



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:51 PM UTC

PDB ID : 2BN4 / pdb_00002bn4
Title : A second FMN-binding site in yeast NADPH-cytochrome P450 reductase suggests a novel mechanism of electron transfer by diflavin reductase
Authors : Podust, L.M.; Lepesheva, G.I.; Kim, Y.; Yermalitskaya, L.V.; Yermalitsky, V.N.; Lamb, D.C.; Kelly, S.L.; Waterman, M.R.
Deposited on : 2005-03-18
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

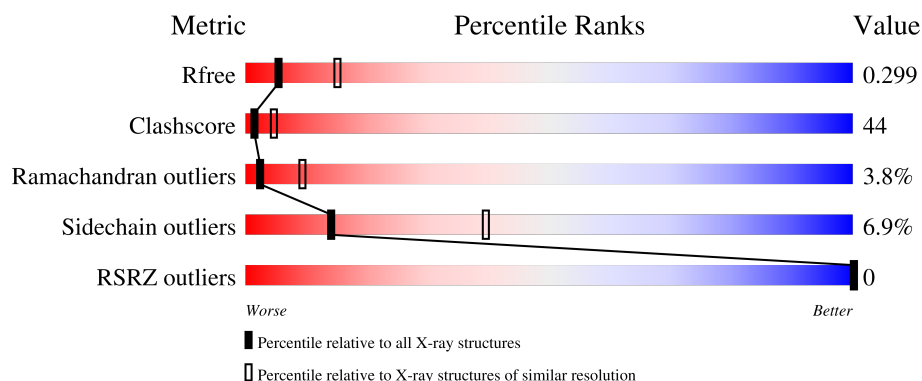
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	682	
1	B	682	

2 Entry composition [i](#)

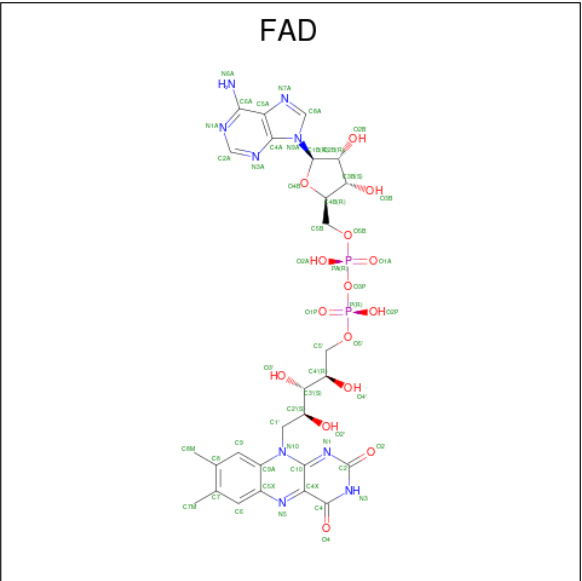
There are 5 unique types of molecules in this entry. The entry contains 10331 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADPH CYTOCHROME P450 REDUCTASE.

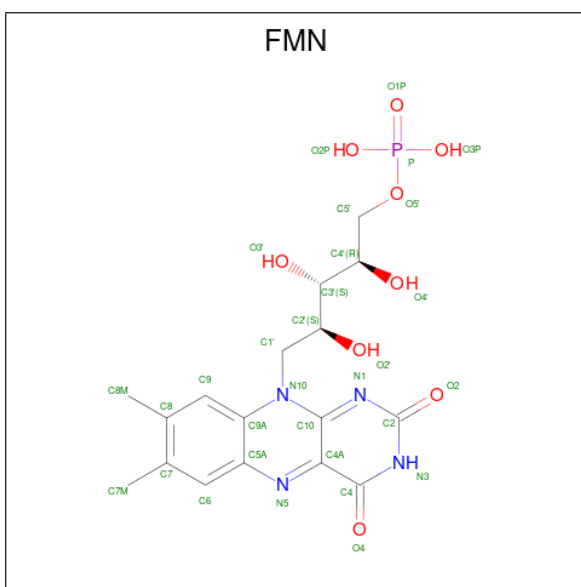
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	0	0
			5021	3202	827	977	15			
1	B	641	Total	C	N	O	S	0	0	0
			5007	3191	825	976	15			

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



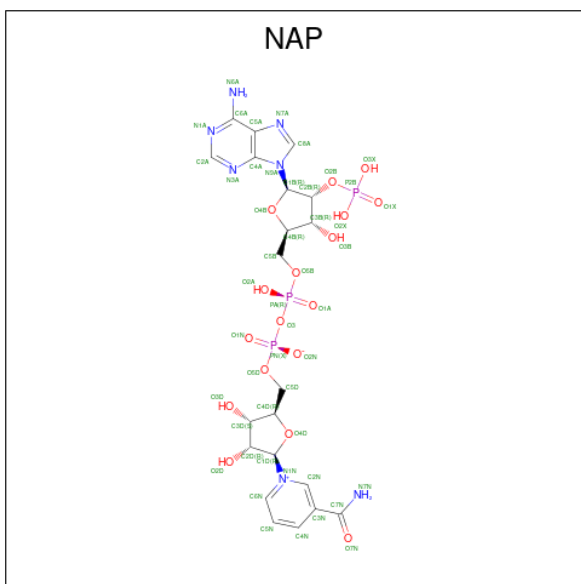
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	22	Total	O	0	0
			22	22		

Y666 Q697 V690 W691	Q621	L562	L482	K420	A354	C287	Q216	L142	GLY	MET
	D622	R553	R483	W421	A355	I288	K77	S143	SER	
	K623	E554	M484	D422	I356	A218	N144	L144	GLY	
	L624	R555	I485	T423	K357	K219	S80	R446	SER	
	K625	V556	Q486	W424	H358	F220	E82	L147	HIS	
	D626	A557	L487	P425	Y359	D293	E21	L148	HIS	
	Y627	Q562	M493	M426	L360	L294	Q223	L83	HIS	
	E628	Q562	Q427	Q426	E361	F224	M49	V84	HIS	
	V631	N568	I494	F428	I362	S295	Q225	L51	HIS	
	F632	V669	E496	L429	T363	Y301	E231	F150	HIS	
E633	S570	T497	E431	G364	D305	I232	L152	SER		
M634	L571	M498	S432	Q369	H306	T233	G153	SER		
L635	G572	L499	W433	L370	D234	S155	N154	LEU		
M636	K573	P500	P434	F371	A308	T156	M92	VAL		
N637	H574	V501	Q435	S372	V309	M236	C93	VAL		
G638	I575	H502	M436	S373	K310	E237	E157	PRO		
A639	L576	Y503	T437	L374	P311	L238	E458	ARG		
F640	F577	P508	P438	L375	S312	G239	D95	GLY		
L641	Y578	R509	R439	Q376	N313	E240	V96	SER		
W642	G579	S580	Y440	F377	P314	P241	E97	HIS		
V643	S581	K510	Y441	A378	L315	G162	N98	LEU		
C644	R581	L511	S442	R379	E316	A163	Y99	LEU		
G645	N582	F512	I443	N380	K317	A164	D100	ASP		
D646	T583	A513	S444	A381	V318	K165	F101	ASP		
A647	D584	M514	S445	D382	E319	K166	E102	ILE		
K648	D585	Y515	S446	Q320	S248	A167	S103	MET		
G649	F586	K516	S447	K384	E168	E168	L104	SER		
M650		L517	I448	F321	F321	K169	N105	ASP		
A651	Q589	P518	S449	R385	L322	H170	D106	GLY		
K652	D590	V519	E450	ASN	S223	ASN	V107	ASP		
E591	H520	H520	K451	ASN	I324	ARG	P108	ILE		
W592	F592	H521	Q452	F325	A174	V109	E108	THR		
S593	P593	R522	T453	N326	G175	I110	I111	ALA		
E594	V594	V522	W454	K392	D256	L179	S112	VAL		
Y595	R527		H455	D395	L327	G257	E113	SER		
A596	L528		V456	E330	P329	I258	I113	SER		
L598	P529			Q396	E330	Q259	F114	GLY		
K597	S530			F397	T331	L260	A185			
S598	P530	I459	T459	D397	I332	F263	D186	M47		
L599	N531	V460	V460	A398	I332	D264	S116	R48		
S600	P532	E461	E461	V399	F333	A189	Y117	D49		
G601	S533		N462	E400	D334	G190	G119	I50		
S602	T534			I401	L335	L265	E120	A51		
F603	V536			T402	K336	S266	T191	Q52		
E604	V537			S403	P337	Q267	T192	Q52		
M605	I537			K404	D339	Y269	F123	V54		
V606	M538			Y405	L338	P268	Y196			
L607	I539			F406	D339	I270	P124			
A608	G540			T341	P340	Z271	W199	K59		
H609	P541			N407	T342	P272	K200	R60		
W674	S610			I408	V342	I273	F130	Y61		
E575	G542			A409	K343	S202	E131	L62		
R611	T543			P472	V344	Z274	D132	V63		
L612	G			D410	P345	I203	F133			
P613	V545			W474	P346	T134	I134	A66		
	A546			V475	P347	L207	C135	S67		
	P547			G476	T348	E210	N136	Q88		
	F548			V477	P349	E210	A137	T69		
	R549			T478	Y414	L211	E138			
	V618			T479	T350	H212	A139	A72		
	G684			S416	T351	H212	A139	E73		
	V620			N480	I352	L213	G140	D74		
	E551			L481	C552	A141	N386			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 77.84Å 261.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.41 – 2.91 43.41 – 2.91	Depositor EDS
% Data completeness (in resolution range)	82.1 (43.41-2.91) 91.7 (43.41-2.91)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.300 0.239 , 0.299	Depositor DCC
R_{free} test set	3371 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.135 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10331	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/5137	1.09	41/6978 (0.6%)
1	B	0.49	0/5120	1.07	41/6952 (0.6%)
All	All	0.50	0/10257	1.08	82/13930 (0.6%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ASN	N-CA-C	-13.54	92.66	110.53
1	B	499	LEU	CA-C-N	8.38	127.98	118.85
1	B	499	LEU	C-N-CA	8.38	127.98	118.85
1	A	158	GLU	N-CA-C	-8.36	100.12	110.41
1	A	591	GLU	N-CA-C	8.31	120.42	111.36
1	B	607	VAL	N-CA-C	8.26	119.80	107.75
1	A	648	LYS	N-CA-C	-8.17	102.38	111.28
1	A	84	VAL	N-CA-C	-8.08	104.62	113.43
1	B	158	GLU	N-CA-C	-7.84	99.96	110.55
1	A	244	HIS	N-CA-C	-7.73	104.07	113.97
1	A	288	ILE	N-CA-C	7.64	119.58	108.58
1	B	399	VAL	N-CA-C	7.32	118.05	110.36
1	B	312	SER	N-CA-C	-7.31	97.21	108.76
1	B	407	ASN	N-CA-C	-7.20	100.16	110.59
1	B	288	ILE	N-CA-C	7.18	118.22	108.17
1	A	183	GLY	N-CA-C	7.02	121.08	111.54
1	A	612	LEU	CA-C-N	6.98	128.57	119.84
1	A	612	LEU	C-N-CA	6.98	128.57	119.84
1	B	591	GLU	N-CA-C	6.86	120.12	111.69
1	A	111	VAL	N-CA-C	6.82	118.31	108.48
1	A	149	MET	N-CA-C	6.64	119.52	109.23
1	B	111	VAL	N-CA-C	6.59	117.97	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	648	LYS	N-CA-C	-6.53	104.21	111.71
1	A	463	PHE	CA-C-N	6.48	126.24	119.76
1	A	463	PHE	C-N-CA	6.48	126.24	119.76
1	A	169	LYS	N-CA-C	-6.31	103.70	111.40
1	B	123	PHE	N-CA-C	-6.26	102.25	110.39
1	A	476	GLY	N-CA-C	-6.16	103.23	113.02
1	A	101	PHE	N-CA-C	6.11	119.45	112.97
1	A	231	GLU	N-CA-C	6.09	119.43	107.98
1	B	584	ASP	N-CA-C	-6.09	106.83	114.56
1	B	485	ILE	CB-CA-C	-5.97	104.06	111.70
1	A	127	ALA	N-CA-C	-5.94	98.15	110.80
1	B	146	ARG	N-CA-C	-5.90	99.63	109.24
1	A	549	ARG	N-CA-C	-5.87	104.96	111.36
1	A	235	SER	N-CA-C	-5.79	105.88	113.17
1	B	149	MET	N-CA-C	5.78	118.19	109.23
1	A	121	GLY	N-CA-C	-5.71	107.09	115.72
1	B	433	VAL	CA-C-N	5.68	126.94	119.84
1	B	433	VAL	C-N-CA	5.68	126.94	119.84
1	A	503	TYR	N-CA-C	5.68	118.98	109.95
1	B	187	ASP	N-CA-C	-5.68	106.19	113.01
1	B	540	GLY	CA-C-N	5.67	126.56	119.98
1	B	540	GLY	C-N-CA	5.67	126.56	119.98
1	B	476	GLY	N-CA-C	-5.63	104.48	112.37
1	A	471	ALA	CA-C-N	5.60	126.15	120.38
1	A	471	ALA	C-N-CA	5.60	126.15	120.38
1	B	145	LEU	N-CA-C	5.60	117.86	108.96
1	B	148	ASN	N-CA-C	-5.57	100.88	109.52
1	A	364	GLY	CA-C-N	5.55	125.56	119.89
1	A	364	GLY	C-N-CA	5.55	125.56	119.89
1	B	235	SER	N-CA-C	-5.55	106.51	113.28
1	A	407	ASN	N-CA-C	-5.50	101.61	110.14
1	B	94	ALA	N-CA-C	5.50	118.51	109.72
1	A	413	LYS	N-CA-C	-5.47	105.39	111.36
1	B	323	SER	N-CA-C	5.40	117.25	111.36
1	B	511	LEU	N-CA-C	-5.35	106.59	113.23
1	B	637	ASN	N-CA-C	-5.35	104.46	112.54
1	A	521	VAL	N-CA-C	5.33	115.53	107.75
1	A	281	SER	N-CA-C	-5.28	106.69	113.02
1	A	395	ASP	N-CA-C	5.25	116.70	110.97
1	B	628	GLU	N-CA-C	5.25	118.47	111.75
1	A	179	LEU	N-CA-C	5.24	119.57	111.56
1	B	223	GLN	N-CA-C	-5.21	106.77	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	VAL	N-CA-C	5.19	116.06	108.53
1	A	273	ILE	N-CA-C	-5.17	100.88	108.54
1	B	344	VAL	CA-C-N	5.17	124.97	119.28
1	B	344	VAL	C-N-CA	5.17	124.97	119.28
1	B	402	THR	N-CA-C	5.17	116.99	111.36
1	B	400	GLU	N-CA-C	5.16	118.60	112.72
1	A	399	VAL	N-CA-C	5.15	115.59	110.23
1	B	60	ASN	N-CA-C	5.14	118.66	112.38
1	B	521	VAL	N-CA-C	5.14	115.37	108.17
1	A	278	GLU	N-CA-C	-5.13	103.62	110.55
1	A	360	LEU	N-CA-C	5.12	116.87	108.52
1	A	177	ILE	N-CA-C	5.10	115.39	107.28
1	A	553	ARG	N-CA-C	-5.10	104.99	111.11
1	B	360	LEU	N-CA-C	5.09	117.02	108.73
1	B	676	LEU	N-CA-C	-5.04	105.06	111.11
1	A	626	ASP	N-CA-C	-5.02	105.46	111.03
1	A	234	ASP	N-CA-C	-5.00	106.77	112.92
1	B	99	TYR	N-CA-C	5.00	118.11	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5021	0	4876	383	0
1	B	5007	0	4880	507	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
3	A	31	0	19	2	0
3	B	31	0	19	1	0
4	A	40	0	19	5	0
4	B	40	0	19	1	0
5	A	33	0	0	3	0
5	B	22	0	0	5	0
All	All	10331	0	9894	886	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 44.

All (886) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLU:HG2	1:A:436:MET:HA	1.30	1.13
1:A:528:LEU:HD23	1:A:529:PRO:HD2	1.28	1.11
1:B:59:LYS:HD3	1:B:92:MET:HB2	1.22	1.10
1:A:67:SER:HB2	1:A:72:ALA:HB3	1.39	1.05
1:B:482:LEU:HA	1:B:485:ILE:HD12	1.42	1.01
1:A:60:ASN:HD21	1:A:89:LEU:HB3	1.28	0.99
1:A:449:SER:HB3	1:A:557:ALA:HB2	1.45	0.98
1:B:327:LEU:HD11	1:B:352:ILE:HD13	1.46	0.96
1:A:379:PRO:HD2	1:A:383:VAL:HG11	1.46	0.95
1:B:225:GLN:HB3	1:B:336:LYS:HB3	1.48	0.95
1:A:311:PRO:HG2	1:A:436:MET:HE2	1.48	0.95
1:A:60:ASN:ND2	1:A:89:LEU:HB3	1.82	0.94
1:A:322:LEU:HD13	1:A:329:PRO:HG3	1.49	0.94
1:B:467:GLU:O	1:B:469:PRO:HD3	1.68	0.93
1:B:449:SER:HB3	1:B:557:ALA:HB2	1.49	0.93
1:B:623:LYS:HE2	1:B:623:LYS:HA	1.53	0.91
1:A:612:LEU:HD23	1:A:613:PRO:HD2	1.51	0.91
1:A:647:ALA:CB	1:A:690:VAL:HG11	2.01	0.91
1:B:633:GLU:HG2	1:B:637:ASN:HD21	1.36	0.90
1:A:178:ARG:HH21	1:A:181:LYS:HA	1.34	0.90
1:A:50:ILE:HG23	1:A:51:ALA:H	1.37	0.90
1:B:278:GLU:OE2	1:B:286:ASN:HB3	1.71	0.90
1:B:313:ASN:ND2	1:B:436:MET:HE1	1.86	0.90
1:B:105:ASN:ND2	1:B:142:LEU:HA	1.87	0.90
1:A:647:ALA:HB2	1:A:690:VAL:HG11	1.54	0.89
1:B:659:VAL:HG22	1:B:677:ILE:HG13	1.52	0.89
1:A:529:PRO:HD3	1:A:642:TYR:OH	1.72	0.89
1:B:361:GLU:HA	1:B:436:MET:HE3	1.55	0.88
1:B:273:ILE:HD12	1:B:485:ILE:HG21	1.55	0.88
1:B:380:ASN:ND2	1:B:382:ASP:H	1.73	0.87
1:B:67:SER:HB2	1:B:72:ALA:HB3	1.57	0.86
1:A:246:LEU:HB2	1:A:249:HIS:HD2	1.40	0.86
1:B:647:ALA:HA	1:B:650:MET:HB3	1.57	0.85
1:A:361:GLU:OE2	1:A:436:MET:HG3	1.77	0.84
1:A:467:GLU:O	1:A:469:PRO:HD3	1.77	0.84
1:B:416:SER:HB2	1:B:419:ALA:HB3	1.60	0.84
1:B:640:PHE:HB3	1:B:642:TYR:HE1	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASN:HD22	1:B:142:LEU:HA	1.39	0.84
1:A:493:ASN:ND2	1:A:496:GLU:HB2	1.91	0.84
1:B:379:PRO:HD2	1:B:383:VAL:HB	1.60	0.83
1:B:87:PHE:HB2	1:B:89:LEU:HD12	1.60	0.83
1:A:648:LYS:HE3	4:A:753:NAP:N1N	1.93	0.82
1:B:185:ALA:HB1	1:B:192:THR:HG23	1.62	0.82
1:A:599:LEU:HD12	1:A:603:PHE:HB2	1.61	0.81
1:B:247:PRO:HG2	1:B:509:ARG:NH1	1.93	0.81
1:A:666:LYS:HE3	1:A:676:LEU:HD21	1.62	0.81
1:B:562:GLN:CB	1:B:568:ASN:HB3	2.11	0.80
1:A:416:SER:HB3	1:A:419:ALA:HB3	1.63	0.80
1:A:105:ASN:ND2	1:A:142:LEU:HA	1.96	0.80
1:B:327:LEU:HD11	1:B:352:ILE:CD1	2.11	0.79
1:A:247:PRO:HG2	1:A:509:ARG:NH1	1.96	0.79
1:B:540:GLY:HA3	1:B:548:PHE:HE1	1.47	0.79
1:B:238:LEU:HD12	1:B:509:ARG:HE	1.48	0.79
1:B:220:PHE:H	1:B:376:GLN:HE22	1.29	0.79
1:A:623:LYS:HE2	1:A:623:LYS:HA	1.65	0.79
1:A:130:PHE:CE1	1:A:134:ILE:HD11	2.19	0.78
1:A:54:VAL:HG13	1:A:59:LYS:HB2	1.66	0.78
1:A:130:PHE:CZ	1:A:134:ILE:HD11	2.19	0.78
1:A:318:VAL:HG13	1:A:356:ILE:HG22	1.65	0.78
1:B:68:GLN:HB2	1:B:124:PRO:HB3	1.65	0.78
1:B:640:PHE:HB3	1:B:642:TYR:CE1	2.18	0.78
1:A:49:ASP:O	1:A:53:VAL:HG23	1.84	0.78
1:B:220:PHE:H	1:B:376:GLN:NE2	1.82	0.77
1:A:311:PRO:CG	1:A:436:MET:HE2	2.15	0.77
1:B:508:PRO:O	1:B:511:LEU:HB2	1.87	0.75
1:A:115:ILE:HD11	1:A:163:ALA:HB1	1.67	0.75
1:A:211:LEU:HB2	1:A:213:LEU:HG	1.69	0.75
1:B:328:ASP:OD2	1:B:330:GLU:HB2	1.85	0.75
1:B:465:ASN:HB2	5:B:2016:HOH:O	1.86	0.75
1:A:260:LEU:HA	1:A:298:ASN:OD1	1.85	0.75
1:B:372:SER:HB2	1:B:391:SER:HB2	1.69	0.75
1:B:96:VAL:HG21	1:B:130:PHE:CD2	2.21	0.75
1:B:313:ASN:HD21	1:B:436:MET:HE1	1.50	0.75
1:A:528:LEU:HD23	1:A:529:PRO:CD	2.14	0.75
1:A:226:TYR:HB2	1:A:427:GLN:HG2	1.69	0.74
1:B:322:LEU:HD13	1:B:329:PRO:HG3	1.69	0.74
1:A:95:ASP:HB3	1:A:98:ASN:ND2	2.03	0.73
1:B:323:SER:O	1:B:420:LYS:HE3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:HD12	1:B:328:ASP:N	2.03	0.73
1:A:398:ALA:HA	1:A:402:THR:HB	1.70	0.73
1:B:59:LYS:HE2	1:B:341:THR:HG21	1.68	0.73
1:A:449:SER:HB3	1:A:557:ALA:CB	2.19	0.73
1:B:263:PHE:HD2	1:B:268:PRO:O	1.72	0.73
1:B:327:LEU:CD1	1:B:352:ILE:HD13	2.18	0.73
1:A:326:ASN:HB2	1:A:420:LYS:HD3	1.71	0.73
1:A:346:PHE:CD2	1:A:359:TYR:HB3	2.23	0.73
1:B:449:SER:O	1:B:450:GLU:HG3	1.89	0.73
1:A:230:ASN:HD22	1:A:231:GLU:HG2	1.54	0.72
1:B:535:PRO:HB2	1:B:639:ALA:HB2	1.69	0.72
1:B:437:THR:HG22	1:B:438:PRO:O	1.89	0.72
1:A:154:ASN:OD1	1:A:156:THR:HG22	1.89	0.72
1:A:426:MET:O	1:A:430:VAL:HG23	1.89	0.72
1:B:113:ILE:O	1:B:149:MET:HG3	1.89	0.72
1:A:59:LYS:HE2	1:A:92:MET:HB2	1.70	0.72
1:A:78:LYS:HE2	1:A:367:SER:OG	1.89	0.72
1:B:535:PRO:HB2	1:B:639:ALA:CB	2.19	0.72
1:A:233:THR:HG22	1:A:234:ASP:H	1.54	0.72
1:B:88:ASN:HD21	1:B:216:GLN:NE2	1.87	0.71
1:B:400:GLU:C	1:B:401:ILE:HD12	2.15	0.71
1:B:573:LYS:HG3	1:B:634:MET:HE3	1.72	0.71
1:A:628:GLU:HG3	1:A:629:ASP:N	2.05	0.71
1:B:220:PHE:N	1:B:376:GLN:HE22	1.88	0.71
1:A:138:GLU:HG3	1:A:139:ALA:H	1.56	0.70
1:B:633:GLU:HG2	1:B:637:ASN:ND2	2.04	0.70
1:B:50:ILE:HG23	1:B:51:ALA:H	1.55	0.70
1:B:473:PRO:O	1:B:475:VAL:HG13	1.91	0.70
1:B:528:LEU:H	1:B:528:LEU:HD12	1.57	0.70
1:A:535:PRO:HB2	1:A:639:ALA:HB2	1.72	0.70
1:B:562:GLN:HB2	1:B:568:ASN:HB3	1.73	0.70
1:B:576:LEU:HD12	1:B:577:PHE:N	2.07	0.70
1:B:154:ASN:OD1	1:B:156:THR:HB	1.93	0.69
1:B:361:GLU:HG2	1:B:436:MET:HA	1.73	0.69
1:B:547:PRO:HG2	1:B:644:CYS:SG	2.32	0.69
1:A:233:THR:HG22	1:A:234:ASP:N	2.07	0.69
1:B:581:ARG:HD3	1:B:611:ARG:NH1	2.08	0.69
1:A:50:ILE:HG23	1:A:51:ALA:N	2.07	0.68
1:A:51:ALA:HB2	1:A:103:SER:O	1.93	0.68
1:A:565:GLY:O	1:A:567:ASN:N	2.27	0.68
1:A:144:ASN:OD1	1:B:109:VAL:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLU:HG3	1:B:401:ILE:HD12	1.75	0.68
1:A:273:ILE:HD12	1:A:485:ILE:HG21	1.76	0.68
1:B:279:LEU:HD11	1:B:289:HIS:HB2	1.76	0.68
1:A:361:GLU:HG2	1:A:436:MET:CA	2.17	0.68
1:B:528:LEU:HG	1:B:551:PHE:CD2	2.28	0.67
1:A:97:GLU:HB2	1:A:126:GLY:O	1.94	0.67
1:A:292:PHE:O	1:A:453:THR:HG22	1.95	0.67
1:B:62:LEU:CD1	1:B:92:MET:HE2	2.23	0.67
1:B:295:SER:HA	1:B:452:GLN:NE2	2.09	0.67
1:A:236:MET:O	1:A:246:LEU:HD22	1.95	0.67
1:B:288:ILE:HD11	1:B:483:ARG:HD2	1.76	0.67
1:A:322:LEU:HD13	1:A:329:PRO:CG	2.23	0.67
1:B:380:ASN:OD1	1:B:383:VAL:HG23	1.94	0.67
1:B:445:SER:HB3	1:B:455:HIS:CG	2.29	0.67
1:A:152:LEU:HD12	1:A:152:LEU:H	1.59	0.67
1:A:370:LEU:HD13	1:A:370:LEU:O	1.95	0.67
1:B:514:ASN:HB2	1:B:516:LYS:HE3	1.77	0.67
1:A:100:ASP:OD1	1:A:102:GLU:HG2	1.95	0.67
1:A:476:GLY:HA3	2:A:750:FAD:O2P	1.94	0.67
1:B:481:LEU:HD13	1:B:503:TYR:CG	2.30	0.66
1:A:95:ASP:C	1:A:97:GLU:H	2.03	0.66
1:A:95:ASP:OD2	1:A:97:GLU:HB3	1.95	0.66
1:B:573:LYS:HE3	1:B:634:MET:HG2	1.77	0.66
1:A:270:ILE:HD13	1:A:511:LEU:HD22	1.77	0.66
1:A:322:LEU:CD1	1:A:329:PRO:HG3	2.26	0.66
1:B:225:GLN:NE2	1:B:336:LYS:HD3	2.09	0.66
1:B:538:MET:HE3	1:B:576:LEU:HB2	1.77	0.66
1:A:246:LEU:HB2	1:A:249:HIS:CD2	2.28	0.66
1:A:547:PRO:HG2	1:A:644:CYS:SG	2.36	0.66
1:A:625:LYS:HG3	1:A:664:ARG:HH12	1.61	0.66
1:B:130:PHE:CZ	1:B:134:ILE:HD11	2.30	0.66
1:A:646:ASP:OD1	1:A:648:LYS:HG3	1.96	0.66
1:B:352:ILE:HD11	1:B:426:MET:HG3	1.75	0.66
1:B:487:LEU:HD12	1:B:499:LEU:HD22	1.77	0.66
1:B:632:PHE:CE1	1:B:665:GLY:HA3	2.30	0.65
1:A:240:GLU:OE2	1:A:508:PRO:HB3	1.95	0.65
1:B:541:PRO:HD2	1:B:650:MET:HE2	1.77	0.65
1:A:677:ILE:HG22	1:A:681:LYS:HE3	1.77	0.65
1:A:69:THR:HB	3:A:751:FMN:O1P	1.96	0.65
1:A:194:GLU:OE1	1:A:368:ARG:NH1	2.30	0.65
1:B:82:GLU:OE1	1:B:200:LYS:HD2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASP:HB3	1:B:98:ASN:ND2	2.11	0.65
1:B:449:SER:HB3	1:B:557:ALA:CB	2.26	0.65
1:B:51:ALA:HB2	1:B:103:SER:O	1.97	0.65
1:B:59:LYS:HD3	1:B:92:MET:CB	2.15	0.64
1:B:152:LEU:HD12	1:B:152:LEU:H	1.62	0.64
1:B:265:LEU:HG	1:B:522:ARG:HH12	1.62	0.64
1:B:609:HIS:HB3	1:B:612:LEU:HG	1.80	0.64
1:B:327:LEU:HG	1:B:352:ILE:HG21	1.78	0.64
1:B:600:ASP:OD1	1:B:601:GLY:N	2.28	0.64
1:A:278:GLU:OE2	1:A:286:ASN:HB3	1.97	0.64
1:A:425:PRO:HB3	1:A:427:GLN:OE1	1.98	0.64
1:B:100:ASP:OD1	1:B:102:GLU:HG2	1.97	0.64
1:B:400:GLU:O	1:B:401:ILE:HD12	1.98	0.64
1:A:576:LEU:HD21	1:A:605:MET:HE3	1.79	0.64
1:A:562:GLN:HB3	1:A:568:ASN:HA	1.79	0.63
1:B:546:ALA:HB3	1:B:547:PRO:HD3	1.80	0.63
1:A:407:ASN:H	1:A:410:ASP:HB2	1.62	0.63
1:B:327:LEU:HD12	1:B:328:ASP:H	1.62	0.63
1:A:528:LEU:HD22	1:A:555:ARG:NH2	2.14	0.63
1:A:647:ALA:HB3	1:A:690:VAL:HG11	1.79	0.63
1:B:232:ILE:HG22	1:B:232:ILE:O	1.99	0.63
1:A:576:LEU:CD2	1:A:605:MET:HE3	2.29	0.62
1:B:233:THR:HG22	1:B:235:SER:H	1.62	0.62
1:B:327:LEU:CG	1:B:352:ILE:HG21	2.29	0.62
1:A:236:MET:HG2	1:A:349:PRO:HB2	1.81	0.62
1:B:234:ASP:HB3	1:B:247:PRO:HB2	1.79	0.62
1:B:459:ILE:HD13	4:B:753:NAP:H52N	1.81	0.62
1:A:226:TYR:HB2	1:A:427:GLN:CG	2.28	0.62
1:A:489:GLN:HA	1:A:515:TYR:CE1	2.34	0.62
1:B:268:PRO:HD3	1:B:310:TRP:CH2	2.35	0.62
1:B:322:LEU:HD21	1:B:356:ILE:HD12	1.81	0.62
1:B:439:ARG:HB2	1:B:441:TYR:HE1	1.64	0.62
1:B:513:ALA:O	1:B:514:ASN:HB2	2.00	0.62
1:A:288:ILE:HD12	1:A:288:ILE:N	2.15	0.62
1:B:50:ILE:HG23	1:B:51:ALA:N	2.15	0.62
1:B:421:TRP:CD1	1:B:421:TRP:N	2.68	0.62
1:A:363:THR:HG21	1:A:477:VAL:CG2	2.30	0.61
1:A:60:ASN:HD21	1:A:89:LEU:CB	2.07	0.61
1:B:247:PRO:CG	1:B:509:ARG:NH1	2.62	0.61
1:B:274:VAL:CG1	1:B:293:ASP:HB2	2.30	0.61
1:A:59:LYS:HD2	1:A:90:ASN:OD1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG21	1:A:80:SER:OG	2.00	0.61
1:B:544:GLY:O	1:B:547:PRO:HD2	1.99	0.61
1:A:291:GLU:HG2	1:A:455:HIS:CE1	2.35	0.61
1:B:263:PHE:CD2	1:B:269:TYR:HB2	2.36	0.61
1:B:351:THR:HG23	1:B:354:ALA:H	1.66	0.61
1:A:305:ASP:OD1	1:A:523:ARG:HA	2.00	0.61
1:A:371:PHE:HE1	1:A:390:LEU:HD13	1.64	0.61
1:A:535:PRO:HB2	1:A:639:ALA:CB	2.29	0.61
1:A:152:LEU:HD12	1:A:152:LEU:N	2.15	0.61
1:B:301:TYR:CE2	1:B:454:VAL:HG22	2.36	0.61
1:B:179:LEU:HD22	1:B:210:GLU:HG3	1.80	0.61
1:B:307:LEU:HD11	1:B:519:VAL:HG11	1.83	0.61
1:A:228:VAL:O	1:A:229:LEU:HD23	2.01	0.61
1:B:640:PHE:CB	1:B:642:TYR:HE1	2.12	0.61
1:A:118:TYR:O	1:A:119:GLY:C	2.44	0.61
1:B:307:LEU:HD11	1:B:519:VAL:CG1	2.31	0.60
1:B:135:CYS:HA	1:B:170:HIS:CD2	2.36	0.60
1:B:331:THR:HB	1:B:352:ILE:HD12	1.82	0.60
1:B:379:PRO:HD2	1:B:383:VAL:CB	2.31	0.60
1:B:481:LEU:O	1:B:485:ILE:HG13	2.01	0.60
1:A:370:LEU:HD13	1:A:370:LEU:C	2.26	0.60
1:A:279:LEU:HD23	1:A:587:LEU:HD22	1.83	0.60
1:A:628:GLU:HG3	1:A:629:ASP:H	1.67	0.60
1:B:273:ILE:HG12	1:B:292:PHE:CE2	2.36	0.60
1:B:573:LYS:NZ	1:B:633:GLU:OE1	2.35	0.60
1:B:152:LEU:HD12	1:B:152:LEU:N	2.17	0.60
1:B:310:TRP:HB2	1:B:518:PRO:HB2	1.83	0.60
1:B:316:GLU:OE1	1:B:502:HIS:HD2	1.84	0.60
1:B:231:GLU:C	1:B:232:ILE:HD12	2.27	0.60
1:B:339:ASP:OD2	1:B:341:THR:HB	2.01	0.60
1:A:318:VAL:HG13	1:A:356:ILE:CG2	2.32	0.60
1:A:94:ALA:HB1	1:A:99:TYR:CE1	2.37	0.59
1:A:335:LEU:HD11	1:A:430:VAL:HG11	1.84	0.59
1:B:247:PRO:HG2	1:B:509:ARG:HH11	1.66	0.59
1:A:96:VAL:HG21	1:A:130:PHE:CD2	2.37	0.59
1:B:136:ASN:O	1:B:137:ALA:C	2.45	0.59
1:A:105:ASN:OD1	1:A:144:ASN:HB2	2.02	0.59
1:B:185:ALA:CB	1:B:192:THR:HG23	2.31	0.59
1:A:230:ASN:ND2	1:A:231:GLU:HG2	2.16	0.59
1:B:69:THR:HG22	1:B:69:THR:O	2.03	0.59
1:B:528:LEU:HD23	1:B:555:ARG:NH1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:C	1:A:401:ILE:HD12	2.28	0.59
1:A:640:PHE:HB3	1:A:642:TYR:CE1	2.38	0.59
1:B:452:GLN:HB2	5:B:2014:HOH:O	2.03	0.59
1:B:240:GLU:HG2	1:B:245:TYR:O	2.02	0.58
1:B:531:ASN:ND2	1:B:533:SER:HB2	2.18	0.58
1:B:327:LEU:HD21	1:B:352:ILE:HD13	1.85	0.58
1:B:374:LEU:HB2	1:B:387:LEU:HD11	1.84	0.58
1:B:658:LEU:O	1:B:662:LEU:HD13	2.03	0.58
1:A:379:PRO:CD	1:A:383:VAL:HG11	2.25	0.58
1:B:62:LEU:HD11	1:B:92:MET:HE2	1.83	0.58
1:A:232:ILE:HB	1:A:332:ILE:HD11	1.86	0.58
1:B:555:ARG:HG3	1:B:574:HIS:CE1	2.38	0.58
1:B:603:PHE:CD2	1:B:604:GLU:N	2.72	0.58
1:B:363:THR:HG21	1:B:477:VAL:CG2	2.33	0.58
1:B:582:ASN:HD21	1:B:584:ASP:HB2	1.68	0.58
1:A:209:ASP:O	1:A:210:GLU:C	2.46	0.58
1:B:277:ARG:CA	1:B:486:GLN:HE21	2.17	0.58
1:B:346:PHE:HB2	1:B:347:PRO:HD2	1.85	0.58
1:B:60:ASN:O	1:B:109:VAL:HB	2.03	0.57
1:B:276:SER:OG	1:B:486:GLN:HG2	2.03	0.57
1:B:580:SER:HB2	1:B:585:ASP:OD2	2.05	0.57
1:B:95:ASP:OD2	1:B:97:GLU:HB2	2.04	0.57
1:B:484:ASN:ND2	1:B:502:HIS:HA	2.19	0.57
1:A:149:MET:HE1	1:A:168:GLU:HB2	1.86	0.57
1:B:380:ASN:ND2	1:B:382:ASP:N	2.49	0.57
1:A:481:LEU:HB2	1:A:503:TYR:CE2	2.40	0.57
1:B:456:VAL:HG12	1:B:456:VAL:O	2.05	0.57
1:B:646:ASP:O	1:B:647:ALA:CB	2.52	0.57
1:B:600:ASP:C	1:B:602:SER:H	2.13	0.56
1:A:484:ASN:HD22	1:A:503:TYR:H	1.53	0.56
1:A:523:ARG:NH2	5:A:2023:HOH:O	2.37	0.56
1:B:158:GLU:O	1:B:159:PHE:HB2	2.03	0.56
1:A:647:ALA:HB1	1:A:651:ALA:H	1.69	0.56
1:B:88:ASN:HD21	1:B:216:GLN:HE22	1.52	0.56
1:B:139:ALA:O	1:B:141:ALA:N	2.38	0.56
1:B:139:ALA:C	1:B:141:ALA:H	2.13	0.56
1:B:239:GLY:HA3	1:B:358:HIS:CD2	2.40	0.56
1:B:263:PHE:HA	1:B:267:GLN:O	2.05	0.56
1:B:380:ASN:HD21	1:B:382:ASP:H	1.53	0.56
1:A:182:LEU:C	1:A:182:LEU:HD12	2.30	0.56
1:B:59:LYS:HE2	1:B:341:THR:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:O	1:B:471:ALA:HB3	2.06	0.56
1:A:138:GLU:CG	1:A:139:ALA:H	2.19	0.56
1:A:238:LEU:HD12	1:A:509:ARG:NE	2.20	0.55
1:A:375:ILE:HG22	1:A:384:LYS:HG3	1.88	0.55
1:A:513:ALA:O	1:A:516:LYS:HG3	2.06	0.55
1:B:247:PRO:CG	1:B:509:ARG:HH11	2.19	0.55
1:B:352:ILE:CD1	1:B:426:MET:HG3	2.36	0.55
1:B:301:TYR:CD1	1:B:301:TYR:C	2.84	0.55
1:B:322:LEU:CD2	1:B:356:ILE:HD12	2.36	0.55
1:B:474:VAL:HG12	2:B:750:FAD:O2B	2.06	0.55
1:B:562:GLN:HB3	1:B:568:ASN:HB3	1.88	0.55
1:B:625:LYS:HG3	1:B:664:ARG:HH22	1.71	0.55
1:A:537:ILE:HA	1:A:575:ILE:CG2	2.37	0.55
1:B:50:ILE:CD1	1:B:92:MET:HE1	2.37	0.55
1:A:115:ILE:HG23	1:A:164:ALA:HB2	1.88	0.55
1:B:110:ILE:HD12	1:B:211:LEU:HD21	1.87	0.55
1:B:130:PHE:CE1	1:B:134:ILE:HD11	2.42	0.55
1:B:277:ARG:HA	1:B:486:GLN:HE21	1.72	0.55
1:B:620:VAL:O	1:B:624:LEU:HG	2.07	0.55
1:A:50:ILE:CG2	1:A:51:ALA:H	2.16	0.54
1:A:65:TYR:CZ	1:A:73:GLU:HG3	2.42	0.54
1:B:60:ASN:OD1	1:B:90:ASN:N	2.39	0.54
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.07	0.54
1:A:270:ILE:CD1	1:A:511:LEU:HD22	2.37	0.54
1:A:473:PRO:O	1:A:475:VAL:HG13	2.08	0.54
1:B:220:PHE:N	1:B:376:GLN:NE2	2.51	0.54
1:B:231:GLU:OE1	1:B:231:GLU:N	2.37	0.54
1:B:313:ASN:CG	1:B:436:MET:HE1	2.31	0.54
1:B:635:ILE:C	1:B:637:ASN:H	2.15	0.54
1:A:48:ARG:NH1	1:A:100:ASP:HB2	2.22	0.54
1:B:247:PRO:O	1:B:249:HIS:N	2.39	0.54
1:A:85:ALA:O	1:A:218:ALA:HA	2.07	0.54
1:A:280:PHE:CD2	1:A:585:ASP:HA	2.43	0.54
1:A:322:LEU:HD21	1:A:356:ILE:HD12	1.89	0.54
1:B:346:PHE:HB2	1:B:347:PRO:CD	2.37	0.54
1:A:211:LEU:CB	1:A:213:LEU:HG	2.36	0.54
1:A:445:SER:HB3	1:A:455:HIS:CG	2.43	0.54
1:A:355:ALA:HA	1:A:359:TYR:CD1	2.43	0.54
1:B:314:PRO:HB3	1:B:501:VAL:HB	1.89	0.54
1:B:576:LEU:CD2	1:B:605:MET:HE3	2.38	0.54
1:B:199:TRP:CZ2	1:B:203:ILE:HG13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD11	1:B:430:VAL:HG11	1.88	0.54
1:B:449:SER:C	1:B:450:GLU:HG3	2.33	0.54
1:B:476:GLY:HA3	2:B:750:FAD:O2P	2.07	0.54
1:B:594:GLU:O	1:B:597:LYS:HB2	2.07	0.54
1:B:627:TYR:O	1:B:631:VAL:HG23	2.08	0.54
1:B:161:ASN:ND2	1:B:164:ALA:HB3	2.22	0.54
1:B:330:GLU:O	1:B:331:THR:C	2.49	0.54
1:A:279:LEU:HB2	1:A:287:CYS:O	2.07	0.54
1:A:310:TRP:HB2	1:A:518:PRO:HB2	1.90	0.54
1:B:92:MET:HG3	1:B:341:THR:OG1	2.07	0.54
1:B:363:THR:HA	1:B:407:ASN:OD1	2.08	0.54
1:B:623:LYS:HE2	1:B:623:LYS:CA	2.32	0.54
1:A:346:PHE:HB2	1:A:347:PRO:CD	2.39	0.53
1:A:462:ASN:OD1	1:A:475:VAL:HG12	2.08	0.53
1:B:533:SER:O	1:B:572:GLY:HA3	2.08	0.53
1:A:460:VAL:HA	1:A:479:THR:HB	1.88	0.53
1:A:485:ILE:HG23	1:A:515:TYR:CD2	2.43	0.53
1:A:529:PRO:HG3	1:A:640:PHE:CG	2.43	0.53
1:B:555:ARG:HG3	1:B:574:HIS:HE1	1.72	0.53
1:A:105:ASN:ND2	1:A:142:LEU:CA	2.70	0.53
1:A:289:HIS:HD1	1:A:588:TYR:HE2	1.55	0.53
1:A:324:ILE:HG23	1:A:325:PHE:CD2	2.44	0.53
1:B:364:GLY:N	1:B:407:ASN:OD1	2.41	0.53
1:B:407:ASN:H	1:B:410:ASP:HB2	1.72	0.53
1:B:487:LEU:HD22	1:B:497:THR:HG21	1.89	0.53
1:A:580:SER:O	1:A:609:HIS:HA	2.09	0.53
1:B:156:THR:HG21	1:B:647:ALA:O	2.08	0.53
1:B:540:GLY:HA2	1:B:644:CYS:O	2.09	0.53
1:A:96:VAL:HG21	1:A:130:PHE:CG	2.43	0.53
1:A:501:VAL:HG23	1:A:503:TYR:CE1	2.44	0.53
1:A:647:ALA:HA	1:A:650:MET:HB3	1.89	0.53
1:B:623:LYS:HA	1:B:626:ASP:HB2	1.90	0.53
1:B:173:ALA:C	1:B:175:GLY:H	2.15	0.53
1:B:333:PHE:CD2	1:B:352:ILE:HG13	2.43	0.53
1:B:430:VAL:HG12	1:B:430:VAL:O	2.09	0.53
1:A:191:THR:O	1:A:192:THR:C	2.52	0.53
1:A:258:ILE:HG22	1:A:258:ILE:O	2.08	0.53
1:B:265:LEU:CD2	1:B:522:ARG:HH12	2.21	0.53
1:A:390:LEU:CD2	1:A:396:GLN:HG2	2.39	0.52
1:A:612:LEU:HD23	1:A:613:PRO:CD	2.32	0.52
1:B:98:ASN:HB2	1:B:99:TYR:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:VAL:HG23	1:B:275:LYS:N	2.24	0.52
1:A:599:LEU:O	1:A:600:ASP:HB2	2.10	0.52
1:B:519:VAL:HG12	1:B:520:HIS:N	2.23	0.52
1:B:330:GLU:O	1:B:332:ILE:HD12	2.09	0.52
1:A:109:VAL:HG12	1:B:144:ASN:HD21	1.74	0.52
1:A:240:GLU:HG2	1:A:245:TYR:O	2.08	0.52
1:B:104:LEU:O	1:B:107:VAL:HG23	2.10	0.52
1:B:105:ASN:OD1	1:B:144:ASN:HB2	2.08	0.52
1:A:407:ASN:HB2	1:A:410:ASP:OD2	2.10	0.52
1:A:363:THR:HG21	1:A:477:VAL:HG21	1.91	0.52
1:B:310:TRP:CD1	1:B:310:TRP:N	2.77	0.52
1:B:611:ARG:NH1	1:B:611:ARG:HG3	2.25	0.52
1:A:247:PRO:C	1:A:249:HIS:H	2.17	0.52
1:A:578:TYR:CG	1:A:579:GLY:N	2.77	0.52
1:B:49:ASP:O	1:B:53:VAL:HG23	2.09	0.52
1:B:66:ALA:HB2	1:B:96:VAL:HG11	1.92	0.52
1:B:539:ILE:HD13	1:B:624:LEU:HD11	1.92	0.52
1:B:576:LEU:HD12	1:B:576:LEU:C	2.35	0.52
1:A:113:ILE:O	1:A:149:MET:HG3	2.09	0.52
1:A:621:GLN:NE2	4:A:753:NAP:N1A	2.58	0.52
1:B:357:LYS:HG2	1:B:358:HIS:CE1	2.45	0.52
1:B:437:THR:HG23	1:B:438:PRO:HD2	1.91	0.52
1:A:374:LEU:O	1:A:375:ILE:C	2.53	0.52
1:A:529:PRO:HD3	1:A:642:TYR:HH	1.75	0.52
1:B:59:LYS:HG2	1:B:90:ASN:HD22	1.75	0.52
1:B:73:GLU:CG	1:B:77:LYS:HE3	2.39	0.52
1:B:117:THR:HA	1:B:163:ALA:HB2	1.92	0.52
1:B:223:GLN:HB2	1:B:342:VAL:HG21	1.92	0.52
1:A:240:GLU:CD	1:A:240:GLU:H	2.18	0.51
1:A:406:PHE:HD1	1:A:411:ALA:HA	1.76	0.51
1:B:59:LYS:CG	1:B:90:ASN:HD22	2.22	0.51
1:B:646:ASP:O	1:B:647:ALA:HB3	2.11	0.51
1:A:268:PRO:HB3	1:A:310:TRP:CE2	2.46	0.51
1:B:260:LEU:O	1:B:263:PHE:CZ	2.63	0.51
1:A:677:ILE:CG2	1:A:681:LYS:HE3	2.40	0.51
1:B:61:TYR:HD2	1:B:62:LEU:N	2.09	0.51
1:B:274:VAL:HG13	1:B:293:ASP:HB2	1.91	0.51
1:B:513:ALA:O	1:B:516:LYS:HE3	2.10	0.51
1:A:209:ASP:O	1:A:212:HIS:HD2	1.93	0.51
1:A:390:LEU:HD23	1:A:396:GLN:HG2	1.91	0.51
1:A:538:MET:HE1	1:A:552:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:CD1	1:B:211:LEU:HD21	2.40	0.51
1:B:528:LEU:HD23	1:B:555:ARG:HH11	1.75	0.51
1:B:568:ASN:O	1:B:569:VAL:C	2.54	0.51
1:B:674:THR:O	1:B:677:ILE:HB	2.09	0.51
1:A:345:PRO:HB3	1:A:435:GLN:OE1	2.11	0.51
1:B:316:GLU:OE1	1:B:502:HIS:CD2	2.64	0.51
1:B:247:PRO:HG2	1:B:509:ARG:HH12	1.74	0.51
1:B:390:LEU:HD21	1:B:400:GLU:CG	2.41	0.51
1:A:548:PHE:O	1:A:552:ILE:HD13	2.10	0.51
1:B:519:VAL:CG1	1:B:520:HIS:N	2.74	0.51
1:B:265:LEU:CG	1:B:522:ARG:HH12	2.22	0.51
1:B:531:ASN:HD21	1:B:533:SER:HB2	1.76	0.51
1:A:437:THR:HG22	1:A:438:PRO:O	2.11	0.51
1:B:603:PHE:HD2	1:B:604:GLU:N	2.07	0.51
1:A:95:ASP:O	1:A:97:GLU:N	2.43	0.50
1:A:484:ASN:ND2	1:A:503:TYR:H	2.07	0.50
1:A:599:LEU:CD1	1:A:603:PHE:HB2	2.37	0.50
1:A:621:GLN:HE21	4:A:753:NAP:C2A	2.23	0.50
1:A:95:ASP:CB	1:A:98:ASN:ND2	2.74	0.50
1:A:324:ILE:HD11	1:A:413:LYS:HA	1.92	0.50
1:A:407:ASN:O	1:A:408:ILE:C	2.54	0.50
1:B:62:LEU:HD12	1:B:92:MET:O	2.11	0.50
1:B:148:ASN:ND2	1:B:207:LEU:HD21	2.25	0.50
1:A:518:PRO:C	1:A:519:VAL:HG23	2.36	0.50
1:A:519:VAL:HG12	1:A:520:HIS:N	2.25	0.50
1:A:611:ARG:NE	4:A:753:NAP:O3X	2.44	0.50
1:B:577:PHE:CE2	1:B:624:LEU:HD23	2.46	0.50
1:B:666:LYS:HE3	1:B:676:LEU:HD21	1.92	0.50
1:A:149:MET:CE	1:A:168:GLU:HB2	2.41	0.50
1:A:565:GLY:C	1:A:567:ASN:H	2.20	0.50
1:A:647:ALA:CB	1:A:690:VAL:CG1	2.83	0.50
1:B:313:ASN:ND2	1:B:362:ILE:HG12	2.26	0.50
1:B:632:PHE:CZ	1:B:665:GLY:HA3	2.45	0.50
1:A:259:GLN:O	1:A:297:SER:HA	2.11	0.50
1:B:531:ASN:C	1:B:533:SER:H	2.20	0.50
1:B:534:THR:HG23	1:B:638:GLY:O	2.11	0.50
1:A:233:THR:HB	1:A:236:MET:SD	2.51	0.50
1:B:400:GLU:HG3	1:B:401:ILE:CD1	2.41	0.50
1:B:460:VAL:HA	1:B:479:THR:HB	1.94	0.50
1:B:118:TYR:O	1:B:119:GLY:C	2.55	0.50
1:B:379:PRO:CD	1:B:383:VAL:HG11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ARG:O	1:B:510:LYS:C	2.55	0.50
1:B:595:TYR:C	1:B:597:LYS:H	2.20	0.50
1:A:107:VAL:HG12	1:A:109:VAL:H	1.77	0.50
1:A:508:PRO:HD2	1:A:511:LEU:HB3	1.94	0.50
1:A:596:ALA:HA	1:A:603:PHE:HD1	1.77	0.50
1:A:645:GLY:O	1:A:690:VAL:HG13	2.12	0.50
1:B:576:LEU:HD23	1:B:605:MET:HE3	1.93	0.50
1:A:288:ILE:N	1:A:288:ILE:CD1	2.74	0.49
1:A:316:GLU:O	1:A:320:GLN:HG3	2.12	0.49
1:A:319:GLU:HA	1:A:319:GLU:OE1	2.12	0.49
1:B:450:GLU:OE2	1:B:553:ARG:CZ	2.60	0.49
1:B:579:GLY:O	1:B:580:SER:HB3	2.11	0.49
1:B:99:TYR:CD1	1:B:99:TYR:N	2.80	0.49
1:A:352:ILE:HG12	1:A:426:MET:HE2	1.94	0.49
1:A:570:SER:O	1:A:571:LEU:HB2	2.12	0.49
1:B:551:PHE:CE2	1:B:642:TYR:CE2	3.00	0.49
1:B:611:ARG:HG3	1:B:611:ARG:HH11	1.78	0.49
1:A:119:GLY:HA3	1:A:122:ASP:OD1	2.12	0.49
1:A:485:ILE:HG12	1:A:505:LEU:HD22	1.95	0.49
1:A:608:ALA:HB1	1:A:618:VAL:CG1	2.43	0.49
1:B:264:ASP:CG	1:B:265:LEU:HD12	2.38	0.49
1:B:361:GLU:CG	1:B:436:MET:HA	2.41	0.49
1:B:551:PHE:HE2	1:B:642:TYR:CE2	2.30	0.49
1:B:646:ASP:O	1:B:691:TRP:O	2.30	0.49
1:A:239:GLY:HA3	1:A:358:HIS:CD2	2.48	0.49
1:A:548:PHE:HA	1:A:551:PHE:HB2	1.93	0.49
1:B:684:GLY:O	1:B:687:GLN:HG3	2.12	0.49
1:A:138:GLU:HG3	1:A:139:ALA:N	2.24	0.49
1:A:233:THR:CG2	1:A:234:ASP:N	2.76	0.49
1:B:61:TYR:HE1	1:B:207:LEU:HD13	1.77	0.49
1:B:161:ASN:HD21	1:B:164:ALA:HB3	1.76	0.49
1:B:548:PHE:HA	1:B:551:PHE:HB2	1.93	0.49
1:B:655:SER:O	1:B:659:VAL:HG23	2.12	0.49
1:B:534:THR:HG21	1:B:640:PHE:CE1	2.47	0.49
1:B:263:PHE:O	1:B:264:ASP:HB3	2.12	0.49
1:B:443:ILE:HD13	1:B:454:VAL:HG13	1.94	0.48
1:A:478:THR:N	2:A:750:FAD:O1P	2.44	0.48
1:A:542:GLY:O	1:A:543:THR:C	2.56	0.48
1:B:264:ASP:HA	1:B:520:HIS:CG	2.48	0.48
1:B:540:GLY:HA3	1:B:548:PHE:CE1	2.37	0.48
1:B:651:ALA:O	1:B:655:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HA	1:A:185:ALA:HB3	1.95	0.48
1:B:369:GLN:O	1:B:373:SER:OG	2.32	0.48
1:B:455:HIS:CD2	1:B:549:ARG:HH12	2.31	0.48
1:B:591:GLU:O	1:B:594:GLU:HB2	2.14	0.48
1:A:323:SER:O	1:A:326:ASN:N	2.44	0.48
1:B:238:LEU:HD23	1:B:351:THR:HG22	1.94	0.48
1:B:352:ILE:HG12	1:B:426:MET:HE2	1.94	0.48
1:B:277:ARG:C	1:B:486:GLN:HE21	2.22	0.48
1:B:321:PHE:HD2	1:B:356:ILE:HD13	1.78	0.48
1:A:314:PRO:HB3	1:A:501:VAL:HB	1.95	0.48
1:A:532:PRO:HA	1:A:555:ARG:NH2	2.28	0.48
1:A:238:LEU:HD12	1:A:509:ARG:CD	2.43	0.48
1:A:263:PHE:HA	1:A:267:GLN:O	2.14	0.48
1:A:475:VAL:HB	1:A:480:ASN:ND2	2.28	0.48
1:A:582:ASN:HD22	1:A:582:ASN:N	2.12	0.48
1:A:609:HIS:HB2	1:A:612:LEU:HD12	1.95	0.48
1:A:95:ASP:C	1:A:97:GLU:N	2.67	0.48
1:A:272:PRO:HB3	1:A:516:LYS:HE3	1.96	0.48
1:A:325:PHE:CE1	1:A:429:LEU:HD21	2.49	0.48
1:A:355:ALA:O	1:A:360:LEU:HG	2.13	0.48
1:A:552:ILE:O	1:A:556:VAL:HG23	2.14	0.48
1:B:216:GLN:HG3	1:B:217:GLU:N	2.29	0.48
1:B:539:ILE:CD1	1:B:624:LEU:HD11	2.44	0.48
1:A:123:PHE:CD1	1:A:123:PHE:N	2.82	0.48
1:A:211:LEU:HD12	1:A:213:LEU:HD11	1.95	0.48
1:A:379:PRO:HD2	1:A:383:VAL:CG1	2.30	0.48
1:A:440:TYR:CD1	1:A:440:TYR:N	2.82	0.48
1:A:594:GLU:HA	1:A:594:GLU:OE2	2.14	0.48
1:B:301:TYR:CD2	1:B:454:VAL:HG22	2.49	0.48
1:B:542:GLY:O	1:B:544:GLY:N	2.46	0.48
1:A:537:ILE:HA	1:A:575:ILE:HG23	1.96	0.47
1:A:588:TYR:O	1:A:589:GLN:C	2.57	0.47
1:B:117:THR:C	1:B:118:TYR:CD1	2.92	0.47
1:B:529:PRO:HG3	1:B:640:PHE:CG	2.49	0.47
1:B:531:ASN:C	1:B:533:SER:N	2.71	0.47
1:B:582:ASN:CG	1:B:583:THR:N	2.68	0.47
1:A:158:GLU:HB3	1:A:159:PHE:HD1	1.78	0.47
1:B:164:ALA:O	1:B:165:LYS:C	2.58	0.47
1:B:117:THR:O	1:B:118:TYR:CD1	2.67	0.47
1:A:274:VAL:CG1	1:A:293:ASP:HB2	2.44	0.47
1:B:578:TYR:CG	1:B:579:GLY:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MET:HE3	1:A:164:ALA:HB1	1.97	0.47
1:A:233:THR:HG22	1:A:235:SER:H	1.78	0.47
1:B:241:PRO:O	1:B:347:PRO:HG2	2.14	0.47
1:B:411:ALA:O	1:B:414:TYR:HB3	2.14	0.47
1:B:484:ASN:ND2	1:B:503:TYR:H	2.13	0.47
1:A:404:LYS:HB3	1:A:406:PHE:CE2	2.50	0.47
1:B:50:ILE:HD12	1:B:92:MET:HE1	1.96	0.47
1:B:73:GLU:HG2	1:B:77:LYS:HE3	1.97	0.47
1:B:224:PHE:CZ	1:B:345:PRO:HD3	2.49	0.47
1:A:216:GLN:HG3	1:A:217:GLU:O	2.15	0.47
1:A:325:PHE:HE2	1:A:412:LEU:HD12	1.79	0.47
1:A:494:ILE:O	1:A:497:THR:OG1	2.30	0.47
1:A:528:LEU:HD22	1:A:555:ARG:CZ	2.44	0.47
1:B:62:LEU:HD13	1:B:92:MET:HE2	1.95	0.47
1:B:84:VAL:HG22	1:B:89:LEU:O	2.15	0.47
1:B:265:LEU:CD2	1:B:522:ARG:NH1	2.78	0.47
1:B:294:LEU:HG	1:B:454:VAL:HG23	1.96	0.47
1:A:333:PHE:CD1	1:A:333:PHE:C	2.92	0.47
1:B:272:PRO:HB3	1:B:516:LYS:HG2	1.95	0.47
1:B:324:ILE:HD11	1:B:413:LYS:HA	1.96	0.47
1:B:347:PRO:HD2	1:B:359:TYR:CZ	2.49	0.47
1:B:400:GLU:O	1:B:401:ILE:CD1	2.63	0.47
1:B:501:VAL:HG23	1:B:503:TYR:CE1	2.50	0.47
1:A:372:SER:HB2	1:A:391:SER:HB2	1.95	0.47
1:A:499:LEU:HD12	1:A:500:PRO:HD2	1.96	0.47
1:A:686:TYR:C	1:A:686:TYR:CD2	2.92	0.47
1:B:647:ALA:HB2	1:B:690:VAL:CG2	2.45	0.47
1:B:63:VAL:HG23	1:B:91:VAL:CG1	2.44	0.47
1:B:257:GLY:O	1:B:258:ILE:C	2.58	0.47
1:A:87:PHE:CD2	1:A:213:LEU:HB3	2.49	0.46
1:B:380:ASN:HD21	1:B:382:ASP:CB	2.28	0.46
1:B:483:ARG:NH2	1:B:498:ASN:OD1	2.46	0.46
1:B:493:ASN:OD1	1:B:495:ALA:HB3	2.14	0.46
1:A:70:GLY:O	1:A:74:ASP:N	2.46	0.46
1:A:422:ASP:OD1	1:A:422:ASP:O	2.31	0.46
1:B:247:PRO:C	1:B:249:HIS:N	2.73	0.46
1:B:499:LEU:HD12	1:B:500:PRO:HD2	1.97	0.46
1:B:633:GLU:O	1:B:634:MET:C	2.58	0.46
1:A:233:THR:CG2	1:A:234:ASP:H	2.25	0.46
1:A:660:GLY:HA3	1:A:664:ARG:HH21	1.80	0.46
1:B:59:LYS:HE2	1:B:341:THR:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLY:HA2	5:B:2001:HOH:O	2.15	0.46
1:B:619:TYR:O	1:B:622:ASP:HB2	2.15	0.46
1:B:673:ALA:O	1:B:677:ILE:HG12	2.15	0.46
1:A:563:LYS:C	1:A:565:GLY:H	2.24	0.46
1:A:69:THR:O	1:A:69:THR:HG22	2.16	0.46
1:A:393:ASP:O	1:A:394:LYS:C	2.57	0.46
1:B:156:THR:O	1:B:652:LYS:HG3	2.16	0.46
1:B:310:TRP:O	1:B:518:PRO:HD2	2.15	0.46
1:B:333:PHE:C	1:B:333:PHE:CD1	2.93	0.46
1:B:390:LEU:C	1:B:392:LYS:N	2.73	0.46
1:A:136:ASN:O	1:A:137:ALA:C	2.58	0.46
1:A:268:PRO:HB3	1:A:310:TRP:CZ2	2.51	0.46
1:A:541:PRO:HG3	1:A:620:VAL:HG21	1.97	0.46
1:A:552:ILE:HD12	1:A:552:ILE:N	2.31	0.46
1:A:197:MET:O	1:A:200:LYS:HB3	2.15	0.46
1:B:482:LEU:HA	1:B:485:ILE:CD1	2.31	0.46
1:A:406:PHE:CD1	1:A:411:ALA:HA	2.51	0.46
1:A:485:ILE:O	1:A:486:GLN:C	2.58	0.46
1:B:87:PHE:CB	1:B:89:LEU:HD12	2.39	0.46
1:A:531:ASN:C	1:A:533:SER:H	2.22	0.46
1:A:582:ASN:N	1:A:582:ASN:ND2	2.62	0.46
1:B:105:ASN:HB2	5:B:2002:HOH:O	2.16	0.46
1:B:154:ASN:ND2	1:B:188:GLY:HA2	2.31	0.46
1:B:265:LEU:HD23	1:B:522:ARG:HH22	1.81	0.46
1:B:533:SER:HA	1:B:572:GLY:H	1.81	0.46
1:B:662:LEU:HD22	1:B:677:ILE:HD11	1.96	0.46
1:A:481:LEU:HD13	1:A:503:TYR:CD2	2.51	0.46
1:B:48:ARG:HG2	1:B:98:ASN:O	2.16	0.46
1:B:66:ALA:O	1:B:124:PRO:HG2	2.16	0.46
1:B:374:LEU:O	1:B:375:ILE:C	2.59	0.46
1:B:440:TYR:CD1	1:B:440:TYR:N	2.83	0.46
1:A:82:GLU:HA	1:A:85:ALA:HB3	1.98	0.45
1:A:274:VAL:O	1:A:275:LYS:HG3	2.15	0.45
1:A:541:PRO:HG3	1:A:620:VAL:CG2	2.46	0.45
1:B:50:ILE:O	1:B:54:VAL:HG23	2.16	0.45
1:B:63:VAL:HG21	1:B:80:SER:HB2	1.98	0.45
1:B:91:VAL:HG12	1:B:92:MET:N	2.31	0.45
1:A:88:ASN:ND2	1:A:216:GLN:OE1	2.48	0.45
1:A:291:GLU:HG2	1:A:455:HIS:ND1	2.30	0.45
1:A:493:ASN:HD22	1:A:496:GLU:HB2	1.74	0.45
1:B:404:LYS:HB3	1:B:406:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:CG2	1:B:130:PHE:CG	3.00	0.45
1:B:327:LEU:CD2	1:B:352:ILE:HD13	2.47	0.45
1:A:135:CYS:HA	1:A:170:HIS:CD2	2.52	0.45
1:A:455:HIS:HD2	1:A:549:ARG:HH12	1.64	0.45
1:A:644:CYS:SG	1:A:645:GLY:N	2.89	0.45
1:B:95:ASP:OD2	1:B:97:GLU:CB	2.64	0.45
1:B:390:LEU:C	1:B:392:LYS:H	2.24	0.45
1:A:65:TYR:CE1	1:A:73:GLU:HG3	2.51	0.45
1:A:158:GLU:HB3	1:A:159:PHE:CD1	2.51	0.45
1:A:487:LEU:HD22	1:A:497:THR:HG21	1.98	0.45
1:B:223:GLN:C	1:B:338:LEU:HD12	2.41	0.45
1:B:223:GLN:HA	1:B:338:LEU:HD12	1.97	0.45
1:B:321:PHE:CD2	1:B:356:ILE:HD13	2.51	0.45
1:A:62:LEU:HD11	1:A:64:LEU:HD21	1.99	0.45
1:A:298:ASN:OD1	1:A:298:ASN:N	2.46	0.45
1:A:522:ARG:NH2	5:A:2022:HOH:O	2.33	0.45
1:B:69:THR:HB	3:B:751:FMN:O1P	2.17	0.45
1:B:379:PRO:HD3	1:B:383:VAL:HG11	1.99	0.45
1:A:263:PHE:CD2	1:A:269:TYR:HB2	2.51	0.45
1:A:316:GLU:OE2	1:A:316:GLU:N	2.42	0.45
1:A:481:LEU:O	1:A:485:ILE:HG13	2.17	0.45
1:A:647:ALA:HB2	1:A:690:VAL:CG1	2.37	0.45
1:B:150:PHE:CZ	1:B:196:TYR:HA	2.52	0.45
1:B:484:ASN:HD22	1:B:503:TYR:HD1	1.63	0.45
1:B:586:PHE:CE2	1:B:589:GLN:HA	2.52	0.45
1:B:600:ASP:CG	1:B:601:GLY:H	2.24	0.45
1:A:123:PHE:N	1:A:123:PHE:HD1	2.14	0.45
1:A:153:GLY:HA2	3:A:751:FMN:O2'	2.16	0.45
1:A:274:VAL:HG11	1:A:293:ASP:HB2	1.99	0.45
1:A:343:LYS:HE3	5:A:2002:HOH:O	2.17	0.45
1:A:346:PHE:HB2	1:A:347:PRO:HD2	1.99	0.45
1:B:218:ALA:O	1:B:219:LYS:HG3	2.17	0.45
1:B:324:ILE:HG23	1:B:325:PHE:CD2	2.51	0.45
1:B:356:ILE:HG22	1:B:356:ILE:O	2.15	0.45
1:B:96:VAL:HG21	1:B:130:PHE:CG	2.51	0.44
1:B:425:PRO:O	1:B:428:PHE:HB3	2.17	0.44
1:B:597:LYS:C	1:B:599:LEU:H	2.26	0.44
1:B:597:LYS:C	1:B:599:LEU:N	2.75	0.44
1:B:616:LYS:O	1:B:618:VAL:HG23	2.16	0.44
1:A:115:ILE:CD1	1:A:163:ALA:HB1	2.44	0.44
1:A:421:TRP:N	1:A:421:TRP:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ALA:O	1:B:191:THR:HG23	2.17	0.44
1:B:669:THR:OG1	1:B:672:GLU:HG3	2.17	0.44
1:A:423:THR:O	1:A:425:PRO:HD3	2.17	0.44
1:B:166:LYS:O	1:B:167:ALA:C	2.61	0.44
1:B:276:SER:CB	1:B:486:GLN:HG2	2.47	0.44
1:A:74:ASP:OD1	1:A:434:PRO:HG3	2.17	0.44
1:A:226:TYR:CB	1:A:427:GLN:CG	2.95	0.44
1:A:333:PHE:O	1:A:349:PRO:HB3	2.17	0.44
1:A:690:VAL:HG12	1:A:691:TRP:N	2.32	0.44
1:B:412:LEU:O	1:B:413:LYS:C	2.60	0.44
1:B:450:GLU:OE2	1:B:553:ARG:NH1	2.49	0.44
1:B:380:ASN:HD21	1:B:382:ASP:HB3	1.82	0.44
1:B:445:SER:HB3	1:B:455:HIS:ND1	2.32	0.44
1:B:538:MET:HE3	1:B:538:MET:HB2	1.80	0.44
1:A:107:VAL:HA	1:A:108:PRO:HD3	1.74	0.44
1:A:232:ILE:O	1:A:232:ILE:HG13	2.18	0.44
1:A:275:LYS:HD2	1:A:291:GLU:OE1	2.17	0.44
1:A:546:ALA:HB3	1:A:547:PRO:HD3	2.00	0.44
1:B:138:GLU:H	1:B:138:GLU:CD	2.26	0.44
1:B:232:ILE:HA	1:B:236:MET:HE1	1.99	0.44
1:A:350:THR:OG1	1:A:351:THR:N	2.51	0.44
1:B:185:ALA:HB1	1:B:192:THR:HA	2.00	0.44
1:B:223:GLN:HG2	1:B:431:GLU:CD	2.43	0.44
1:B:247:PRO:C	1:B:249:HIS:H	2.26	0.44
1:B:289:HIS:CE1	1:B:455:HIS:CD2	3.06	0.44
1:B:333:PHE:HD2	1:B:352:ILE:HG13	1.82	0.44
1:A:50:ILE:HD12	1:A:92:MET:HE1	1.99	0.44
1:A:54:VAL:O	1:A:59:LYS:HG2	2.18	0.44
1:A:173:ALA:C	1:A:175:GLY:H	2.24	0.44
1:A:518:PRO:O	1:A:519:VAL:CG2	2.66	0.44
1:B:129:ASN:ND2	1:B:129:ASN:H	2.16	0.44
1:B:211:LEU:HB2	1:B:213:LEU:HG	1.99	0.44
1:A:240:GLU:OE2	1:A:508:PRO:CB	2.65	0.44
1:A:322:LEU:HD22	1:A:329:PRO:HG3	1.99	0.44
1:B:157:TYR:CE2	1:B:690:VAL:HG12	2.53	0.44
1:A:87:PHE:HD2	1:A:213:LEU:HB3	1.83	0.43
1:A:96:VAL:CG2	1:A:130:PHE:CG	3.01	0.43
1:B:405:TYR:CD1	1:B:405:TYR:N	2.86	0.43
1:B:483:ARG:O	1:B:484:ASN:C	2.60	0.43
1:A:61:TYR:HB3	1:A:91:VAL:HG22	2.01	0.43
1:A:224:PHE:CZ	1:A:345:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:PHE:HE1	1:B:390:LEU:HD13	1.84	0.43
1:B:594:GLU:O	1:B:595:TYR:C	2.62	0.43
1:A:411:ALA:O	1:A:414:TYR:HB3	2.17	0.43
1:A:436:MET:CE	1:A:477:VAL:HG11	2.49	0.43
1:B:332:ILE:HD12	1:B:332:ILE:N	2.33	0.43
1:B:599:LEU:O	1:B:602:SER:HB2	2.18	0.43
1:A:51:ALA:O	1:A:55:THR:HG23	2.19	0.43
1:A:132:ASP:O	1:A:133:PHE:C	2.61	0.43
1:A:170:HIS:O	1:A:171:LEU:C	2.59	0.43
1:B:487:LEU:CD2	1:B:497:THR:HG21	2.48	0.43
1:B:528:LEU:HB3	1:B:555:ARG:HH12	1.83	0.43
1:B:536:VAL:HB	1:B:574:HIS:CD2	2.53	0.43
1:A:531:ASN:C	1:A:533:SER:N	2.76	0.43
1:A:608:ALA:HB1	1:A:618:VAL:HG13	2.00	0.43
1:B:441:TYR:HH	2:B:750:FAD:HO4'	1.64	0.43
1:B:654:VAL:O	1:B:657:ALA:HB3	2.18	0.43
1:A:385:GLU:O	1:A:389:LEU:HG	2.18	0.43
1:A:404:LYS:HD3	1:A:406:PHE:CZ	2.54	0.43
1:A:581:ARG:NH1	1:A:611:ARG:HH12	2.17	0.43
1:A:686:TYR:C	1:A:686:TYR:HD2	2.25	0.43
1:B:329:PRO:O	1:B:351:THR:OG1	2.36	0.43
1:B:603:PHE:HD2	1:B:604:GLU:H	1.65	0.43
1:A:209:ASP:O	1:A:212:HIS:CD2	2.72	0.43
1:A:519:VAL:CG1	1:A:520:HIS:N	2.81	0.43
1:B:440:TYR:OH	1:B:522:ARG:NH2	2.51	0.43
1:B:595:TYR:C	1:B:597:LYS:N	2.77	0.43
1:B:609:HIS:CB	1:B:612:LEU:HG	2.46	0.43
1:B:675:GLU:O	1:B:676:LEU:C	2.59	0.43
1:A:108:PRO:HB2	1:B:144:ASN:HD22	1.84	0.43
1:A:226:TYR:CB	1:A:427:GLN:HG2	2.46	0.43
1:A:338:LEU:O	1:A:339:ASP:HB3	2.18	0.43
1:A:558:PHE:CE2	1:A:562:GLN:HG3	2.54	0.43
1:B:138:GLU:O	1:B:141:ALA:CB	2.67	0.43
1:B:173:ALA:C	1:B:175:GLY:N	2.74	0.43
1:B:317:LYS:O	1:B:318:VAL:C	2.62	0.43
1:B:646:ASP:OD1	1:B:648:LYS:HB3	2.19	0.43
1:B:686:TYR:C	1:B:686:TYR:CD2	2.96	0.43
1:A:159:PHE:CD1	1:A:159:PHE:N	2.86	0.43
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.92	0.43
1:B:305:ASP:OD1	1:B:527:ARG:NH2	2.48	0.43
1:B:597:LYS:O	1:B:599:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASP:N	1:A:267:GLN:O	2.48	0.42
1:A:440:TYR:CE2	1:A:522:ARG:NH2	2.87	0.42
1:A:556:VAL:O	1:A:560:GLU:HB2	2.19	0.42
1:B:265:LEU:HG	1:B:522:ARG:NH1	2.33	0.42
1:B:308:ALA:HA	1:B:439:ARG:O	2.19	0.42
1:B:378:ALA:CB	1:B:384:LYS:HB2	2.49	0.42
1:B:383:VAL:O	1:B:384:LYS:C	2.62	0.42
1:B:395:ASP:O	1:B:398:ALA:HB3	2.18	0.42
1:B:503:TYR:CD1	1:B:503:TYR:N	2.87	0.42
1:B:582:ASN:OD1	1:B:583:THR:N	2.52	0.42
1:A:84:VAL:HG13	1:A:88:ASN:HA	2.01	0.42
1:B:233:THR:HG22	1:B:234:ASP:N	2.33	0.42
1:B:333:PHE:O	1:B:349:PRO:HB3	2.18	0.42
1:B:348:THR:HA	1:B:349:PRO:C	2.44	0.42
1:B:377:PHE:HE2	1:B:428:PHE:CD1	2.36	0.42
1:B:390:LEU:HD22	1:B:397:PHE:HA	2.01	0.42
1:A:390:LEU:CD1	1:A:415:LEU:HD21	2.49	0.42
1:A:513:ALA:O	1:A:514:ASN:HB2	2.20	0.42
1:A:638:GLY:HA2	1:A:685:ARG:CZ	2.49	0.42
1:B:105:ASN:ND2	1:B:142:LEU:CA	2.72	0.42
1:B:132:ASP:O	1:B:133:PHE:C	2.62	0.42
1:B:439:ARG:HG3	1:B:478:THR:OG1	2.19	0.42
1:B:633:GLU:O	1:B:636:ASN:N	2.53	0.42
1:A:325:PHE:O	1:A:326:ASN:HB3	2.19	0.42
1:A:508:PRO:HD2	1:A:511:LEU:CB	2.49	0.42
1:A:528:LEU:O	1:A:529:PRO:C	2.62	0.42
1:B:95:ASP:OD2	1:B:97:GLU:HG3	2.19	0.42
1:B:276:SER:HA	1:B:289:HIS:O	2.19	0.42
1:B:329:PRO:HA	1:B:352:ILE:HG22	2.01	0.42
1:B:362:ILE:HG13	1:B:363:THR:N	2.33	0.42
1:B:542:GLY:C	1:B:544:GLY:N	2.75	0.42
1:A:390:LEU:C	1:A:392:LYS:N	2.75	0.42
1:A:459:ILE:HD13	4:A:753:NAP:H52N	2.02	0.42
1:A:528:LEU:HD13	1:A:555:ARG:NH1	2.35	0.42
1:A:607:VAL:CG1	1:A:608:ALA:N	2.82	0.42
1:B:94:ALA:HB1	1:B:99:TYR:CE1	2.55	0.42
1:B:139:ALA:C	1:B:141:ALA:N	2.77	0.42
1:B:360:LEU:O	1:B:362:ILE:N	2.50	0.42
1:B:468:LEU:O	1:B:469:PRO:C	2.61	0.42
1:B:642:TYR:CD1	1:B:642:TYR:N	2.87	0.42
1:B:327:LEU:HD21	1:B:352:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LEU:H	1:B:528:LEU:CD1	2.28	0.42
1:B:223:GLN:HG2	1:B:431:GLU:OE1	2.20	0.42
1:B:424:VAL:HG11	1:B:429:LEU:HD21	2.01	0.42
1:B:346:PHE:CD2	1:B:359:TYR:HB3	2.55	0.42
1:B:442:SER:HB3	1:B:547:PRO:HG3	2.01	0.42
1:B:528:LEU:HD12	1:B:528:LEU:N	2.31	0.42
1:B:603:PHE:CD2	1:B:603:PHE:C	2.96	0.42
1:A:74:ASP:OD2	1:A:78:LYS:NZ	2.53	0.42
1:A:286:ASN:O	1:A:460:VAL:HG23	2.20	0.42
1:A:528:LEU:HD11	1:A:555:ARG:HG2	2.02	0.42
1:A:194:GLU:CG	1:A:394:LYS:HG3	2.50	0.42
1:B:268:PRO:HB3	1:B:310:TRP:CE2	2.55	0.42
1:B:528:LEU:CD2	1:B:555:ARG:HH11	2.33	0.42
1:A:390:LEU:C	1:A:392:LYS:H	2.28	0.41
1:A:504:ASP:OD1	1:A:504:ASP:C	2.62	0.41
1:B:95:ASP:C	1:B:97:GLU:H	2.28	0.41
1:B:325:PHE:CE1	1:B:429:LEU:HD11	2.54	0.41
1:B:534:THR:HG21	1:B:640:PHE:CD1	2.55	0.41
1:B:676:LEU:O	1:B:680:LEU:HG	2.20	0.41
1:B:160:PHE:C	1:B:160:PHE:CD2	2.92	0.41
1:B:481:LEU:HD13	1:B:503:TYR:CD2	2.56	0.41
1:B:542:GLY:O	1:B:543:THR:C	2.61	0.41
1:B:581:ARG:HD3	1:B:611:ARG:HH12	1.83	0.41
1:A:247:PRO:C	1:A:249:HIS:N	2.78	0.41
1:A:618:VAL:O	1:A:618:VAL:HG12	2.20	0.41
1:B:289:HIS:CE1	1:B:455:HIS:HD2	2.39	0.41
1:B:592:TRP:CE2	1:B:605:MET:HE1	2.55	0.41
1:A:138:GLU:CG	1:A:139:ALA:N	2.83	0.41
1:A:371:PHE:O	1:A:387:LEU:HD22	2.19	0.41
1:B:74:ASP:OD1	1:B:434:PRO:HG3	2.20	0.41
1:B:319:GLU:C	1:B:321:PHE:N	2.78	0.41
1:B:453:THR:HG22	1:B:454:VAL:N	2.34	0.41
1:A:158:GLU:O	1:A:159:PHE:C	2.63	0.41
1:A:346:PHE:CZ	1:A:430:VAL:HG13	2.55	0.41
1:B:63:VAL:HB	1:B:93:CYS:HA	2.02	0.41
1:B:95:ASP:C	1:B:97:GLU:N	2.78	0.41
1:B:267:GLN:O	1:B:268:PRO:O	2.38	0.41
1:B:356:ILE:HG23	1:B:362:ILE:HG21	2.03	0.41
1:B:371:PHE:CE1	1:B:390:LEU:HD13	2.56	0.41
1:B:408:ILE:HD13	1:B:433:VAL:HG22	2.03	0.41
1:B:586:PHE:CD2	1:B:589:GLN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:LEU:HA	1:B:613:PRO:HD3	1.89	0.41
1:A:393:ASP:HB3	1:A:396:GLN:HB3	2.02	0.41
1:A:550:GLY:O	1:A:551:PHE:C	2.64	0.41
1:B:423:THR:O	1:B:425:PRO:HD3	2.21	0.41
1:B:499:LEU:HA	1:B:500:PRO:HD3	1.74	0.41
1:B:536:VAL:HG12	1:B:538:MET:HG3	2.02	0.41
1:A:555:ARG:HD2	1:A:571:LEU:HD11	2.02	0.41
1:B:87:PHE:HB2	1:B:89:LEU:CD1	2.42	0.41
1:B:336:LYS:HA	1:B:337:PRO:HD3	1.85	0.41
1:A:57:ASN:HB3	1:A:59:LYS:HD3	2.03	0.41
1:A:82:GLU:HA	1:A:85:ALA:CB	2.50	0.41
1:A:239:GLY:O	1:A:240:GLU:C	2.63	0.41
1:A:363:THR:HG21	1:A:477:VAL:HG23	2.02	0.41
1:A:581:ARG:HD3	1:A:611:ARG:HG3	2.02	0.41
1:A:666:LYS:HE3	1:A:676:LEU:CD2	2.40	0.41
1:B:224:PHE:HA	1:B:336:LYS:O	2.19	0.41
1:B:240:GLU:O	1:B:241:PRO:C	2.64	0.41
1:B:337:PRO:HB3	1:B:342:VAL:O	2.20	0.41
1:A:62:LEU:C	1:A:62:LEU:HD22	2.45	0.41
1:A:123:PHE:CD2	1:A:131:GLU:HB2	2.55	0.41
1:A:223:GLN:NE2	1:A:342:VAL:HG22	2.35	0.41
1:A:229:LEU:HB2	1:A:332:ILE:HG22	2.03	0.41
1:A:403:SER:O	1:A:467:GLU:HG3	2.20	0.41
1:A:552:ILE:O	1:A:553:ARG:C	2.60	0.41
1:A:578:TYR:CD1	1:A:579:GLY:N	2.86	0.41
1:A:632:PHE:CE2	1:A:636:ASN:ND2	2.89	0.41
1:B:87:PHE:O	1:B:88:ASN:HB2	2.21	0.41
1:B:98:ASN:HB2	1:B:99:TYR:CE1	2.55	0.41
1:B:240:GLU:HB3	1:B:245:TYR:CB	2.51	0.41
1:B:344:VAL:HA	1:B:345:PRO:HD3	1.83	0.41
1:B:374:LEU:CB	1:B:387:LEU:HD11	2.50	0.41
1:B:377:PHE:HB3	1:B:423:THR:HB	2.02	0.41
1:B:433:VAL:HA	1:B:434:PRO:HD3	1.80	0.41
1:B:539:ILE:HG23	1:B:620:VAL:HG21	2.02	0.41
1:B:592:TRP:O	1:B:593:PRO:C	2.63	0.41
1:B:686:TYR:C	1:B:686:TYR:HD2	2.28	0.41
1:A:146:ARG:HD3	1:B:146:ARG:NH1	2.35	0.41
1:A:240:GLU:CG	1:A:245:TYR:O	2.68	0.41
1:A:380:ASN:O	1:A:383:VAL:HB	2.21	0.41
1:A:609:HIS:CB	1:A:612:LEU:HD12	2.49	0.41
1:B:95:ASP:HB3	1:B:98:ASN:HD21	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:O	1:B:374:LEU:HG	2.20	0.41
1:B:485:ILE:HG23	1:B:515:TYR:HD2	1.85	0.41
1:A:62:LEU:C	1:A:62:LEU:CD2	2.94	0.40
1:A:316:GLU:OE1	1:A:501:VAL:HA	2.21	0.40
1:B:202:SER:OG	1:B:203:ILE:N	2.53	0.40
1:B:301:TYR:CE1	1:B:447:SER:HA	2.55	0.40
1:B:157:TYR:OH	1:B:691:TRP:HA	2.22	0.40
1:B:161:ASN:ND2	5:B:2003:HOH:O	2.54	0.40
1:B:166:LYS:O	1:B:169:LYS:HB3	2.21	0.40
1:B:264:ASP:OD2	1:B:264:ASP:C	2.63	0.40
1:B:514:ASN:O	1:B:515:TYR:C	2.64	0.40
1:B:572:GLY:O	1:B:574:HIS:CD2	2.73	0.40
1:B:621:GLN:OE1	1:B:653:GLY:HA3	2.22	0.40
1:A:362:ILE:HG13	1:A:363:THR:N	2.36	0.40
1:A:493:ASN:O	1:A:494:ILE:C	2.65	0.40
1:A:607:VAL:HG12	1:A:608:ALA:N	2.36	0.40
1:B:269:TYR:N	1:B:519:VAL:O	2.55	0.40
1:B:313:ASN:HD21	1:B:436:MET:CE	2.26	0.40
1:A:553:ARG:HG2	1:A:553:ARG:NH1	2.36	0.40
1:A:677:ILE:HD13	1:A:677:ILE:HA	1.86	0.40
1:B:223:GLN:CA	1:B:338:LEU:HD12	2.52	0.40
1:B:301:TYR:C	1:B:301:TYR:HD1	2.28	0.40
1:B:620:VAL:HG23	1:B:621:GLN:N	2.37	0.40
1:B:662:LEU:HD22	1:B:677:ILE:CD1	2.50	0.40
1:A:582:ASN:HB2	1:A:583:THR:H	1.74	0.40
1:B:107:VAL:HG12	1:B:109:VAL:H	1.86	0.40
1:B:550:GLY:O	1:B:551:PHE:C	2.64	0.40
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.84	0.40
1:B:609:HIS:HB2	1:B:612:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	639/682 (94%)	513 (80%)	105 (16%)	21 (3%)	3	11
1	B	637/682 (93%)	504 (79%)	106 (17%)	27 (4%)	2	7
All	All	1276/1364 (94%)	1017 (80%)	211 (16%)	48 (4%)	2	9

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ASP
1	A	508	PRO
1	A	566	GLY
1	B	233	THR
1	B	241	PRO
1	B	571	LEU
1	B	646	ASP
1	B	647	ALA
1	A	127	ALA
1	A	232	ILE
1	A	331	THR
1	A	526	PHE
1	A	571	LEU
1	B	119	GLY
1	B	140	GLY
1	B	248	SER
1	B	268	PRO
1	B	497	THR
1	B	570	SER
1	A	143	SER
1	A	241	PRO
1	A	261	GLY
1	A	529	PRO
1	B	264	ASP
1	B	331	THR
1	B	401	ILE
1	B	543	THR
1	B	594	GLU
1	A	50	ILE
1	A	96	VAL
1	A	192	THR
1	A	253	ARG
1	A	462	ASN
1	A	639	ALA
1	B	133	PHE

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Mol	Chain	Res	Type
1	B	137	ALA
1	B	379	PRO
1	B	569	VAL
1	A	613	PRO
1	B	311	PRO
1	B	514	ASN
1	B	596	ALA
1	B	598	LYS
1	B	636	ASN
1	B	649	GLY
1	A	500	PRO
1	A	311	PRO
1	B	468	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	548/592 (93%)	503 (92%)	45 (8%)	10	31
1	B	549/592 (93%)	518 (94%)	31 (6%)	19	48
All	All	1097/1184 (93%)	1021 (93%)	76 (7%)	14	39

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	62	LEU
1	A	97	GLU
1	A	104	LEU
1	A	115	ILE
1	A	120	GLU
1	A	161	ASN
1	A	182	LEU
1	A	194	GLU
1	A	203	ILE

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Mol	Chain	Res	Type
1	A	232	ILE
1	A	236	MET
1	A	272	PRO
1	A	283	ASN
1	A	284	ASP
1	A	285	ARG
1	A	286	ASN
1	A	288	ILE
1	A	319	GLU
1	A	330	GLU
1	A	341	THR
1	A	344	VAL
1	A	350	THR
1	A	371	PHE
1	A	375	ILE
1	A	387	LEU
1	A	402	THR
1	A	416	SER
1	A	423	THR
1	A	426	MET
1	A	427	GLN
1	A	443	ILE
1	A	453	THR
1	A	457	THR
1	A	511	LEU
1	A	526	PHE
1	A	582	ASN
1	A	612	LEU
1	A	613	PRO
1	A	618	VAL
1	A	662	LEU
1	A	667	SER
1	A	668	ILE
1	A	670	THR
1	A	682	THR
1	B	48	ARG
1	B	60	ASN
1	B	104	LEU
1	B	115	ILE
1	B	120	GLU
1	B	156	THR
1	B	265	LEU

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Mol	Chain	Res	Type
1	B	270	ILE
1	B	283	ASN
1	B	341	THR
1	B	344	VAL
1	B	352	ILE
1	B	369	GLN
1	B	373	SER
1	B	385	GLU
1	B	387	LEU
1	B	402	THR
1	B	422	ASP
1	B	423	THR
1	B	462	ASN
1	B	470	ASP
1	B	483	ARG
1	B	511	LEU
1	B	528	LEU
1	B	576	LEU
1	B	583	THR
1	B	590	ASP
1	B	626	ASP
1	B	676	LEU
1	B	682	THR
1	B	690	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	68	GLN
1	A	88	ASN
1	A	98	ASN
1	A	129	ASN
1	A	148	ASN
1	A	161	ASN
1	A	170	HIS
1	A	212	HIS
1	A	216	GLN
1	A	223	GLN
1	A	230	ASN
1	A	249	HIS
1	A	267	GLN

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Mol	Chain	Res	Type
1	A	320	GLN
1	A	326	ASN
1	A	396	GLN
1	A	455	HIS
1	A	480	ASN
1	A	484	ASN
1	A	502	HIS
1	A	531	ASN
1	A	582	ASN
1	A	621	GLN
1	A	630	GLN
1	A	637	ASN
1	B	68	GLN
1	B	90	ASN
1	B	98	ASN
1	B	129	ASN
1	B	144	ASN
1	B	161	ASN
1	B	170	HIS
1	B	212	HIS
1	B	216	GLN
1	B	225	GLN
1	B	267	GLN
1	B	320	GLN
1	B	326	ASN
1	B	358	HIS
1	B	369	GLN
1	B	376	GLN
1	B	380	ASN
1	B	435	GLN
1	B	452	GLN
1	B	455	HIS
1	B	484	ASN
1	B	486	GLN
1	B	502	HIS
1	B	531	ASN
1	B	567	ASN
1	B	574	HIS
1	B	589	GLN
1	B	621	GLN
1	B	637	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	A	753	-	42,43,52	1.40	6 (14%)	62,67,80	1.87	15 (24%)
2	FAD	A	750	-	58,58,58	1.63	9 (15%)	85,89,89	0.95	4 (4%)
2	FAD	B	750	-	58,58,58	1.61	10 (17%)	85,89,89	0.86	2 (2%)
3	FMN	A	751	-	33,33,33	1.55	6 (18%)	48,50,50	1.39	7 (14%)
3	FMN	B	751	-	33,33,33	1.66	9 (27%)	48,50,50	1.38	6 (12%)
4	NAP	B	753	-	42,43,52	1.33	4 (9%)	62,67,80	1.90	17 (27%)

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	NAP	A	753	-	-	11/27/59/67	0/4/4/5
2	FAD	A	750	-	-	11/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	750	-	-	11/34/50/50	0/6/6/6
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3
3	FMN	B	751	-	-	2/18/18/18	0/3/3/3
4	NAP	B	753	-	-	7/27/59/67	0/4/4/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	FAD	C4X-N5	5.34	1.42	1.30
2	A	750	FAD	PA-O3P	-5.22	1.53	1.59
2	B	750	FAD	C9-C8	4.72	1.46	1.39
2	A	750	FAD	C4X-N5	4.63	1.40	1.30
2	A	750	FAD	C9-C8	4.35	1.45	1.39
3	A	751	FMN	C4A-N5	4.23	1.39	1.30
4	A	753	NAP	C5A-N7A	-3.87	1.32	1.39
3	A	751	FMN	C9-C8	-3.74	1.34	1.39
3	B	751	FMN	C4A-N5	3.70	1.38	1.30
3	B	751	FMN	C5'-C4'	3.57	1.56	1.51
3	A	751	FMN	C10-N10	3.53	1.44	1.37
2	B	750	FAD	C9A-C5X	3.52	1.46	1.41
4	A	753	NAP	C2B-C1B	-3.51	1.44	1.53
4	B	753	NAP	C2B-C1B	-3.49	1.44	1.53
4	B	753	NAP	C5A-N7A	-3.47	1.32	1.39
3	B	751	FMN	C10-N10	3.42	1.44	1.37
2	A	750	FAD	C4A-N3A	3.29	1.40	1.34
2	B	750	FAD	C9A-N10	3.25	1.46	1.41
2	A	750	FAD	P-O3P	-3.19	1.56	1.59
2	A	750	FAD	C6-C5X	3.12	1.44	1.40
4	B	753	NAP	C4A-N3A	3.10	1.40	1.34
2	B	750	FAD	C6-C5X	2.99	1.44	1.40
2	B	750	FAD	C4A-N3A	2.96	1.39	1.34
2	B	750	FAD	C10-N1	2.84	1.39	1.33
4	A	753	NAP	C4A-N3A	2.84	1.39	1.34
2	A	750	FAD	C10-N1	2.83	1.38	1.33
2	A	750	FAD	C9A-N10	2.79	1.46	1.41
2	A	750	FAD	C9A-C5X	2.76	1.45	1.41
4	A	753	NAP	C4A-N9A	-2.53	1.32	1.37
3	B	751	FMN	C9A-C5A	2.48	1.45	1.41
3	B	751	FMN	C6-C5A	2.48	1.43	1.40
3	A	751	FMN	C6-C5A	2.38	1.43	1.40
3	B	751	FMN	P-O2P	-2.38	1.46	1.54
3	B	751	FMN	C9-C8	-2.35	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	751	FMN	P-O2P	-2.24	1.46	1.54
3	B	751	FMN	P-O3P	-2.17	1.46	1.54
3	A	751	FMN	C5'-C4'	2.12	1.54	1.51
4	A	753	NAP	P2B-O3X	-2.11	1.47	1.54
3	B	751	FMN	C9A-N10	2.09	1.44	1.41
4	A	753	NAP	C3D-C4D	2.06	1.58	1.53
2	B	750	FAD	C1'-C2'	2.05	1.55	1.52
2	B	750	FAD	C5'-C4'	-2.04	1.49	1.51
2	B	750	FAD	C5A-C4A	-2.01	1.35	1.39
4	B	753	NAP	C4A-N9A	-2.01	1.33	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	753	NAP	O4D-C1D-N1N	-5.34	102.07	110.57
4	B	753	NAP	O4D-C1D-N1N	-5.28	102.16	110.57
4	A	753	NAP	C5A-C4A-N3A	-5.04	119.78	126.72
4	A	753	NAP	N3A-C2A-N1A	-4.94	121.11	128.58
4	B	753	NAP	C5A-C4A-N3A	-4.91	119.95	126.72
4	B	753	NAP	N3A-C4A-N9A	4.81	135.34	127.17
4	B	753	NAP	N3A-C2A-N1A	-4.75	121.39	128.58
4	A	753	NAP	N3A-C4A-N9A	4.67	135.11	127.17
3	B	751	FMN	C9A-C5A-N5	4.02	126.72	122.45
3	A	751	FMN	C9A-C5A-N5	3.93	126.62	122.45
4	A	753	NAP	C4A-N9A-C1B	-3.70	117.97	126.63
4	B	753	NAP	C4A-N9A-C1B	-3.35	118.79	126.63
3	B	751	FMN	C5A-N5-C4A	-3.25	112.83	118.09
3	A	751	FMN	C5A-N5-C4A	-3.23	112.87	118.09
4	A	753	NAP	C2A-N3A-C4A	3.08	119.36	111.83
4	A	753	NAP	C1B-N9A-C8A	3.05	133.85	127.09
4	B	753	NAP	C2A-N3A-C4A	3.02	119.20	111.83
3	A	751	FMN	O2-C2-N3	2.91	124.16	118.58
3	B	751	FMN	O2-C2-N3	2.78	123.91	118.58
4	B	753	NAP	C1B-N9A-C8A	2.76	133.22	127.09
3	A	751	FMN	C10-N1-C2	2.74	122.78	116.85
4	B	753	NAP	O3X-P2B-O2X	2.63	117.67	107.80
3	B	751	FMN	C10-N1-C2	2.60	122.48	116.85
2	A	750	FAD	C5'-C4'-C3'	-2.58	107.35	112.22
2	B	750	FAD	C4X-C10-N10	2.56	120.14	116.48
4	A	753	NAP	O3X-P2B-O2X	2.55	117.36	107.80
3	A	751	FMN	O3'-C3'-C2'	2.53	114.69	108.93
2	A	750	FAD	C4X-C10-N10	2.51	120.08	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	FAD	O2B-C2B-C3B	2.46	119.71	111.82
4	B	753	NAP	O2A-PA-O3	2.41	113.79	107.27
2	A	750	FAD	O5'-C5'-C4'	-2.33	103.14	109.36
4	A	753	NAP	C4A-N9A-C8A	2.31	108.17	105.74
4	A	753	NAP	P2B-O2B-C2B	2.31	129.59	123.43
4	B	753	NAP	C2D-C3D-C4D	2.30	107.06	102.61
4	A	753	NAP	C2B-C1B-N9A	2.30	117.54	113.75
3	B	751	FMN	O2P-P-O5'	-2.28	100.73	106.67
4	B	753	NAP	O4B-C1B-C2B	-2.28	102.67	106.59
4	B	753	NAP	C3D-C2D-C1D	2.23	105.67	101.46
2	A	750	FAD	O2B-C2B-C3B	2.18	118.81	111.82
4	B	753	NAP	C6A-C5A-N7A	-2.17	127.90	132.09
4	B	753	NAP	C4A-N9A-C8A	2.14	107.99	105.74
4	A	753	NAP	N9A-C8A-N7A	-2.13	110.91	113.94
4	A	753	NAP	C6A-C5A-N7A	-2.09	128.06	132.09
3	A	751	FMN	N3-C2-N1	-2.09	115.06	119.50
4	B	753	NAP	O3B-C3B-C2B	2.08	117.01	111.19
4	B	753	NAP	O5D-C5D-C4D	2.06	116.00	108.99
4	A	753	NAP	C6A-C5A-C4A	2.04	119.97	117.18
4	B	753	NAP	C6A-C5A-C4A	2.01	119.93	117.18
3	B	751	FMN	O3'-C3'-C2'	2.01	113.50	108.93
4	A	753	NAP	O3B-C3B-C4B	-2.01	105.32	111.08
3	A	751	FMN	O2P-P-O5'	-2.00	101.45	106.67

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	750	FAD	C1'-C2'-C3'-C4'
2	B	750	FAD	C1'-C2'-C3'-C4'
2	B	750	FAD	O4'-C4'-C5'-O5'
3	B	751	FMN	C5'-O5'-P-O1P
4	A	753	NAP	C5B-O5B-PA-O1A
4	A	753	NAP	C5B-O5B-PA-O3
4	A	753	NAP	C2B-C1B-N9A-C8A
4	A	753	NAP	C2B-C1B-N9A-C4A
4	B	753	NAP	C5B-O5B-PA-O1A
4	B	753	NAP	C5B-O5B-PA-O3
4	B	753	NAP	C2B-C1B-N9A-C8A
4	B	753	NAP	C2B-C1B-N9A-C4A
4	A	753	NAP	O4D-C4D-C5D-O5D
4	A	753	NAP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	B	750	FAD	O2'-C2'-C3'-O3'
2	A	750	FAD	O2'-C2'-C3'-C4'
2	A	750	FAD	O2'-C2'-C3'-O3'
2	B	750	FAD	O2'-C2'-C3'-C4'
2	A	750	FAD	C3'-C4'-C5'-O5'
2	B	750	FAD	C3'-C4'-C5'-O5'
4	A	753	NAP	PN-O3-PA-O5B
2	B	750	FAD	C2B-C1B-N9A-C8A
3	B	751	FMN	C5'-O5'-P-O2P
2	A	750	FAD	C2B-C1B-N9A-C8A
2	A	750	FAD	P-O3P-PA-O1A
2	B	750	FAD	P-O3P-PA-O1A
2	A	750	FAD	O4'-C4'-C5'-O5'
4	A	753	NAP	C5B-O5B-PA-O2A
4	A	753	NAP	C5D-O5D-PN-O1N
4	B	753	NAP	C5B-O5B-PA-O2A
4	B	753	NAP	C5D-O5D-PN-O1N
2	B	750	FAD	C2B-C1B-N9A-C4A
2	A	750	FAD	C2B-C1B-N9A-C4A
4	A	753	NAP	C4B-C5B-O5B-PA
2	A	750	FAD	O4B-C1B-N9A-C8A
2	A	750	FAD	C1'-C2'-C3'-O3'
2	B	750	FAD	C1'-C2'-C3'-O3'
2	A	750	FAD	P-O3P-PA-O2A
2	B	750	FAD	O4B-C1B-N9A-C8A
4	A	753	NAP	C2B-O2B-P2B-O1X
4	B	753	NAP	C2B-O2B-P2B-O1X
2	B	750	FAD	P-O3P-PA-O2A

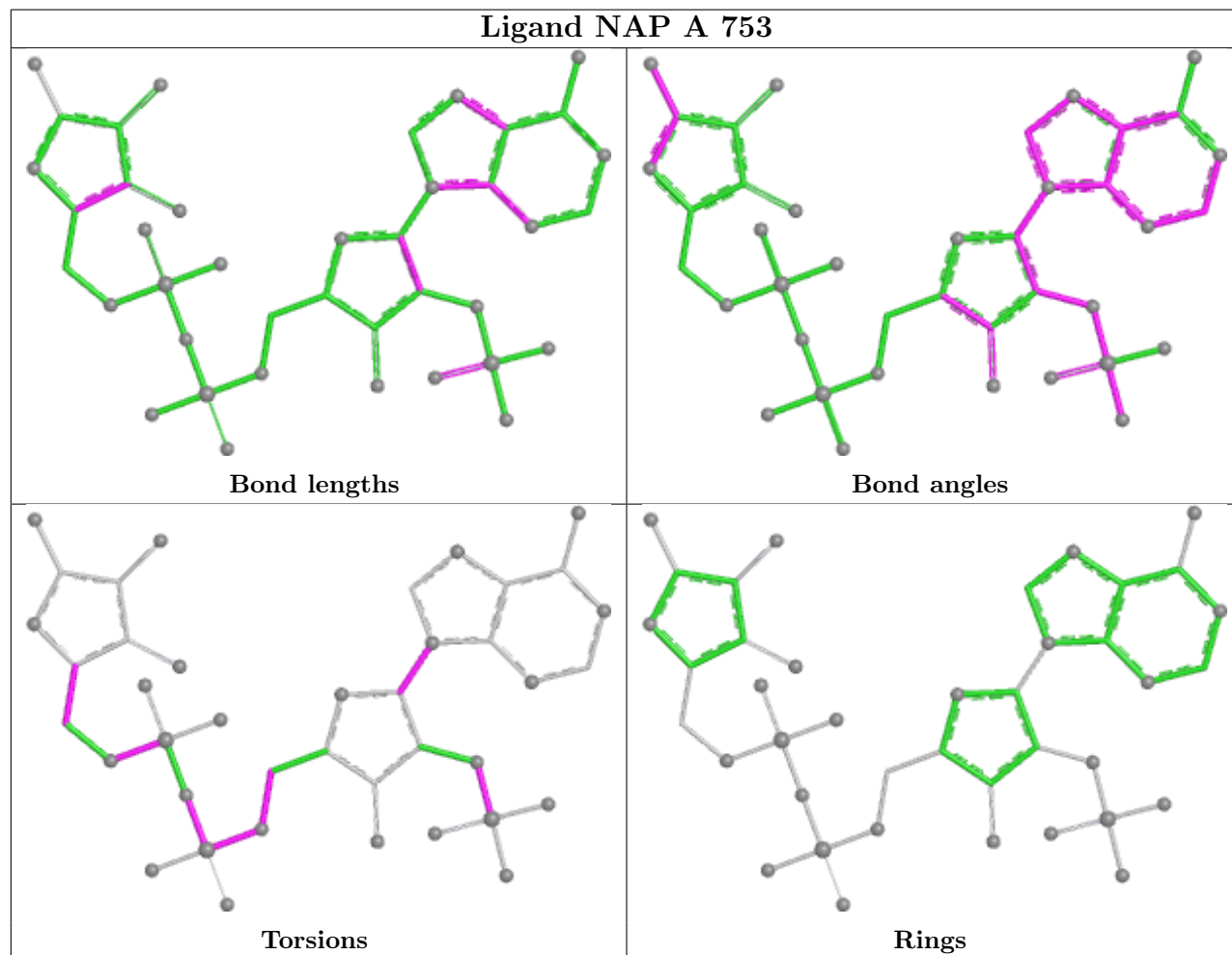
There are no ring outliers.

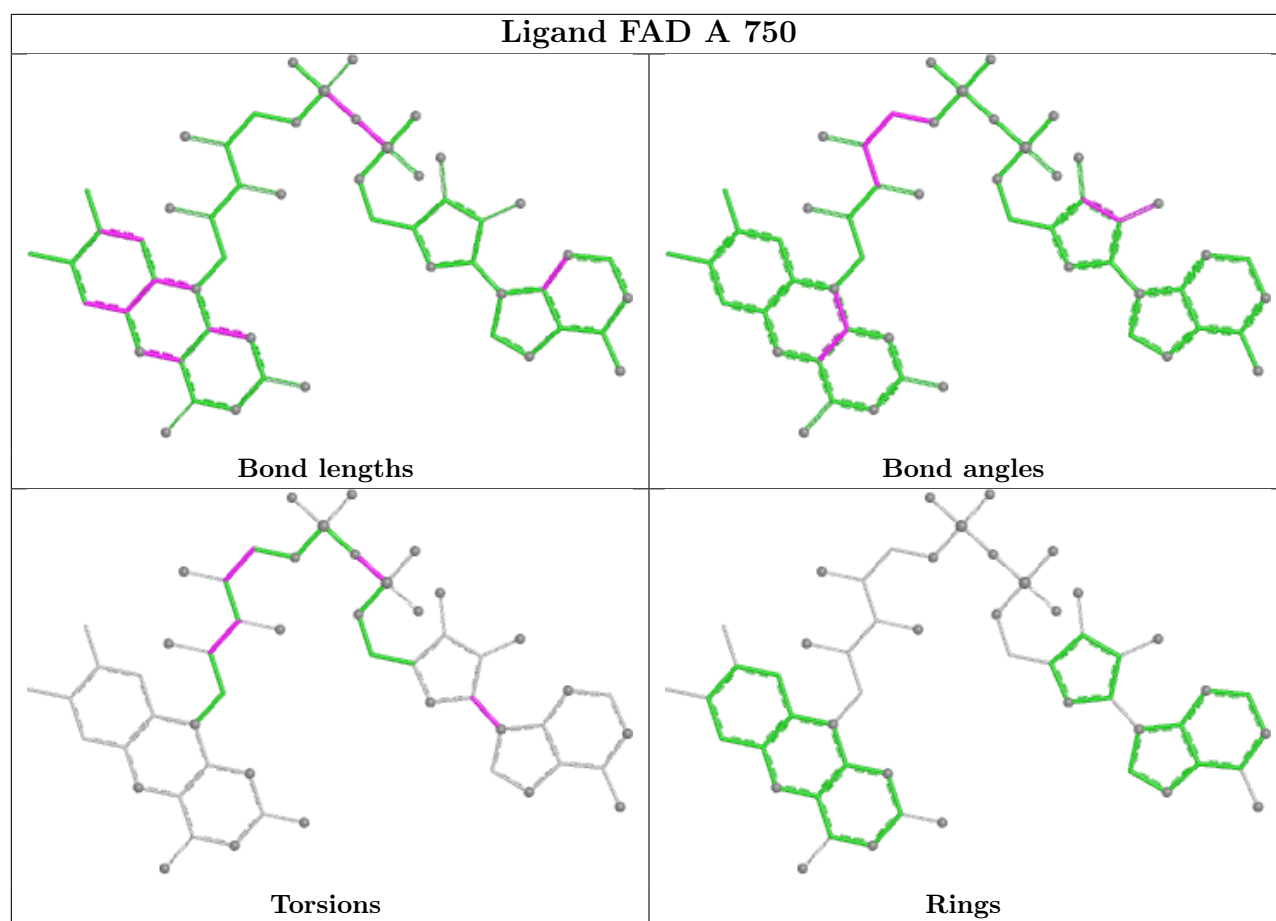
6 monomers are involved in 14 short contacts:

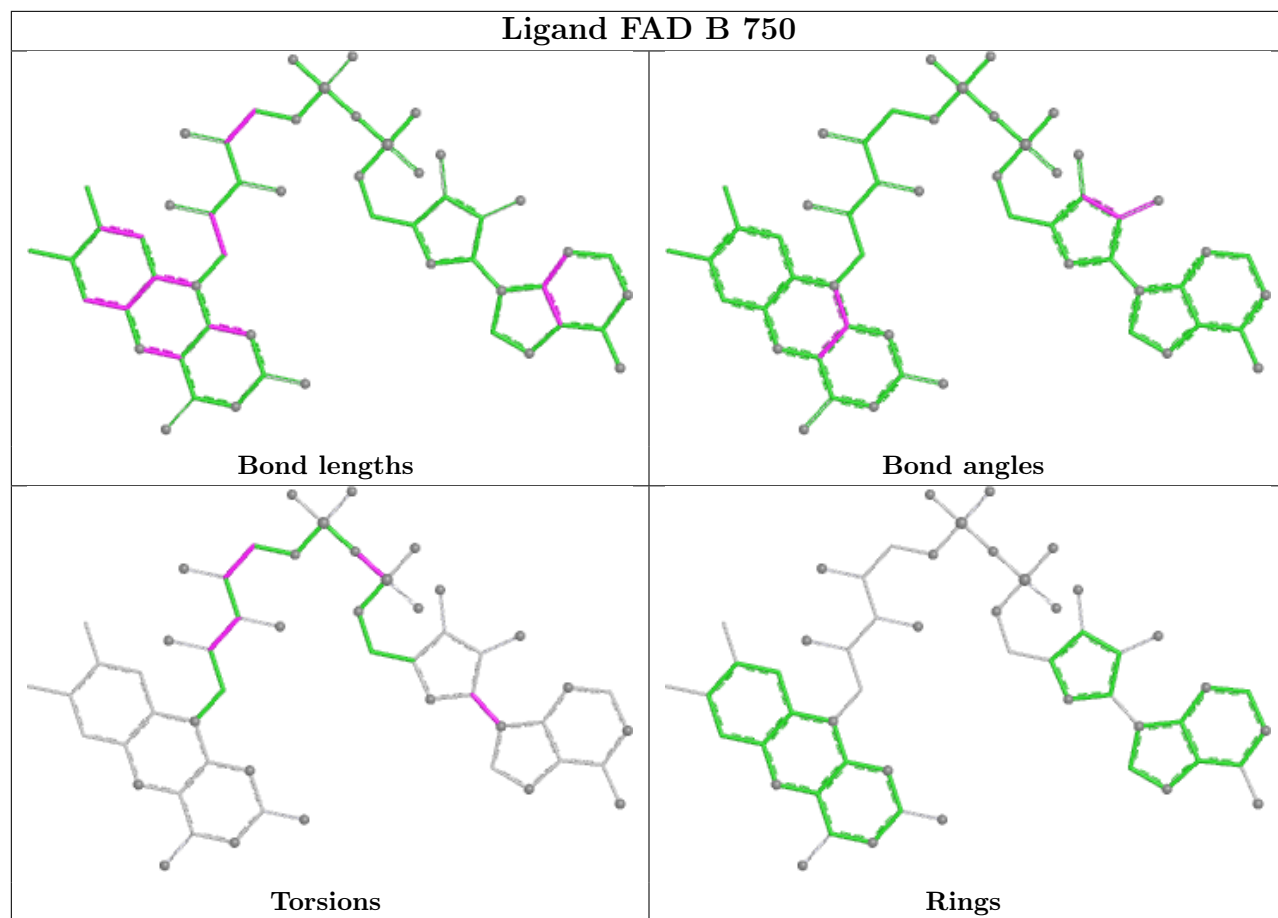
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	753	NAP	5	0
2	A	750	FAD	2	0
2	B	750	FAD	3	0
3	A	751	FMN	2	0
3	B	751	FMN	1	0
4	B	753	NAP	1	0

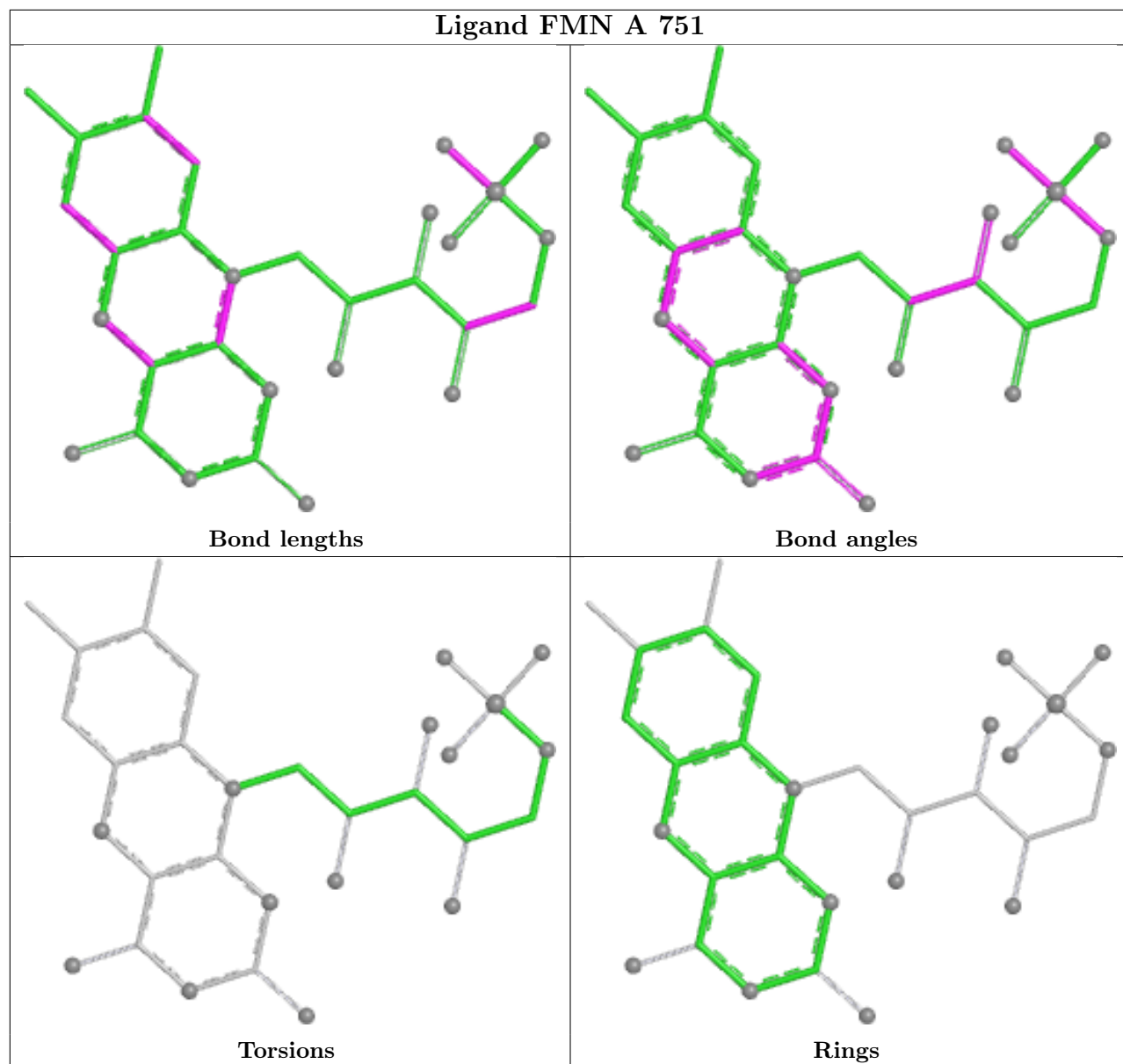
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

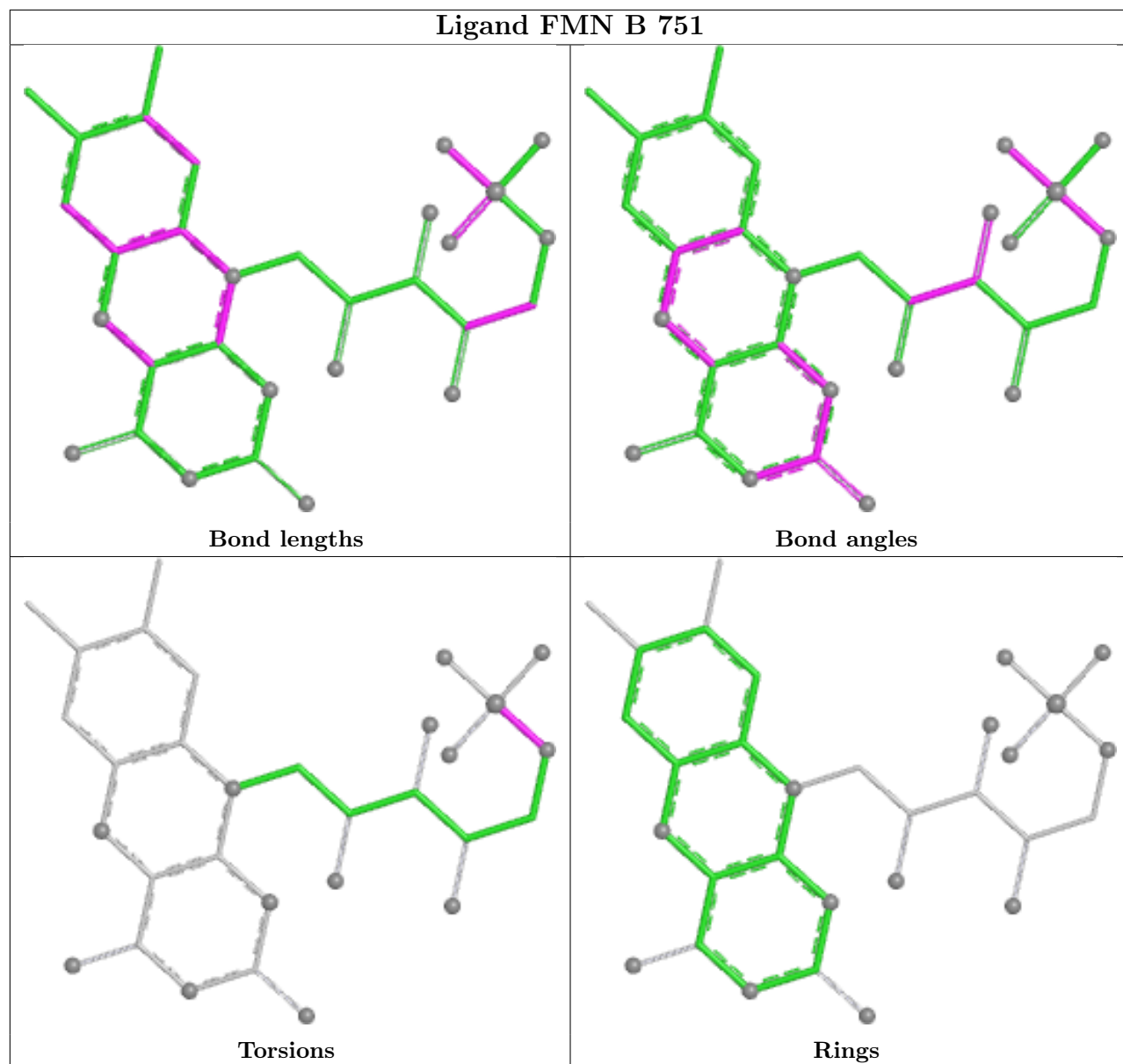
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

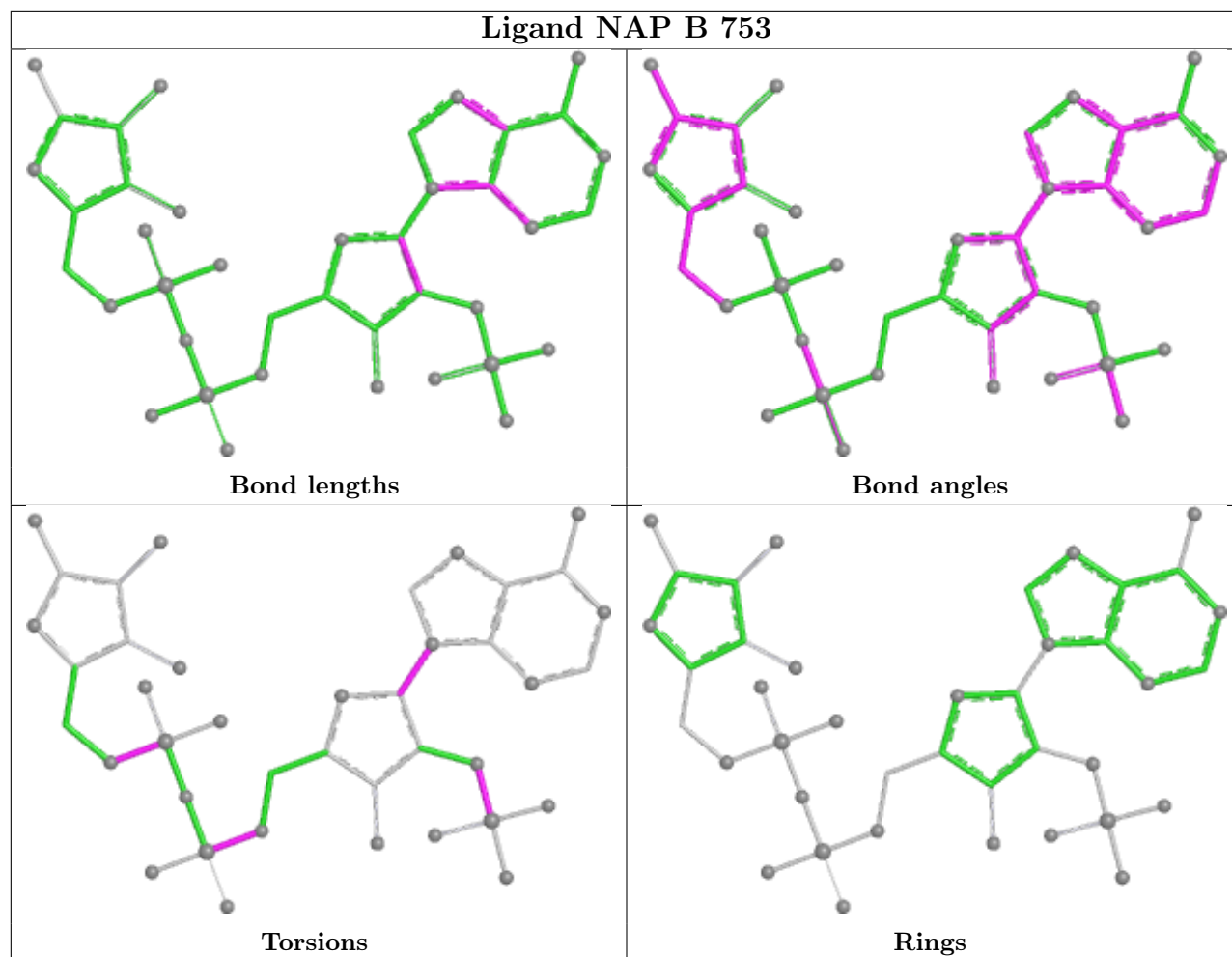












5.7 Other polymers [i](#)

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	643/682 (94%)	-1.45	0 100 100	35, 62, 89, 109	0
1	B	641/682 (93%)	-1.43	0 100 100	42, 69, 91, 118	0
All	All	1284/1364 (94%)	-1.44	0 100 100	35, 66, 90, 118	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

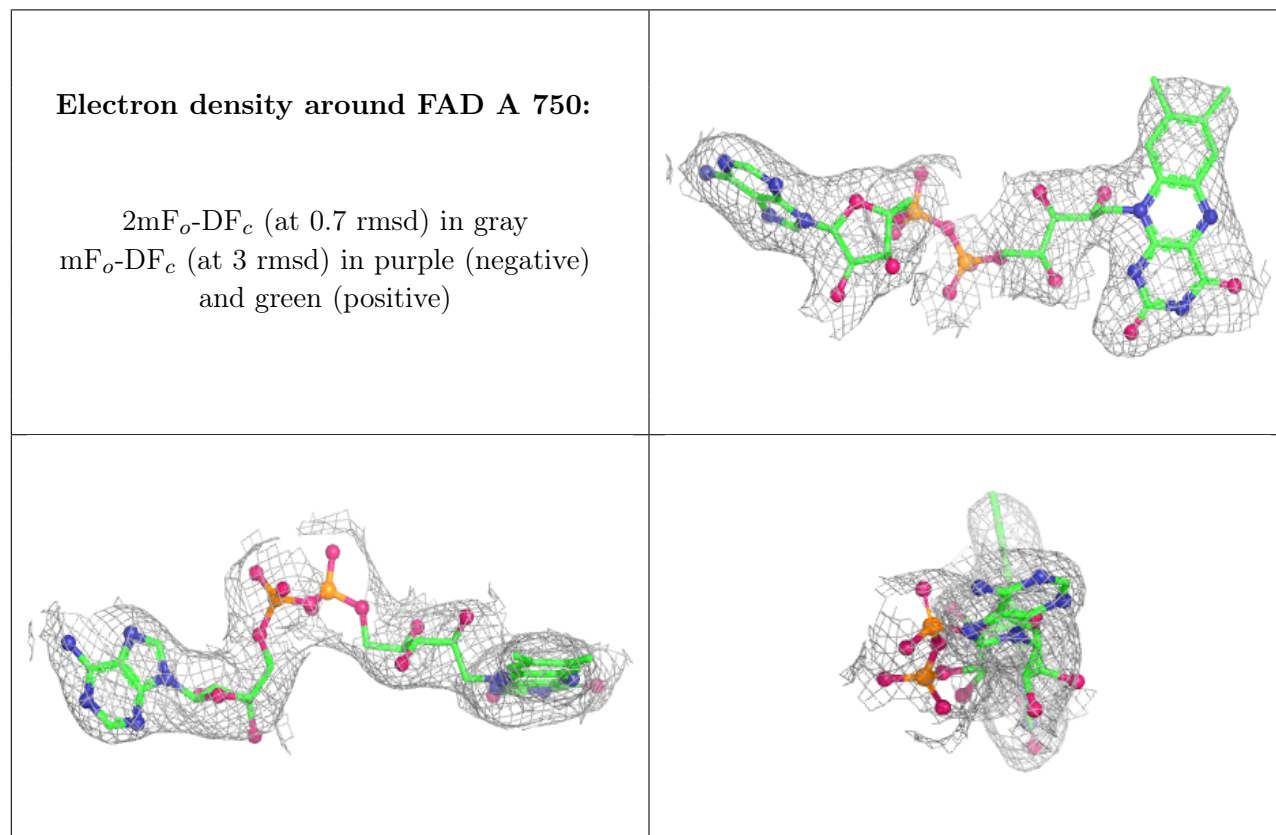
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

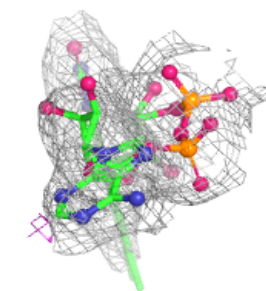
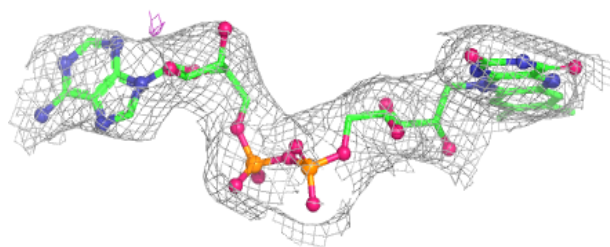
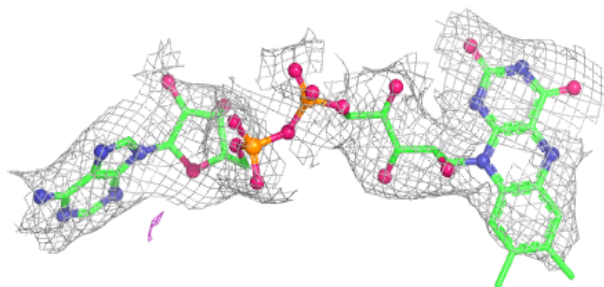
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	750	53/53	0.99	0.03	29,47,58,60	0
2	FAD	B	750	53/53	0.99	0.04	49,60,67,69	0
4	NAP	A	753	40/48	0.99	0.03	52,59,79,82	0
4	NAP	B	753	40/48	0.99	0.04	88,92,112,112	0
3	FMN	A	751	31/31	1.00	0.03	39,52,56,57	0
3	FMN	B	751	31/31	1.00	0.02	49,60,66,66	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.

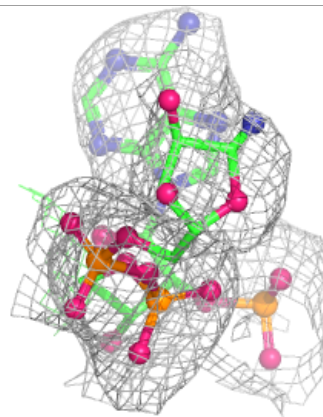
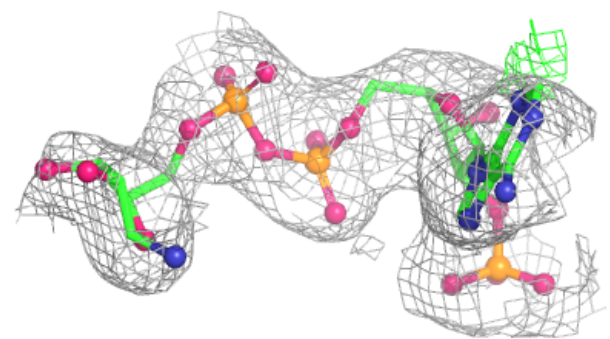
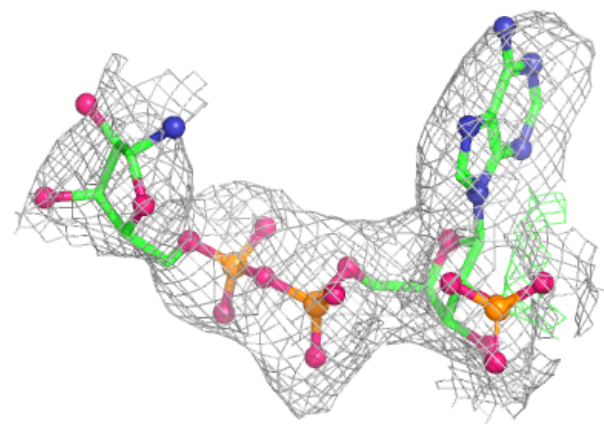


Electron density around FAD B 750:

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

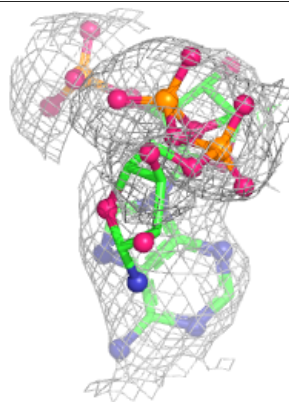
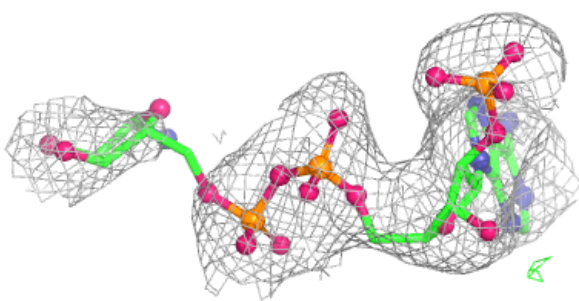
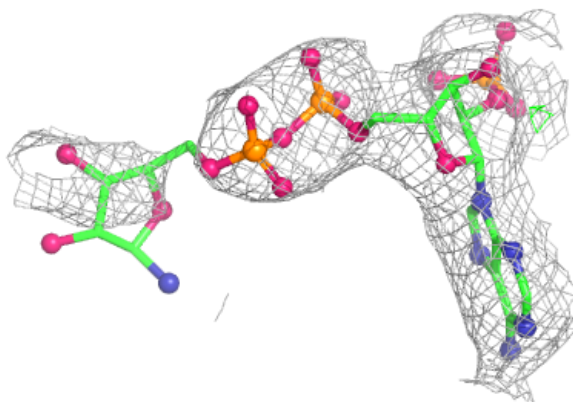
**Electron density around NAP A 753:**

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



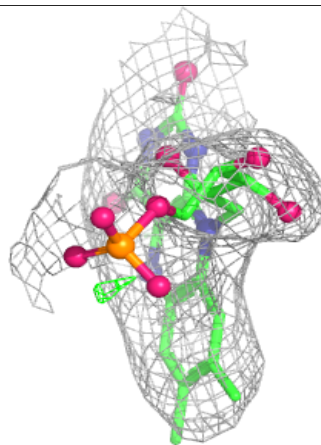
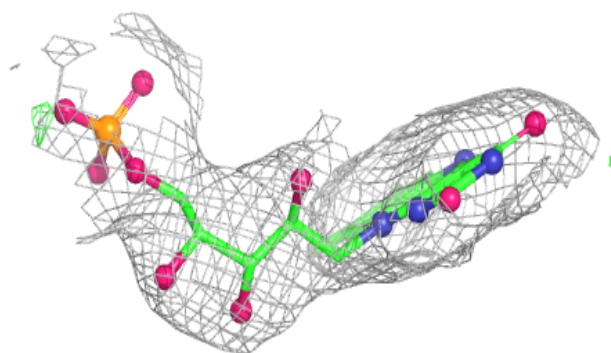
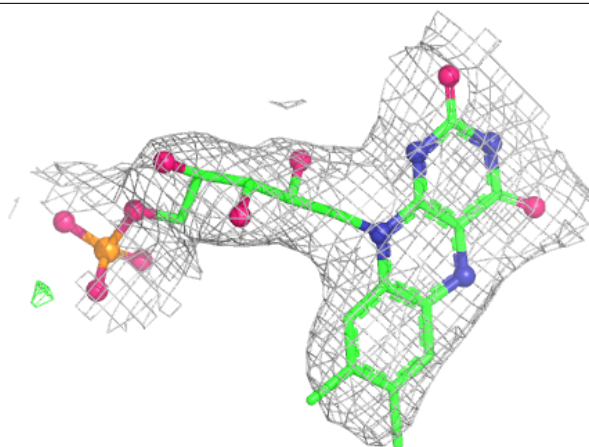
Electron density around NAP B 753:

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



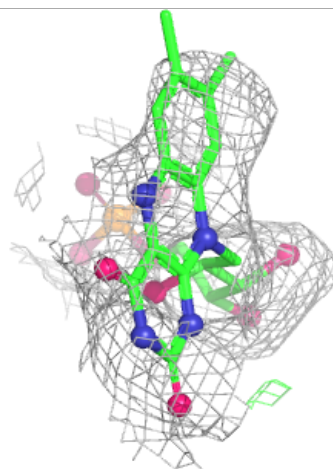
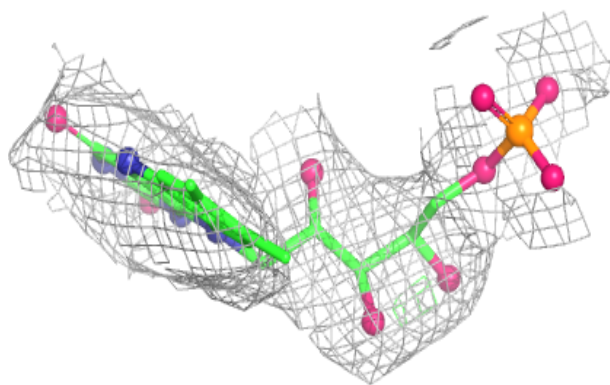
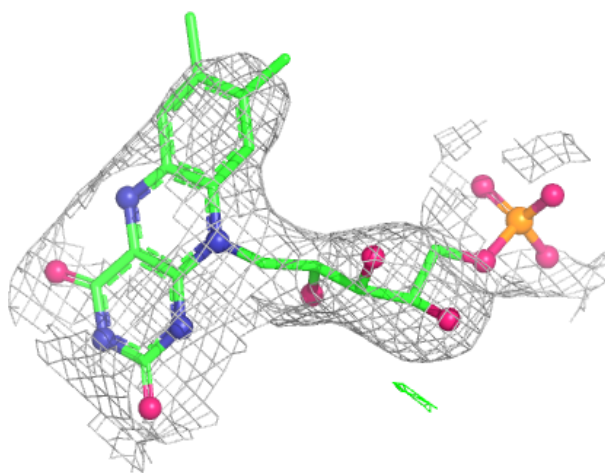
Electron density around FMN A 751:

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



Electron density around FMN B 751:

$2mF_o-DF_c$ (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.