Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 12:57 PM EDT

PDB ID	:	1O95
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 (i) 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 (i)) were used in the production of this report:

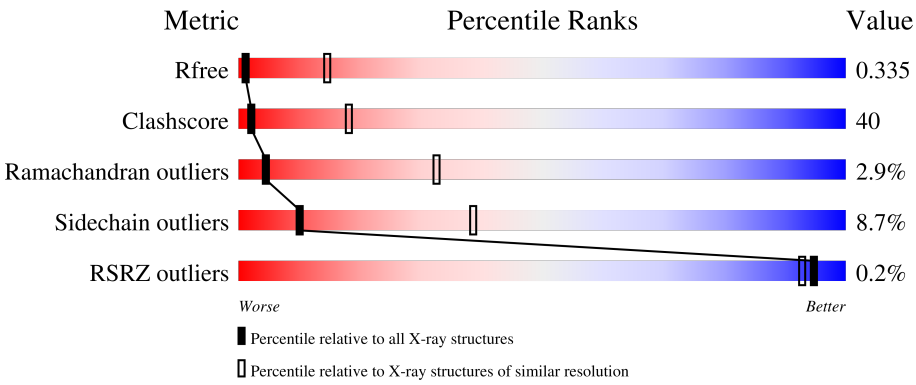
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (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}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 <=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	36% 48% 14% •
1	B	729	33% 53% 11% •
2	C	264	42% 34% 11% • 12%
2	E	264	39% 35% 14% • 11%
3	D	320	27% 23% 7% • 41%

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Mol	Chain	Length	Quality of chain
3	F	320	% 22% 27% 9% • 41%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	729	5692	3589	996	1079	28	0	0	0
1	B	729	5676	3583	994	1071	28	0	0	0

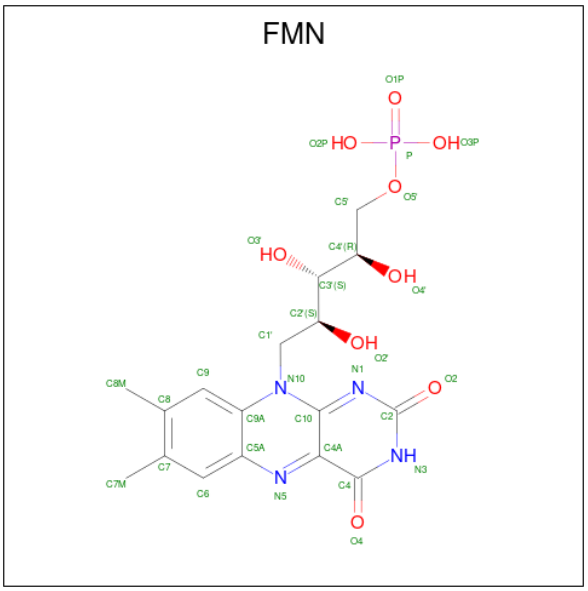
- Molecule 2 is a protein called ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT.

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

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

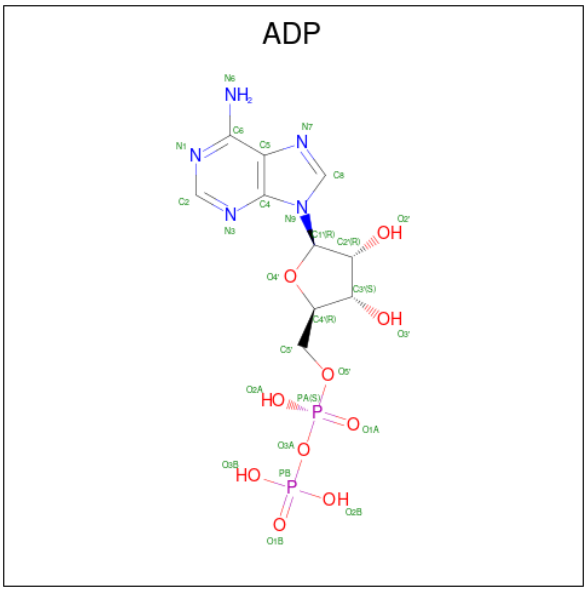
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	189	1354	857	230	267	0	0	0
3	F	189	1376	870	232	274	0	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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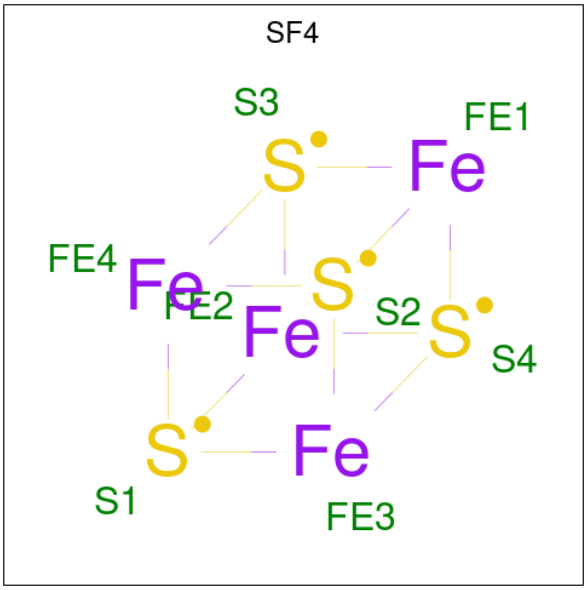
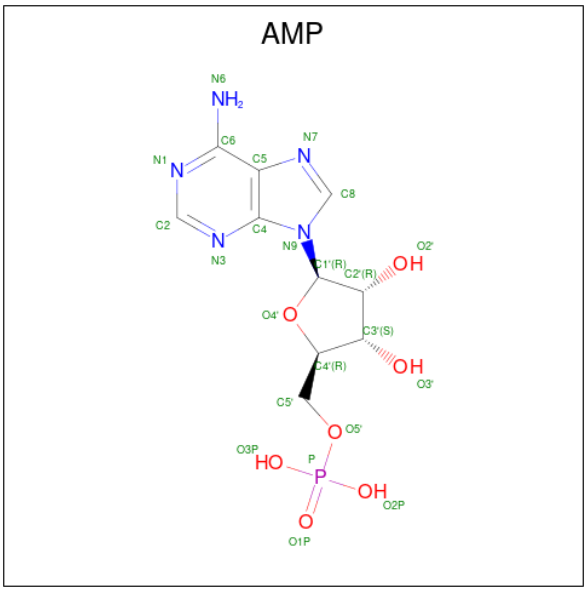
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	27	10	5	10	2	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



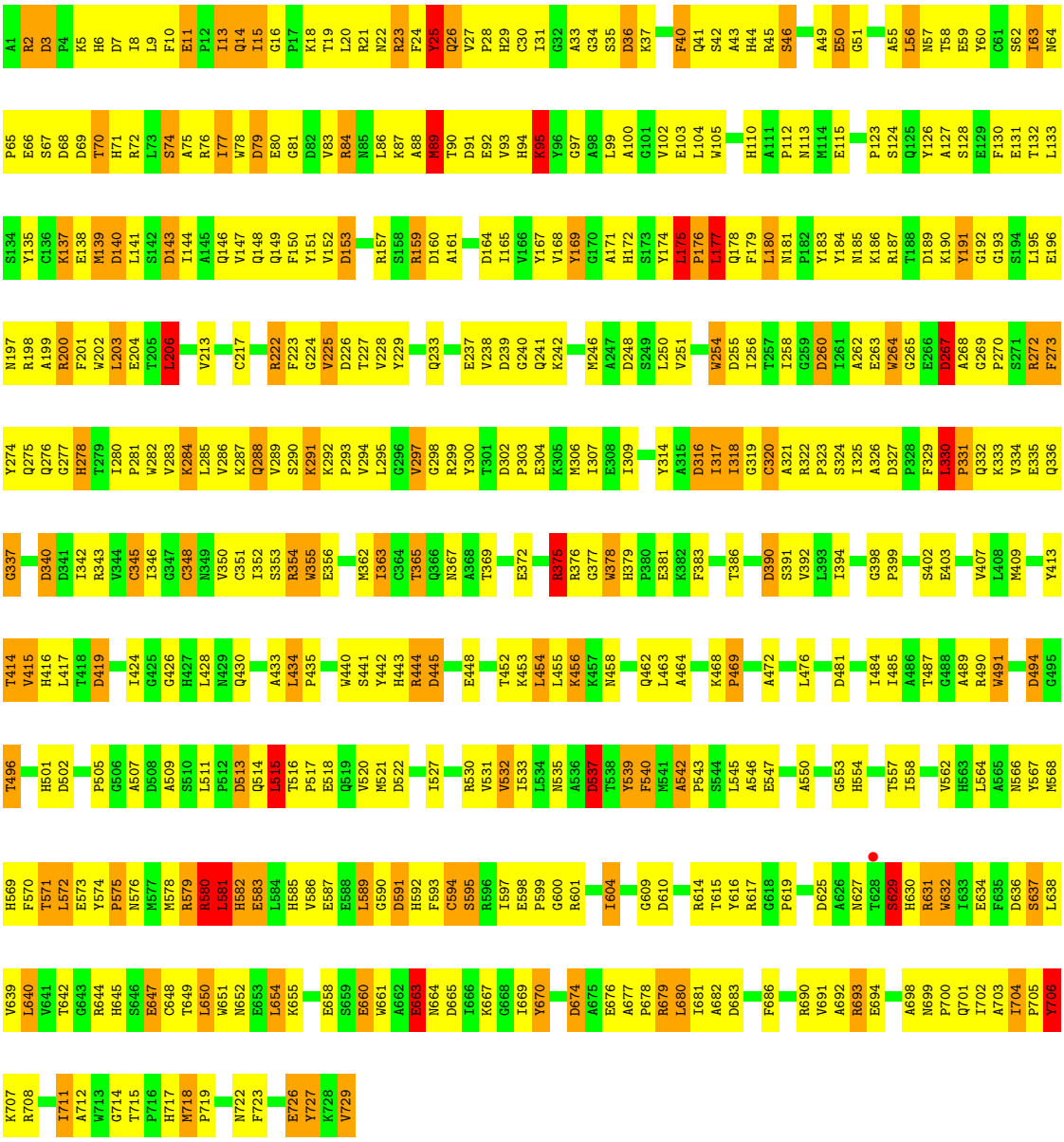
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	C	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
7	E	1	23	10	5	7	1	0	0

3 Residue-property plots (i)

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

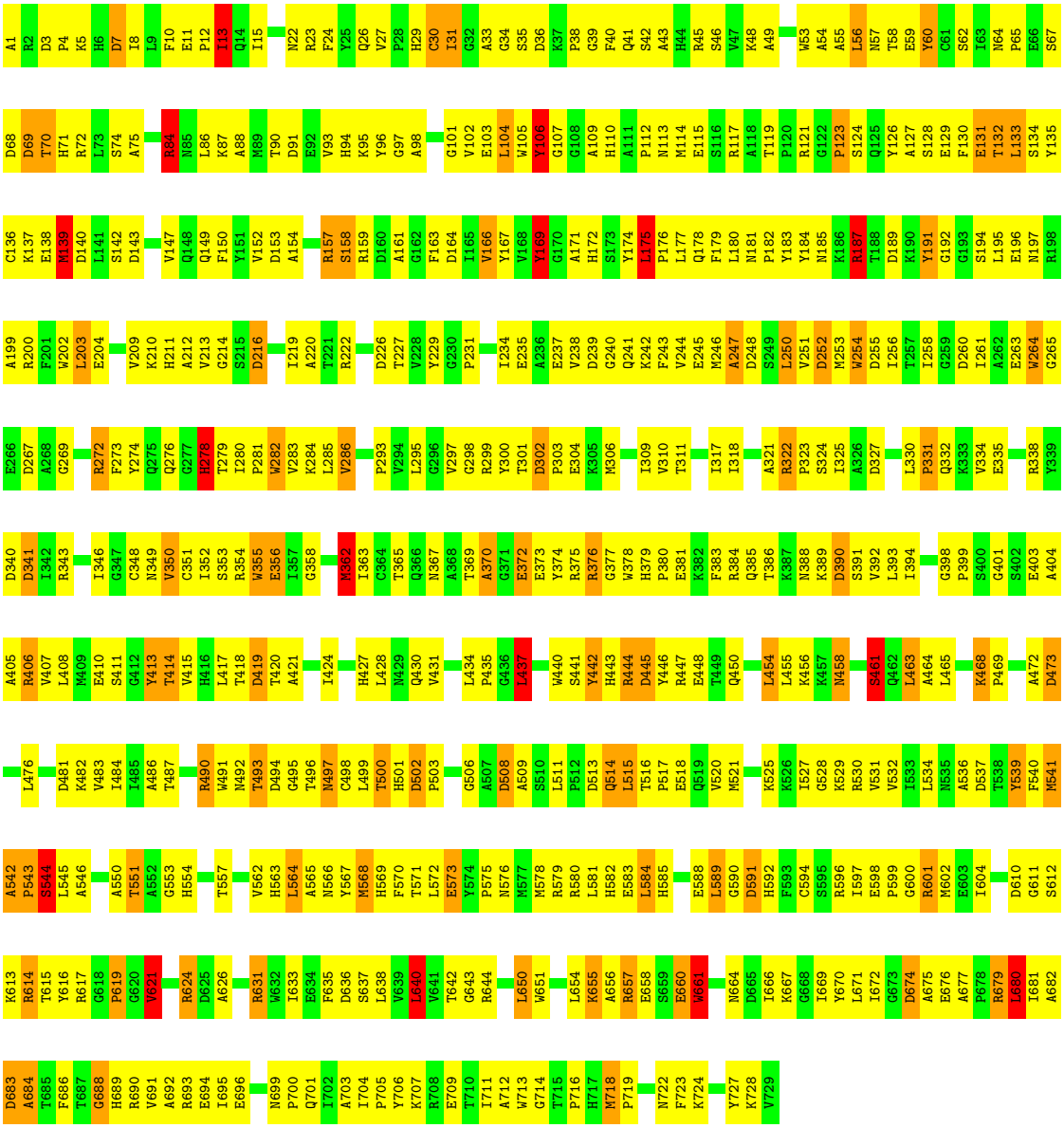
- Molecule 1: TRIMETHYLAMINE DEHYDROGENASE

Chain A: 36% 48% 14% •



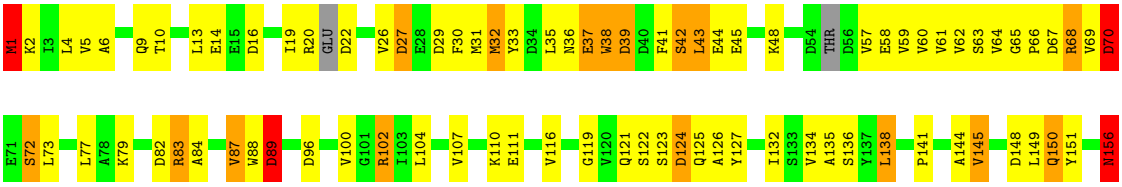
• Molecule 1: TRIMETHYLAMINE DEHYDROGENASE

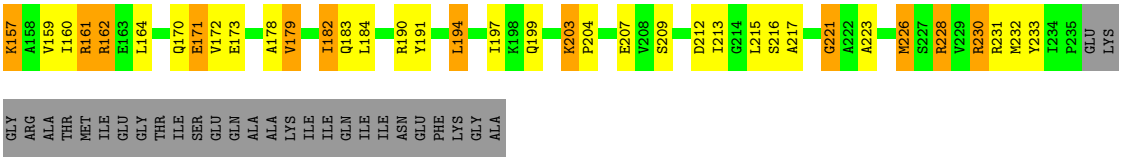
Chain B: 33% 53% 11% •



• Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT

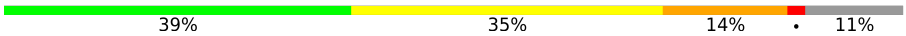
Chain C: 42% 34% 11% • 12%

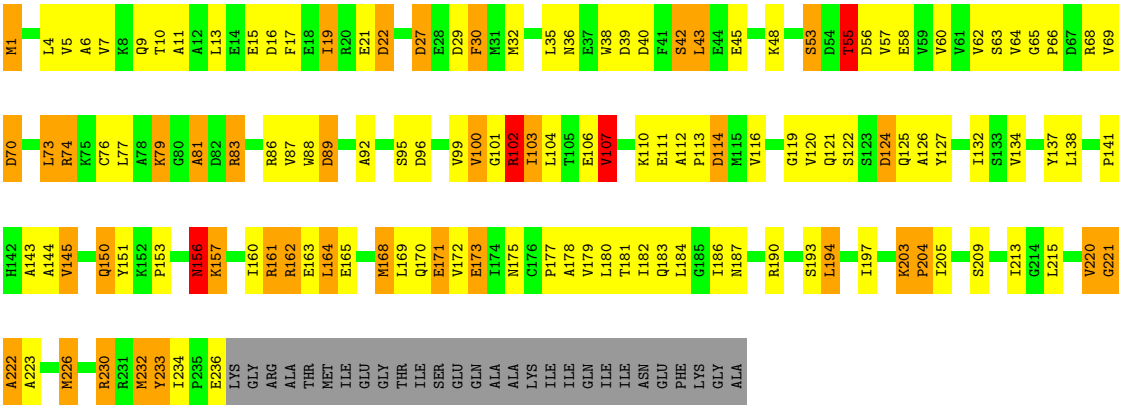




• Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT

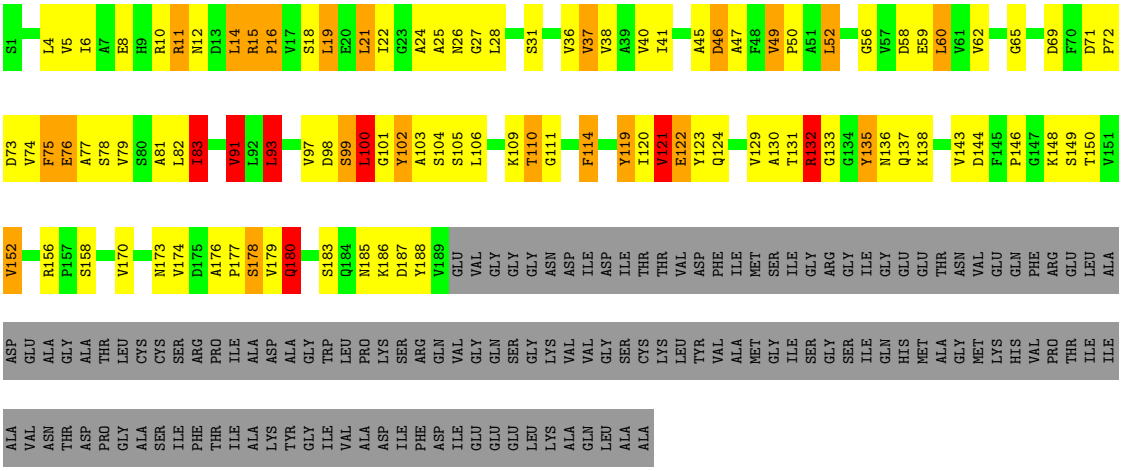
Chain E:





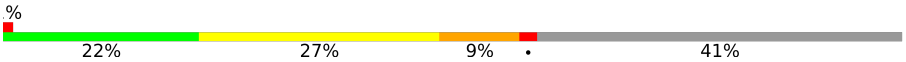
• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT

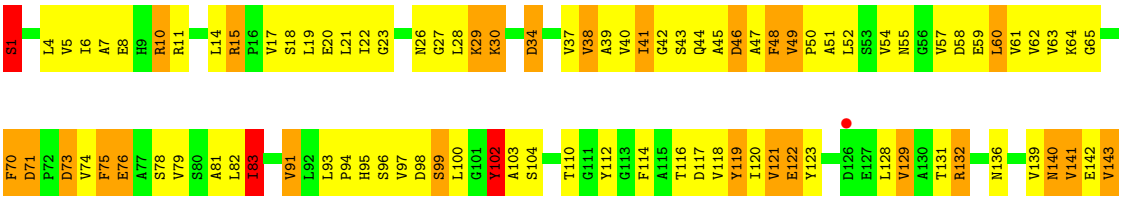
Chain D:

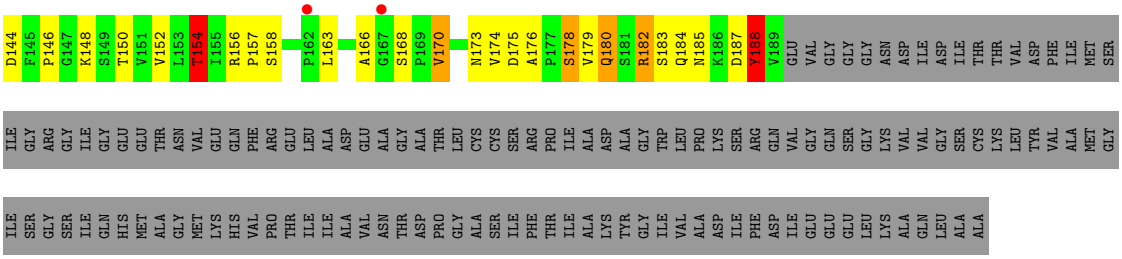


• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT

Chain F:






D144 F145 P146 G147 K148 S149 T150 V151 V152 L153 T154 I155 R156 P157 S158 P162 L163 A166 G167 S168 P169 V170 N173 V174 D175 A176 P177 S178 V179 Q180 S181 R182 S183 Q184 N185 K186 D187 Y188 V189 GLU VAL GLY GLY GLY ASN ASP ILE ASP ILE THR THR VAL ASP PHE ILE MET SER
ILE GLY ARG GLY ILE GLY GLU GLU THR ASN VAL GLU GLN PHE ARG GLU LEU ALA ASP GLU ALA GLY ALA THR LEU CYS CYS SER ARG PRO ILE ALA ASP ALA GLY TRP LEU PRO LYS SER ARG GLN VAL GLY GLN SER GLY LYS VAL VAL GLY SER CYS LYS LEU TYR VAL ALA MET GLY
ILE SER GLY SER ILE GLN HIS MET ALA GLY MET LYS HIS VAL PRO THR ILE ILE ALA VAL ASN THR ASP PRO GLY ALA SER ILE PHE THR ILE ALA LYS TYR GLY ILE VAL ALA ASP ILE PHE ASP ILE GLU GLU GLU LEU LYS ALA GLN LEU ALA ALA

4 Data and refinement statistics (i)

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 19.98 – 3.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.70) 96.9 (19.98-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.71Å)	Xtriage
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	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, AMP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.61	53/5834 (0.9%)	1.66	102/7918 (1.3%)
1	B	1.63	49/5818 (0.8%)	1.66	97/7902 (1.2%)
2	C	1.60	22/1771 (1.2%)	1.54	24/2399 (1.0%)
2	E	1.70	22/1775 (1.2%)	1.65	34/2408 (1.4%)
3	D	1.61	13/1378 (0.9%)	1.59	21/1884 (1.1%)
3	F	2.01	34/1400 (2.4%)	1.77	26/1913 (1.4%)
All	All	1.66	193/17976 (1.1%)	1.65	304/24424 (1.2%)

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 (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	718	MET	SD-CE	12.45	2.47	1.77
3	F	188	TYR	CE1-CZ	9.02	1.50	1.38
1	B	254	TRP	CB-CG	-8.99	1.34	1.50
2	E	232	MET	C-O	8.98	1.40	1.23
3	D	180	GLN	CB-CG	8.94	1.76	1.52
1	B	500	THR	CA-CB	8.44	1.75	1.53
3	F	121	VAL	CB-CG2	-8.27	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	651	TRP	CB-CG	-8.18	1.35	1.50
1	A	663	GLU	CG-CD	8.11	1.64	1.51
2	E	168	MET	SD-CE	8.03	2.22	1.77
1	B	468	LYS	CB-CG	8.02	1.74	1.52
1	A	355	TRP	CB-CG	-7.99	1.35	1.50
2	C	38	TRP	CB-CG	-7.81	1.36	1.50
2	C	156	ASN	CB-CG	7.76	1.69	1.51
1	A	567	TYR	CD2-CE2	-7.57	1.27	1.39
1	B	350	VAL	CA-CB	-7.44	1.39	1.54
2	E	171	GLU	CD-OE2	7.37	1.33	1.25
3	F	143	VAL	CB-CG2	7.35	1.68	1.52
3	F	180	GLN	CB-CG	7.34	1.72	1.52
1	A	46	SER	CA-CB	7.33	1.64	1.52
1	A	670	TYR	CD1-CE1	-7.14	1.28	1.39
1	B	601	ARG	CG-CD	7.14	1.69	1.51
3	F	102	TYR	CE1-CZ	7.06	1.47	1.38
2	C	150	GLN	CG-CD	7.00	1.67	1.51
1	B	331	PRO	CA-C	6.98	1.66	1.52
3	F	140	ASN	CB-CG	6.92	1.67	1.51
1	A	248	ASP	CB-CG	6.86	1.66	1.51
1	A	320	CYS	CB-SG	-6.85	1.70	1.82
1	B	13	ILE	CA-CB	6.83	1.70	1.54
1	A	25	TYR	CE1-CZ	6.82	1.47	1.38
3	F	180	GLN	CG-CD	6.78	1.66	1.51
3	F	15	ARG	CB-CG	6.71	1.70	1.52
2	C	135	ALA	CA-CB	-6.62	1.38	1.52
1	A	275	GLN	CG-CD	6.61	1.66	1.51
2	C	14	GLU	CG-CD	-6.58	1.42	1.51
2	E	156	ASN	CB-CG	6.58	1.66	1.51
3	D	83	ILE	CB-CG2	-6.58	1.32	1.52
3	D	178	SER	CA-CB	6.56	1.62	1.52
2	C	29	ASP	CB-CG	6.54	1.65	1.51
1	A	291	LYS	CD-CE	6.50	1.67	1.51
1	B	355	TRP	CE3-CZ3	6.48	1.49	1.38
1	A	25	TYR	CD1-CE1	6.45	1.49	1.39
1	B	442	TYR	CD2-CE2	-6.39	1.29	1.39
3	F	129	VAL	CA-CB	6.37	1.68	1.54
1	A	225	VAL	CB-CG1	6.36	1.66	1.52
1	B	169	TYR	CD2-CE2	-6.36	1.29	1.39
1	B	728	LYS	CD-CE	6.35	1.67	1.51
1	A	275	GLN	CB-CG	6.33	1.69	1.52
2	C	1	MET	SD-CE	6.32	2.13	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	38	TRP	CB-CG	-6.32	1.38	1.50
3	D	180	GLN	CG-CD	6.30	1.65	1.51
3	F	170	VAL	CB-CG1	6.29	1.66	1.52
2	C	6	ALA	CA-CB	-6.28	1.39	1.52
1	B	282	TRP	CB-CG	-6.26	1.39	1.50
1	B	509	ALA	CA-CB	6.23	1.65	1.52
2	E	106	GLU	CD-OE2	6.21	1.32	1.25
1	A	331	PRO	CA-C	6.20	1.65	1.52
1	A	567	TYR	CE2-CZ	-6.20	1.30	1.38
1	A	663	GLU	CD-OE1	6.19	1.32	1.25
2	E	100	VAL	CA-CB	6.17	1.67	1.54
3	D	121	VAL	CB-CG1	-6.15	1.40	1.52
3	D	114	PHE	CD2-CE2	-6.14	1.26	1.39
1	A	704	ILE	CA-CB	6.13	1.69	1.54
2	E	30	PHE	CD2-CE2	6.13	1.51	1.39
2	E	233	TYR	CE2-CZ	6.12	1.46	1.38
1	A	314	TYR	CD1-CE1	6.12	1.48	1.39
2	C	171	GLU	CD-OE1	6.12	1.32	1.25
1	A	153	ASP	CB-CG	6.11	1.64	1.51
1	B	621	VAL	CA-CB	6.11	1.67	1.54
2	C	42	SER	CB-OG	-6.08	1.34	1.42
1	B	286	VAL	CB-CG1	6.06	1.65	1.52
3	D	114	PHE	CD1-CE1	-6.01	1.27	1.39
1	B	562	VAL	CB-CG1	6.01	1.65	1.52
1	A	196	GLU	CD-OE1	6.00	1.32	1.25
3	F	58	ASP	CB-CG	5.99	1.64	1.51
1	B	355	TRP	CG-CD1	-5.99	1.28	1.36
3	F	38	VAL	CB-CG2	5.97	1.65	1.52
1	B	191	TYR	CD2-CE2	-5.97	1.30	1.39
1	B	372	GLU	CD-OE2	-5.97	1.19	1.25
1	A	11	GLU	CG-CD	5.95	1.60	1.51
2	E	22	ASP	CA-C	5.95	1.68	1.52
2	E	171	GLU	CG-CD	5.95	1.60	1.51
1	A	250	LEU	CG-CD1	5.91	1.73	1.51
3	F	175	ASP	CB-CG	5.91	1.64	1.51
3	F	170	VAL	CB-CG2	5.90	1.65	1.52
1	A	159	ARG	CG-CD	5.90	1.66	1.51
1	A	711	ILE	CA-CB	-5.89	1.41	1.54
2	C	207	GLU	CD-OE2	5.88	1.32	1.25
2	E	30	PHE	CE2-CZ	5.86	1.48	1.37
1	B	166	VAL	CB-CG2	-5.85	1.40	1.52
3	F	34	ASP	CB-CG	5.84	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	CYS	CB-SG	-5.81	1.72	1.81
1	A	262	ALA	CA-CB	-5.80	1.40	1.52
1	A	196	GLU	CD-OE2	5.79	1.32	1.25
1	B	169	TYR	CD1-CE1	-5.79	1.30	1.39
2	E	107	VAL	CB-CG1	-5.77	1.40	1.52
1	B	169	TYR	CE2-CZ	-5.72	1.31	1.38
1	B	191	TYR	CZ-OH	5.72	1.47	1.37
2	E	30	PHE	CE1-CZ	5.72	1.48	1.37
3	F	48	PHE	CE1-CZ	5.72	1.48	1.37
2	E	150	GLN	CG-CD	5.70	1.64	1.51
3	D	8	GLU	CD-OE2	5.70	1.31	1.25
1	B	684	ALA	CA-CB	-5.69	1.40	1.52
3	F	1	SER	CA-CB	5.69	1.61	1.52
1	A	89	MET	SD-CE	5.69	2.09	1.77
1	A	567	TYR	CD1-CE1	-5.67	1.30	1.39
3	D	152	VAL	CA-CB	-5.67	1.42	1.54
1	B	655	LYS	CE-NZ	5.66	1.63	1.49
3	D	158	SER	CB-OG	5.65	1.49	1.42
2	C	32	MET	CG-SD	-5.65	1.66	1.81
1	B	656	ALA	CA-CB	5.64	1.64	1.52
1	B	537	ASP	CB-CG	5.63	1.63	1.51
3	F	178	SER	CA-CB	5.58	1.61	1.52
1	A	693	ARG	NE-CZ	-5.57	1.25	1.33
1	B	370	ALA	CA-CB	-5.56	1.40	1.52
2	C	191	TYR	CE2-CZ	-5.56	1.31	1.38
1	A	345	CYS	CB-SG	-5.55	1.72	1.81
1	B	601	ARG	CB-CG	5.54	1.67	1.52
3	F	168	SER	CA-CB	5.53	1.61	1.52
3	F	44	GLN	CB-CG	5.52	1.67	1.52
3	F	10	ARG	CZ-NH1	5.51	1.40	1.33
1	B	410	GLU	CD-OE2	5.50	1.31	1.25
2	C	179	VAL	CB-CG2	-5.50	1.41	1.52
1	A	204	GLU	CD-OE2	5.50	1.31	1.25
1	A	456	LYS	CB-CG	5.49	1.67	1.52
1	B	543	PRO	CB-CG	-5.49	1.22	1.50
1	A	647	GLU	CD-OE1	5.47	1.31	1.25
1	A	540	PHE	CB-CG	-5.46	1.42	1.51
2	E	163	GLU	CD-OE2	5.46	1.31	1.25
1	A	727	TYR	CD1-CE1	-5.46	1.31	1.39
3	F	75	PHE	CE2-CZ	5.43	1.47	1.37
1	B	514	GLN	CG-CD	5.42	1.63	1.51
1	A	126	TYR	CB-CG	-5.42	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	ALA	CA-CB	-5.41	1.41	1.52
1	A	540	PHE	CG-CD1	-5.38	1.30	1.38
1	B	1	ALA	CA-CB	5.38	1.63	1.52
2	E	30	PHE	CD1-CE1	5.38	1.50	1.39
1	B	580	ARG	NE-CZ	5.37	1.40	1.33
3	F	55	ASN	CB-CG	5.37	1.63	1.51
2	C	151	TYR	CD2-CE2	5.37	1.47	1.39
1	B	588	GLU	CD-OE1	5.36	1.31	1.25
1	B	350	VAL	CB-CG1	-5.36	1.41	1.52
3	F	41	ILE	CA-CB	5.36	1.67	1.54
1	A	670	TYR	CB-CG	-5.35	1.43	1.51
3	D	135	TYR	CD2-CE2	5.34	1.47	1.39
3	D	76	GLU	CD-OE1	5.33	1.31	1.25
2	C	30	PHE	CE1-CZ	5.33	1.47	1.37
2	C	16	ASP	CB-CG	5.33	1.62	1.51
3	F	136	ASN	CB-CG	5.30	1.63	1.51
1	B	551	THR	CA-CB	5.29	1.67	1.53
2	C	87	VAL	CB-CG2	-5.29	1.41	1.52
3	F	70	PHE	CE2-CZ	5.29	1.47	1.37
3	F	182	ARG	NE-CZ	5.28	1.40	1.33
1	A	629	SER	CA-CB	5.27	1.60	1.52
1	B	348	CYS	CB-SG	-5.26	1.73	1.81
1	B	383	PHE	CD2-CE2	-5.25	1.28	1.39
1	A	583	GLU	CD-OE1	5.23	1.31	1.25
1	A	625	ASP	CB-CG	-5.23	1.40	1.51
2	C	5	VAL	CA-CB	-5.19	1.43	1.54
1	B	727	TYR	CB-CG	-5.19	1.43	1.51
1	A	708	ARG	CB-CG	-5.18	1.38	1.52
1	B	626	ALA	CA-CB	5.18	1.63	1.52
1	A	599	PRO	CA-C	5.17	1.63	1.52
1	A	706	TYR	CD1-CE1	-5.16	1.31	1.39
1	A	13	ILE	CA-CB	5.15	1.66	1.54
1	A	632	TRP	CB-CG	-5.14	1.41	1.50
2	C	162	ARG	CZ-NH1	-5.14	1.26	1.33
2	E	151	TYR	CB-CG	5.14	1.59	1.51
1	A	532	VAL	C-O	5.14	1.33	1.23
1	B	468	LYS	CG-CD	5.14	1.70	1.52
3	F	48	PHE	CD2-CE2	5.12	1.49	1.39
3	F	154	THR	CA-CB	5.12	1.66	1.53
3	D	123	TYR	CE1-CZ	5.10	1.45	1.38
2	E	95	SER	CB-OG	5.09	1.48	1.42
1	B	140	ASP	CB-CG	5.08	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	139	VAL	CA-CB	-5.08	1.44	1.54
1	A	378	TRP	CB-CG	-5.08	1.41	1.50
2	E	103	ILE	CA-CB	-5.08	1.43	1.54
3	F	102	TYR	CG-CD2	5.07	1.45	1.39
1	B	573	GLU	CG-CD	5.07	1.59	1.51
1	A	50	GLU	CG-CD	5.06	1.59	1.51
1	A	496	THR	CA-CB	5.05	1.66	1.53
1	B	656	ALA	CA-C	5.05	1.66	1.52
1	A	604	ILE	CA-CB	-5.04	1.43	1.54
1	A	699	ASN	CB-CG	5.04	1.62	1.51
1	B	202	TRP	CB-CG	-5.03	1.41	1.50
2	E	232	MET	CG-SD	5.03	1.94	1.81
3	F	76	GLU	CD-OE2	5.03	1.31	1.25
2	C	37	GLU	CD-OE1	5.03	1.31	1.25
3	F	139	VAL	CB-CG1	-5.02	1.42	1.52
3	F	132	ARG	NE-CZ	5.02	1.39	1.33
1	A	539	TYR	CG-CD2	-5.01	1.32	1.39
2	C	171	GLU	CD-OE2	5.00	1.31	1.25

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	ASP	CB-CG-OD2	13.04	130.03	118.30
1	B	272	ARG	NE-CZ-NH1	-12.16	114.22	120.30
3	F	15	ARG	NE-CZ-NH2	11.80	126.20	120.30
1	A	302	ASP	CB-CG-OD2	11.78	128.90	118.30
1	A	665	ASP	CB-CG-OD2	11.31	128.48	118.30
1	B	272	ARG	NE-CZ-NH2	11.27	125.93	120.30
2	E	16	ASP	CB-CG-OD2	11.26	128.44	118.30
3	F	10	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	B	680	LEU	CB-CG-CD2	-10.42	93.28	111.00
1	A	302	ASP	CB-CG-OD1	-10.23	109.09	118.30
1	B	454	LEU	CA-CB-CG	-10.12	92.03	115.30
3	F	83	ILE	CG1-CB-CG2	-10.06	89.27	111.40
1	B	473	ASP	CB-CG-OD2	9.82	127.14	118.30
1	B	239	ASP	CB-CG-OD2	9.81	127.13	118.30
1	A	419	ASP	CB-CG-OD2	9.81	127.13	118.30
3	D	83	ILE	CG1-CB-CG2	-9.79	89.87	111.40
1	A	469	PRO	N-CD-CG	-9.71	88.64	103.20
2	E	27	ASP	CB-CG-OD1	9.63	126.97	118.30
1	A	494	ASP	CB-CG-OD2	9.61	126.95	118.30
1	B	140	ASP	CB-CG-OD1	9.54	126.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	15	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	B	302	ASP	CB-CG-OD2	9.28	126.65	118.30
1	A	69	ASP	CB-CG-OD2	9.17	126.56	118.30
1	A	537	ASP	CB-CG-OD2	9.13	126.52	118.30
1	B	177	LEU	CA-CB-CG	9.01	136.01	115.30
1	B	157	ARG	NE-CZ-NH2	-8.87	115.86	120.30
3	F	10	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	A	3	ASP	CB-CG-OD1	8.76	126.18	118.30
1	B	338	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	B	419	ASP	CB-CG-OD2	8.62	126.06	118.30
1	A	640	LEU	CB-CG-CD1	-8.46	96.62	111.00
3	D	15	ARG	NE-CZ-NH1	8.41	124.51	120.30
2	C	27	ASP	CB-CG-OD2	8.37	125.84	118.30
2	E	83	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	522	ASP	CB-CG-OD1	-8.29	110.83	118.30
3	D	15	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	338	ARG	NE-CZ-NH2	8.22	124.41	120.30
2	E	162	ARG	NE-CZ-NH1	8.21	124.41	120.30
2	E	102	ARG	NE-CZ-NH2	8.17	124.38	120.30
3	D	19	LEU	CB-CG-CD1	8.17	124.88	111.00
1	A	591	ASP	CB-CG-OD2	8.15	125.63	118.30
1	B	601	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	25	TYR	CB-CG-CD2	-8.07	116.16	121.00
1	B	437	LEU	CB-CG-CD1	-8.04	97.32	111.00
3	D	93	LEU	CB-CG-CD2	8.02	124.63	111.00
1	A	2	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	644	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	203	LEU	CA-CB-CG	-7.87	97.20	115.30
1	A	434	LEU	CA-CB-CG	-7.87	97.20	115.30
3	F	117	ASP	CB-CG-OD2	7.83	125.35	118.30
1	B	502	ASP	CB-CG-OD2	7.80	125.32	118.30
1	B	455	LEU	CA-CB-CG	7.74	133.11	115.30
1	A	190	LYS	CD-CE-NZ	-7.70	94.00	111.70
3	F	187	ASP	CB-CG-OD2	7.65	125.19	118.30
1	A	248	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	522	ASP	CB-CG-OD2	7.60	125.14	118.30
3	D	11	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	250	LEU	CA-CB-CG	-7.51	98.02	115.30
2	E	194	LEU	CB-CG-CD2	-7.51	98.24	111.00
2	E	114	ASP	CB-CG-OD2	7.49	125.04	118.30
1	B	252	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	362	MET	CG-SD-CE	7.38	112.02	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	LEU	CB-CG-CD1	-7.38	98.46	111.00
3	D	69	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	B	683	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	330	LEU	CA-CB-CG	7.34	132.17	115.30
1	A	327	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	143	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	508	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	140	ASP	CB-CG-OD2	7.29	124.86	118.30
2	C	102	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	343	ARG	NE-CZ-NH2	7.27	123.93	120.30
3	D	69	ASP	CB-CG-OD2	7.22	124.80	118.30
1	B	69	ASP	CB-CG-OD1	-7.20	111.82	118.30
2	C	83	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	F	73	ASP	CB-CG-OD2	7.12	124.70	118.30
1	A	25	TYR	CB-CG-CD1	7.09	125.25	121.00
1	B	376	ARG	NE-CZ-NH1	7.07	123.83	120.30
3	F	143	VAL	CB-CA-C	-7.06	97.98	111.40
1	A	617	ARG	CG-CD-NE	7.06	126.62	111.80
2	E	230	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	A	206	LEU	CA-CB-CG	-7.05	99.08	115.30
1	B	481	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	187	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	A	36	ASP	CB-CG-OD2	7.00	124.60	118.30
2	E	230	ARG	NE-CZ-NH1	6.99	123.80	120.30
3	D	91	VAL	CB-CA-C	6.96	124.62	111.40
1	A	180	LEU	CA-CB-CG	6.95	131.29	115.30
3	F	175	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	169	TYR	N-CA-C	-6.91	92.35	111.00
2	E	230	ARG	CG-CD-NE	6.88	126.24	111.80
1	A	683	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	624	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	160	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	693	ARG	CG-CD-NE	-6.85	97.41	111.80
1	A	494	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	B	445	ASP	CB-CG-OD2	6.83	124.44	118.30
2	E	161	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	455	LEU	CB-CG-CD2	6.81	122.58	111.00
1	A	654	LEU	CA-CB-CG	-6.81	99.64	115.30
1	A	340	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	579	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	A	455	LEU	CB-CG-CD1	-6.79	99.46	111.00
1	B	254	TRP	CA-CB-CG	-6.78	100.81	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	564	LEU	CB-CG-CD1	-6.75	99.52	111.00
3	F	58	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	25	TYR	CA-CB-CG	6.70	126.14	113.40
2	C	16	ASP	N-CA-C	-6.70	92.92	111.00
2	C	67	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	693	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	203	LEU	CB-CG-CD2	-6.63	99.73	111.00
1	A	153	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	621	VAL	CB-CA-C	6.62	123.99	111.40
1	A	18	LYS	CD-CE-NZ	6.62	126.91	111.70
1	A	222	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	A	515	LEU	CB-CG-CD1	-6.57	99.84	111.00
2	E	70	ASP	CB-CG-OD2	6.55	124.20	118.30
1	B	568	MET	CG-SD-CE	6.50	110.61	100.20
2	C	39	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	291	LYS	CD-CE-NZ	6.49	126.62	111.70
1	B	406	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	275	GLN	CA-CB-CG	6.48	127.66	113.40
1	B	614	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	E	102	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	B	327	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	B	267	ASP	CB-CG-OD2	6.43	124.08	118.30
2	E	230	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	B	187	ARG	CG-CD-NE	-6.37	98.42	111.80
1	A	239	ASP	CB-CG-OD1	6.36	124.03	118.30
2	E	204	PRO	N-CD-CG	-6.33	93.70	103.20
1	A	74	SER	CB-CA-C	-6.33	98.08	110.10
1	B	644	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	B	216	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	79	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	106	TYR	N-CA-C	-6.29	94.03	111.00
3	D	46	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	30	CYS	CA-CB-SG	-6.28	102.69	114.00
1	B	616	TYR	CB-CG-CD2	-6.27	117.24	121.00
3	D	28	LEU	CA-CB-CG	6.26	129.69	115.30
3	F	175	ASP	CB-CG-OD1	6.26	123.93	118.30
3	D	93	LEU	CA-CB-CG	6.25	129.67	115.30
1	B	260	ASP	CB-CG-OD1	6.25	123.92	118.30
2	C	68	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	661	TRP	N-CA-CB	6.23	121.81	110.60
3	F	175	ASP	OD1-CG-OD2	-6.20	111.52	123.30
1	A	168	VAL	N-CA-C	-6.15	94.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	363	ILE	N-CA-C	-6.14	94.43	111.00
1	B	248	ASP	CB-CG-OD2	6.07	123.77	118.30
3	F	121	VAL	CG1-CB-CG2	-6.07	101.19	110.90
1	B	616	TYR	CB-CG-CD1	6.07	124.64	121.00
2	E	124	ASP	CB-CG-OD2	6.06	123.75	118.30
2	C	16	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	456	LYS	CD-CE-NZ	6.05	125.61	111.70
1	B	327	ASP	CB-CG-OD2	6.00	123.70	118.30
2	C	162	ARG	CG-CD-NE	5.99	124.38	111.80
1	A	70	THR	OG1-CB-CG2	-5.99	96.22	110.00
1	A	445	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	591	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	372	GLU	OE1-CD-OE2	-5.99	116.12	123.30
2	E	89	ASP	N-CA-C	-5.96	94.90	111.00
1	A	7	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	496	THR	OG1-CB-CG2	-5.94	96.34	110.00
1	A	189	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	267	ASP	CB-CG-OD2	5.87	123.58	118.30
3	D	187	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	564	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	B	544	SER	CB-CA-C	5.83	121.19	110.10
1	B	728	LYS	CD-CE-NZ	5.81	125.07	111.70
3	F	180	GLN	N-CA-CB	5.80	121.05	110.60
1	B	610	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	177	LEU	CA-CB-CG	5.79	128.61	115.30
2	C	43	LEU	CB-CG-CD1	-5.78	101.18	111.00
1	B	380	PRO	N-CD-CG	-5.78	94.54	103.20
3	D	133	GLY	N-CA-C	-5.78	98.66	113.10
1	B	601	ARG	CA-CB-CG	5.77	126.09	113.40
1	B	511	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	375	ARG	NE-CZ-NH2	-5.75	117.43	120.30
3	F	143	VAL	CG1-CB-CG2	5.74	120.08	110.90
3	F	139	VAL	CB-CA-C	-5.73	100.51	111.40
1	A	250	LEU	CB-CG-CD1	5.72	120.73	111.00
3	F	46	ASP	CB-CA-C	-5.71	98.97	110.40
1	B	123	PRO	N-CD-CG	-5.71	94.64	103.20
2	C	89	ASP	CB-CG-OD2	5.71	123.44	118.30
3	F	71	ASP	CB-CG-OD2	5.71	123.44	118.30
2	E	15	GLU	N-CA-C	-5.70	95.62	111.00
1	A	272	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	A	333	LYS	CD-CE-NZ	-5.69	98.61	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	182	ILE	CB-CA-C	-5.69	100.23	111.60
3	F	188	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	A	365	THR	OG1-CB-CG2	-5.68	96.94	110.00
1	B	53	TRP	N-CA-C	-5.67	95.68	111.00
1	A	348	CYS	CA-CB-SG	-5.67	103.80	114.00
2	C	231	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	B	189	ASP	CB-CG-OD1	5.66	123.39	118.30
3	D	106	LEU	CA-CB-CG	5.66	128.31	115.30
2	E	107	VAL	CG1-CB-CG2	-5.65	101.86	110.90
2	E	232	MET	CA-CB-CG	5.65	122.91	113.30
1	A	637	SER	CB-CA-C	5.64	120.82	110.10
1	B	502	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	B	164	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	133	LEU	CB-CG-CD2	-5.62	101.44	111.00
2	E	169	LEU	CB-CG-CD1	-5.62	101.45	111.00
2	E	76	CYS	CA-CB-SG	-5.61	103.89	114.00
2	C	138	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	B	196	GLU	N-CA-CB	5.59	120.66	110.60
3	D	52	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	A	456	LYS	CB-CA-C	5.59	121.58	110.40
1	B	494	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	610	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	23	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	317	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	A	581	LEU	CB-CG-CD1	-5.58	101.52	111.00
3	D	143	VAL	CB-CA-C	-5.57	100.81	111.40
3	F	30	LYS	CA-CB-CG	5.57	125.66	113.40
1	B	640	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	A	225	VAL	CB-CA-C	-5.55	100.86	111.40
1	B	311	THR	CA-CB-CG2	5.54	120.16	112.40
2	C	194	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	B	584	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	A	254	TRP	CA-CB-CG	-5.53	103.19	113.70
2	C	5	VAL	CB-CA-C	-5.53	100.90	111.40
1	A	141	LEU	CB-CG-CD2	5.52	120.39	111.00
1	A	222	ARG	CB-CA-C	5.52	121.43	110.40
3	D	14	LEU	CA-CB-CG	-5.50	102.66	115.30
1	B	363	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	A	674	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	406	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	C	124	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	341	ASP	CB-CG-OD1	5.46	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	LEU	CA-CB-CG	-5.45	102.77	115.30
1	A	187	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	E	16	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	248	ASP	OD1-CG-OD2	-5.42	113.00	123.30
1	B	484	ILE	CG1-CB-CG2	-5.41	99.50	111.40
1	A	718	MET	CG-SD-CE	5.41	108.85	100.20
1	B	250	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	A	652	ASN	N-CA-CB	5.40	120.31	110.60
1	B	70	THR	OG1-CB-CG2	-5.39	97.59	110.00
2	E	236	GLU	N-CA-C	5.38	125.52	111.00
3	F	170	VAL	CG1-CB-CG2	5.36	119.47	110.90
1	A	273	PHE	CB-CA-C	-5.35	99.70	110.40
2	E	164	LEU	CB-CG-CD1	5.35	120.09	111.00
1	B	177	LEU	CB-CG-CD2	5.34	120.08	111.00
2	C	148	ASP	CB-CG-OD2	5.34	123.11	118.30
2	E	114	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	B	131	GLU	N-CA-C	-5.34	96.59	111.00
1	A	711	ILE	CB-CA-C	-5.33	100.93	111.60
1	A	316	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	680	LEU	CB-CG-CD1	5.31	120.03	111.00
2	E	32	MET	CB-CG-SD	5.30	128.31	112.40
1	B	348	CYS	CA-CB-SG	-5.30	104.46	114.00
3	D	150	THR	N-CA-C	-5.29	96.71	111.00
1	A	513	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	452	THR	OG1-CB-CG2	-5.29	97.84	110.00
1	A	363	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	B	688	GLY	N-CA-C	-5.24	99.99	113.10
2	C	14	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	A	95	LYS	CD-CE-NZ	5.24	123.76	111.70
1	B	601	ARG	CD-NE-CZ	5.24	130.94	123.60
2	C	149	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	B	525	LYS	CD-CE-NZ	5.23	123.73	111.70
2	C	14	GLU	CA-CB-CG	-5.21	101.94	113.40
2	C	161	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	F	179	VAL	CB-CA-C	-5.20	101.53	111.40
1	B	463	LEU	N-CA-C	5.19	125.02	111.00
3	F	168	SER	N-CA-CB	5.18	118.28	110.50
1	B	718	MET	CG-SD-CE	-5.18	91.92	100.20
2	E	43	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	A	15	ILE	CG1-CB-CG2	5.17	122.78	111.40
1	A	153	ASP	OD1-CG-OD2	-5.17	113.48	123.30
1	A	226	ASP	N-CA-C	-5.16	97.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	343	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	E	194	LEU	CA-CB-CG	-5.15	103.45	115.30
1	A	580	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	E	74	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	37	LYS	CD-CE-NZ	5.13	123.50	111.70
3	F	132	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	139	MET	CG-SD-CE	-5.12	92.00	100.20
2	E	73	LEU	CA-CB-CG	-5.12	103.53	115.30
1	B	515	LEU	CB-CG-CD2	-5.11	102.31	111.00
2	C	70	ASP	CB-CG-OD2	5.11	122.90	118.30
3	F	34	ASP	CB-CG-OD2	5.11	122.90	118.30
3	D	6	ILE	N-CA-C	-5.10	97.23	111.00
2	E	173	GLU	N-CA-C	-5.08	97.28	111.00
1	B	534	LEU	CA-CB-CG	-5.08	103.62	115.30
3	D	132	ARG	CA-CB-CG	5.08	124.57	113.40
1	B	458	ASN	N-CA-CB	5.07	119.73	110.60
1	A	69	ASP	OD1-CG-OD2	-5.06	113.68	123.30
2	E	86	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	502	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	461	SER	N-CA-C	-5.05	97.36	111.00
1	A	454	LEU	CB-CG-CD2	5.04	119.57	111.00
1	A	63	ILE	CG1-CB-CG2	-5.04	100.31	111.40
1	A	222	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	647	GLU	C-N-CA	-5.04	109.11	121.70
1	B	498	CYS	CA-CB-SG	5.03	123.05	114.00
1	A	200	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	674	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	491	TRP	CA-CB-CG	-5.01	104.18	113.70
1	B	340	ASP	CB-CG-OD2	5.01	122.81	118.30
2	C	72	SER	CA-CB-OG	-5.01	97.67	111.20
2	E	29	ASP	CB-CA-C	5.01	120.42	110.40
1	A	191	TYR	CA-CB-CG	-5.01	103.89	113.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	MET	Peptide
1	A	320	CYS	Peptide
1	A	539	TYR	Peptide
1	A	66	GLU	Peptide
1	B	139	MET	Peptide

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Mol	Chain	Res	Type	Group
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 (i)

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	505	0
1	B	5676	0	5424	519	0
2	C	1749	0	1722	121	0
2	E	1751	0	1716	129	0
3	D	1354	0	1311	85	0
3	F	1376	0	1358	129	0
4	A	31	0	18	5	0
4	B	31	0	18	6	0
5	A	27	0	12	6	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	1402	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 40.

All (1402) 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
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: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:A:139:MET:HE3	1:A:147:VAL:HG21	1.43	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:A:195:LEU:HD23	1:A:246:MET:HE1	1.46	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:24:PHE:CE2	1:A:306:MET:SD	2.63	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: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: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
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:B:26:GLN:NE2	1:B:48:LYS:HZ3	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:692:ALA:O	1:A:693:ARG:C	2.13	0.85
1:A:589:LEU:HD22	1:A:592:HIS:ND1	1.91	0.85
2:C:31:MET:HE2	2:C:33:TYR:OH	1.76	0.85
1:B:589:LEU:HD23	1:B:592:HIS:CG	2.10	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
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:B:26:GLN:HE21	1:B:48:LYS:HZ3	0.87	0.83
1:A:195:LEU:HD23	1:A:246:MET:HE3	1.60	0.82
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:711:ILE:HG12	1:A:712:ALA:N	1.98	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
2:C:226:MET:HE2	3:D:111:GLY:HA2	1.64	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: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: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
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:350:VAL:O	1:B:353:SER:OG	2.02	0.76
1:A:419:ASP:OD1	5:A:1731:ADP:O2'	2.02	0.76
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:B:26:GLN:NE2	1:B:48:LYS:NZ	2.31	0.75
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
2:E:1:MET:HB2	2:E:1:MET:HE3	1.67	0.75
2:C:136:SER:OG	3:D:109:LYS:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:660:GLU:HB3	1:A:663:GLU:CD	2.08	0.73
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
1:A:164:ASP:C	1:A:165:ILE:HG13	2.09	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
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: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
2:E:7:VAL:O	7:E:1237:AMP:C2	2.43	0.72
1:A:287:LYS:O	1:A:289:VAL:N	2.23	0.72
1:A:35:SER:HG	1:A:76:ARG:H	1.35	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
1:B:55:ALA:C	1:B:56:LEU:HD13	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:276:GLN:HE22	1:B:301:THR:H	1.40	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:B:68:ASP:OD2	1:B:68:ASP:C	2.30	0.69
2:C:226:MET:HE2	3:D:111:GLY:CA	2.23	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
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: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
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
2:C:125:GLN:O	2:C:126:ALA:C	2.30	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:226:MET:CE	3:F:148:LYS:HZ3	2.06	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:167:TYR:CD1	1:A:222:ARG:HB2	2.29	0.67
1:A:195:LEU:CD2	1:A:246:MET:HE3	2.22	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
1:B:330:LEU:C	1:B:330:LEU:HD23	2.15	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
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:C:1:MET:HB2	2:C:1:MET:HE2	1.77	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: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
3:F:102:TYR:O	3:F:103:ALA:C	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:195:LEU:CD2	1:A:246:MET:HE1	2.24	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:B:374:TYR:CE1	1:B:707:LYS:HD2	2.31	0.64
2:E:45:GLU:O	2:E:48:LYS:HB2	1.97	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
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
1:B:367:ASN:OD1	1:B:367:ASN:C	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:136:SER:CB	3:D:109:LYS:HZ2	2.12	0.63
2:C:230:ARG:HH22	3:D:124:GLN:CD	2.01	0.63
3:F:46:ASP:C	3:F:48:PHE:H	2.00	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:A:22:ASN:OD1	1:A:22:ASN:C	2.36	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: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
1:B:699:ASN:OD1	1:B:701:GLN:HB3	1.99	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:B:264:TRP:CH2	1:B:352:ILE:CD1	2.83	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:598:GLU:HB2	1:A:601:ARG:HG3	1.81	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
1:B:398:GLY:O	1:B:399:PRO:C	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLY:HA2	1:A:300:TYR:CE1	2.34	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: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:350:VAL:O	1:A:353:SER:OG	2.10	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
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
1:B:295:LEU:C	1:B:295:LEU:HD12	2.21	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
2:E:1:MET:HB2	2:E:1:MET:HE2	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:A:222:ARG:HG3	1:A:255:ASP:CG	2.22	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
1:A:329:PHE:O	1:A:330:LEU:C	2.40	0.60
2:E:226:MET:CE	3:F:148:LYS:NZ	2.65	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:B:352:ILE:HG13	4:B:1730:FMN:HM82	1.84	0.60
2:C:69:VAL:O	2:C:72:SER:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:287:LYS:O	1:A:288:GLN:C	2.39	0.60
1:B:34:GLY:HA2	1:B:59:GLU:OE2	2.02	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:A:679:ARG:C	1:A:680:LEU:O	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
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:A:367:ASN:OD1	1:A:367:ASN:C	2.39	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: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: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
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:B:441:SER:O	1:B:444:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:87:LYS:O	1:A:88:ALA:C	2.42	0.59
1:A:202:TRP:CD1	1:A:206:LEU:CD1	2.86	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
1:B:492:ASN:ND2	1:B:643:GLY:C	2.56	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:571:THR:C	1:A:572:LEU:HG	2.23	0.58
1:A:619:PRO:HG3	1:B:237:GLU:HB3	1.82	0.58
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
3:D:71:ASP:OD1	3:D:74:VAL:HG23	2.02	0.58
2:E:226:MET:HE3	3:F:148:LYS:NZ	2.17	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:59:GLU:O	1:B:60:TYR:C	2.39	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
1:B:517:PRO:O	1:B:521:MET:HE2	2.04	0.58
2:C:69:VAL:O	2:C:70:ASP:C	2.41	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
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
3:F:46:ASP:C	3:F:48:PHE:N	2.57	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
1:A:443:HIS:ND1	1:A:443:HIS:C	2.57	0.57
2:E:19:ILE:HD11	2:E:233:TYR:HA	1.86	0.57
1:A:568:MET:O	1:A:569:HIS:C	2.43	0.57
1:A:681:ILE:O	1:A:682:ALA:C	2.41	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:96:ASP:OD1	2:E:96:ASP:C	2.42	0.57
1:A:14:GLN:NE2	1:A:16:GLY:O	2.38	0.57
1:B:497:ASN:OD1	1:B:499:LEU:HB2	2.04	0.57
2:C:88:TRP:CG	2:C:89:ASP:N	2.68	0.57
1:A:409:MET:HE3	1:A:454:LEU:CB	2.35	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
1:B:690:ARG:O	1:B:691:VAL:C	2.39	0.57
2:C:36:ASN:HB3	2:C:39:ASP:OD2	2.05	0.57
2:E:35:LEU:O	2:E:36:ASN:C	2.44	0.56
2:E:226:MET:HE3	3:F:148:LYS:HZ3	1.69	0.56
1:A:568:MET:HE3	1:A:573:GLU:OE1	2.05	0.56
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
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:183:TYR:O	1:A:186:LYS:NZ	2.30	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:22:ASN:OD1	1:B:22:ASN:C	2.43	0.56
2:C:2:LYS:CE	2:C:111:GLU:OE1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:213:ILE:HG13	2:C:215:LEU:HD12	1.85	0.56
1:A:540:PHE:C	1:A:540:PHE:CD2	2.80	0.55
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
1:A:280:ILE:O	1:A:281:PRO:C	2.44	0.55
2:E:226:MET:HE2	3:F:148:LYS:HZ3	1.71	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: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
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: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:1:MET:HB2	2:C:1:MET:HE3	1.86	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
3:D:93:LEU:CD1	3:D:102:TYR:OH	2.55	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
1:B:571:THR:C	1:B:572:LEU:HG	2.27	0.54
2:C:144:ALA:C	2:C:145:VAL:HG23	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:LEU:C	2:E:4:LEU:HD23	2.27	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:20:ARG:C	2:C:22:ASP:N	2.60	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:674:ASP:OD1	5:B:1731:ADP:O1B	2.26	0.54
1:B:692:ALA:O	1:B:693:ARG:C	2.45	0.54
2:E:172:VAL:HG12	3:F:183:SER:HB2	1.89	0.54
1:B:263:GLU:C	1:B:265:GLY:H	2.09	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:A:398:GLY:O	1:A:399:PRO:C	2.45	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
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:A:568:MET:HE2	1:A:573:GLU:HB3	1.90	0.54
1:A:629:SER:O	1:A:630:HIS:C	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:C:42:SER:O	2:C:43:LEU:C	2.46	0.53
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
1:B:321:ALA:O	1:B:322:ARG:C	2.47	0.53
1:B:430:GLN:O	1:B:431:VAL:C	2.45	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:B:131:GLU:O	1:B:133:LEU:N	2.42	0.53
1:B:540:PHE:C	1:B:543:PRO:HD2	2.28	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: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:564:LEU:O	1:B:565:ALA:HB3	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:174:TYR:O	1:A:175:LEU:C	2.47	0.52
1:B:174:TYR:O	1:B:175:LEU:C	2.47	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:89:MET:SD	1:A:89:MET:C	2.88	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
3:F:46:ASP:N	3:F:62:VAL:HG11	2.24	0.52
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
2:E:125:GLN:O	2:E:126:ALA:C	2.47	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
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:B:706:TYR:O	1:B:707:LYS:C	2.46	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
2:E:116:VAL:HG12	2:E:179:VAL:HG13	1.91	0.52
1:A:287:LYS:C	1:A:289:VAL:N	2.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:ARG:O	2:C:22:ASP:N	2.43	0.52
1:A:542:ALA:CB	1:A:543:PRO:CD	2.88	0.51
1:B:434:LEU:O	1:B:435:PRO:C	2.45	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:A:409:MET:HE3	1:A:454:LEU:HB2	1.92	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
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
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:A:700:PRO:O	1:A:701:GLN:C	2.47	0.51
1:B:671:LEU:CD2	1:B:676:GLU:HA	2.39	0.51
1:B:683:ASP:O	1:B:684:ALA:C	2.47	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:542:ALA:O	1:B:543:PRO:C	2.47	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:322:ARG:O	1:B:323:PRO:C	2.47	0.50
2:C:226:MET:CE	3:D:111:GLY:CA	2.89	0.50
1:A:535:ASN:HD21	1:A:537:ASP:H	1.56	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
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
1:B:90:THR:O	1:B:91:ASP:C	2.50	0.50
1:B:302:ASP:OD2	1:B:303:PRO:N	2.45	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
3:F:79:VAL:C	3:F:82:LEU:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:216:SER:O	2:C:217:ALA:C	2.51	0.49
3:F:51:ALA:O	3:F:54:VAL:HG13	2.11	0.49
1:B:42:SER:O	1:B:43:ALA:C	2.47	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
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:362:MET:HE2	1:B:370:ALA:HB1	1.94	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:B:303:PRO:O	1:B:306:MET:HB2	2.12	0.49
1:B:568:MET:O	1:B:569:HIS:C	2.50	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:568:MET:CE	1:A:573:GLU:OE1	2.60	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: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:B:210:LYS:O	1:B:211:HIS:C	2.50	0.49
1:B:269:GLY:O	1:B:299:ARG:NH2	2.45	0.49
3:D:37:VAL:HB	3:D:59:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:6:HIS:NE2	1:A:304:GLU:OE1	2.46	0.49
1:A:139:MET:HE2	1:A:147:VAL:HG21	1.90	0.49
1:A:386:THR:HB	1:A:413:TYR:CZ	2.48	0.49
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:CG	1:B:332:GLN:O	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
3:D:75:PHE:O	3:D:76:GLU:C	2.51	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: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:456:LYS:CD	1:A:456:LYS:NZ	2.76	0.48
1:B:87:LYS:O	1:B:88:ALA:C	2.52	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:A:669:ILE:C	1:A:670:TYR:CD1	2.87	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
1:A:148:GLN:O	1:A:149:GLN:C	2.49	0.48
1:A:424:ILE:CD1	1:A:448:GLU:HA	2.43	0.48
1:A:582:HIS:O	1:A:583:GLU:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:6:ILE:HB	3:F:93:LEU:HD12	1.95	0.48
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
1:B:718:MET:HG3	1:B:719:PRO:N	2.27	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:405:ALA:O	1:B:406:ARG:C	2.49	0.48
1:B:714:GLY:HA2	1:B:723:PHE:CG	2.49	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
1:B:468:LYS:O	1:B:469:PRO:C	2.51	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:171:ALA:O	1:A:172:HIS:C	2.52	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: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:B:450:GLN:O	1:B:454:LEU:HD12	2.14	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:194:SER:O	1:B:195:LEU:C	2.52	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)
1:A:148:GLN:O	1:A:151:TYR:HB2	2.14	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:D:99:SER:C	3:D:101:GLY:H	2.17	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
3:D:99:SER:C	3:D:101:GLY:N	2.67	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: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: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: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: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: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
1:B:403:GLU:O	1:B:404:ALA:C	2.50	0.47
1:B:578:MET:O	1:B:579:ARG:C	2.51	0.47
2:C:173:GLU:O	3:D:183:SER:HA	2.15	0.47
3:D:99:SER:O	3:D:100:LEU:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:660:GLU:HA	1:A:663:GLU:HG3	1.97	0.47
1:B:280:ILE:O	1:B:283:VAL:N	2.47	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:A:290:SER:OG	1:A:291:LYS:N	2.47	0.46
2:E:143:ALA:HB1	2:E:160:ILE:CD1	2.45	0.46
1:A:77:ILE:HG23	1:A:77:ILE:O	2.15	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
2:E:111:GLU:O	2:E:112:ALA:C	2.51	0.46
3:F:40:VAL:HG11	3:F:45:ALA:O	2.15	0.46
1:A:414:THR:O	1:A:414:THR:HG22	2.15	0.46
1:A:676:GLU:CD	1:B:119:THR:HG21	2.36	0.46
1:B:27:VAL:HG21	1:B:222:ARG:NH1	2.30	0.46
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:407:VAL:CG2	1:B:689:HIS:CE1	2.98	0.46
1:B:568:MET:HE2	1:B:573:GLU:HB3	1.98	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:184:GLN:O	3:F:185:ASN:C	2.54	0.46
1:A:72:ARG:HD2	1:A:355:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:317:ILE:HG22	1:B:318:ILE:N	2.31	0.46
2:C:35:LEU:O	2:C:36:ASN:C	2.52	0.46
1:A:87:LYS:NZ	1:A:91:ASP:OD2	2.42	0.46
1:A:463:LEU:HG	1:A:464:ALA:N	2.30	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: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
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
1:B:598:GLU:O	1:B:599:PRO:C	2.54	0.46
1:B:692:ALA:C	1:B:694:GLU:N	2.68	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
1:A:55:ALA:O	1:A:56:LEU:HD13	2.16	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
1:B:545:LEU:O	1:B:546:ALA:C	2.54	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
3:D:135:TYR:O	3:D:136:ASN:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:60:VAL:HG13	2:C:60:VAL:O	2.16	0.45
3:D:144:ASP:OD1	3:D:144:ASP:C	2.55	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: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:568:MET:HE3	1:A:573:GLU:CB	2.46	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
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
3:F:22:ILE:O	3:F:23:GLY:C	2.55	0.45
1:A:51:GLY:HA2	1:A:329:PHE:CD2	2.52	0.45
1:A:51:GLY:HA2	1:A:329:PHE:CE2	2.52	0.45
1:A:322:ARG:O	1:A:323:PRO:C	2.54	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:679:ARG:C	1:B:680:LEU:O	2.54	0.45
2:E:111:GLU:O	2:E:112:ALA:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ARG:O	1:A:691:VAL:C	2.54	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
2:E:69:VAL:O	2:E:70:ASP:C	2.53	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:62:VAL:HG12	2:C:63:SER:N	2.32	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: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:434:LEU:O	1:A:435:PRO:C	2.55	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
1:A:348:CYS:SG	6:A:1732:SF4:S1	3.15	0.44
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
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:265:GLY:O	1:A:268:ALA:C	2.55	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:568:MET:HE3	1:B:573:GLU:CB	2.47	0.44
1:B:713:TRP:CE2	1:B:723:PHE:HE2	2.33	0.44
3:D:16:PRO:C	3:D:18:SER:N	2.71	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
2:C:96:ASP:OD1	2:C:96:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:21:LEU:HD11	3:D:93:LEU:C	2.37	0.44
3:F:70:PHE:C	3:F:70:PHE:CD2	2.91	0.44
1:A:203:LEU:HA	1:A:203:LEU:HD23	1.13	0.44
1:A:287:LYS:C	1:A:289:VAL:H	2.21	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
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:76:GLU:O	3:D:77:ALA:C	2.52	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:A:354:ARG:O	1:A:355:TRP:C	2.55	0.44
1:B:352:ILE:HG21	1:B:352:ILE:HD13	1.50	0.44
1:B:704:ILE:C	1:B:705:PRO:O	2.54	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
1:B:517:PRO:O	1:B:521:MET:CE	2.66	0.44
3:F:75:PHE:O	3:F:76:GLU:C	2.56	0.44
1:A:391:SER:H	1:A:481:ASP:HB2	1.82	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:695:ILE:CG2	1:B:696:GLU:HG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:PHE:HA	3:D:152:VAL:O	2.17	0.44
2:E:144:ALA:C	2:E:145:VAL:HG23	2.37	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
2:C:226:MET:HE2	3:D:111:GLY:C	2.39	0.43
3:F:144:ASP:CG	3:F:146:PRO:HD3	2.39	0.43
1:A:376:ARG:O	1:A:377:GLY:C	2.55	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
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: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: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:A:679:ARG:O	1:A:680:LEU:C	2.56	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
1:A:86:LEU:O	1:A:87:LYS:C	2.55	0.43
1:A:175:LEU:O	1:A:176:PRO:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ASN:O	1:B:567:TYR:C	2.56	0.43
2:C:13:LEU:HD22	2:C:26:VAL:HG11	2.00	0.43
3:D:24:ALA:O	3:D:25:ALA:C	2.57	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:102:TYR:O	3:D:103:ALA:C	2.55	0.43
1:A:290:SER:OG	1:A:292:LYS:N	2.43	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: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:A:700:PRO:C	1:A:702:ILE:H	2.23	0.42
1:B:263:GLU:C	1:B:265:GLY:N	2.72	0.42
1:B:330:LEU:C	1:B:330:LEU:CD2	2.87	0.42
1:B:539:TYR:CE2	1:B:540:PHE:HB3	2.54	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: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:349:ASN:O	1:B:350:VAL:C	2.48	0.42
1:B:672:ILE:O	1:B:672:ILE:HG13	2.16	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:B:532:VAL:HG11	1:B:602:MET:SD	2.59	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
3:F:173:ASN:C	3:F:174:VAL:CG1	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:MET:CE	3:F:11:ARG:HD2	2.50	0.42
1:A:79:ASP:OD1	1:A:79:ASP:C	2.56	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:A:545:LEU:O	1:A:546:ALA:C	2.58	0.42
1:A:700:PRO:C	1:A:702:ILE:N	2.71	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:325:ILE:CD1	1:A:362:MET:SD	3.08	0.42
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:568:MET:C	1:B:570:PHE:N	2.72	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:171:ALA:O	1:B:172:HIS:C	2.58	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
2:E:100:VAL:O	2:E:101:GLY:C	2.56	0.42
3:F:10:ARG:O	3:F:11:ARG:C	2.59	0.42
3:F:17:VAL:HG23	3:F:20:GLU:OE1	2.19	0.42
1:A:13:ILE:HG23	1:A:20:LEU:HD12	2.02	0.42
1:A:33:ALA:O	1:A:34:GLY:C	2.58	0.42
1:A:496:THR:O	1:A:642:THR:OG1	2.19	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
1:B:443:HIS:O	1:B:443:HIS:CG	2.72	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:42:SER:O	1:A:43:ALA:C	2.58	0.41
1:A:56:LEU:HD23	1:A:93:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:302:ASP:OD2	1:B:302:ASP:C	2.57	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
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: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
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
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:A:468:LYS:O	1:A:469:PRO:C	2.58	0.41
1:B:152:VAL:O	1:B:153:ASP:C	2.57	0.41
1:B:185:ASN:CG	1:B:187:ARG:HG3	2.38	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
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:29:HIS:ND1	1:B:29:HIS:C	2.73	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
1:B:681:ILE:O	1:B:682:ALA:C	2.58	0.41
2:C:62:VAL:CG1	2:C:63:SER:N	2.84	0.41
2:C:144:ALA:HB2	3:D:101:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:THR:CA	2:E:124:ASP:OD2	2.68	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: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
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
2:E:221:GLY:O	2:E:222:ALA:C	2.58	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:169:TYR:C	1:A:169:TYR:CD2	2.93	0.41
1:A:282:TRP:CH2	1:B:614:ARG:NE	2.89	0.41
2:E:64:VAL:CG2	2:E:87:VAL:HB	2.36	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: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: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: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
1:B:686:PHE:C	1:B:688:GLY:H	2.23	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
2:C:221:GLY:C	2:C:223:ALA:N	2.74	0.41
3:D:16:PRO:C	3:D:18:SER:H	2.23	0.41
3:D:45:ALA:CB	3:D:62:VAL:HG13	2.50	0.41
3:D:72:PRO:O	3:D:73:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:530:ARG:HH11	1:A:634:GLU:CB	2.34	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:502:ASP:HB3	1:B:503:PRO:HD2	2.01	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:40:PHE:C	1:A:40:PHE:CD2	2.91	0.40
1:A:269:GLY:HA2	1:A:270:PRO:HD2	1.83	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
3:D:58:ASP:O	3:D:59:GLU:CG	2.69	0.40
2:E:42:SER:O	2:E:43:LEU:C	2.57	0.40
1:A:419:ASP:CG	5:A:1731:ADP:O2'	2.60	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: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: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: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
2:C:44:GLU:O	2:C:45:GLU:C	2.58	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: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:704:ILE:O	1:B:705:PRO:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:226:MET:HE2	3:F:148:LYS:NZ	2.32	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%)	5	33
1	B	727/729 (100%)	614 (84%)	98 (14%)	15 (2%)	7	38
2	C	227/264 (86%)	202 (89%)	21 (9%)	4 (2%)	8	41
2	E	234/264 (89%)	210 (90%)	14 (6%)	10 (4%)	2	24
3	D	187/320 (58%)	153 (82%)	24 (13%)	10 (5%)	2	21
3	F	187/320 (58%)	162 (87%)	18 (10%)	7 (4%)	3	28
All	All	2289/2626 (87%)	1965 (86%)	258 (11%)	66 (3%)	4	32

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%)	537 (92%)	47 (8%)	12	42
1	B	578/602 (96%)	527 (91%)	51 (9%)	10	38
2	C	180/216 (83%)	167 (93%)	13 (7%)	14	45
2	E	177/216 (82%)	161 (91%)	16 (9%)	9	37
3	D	143/258 (55%)	123 (86%)	20 (14%)	3	20
3	F	150/258 (58%)	139 (93%)	11 (7%)	14	44
All	All	1812/2152 (84%)	1654 (91%)	158 (9%)	10	38

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	25	TYR
1	A	26	GLN
1	A	36	ASP
1	A	40	PHE
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	169	TYR
1	A	176	PRO
1	A	177	LEU
1	A	206	LEU
1	A	260	ASP
1	A	267	ASP
1	A	284	LYS
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	414	THR
1	A	415	VAL
1	A	444	ARG
1	A	515	LEU
1	A	537	ASP
1	A	571	THR
1	A	572	LEU
1	A	580	ARG
1	A	581	LEU
1	A	589	LEU
1	A	593	PHE
1	A	594	CYS
1	A	595	SER
1	A	629	SER
1	A	631	ARG
1	A	650	LEU
1	A	660	GLU
1	A	663	GLU
1	A	667	LYS

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Mol	Chain	Res	Type
1	A	679	ARG
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	40	PHE
1	B	41	GLN
1	B	56	LEU
1	B	60	TYR
1	B	84	ARG
1	B	104	LEU
1	B	106	TYR
1	B	134	SER
1	B	142	SER
1	B	158	SER
1	B	169	TYR
1	B	187	ARG
1	B	203	LEU
1	B	216	ASP
1	B	278	HIS
1	B	304	GLU
1	B	322	ARG
1	B	351	CYS
1	B	356	GLU
1	B	362	MET
1	B	389	LYS
1	B	414	THR
1	B	437	LEU
1	B	444	ARG
1	B	447	ARG
1	B	461	SER
1	B	487	THR
1	B	490	ARG
1	B	493	THR
1	B	497	ASN
1	B	539	TYR
1	B	541	MET
1	B	544	SER
1	B	589	LEU
1	B	594	CYS

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Mol	Chain	Res	Type
1	B	596	ARG
1	B	613	LYS
1	B	615	THR
1	B	619	PRO
1	B	621	VAL
1	B	631	ARG
1	B	640	LEU
1	B	650	LEU
1	B	657	ARG
1	B	660	GLU
1	B	661	TRP
1	B	667	LYS
1	B	679	ARG
2	C	1	MET
2	C	32	MET
2	C	89	ASP
2	C	110	LYS
2	C	150	GLN
2	C	156	ASN
2	C	157	LYS
2	C	171	GLU
2	C	199	GLN
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	75	PHE
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	132	ARG
3	D	138	LYS

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Mol	Chain	Res	Type
3	D	149	SER
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	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	150	GLN
2	E	156	ASN
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	49	VAL
3	F	60	LEU
3	F	83	ILE
3	F	91	VAL
3	F	99	SER
3	F	141	VAL
3	F	154	THR
3	F	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	241	GLN
1	A	332	GLN
1	A	501	HIS
1	A	535	ASN
1	A	554	HIS
1	A	563	HIS

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Mol	Chain	Res	Type
1	A	569	HIS
1	A	630	HIS
1	A	717	HIS
1	B	26	GLN
1	B	276	GLN
1	B	429	ASN
1	B	501	HIS
1	B	554	HIS
1	B	563	HIS
1	B	652	ASN
2	C	121	GLN
2	C	125	GLN
2	C	150	GLN
2	C	170	GLN
2	C	175	ASN
2	C	183	GLN
2	C	199	GLN
3	D	26	ASN
3	D	44	GLN
3	D	124	GLN
3	D	137	GLN
3	D	180	GLN
2	E	150	GLN
2	E	170	GLN
2	E	175	ASN
2	E	183	GLN
3	F	26	ASN
3	F	124	GLN
3	F	137	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 monosaccharides 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	$\#\|Z\| > 2$
6	SF4	A	1732	1	0,12,12	-	-	-		
4	FMN	B	1730	1	33,33,33	1.68	4 (12%)	48,50,50	2.44	23 (47%)
7	AMP	C	1236	-	22,25,25	2.01	7 (31%)	25,38,38	3.15	14 (56%)
5	ADP	B	1731	-	24,29,29	1.58	4 (16%)	29,45,45	2.43	9 (31%)
5	ADP	A	1731	-	24,29,29	1.83	7 (29%)	29,45,45	2.33	11 (37%)
6	SF4	B	1732	1	0,12,12	-	-	-		
7	AMP	E	1237	-	22,25,25	2.30	6 (27%)	25,38,38	2.92	11 (44%)
4	FMN	A	1730	1	33,33,33	1.67	6 (18%)	48,50,50	2.48	17 (35%)

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
4	FMN	B	1730	1	-	1/18/18/18	0/3/3/3
6	SF4	A	1732	1	-	-	0/6/5/5
7	AMP	C	1236	-	-	3/6/26/26	0/3/3/3
5	ADP	B	1731	-	-	3/12/32/32	0/3/3/3
5	ADP	A	1731	-	-	4/12/32/32	0/3/3/3
6	SF4	B	1732	1	-	-	0/6/5/5
7	AMP	E	1237	-	-	3/6/26/26	0/3/3/3
4	FMN	A	1730	1	-	7/18/18/18	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1237	AMP	C2-N3	5.37	1.40	1.32
4	B	1730	FMN	C4A-N5	5.24	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1237	AMP	C2'-C1'	-5.04	1.46	1.53
4	A	1730	FMN	C4A-N5	5.01	1.40	1.30
7	E	1237	AMP	C4-N3	4.99	1.42	1.35
5	A	1731	ADP	C2-N3	4.57	1.39	1.32
7	C	1236	AMP	C2-N3	4.39	1.39	1.32
5	A	1731	ADP	C2'-C1'	-4.34	1.47	1.53
5	B	1731	ADP	O4'-C4'	-4.06	1.35	1.45
4	B	1730	FMN	C10-N1	3.86	1.41	1.33
5	A	1731	ADP	C2-N1	3.67	1.40	1.33
4	A	1730	FMN	C10-N1	3.62	1.40	1.33
7	C	1236	AMP	O4'-C4'	-3.59	1.37	1.45
5	B	1731	ADP	C2-N3	3.58	1.37	1.32
7	C	1236	AMP	C2-N1	3.41	1.40	1.33
5	B	1731	ADP	C2'-C1'	-3.35	1.48	1.53
7	C	1236	AMP	C4-N3	3.34	1.40	1.35
7	E	1237	AMP	P-O1P	3.22	1.60	1.50
4	B	1730	FMN	C2'-C3'	3.19	1.59	1.53
7	C	1236	AMP	C2'-C1'	-3.01	1.49	1.53
7	C	1236	AMP	O3'-C3'	-2.82	1.36	1.43
4	A	1730	FMN	C2-N3	2.68	1.45	1.39
7	E	1237	AMP	C2-N1	2.67	1.38	1.33
7	C	1236	AMP	C2'-C3'	-2.65	1.46	1.53
4	A	1730	FMN	C9-C9A	-2.56	1.35	1.39
5	B	1731	ADP	C2-N1	2.48	1.38	1.33
5	A	1731	ADP	O4'-C4'	-2.43	1.39	1.45
7	E	1237	AMP	O4'-C4'	-2.41	1.39	1.45
4	A	1730	FMN	C4'-C3'	2.28	1.57	1.53
5	A	1731	ADP	O2'-C2'	-2.06	1.38	1.43
5	A	1731	ADP	C6-C5	-2.06	1.35	1.43
5	A	1731	ADP	PB-O3B	-2.05	1.46	1.54
4	A	1730	FMN	C9-C8	-2.05	1.36	1.39
4	B	1730	FMN	P-O5'	2.04	1.66	1.60

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1730	FMN	C8M-C8-C9	-8.08	104.55	119.49
7	E	1237	AMP	N3-C2-N1	-7.87	116.38	128.68
5	B	1731	ADP	N3-C2-N1	-7.01	117.73	128.68
7	C	1236	AMP	O3'-C3'-C2'	-7.00	89.16	111.82
5	A	1731	ADP	O2'-C2'-C1'	-6.37	87.33	110.85
5	B	1731	ADP	PA-O3A-PB	-6.07	111.98	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1236	AMP	N3-C2-N1	-5.99	119.31	128.68
7	E	1237	AMP	O4'-C1'-C2'	5.81	115.41	106.93
7	C	1236	AMP	O2P-P-O5'	5.69	121.87	106.73
4	B	1730	FMN	O4-C4-N3	-5.46	109.66	120.12
7	E	1237	AMP	C1'-N9-C4	-5.27	117.38	126.64
4	B	1730	FMN	C5A-C9A-N10	5.13	123.25	117.95
4	A	1730	FMN	O4'-C4'-C5'	-4.80	99.13	109.92
4	A	1730	FMN	C5'-C4'-C3'	4.69	121.27	112.20
7	C	1236	AMP	C1'-N9-C4	-4.64	118.49	126.64
4	A	1730	FMN	C7M-C7-C6	-4.61	110.96	119.49
7	E	1237	AMP	O3'-C3'-C2'	-4.60	96.95	111.82
4	A	1730	FMN	C4A-C10-N10	4.59	123.20	116.48
4	B	1730	FMN	P-O5'-C5'	4.50	130.68	118.30
7	C	1236	AMP	C5-C6-N6	-4.39	113.67	120.35
4	B	1730	FMN	C7M-C7-C8	-4.34	111.83	120.74
4	B	1730	FMN	C9A-C5A-N5	-4.29	117.77	122.43
5	A	1731	ADP	C3'-C2'-C1'	4.18	107.28	100.98
4	A	1730	FMN	O4-C4-N3	-3.89	112.66	120.12
5	A	1731	ADP	N6-C6-N1	3.77	126.39	118.57
5	A	1731	ADP	N3-C2-N1	-3.74	122.83	128.68
5	B	1731	ADP	C1'-N9-C4	-3.68	120.17	126.64
4	A	1730	FMN	C10-C4A-N5	-3.67	117.07	124.86
5	A	1731	ADP	C5-C6-N6	-3.66	114.79	120.35
5	A	1731	ADP	PA-O3A-PB	-3.56	120.61	132.83
4	A	1730	FMN	O2-C2-N1	-3.53	115.98	121.83
4	B	1730	FMN	C4'-C3'-C2'	3.40	120.44	113.36
7	C	1236	AMP	O5'-P-O1P	-3.37	97.01	106.47
4	B	1730	FMN	C4-C4A-N5	3.35	123.01	118.23
7	E	1237	AMP	O2P-P-O5'	-3.30	97.95	106.73
7	C	1236	AMP	O4'-C1'-C2'	3.25	111.68	106.93
4	A	1730	FMN	O3'-C3'-C2'	-3.24	100.98	108.81
5	A	1731	ADP	O2'-C2'-C3'	-3.24	101.36	111.82
4	A	1730	FMN	O4-C4-C4A	-3.21	118.07	126.60
7	C	1236	AMP	N6-C6-N1	3.21	125.24	118.57
7	C	1236	AMP	O4'-C4'-C5'	-3.12	99.10	109.37
7	E	1237	AMP	O5'-P-O1P	3.11	115.20	106.47
7	C	1236	AMP	C3'-C2'-C1'	-3.11	96.29	100.98
4	B	1730	FMN	O3P-P-O1P	-3.09	98.60	110.68
4	B	1730	FMN	O3P-P-O5'	3.08	114.93	106.73
4	B	1730	FMN	C8M-C8-C7	-3.08	114.43	120.74
5	B	1731	ADP	C2'-C3'-C4'	3.05	108.56	102.64
4	A	1730	FMN	C4-C4A-C10	3.03	121.88	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1730	FMN	C8M-C8-C9	-3.01	113.92	119.49
5	B	1731	ADP	O5'-PA-O1A	2.96	120.65	109.07
5	A	1731	ADP	O3'-C3'-C2'	-2.93	102.34	111.82
7	C	1236	AMP	O2'-C2'-C3'	-2.93	102.36	111.82
4	B	1730	FMN	C4A-C4-N3	2.90	120.56	113.19
4	B	1730	FMN	C6-C7-C8	-2.87	115.56	119.67
4	B	1730	FMN	C10-N1-C2	2.83	122.57	116.90
5	A	1731	ADP	O5'-C5'-C4'	-2.83	99.24	108.99
4	A	1730	FMN	O5'-P-O1P	-2.82	98.56	106.47
7	E	1237	AMP	C5'-C4'-C3'	2.77	125.56	115.18
5	B	1731	ADP	O4'-C4'-C5'	-2.70	100.50	109.37
7	C	1236	AMP	C2'-C3'-C4'	-2.65	97.49	102.64
7	E	1237	AMP	O3'-C3'-C4'	2.60	118.58	111.05
5	B	1731	ADP	C2-N1-C6	2.60	123.20	118.75
4	A	1730	FMN	C5A-C9A-N10	2.59	120.62	117.95
4	B	1730	FMN	O3'-C3'-C4'	-2.51	102.75	108.81
4	B	1730	FMN	C6-C5A-N5	2.49	122.85	118.51
4	B	1730	FMN	C9-C9A-N10	-2.46	118.50	121.84
4	B	1730	FMN	O5'-C5'-C4'	2.46	115.93	109.36
7	E	1237	AMP	O2'-C2'-C1'	-2.46	101.79	110.85
7	C	1236	AMP	C4-C5-N7	2.41	111.91	109.40
4	B	1730	FMN	C10-C4A-N5	-2.37	119.82	124.86
4	B	1730	FMN	O2'-C2'-C3'	2.29	114.67	109.10
4	A	1730	FMN	C8M-C8-C7	-2.28	116.07	120.74
5	B	1731	ADP	C5-C6-N6	-2.27	116.90	120.35
4	A	1730	FMN	O3'-C3'-C4'	2.25	114.24	108.81
5	A	1731	ADP	O4'-C1'-C2'	-2.19	103.73	106.93
4	A	1730	FMN	O2-C2-N3	2.17	122.87	118.65
7	E	1237	AMP	C3'-C2'-C1'	-2.14	97.75	100.98
4	B	1730	FMN	O5'-P-O1P	2.13	112.45	106.47
4	B	1730	FMN	C4A-C10-N10	2.09	119.54	116.48
5	B	1731	ADP	O3B-PB-O1B	2.08	118.84	110.68
7	C	1236	AMP	P-O5'-C5'	2.08	124.03	118.30
7	E	1237	AMP	C5-C6-N6	-2.07	117.20	120.35
4	B	1730	FMN	C4A-C10-N1	-2.04	120.00	124.73
5	A	1731	ADP	O3B-PB-O2B	2.02	115.35	107.64
4	A	1730	FMN	O3P-P-O2P	2.02	115.34	107.64

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'
5	A	1731	ADP	C3'-C4'-C5'-O5'
4	A	1730	FMN	C2'-C3'-C4'-O4'
5	A	1731	ADP	O4'-C4'-C5'-O5'
4	A	1730	FMN	C5'-O5'-P-O1P
7	C	1236	AMP	C5'-O5'-P-O1P
4	B	1730	FMN	C4'-C5'-O5'-P
4	A	1730	FMN	C5'-O5'-P-O2P
7	C	1236	AMP	C5'-O5'-P-O2P
5	B	1731	ADP	PB-O3A-PA-O2A
5	B	1731	ADP	O4'-C4'-C5'-O5'
5	A	1731	ADP	PB-O3A-PA-O2A
5	B	1731	ADP	PB-O3A-PA-O1A

There are no ring outliers.

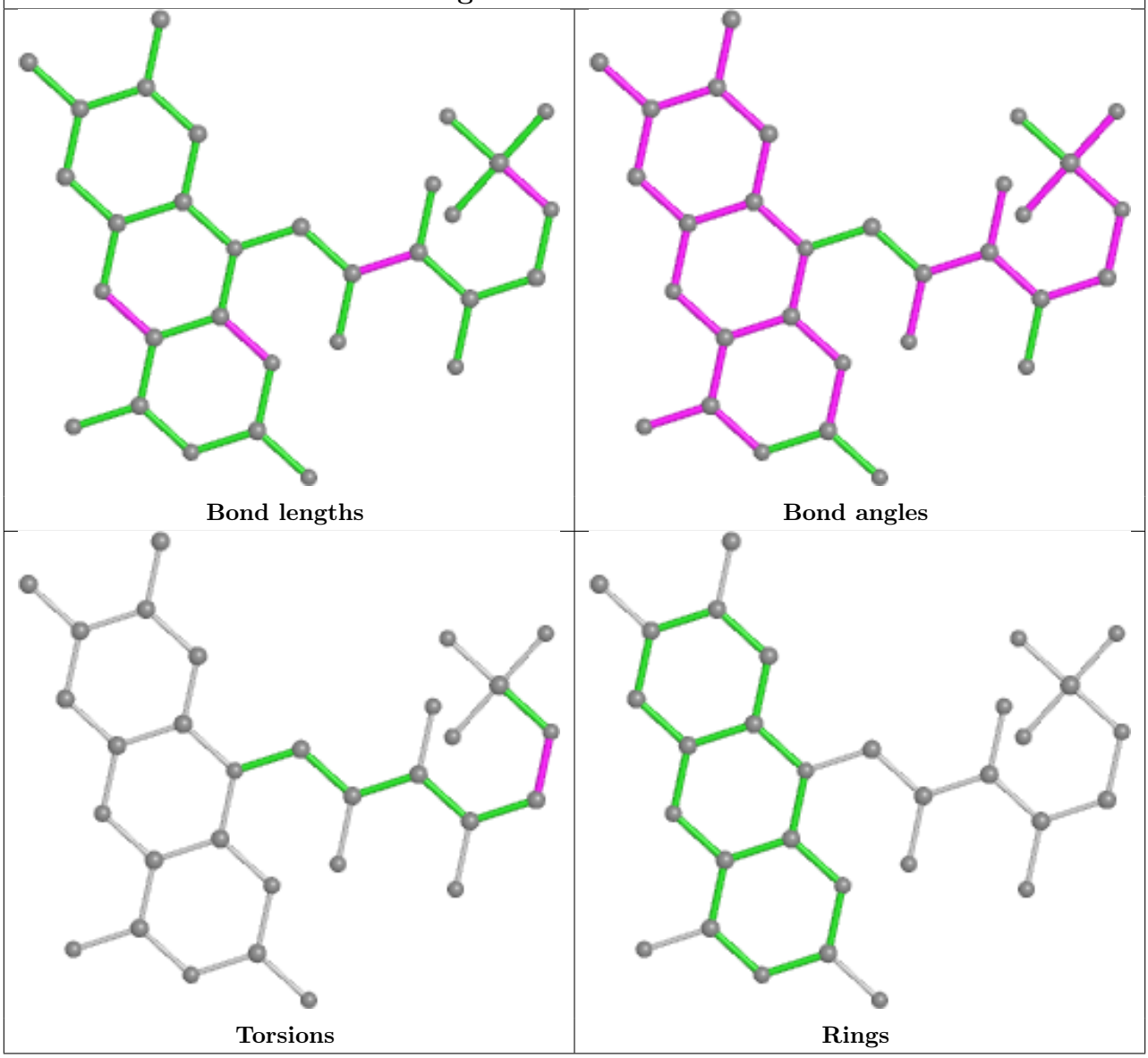
7 monomers are involved in 30 short contacts:

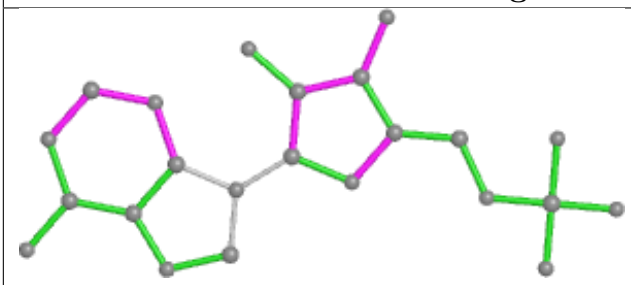
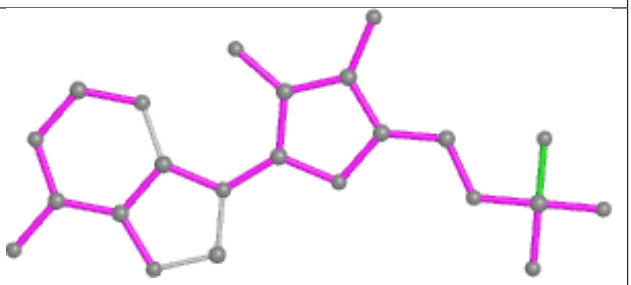
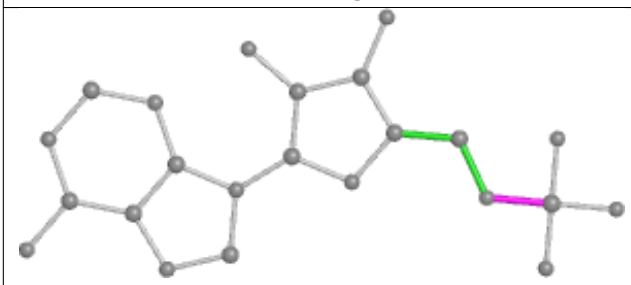
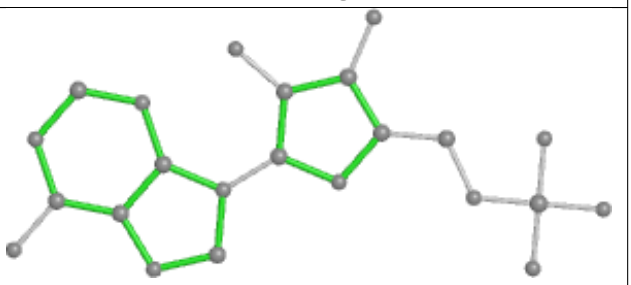
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1732	SF4	1	0
4	B	1730	FMN	6	0
7	C	1236	AMP	6	0
5	B	1731	ADP	2	0
5	A	1731	ADP	6	0
7	E	1237	AMP	4	0
4	A	1730	FMN	5	0

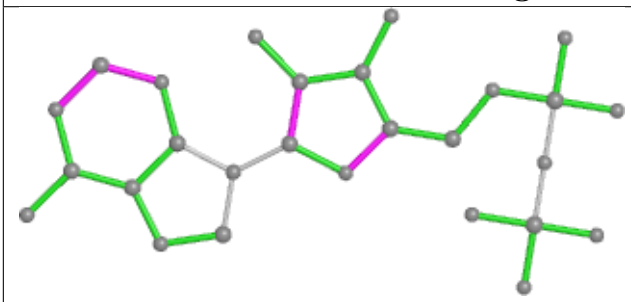
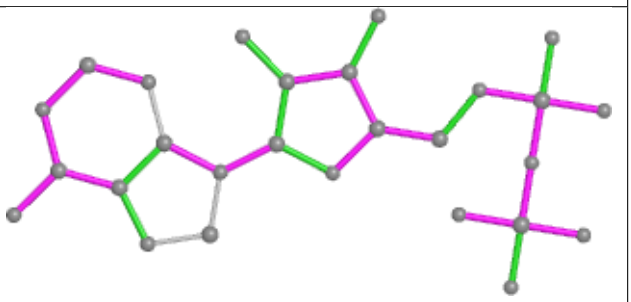
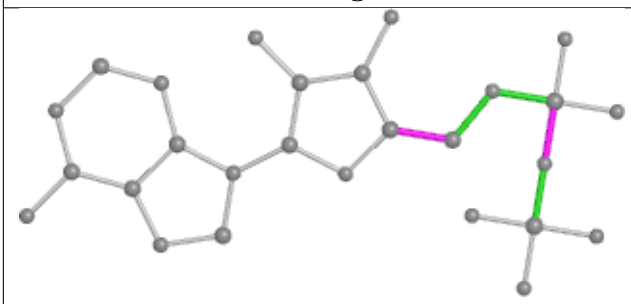
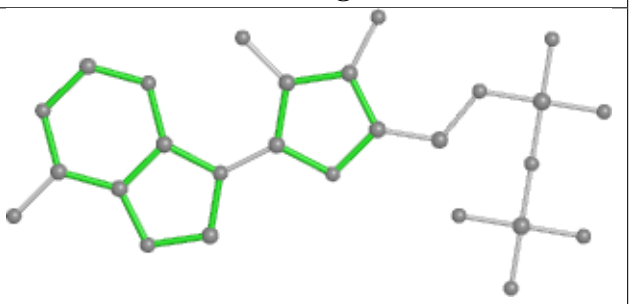
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

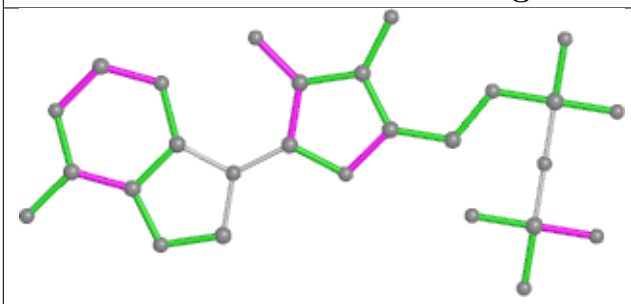
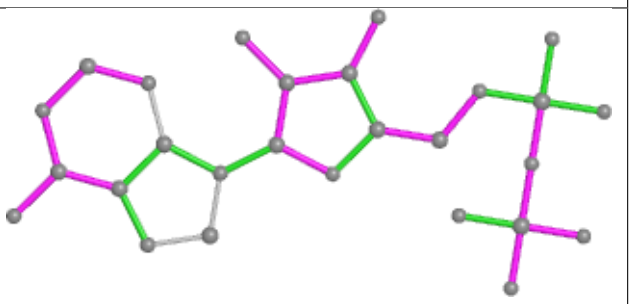
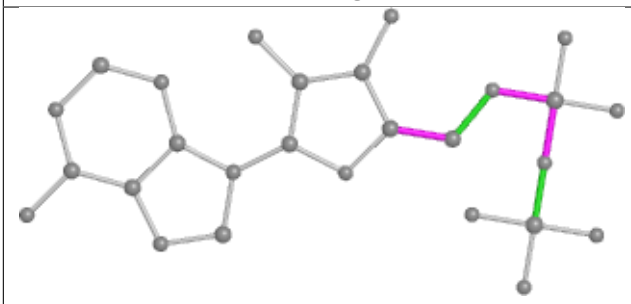
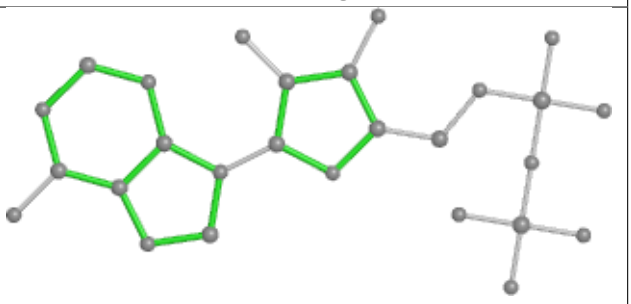
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

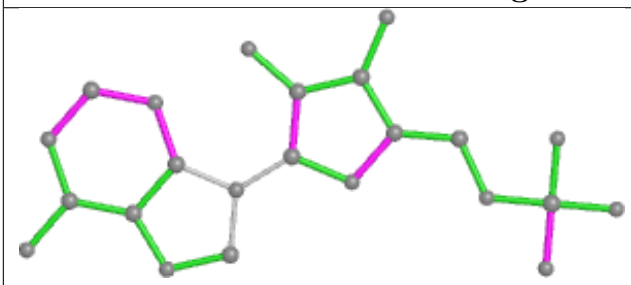
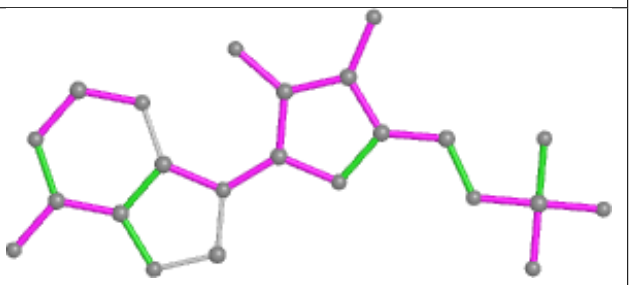
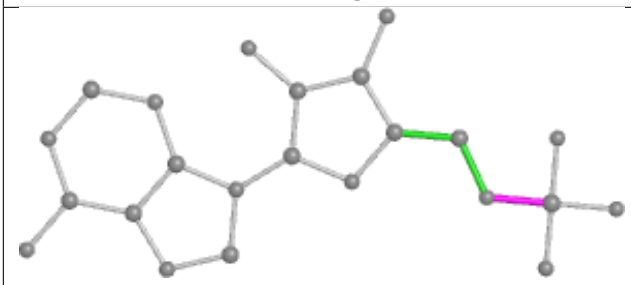
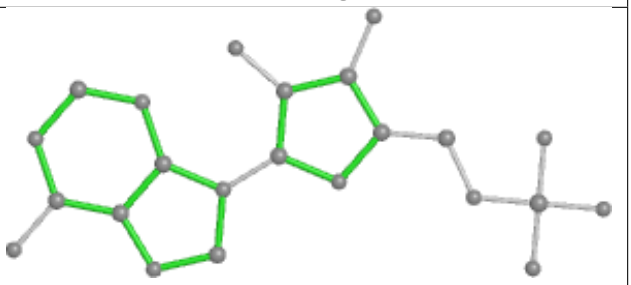
Ligand FMN B 1730



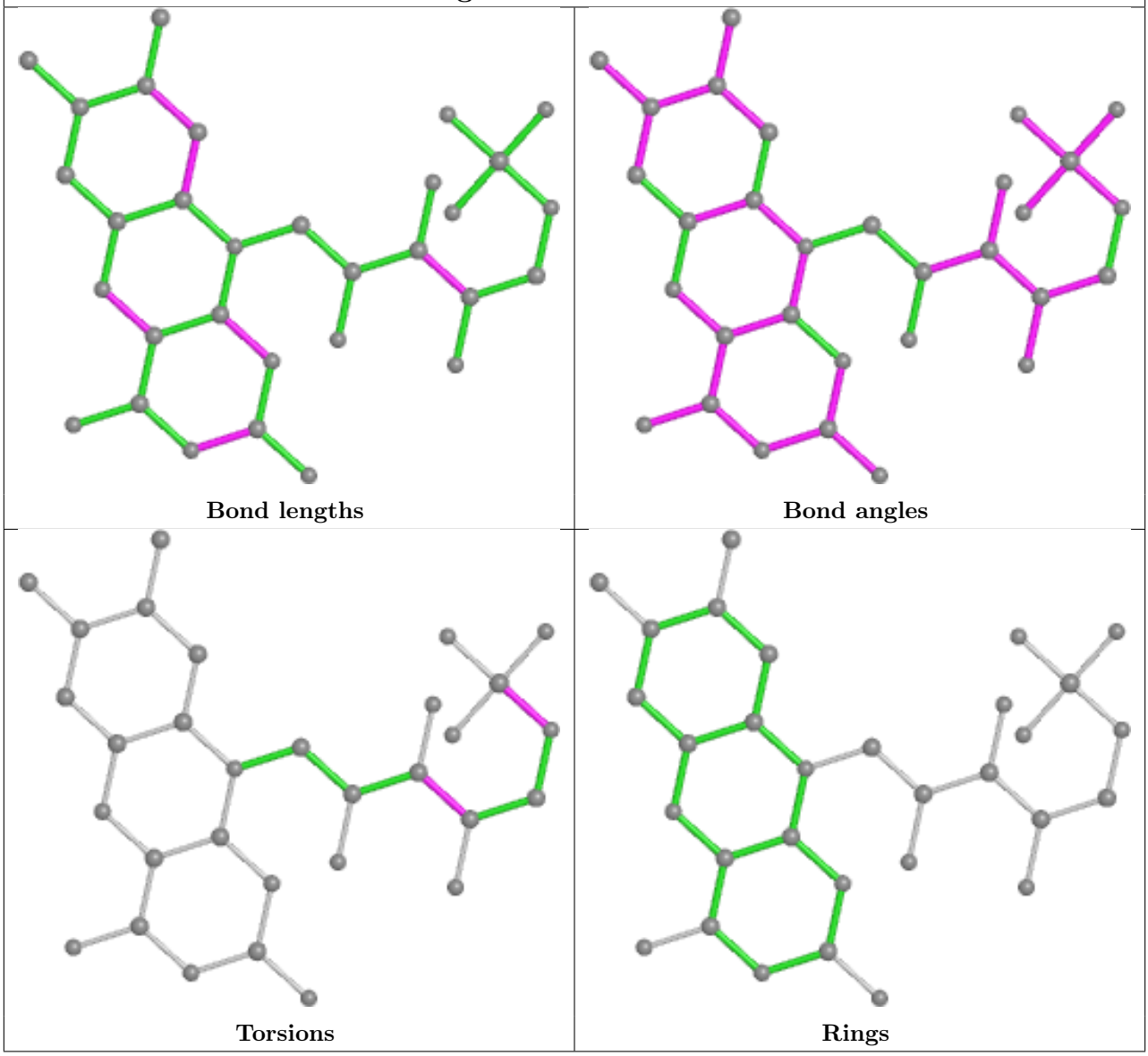
Ligand AMP C 1236	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 1731	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 1731	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP E 1237	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN A 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	729/729 (100%)	-0.60	1 (0%)	95	94	39, 57, 67, 73	0
1	B	729/729 (100%)	-0.62	0	100	100	38, 57, 67, 73	0
2	C	233/264 (88%)	-0.63	0	100	100	49, 58, 65, 71	0
2	E	236/264 (89%)	-0.55	0	100	100	50, 59, 65, 70	0
3	D	189/320 (59%)	-0.56	0	100	100	55, 61, 69, 75	0
3	F	189/320 (59%)	-0.11	3 (1%)	72	61	56, 62, 70, 76	0
All	All	2305/2626 (87%)	-0.56	4 (0%)	95	93	38, 59, 67, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	126	ASP	3.6
1	A	628	THR	2.8
3	F	162	PRO	2.2
3	F	167	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

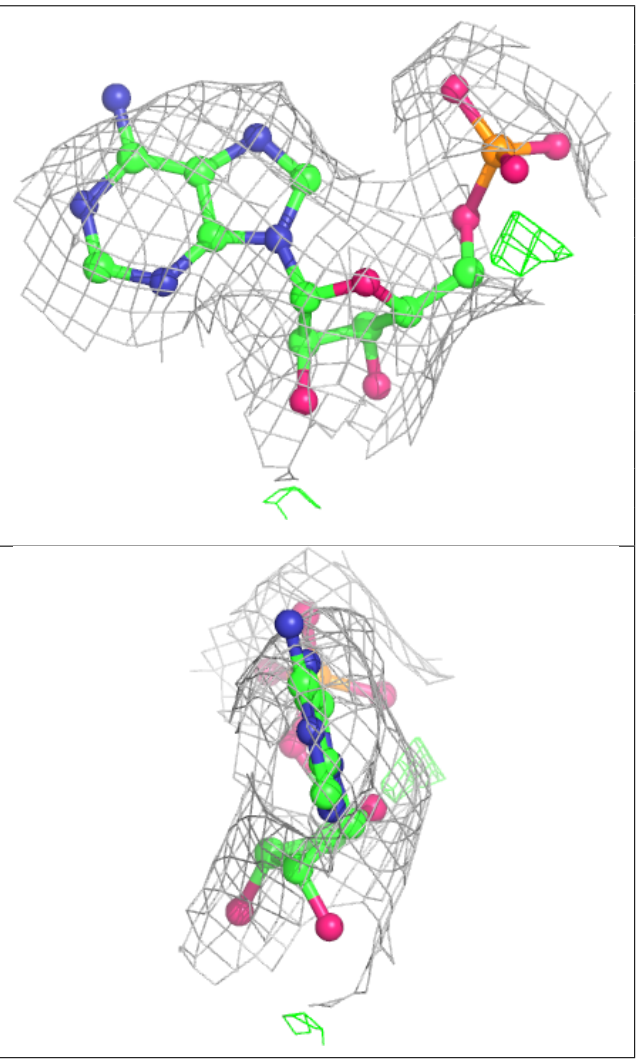
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	AMP	E	1237	23/23	0.93	0.22	33,52,63,66	0
5	ADP	A	1731	27/27	0.94	0.18	40,47,52,53	0
4	FMN	B	1730	31/31	0.94	0.20	23,39,46,52	0
7	AMP	C	1236	23/23	0.95	0.17	34,50,56,60	0
4	FMN	A	1730	31/31	0.95	0.16	35,47,60,61	0
5	ADP	B	1731	27/27	0.96	0.16	45,52,59,61	0
6	SF4	A	1732	8/8	1.00	0.11	31,36,40,41	0
6	SF4	B	1732	8/8	1.00	0.12	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.

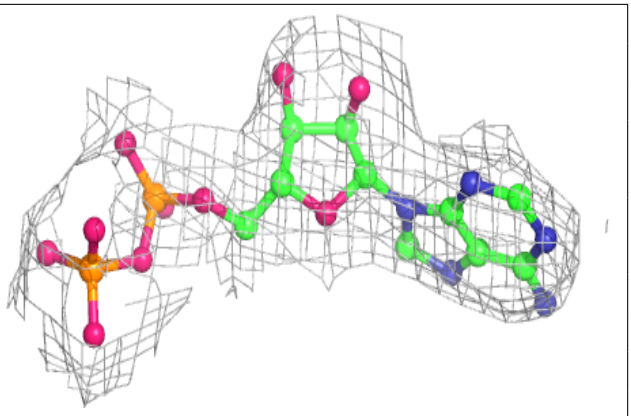
Electron density around AMP E 1237:

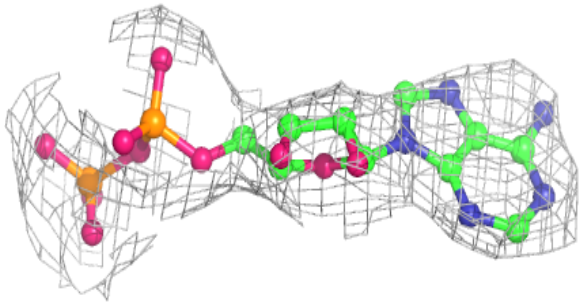
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

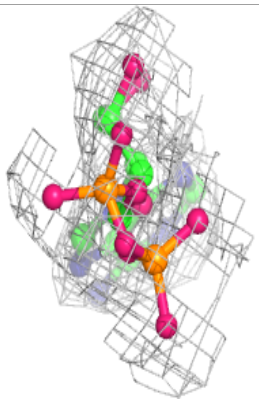


Electron density around ADP A 1731:

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

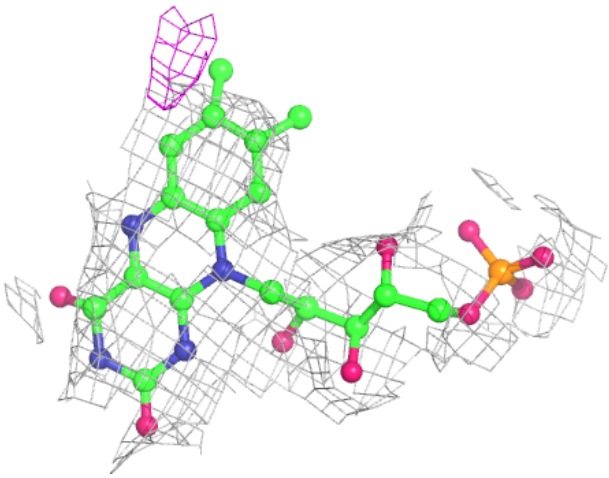


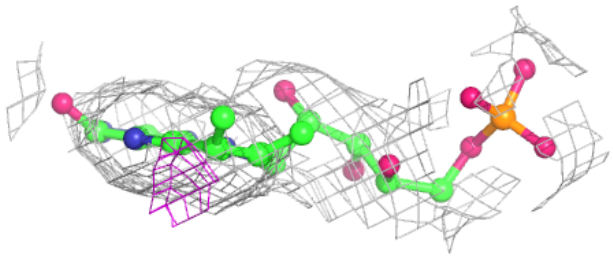


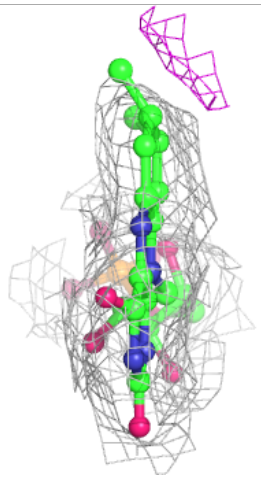


Electron density around FMN B 1730:

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

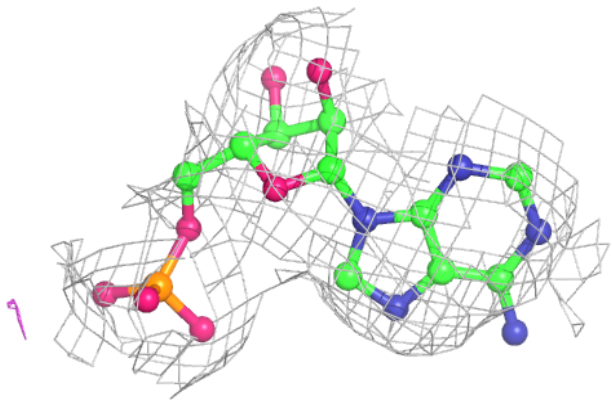


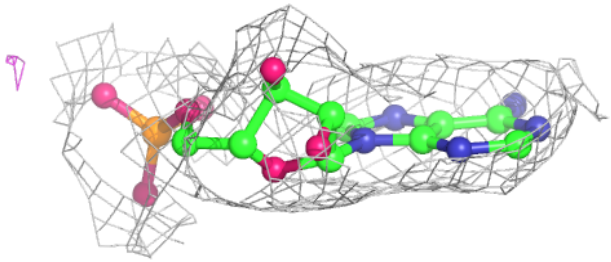


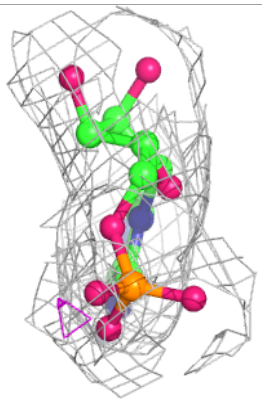


Electron density around AMP C 1236:

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

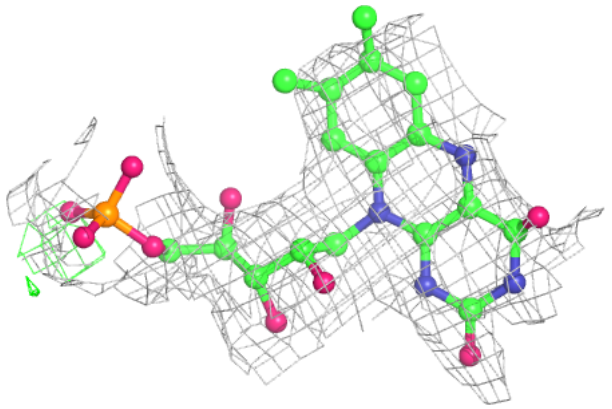


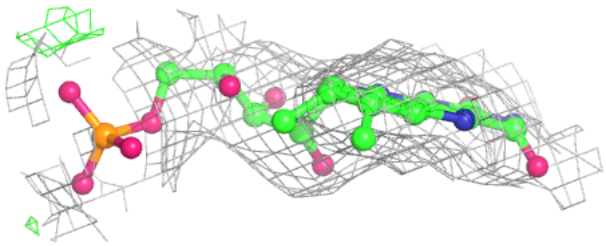


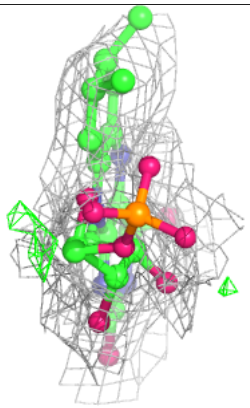


Electron density around FMN A 1730:

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

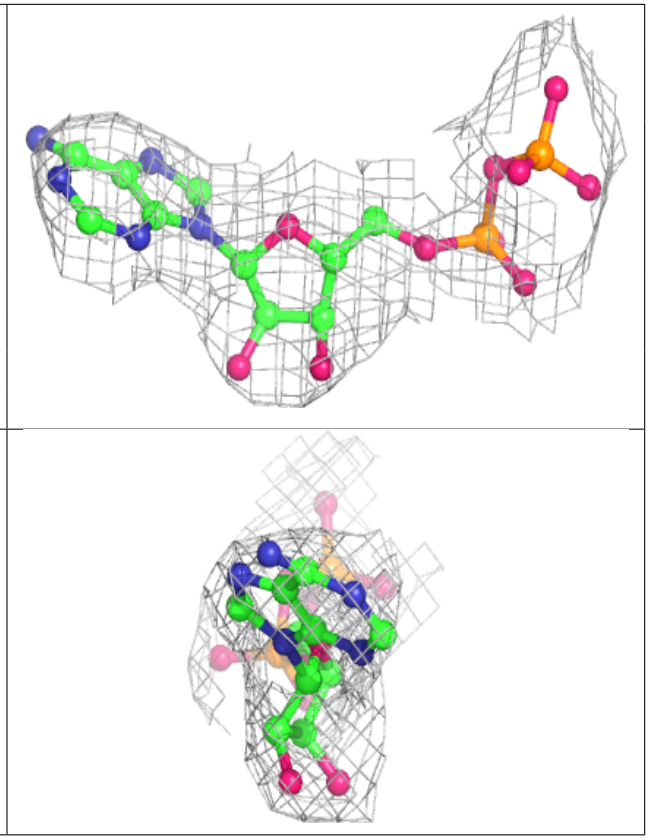






Electron density around ADP B 1731:

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



6.5 Other polymers (i)

There are no such residues in this entry.