HG2	3:F:141:VAL:HG13	1.82	0.62
1:A:251:VAL:HG21	1:A:254:TRP:HE1	1.63	0.61
3:F:94:PRO:O	3:F:96:SER:N	2.33	0.61
3:F:143:VAL:HG23	3:F:143:VAL:O	1.99	0.61
1:A:24:PHE:CD1	1:A:331:PRO:CB	2.67	0.61
1:B:210:LYS:HD2	1:B:250:LEU:HD23	1.82	0.61
1:B:690:ARG:O	1:B:691:VAL:C	2.39	0.61
2:E:125:GLN:O	3:F:132:ARG:NH1	2.29	0.61
3:F:173:ASN:O	3:F:174:VAL:CG1	2.48	0.61
1:A:277:GLY:HA2	1:A:300:TYR:CE1	2.34	0.61
2:E:35:LEU:O	2:E:36:ASN:C	2.44	0.61
1:A:229:TYR:CD2	1:A:233:GLN:NE2	2.68	0.61
1:B:251:VAL:HG21	1:B:254:TRP:CD1	2.30	0.61
1:B:713:TRP:CH2	1:B:723:PHE:HD2	2.17	0.61
1:A:589:LEU:CD2	1:A:592:HIS:HD1	2.13	0.61
1:B:671:LEU:HD21	1:B:676:GLU:HA	1.82	0.61
3:D:119:TYR:CD2	3:D:156:ARG:CZ	2.83	0.61
1:A:568:MET:CE	1:A:573:GLU:HB3	2.30	0.61
1:B:167:TYR:HA	1:B:220:ALA:O	2.00	0.61
1:B:476:LEU:HD23	1:B:666:ILE:CD1	2.31	0.61
3:F:144:ASP:OD1	3:F:146:PRO:HD3	2.00	0.61
3:F:14:LEU:HD21	3:F:18:SER:HB2	1.82	0.61
1:A:598:GLU:HG3	1:A:632:TRP:CZ3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:SER:O	1:B:67:SER:OG	2.15	0.61
3:F:17:VAL:O	3:F:20:GLU:HB2	2.01	0.61
1:B:30:CYS:H	4:B:1730:FMN:C5A	2.13	0.61
2:C:2:LYS:NZ	2:C:111:GLU:OE1	2.34	0.61
2:C:100:VAL:HG12	2:C:104:LEU:CD1	2.31	0.61
1:A:80:GLU:HB2	1:A:719:PRO:HG2	1.83	0.60
1:A:594:CYS:HB2	1:A:604:ILE:HG22	1.82	0.60
2:E:9:GLN:OE1	2:E:68:ARG:NH1	2.25	0.60
3:F:30:LYS:HE2	3:F:123:TYR:CE2	2.35	0.60
1:A:516:THR:HB	1:A:517:PRO:HD2	1.83	0.60
3:F:1:SER:O	3:F:34:ASP:HB3	2.02	0.60
3:F:28:LEU:HD21	3:F:128:LEU:HD11	1.84	0.60
1:B:22:ASN:C	1:B:22:ASN:OD1	2.43	0.60
1:A:540:PHE:C	1:A:540:PHE:CD2	2.80	0.60
1:B:713:TRP:CZ2	1:B:723:PHE:CE2	2.89	0.60
1:A:13:ILE:HG22	1:A:23:ARG:HD3	1.84	0.60
3:F:121:VAL:HA	3:F:129:VAL:O	2.02	0.60
1:A:177:LEU:CD1	1:A:181:ASN:HD22	2.15	0.60
1:B:272:ARG:CD	1:B:273:PHE:CZ	2.85	0.60
1:B:539:TYR:CD2	1:B:540:PHE:N	2.69	0.60
2:C:45:GLU:O	2:C:48:LYS:HB2	2.01	0.60
1:A:29:HIS:CD2	1:A:321:ALA:HB1	2.36	0.60
1:A:251:VAL:CG2	1:A:254:TRP:HE1	2.14	0.60
1:A:280:ILE:O	1:A:281:PRO:C	2.44	0.60
2:C:69:VAL:O	2:C:72:SER:N	2.35	0.60
1:A:139:MET:HE3	1:A:147:VAL:CG2	2.22	0.60
1:A:566:ASN:O	1:A:569:HIS:HB2	2.01	0.60
1:A:680:LEU:HD12	1:A:680:LEU:H	1.65	0.60
2:C:19:ILE:CD1	2:C:233:TYR:HA	2.32	0.60
1:A:197:ASN:OD1	1:A:200:ARG:NH1	2.34	0.60
1:A:334:VAL:O	1:A:337:GLY:N	2.33	0.60
1:A:9:LEU:HD11	1:A:306:MET:HB3	1.83	0.60
1:B:34:GLY:HA2	1:B:59:GLU:OE2	2.02	0.60
1:B:571:THR:C	1:B:572:LEU:HG	2.27	0.60
3:D:79:VAL:O	3:D:82:LEU:N	2.35	0.60
1:A:191:TYR:CE1	1:A:200:ARG:HD2	2.37	0.59
1:B:13:ILE:HG21	1:B:23:ARG:NH2	2.17	0.59
1:B:486:ALA:HB2	1:B:672:ILE:HD11	1.83	0.59
1:A:127:ALA:O	1:B:501:HIS:HE1	1.85	0.59
1:A:379:HIS:CE1	1:A:381:GLU:H	2.20	0.59
1:B:3:ASP:OD1	1:B:4:PRO:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:TRP:CZ2	1:B:541:MET:HG2	2.37	0.59
1:B:554:HIS:CD2	1:B:554:HIS:H	2.20	0.59
1:B:657:ARG:HB3	1:B:660:GLU:OE2	2.02	0.59
2:E:19:ILE:CD1	2:E:233:TYR:HA	2.31	0.59
1:A:144:ILE:HG23	1:A:201:PHE:CE1	2.37	0.59
1:B:272:ARG:O	1:B:272:ARG:HG2	2.02	0.59
1:B:679:ARG:O	1:B:680:LEU:O	2.21	0.59
3:D:75:PHE:O	3:D:78:SER:N	2.34	0.59
1:B:23:ARG:O	1:B:317:ILE:HG22	2.01	0.59
1:B:123:PRO:HG2	1:B:124:SER:H	1.67	0.59
1:B:515:LEU:O	1:B:640:LEU:N	2.33	0.59
1:A:10:PHE:CE2	1:A:335:GLU:HB2	2.38	0.59
1:B:302:ASP:O	1:B:306:MET:HG3	2.01	0.59
3:F:10:ARG:HD3	3:F:188:TYR:HE2	1.67	0.59
2:C:20:ARG:C	2:C:22:ASP:N	2.60	0.59
2:C:144:ALA:C	2:C:145:VAL:HG23	2.27	0.59
2:E:4:LEU:C	2:E:4:LEU:HD23	2.27	0.59
2:E:116:VAL:O	2:E:179:VAL:HA	2.02	0.59
1:A:10:PHE:N	1:A:10:PHE:CD1	2.71	0.59
1:A:378:TRP:CD1	1:A:693:ARG:HD2	2.38	0.59
1:A:700:PRO:O	1:A:702:ILE:N	2.36	0.59
1:B:175:LEU:O	1:B:178:GLN:N	2.33	0.59
1:B:263:GLU:C	1:B:265:GLY:H	2.09	0.59
1:B:341:ASP:HA	1:B:450:GLN:NE2	2.18	0.59
1:B:529:LYS:HB3	1:B:636:ASP:OD2	2.03	0.59
1:B:692:ALA:O	1:B:693:ARG:C	2.45	0.59
3:F:17:VAL:O	3:F:21:LEU:HG	2.01	0.59
1:A:80:GLU:OE2	1:A:80:GLU:N	2.24	0.59
1:A:398:GLY:O	1:A:399:PRO:C	2.45	0.59
1:B:441:SER:O	1:B:444:ARG:HG3	2.02	0.59
1:A:31:ILE:HG21	1:A:44:HIS:HD2	1.67	0.59
1:A:34:GLY:N	1:A:59:GLU:OE2	2.36	0.59
1:A:202:TRP:CD1	1:A:206:LEU:CD1	2.86	0.59
1:B:540:PHE:C	1:B:543:PRO:HD2	2.28	0.59
1:B:31:ILE:CD1	1:B:33:ALA:CB	2.81	0.58
1:B:199:ALA:O	1:B:203:LEU:HB2	2.03	0.58
2:E:120:VAL:HG22	2:E:181:THR:OG1	2.03	0.58
1:A:375:ARG:HG3	1:A:706:TYR:HB2	1.85	0.58
2:E:60:VAL:HG13	2:E:60:VAL:O	2.02	0.58
1:A:619:PRO:HG3	1:B:237:GLU:HB3	1.82	0.58
1:A:629:SER:O	1:A:630:HIS:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:ARG:HG2	2:E:205:ILE:HD11	1.85	0.58
2:E:186:ILE:HG23	2:E:187:ASN:ND2	2.18	0.58
1:A:195:LEU:CD2	1:A:246:MET:HE1	2.30	0.58
3:D:71:ASP:OD1	3:D:74:VAL:HG23	2.02	0.58
1:A:263:GLU:O	1:A:265:GLY:N	2.36	0.58
1:A:391:SER:O	1:A:481:ASP:HB2	2.03	0.58
2:E:173:GLU:O	3:F:183:SER:HA	2.03	0.58
2:C:2:LYS:HE3	2:C:111:GLU:OE1	2.03	0.58
3:D:52:LEU:HB2	3:D:60:LEU:HD11	1.86	0.58
1:B:149:GLN:O	1:B:152:VAL:HB	2.03	0.58
2:C:1:MET:CE	2:C:1:MET:CB	2.78	0.58
1:B:280:ILE:HD11	1:B:309:ILE:HG21	1.85	0.58
1:B:476:LEU:HD23	1:B:666:ILE:HD12	1.86	0.58
2:E:89:ASP:O	2:E:92:ALA:HB3	2.03	0.58
3:F:119:TYR:CD2	3:F:156:ARG:NH1	2.72	0.58
1:B:30:CYS:HA	1:B:59:GLU:CB	2.33	0.57
1:B:272:ARG:HD2	1:B:273:PHE:CZ	2.39	0.57
1:B:321:ALA:O	1:B:322:ARG:C	2.47	0.57
1:B:430:GLN:O	1:B:431:VAL:C	2.45	0.57
2:C:64:VAL:HG22	2:C:87:VAL:HB	1.86	0.57
3:D:49:VAL:HB	3:D:50:PRO:HD3	1.86	0.57
1:B:60:TYR:CE2	1:B:74:SER:HA	2.38	0.57
1:A:183:TYR:CE1	1:B:501:HIS:CD2	2.93	0.57
2:E:19:ILE:HD11	2:E:233:TYR:HA	1.86	0.57
1:B:706:TYR:HD2	1:B:707:LYS:O	1.86	0.57
1:B:713:TRP:CZ2	1:B:723:PHE:CD2	2.92	0.57
2:C:65:GLY:HA2	2:C:88:TRP:CZ3	2.39	0.57
2:C:121:GLN:HA	7:C:1236:AMP:O3P	2.04	0.57
3:F:51:ALA:O	3:F:54:VAL:CG1	2.51	0.57
1:A:174:TYR:O	1:A:175:LEU:C	2.47	0.57
1:B:174:TYR:O	1:B:175:LEU:C	2.47	0.57
1:A:14:GLN:NE2	1:A:16:GLY:O	2.38	0.57
1:A:89:MET:SD	1:A:89:MET:C	2.88	0.57
2:E:1:MET:HB2	2:E:1:MET:HE3	1.86	0.57
1:B:497:ASN:OD1	1:B:499:LEU:HB2	2.04	0.57
2:E:125:GLN:O	2:E:126:ALA:C	2.47	0.57
1:B:251:VAL:HG11	1:B:254:TRP:CZ2	2.39	0.57
2:E:221:GLY:O	2:E:223:ALA:N	2.38	0.57
1:A:505:PRO:HG2	1:A:595:SER:O	2.04	0.57
2:C:36:ASN:HB3	2:C:39:ASP:OD2	2.05	0.57
1:A:287:LYS:C	1:A:289:VAL:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:THR:HG21	1:B:115:GLU:HB2	1.86	0.56
2:E:175:ASN:HB2	3:F:182:ARG:HB3	1.87	0.56
1:A:74:SER:OG	1:A:75:ALA:N	2.31	0.56
1:A:93:VAL:HG11	1:A:99:LEU:O	2.05	0.56
1:B:24:PHE:CD1	1:B:331:PRO:HB3	2.41	0.56
1:B:67:SER:OG	1:B:105:TRP:CZ3	2.58	0.56
1:B:231:PRO:HA	1:B:235:GLU:OE1	2.04	0.56
2:C:102:ARG:HH11	2:C:102:ARG:CG	2.19	0.56
2:C:209:SER:O	2:C:212:ASP:HB2	2.05	0.56
3:D:121:VAL:HA	3:D:129:VAL:O	2.05	0.56
1:B:527:ILE:CG2	1:B:554:HIS:CE1	2.88	0.56
2:C:162:ARG:NH2	3:D:98:ASP:OD1	2.38	0.56
1:B:280:ILE:HD11	1:B:300:TYR:OH	2.06	0.56
1:B:706:TYR:O	1:B:707:LYS:C	2.46	0.56
2:E:40:ASP:OD2	2:E:79:LYS:HE2	2.06	0.56
2:E:125:GLN:HB2	2:E:127:TYR:CE1	2.40	0.56
3:F:26:ASN:O	3:F:29:LYS:CD	2.52	0.56
1:A:325:ILE:HD13	1:A:362:MET:SD	2.46	0.56
1:A:379:HIS:ND1	1:A:381:GLU:N	2.49	0.56
1:A:700:PRO:O	1:A:701:GLN:C	2.47	0.56
1:B:22:ASN:OD1	1:B:54:ALA:HB2	2.05	0.56
1:B:482:LYS:HD3	1:B:695:ILE:HD11	1.87	0.56
1:B:683:ASP:O	1:B:684:ALA:C	2.47	0.56
2:C:2:LYS:CE	2:C:111:GLU:OE1	2.53	0.56
2:C:213:ILE:HG13	2:C:215:LEU:HD12	1.85	0.56
1:B:199:ALA:HB1	1:B:243:PHE:HE1	1.71	0.55
1:B:385:GLN:HA	1:B:411:SER:O	2.06	0.55
1:B:476:LEU:HA	1:B:666:ILE:HD11	1.88	0.55
2:C:88:TRP:CG	2:C:89:ASP:N	2.68	0.55
1:A:630:HIS:CD2	1:A:630:HIS:H	2.24	0.55
1:A:569:HIS:CE1	1:A:574:TYR:CD2	2.94	0.55
1:A:722:ASN:HB3	1:A:726:GLU:OE2	2.07	0.55
1:B:417:LEU:HD23	1:B:463:LEU:HD13	1.87	0.55
1:B:542:ALA:O	1:B:543:PRO:C	2.47	0.55
1:B:124:SER:HA	1:B:138:GLU:HG3	1.88	0.55
1:B:568:MET:CE	1:B:573:GLU:HB3	2.37	0.55
2:C:122:SER:N	7:C:1236:AMP:O3P	2.38	0.55
2:C:221:GLY:O	2:C:223:ALA:N	2.40	0.55
2:E:134:VAL:CG1	2:E:138:LEU:HD12	2.34	0.55
1:A:104:LEU:N	1:A:104:LEU:HD23	2.21	0.55
1:A:180:LEU:HD22	1:A:202:TRP:CZ3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:OE2	1:A:403:GLU:HA	2.07	0.55
1:B:254:TRP:HB3	1:B:256:ILE:HD11	1.88	0.55
3:D:99:SER:O	3:D:101:GLY:N	2.40	0.55
1:A:84:ARG:O	1:A:87:LYS:N	2.38	0.55
1:B:90:THR:O	1:B:91:ASP:C	2.50	0.55
1:A:149:GLN:O	1:A:152:VAL:HB	2.07	0.55
1:A:199:ALA:O	1:A:203:LEU:HG	2.07	0.55
1:A:254:TRP:HB3	1:A:256:ILE:CD1	2.24	0.55
1:B:441:SER:HB3	1:B:445:ASP:OD2	2.06	0.55
2:C:42:SER:O	2:C:43:LEU:C	2.46	0.55
3:F:119:TYR:O	3:F:120:ILE:HG13	2.06	0.55
1:A:515:LEU:N	1:A:515:LEU:CD1	2.66	0.55
1:A:576:ASN:OD1	1:B:624:ARG:NH1	2.40	0.55
1:B:179:PHE:HA	1:B:185:ASN:HD22	1.71	0.55
1:B:434:LEU:O	1:B:435:PRO:C	2.45	0.55
3:D:93:LEU:CD1	3:D:102:TYR:OH	2.55	0.55
3:F:79:VAL:C	3:F:82:LEU:H	2.15	0.55
1:A:580:ARG:NH1	1:B:612:SER:OG	2.29	0.54
1:B:10:PHE:CE2	1:B:335:GLU:HB2	2.42	0.54
1:B:57:ASN:OD1	1:B:101:GLY:CA	2.51	0.54
2:C:59:VAL:O	2:C:82:ASP:HB2	2.07	0.54
1:A:574:TYR:N	1:A:575:PRO:HD3	2.22	0.54
1:A:647:GLU:O	1:A:647:GLU:CG	2.52	0.54
1:B:476:LEU:HD22	1:B:664:ASN:ND2	2.22	0.54
2:E:141:PRO:O	2:E:178:ALA:HB1	2.07	0.54
1:A:222:ARG:HG3	1:A:255:ASP:HB3	1.89	0.54
1:A:647:GLU:OE2	1:A:649:THR:CB	2.55	0.54
2:C:216:SER:O	2:C:217:ALA:C	2.51	0.54
2:E:17:PHE:HA	2:E:30:PHE:CG	2.42	0.54
1:A:569:HIS:CE1	1:A:574:TYR:CE2	2.96	0.54
1:B:42:SER:O	1:B:43:ALA:C	2.47	0.54
1:B:674:ASP:OD1	5:B:1731:ADP:O1B	2.26	0.54
2:E:172:VAL:HG12	3:F:183:SER:HB2	1.89	0.54
1:B:322:ARG:O	1:B:324:SER:N	2.40	0.54
2:C:136:SER:HB2	3:D:105:SER:HB2	1.90	0.54
2:E:143:ALA:HB3	2:E:180:LEU:CD2	2.38	0.54
1:B:58:THR:HG23	1:B:102:VAL:HA	1.89	0.54
1:B:71:HIS:ND1	1:B:358:GLY:HA3	2.23	0.54
1:B:200:ARG:O	1:B:204:GLU:HG3	2.08	0.54
1:B:500:THR:CA	1:B:500:THR:CG2	2.79	0.54
1:B:568:MET:O	1:B:569:HIS:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:MET:CE	2:E:1:MET:CG	2.86	0.54
2:E:79:LYS:O	2:E:190:ARG:HD2	2.08	0.54
2:C:162:ARG:HE	2:C:170:GLN:NE2	2.06	0.54
1:A:62:SER:OG	1:A:78:TRP:NE1	2.29	0.54
1:A:123:PRO:O	1:A:138:GLU:HG3	2.08	0.54
1:B:365:THR:HG23	1:B:682:ALA:CA	2.38	0.54
1:B:692:ALA:O	1:B:694:GLU:N	2.41	0.54
2:C:26:VAL:HG12	2:C:27:ASP:O	2.07	0.54
2:E:161:ARG:HG2	2:E:171:GLU:HG3	1.90	0.54
1:B:107:GLY:CA	1:B:174:TYR:CD1	2.87	0.54
3:D:120:ILE:HG22	3:D:121:VAL:N	2.21	0.54
1:A:444:ARG:NH2	1:A:445:ASP:HA	2.23	0.54
1:A:527:ILE:O	1:A:554:HIS:HE1	1.91	0.54
1:B:210:LYS:O	1:B:211:HIS:C	2.50	0.54
3:D:75:PHE:O	3:D:76:GLU:C	2.51	0.54
2:E:58:GLU:OE2	2:E:83:ARG:NH1	2.39	0.54
2:E:77:LEU:HA	2:E:81:ALA:HB3	1.90	0.54
1:A:331:PRO:O	1:A:334:VAL:N	2.41	0.53
1:A:650:LEU:CD2	1:A:654:LEU:CD1	2.84	0.53
1:B:102:VAL:HG12	1:B:163:PHE:CG	2.42	0.53
1:B:309:ILE:HD11	1:B:318:ILE:CD1	2.37	0.53
1:A:144:ILE:HG23	1:A:201:PHE:HE1	1.73	0.53
1:B:87:LYS:O	1:B:88:ALA:C	2.52	0.53
2:E:53:SER:HB3	2:E:55:THR:O	2.08	0.53
1:B:39:GLY:HA3	1:B:374:TYR:CE2	2.43	0.53
1:B:386:THR:HB	1:B:413:TYR:CZ	2.44	0.53
1:B:513:ASP:HB2	1:B:636:ASP:O	2.08	0.53
1:A:14:GLN:OE1	1:A:19:THR:OG1	2.23	0.53
1:A:169:TYR:OH	1:A:172:HIS:ND1	2.42	0.53
1:A:330:LEU:HD23	1:A:342:ILE:CG2	2.38	0.53
1:A:443:HIS:C	1:A:443:HIS:HD1	2.16	0.53
1:B:26:GLN:HE22	1:B:45:ARG:HH21	1.56	0.53
1:B:227:THR:HG22	1:B:229:TYR:HB2	1.90	0.53
2:C:100:VAL:O	2:C:104:LEU:HD12	2.09	0.53
2:E:230:ARG:HB2	3:F:142:GLU:O	2.09	0.53
1:A:369:THR:HA	1:A:372:GLU:HB2	1.89	0.53
1:A:582:HIS:O	1:A:583:GLU:C	2.52	0.53
1:A:669:ILE:C	1:A:670:TYR:CD1	2.87	0.53
1:B:353:SER:OG	1:B:354:ARG:N	2.40	0.53
1:B:365:THR:HG23	1:B:682:ALA:N	2.24	0.53
1:B:589:LEU:HD23	1:B:592:HIS:HD1	1.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:LEU:HB3	3:D:10:ARG:NH1	2.23	0.53
1:B:272:ARG:NH2	1:B:544:SER:OG	2.40	0.53
1:B:341:ASP:HA	1:B:450:GLN:HE22	1.74	0.53
1:A:260:ASP:OD1	1:A:260:ASP:N	2.42	0.53
1:A:568:MET:HA	1:A:571:THR:OG1	2.08	0.53
2:C:10:THR:HB	2:C:124:ASP:OD2	2.08	0.53
1:A:74:SER:OG	1:A:75:ALA:O	2.26	0.53
1:A:148:GLN:O	1:A:149:GLN:C	2.49	0.53
1:B:131:GLU:O	1:B:133:LEU:N	2.42	0.53
1:B:405:ALA:O	1:B:406:ARG:C	2.49	0.53
2:E:145:VAL:HG22	3:F:100:LEU:HD12	1.90	0.53
3:F:10:ARG:HD3	3:F:188:TYR:CE2	2.44	0.53
3:F:14:LEU:HG	3:F:15:ARG:N	2.24	0.53
1:B:39:GLY:HA3	1:B:374:TYR:CD2	2.44	0.53
1:B:295:LEU:HD12	1:B:295:LEU:O	2.09	0.53
1:B:322:ARG:O	1:B:323:PRO:C	2.47	0.53
1:B:394:ILE:CG2	1:B:417:LEU:HD12	2.39	0.53
1:A:132:THR:O	1:A:133:LEU:HD23	2.08	0.53
1:A:241:GLN:HE21	1:A:289:VAL:HG11	1.74	0.53
1:B:468:LYS:O	1:B:469:PRO:C	2.51	0.53
1:B:658:GLU:HA	1:B:661:TRP:NE1	2.23	0.53
2:C:119:GLY:H	7:C:1236:AMP:H4'	1.73	0.53
1:A:28:PRO:HG2	1:A:103:GLU:OE2	2.09	0.52
1:A:171:ALA:O	1:A:172:HIS:C	2.52	0.52
1:A:199:ALA:O	1:A:203:LEU:CG	2.57	0.52
1:A:515:LEU:HD21	1:A:527:ILE:HG13	1.91	0.52
1:B:564:LEU:O	1:B:565:ALA:HB3	2.09	0.52
2:C:65:GLY:HA2	2:C:88:TRP:CE3	2.44	0.52
3:F:188:TYR:HD1	3:F:188:TYR:H	1.57	0.52
1:A:21:ARG:NH1	1:A:97:GLY:O	2.42	0.52
1:B:280:ILE:CD1	1:B:300:TYR:OH	2.57	0.52
1:B:330:LEU:HD23	1:B:330:LEU:O	2.09	0.52
1:B:392:VAL:HG11	1:B:408:LEU:CD1	2.39	0.52
1:B:713:TRP:CH2	1:B:723:PHE:CD2	2.97	0.52
3:F:83:ILE:HD11	3:F:112:TYR:CZ	2.45	0.52
3:F:188:TYR:CD1	3:F:188:TYR:N	2.73	0.52
1:A:409:MET:HG2	1:A:415:VAL:CG1	2.36	0.52
1:B:31:ILE:HD12	1:B:33:ALA:HB2	1.91	0.52
1:B:68:ASP:HB3	1:B:113:ASN:OD1	2.08	0.52
1:B:194:SER:O	1:B:195:LEU:C	2.52	0.52
3:F:46:ASP:N	3:F:62:VAL:HG11	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HB2	1:B:619:PRO:CG	2.12	0.52
1:B:181:ASN:OD1	1:B:182:PRO:CD	2.56	0.52
1:B:251:VAL:CG2	1:B:254:TRP:NE1	2.36	0.52
2:C:156:ASN:OD1	2:C:157:LYS:HD2	2.08	0.52
1:B:276:GLN:HE22	1:B:302:ASP:H	1.58	0.52
1:B:490:ARG:HH22	1:B:518:GLU:HG2	1.75	0.52
3:D:99:SER:C	3:D:101:GLY:H	2.17	0.52
1:A:139:MET:HB3	1:A:143:ASP:HB3	1.89	0.52
1:B:252:ASP:O	1:B:293:PRO:HD2	2.10	0.52
1:B:473:ASP:OD2	1:B:657:ARG:NH1	2.43	0.52
1:A:272:ARG:O	1:A:273:PHE:CD2	2.62	0.52
1:B:528:GLY:HA3	1:B:636:ASP:HB3	1.91	0.52
2:C:4:LEU:HD11	2:C:62:VAL:CG2	2.38	0.52
2:C:9:GLN:OE1	2:C:68:ARG:NH1	2.30	0.52
1:A:24:PHE:HE2	1:A:306:MET:CE	2.23	0.52
1:B:8:ILE:O	1:B:11:GLU:HG3	2.09	0.52
3:D:99:SER:C	3:D:101:GLY:N	2.67	0.52
2:E:116:VAL:HG12	2:E:179:VAL:HG13	1.91	0.52
1:A:582:HIS:O	1:A:585:HIS:N	2.39	0.52
1:A:712:ALA:CB	1:B:84:ARG:CZ	2.88	0.52
1:B:272:ARG:CG	1:B:273:PHE:CE2	2.93	0.52
1:B:578:MET:O	1:B:579:ARG:C	2.51	0.52
1:A:583:GLU:OE2	1:B:612:SER:OG	2.19	0.52
1:A:670:TYR:CE2	1:A:700:PRO:HG2	2.44	0.52
1:B:199:ALA:HB1	1:B:243:PHE:CE1	2.45	0.52
1:B:403:GLU:O	1:B:404:ALA:C	2.50	0.52
1:B:568:MET:HE2	1:B:573:GLU:HB3	1.91	0.52
2:C:20:ARG:O	2:C:22:ASP:N	2.43	0.52
3:D:99:SER:O	3:D:100:LEU:C	2.52	0.52
1:A:542:ALA:CB	1:A:543:PRO:CD	2.88	0.51
1:B:500:THR:CB	1:B:500:THR:N	2.64	0.51
2:C:125:GLN:CB	2:C:127:TYR:CE1	2.92	0.51
1:A:24:PHE:HZ	1:A:334:VAL:HG21	1.74	0.51
1:A:147:VAL:O	1:A:150:PHE:HB2	2.11	0.51
1:A:416:HIS:CE1	2:E:197:ILE:HD11	2.46	0.51
1:A:45:ARG:CZ	1:A:57:ASN:O	2.57	0.51
1:A:507:ALA:HB2	1:A:597:ILE:HD12	1.92	0.51
1:B:242:LYS:O	1:B:246:MET:HG3	2.09	0.51
2:C:226:MET:CE	3:D:111:GLY:HA2	2.36	0.51
1:B:104:LEU:HB2	1:B:167:TYR:O	2.10	0.51
1:B:458:ASN:HB3	1:B:461:SER:CB	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASP:HB2	2:C:125:GLN:NE2	2.25	0.51
3:D:173:ASN:O	3:D:174:VAL:CG1	2.59	0.51
3:F:102:TYR:O	3:F:103:ALA:O	2.27	0.51
1:A:413:TYR:O	1:A:458:ASN:ND2	2.39	0.51
1:B:378:TRP:CD1	1:B:378:TRP:N	2.76	0.51
1:B:428:LEU:HD12	1:B:431:VAL:HB	1.92	0.51
2:C:39:ASP:OD1	7:C:1236:AMP:O3'	2.29	0.51
2:C:159:VAL:HA	2:C:172:VAL:O	2.10	0.51
2:E:168:MET:HE1	3:F:11:ARG:HD2	1.93	0.51
1:A:15:ILE:CG2	1:A:293:PRO:HG2	2.40	0.51
1:A:277:GLY:CA	1:A:300:TYR:HE1	2.23	0.51
1:B:671:LEU:CD2	1:B:676:GLU:HA	2.39	0.51
2:E:111:GLU:O	2:E:112:ALA:C	2.51	0.51
1:B:39:GLY:CA	1:B:374:TYR:CD2	2.93	0.51
3:F:71:ASP:O	3:F:75:PHE:HB2	2.10	0.51
3:F:123:TYR:CZ	3:F:128:LEU:HD13	2.45	0.51
1:A:169:TYR:OH	4:A:1730:FMN:O2	2.29	0.51
1:A:430:GLN:OE1	1:A:521:MET:HE3	2.11	0.51
1:A:527:ILE:HG22	1:A:554:HIS:CE1	2.46	0.51
1:B:38:PRO:HD2	1:B:709:GLU:OE1	2.11	0.51
3:F:52:LEU:HB2	3:F:60:LEU:HD11	1.92	0.51
3:F:184:GLN:O	3:F:185:ASN:C	2.54	0.51
1:A:225:VAL:HG22	1:A:240:GLY:HA3	1.92	0.51
1:A:274:TYR:HB3	1:A:278:HIS:CG	2.45	0.51
1:A:676:GLU:CD	1:B:119:THR:HG21	2.36	0.51
2:C:35:LEU:O	2:C:36:ASN:C	2.52	0.51
2:C:183:GLN:HG3	2:C:184:LEU:N	2.25	0.51
2:E:164:LEU:HD23	2:E:164:LEU:N	2.26	0.51
3:F:51:ALA:O	3:F:54:VAL:HG11	2.10	0.51
1:A:41:GLN:OE1	1:A:45:ARG:NE	2.33	0.51
1:A:409:MET:CE	1:A:454:LEU:HB2	2.41	0.51
1:A:569:HIS:HE1	1:A:574:TYR:CE2	2.29	0.51
1:A:615:THR:HG22	1:A:616:TYR:O	2.11	0.51
1:B:350:VAL:O	1:B:353:SER:CB	2.59	0.51
2:C:161:ARG:HA	2:C:170:GLN:O	2.11	0.51
2:C:230:ARG:NH2	3:D:124:GLN:NE2	2.42	0.51
3:F:78:SER:O	3:F:81:ALA:HB3	2.11	0.51
1:B:29:HIS:HA	4:B:1730:FMN:C4A	2.40	0.50
1:B:234:ILE:HD13	1:B:234:ILE:N	2.25	0.50
1:B:692:ALA:C	1:B:694:GLU:N	2.68	0.50
2:C:226:MET:CE	3:D:111:GLY:CA	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ASN:HD21	1:A:537:ASP:H	1.56	0.50
1:B:598:GLU:O	1:B:599:PRO:C	2.54	0.50
1:A:416:HIS:CE1	2:E:197:ILE:CD1	2.94	0.50
1:A:711:ILE:HG13	1:A:712:ALA:N	2.25	0.50
1:B:545:LEU:O	1:B:546:ALA:C	2.54	0.50
2:E:127:TYR:HD1	7:E:1237:AMP:O1P	1.95	0.50
2:E:161:ARG:HA	2:E:170:GLN:O	2.11	0.50
1:A:15:ILE:HG22	1:A:293:PRO:HG2	1.93	0.50
1:A:242:LYS:O	1:A:246:MET:HG3	2.11	0.50
3:D:135:TYR:O	3:D:136:ASN:C	2.53	0.50
1:B:302:ASP:OD2	1:B:303:PRO:N	2.45	0.50
3:D:144:ASP:C	3:D:144:ASP:OD1	2.55	0.50
2:E:96:ASP:O	2:E:99:VAL:N	2.44	0.50
1:A:532:VAL:HA	1:A:557:THR:O	2.11	0.50
1:B:110:HIS:CD2	1:B:261:ILE:HG21	2.47	0.50
1:B:419:ASP:OD1	1:B:421:ALA:N	2.41	0.50
2:C:10:THR:HG21	2:C:123:SER:OG	2.12	0.50
2:C:87:VAL:HG21	2:C:107:VAL:HG21	1.94	0.50
1:A:159:ARG:NH2	1:A:213:VAL:HG12	2.27	0.50
1:A:490:ARG:CZ	1:A:518:GLU:HG2	2.41	0.50
1:B:241:GLN:O	1:B:244:VAL:HB	2.12	0.50
1:B:355:TRP:CE3	1:B:356:GLU:HG2	2.47	0.50
1:B:713:TRP:CE2	1:B:723:PHE:CE2	3.00	0.50
3:F:49:VAL:CG2	3:F:50:PRO:HD3	2.35	0.50
1:A:183:TYR:CE1	1:B:501:HIS:HD2	2.29	0.50
1:A:303:PRO:HA	1:A:306:MET:HB2	1.94	0.50
1:B:167:TYR:OH	1:B:255:ASP:OD2	2.23	0.50
3:D:144:ASP:OD1	3:D:146:PRO:HD3	2.11	0.50
2:E:17:PHE:HA	2:E:30:PHE:CD2	2.47	0.50
1:A:714:GLY:HA2	1:A:723:PHE:CG	2.46	0.50
3:F:1:SER:N	3:F:34:ASP:OD1	2.45	0.50
3:F:22:ILE:O	3:F:23:GLY:C	2.55	0.50
1:A:222:ARG:HG3	1:A:255:ASP:CB	2.42	0.49
1:A:227:THR:O	1:A:228:VAL:CG2	2.60	0.49
1:A:322:ARG:O	1:A:323:PRO:C	2.54	0.49
1:B:679:ARG:C	1:B:680:LEU:O	2.54	0.49
3:F:51:ALA:O	3:F:54:VAL:HG13	2.11	0.49
1:A:690:ARG:O	1:A:691:VAL:C	2.54	0.49
2:E:69:VAL:O	2:E:70:ASP:C	2.53	0.49
3:F:10:ARG:HG2	3:F:11:ARG:HG3	1.94	0.49
3:F:46:ASP:O	3:F:48:PHE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LEU:O	1:A:435:PRO:C	2.55	0.49
1:A:494:ASP:OD1	1:A:494:ASP:N	2.27	0.49
1:B:661:TRP:CE2	1:B:669:ILE:HD12	2.46	0.49
1:B:722:ASN:OD1	1:B:724:LYS:HB2	2.12	0.49
1:A:192:GLY:O	1:A:197:ASN:ND2	2.31	0.49
1:A:256:ILE:HD12	1:A:286:VAL:HG21	1.93	0.49
1:A:520:VAL:HG12	1:A:521:MET:N	2.26	0.49
1:B:420:THR:CG2	1:B:469:PRO:HA	2.42	0.49
1:B:714:GLY:HA2	1:B:723:PHE:CD2	2.48	0.49
2:E:11:ALA:N	2:E:124:ASP:OD2	2.40	0.49
3:F:8:GLU:O	3:F:15:ARG:HG3	2.13	0.49
1:A:13:ILE:HG22	1:A:23:ARG:CD	2.42	0.49
1:A:295:LEU:HB3	1:A:317:ILE:HB	1.93	0.49
1:A:430:GLN:HB3	1:A:521:MET:HE3	1.94	0.49
1:B:303:PRO:O	1:B:306:MET:HB2	2.12	0.49
1:B:589:LEU:HD23	1:B:592:HIS:CB	2.41	0.49
2:E:120:VAL:HG23	2:E:182:ILE:O	2.12	0.49
1:A:26:GLN:NE2	1:A:27:VAL:O	2.40	0.49
1:A:321:ALA:O	1:A:324:SER:N	2.46	0.49
1:A:609:GLY:HA3	1:A:627:ASN:OD1	2.13	0.49
1:B:502:ASP:HB3	1:B:503:PRO:CD	2.42	0.49
2:C:41:PHE:CD1	2:C:184:LEU:HD23	2.48	0.49
2:E:172:VAL:HG12	2:E:173:GLU:N	2.28	0.49
1:A:293:PRO:HA	1:A:316:ASP:OD2	2.12	0.49
1:A:515:LEU:HD22	1:A:527:ILE:CD1	2.37	0.49
1:A:650:LEU:O	1:A:654:LEU:HD12	2.13	0.49
1:B:276:GLN:NE2	1:B:301:THR:N	2.55	0.49
2:C:96:ASP:OD1	2:C:96:ASP:C	2.56	0.49
2:E:9:GLN:NE2	2:E:69:VAL:HA	2.28	0.49
3:F:120:ILE:HB	3:F:131:THR:CB	2.42	0.49
1:A:222:ARG:HA	1:A:255:ASP:HB3	1.95	0.49
1:A:265:GLY:O	1:A:268:ALA:C	2.55	0.49
1:B:269:GLY:O	1:B:299:ARG:NH2	2.45	0.49
3:D:21:LEU:HD11	3:D:93:LEU:C	2.37	0.49
3:D:37:VAL:HB	3:D:59:GLU:HB2	1.95	0.49
3:D:173:ASN:O	3:D:174:VAL:HG12	2.13	0.49
2:E:173:GLU:O	3:F:183:SER:CA	2.61	0.49
3:F:70:PHE:CD2	3:F:70:PHE:C	2.91	0.49
1:A:6:HIS:NE2	1:A:304:GLU:OE1	2.46	0.49
1:A:287:LYS:C	1:A:289:VAL:H	2.21	0.49
1:A:386:THR:HB	1:A:413:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:TYR:N	1:A:575:PRO:CD	2.76	0.49
1:A:677:ALA:O	1:A:679:ARG:HG2	2.12	0.49
1:B:180:LEU:HD23	1:B:234:ILE:HG13	1.95	0.49
1:B:273:PHE:CE1	1:B:576:ASN:HB2	2.47	0.49
1:B:332:GLN:O	1:B:332:GLN:CG	2.61	0.49
1:B:418:THR:HA	1:B:464:ALA:O	2.13	0.49
1:B:631:ARG:HH21	1:B:631:ARG:CG	2.05	0.49
1:B:690:ARG:HD2	1:B:703:ALA:HB2	1.94	0.49
3:D:14:LEU:HG	3:D:15:ARG:N	2.27	0.49
2:E:100:VAL:HG12	2:E:104:LEU:CD1	2.43	0.49
1:A:286:VAL:HG12	1:A:294:VAL:HG21	1.95	0.49
1:A:511:LEU:N	1:A:511:LEU:HD23	2.28	0.49
1:A:676:GLU:O	1:A:677:ALA:HB2	2.12	0.49
1:B:126:TYR:CD1	1:B:126:TYR:N	2.80	0.49
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.62	0.49
1:B:178:GLN:O	1:B:184:TYR:HB2	2.13	0.49
1:B:369:THR:HA	1:B:372:GLU:HB2	1.94	0.49
1:B:483:VAL:HB	1:B:669:ILE:HG12	1.94	0.49
3:D:76:GLU:O	3:D:77:ALA:C	2.52	0.49
3:F:116:THR:HG22	3:F:154:THR:HG23	1.95	0.49
1:A:60:TYR:CE2	1:A:74:SER:HA	2.48	0.48
1:A:354:ARG:O	1:A:355:TRP:C	2.55	0.48
1:A:456:LYS:CD	1:A:456:LYS:NZ	2.76	0.48
2:E:144:ALA:HB1	2:E:145:VAL:HG23	1.95	0.48
1:A:25:TYR:CD2	1:A:55:ALA:HB3	2.48	0.48
1:A:354:ARG:NH2	1:A:354:ARG:CG	2.59	0.48
1:A:417:LEU:HD23	1:A:463:LEU:HD11	1.93	0.48
1:B:392:VAL:HG12	1:B:394:ILE:HG13	1.95	0.48
1:B:473:ASP:OD2	1:B:657:ARG:NH2	2.45	0.48
3:D:65:GLY:HA2	3:D:176:ALA:HB3	1.95	0.48
2:E:168:MET:HE1	3:F:11:ARG:CD	2.43	0.48
3:F:75:PHE:O	3:F:76:GLU:C	2.56	0.48
1:A:424:ILE:CD1	1:A:448:GLU:HA	2.43	0.48
1:A:568:MET:HE2	1:A:573:GLU:CB	2.41	0.48
1:B:394:ILE:HD12	1:B:405:ALA:HB2	1.94	0.48
1:B:444:ARG:HD3	1:B:445:ASP:OD1	2.13	0.48
2:C:10:THR:CB	2:C:124:ASP:OD2	2.61	0.48
3:D:36:VAL:N	3:D:58:ASP:OD1	2.36	0.48
2:E:53:SER:OG	2:E:153:PRO:HG2	2.14	0.48
2:E:144:ALA:C	2:E:145:VAL:HG23	2.37	0.48
3:F:6:ILE:HB	3:F:93:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ARG:HB2	1:A:707:LYS:O	2.13	0.48
1:A:375:ARG:HH11	1:A:376:ARG:HH11	1.59	0.48
1:B:5:LYS:O	1:B:8:ILE:HG22	2.13	0.48
1:B:670:TYR:CZ	1:B:700:PRO:HG2	2.49	0.48
1:B:704:ILE:O	1:B:705:PRO:O	2.31	0.48
2:C:226:MET:HE2	3:D:111:GLY:C	2.38	0.48
3:F:144:ASP:CG	3:F:146:PRO:HD3	2.39	0.48
1:A:277:GLY:CA	1:A:300:TYR:CE1	2.96	0.48
1:A:714:GLY:HA2	1:A:723:PHE:CE2	2.49	0.48
1:B:528:GLY:HA3	1:B:636:ASP:CB	2.44	0.48
1:B:543:PRO:O	1:B:546:ALA:HB3	2.14	0.48
3:F:40:VAL:CG1	3:F:45:ALA:O	2.61	0.48
3:F:118:VAL:HG13	3:F:120:ILE:O	2.14	0.48
1:B:62:SER:OG	1:B:67:SER:O	2.24	0.48
1:B:714:GLY:HA2	1:B:723:PHE:CG	2.49	0.48
3:F:49:VAL:O	3:F:53:SER:OG	2.30	0.48
3:F:57:VAL:HG12	3:F:59:GLU:O	2.14	0.48
1:A:533:ILE:HG12	1:A:639:VAL:HB	1.95	0.48
1:A:658:GLU:HA	1:A:661:TRP:NE1	2.29	0.48
3:D:132:ARG:HG3	3:D:132:ARG:NH1	2.24	0.48
1:A:21:ARG:CG	1:A:22:ASN:ND2	2.75	0.48
1:A:83:VAL:O	1:A:84:ARG:O	2.32	0.48
1:A:169:TYR:HE2	1:A:171:ALA:HB3	1.77	0.48
1:A:179:PHE:HA	1:A:185:ASN:HD22	1.77	0.48
1:A:322:ARG:HB2	1:A:323:PRO:HD3	1.96	0.48
1:A:363:ILE:HG21	1:A:363:ILE:HD13	1.45	0.48
1:A:679:ARG:O	1:A:680:LEU:C	2.56	0.48
1:B:222:ARG:HG3	1:B:255:ASP:O	2.13	0.48
1:B:303:PRO:HA	1:B:306:MET:HG3	1.96	0.48
1:A:86:LEU:O	1:A:87:LYS:C	2.55	0.48
1:A:175:LEU:O	1:A:176:PRO:C	2.57	0.48
1:B:450:GLN:O	1:B:454:LEU:HD12	2.14	0.48
1:B:566:ASN:O	1:B:567:TYR:C	2.56	0.48
1:B:718:MET:HG3	1:B:719:PRO:N	2.27	0.48
3:D:16:PRO:C	3:D:18:SER:N	2.71	0.48
3:D:83:ILE:HD11	3:D:91:VAL:HG11	1.94	0.48
3:F:73:ASP:OD2	3:F:182:ARG:N	2.41	0.48
1:A:701:GLN:O	1:A:701:GLN:HG3	2.13	0.47
1:A:711:ILE:HD11	1:A:715:THR:O	2.14	0.47
1:B:13:ILE:HD11	1:B:293:PRO:HB3	1.94	0.47
1:B:513:ASP:O	1:B:637:SER:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:TYR:O	3:D:103:ALA:C	2.55	0.47
1:A:148:GLN:O	1:A:151:TYR:HB2	2.14	0.47
1:A:376:ARG:O	1:A:377:GLY:C	2.55	0.47
1:B:45:ARG:HA	1:B:48:LYS:HD2	1.96	0.47
1:B:49:ALA:HB1	1:B:96:TYR:HB2	1.96	0.47
2:C:10:THR:HA	2:C:124:ASP:OD2	2.14	0.47
2:C:228:ARG:N	3:D:144:ASP:O	2.47	0.47
2:E:100:VAL:HG12	2:E:104:LEU:HD11	1.96	0.47
2:E:145:VAL:CG2	3:F:100:LEU:HD12	2.44	0.47
3:F:83:ILE:CD1	3:F:150:THR:HG21	2.44	0.47
3:D:26:ASN:HD21	3:D:56:GLY:HA2	1.79	0.47
3:F:114:PHE:HA	3:F:152:VAL:O	2.15	0.47
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.61	0.47
1:A:130:PHE:CD1	1:A:131:GLU:HG2	2.49	0.47
1:A:576:ASN:OD1	1:A:579:ARG:NH2	2.46	0.47
1:A:700:PRO:C	1:A:702:ILE:H	2.23	0.47
2:E:164:LEU:HB3	3:F:10:ARG:CZ	2.45	0.47
3:F:63:VAL:HG12	3:F:176:ALA:HB2	1.96	0.47
1:A:40:PHE:C	1:A:40:PHE:CD2	2.91	0.47
1:B:45:ARG:NH1	1:B:59:GLU:OE1	2.48	0.47
1:B:128:SER:O	1:B:132:THR:HA	2.14	0.47
1:B:158:SER:O	1:B:161:ALA:HB3	2.14	0.47
1:B:330:LEU:C	1:B:330:LEU:CD2	2.87	0.47
1:B:330:LEU:N	1:B:331:PRO:CD	2.78	0.47
3:D:120:ILE:O	3:D:131:THR:N	2.42	0.47
3:F:41:ILE:HA	3:F:63:VAL:O	2.15	0.47
1:B:103:GLU:OE2	1:B:169:TYR:CD2	2.67	0.47
1:B:349:ASN:O	1:B:350:VAL:C	2.48	0.47
1:B:394:ILE:CG2	1:B:417:LEU:CD1	2.92	0.47
1:B:424:ILE:CD1	1:B:448:GLU:HA	2.42	0.47
2:E:114:ASP:O	2:E:177:PRO:HB3	2.15	0.47
1:A:62:SER:HG	1:A:78:TRP:HE1	1.56	0.47
1:A:124:SER:HB2	1:A:184:TYR:O	2.15	0.47
1:A:177:LEU:HD13	1:A:181:ASN:HB2	1.96	0.47
1:A:409:MET:CG	1:A:415:VAL:HG13	2.42	0.47
1:A:409:MET:HE3	1:A:454:LEU:CB	2.45	0.47
1:A:513:ASP:HB2	1:A:636:ASP:O	2.15	0.47
1:A:680:LEU:HD12	1:A:680:LEU:N	2.30	0.47
1:B:278:HIS:CD2	1:B:279:THR:HG23	2.49	0.47
1:B:367:ASN:OD1	1:B:367:ASN:O	2.31	0.47
1:B:375:ARG:HA	1:B:707:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1730:FMN:HM73	4:B:1730:FMN:HM81	1.78	0.47
2:C:173:GLU:O	3:D:183:SER:HA	2.15	0.47
2:E:121:GLN:HA	7:E:1237:AMP:H5'2	1.96	0.47
3:F:39:ALA:HA	3:F:61:VAL:O	2.14	0.47
1:A:2:ARG:NH1	1:A:335:GLU:O	2.48	0.47
1:A:489:ALA:CB	1:A:645:HIS:O	2.62	0.47
1:A:545:LEU:O	1:A:546:ALA:C	2.58	0.47
1:A:660:GLU:HA	1:A:663:GLU:HG3	1.97	0.47
1:A:700:PRO:C	1:A:702:ILE:N	2.71	0.47
1:B:280:ILE:O	1:B:283:VAL:N	2.47	0.47
1:B:568:MET:HE2	1:B:573:GLU:CB	2.45	0.47
2:C:197:ILE:O	2:C:197:ILE:HG22	2.15	0.47
3:D:83:ILE:HD13	3:D:83:ILE:HG21	1.31	0.47
1:B:242:LYS:O	1:B:245:GLU:HB2	2.14	0.47
1:B:282:TRP:HA	1:B:285:LEU:HD12	1.95	0.47
1:B:362:MET:HE3	1:B:370:ALA:HB1	1.96	0.47
1:B:568:MET:C	1:B:570:PHE:N	2.72	0.47
1:A:290:SER:OG	1:A:291:LYS:N	2.47	0.46
1:B:171:ALA:O	1:B:172:HIS:C	2.58	0.46
1:B:263:GLU:C	1:B:265:GLY:N	2.72	0.46
1:B:704:ILE:C	1:B:705:PRO:O	2.54	0.46
2:E:100:VAL:O	2:E:101:GLY:C	2.56	0.46
2:E:143:ALA:HB1	2:E:160:ILE:CD1	2.45	0.46
1:A:33:ALA:O	1:A:34:GLY:C	2.58	0.46
1:A:79:ASP:OD1	1:A:79:ASP:C	2.56	0.46
1:A:167:TYR:HD1	1:A:222:ARG:HB2	1.79	0.46
1:B:109:ALA:HB3	1:B:126:TYR:CZ	2.51	0.46
1:B:139:MET:HB3	1:B:143:ASP:CB	2.36	0.46
1:B:463:LEU:HD21	1:B:465:LEU:HD11	1.96	0.46
1:B:661:TRP:HB3	1:B:666:ILE:CB	2.41	0.46
3:F:26:ASN:O	3:F:29:LYS:HD2	2.15	0.46
1:A:223:PHE:CD1	1:A:224:GLY:N	2.83	0.46
1:A:531:VAL:HG13	1:A:637:SER:O	2.15	0.46
1:A:558:ILE:HD11	1:A:586:VAL:HG11	1.97	0.46
2:C:77:LEU:HA	2:C:77:LEU:HD23	1.69	0.46
2:C:100:VAL:HG11	7:C:1236:AMP:C5	2.50	0.46
3:F:40:VAL:HG11	3:F:45:ALA:O	2.15	0.46
1:A:42:SER:O	1:A:43:ALA:C	2.58	0.46
1:A:77:ILE:HG23	1:A:77:ILE:O	2.15	0.46
1:A:414:THR:O	1:A:414:THR:HG22	2.15	0.46
1:B:27:VAL:HG21	1:B:222:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.59	0.46
1:B:297:VAL:HG21	4:B:1730:FMN:H5'1	1.97	0.46
1:B:302:ASP:OD2	1:B:302:ASP:C	2.57	0.46
1:B:407:VAL:CG2	1:B:689:HIS:CE1	2.98	0.46
2:E:119:GLY:O	2:E:181:THR:HB	2.16	0.46
2:E:164:LEU:HD23	3:F:97:VAL:HG11	1.97	0.46
1:A:530:ARG:NH1	1:A:634:GLU:OE1	2.49	0.46
1:A:550:ALA:O	1:A:553:GLY:N	2.43	0.46
1:B:372:GLU:OE1	1:B:376:ARG:NE	2.39	0.46
1:B:434:LEU:HD21	1:B:521:MET:SD	2.55	0.46
2:E:143:ALA:HB1	2:E:160:ILE:HD11	1.98	0.46
3:F:30:LYS:HE2	3:F:123:TYR:CD2	2.50	0.46
3:F:173:ASN:C	3:F:174:VAL:CG1	2.88	0.46
1:A:72:ARG:HD2	1:A:355:TRP:CZ2	2.51	0.46
1:A:267:ASP:OD2	4:A:1730:FMN:H4'	2.16	0.46
1:A:284:LYS:HG3	1:A:285:LEU:HD23	1.98	0.46
1:A:383:PHE:N	1:A:383:PHE:CD1	2.84	0.46
1:A:729:VAL:C	1:B:384:ARG:HA	2.41	0.46
1:B:152:VAL:O	1:B:153:ASP:C	2.57	0.46
1:B:317:ILE:HG22	1:B:318:ILE:N	2.31	0.46
1:A:463:LEU:HG	1:A:464:ALA:N	2.30	0.46
1:A:468:LYS:O	1:A:469:PRO:C	2.58	0.46
1:B:185:ASN:CG	1:B:187:ARG:HG3	2.38	0.46
1:B:568:MET:CE	1:B:573:GLU:CB	2.94	0.46
1:B:686:PHE:O	1:B:689:HIS:N	2.48	0.46
1:A:95:LYS:O	1:A:95:LYS:HG2	2.15	0.46
1:A:112:PRO:O	1:A:113:ASN:HB2	2.16	0.46
1:A:355:TRP:HZ3	1:A:356:GLU:CG	2.25	0.46
1:B:29:HIS:ND1	1:B:29:HIS:C	2.73	0.46
1:B:253:MET:HG2	1:B:254:TRP:O	2.16	0.46
1:B:655:LYS:HD2	1:B:655:LYS:HA	1.74	0.46
1:B:681:ILE:O	1:B:682:ALA:C	2.58	0.46
2:E:164:LEU:HD11	2:E:170:GLN:CB	2.42	0.46
1:A:202:TRP:HD1	1:A:206:LEU:CD1	2.29	0.46
1:B:183:TYR:CD1	1:B:184:TYR:CZ	3.03	0.46
1:B:506:GLY:HA3	1:B:597:ILE:O	2.15	0.46
2:C:4:LEU:HA	2:C:60:VAL:HG13	1.98	0.46
3:D:119:TYR:CE2	3:D:156:ARG:NH1	2.83	0.46
2:E:221:GLY:O	2:E:222:ALA:C	2.58	0.46
3:F:10:ARG:O	3:F:11:ARG:C	2.59	0.46
1:A:55:ALA:O	1:A:56:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:C	1:A:169:TYR:CD2	2.93	0.46
1:A:193:GLY:O	1:A:198:ARG:NE	2.38	0.46
1:A:383:PHE:CE2	1:A:407:VAL:HG13	2.51	0.46
1:A:727:TYR:O	1:A:729:VAL:HG22	2.15	0.46
1:B:34:GLY:CA	1:B:59:GLU:OE2	2.64	0.46
1:B:192:GLY:O	1:B:197:ASN:ND2	2.48	0.46
3:D:45:ALA:HB3	3:D:62:VAL:CG1	2.46	0.46
3:D:45:ALA:HB3	3:D:62:VAL:HG13	1.96	0.46
3:D:132:ARG:HH11	3:D:132:ARG:CG	2.22	0.46
2:E:1:MET:HG3	2:E:57:VAL:HG13	1.98	0.46
1:A:390:ASP:HA	1:A:481:ASP:OD1	2.16	0.45
1:B:406:ARG:NH2	1:B:446:TYR:OH	2.49	0.45
1:B:415:VAL:O	1:B:461:SER:HA	2.17	0.45
1:B:713:TRP:CZ2	1:B:723:PHE:HE2	2.33	0.45
2:C:1:MET:CE	2:C:1:MET:CG	2.91	0.45
1:A:398:GLY:O	1:A:402:SER:OG	2.32	0.45
1:A:547:GLU:OE2	1:A:580:ARG:HD2	2.15	0.45
1:B:417:LEU:HD23	1:B:463:LEU:CD1	2.46	0.45
1:B:443:HIS:O	1:B:443:HIS:ND1	2.50	0.45
1:B:686:PHE:C	1:B:688:GLY:H	2.23	0.45
2:C:60:VAL:HG13	2:C:60:VAL:O	2.16	0.45
3:D:16:PRO:C	3:D:18:SER:H	2.23	0.45
3:D:72:PRO:O	3:D:73:ASP:C	2.59	0.45
2:E:102:ARG:HB2	2:E:137:TYR:CE1	2.51	0.45
1:A:309:ILE:HD11	1:A:318:ILE:HD13	1.98	0.45
1:B:69:ASP:OD1	1:B:72:ARG:HB2	2.16	0.45
2:C:66:PRO:HD3	2:C:88:TRP:CZ2	2.52	0.45
2:E:45:GLU:OE2	2:E:48:LYS:HE2	2.16	0.45
1:A:254:TRP:N	1:A:254:TRP:CD1	2.84	0.45
1:A:444:ARG:HG3	1:A:444:ARG:H	1.61	0.45
1:B:102:VAL:CG1	1:B:163:PHE:CG	2.99	0.45
1:B:183:TYR:CD1	1:B:184:TYR:CE2	2.95	0.45
1:B:617:ARG:HB3	1:B:621:VAL:CG1	2.46	0.45
2:E:42:SER:O	2:E:43:LEU:C	2.57	0.45
2:E:173:GLU:O	3:F:183:SER:CB	2.65	0.45
3:F:143:VAL:O	3:F:143:VAL:CG2	2.63	0.45
1:A:58:THR:OG1	1:A:102:VAL:HG23	2.17	0.45
1:A:419:ASP:CG	5:A:1731:ADP:O2'	2.60	0.45
1:B:394:ILE:HG21	1:B:417:LEU:CD1	2.46	0.45
1:A:213:VAL:HG23	1:A:217:CYS:HB2	1.98	0.45
1:A:264:TRP:CH2	1:A:352:ILE:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLN:CB	1:A:521:MET:HE3	2.47	0.45
1:A:692:ALA:O	1:A:694:GLU:N	2.49	0.45
1:B:109:ALA:HB3	1:B:126:TYR:CE2	2.51	0.45
1:B:472:ALA:HB1	1:B:654:LEU:CD2	2.46	0.45
1:B:671:LEU:HD21	1:B:675:ALA:O	2.17	0.45
2:C:160:ILE:N	2:C:172:VAL:O	2.48	0.45
3:F:5:VAL:HG12	3:F:6:ILE:N	2.31	0.45
1:A:51:GLY:HA2	1:A:329:PHE:CE2	2.52	0.45
1:A:51:GLY:HA2	1:A:329:PHE:CD2	2.52	0.45
1:B:280:ILE:HG13	1:B:300:TYR:OH	2.17	0.45
1:B:297:VAL:HG21	4:B:1730:FMN:C5'	2.47	0.45
1:B:369:THR:O	1:B:372:GLU:N	2.39	0.45
1:B:408:LEU:O	1:B:411:SER:HB2	2.17	0.45
1:B:590:GLY:O	1:B:591:ASP:HB2	2.17	0.45
1:B:704:ILE:O	1:B:705:PRO:C	2.58	0.45
2:E:111:GLU:O	2:E:112:ALA:O	2.34	0.45
2:E:115:MET:HE2	2:E:151:TYR:CD1	2.52	0.45
2:E:203:LYS:HA	2:E:204:PRO:HD2	1.62	0.45
1:A:147:VAL:O	1:A:151:TYR:HD2	2.00	0.45
1:A:228:VAL:HG11	1:A:258:ILE:HD12	1.98	0.45
1:B:7:ASP:O	1:B:10:PHE:N	2.44	0.45
1:B:94:HIS:O	1:B:97:GLY:N	2.47	0.45
1:B:373:GLU:O	1:B:377:GLY:HA2	2.16	0.45
1:B:472:ALA:HB1	1:B:654:LEU:HD23	1.99	0.45
1:A:139:MET:CE	1:A:147:VAL:CG2	2.85	0.45
1:A:491:TRP:HB2	1:A:517:PRO:HD2	1.99	0.45
1:B:272:ARG:O	1:B:273:PHE:CD2	2.70	0.45
1:B:388:ASN:OD1	1:B:390:ASP:HB2	2.16	0.45
1:B:690:ARG:HD2	1:B:703:ALA:CB	2.47	0.45
2:C:172:VAL:HG12	3:D:183:SER:HB2	1.98	0.45
3:F:122:GLU:O	3:F:129:VAL:N	2.35	0.45
1:A:8:ILE:CG2	1:A:307:ILE:HG22	2.46	0.45
1:A:191:TYR:C	1:A:197:ASN:HB3	2.42	0.45
1:A:241:GLN:HE21	1:A:289:VAL:HG13	1.83	0.45
1:A:332:GLN:O	1:A:336:GLN:HB2	2.17	0.45
1:A:683:ASP:O	1:A:684:ALA:C	2.58	0.45
1:B:226:ASP:OD2	1:B:235:GLU:HA	2.16	0.45
2:E:19:ILE:HD13	2:E:233:TYR:HA	1.97	0.45
3:F:4:LEU:HB3	3:F:91:VAL:HB	1.99	0.45
3:F:17:VAL:HA	3:F:20:GLU:CD	2.42	0.45
1:A:348:CYS:SG	6:A:1732:SF4:S1	3.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLN:NE2	1:A:597:ILE:HG21	2.33	0.44
1:B:516:THR:O	1:B:520:VAL:HG23	2.17	0.44
1:B:531:VAL:HG12	1:B:532:VAL:N	2.32	0.44
1:B:650:LEU:O	1:B:654:LEU:HG	2.17	0.44
1:B:691:VAL:O	1:B:692:ALA:C	2.60	0.44
2:C:44:GLU:O	2:C:45:GLU:C	2.58	0.44
2:C:221:GLY:C	2:C:223:ALA:N	2.74	0.44
2:E:65:GLY:HA2	2:E:88:TRP:CZ3	2.52	0.44
1:A:87:LYS:O	1:A:90:THR:N	2.49	0.44
1:A:303:PRO:C	1:A:306:MET:HB2	2.41	0.44
1:A:470:MET:HE3	1:A:470:MET:HB3	1.55	0.44
1:A:501:HIS:CD2	1:B:183:TYR:CE1	3.06	0.44
1:A:515:LEU:HD21	1:A:527:ILE:CG1	2.47	0.44
1:B:563:HIS:HE1	1:B:569:HIS:NE2	2.15	0.44
1:B:713:TRP:CE2	1:B:723:PHE:HE2	2.33	0.44
3:F:79:VAL:O	3:F:83:ILE:N	2.50	0.44
1:A:139:MET:HA	1:A:143:ASP:OD2	2.17	0.44
1:B:39:GLY:CA	1:B:374:TYR:CE2	3.01	0.44
1:B:539:TYR:HD2	1:B:540:PHE:N	2.15	0.44
1:B:704:ILE:HB	1:B:705:PRO:CD	2.47	0.44
1:A:222:ARG:NH1	4:A:1730:FMN:O3'	2.42	0.44
1:B:210:LYS:O	1:B:214:GLY:N	2.49	0.44
1:B:599:PRO:O	1:B:601:ARG:N	2.51	0.44
3:D:8:GLU:OE1	3:D:96:SER:OG	2.33	0.44
1:A:203:LEU:HA	1:A:203:LEU:HD23	1.13	0.44
1:A:491:TRP:CB	1:A:517:PRO:HD2	2.48	0.44
1:B:175:LEU:HA	1:B:175:LEU:HD12	1.48	0.44
1:B:352:ILE:O	1:B:356:GLU:HB2	2.17	0.44
1:B:635:PHE:O	1:B:635:PHE:CD1	2.71	0.44
2:C:87:VAL:CG2	2:C:107:VAL:HG21	2.48	0.44
3:D:24:ALA:O	3:D:25:ALA:C	2.57	0.44
1:A:139:MET:HG2	1:A:143:ASP:HB3	2.00	0.44
1:B:137:LYS:HG2	1:B:138:GLU:N	2.32	0.44
1:B:139:MET:CB	1:B:143:ASP:HB2	2.35	0.44
1:B:247:ALA:O	1:B:250:LEU:HB2	2.18	0.44
2:C:102:ARG:CG	2:C:102:ARG:NH1	2.81	0.44
2:C:203:LYS:HA	2:C:204:PRO:HD2	1.63	0.44
3:D:148:LYS:HA	3:D:148:LYS:HD3	1.71	0.44
3:F:17:VAL:HG21	3:F:157:PRO:HB3	1.99	0.44
1:B:7:ASP:O	1:B:8:ILE:C	2.59	0.44
1:B:128:SER:C	1:B:130:PHE:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:O	1:B:176:PRO:C	2.60	0.44
1:B:197:ASN:O	1:B:198:ARG:C	2.60	0.44
1:B:352:ILE:HG21	1:B:352:ILE:HD13	1.50	0.44
3:F:29:LYS:HG3	3:F:29:LYS:H	1.37	0.44
1:A:241:GLN:NE2	1:A:289:VAL:HG11	2.32	0.44
1:A:590:GLY:O	1:A:591:ASP:HB2	2.17	0.44
1:A:704:ILE:HB	1:A:705:PRO:HD2	1.99	0.44
1:B:376:ARG:O	1:B:378:TRP:CD1	2.71	0.44
2:C:4:LEU:HD23	2:C:4:LEU:C	2.43	0.44
1:A:391:SER:H	1:A:481:ASP:HB2	1.82	0.44
1:A:487:THR:C	5:A:1731:ADP:H5'2	2.43	0.44
1:A:655:LYS:HD2	1:A:661:TRP:CH2	2.53	0.44
1:B:102:VAL:HB	1:B:163:PHE:CE2	2.53	0.44
1:B:183:TYR:HD1	1:B:184:TYR:CZ	2.36	0.44
1:B:280:ILE:N	1:B:281:PRO:CD	2.81	0.44
1:B:303:PRO:HG3	1:B:334:VAL:CG2	2.48	0.44
1:B:532:VAL:HA	1:B:557:THR:O	2.18	0.44
1:B:635:PHE:CD1	1:B:635:PHE:C	2.95	0.44
1:B:686:PHE:C	1:B:688:GLY:N	2.75	0.44
1:B:695:ILE:CG2	1:B:696:GLU:HG2	2.39	0.44
2:C:47:MET:O	2:C:48:LYS:C	2.60	0.44
2:C:79:LYS:O	2:C:190:ARG:HD2	2.18	0.44
3:D:91:VAL:HG13	3:D:152:VAL:HG22	1.99	0.44
3:D:114:PHE:HA	3:D:152:VAL:O	2.17	0.44
1:A:169:TYR:CZ	4:A:1730:FMN:O2	2.71	0.43
1:A:179:PHE:CE1	1:A:201:PHE:CG	3.05	0.43
1:A:416:HIS:HE1	2:E:197:ILE:CD1	2.29	0.43
1:B:258:ILE:HD13	1:B:258:ILE:HG21	1.61	0.43
1:B:355:TRP:HZ3	1:B:356:GLU:HG2	1.79	0.43
1:B:476:LEU:HA	1:B:666:ILE:CD1	2.48	0.43
1:B:551:THR:HG22	1:B:584:LEU:HD21	1.99	0.43
1:A:79:ASP:HB2	1:A:80:GLU:OE2	2.18	0.43
1:A:332:GLN:O	1:A:332:GLN:HG2	2.18	0.43
1:B:64:ASN:HA	1:B:65:PRO:HD3	1.93	0.43
1:B:303:PRO:HG3	1:B:334:VAL:HG21	2.00	0.43
1:B:386:THR:OG1	1:B:413:TYR:CE1	2.71	0.43
1:B:427:HIS:HD1	1:B:427:HIS:H	1.66	0.43
1:B:550:ALA:O	1:B:553:GLY:N	2.41	0.43
1:B:674:ASP:HA	1:B:677:ALA:O	2.18	0.43
1:A:724:LYS:O	1:A:725:ILE:C	2.60	0.43
1:B:3:ASP:OD1	1:B:3:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLU:O	1:B:12:PRO:C	2.59	0.43
1:B:68:ASP:OD2	1:B:69:ASP:N	2.51	0.43
2:E:164:LEU:HD12	2:E:168:MET:HG2	2.00	0.43
3:F:16:PRO:C	3:F:18:SER:H	2.24	0.43
1:A:103:GLU:HG3	1:A:169:TYR:HB2	1.99	0.43
1:A:258:ILE:O	1:A:267:ASP:HB2	2.19	0.43
1:A:444:ARG:O	1:A:445:ASP:C	2.60	0.43
1:B:34:GLY:HA2	1:B:75:ALA:HB2	2.01	0.43
1:B:56:LEU:N	1:B:56:LEU:HD22	2.33	0.43
1:B:244:VAL:HG23	1:B:244:VAL:H	1.54	0.43
2:C:36:ASN:OD1	2:C:37:GLU:N	2.52	0.43
1:B:11:GLU:C	1:B:12:PRO:O	2.59	0.43
1:B:34:GLY:N	1:B:59:GLU:OE2	2.51	0.43
1:B:272:ARG:NH1	1:B:437:LEU:HD21	2.33	0.43
3:D:49:VAL:HG13	3:D:60:LEU:HD13	2.00	0.43
3:F:96:SER:H	3:F:99:SER:HB2	1.82	0.43
1:B:166:VAL:O	1:B:219:ILE:HA	2.18	0.43
1:B:331:PRO:O	1:B:335:GLU:N	2.50	0.43
1:B:392:VAL:HA	1:B:482:LYS:O	2.18	0.43
3:F:157:PRO:O	3:F:158:SER:C	2.60	0.43
3:F:173:ASN:C	3:F:174:VAL:HG13	2.44	0.43
1:A:199:ALA:O	1:A:203:LEU:HD12	2.18	0.43
1:A:589:LEU:CD2	1:A:592:HIS:CE1	3.02	0.43
1:B:70:THR:O	1:B:114:MET:HG3	2.17	0.43
2:C:13:LEU:HD22	2:C:26:VAL:HG11	2.00	0.43
1:A:340:ASP:OD1	1:A:340:ASP:C	2.61	0.43
1:B:3:ASP:OD1	1:B:5:LYS:N	2.41	0.43
1:B:508:ASP:N	1:B:514:GLN:OE1	2.39	0.43
2:C:19:ILE:HD13	2:C:232:MET:O	2.18	0.43
3:D:46:ASP:C	3:D:48:PHE:H	2.27	0.43
1:A:290:SER:OG	1:A:292:LYS:N	2.43	0.43
1:B:171:ALA:C	1:B:173:SER:N	2.73	0.43
1:B:470:MET:HE3	1:B:470:MET:HB3	1.89	0.43
1:B:680:LEU:HA	1:B:680:LEU:HD23	1.60	0.43
2:C:65:GLY:CA	2:C:88:TRP:CE3	3.01	0.43
3:F:17:VAL:CG2	3:F:157:PRO:HB3	2.48	0.43
3:F:119:TYR:CD2	3:F:156:ARG:CZ	3.02	0.43
3:F:163:LEU:HD23	3:F:163:LEU:HA	1.85	0.43
1:A:202:TRP:CD1	1:A:206:LEU:HD12	2.54	0.43
1:A:578:MET:O	1:A:581:LEU:N	2.52	0.43
1:B:284:LYS:C	1:B:286:VAL:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:HD23	1:B:483:VAL:CG1	2.46	0.43
1:B:520:VAL:O	1:B:520:VAL:HG12	2.16	0.43
1:B:657:ARG:NE	1:B:660:GLU:OE2	2.52	0.43
1:A:179:PHE:CD1	1:A:201:PHE:CD2	3.07	0.42
1:A:277:GLY:HA2	1:A:300:TYR:CZ	2.53	0.42
1:A:394:ILE:HG12	1:A:484:ILE:HB	2.01	0.42
1:B:530:ARG:H	1:B:636:ASP:CG	2.23	0.42
1:B:539:TYR:CE2	1:B:540:PHE:HB3	2.54	0.42
1:A:87:LYS:NZ	1:A:91:ASP:OD2	2.42	0.42
1:B:105:TRP:HB2	1:B:169:TYR:HD1	1.83	0.42
1:B:434:LEU:H	1:B:434:LEU:HG	1.60	0.42
2:E:4:LEU:HD23	2:E:5:VAL:N	2.33	0.42
1:A:59:GLU:O	1:A:60:TYR:C	2.62	0.42
1:A:579:ARG:HD3	1:B:611:GLY:O	2.19	0.42
1:B:346:ILE:CD1	1:B:346:ILE:CB	2.84	0.42
1:B:599:PRO:C	1:B:601:ARG:H	2.28	0.42
1:B:672:ILE:O	1:B:672:ILE:HG13	2.16	0.42
2:E:98:ILE:O	2:E:99:VAL:C	2.61	0.42
1:A:139:MET:CB	1:A:143:ASP:HB3	2.49	0.42
1:A:180:LEU:HD22	1:A:202:TRP:CE3	2.54	0.42
1:A:566:ASN:O	1:A:567:TYR:C	2.58	0.42
1:B:532:VAL:HG11	1:B:602:MET:SD	2.59	0.42
2:E:120:VAL:HG23	2:E:181:THR:C	2.45	0.42
3:F:7:ALA:HB1	3:F:14:LEU:HD11	2.01	0.42
3:F:118:VAL:CG1	3:F:120:ILE:O	2.67	0.42
1:A:515:LEU:CD2	1:A:527:ILE:CD1	2.97	0.42
1:A:686:PHE:HB2	1:B:117:ARG:NH1	2.35	0.42
2:C:132:ILE:HD12	2:C:132:ILE:HG23	1.85	0.42
2:E:168:MET:CE	3:F:11:ARG:HD2	2.50	0.42
1:A:237:GLU:OE2	1:B:619:PRO:HD3	2.19	0.42
1:A:326:ALA:CB	1:A:345:CYS:HB2	2.47	0.42
1:B:209:VAL:O	1:B:212:ALA:HB3	2.20	0.42
1:B:428:LEU:HD21	1:B:440:TRP:O	2.20	0.42
2:C:36:ASN:HD21	2:C:38:TRP:HB2	1.85	0.42
2:E:62:VAL:HG11	2:E:107:VAL:HG11	2.01	0.42
1:A:46:SER:OG	1:A:92:GLU:HG2	2.20	0.42
1:A:63:ILE:HD13	1:A:63:ILE:HG21	1.87	0.42
1:A:83:VAL:O	1:A:84:ARG:C	2.60	0.42
1:A:325:ILE:CD1	1:A:362:MET:SD	3.08	0.42
1:A:496:THR:O	1:A:642:THR:OG1	2.19	0.42
1:B:40:PHE:C	1:B:40:PHE:CD2	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:OE1	1:B:59:GLU:N	2.32	0.42
1:A:77:ILE:HA	1:A:77:ILE:HD12	1.32	0.42
1:B:60:TYR:CZ	1:B:74:SER:HB3	2.55	0.42
1:B:94:HIS:O	1:B:96:TYR:N	2.52	0.42
1:B:616:TYR:C	1:B:616:TYR:CD2	2.93	0.42
1:B:672:ILE:HG22	1:B:691:VAL:HG11	2.02	0.42
1:A:3:ASP:O	1:A:6:HIS:HB2	2.20	0.42
1:A:127:ALA:HB2	1:A:135:TYR:CD1	2.53	0.42
1:A:424:ILE:HD13	1:A:448:GLU:HA	2.02	0.42
1:B:200:ARG:O	1:B:201:PHE:C	2.63	0.42
1:B:530:ARG:N	1:B:636:ASP:OD2	2.33	0.42
2:C:194:LEU:HD23	2:C:194:LEU:HA	1.71	0.42
3:F:17:VAL:HG23	3:F:20:GLU:OE1	2.19	0.42
3:F:167:GLY:C	3:F:169:PRO:HD2	2.45	0.42
1:A:13:ILE:HG23	1:A:20:LEU:HD12	2.02	0.42
1:A:580:ARG:HD2	1:A:580:ARG:HH21	1.68	0.42
1:A:658:GLU:HA	1:A:661:TRP:CE2	2.54	0.42
1:A:660:GLU:O	1:A:664:ASN:ND2	2.40	0.42
1:A:670:TYR:CD1	1:A:670:TYR:N	2.80	0.42
2:E:47:MET:HE3	2:E:47:MET:HB3	1.84	0.42
2:E:89:ASP:O	2:E:92:ALA:CB	2.67	0.42
2:E:122:SER:N	7:E:1237:AMP:O3P	2.42	0.42
3:F:157:PRO:O	3:F:158:SER:HB2	2.20	0.42
1:A:56:LEU:HD23	1:A:93:VAL:HG13	2.02	0.41
1:A:84:ARG:CZ	1:B:712:ALA:HB1	2.50	0.41
1:A:268:ALA:O	1:A:270:PRO:CD	2.64	0.41
1:A:399:PRO:CD	5:A:1731:ADP:O3B	2.56	0.41
1:A:516:THR:CB	1:A:517:PRO:CD	2.92	0.41
1:A:638:LEU:CD2	1:A:640:LEU:HD21	2.49	0.41
1:B:546:ALA:O	1:B:547:GLU:C	2.62	0.41
2:C:119:GLY:N	7:C:1236:AMP:H4'	2.35	0.41
3:D:41:ILE:HD12	3:D:75:PHE:CE2	2.55	0.41
2:E:143:ALA:CB	2:E:160:ILE:CD1	2.98	0.41
1:A:80:GLU:HB2	1:A:719:PRO:CG	2.49	0.41
1:A:146:GLN:O	1:A:149:GLN:HB3	2.20	0.41
1:A:175:LEU:CB	1:A:176:PRO:CD	2.98	0.41
1:A:204:GLU:O	1:A:205:THR:C	2.63	0.41
1:B:332:GLN:O	1:B:332:GLN:HG2	2.18	0.41
1:B:346:ILE:CG2	1:B:442:TYR:HB2	2.48	0.41
1:B:407:VAL:HG22	1:B:689:HIS:CE1	2.54	0.41
1:B:424:ILE:HD13	1:B:424:ILE:HG21	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:TRP:H	2:C:38:TRP:HE3	1.68	0.41
1:A:199:ALA:HB1	1:A:203:LEU:CD1	2.50	0.41
1:A:532:VAL:HG22	1:A:557:THR:HB	2.01	0.41
1:A:575:PRO:O	1:A:576:ASN:C	2.61	0.41
1:A:589:LEU:HD23	1:A:592:HIS:HD1	1.82	0.41
1:B:10:PHE:N	1:B:10:PHE:CD1	2.87	0.41
1:B:10:PHE:CZ	1:B:335:GLU:N	2.89	0.41
1:B:391:SER:HA	1:B:414:THR:O	2.21	0.41
1:B:443:HIS:O	1:B:443:HIS:CG	2.72	0.41
2:C:100:VAL:O	2:C:101:GLY:C	2.59	0.41
2:C:145:VAL:HG11	3:D:97:VAL:HG13	2.02	0.41
1:A:64:ASN:O	1:A:67:SER:N	2.40	0.41
1:A:279:THR:O	1:A:280:ILE:C	2.61	0.41
1:B:354:ARG:O	1:B:355:TRP:C	2.61	0.41
2:E:63:SER:HB2	2:E:73:LEU:HD21	2.02	0.41
1:A:409:MET:CG	1:A:415:VAL:CG1	2.98	0.41
1:B:222:ARG:CG	1:B:255:ASP:O	2.69	0.41
1:B:306:MET:O	1:B:310:VAL:HG23	2.20	0.41
1:B:582:HIS:O	1:B:583:GLU:C	2.64	0.41
2:C:69:VAL:C	2:C:71:GLU:N	2.76	0.41
3:D:46:ASP:C	3:D:48:PHE:N	2.78	0.41
2:E:193:SER:O	2:E:197:ILE:N	2.53	0.41
3:F:42:GLY:N	3:F:45:ALA:HB2	2.35	0.41
1:A:277:GLY:HA2	1:A:300:TYR:OH	2.21	0.41
1:A:594:CYS:HA	1:A:604:ILE:HA	2.02	0.41
1:B:258:ILE:O	1:B:258:ILE:HG13	2.21	0.41
1:B:407:VAL:HG21	1:B:689:HIS:ND1	2.35	0.41
2:C:144:ALA:HB2	3:D:101:GLY:HA2	2.01	0.41
2:E:10:THR:CA	2:E:124:ASP:OD2	2.68	0.41
2:E:70:ASP:O	2:E:71:GLU:C	2.62	0.41
2:E:73:LEU:O	2:E:74:ARG:C	2.62	0.41
3:F:5:VAL:HB	3:F:38:VAL:HG22	2.03	0.41
1:A:376:ARG:O	1:A:378:TRP:CD1	2.74	0.41
1:A:416:HIS:HE1	2:E:197:ILE:HD11	1.82	0.41
1:A:614:ARG:NH2	1:B:274:TYR:CE1	2.88	0.41
1:A:631:ARG:HH21	1:A:631:ARG:HD3	1.72	0.41
1:A:711:ILE:HA	1:B:711:ILE:HG13	2.03	0.41
1:B:16:GLY:C	1:B:18:LYS:H	2.29	0.41
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.90	0.41
1:B:256:ILE:HD12	1:B:286:VAL:HG21	2.02	0.41
1:B:386:THR:CB	1:B:413:TYR:CE1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:MET:O	1:B:581:LEU:N	2.53	0.41
1:B:706:TYR:CD2	1:B:707:LYS:O	2.72	0.41
3:D:188:TYR:CD1	3:D:188:TYR:N	2.87	0.41
2:E:10:THR:HA	2:E:124:ASP:OD2	2.20	0.41
2:E:220:VAL:O	2:E:221:GLY:O	2.38	0.41
1:A:25:TYR:O	1:A:319:GLY:HA2	2.20	0.41
1:A:84:ARG:O	1:A:87:LYS:HB3	2.20	0.41
1:A:282:TRP:CH2	1:B:614:ARG:NE	2.89	0.41
1:A:284:LYS:C	1:A:286:VAL:N	2.79	0.41
2:E:64:VAL:CG2	2:E:87:VAL:HB	2.36	0.41
3:F:16:PRO:C	3:F:18:SER:N	2.77	0.41
1:A:90:THR:HG22	1:A:100:ALA:HB1	2.03	0.41
1:A:90:THR:O	1:A:94:HIS:CG	2.74	0.41
1:A:128:SER:C	1:A:130:PHE:H	2.28	0.41
1:A:175:LEU:O	1:A:178:GLN:HB2	2.21	0.41
1:A:297:VAL:HG12	1:A:319:GLY:O	2.20	0.41
1:A:365:THR:HG23	1:A:682:ALA:N	2.36	0.41
1:A:426:GLY:HA3	5:A:1731:ADP:O2A	2.21	0.41
1:A:509:ALA:HB1	1:A:514:GLN:O	2.21	0.41
1:A:541:MET:O	1:A:542:ALA:C	2.63	0.41
1:A:677:ALA:HA	1:A:678:PRO:HD3	1.84	0.41
1:B:31:ILE:HD11	1:B:33:ALA:HB3	2.00	0.41
1:B:116:SER:C	1:B:118:ALA:H	2.28	0.41
1:B:174:TYR:OH	1:B:261:ILE:HD13	2.21	0.41
1:B:322:ARG:N	1:B:323:PRO:CD	2.84	0.41
2:C:141:PRO:O	2:C:178:ALA:HB1	2.20	0.41
2:C:182:ILE:N	2:C:182:ILE:HD13	2.35	0.41
3:D:45:ALA:CB	3:D:62:VAL:HG13	2.50	0.41
3:D:177:PRO:O	3:D:178:SER:C	2.64	0.41
2:E:165:GLU:OE2	3:F:96:SER:CB	2.61	0.41
2:E:165:GLU:OE1	2:E:165:GLU:N	2.44	0.41
2:E:175:ASN:ND2	3:F:182:ARG:O	2.54	0.41
3:F:6:ILE:CG1	3:F:93:LEU:HD12	2.51	0.41
1:A:24:PHE:CE1	1:A:331:PRO:CB	2.91	0.41
1:A:264:TRP:O	1:A:265:GLY:C	2.63	0.41
1:A:295:LEU:HD12	1:A:295:LEU:C	2.46	0.41
1:A:530:ARG:HH11	1:A:634:GLU:CB	2.34	0.41
1:B:143:ASP:O	1:B:144:ILE:C	2.63	0.41
1:B:183:TYR:HD1	1:B:184:TYR:CD2	2.39	0.41
1:B:399:PRO:HD2	5:B:1731:ADP:O3B	2.21	0.41
1:B:425:GLY:O	1:B:426:GLY:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:ASP:HB3	1:B:503:PRO:HD2	2.01	0.41
1:B:651:TRP:CD1	1:B:651:TRP:C	2.95	0.41
2:C:44:GLU:O	2:C:48:LYS:N	2.49	0.41
3:F:6:ILE:HG13	3:F:93:LEU:HD11	2.03	0.41
1:A:269:GLY:HA2	1:A:270:PRO:HD2	1.83	0.40
4:A:1730:FMN:HM72	4:A:1730:FMN:HM83	1.90	0.40
1:B:325:ILE:HD13	1:B:362:MET:SD	2.62	0.40
1:B:640:LEU:H	1:B:640:LEU:HG	1.69	0.40
1:B:692:ALA:C	1:B:694:GLU:H	2.29	0.40
3:D:58:ASP:O	3:D:59:GLU:CG	2.69	0.40
1:A:468:LYS:HA	1:A:469:PRO:HD2	1.68	0.40
1:B:330:LEU:N	1:B:331:PRO:HD2	2.36	0.40
1:B:430:GLN:HB3	1:B:521:MET:SD	2.62	0.40
1:B:451:ILE:O	1:B:452:THR:C	2.65	0.40
1:B:515:LEU:HD12	1:B:638:LEU:O	2.21	0.40
1:B:536:ALA:HB3	1:B:642:THR:O	2.21	0.40
1:B:584:LEU:O	1:B:585:HIS:C	2.64	0.40
1:B:638:LEU:HD23	1:B:640:LEU:HD21	2.03	0.40
2:C:39:ASP:O	2:C:42:SER:HB2	2.21	0.40
2:C:62:VAL:HG12	2:C:63:SER:N	2.32	0.40
2:C:116:VAL:O	2:C:179:VAL:HA	2.21	0.40
3:D:4:LEU:HD12	3:D:5:VAL:N	2.37	0.40
1:A:2:ARG:HG2	1:A:3:ASP:O	2.21	0.40
1:A:34:GLY:CA	1:A:59:GLU:OE2	2.69	0.40
1:B:157:ARG:HH21	1:B:157:ARG:HD3	1.58	0.40
1:B:191:TYR:CE1	1:B:200:ARG:HD2	2.56	0.40
1:B:192:GLY:N	1:B:197:ASN:HB3	2.36	0.40
1:B:272:ARG:HG2	1:B:273:PHE:CZ	2.56	0.40
1:B:408:LEU:O	1:B:409:MET:C	2.63	0.40
1:B:494:ASP:OD1	1:B:494:ASP:C	2.61	0.40
2:E:233:TYR:CD1	2:E:233:TYR:O	2.74	0.40
3:F:57:VAL:CG1	3:F:59:GLU:O	2.68	0.40
1:A:50:GLU:HG2	1:A:329:PHE:CZ	2.56	0.40
1:A:84:ARG:NH1	1:B:712:ALA:HB1	2.37	0.40
1:A:183:TYR:HB2	1:A:233:GLN:HG2	2.02	0.40
1:A:199:ALA:C	1:A:203:LEU:HD12	2.46	0.40
1:A:375:ARG:HG3	1:A:706:TYR:CB	2.52	0.40
1:A:416:HIS:ND1	2:E:194:LEU:HG	2.36	0.40
1:B:181:ASN:HA	1:B:182:PRO:HD3	1.61	0.40
1:B:243:PHE:O	1:B:244:VAL:C	2.64	0.40
1:B:517:PRO:O	1:B:521:MET:CE	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ARG:O	1:A:581:LEU:C	2.58	0.40
1:B:251:VAL:HG11	1:B:254:TRP:CE2	2.55	0.40
1:B:375:ARG:HA	1:B:707:LYS:HG3	2.03	0.40
1:B:444:ARG:HG3	1:B:444:ARG:H	1.64	0.40
1:B:495:GLY:HA2	1:B:642:THR:HG21	2.03	0.40
1:B:661:TRP:HB3	1:B:666:ILE:CG2	2.51	0.40
2:C:162:ARG:HH12	3:D:98:ASP:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	727/729 (100%)	624 (86%)	83 (11%)	20 (3%)	4	27
1	B	727/729 (100%)	614 (84%)	98 (14%)	15 (2%)	5	31
2	C	227/264 (86%)	202 (89%)	21 (9%)	4 (2%)	6	34
2	E	234/264 (89%)	210 (90%)	14 (6%)	10 (4%)	2	19
3	D	187/320 (58%)	153 (82%)	24 (13%)	10 (5%)	1	16
3	F	187/320 (58%)	162 (87%)	18 (10%)	7 (4%)	2	22
All	All	2289/2626 (87%)	1965 (86%)	258 (11%)	66 (3%)	3	26

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	GLY
1	A	680	LEU
1	B	264	TRP
1	B	680	LEU
3	D	27	GLY

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Mol	Chain	Res	Type
3	D	31	SER
2	E	22	ASP
2	E	81	ALA
2	E	221	GLY
1	A	5	LYS
1	A	84	ARG
1	A	95	LYS
1	A	264	TRP
1	A	582	HIS
1	B	175	LEU
1	B	238	VAL
1	B	298	GLY
1	B	390	ASP
1	B	413	TYR
1	B	600	GLY
2	C	221	GLY
3	D	47	ALA
3	D	100	LEU
3	D	102	TYR
3	D	122	GLU
2	E	19	ILE
2	E	21	GLU
3	F	47	ALA
3	F	95	HIS
3	F	102	TYR
3	F	170	VAL
3	F	188	TYR
1	A	278	HIS
1	A	288	GLN
1	A	298	GLY
1	A	698	ALA
1	B	84	ARG
1	B	95	LYS
1	B	132	THR
1	B	278	HIS
2	C	70	ASP
2	C	89	ASP
2	E	222	ALA
1	A	337	GLY
2	C	145	VAL
3	D	12	ASN
3	D	178	SER

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Mol	Chain	Res	Type
3	F	27	GLY
3	F	178	SER
1	A	575	PRO
3	D	11	ARG
1	A	65	PRO
1	A	175	LEU
1	A	238	VAL
1	A	390	ASP
1	A	542	ALA
1	B	31	ILE
1	A	297	VAL
1	B	542	ALA
2	E	113	PRO
2	E	145	VAL
3	D	170	VAL
2	E	66	PRO
1	A	562	VAL
1	B	575	PRO
2	E	220	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	584/602 (97%)	530 (91%)	54 (9%)	8	32
1	B	578/602 (96%)	520 (90%)	58 (10%)	7	30
2	C	180/216 (83%)	161 (89%)	19 (11%)	6	27
2	E	177/216 (82%)	157 (89%)	20 (11%)	5	25
3	D	143/258 (55%)	121 (85%)	22 (15%)	2	16
3	F	150/258 (58%)	135 (90%)	15 (10%)	7	30
All	All	1812/2152 (84%)	1624 (90%)	188 (10%)	7	28

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	19	THR
1	A	25	TYR
1	A	26	GLN
1	A	56	LEU
1	A	70	THR
1	A	77	ILE
1	A	89	MET
1	A	95	LYS
1	A	137	LYS
1	A	159	ARG
1	A	176	PRO
1	A	177	LEU
1	A	200	ARG
1	A	206	LEU
1	A	260	ASP
1	A	267	ASP
1	A	284	LYS
1	A	288	GLN
1	A	309	ILE
1	A	318	ILE
1	A	330	LEU
1	A	351	CYS
1	A	354	ARG
1	A	375	ARG
1	A	392	VAL
1	A	399	PRO
1	A	414	THR
1	A	415	VAL
1	A	418	THR
1	A	444	ARG
1	A	485	ILE
1	A	515	LEU
1	A	521	MET
1	A	537	ASP
1	A	545	LEU
1	A	571	THR
1	A	572	LEU
1	A	580	ARG
1	A	581	LEU
1	A	589	LEU
1	A	594	CYS
1	A	595	SER

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Mol	Chain	Res	Type
1	A	629	SER
1	A	631	ARG
1	A	650	LEU
1	A	660	GLU
1	A	663	GLU
1	A	667	LYS
1	A	679	ARG
1	A	681	ILE
1	A	706	TYR
1	A	726	GLU
1	A	729	VAL
1	B	13	ILE
1	B	35	SER
1	B	36	ASP
1	B	41	GLN
1	B	56	LEU
1	B	60	TYR
1	B	65	PRO
1	B	84	ARG
1	B	104	LEU
1	B	106	TYR
1	B	121	ARG
1	B	134	SER
1	B	138	GLU
1	B	142	SER
1	B	152	VAL
1	B	158	SER
1	B	187	ARG
1	B	203	LEU
1	B	216	ASP
1	B	227	THR
1	B	238	VAL
1	B	287	LYS
1	B	317	ILE
1	B	322	ARG
1	B	330	LEU
1	B	342	ILE
1	B	351	CYS
1	B	362	MET
1	B	389	LYS
1	B	414	THR
1	B	437	LEU

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Mol	Chain	Res	Type
1	B	444	ARG
1	B	447	ARG
1	B	452	THR
1	B	475	VAL
1	B	487	THR
1	B	493	THR
1	B	497	ASN
1	B	500	THR
1	B	521	MET
1	B	541	MET
1	B	544	SER
1	B	589	LEU
1	B	594	CYS
1	B	596	ARG
1	B	613	LYS
1	B	615	THR
1	B	621	VAL
1	B	631	ARG
1	B	640	LEU
1	B	649	THR
1	B	650	LEU
1	B	657	ARG
1	B	660	GLU
1	B	661	TRP
1	B	667	LYS
1	B	679	ARG
1	B	691	VAL
2	C	1	MET
2	C	26	VAL
2	C	32	MET
2	C	83	ARG
2	C	86	ARG
2	C	89	ASP
2	C	110	LYS
2	C	120	VAL
2	C	145	VAL
2	C	150	GLN
2	C	156	ASN
2	C	157	LYS
2	C	160	ILE
2	C	171	GLU
2	C	199	GLN

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Mol	Chain	Res	Type
2	C	203	LYS
2	C	226	MET
2	C	228	ARG
2	C	230	ARG
3	D	16	PRO
3	D	21	LEU
3	D	37	VAL
3	D	49	VAL
3	D	60	LEU
3	D	83	ILE
3	D	91	VAL
3	D	93	LEU
3	D	99	SER
3	D	100	LEU
3	D	104	SER
3	D	110	THR
3	D	122	GLU
3	D	129	VAL
3	D	132	ARG
3	D	138	LYS
3	D	149	SER
3	D	174	VAL
3	D	179	VAL
3	D	180	GLN
3	D	185	ASN
3	D	186	LYS
2	E	1	MET
2	E	27	ASP
2	E	42	SER
2	E	48	LYS
2	E	53	SER
2	E	55	THR
2	E	56	ASP
2	E	79	LYS
2	E	102	ARG
2	E	107	VAL
2	E	110	LYS
2	E	120	VAL
2	E	130	THR
2	E	145	VAL
2	E	150	GLN
2	E	156	ASN

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Mol	Chain	Res	Type
2	E	157	LYS
2	E	203	LYS
2	E	209	SER
2	E	226	MET
3	F	1	SER
3	F	29	LYS
3	F	37	VAL
3	F	44	GLN
3	F	49	VAL
3	F	60	LEU
3	F	83	ILE
3	F	91	VAL
3	F	99	SER
3	F	127	GLU
3	F	141	VAL
3	F	154	THR
3	F	174	VAL
3	F	179	VAL
3	F	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	241	GLN
1	A	332	GLN
1	A	336	GLN
1	A	462	GLN
1	A	501	HIS
1	A	535	ASN
1	A	554	HIS
1	A	563	HIS
1	A	569	HIS
1	A	630	HIS
1	B	26	GLN
1	B	241	GLN
1	B	276	GLN
1	B	332	GLN
1	B	429	ASN
1	B	501	HIS
1	B	554	HIS
1	B	563	HIS

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Mol	Chain	Res	Type
1	B	652	ASN
2	C	121	GLN
2	C	150	GLN
2	C	170	GLN
2	C	175	ASN
2	C	183	GLN
3	D	26	ASN
3	D	44	GLN
3	D	124	GLN
3	D	137	GLN
3	D	184	GLN
2	E	150	GLN
2	E	170	GLN
2	E	183	GLN
3	F	26	ASN
3	F	124	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	B	1731	-	28,29,29	1.38	5 (17%)	43,45,45	2.39	20 (46%)
7	AMP	E	1237	-	25,25,25	2.00	8 (32%)	37,38,38	3.03	21 (56%)
6	SF4	B	1732	1	0,12,12	-	-	-	-	-
5	ADP	A	1731	-	28,29,29	1.56	6 (21%)	43,45,45	2.32	18 (41%)
4	FMN	A	1730	1	33,33,33	1.67	6 (18%)	48,50,50	2.56	19 (39%)
4	FMN	B	1730	1	33,33,33	1.68	4 (12%)	48,50,50	2.45	22 (45%)
7	AMP	C	1236	-	25,25,25	1.80	8 (32%)	37,38,38	3.00	19 (51%)
6	SF4	A	1732	1	0,12,12	-	-	-	-	-

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
5	ADP	B	1731	-	-	3/16/32/32	0/3/3/3
7	AMP	E	1237	-	-	3/10/26/26	0/3/3/3
6	SF4	B	1732	1	-	-	0/6/5/5
5	ADP	A	1731	-	-	4/16/32/32	0/3/3/3
4	FMN	A	1730	1	-	7/18/18/18	0/3/3/3
4	FMN	B	1730	1	-	1/18/18/18	0/3/3/3
7	AMP	C	1236	-	-	3/10/26/26	0/3/3/3
6	SF4	A	1732	1	-	-	0/6/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1730	FMN	C4A-N5	4.72	1.40	1.30
4	A	1730	FMN	C4A-N5	4.51	1.40	1.30
7	E	1237	AMP	C4-N3	4.34	1.42	1.34
5	B	1731	ADP	O4'-C4'	-4.08	1.35	1.45
4	B	1730	FMN	C10-N1	3.91	1.41	1.33
7	E	1237	AMP	C2-N3	3.85	1.40	1.33
5	A	1731	ADP	C2-N1	3.83	1.40	1.33
4	A	1730	FMN	C10-N1	3.67	1.40	1.33
7	C	1236	AMP	O4'-C4'	-3.60	1.37	1.45
7	C	1236	AMP	C2-N1	3.56	1.40	1.33
4	B	1730	FMN	C2'-C3'	3.46	1.59	1.53
7	E	1237	AMP	P-O1P	3.36	1.60	1.50
7	C	1236	AMP	C4-N3	3.12	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1731	ADP	C2-N3	3.11	1.39	1.33
7	C	1236	AMP	C2-N3	2.95	1.39	1.33
4	A	1730	FMN	C2-N3	2.86	1.45	1.39
5	A	1731	ADP	C5-N7	-2.83	1.33	1.39
7	E	1237	AMP	C2-N1	2.78	1.38	1.33
7	E	1237	AMP	C6-N1	2.70	1.43	1.35
7	C	1236	AMP	C2'-C3'	-2.69	1.46	1.53
7	C	1236	AMP	O3'-C3'	-2.68	1.36	1.43
5	B	1731	ADP	C2-N1	2.58	1.38	1.33
4	A	1730	FMN	C9-C9A	-2.57	1.35	1.39
4	A	1730	FMN	C4'-C3'	2.49	1.57	1.53
5	A	1731	ADP	O4'-C4'	-2.44	1.39	1.45
7	C	1236	AMP	C6-N1	2.43	1.42	1.35
7	E	1237	AMP	O4'-C4'	-2.42	1.39	1.45
7	E	1237	AMP	C8-N7	2.38	1.36	1.31
7	E	1237	AMP	C2'-C1'	-2.34	1.46	1.53
7	C	1236	AMP	C8-N7	2.28	1.36	1.31
5	B	1731	ADP	C8-N7	2.24	1.36	1.31
4	A	1730	FMN	C9-C8	-2.23	1.36	1.39
5	B	1731	ADP	C2-N3	2.21	1.37	1.33
5	B	1731	ADP	C5-N7	-2.21	1.35	1.39
5	A	1731	ADP	PB-O3B	-2.12	1.46	1.54
4	B	1730	FMN	P-O5'	2.05	1.66	1.60
5	A	1731	ADP	C2'-C1'	-2.01	1.47	1.53

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1730	FMN	C8M-C8-C9	-8.53	104.55	119.57
7	E	1237	AMP	N3-C2-N1	-8.06	116.38	128.58
5	B	1731	ADP	N3-C2-N1	-7.17	117.73	128.58
7	C	1236	AMP	O3'-C3'-C2'	-7.07	89.16	111.82
5	A	1731	ADP	O2'-C2'-C1'	-6.61	87.33	110.10
7	C	1236	AMP	N3-C2-N1	-6.12	119.31	128.58
7	C	1236	AMP	C4-N9-C8	5.93	111.97	105.74
4	B	1730	FMN	C5A-C9A-N10	5.84	123.25	117.97
7	C	1236	AMP	O2P-P-O5'	5.83	121.87	106.67
4	B	1730	FMN	O4-C4-N3	-5.56	109.66	120.11
7	E	1237	AMP	C4-N9-C8	5.46	111.47	105.74
7	E	1237	AMP	C2-N3-C4	4.96	123.95	111.83
4	A	1730	FMN	O4'-C4'-C5'	-4.92	99.13	109.99
4	A	1730	FMN	C7M-C7-C6	-4.89	110.96	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1730	FMN	C5'-C4'-C3'	4.80	121.27	112.22
7	E	1237	AMP	N9-C8-N7	-4.72	107.24	113.94
7	C	1236	AMP	N9-C8-N7	-4.69	107.28	113.94
4	A	1730	FMN	C4A-C10-N10	4.69	123.20	116.48
7	E	1237	AMP	O3'-C3'-C2'	-4.64	96.95	111.82
5	B	1731	ADP	O2A-PA-O3A	4.49	119.41	107.27
4	B	1730	FMN	C9A-C5A-N5	-4.42	117.77	122.45
4	B	1730	FMN	C7M-C7-C8	-4.37	111.83	120.76
5	A	1731	ADP	O2A-PA-O3A	4.28	118.85	107.27
7	E	1237	AMP	N3-C4-N9	4.17	134.26	127.17
4	B	1730	FMN	C4'-C3'-C2'	4.13	120.44	113.57
7	E	1237	AMP	O4'-C1'-C2'	4.11	115.41	106.62
5	B	1731	ADP	C5-C4-N3	-4.08	121.10	126.72
7	E	1237	AMP	C5-C4-N3	-3.98	121.24	126.72
4	A	1730	FMN	O4-C4-N3	-3.96	112.66	120.11
5	A	1731	ADP	C5-C4-N3	-3.96	121.26	126.72
7	E	1237	AMP	C4-N9-C1'	-3.95	117.38	126.63
7	C	1236	AMP	C5-C6-N6	-3.88	113.67	123.29
5	A	1731	ADP	N3-C2-N1	-3.80	122.83	128.58
5	A	1731	ADP	N3-C4-N9	3.79	133.62	127.17
4	A	1730	FMN	C10-C4A-N5	-3.79	117.07	124.81
5	A	1731	ADP	N6-C6-N1	3.60	126.39	118.38
5	A	1731	ADP	C6-C5-C4	3.55	122.03	117.18
5	B	1731	ADP	C2-N3-C4	3.53	120.45	111.83
4	A	1730	FMN	O2-C2-N1	-3.51	115.98	121.80
7	C	1236	AMP	C4'-O4'-C1'	-3.50	101.73	109.47
5	B	1731	ADP	O3A-PA-O1A	-3.50	100.17	110.70
7	C	1236	AMP	N3-C4-N9	3.50	133.12	127.17
4	A	1730	FMN	O3'-C3'-C2'	-3.50	100.98	108.93
7	C	1236	AMP	O5'-P-O1P	-3.49	97.01	106.44
7	C	1236	AMP	C4-N9-C1'	-3.48	118.49	126.63
4	B	1730	FMN	C4-C4A-N5	3.47	123.01	118.21
5	A	1731	ADP	C5-C6-N6	-3.43	114.79	123.29
7	E	1237	AMP	O2P-P-O5'	-3.34	97.95	106.67
7	C	1236	AMP	C5-C4-N9	-3.30	102.22	105.81
5	A	1731	ADP	O2'-C2'-C3'	-3.26	101.36	111.82
7	E	1237	AMP	O5'-P-O1P	3.24	115.20	106.44
4	B	1730	FMN	C8M-C8-C9	-3.21	113.92	119.57
4	A	1730	FMN	O4-C4-C4A	-3.20	118.07	126.53
7	C	1236	AMP	O4'-C4'-C5'	-3.20	99.10	109.33
4	B	1730	FMN	O3P-P-O5'	3.17	114.93	106.67
4	B	1730	FMN	O3P-P-O1P	-3.14	98.60	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1730	FMN	C8M-C8-C7	-3.10	114.43	120.76
5	A	1731	ADP	N9-C8-N7	-3.10	109.54	113.94
5	B	1731	ADP	C2'-C3'-C4'	3.08	108.56	102.61
7	C	1236	AMP	N6-C6-N1	3.08	125.24	118.38
5	A	1731	ADP	C3'-C2'-C1'	3.07	107.28	101.46
5	B	1731	ADP	N9-C8-N7	-3.04	109.63	113.94
7	E	1237	AMP	C5-N7-C8	3.03	108.20	103.45
5	A	1731	ADP	O3'-C3'-C2'	-2.96	102.34	111.82
5	B	1731	ADP	O5'-PA-O1A	2.96	120.65	108.94
7	C	1236	AMP	O2'-C2'-C3'	-2.95	102.36	111.82
4	A	1730	FMN	C5A-C9A-N10	2.94	120.62	117.97
4	A	1730	FMN	O5'-P-O1P	-2.92	98.56	106.44
5	B	1731	ADP	C2'-C1'-N9	2.91	120.53	113.30
4	A	1730	FMN	C4-C4A-C10	2.88	121.88	116.93
7	E	1237	AMP	C5'-C4'-C3'	2.87	125.56	115.21
4	B	1730	FMN	C4A-C4-N3	2.87	120.56	113.25
5	A	1731	ADP	O5'-C5'-C4'	-2.87	99.24	108.99
5	B	1731	ADP	C5-N7-C8	2.81	107.87	103.45
4	B	1730	FMN	C6-C7-C8	-2.81	115.56	119.69
5	B	1731	ADP	C4-N9-C1'	-2.76	120.17	126.63
5	B	1731	ADP	O4'-C4'-C5'	-2.76	100.50	109.33
7	C	1236	AMP	C3'-C2'-C1'	-2.73	96.29	101.46
5	B	1731	ADP	C2-N1-C6	2.72	123.20	118.73
4	B	1730	FMN	O3'-C3'-C4'	-2.72	102.75	108.93
7	E	1237	AMP	C6-C5-N7	2.70	137.30	132.09
5	B	1731	ADP	C1'-N9-C8	2.68	133.04	127.09
4	B	1730	FMN	C6-C5A-N5	2.66	122.85	118.44
7	C	1236	AMP	C2'-C3'-C4'	-2.65	97.49	102.61
4	B	1730	FMN	C10-N1-C2	2.64	122.57	116.85
7	C	1236	AMP	C2-N3-C4	2.62	118.24	111.83
7	E	1237	AMP	O3'-C3'-C4'	2.61	118.58	111.08
5	B	1731	ADP	C5-C6-N6	-2.58	116.90	123.29
4	B	1730	FMN	C9-C9A-N10	-2.49	118.50	121.85
4	B	1730	FMN	O5'-C5'-C4'	2.46	115.93	109.36
7	E	1237	AMP	C5-C6-N6	-2.46	117.20	123.29
4	B	1730	FMN	C10-C4A-N5	-2.44	119.82	124.81
5	B	1731	ADP	C4-C5-N7	-2.44	107.79	110.58
7	E	1237	AMP	O2'-C2'-C1'	-2.42	101.79	110.10
5	B	1731	ADP	C5-C4-N9	2.39	108.42	105.81
7	C	1236	AMP	O4'-C1'-C2'	2.37	111.68	106.62
4	A	1730	FMN	O3'-C3'-C4'	2.34	114.24	108.93
4	B	1730	FMN	O2'-C2'-C3'	2.32	114.67	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1731	ADP	C6-C5-N7	-2.31	127.63	132.09
5	A	1731	ADP	C4-N9-C8	2.30	108.16	105.74
4	A	1730	FMN	C8M-C8-C7	-2.30	116.07	120.76
7	E	1237	AMP	C4'-O4'-C1'	-2.26	104.47	109.47
7	E	1237	AMP	C6-C5-C4	-2.25	114.11	117.18
4	A	1730	FMN	O2-C2-N3	2.23	122.87	118.58
4	B	1730	FMN	O5'-P-O1P	2.22	112.45	106.44
7	E	1237	AMP	C5-C6-N1	2.20	123.09	117.51
5	A	1731	ADP	C2'-C1'-N9	2.19	118.75	113.30
5	A	1731	ADP	C5-N7-C8	2.14	106.81	103.45
4	B	1730	FMN	C4A-C10-N10	2.14	119.54	116.48
5	B	1731	ADP	PA-O5'-C5'	2.08	133.26	121.35
5	B	1731	ADP	O3B-PB-O1B	2.05	118.84	110.83
4	A	1730	FMN	C4-C4A-N5	2.04	121.02	118.21
5	B	1731	ADP	C6-C5-C4	2.03	119.95	117.18
4	A	1730	FMN	O2'-C2'-C3'	-2.03	104.50	109.25
7	C	1236	AMP	C5-N7-C8	2.02	106.62	103.45
5	A	1731	ADP	O3B-PB-O2B	2.01	115.35	107.80
7	E	1237	AMP	C2'-C1'-N9	-2.01	108.31	113.30
4	A	1730	FMN	O3P-P-O2P	2.01	115.34	107.80
4	B	1730	FMN	C5'-C4'-C3'	2.00	115.99	112.22

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1730	FMN	O3'-C3'-C4'-C5'
4	A	1730	FMN	C5'-O5'-P-O3P
5	A	1731	ADP	C5'-O5'-PA-O1A
7	C	1236	AMP	C5'-O5'-P-O3P
7	E	1237	AMP	C5'-O5'-P-O1P
7	E	1237	AMP	C5'-O5'-P-O2P
7	E	1237	AMP	C5'-O5'-P-O3P
4	A	1730	FMN	C2'-C3'-C4'-C5'
4	A	1730	FMN	O3'-C3'-C4'-O4'
4	A	1730	FMN	C2'-C3'-C4'-O4'
4	A	1730	FMN	C5'-O5'-P-O1P
7	C	1236	AMP	C5'-O5'-P-O1P
4	B	1730	FMN	C4'-C5'-O5'-P
5	A	1731	ADP	C3'-C4'-C5'-O5'
4	A	1730	FMN	C5'-O5'-P-O2P
7	C	1236	AMP	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
5	A	1731	ADP	O4'-C4'-C5'-O5'
5	B	1731	ADP	PB-O3A-PA-O2A
5	A	1731	ADP	PB-O3A-PA-O2A
5	B	1731	ADP	PB-O3A-PA-O1A
5	B	1731	ADP	O4'-C4'-C5'-O5'

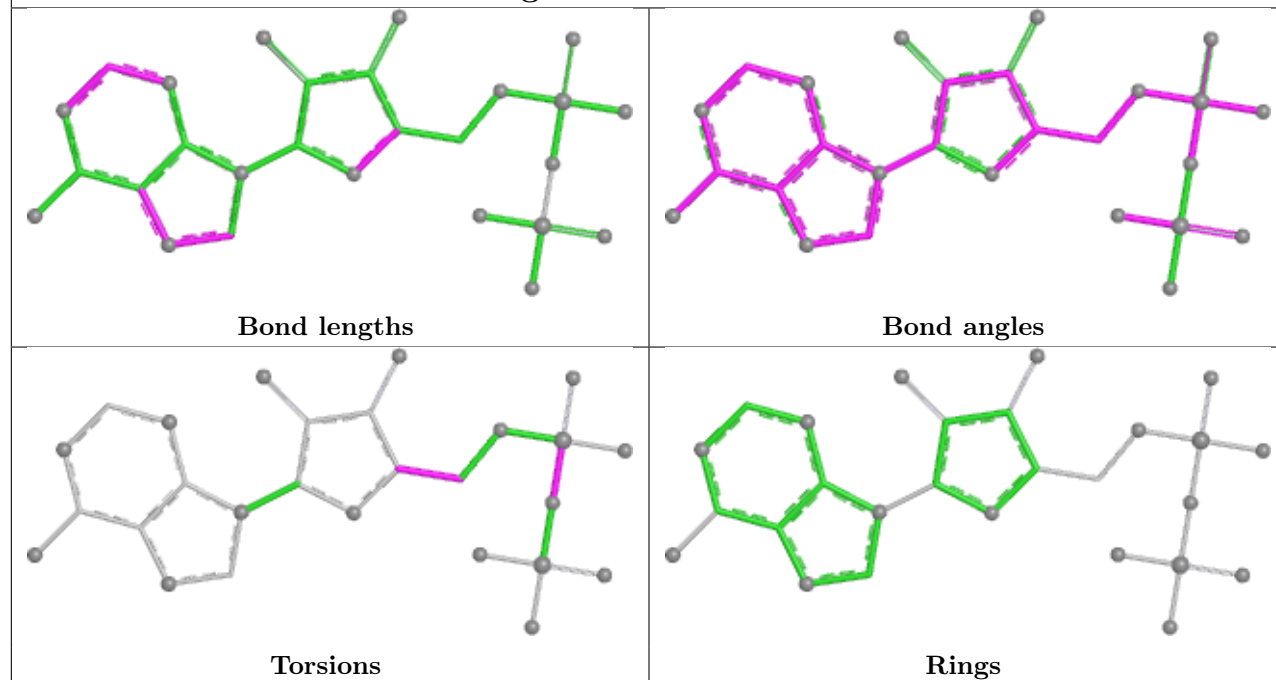
There are no ring outliers.

7 monomers are involved in 32 short contacts:

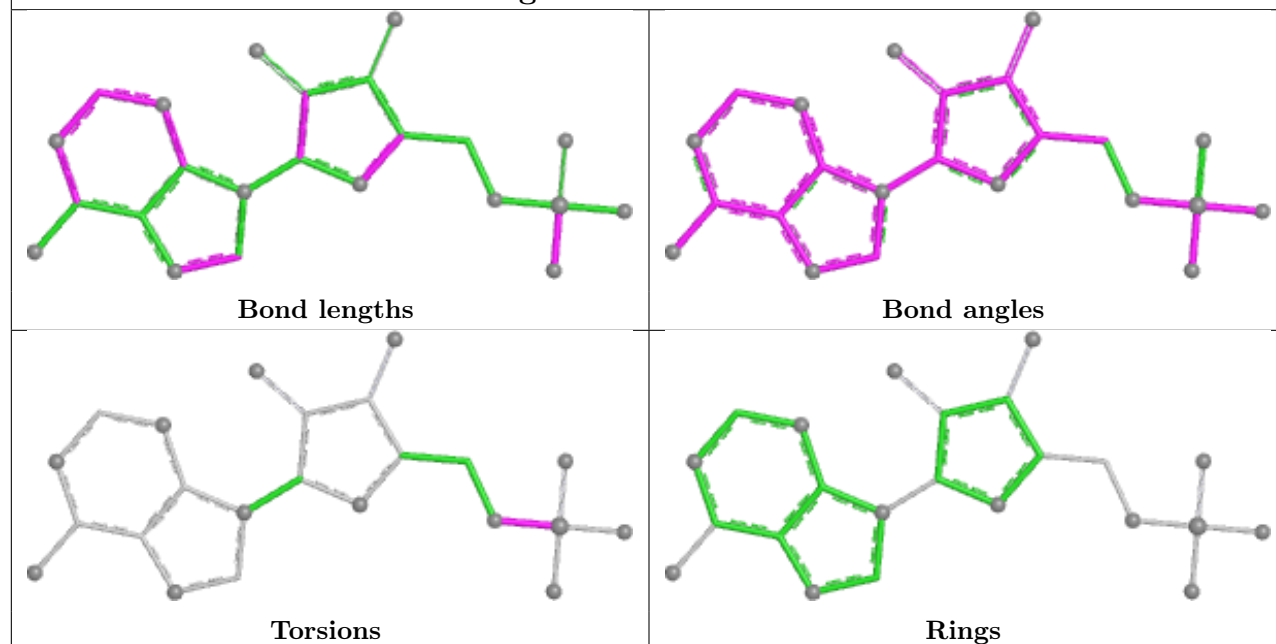
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1731	ADP	2	0
7	E	1237	AMP	4	0
5	A	1731	ADP	7	0
4	A	1730	FMN	6	0
4	B	1730	FMN	6	0
7	C	1236	AMP	6	0
6	A	1732	SF4	1	0

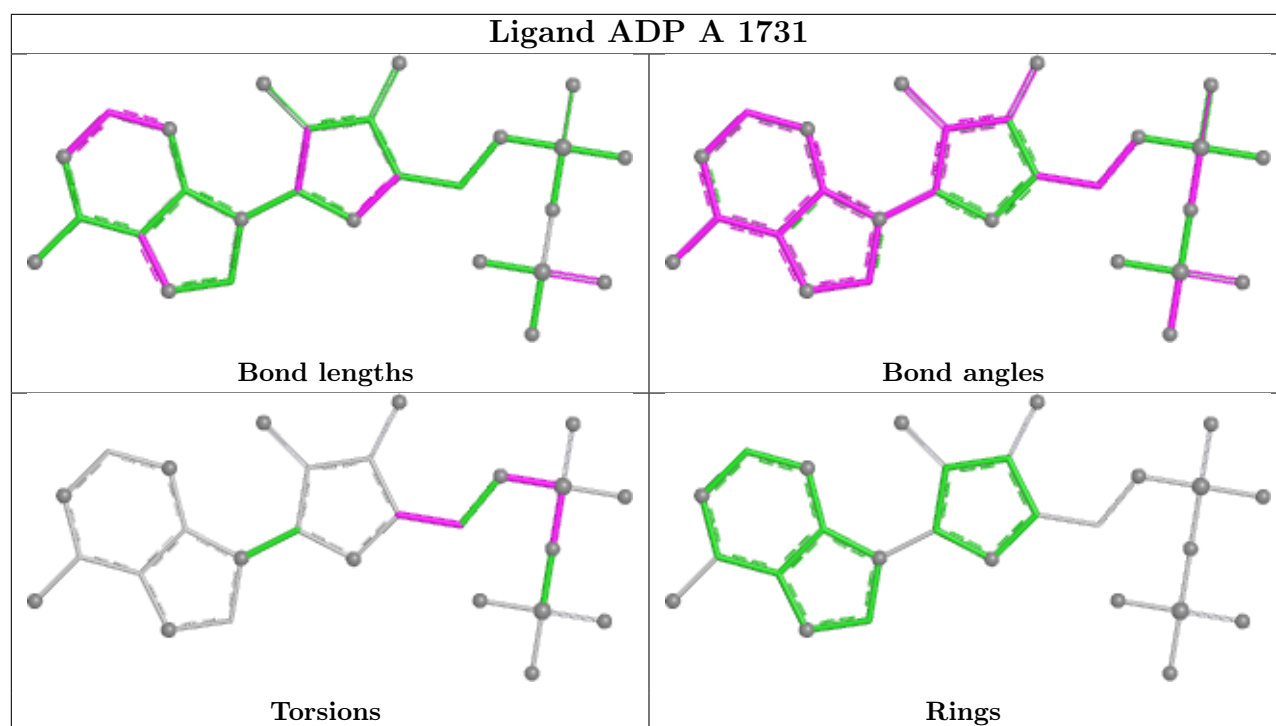
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ADP B 1731

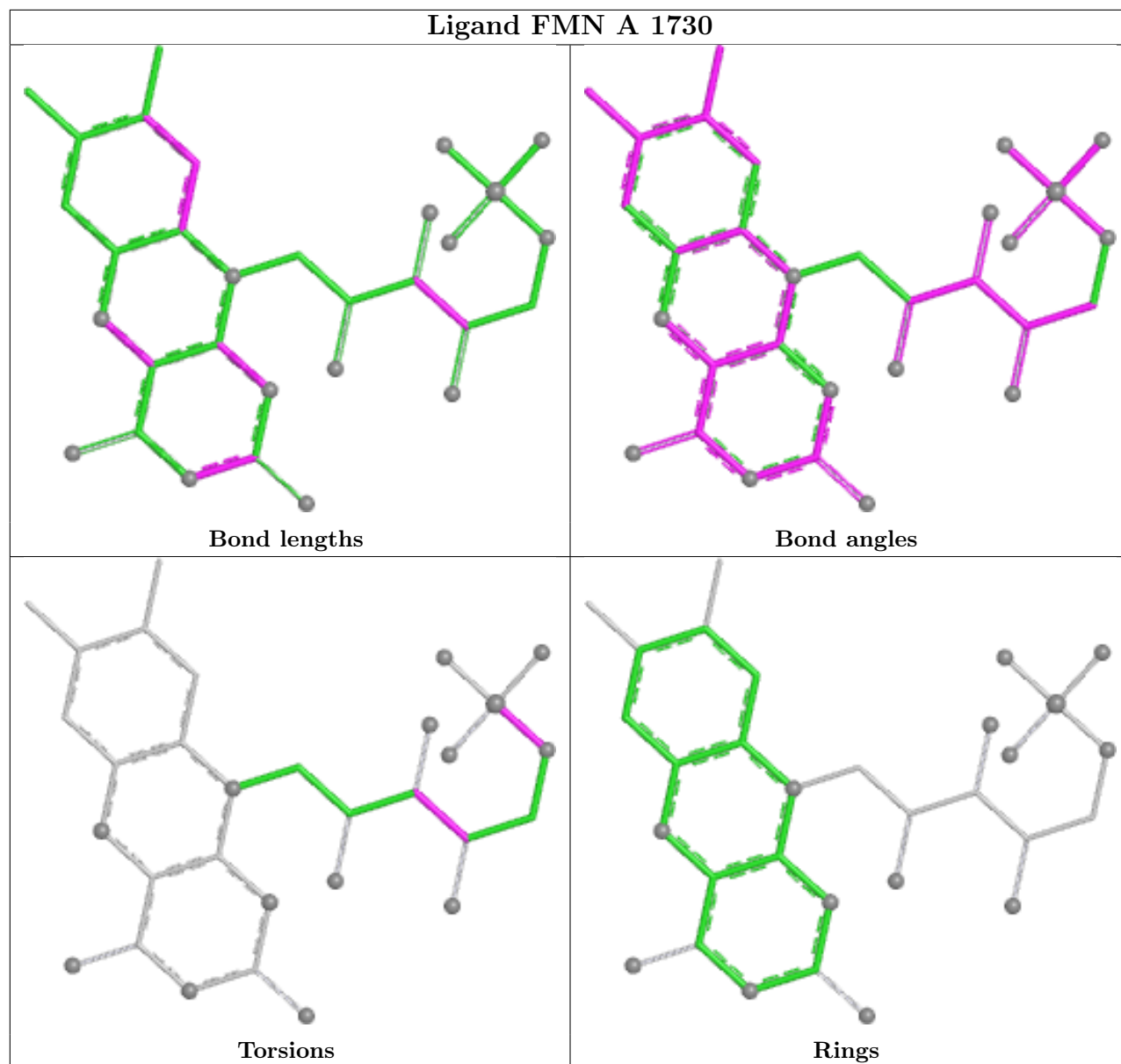


Ligand AMP E 1237

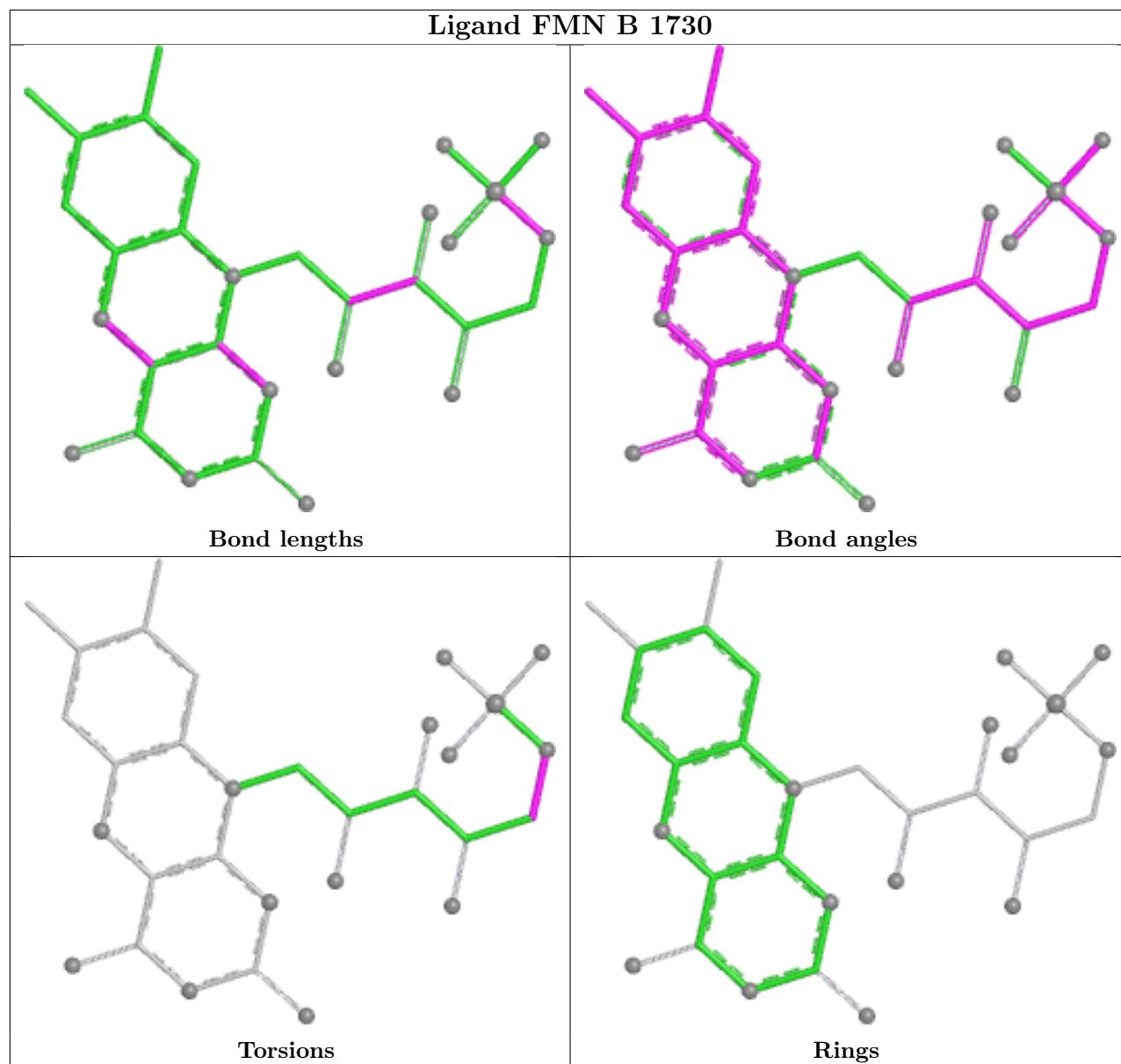


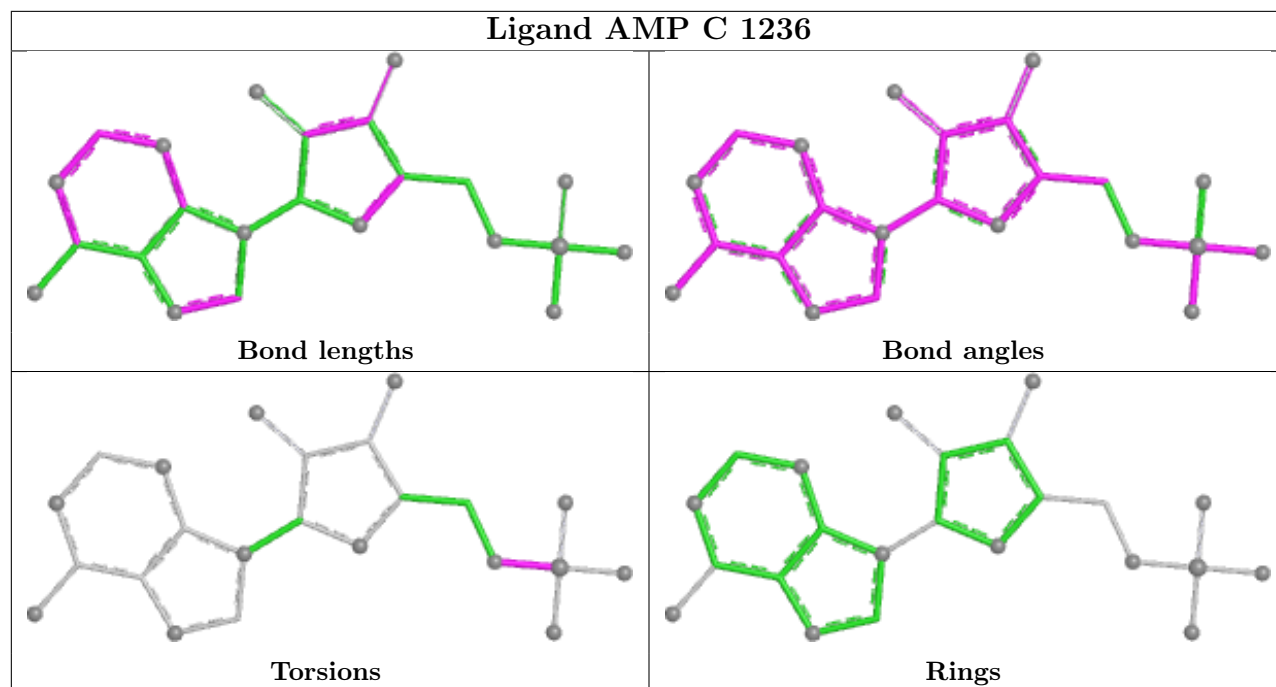


Ligand FMN A 1730



Ligand FMN B 1730





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	729/729 (100%)	0.03	8 (1%)	78 53	39, 57, 67, 73	0
1	B	729/729 (100%)	-0.01	4 (0%)	87 69	38, 57, 67, 73	0
2	C	233/264 (88%)	-0.08	5 (2%)	63 40	49, 58, 65, 71	0
2	E	236/264 (89%)	-0.07	1 (0%)	88 72	50, 59, 65, 70	0
3	D	189/320 (59%)	0.02	3 (1%)	70 45	55, 61, 69, 75	0
3	F	189/320 (59%)	0.38	5 (2%)	57 35	56, 62, 70, 76	0
All	All	2305/2626 (87%)	0.03	26 (1%)	78 53	38, 59, 67, 76	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	6	ILE	3.3
1	B	241	GLN	2.9
1	B	83	VAL	2.8
2	E	11	ALA	2.7
3	F	126	ASP	2.7
1	A	294	VAL	2.6
1	A	239	ASP	2.6
3	D	180	GLN	2.5
1	A	319	GLY	2.5
1	A	609	GLY	2.5
3	F	51	ALA	2.4
1	A	225	VAL	2.4
3	D	126	ASP	2.4
1	B	313	GLY	2.3
2	C	25	ASP	2.3
3	F	143	VAL	2.3
2	C	39	ASP	2.3
1	A	720	GLY	2.2
1	A	628	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	11	ALA	2.2
3	F	61	VAL	2.2
1	B	694	GLU	2.2
1	A	300	TYR	2.2
2	C	22	ASP	2.1
3	D	36	VAL	2.1
2	C	156	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

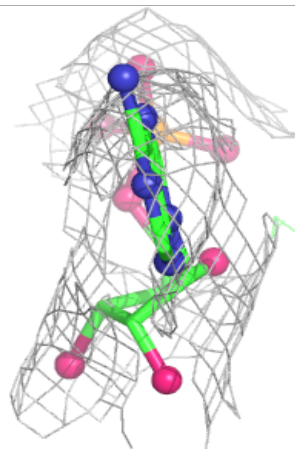
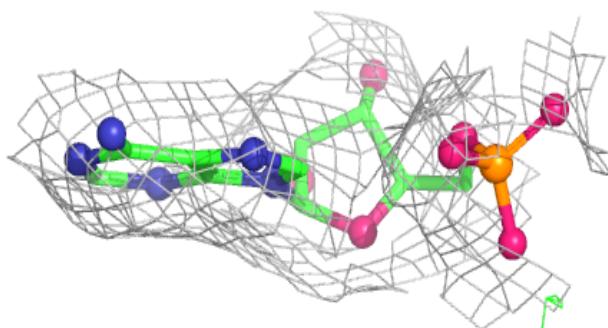
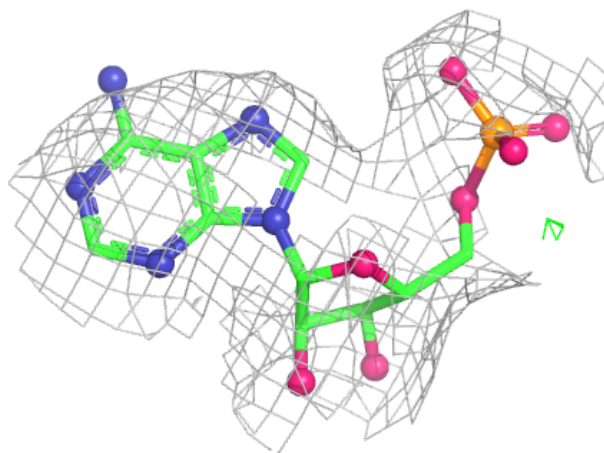
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	AMP	E	1237	23/23	0.92	0.10	33,52,63,66	0
4	FMN	B	1730	31/31	0.93	0.12	23,39,46,52	0
4	FMN	A	1730	31/31	0.93	0.10	35,47,60,61	0
5	ADP	B	1731	27/27	0.94	0.09	45,52,59,61	0
7	AMP	C	1236	23/23	0.94	0.09	34,50,56,60	0
5	ADP	A	1731	27/27	0.94	0.09	40,47,52,53	0
6	SF4	A	1732	8/8	1.00	0.02	31,36,40,41	0
6	SF4	B	1732	8/8	1.00	0.03	33,34,42,44	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.

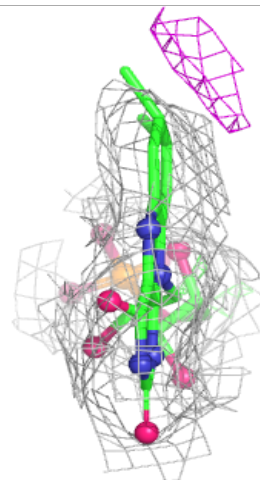
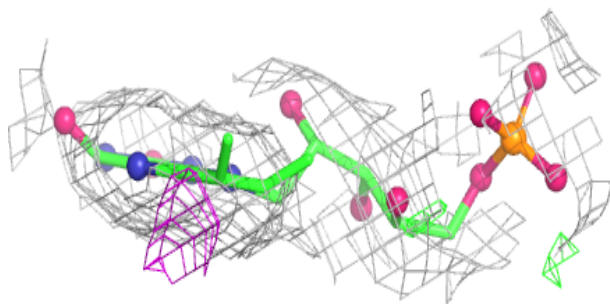
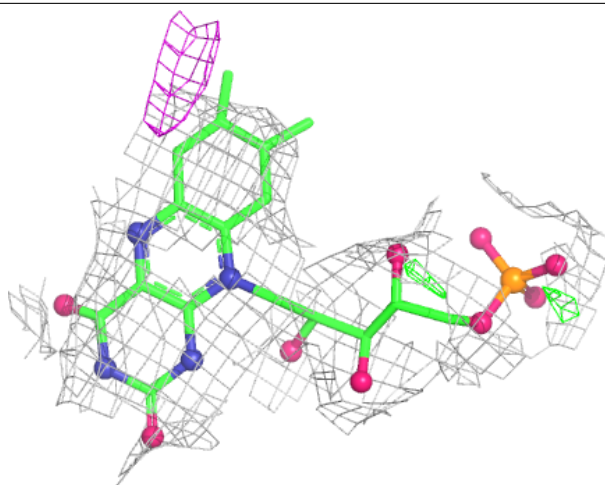
Electron density around AMP E 1237:

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



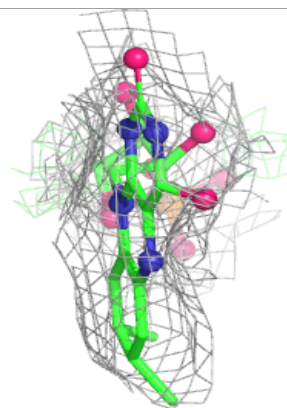
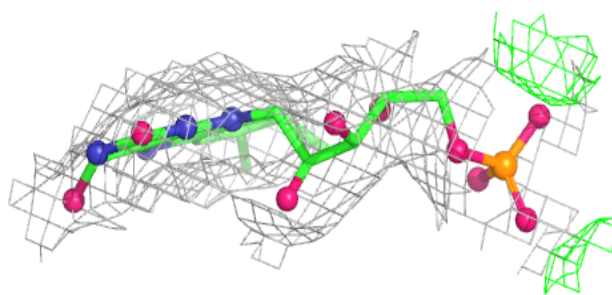
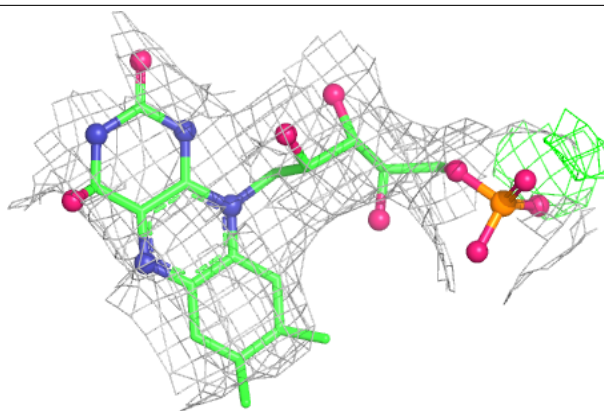
Electron density around FMN B 1730:

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

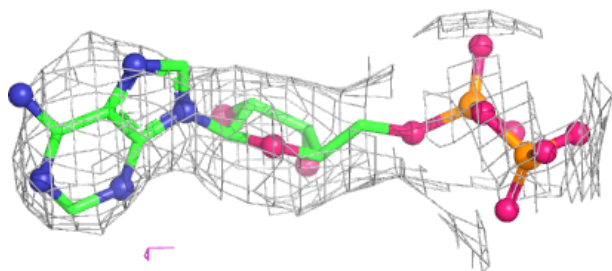
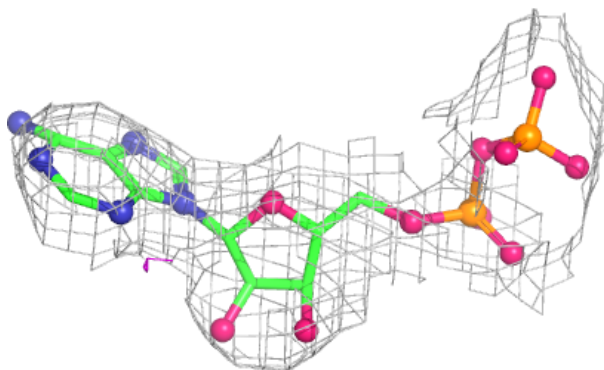


Electron density around FMN A 1730:

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

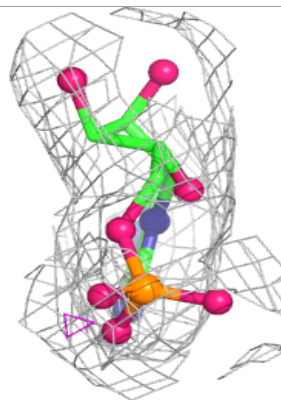
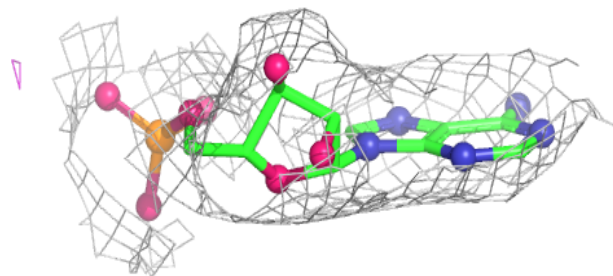
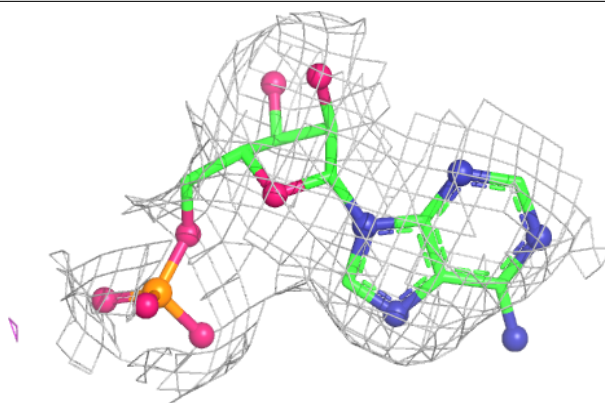
**Electron density around ADP B 1731:**

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

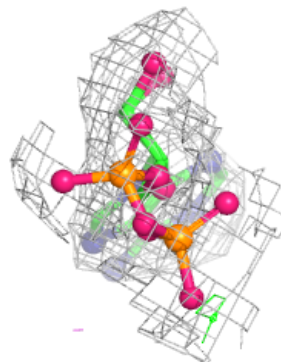
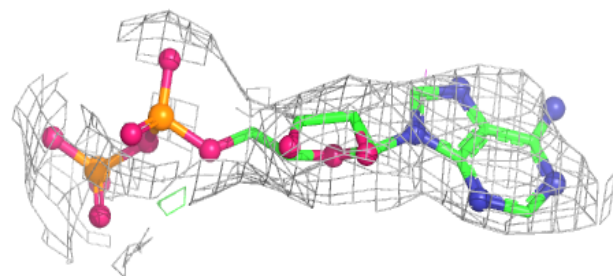
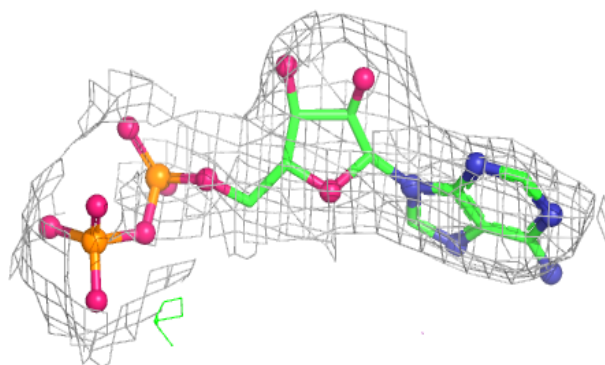


Electron density around AMP C 1236:

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

**Electron density around ADP A 1731:**

$2mF_o-DF_c$ (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.