



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:30 pm GMT

PDB ID : 1AHZ
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH 4-(1-HEPTENYL)PHENOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 3.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

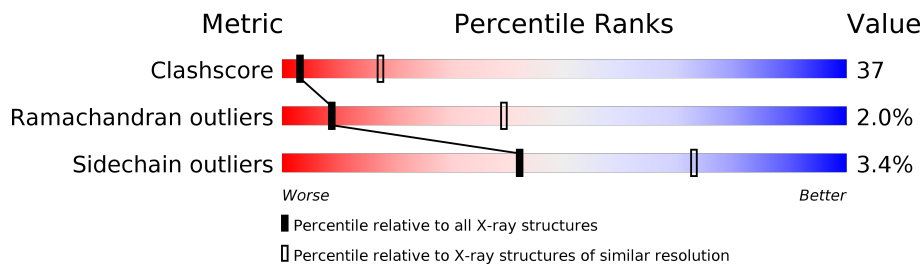
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EPT	A	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8904 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.

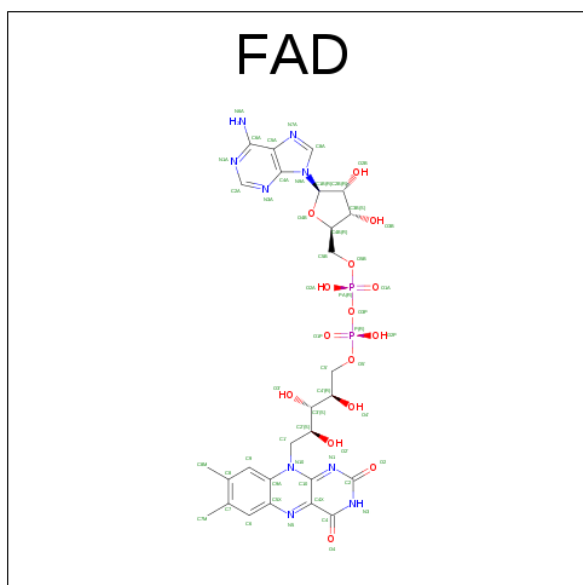
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

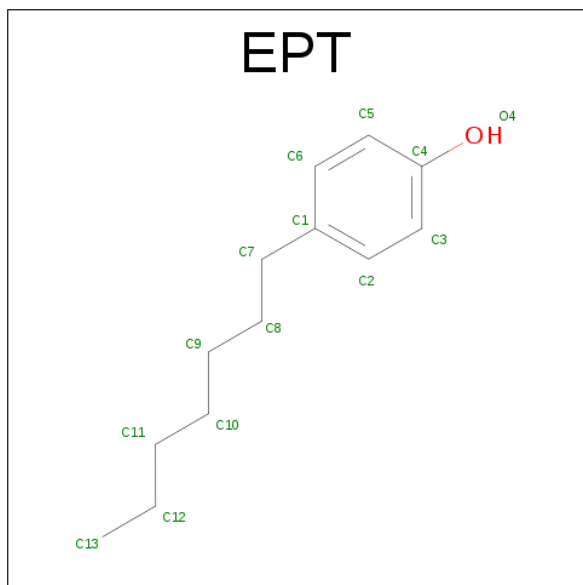
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is HEPTANYL-P-PHENOL (three-letter code: EPT) (formula: $C_{13}H_{20}O$).



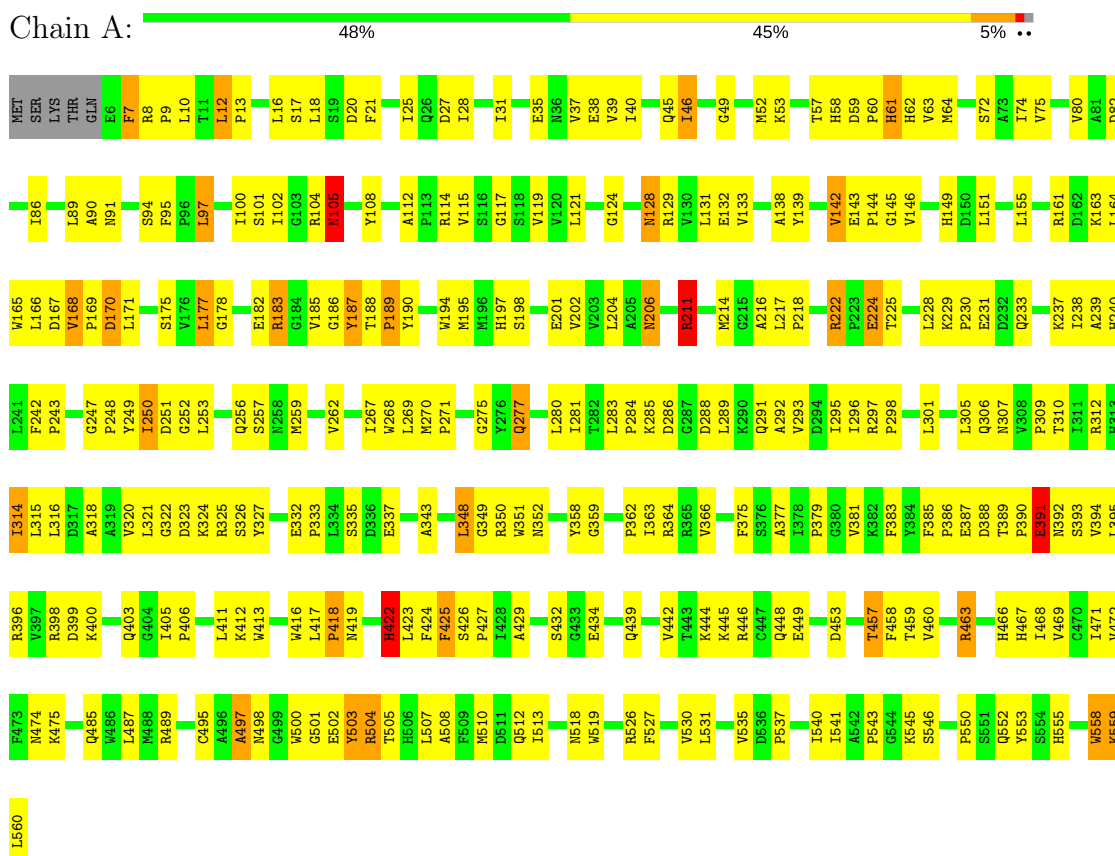
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	13	1		

3 Residue-property plots

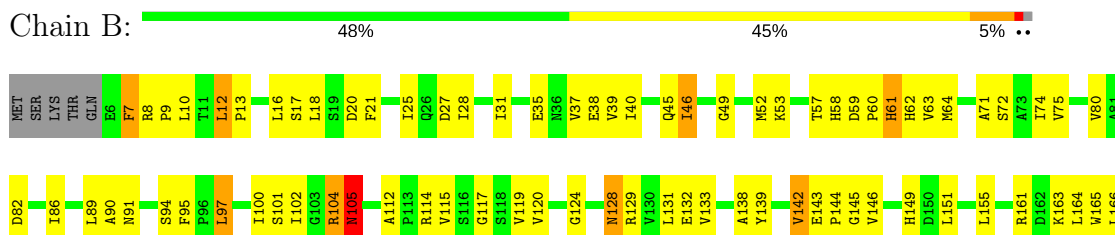
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



D399	Q485	Q486	L487	W488	R489	C495	A496	A497	N498	G499	W500	G501	E502	Y503	W504	T505	W506	L507	F424	A508	F509	W510	D511	G512	T513	S432	G433	E434	Q439	V442	T443	K444	K445	R446	G447	Q448	E449	D453	T457	F458	T459	V460	R463	H466	H467	I468	V469	C470	I471	V472	P473	N474	K475	
K400	W486	Q486	Q403	G404	I405	P406	L411	K412	W413	W416	L417	P418	N419	R422	L423	F424	P425	S426	P427	I428	A429	S432	G433	E434	Q439	V442	T443	K444	K445	R446	G447	Q448	E449	D453	T457	F458	T459	V460	R463	H466	H467	I468	V469	C470	I471	V472	P473	N474	K475					
L316	D317	A318	A319	V320	L321	G322	D323	K324	R325	S326	Y327	E332	P333	L334	S335	D336	E337	A343	L348	G349	R350	K351	N352	Y358	G359	P362	I363	R364	R365	V366	F375	S376	A377	I378	P379	G380	V381	K382	F383	Y384	F385	P386	E387	D388	T389	P390	E391	N392	S393	V394	L395	R396		
F242	P243	G247	P248	Y249	I250	D251	L253	Q256	S257	N258	M259	V262	L267	W268	L269	M270	P271	G275	Y276	Q277	L280	I281	T282	L283	P284	K285	D286	G287	D288	L289	K290	Q291	A292	V293	L295	I296	R297	P298	L301	Q306	N307	V308	P309	D322	P310	Q233	I311	R312	H313	I314	L315			
D167	P168	V169	D170	L171	S175	Y176	L177	G178	E182	R183	G184	V185	G186	Y187	T188	P189	Y190	W194	M195	N196	H197	S198	E201	V202	V203	L204	K205	N206	L209	L210	R211	K214	G215	A216	L217	P218	R222	P223	E224	T225	L228	K229	P230	E231	P309	D322	T310	Q233	I311	R312	H313	I314	H240	L241

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	140.97 Å 140.97 Å 133.45 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30	Depositor
% Data completeness (in resolution range)	90.7 (30.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.224 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.50	0/4511	1.23	26/6131 (0.4%)
1	B	0.50	0/4511	1.23	26/6131 (0.4%)
All	All	0.50	0/9022	1.23	52/12262 (0.4%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	183	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	375	PHE	CB-CG-CD1	7.62	126.13	120.80
1	B	375	PHE	CB-CG-CD1	7.61	126.12	120.80
1	A	97	LEU	CA-CB-CG	-7.36	98.36	115.30
1	B	97	LEU	CA-CB-CG	-7.36	98.37	115.30
1	B	129	ARG	N-CA-C	7.36	130.88	111.00
1	A	129	ARG	N-CA-C	7.34	130.83	111.00
1	A	7	PHE	N-CA-C	6.96	129.80	111.00
1	B	7	PHE	N-CA-C	6.95	129.77	111.00
1	A	211	ARG	N-CA-CB	6.54	122.37	110.60
1	B	211	ARG	N-CA-CB	6.53	122.35	110.60
1	A	457	THR	CB-CA-C	-6.51	94.02	111.60
1	B	457	THR	CB-CA-C	-6.51	94.03	111.60
1	A	463	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	B	463	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	A	187	TYR	N-CA-C	6.20	127.75	111.00
1	B	187	TYR	N-CA-C	6.19	127.72	111.00
1	A	422	HIS	CB-CA-C	6.18	122.77	110.40
1	B	422	HIS	CB-CA-C	6.17	122.73	110.40
1	B	518	ASN	N-CA-C	5.76	126.55	111.00
1	A	518	ASN	N-CA-C	5.74	126.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	B	504	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	314	ILE	CB-CA-C	-5.47	100.66	111.60
1	B	314	ILE	CB-CA-C	-5.46	100.67	111.60
1	A	168	VAL	CB-CA-C	-5.42	101.09	111.40
1	B	168	VAL	CB-CA-C	-5.41	101.12	111.40
1	A	425	PHE	N-CA-C	-5.37	96.51	111.00
1	B	425	PHE	N-CA-C	-5.37	96.51	111.00
1	A	155	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	B	155	LEU	CB-CG-CD2	-5.33	101.93	111.00
1	B	348	LEU	CA-CB-CG	-5.26	103.20	115.30
1	A	348	LEU	CA-CB-CG	-5.26	103.21	115.30
1	A	142	VAL	CB-CA-C	-5.22	101.49	111.40
1	B	142	VAL	CB-CA-C	-5.20	101.52	111.40
1	B	558	TRP	N-CA-C	5.17	124.95	111.00
1	A	558	TRP	N-CA-C	5.16	124.92	111.00
1	B	169	PRO	N-CA-C	-5.11	98.81	112.10
1	A	169	PRO	N-CA-C	-5.11	98.82	112.10
1	B	250	ILE	N-CA-C	5.10	124.78	111.00
1	A	250	ILE	N-CA-C	5.10	124.78	111.00
1	B	124	GLY	N-CA-C	5.06	125.75	113.10
1	A	124	GLY	N-CA-C	5.04	125.70	113.10
1	B	104	ARG	N-CA-C	5.04	124.60	111.00
1	A	104	ARG	N-CA-C	5.03	124.59	111.00
1	A	222	ARG	CB-CA-C	5.03	120.47	110.40
1	B	10	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	B	12	LEU	CA-CB-CG	5.02	126.85	115.30
1	A	12	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	222	ARG	CB-CA-C	5.01	120.43	110.40
1	A	10	LEU	CB-CG-CD1	-5.00	102.50	111.00

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	4391	0	4330	337	0
1	B	4391	0	4330	333	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	29	9	0
3	B	53	0	29	8	0
4	A	14	0	20	14	0
All	All	8904	0	8738	642	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 37.

All (642) 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)
3:A:600:FAD:H8A	3:A:600:FAD:H51A	1.31	1.10
1:A:314:ILE:HD11	1:A:350:ARG:HG3	1.37	1.06
3:B:600:FAD:H51A	3:B:600:FAD:H8A	1.31	1.06
1:B:314:ILE:HD11	1:B:350:ARG:HG3	1.37	1.03
1:A:280:LEU:HD12	1:A:281:ILE:H	1.28	0.99
1:B:280:LEU:HD12	1:B:281:ILE:H	1.28	0.98
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.01	0.94
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.01	0.94
1:A:463:ARG:HH12	1:B:138:ALA:HB3	1.32	0.93
1:B:349:GLY:H	1:B:352:ASN:HD21	1.16	0.92
1:A:138:ALA:HB3	1:B:463:ARG:HH12	1.34	0.91
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.52	0.91
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.52	0.90
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.07	0.90
1:B:314:ILE:HD11	1:B:350:ARG:CG	2.02	0.90
1:A:314:ILE:HD11	1:A:350:ARG:CG	2.02	0.89
1:A:349:GLY:H	1:A:352:ASN:HD21	1.16	0.89
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.07	0.89
1:A:61:HIS:CD2	1:A:422:HIS:HD1	1.91	0.88
1:B:61:HIS:CD2	1:B:422:HIS:HD1	1.91	0.87
1:A:16:LEU:HD11	1:A:20:ASP:HB2	1.56	0.87
1:A:138:ALA:HB3	1:B:463:ARG:NH1	1.90	0.87
1:B:16:LEU:HD11	1:B:20:ASP:HB2	1.56	0.86
1:B:16:LEU:HD11	1:B:20:ASP:CB	2.06	0.86
1:A:16:LEU:HD11	1:A:20:ASP:CB	2.06	0.85
1:A:61:HIS:CD2	1:A:422:HIS:H	1.95	0.84
1:A:510:MET:HE1	1:A:546:SER:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:HIS:CD2	1:B:422:HIS:H	1.95	0.84
1:A:463:ARG:NH1	1:B:138:ALA:HB3	1.93	0.83
1:A:248:PRO:HG3	1:B:257:SER:HB3	1.59	0.83
1:B:80:VAL:HB	1:B:231:GLU:HG3	1.61	0.82
1:A:80:VAL:HB	1:A:231:GLU:HG3	1.61	0.82
1:A:163:LYS:HE2	1:A:163:LYS:HA	1.62	0.82
1:B:280:LEU:HD12	1:B:281:ILE:N	1.95	0.82
1:B:206:ASN:HD22	1:B:206:ASN:H	1.29	0.81
1:B:163:LYS:HA	1:B:163:LYS:HE2	1.62	0.81
1:A:206:ASN:HD22	1:A:206:ASN:H	1.29	0.81
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.61	0.80
1:A:457:THR:HG21	4:A:602:EPT:C13	2.12	0.80
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.63	0.80
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.61	0.80
1:A:280:LEU:HD12	1:A:281:ILE:N	1.95	0.79
1:A:349:GLY:N	1:A:352:ASN:HD21	1.80	0.79
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.63	0.79
1:B:314:ILE:HD11	1:B:350:ARG:HA	1.65	0.79
1:A:257:SER:HB3	1:B:248:PRO:HG3	1.65	0.79
1:B:349:GLY:N	1:B:352:ASN:HD21	1.80	0.78
1:B:312:ARG:HH21	1:B:316:LEU:HD21	1.49	0.78
1:A:211:ARG:HD3	1:B:519:TRP:CH2	2.19	0.78
1:A:416:TRP:HD1	1:A:417:LEU:HD12	1.49	0.78
1:B:510:MET:CE	1:B:546:SER:H	1.97	0.78
1:A:312:ARG:HH21	1:A:316:LEU:HD21	1.49	0.77
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.66	0.77
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.66	0.77
1:A:314:ILE:HD11	1:A:350:ARG:HA	1.65	0.77
1:A:510:MET:CE	1:A:546:SER:H	1.97	0.76
1:B:489:ARG:HG2	1:B:512:GLN:OE1	1.85	0.76
1:A:161:ARG:O	1:A:161:ARG:HD3	1.86	0.76
1:B:161:ARG:O	1:B:161:ARG:HD3	1.86	0.76
1:A:225:THR:O	1:A:228:LEU:HD13	1.86	0.76
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.68	0.76
1:A:40:ILE:HA	1:A:45:GLN:OE1	1.86	0.76
1:A:489:ARG:HG2	1:A:512:GLN:OE1	1.85	0.75
1:B:40:ILE:HA	1:B:45:GLN:OE1	1.86	0.75
1:B:225:THR:O	1:B:228:LEU:HD13	1.86	0.75
1:B:416:TRP:HD1	1:B:417:LEU:HD12	1.49	0.75
1:A:292:ALA:O	1:A:296:ILE:HG13	1.87	0.75
1:B:206:ASN:ND2	1:B:206:ASN:H	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TRP:CH2	1:B:211:ARG:HD3	2.22	0.75
1:A:206:ASN:ND2	1:A:206:ASN:H	1.84	0.75
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.22	0.74
1:B:314:ILE:CD1	1:B:350:ARG:HA	2.18	0.74
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.22	0.74
1:B:292:ALA:O	1:B:296:ILE:HG13	1.87	0.74
1:A:211:ARG:HD3	1:B:519:TRP:CZ3	2.23	0.74
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.68	0.74
1:A:188:THR:HB	1:A:189:PRO:HD2	1.70	0.73
1:B:510:MET:HE1	1:B:546:SER:H	1.53	0.73
1:B:526:ARG:O	1:B:530:VAL:HG23	1.89	0.73
1:B:555:HIS:CD2	1:B:559:LYS:HE3	2.24	0.73
1:A:21:PHE:CE1	1:A:25:ILE:HG13	2.24	0.73
1:A:314:ILE:CD1	1:A:350:ARG:HA	2.17	0.73
1:B:419:ASN:O	1:B:474:ASN:HA	1.88	0.73
1:A:419:ASN:O	1:A:474:ASN:HA	1.88	0.73
1:B:320:VAL:O	1:B:412:LYS:HE2	1.89	0.73
1:A:247:GLY:O	1:B:183:ARG:NH2	2.19	0.73
1:B:349:GLY:H	1:B:352:ASN:ND2	1.87	0.73
1:A:362:PRO:O	1:A:366:VAL:HG23	1.89	0.72
1:B:21:PHE:CE1	1:B:25:ILE:HG13	2.24	0.72
1:B:416:TRP:CD1	1:B:417:LEU:HD12	2.24	0.72
1:B:171:LEU:HD13	1:B:411:LEU:HD21	1.71	0.72
1:A:320:VAL:O	1:A:412:LYS:HE2	1.89	0.72
1:A:555:HIS:CD2	1:A:559:LYS:HE3	2.24	0.72
1:B:362:PRO:O	1:B:366:VAL:HG23	1.90	0.72
1:A:526:ARG:O	1:A:530:VAL:HG23	1.89	0.72
1:A:171:LEU:HD13	1:A:411:LEU:HD21	1.71	0.71
1:A:416:TRP:CD1	1:A:417:LEU:HD12	2.24	0.71
1:B:188:THR:HB	1:B:189:PRO:HD2	1.70	0.71
1:A:359:GLY:O	1:A:364:ARG:HD3	1.90	0.71
1:A:349:GLY:H	1:A:352:ASN:ND2	1.87	0.71
1:B:359:GLY:O	1:B:364:ARG:HD3	1.89	0.70
1:B:128:ASN:HA	1:B:145:GLY:HA3	1.71	0.70
1:A:128:ASN:HA	1:A:145:GLY:HA3	1.72	0.70
1:A:138:ALA:CB	1:B:463:ARG:HH12	2.05	0.69
1:B:418:PRO:HG2	1:B:474:ASN:HD22	1.57	0.69
1:B:427:PRO:HA	1:B:501:GLY:O	1.93	0.69
1:A:427:PRO:HA	1:A:501:GLY:O	1.93	0.69
1:A:503:TYR:CZ	1:A:504:ARG:HD3	2.28	0.69
1:A:363:ILE:HD12	1:B:363:ILE:HD12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:PRO:HG2	1:A:474:ASN:HD22	1.57	0.68
1:A:537:PRO:O	1:A:552:GLN:NE2	2.25	0.68
1:B:503:TYR:CZ	1:B:504:ARG:HD3	2.28	0.68
1:B:555:HIS:HD2	1:B:559:LYS:HE3	1.57	0.68
1:A:297:ARG:HH21	1:A:432:SER:HA	1.59	0.68
1:B:537:PRO:O	1:B:552:GLN:NE2	2.25	0.68
1:B:194:TRP:O	1:B:197:HIS:HD2	1.76	0.68
1:A:390:PRO:HB2	1:A:392:ASN:OD1	1.94	0.68
1:A:555:HIS:HD2	1:A:559:LYS:HE3	1.57	0.68
1:B:297:ARG:HH21	1:B:432:SER:HA	1.58	0.67
1:A:194:TRP:O	1:A:197:HIS:HD2	1.76	0.67
1:B:390:PRO:HB2	1:B:392:ASN:OD1	1.94	0.67
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.76	0.67
1:B:105:ASN:HA	3:B:600:FAD:H5'2	1.77	0.67
1:A:183:ARG:NH2	1:B:247:GLY:O	2.21	0.66
1:B:445:LYS:NZ	1:B:449:GLU:OE2	2.28	0.66
1:A:105:ASN:HA	3:A:600:FAD:H5'2	1.77	0.66
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.25	0.66
1:A:489:ARG:NH2	1:A:508:ALA:O	2.28	0.66
1:A:503:TYR:OH	4:A:602:EPT:O4	2.13	0.66
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.76	0.66
1:A:445:LYS:NZ	1:A:449:GLU:OE2	2.28	0.66
1:B:510:MET:HE1	1:B:545:LYS:HD2	1.78	0.66
1:A:505:THR:HG21	1:A:513:ILE:CD1	2.25	0.66
1:A:463:ARG:HH12	1:B:138:ALA:CB	2.08	0.65
1:A:519:TRP:CZ3	1:B:211:ARG:HD3	2.32	0.65
1:B:489:ARG:NH2	1:B:508:ALA:O	2.28	0.65
1:A:142:VAL:HG12	1:A:143:GLU:O	1.97	0.65
1:A:275:GLY:HA3	1:A:359:GLY:O	1.96	0.65
1:B:275:GLY:HA3	1:B:359:GLY:O	1.96	0.65
1:A:9:PRO:HG2	1:A:12:LEU:HD21	1.79	0.65
1:A:314:ILE:CD1	1:A:350:ARG:HG3	2.21	0.65
1:B:142:VAL:HG12	1:B:143:GLU:O	1.97	0.65
1:A:425:PHE:HB3	1:A:469:VAL:HB	1.78	0.64
1:A:59:ASP:OD2	1:A:62:HIS:HA	1.98	0.64
1:A:108:TYR:OH	4:A:602:EPT:H3	1.97	0.64
1:B:9:PRO:HG2	1:B:12:LEU:HD21	1.78	0.64
1:B:335:SER:HB3	1:B:337:GLU:OE1	1.98	0.64
1:A:335:SER:HB3	1:A:337:GLU:OE1	1.98	0.64
1:A:271:PRO:HG3	1:B:301:LEU:HB3	1.78	0.64
1:B:425:PHE:HB3	1:B:469:VAL:HB	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:OD2	1:B:62:HIS:HA	1.98	0.64
1:A:12:LEU:HB3	1:A:13:PRO:HD2	1.80	0.64
1:B:35:GLU:H	1:B:35:GLU:CD	2.01	0.63
1:B:177:LEU:HD12	1:B:178:GLY:N	2.13	0.63
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.80	0.63
1:B:12:LEU:HB3	1:B:13:PRO:HD2	1.80	0.63
1:A:363:ILE:HD12	1:B:363:ILE:HG23	1.80	0.63
1:B:552:GLN:OE1	1:B:552:GLN:N	2.28	0.63
1:A:13:PRO:HG3	1:A:117:GLY:O	1.99	0.63
1:B:216:ALA:O	1:B:218:PRO:HD3	1.99	0.63
1:A:35:GLU:H	1:A:35:GLU:CD	2.01	0.63
1:A:312:ARG:HH21	1:A:316:LEU:CD2	2.12	0.63
1:A:91:ASN:ND2	1:A:540:ILE:HG13	2.14	0.63
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.80	0.63
1:B:91:ASN:ND2	1:B:540:ILE:HG13	2.14	0.62
1:A:177:LEU:HD12	1:A:178:GLY:N	2.14	0.62
1:A:363:ILE:HG23	1:B:363:ILE:HD12	1.81	0.62
1:A:416:TRP:HD1	1:A:417:LEU:CD1	2.12	0.62
1:A:552:GLN:OE1	1:A:552:GLN:N	2.28	0.62
1:B:425:PHE:HE2	1:B:427:PRO:HG3	1.62	0.62
1:A:216:ALA:O	1:A:218:PRO:HD3	1.98	0.62
1:B:312:ARG:HH21	1:B:316:LEU:CD2	2.12	0.62
1:B:419:ASN:H	1:B:474:ASN:ND2	1.98	0.62
1:B:314:ILE:CG1	1:B:350:ARG:HA	2.30	0.62
1:A:419:ASN:H	1:A:474:ASN:ND2	1.98	0.62
1:B:416:TRP:HD1	1:B:417:LEU:CD1	2.12	0.62
1:A:306:GLN:NE2	1:A:358:TYR:H	1.98	0.62
1:B:13:PRO:HG3	1:B:117:GLY:O	1.99	0.62
1:B:306:GLN:NE2	1:B:358:TYR:H	1.98	0.61
1:B:9:PRO:HG2	1:B:12:LEU:CD2	2.29	0.61
1:B:314:ILE:CD1	1:B:350:ARG:HG3	2.21	0.61
1:B:128:ASN:HD22	1:B:145:GLY:HA3	1.65	0.61
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.29	0.61
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.29	0.61
1:A:9:PRO:HG2	1:A:12:LEU:CD2	2.29	0.61
1:A:314:ILE:CG1	1:A:350:ARG:HA	2.30	0.61
1:A:425:PHE:HE2	1:A:427:PRO:HG3	1.62	0.61
1:B:16:LEU:HD12	1:B:17:SER:H	1.67	0.60
1:B:413:TRP:CZ2	3:B:600:FAD:HM72	2.37	0.60
1:B:28:ILE:HD13	1:B:89:LEU:HD12	1.83	0.60
1:A:16:LEU:HD12	1:A:17:SER:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:HD22	1:A:145:GLY:HA3	1.65	0.60
1:A:413:TRP:CZ2	3:A:600:FAD:HM72	2.37	0.60
1:A:37:VAL:HG12	1:A:38:GLU:N	2.17	0.60
1:A:393:SER:OG	1:A:396:ARG:HG3	2.00	0.60
1:B:417:LEU:HB3	1:B:418:PRO:CD	2.32	0.60
1:A:248:PRO:HG3	1:B:257:SER:CB	2.30	0.60
1:B:21:PHE:CZ	1:B:25:ILE:HG13	2.38	0.59
1:A:28:ILE:HD13	1:A:89:LEU:HD12	1.83	0.59
1:A:503:TYR:HH	4:A:602:EPT:HO4	1.49	0.59
1:A:310:THR:HG22	1:A:459:THR:HA	1.84	0.59
1:B:393:SER:OG	1:B:396:ARG:HG3	2.01	0.59
1:A:12:LEU:HB3	1:A:13:PRO:CD	2.33	0.59
1:B:471:ILE:N	1:B:471:ILE:HD12	2.18	0.59
1:A:471:ILE:HD12	1:A:471:ILE:N	2.18	0.58
1:B:35:GLU:OE1	1:B:35:GLU:N	2.30	0.58
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.32	0.58
1:A:102:ILE:HB	3:A:600:FAD:O2P	2.03	0.58
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.32	0.58
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.18	0.58
1:A:40:ILE:HD11	1:A:57:THR:CG2	2.32	0.58
1:A:429:ALA:HB2	1:A:439:GLN:NE2	2.18	0.58
1:A:495:CYS:HB3	1:A:500:TRP:HB2	1.85	0.58
1:B:310:THR:HG22	1:B:459:THR:HA	1.84	0.58
1:B:7:PHE:O	1:B:18:LEU:HD11	2.04	0.58
1:B:37:VAL:HG12	1:B:38:GLU:N	2.17	0.58
1:B:495:CYS:HB3	1:B:500:TRP:HB2	1.85	0.58
1:B:102:ILE:HB	3:B:600:FAD:O2P	2.03	0.58
1:B:429:ALA:HB2	1:B:439:GLN:HE22	1.69	0.58
1:A:188:THR:HB	1:A:189:PRO:CD	2.33	0.58
1:B:312:ARG:NH1	1:B:394:VAL:HG11	2.19	0.58
1:A:417:LEU:HB3	1:A:418:PRO:CD	2.32	0.58
1:B:188:THR:HB	1:B:189:PRO:CD	2.33	0.58
1:B:312:ARG:NH2	1:B:316:LEU:HG	2.18	0.58
1:B:343:ALA:HB1	1:B:348:LEU:O	2.04	0.58
1:A:21:PHE:CZ	1:A:25:ILE:HG13	2.38	0.57
1:B:12:LEU:HB3	1:B:13:PRO:CD	2.33	0.57
1:B:256:GLN:NE2	1:B:504:ARG:HG2	2.19	0.57
1:A:312:ARG:NH1	1:A:394:VAL:HG11	2.19	0.57
1:A:256:GLN:NE2	1:A:504:ARG:HG2	2.19	0.57
1:A:312:ARG:NH2	1:A:316:LEU:HG	2.18	0.57
1:A:61:HIS:HD2	1:A:422:HIS:HD1	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ALA:HB2	1:A:439:GLN:HE22	1.69	0.57
1:B:314:ILE:HG12	1:B:350:ARG:HA	1.86	0.57
1:B:497:ALA:C	1:B:498:ASN:HD22	2.07	0.57
1:A:343:ALA:HB1	1:A:348:LEU:O	2.04	0.57
1:A:16:LEU:CD1	1:A:20:ASP:HB2	2.33	0.57
1:B:391:GLU:HA	1:B:396:ARG:HD2	1.87	0.57
1:B:151:LEU:HG	1:B:166:LEU:HD21	1.87	0.57
1:B:46:ILE:O	1:B:46:ILE:HG22	2.05	0.57
1:A:222:ARG:HG3	1:A:225:THR:HG23	1.86	0.57
1:A:35:GLU:N	1:A:35:GLU:OE1	2.30	0.56
1:A:391:GLU:HA	1:A:396:ARG:HD2	1.86	0.56
1:A:7:PHE:O	1:A:18:LEU:HD11	2.04	0.56
1:A:46:ILE:HG22	1:A:46:ILE:O	2.05	0.56
1:A:497:ALA:C	1:A:498:ASN:HD22	2.07	0.56
1:A:314:ILE:HG12	1:A:350:ARG:HA	1.86	0.56
1:A:510:MET:HE1	1:A:545:LYS:HD2	1.87	0.56
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.87	0.56
1:A:510:MET:HE1	1:A:546:SER:N	2.15	0.56
1:B:40:ILE:HD11	1:B:57:THR:CG2	2.32	0.56
1:B:82:ASP:O	1:B:86:ILE:HG13	2.06	0.56
1:B:417:LEU:CB	1:B:418:PRO:HD2	2.35	0.56
1:A:214:MET:HB2	1:A:239:ALA:HA	1.87	0.56
1:B:504:ARG:O	1:B:505:THR:HG23	2.06	0.56
1:A:277:GLN:HA	1:A:277:GLN:HE21	1.71	0.56
3:A:600:FAD:C8A	3:A:600:FAD:H51A	2.21	0.56
1:A:82:ASP:O	1:A:86:ILE:HG13	2.06	0.56
1:B:202:VAL:HG12	1:B:262:VAL:HA	1.87	0.55
1:B:214:MET:HB2	1:B:239:ALA:HA	1.87	0.55
1:B:277:GLN:HE21	1:B:277:GLN:HA	1.71	0.55
1:B:434:GLU:HA	1:B:434:GLU:OE1	2.05	0.55
1:A:417:LEU:CB	1:A:418:PRO:HD2	2.35	0.55
1:A:151:LEU:HG	1:A:166:LEU:HD21	1.87	0.55
1:B:161:ARG:NH2	1:B:403:GLN:O	2.39	0.55
1:A:434:GLU:OE1	1:A:434:GLU:HA	2.05	0.55
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.87	0.55
1:B:222:ARG:HG3	1:B:225:THR:HG23	1.86	0.55
1:B:446:ARG:HD3	1:B:449:GLU:OE1	2.06	0.55
1:A:112:ALA:O	1:A:507:LEU:HD11	2.07	0.55
1:A:237:LYS:HE2	1:B:498:ASN:O	2.07	0.55
1:A:202:VAL:HG12	1:A:262:VAL:HA	1.87	0.55
1:A:161:ARG:NH2	1:A:403:GLN:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HD3	1:A:449:GLU:OE1	2.06	0.55
1:A:398:ARG:NH2	4:A:602:EPT:H121	2.21	0.55
1:A:504:ARG:O	1:A:505:THR:HG23	2.06	0.55
1:B:418:PRO:HB2	1:B:474:ASN:ND2	2.23	0.55
1:A:190:TYR:CE1	1:A:270:MET:HB2	2.43	0.54
1:A:281:ILE:HG23	1:A:381:VAL:CG2	2.37	0.54
1:B:8:ARG:HG3	1:B:8:ARG:O	2.06	0.54
1:A:418:PRO:HB2	1:A:474:ASN:ND2	2.22	0.54
1:B:112:ALA:O	1:B:507:LEU:HD11	2.07	0.54
1:B:16:LEU:CD1	1:B:20:ASP:HB2	2.33	0.54
1:B:281:ILE:HG23	1:B:381:VAL:CG2	2.37	0.54
1:A:337:GLU:N	1:A:337:GLU:OE1	2.29	0.54
1:B:9:PRO:HG3	1:B:21:PHE:CE1	2.42	0.54
1:B:190:TYR:CE1	1:B:270:MET:HB2	2.42	0.54
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.37	0.54
1:A:9:PRO:HG3	1:A:21:PHE:CE1	2.42	0.53
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.37	0.53
1:B:61:HIS:HD2	1:B:422:HIS:HD1	1.50	0.53
1:A:301:LEU:HB3	1:B:271:PRO:HG3	1.89	0.53
1:A:519:TRP:HB2	1:B:218:PRO:HG3	1.90	0.53
1:A:61:HIS:HD2	1:A:422:HIS:H	1.54	0.53
1:A:459:THR:OG1	1:A:466:HIS:HB2	2.09	0.53
1:B:309:PRO:HD2	1:B:460:VAL:HB	1.91	0.53
1:A:64:MET:HE2	1:A:485:GLN:HE22	1.74	0.53
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.91	0.53
1:A:309:PRO:HD2	1:A:460:VAL:HB	1.91	0.53
1:B:459:THR:OG1	1:B:466:HIS:HB2	2.09	0.52
1:A:385:PHE:CB	1:A:386:PRO:HD2	2.33	0.52
1:B:324:LYS:HB2	1:B:416:TRP:CE2	2.45	0.52
1:A:324:LYS:HB2	1:A:416:TRP:CE2	2.45	0.52
1:B:187:TYR:O	1:B:307:ASN:HB2	2.09	0.52
1:A:198:SER:O	1:A:240:HIS:HD2	1.92	0.52
1:A:187:TYR:O	1:A:307:ASN:HB2	2.09	0.52
1:A:16:LEU:HD12	1:A:17:SER:N	2.25	0.52
1:B:337:GLU:N	1:B:337:GLU:OE1	2.29	0.52
1:B:423:LEU:HB3	1:B:471:ILE:HB	1.92	0.52
1:A:286:ASP:HB2	1:A:350:ARG:CZ	2.40	0.51
1:B:57:THR:OG1	1:B:58:HIS:ND1	2.41	0.51
1:B:198:SER:O	1:B:240:HIS:HD2	1.92	0.51
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.91	0.51
1:A:57:THR:OG1	1:A:58:HIS:ND1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:SER:CB	1:B:248:PRO:HG3	2.38	0.51
1:B:229:LYS:O	1:B:233:GLN:HG3	2.11	0.51
1:A:177:LEU:C	1:A:177:LEU:HD12	2.31	0.51
1:A:423:LEU:HB3	1:A:471:ILE:HB	1.92	0.51
1:B:16:LEU:HD11	1:B:20:ASP:HB3	1.92	0.51
1:B:286:ASP:HB2	1:B:350:ARG:CZ	2.40	0.51
3:B:600:FAD:H51A	3:B:600:FAD:C8A	2.21	0.51
1:A:238:ILE:O	1:A:238:ILE:HG22	2.11	0.51
1:A:171:LEU:HD22	1:A:411:LEU:HG	1.93	0.51
1:B:238:ILE:HG22	1:B:238:ILE:O	2.11	0.51
1:A:8:ARG:O	1:A:8:ARG:HG3	2.06	0.51
1:B:163:LYS:CA	1:B:163:LYS:HE2	2.36	0.51
1:B:171:LEU:HD22	1:B:411:LEU:HG	1.93	0.51
1:A:163:LYS:HA	1:A:163:LYS:CE	2.38	0.51
1:A:225:THR:C	1:A:228:LEU:HD13	2.31	0.51
1:A:16:LEU:HD11	1:A:20:ASP:HB3	1.92	0.51
1:A:457:THR:HG21	4:A:602:EPT:H133	1.91	0.51
1:A:489:ARG:HH22	1:A:560:LEU:HD22	1.76	0.51
1:A:105:ASN:HD22	3:A:600:FAD:H5'2	1.75	0.51
1:A:163:LYS:HE2	1:A:163:LYS:CA	2.36	0.50
1:A:229:LYS:O	1:A:233:GLN:HG3	2.11	0.50
1:B:16:LEU:HD12	1:B:17:SER:N	2.25	0.50
1:B:318:ALA:O	1:B:322:GLY:N	2.42	0.50
1:B:105:ASN:HD22	3:B:600:FAD:H5'2	1.75	0.50
1:A:386:PRO:HG2	1:A:387:GLU:N	2.27	0.50
1:B:177:LEU:HD12	1:B:177:LEU:C	2.31	0.50
1:A:386:PRO:HG2	1:A:387:GLU:H	1.76	0.50
1:B:386:PRO:HG2	1:B:387:GLU:N	2.27	0.50
1:A:74:ILE:HG22	1:A:75:VAL:N	2.27	0.50
1:B:307:ASN:O	1:B:309:PRO:HD3	2.12	0.50
1:B:386:PRO:HG2	1:B:387:GLU:H	1.76	0.50
1:B:489:ARG:HH22	1:B:560:LEU:HD22	1.76	0.50
1:A:142:VAL:HG13	1:A:146:VAL:CG2	2.41	0.50
1:A:314:ILE:HG13	1:A:350:ARG:O	2.11	0.50
1:B:225:THR:C	1:B:228:LEU:HD13	2.31	0.50
1:B:61:HIS:HD2	1:B:422:HIS:H	1.54	0.50
1:A:444:LYS:O	1:A:448:GLN:HG2	2.11	0.50
1:B:418:PRO:CG	1:B:474:ASN:HD22	2.25	0.50
1:A:231:GLU:OE1	1:A:231:GLU:N	2.36	0.49
1:B:132:GLU:HG2	1:B:133:VAL:N	2.26	0.49
1:B:58:HIS:O	1:B:60:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:O	1:A:309:PRO:HD3	2.12	0.49
1:A:314:ILE:HD11	1:A:350:ARG:CA	2.40	0.49
1:B:510:MET:HE1	1:B:546:SER:N	2.25	0.49
1:B:385:PHE:CB	1:B:386:PRO:HD2	2.33	0.49
1:B:444:LYS:O	1:B:448:GLN:HG2	2.11	0.49
1:B:142:VAL:HG13	1:B:146:VAL:CG2	2.41	0.49
1:B:204:LEU:HB3	1:B:206:ASN:HD21	1.77	0.49
1:B:314:ILE:HG13	1:B:350:ARG:O	2.11	0.49
1:A:142:VAL:HG12	1:A:143:GLU:N	2.28	0.49
1:A:457:THR:OG1	4:A:602:EPT:H132	2.13	0.49
1:B:426:SER:O	1:B:502:GLU:HA	2.13	0.49
1:A:211:ARG:CD	1:B:519:TRP:CH2	2.92	0.49
1:B:163:LYS:HA	1:B:163:LYS:CE	2.38	0.48
1:B:163:LYS:O	1:B:164:LEU:HD23	2.14	0.48
1:A:418:PRO:CG	1:A:474:ASN:HD22	2.25	0.48
1:B:142:VAL:CG1	1:B:143:GLU:N	2.76	0.48
1:B:472:VAL:HG23	1:B:472:VAL:O	2.14	0.48
1:A:142:VAL:CG1	1:A:143:GLU:N	2.76	0.48
1:B:217:LEU:HA	1:B:217:LEU:HD12	1.46	0.48
1:B:74:ILE:HG22	1:B:75:VAL:N	2.27	0.48
1:A:132:GLU:HG2	1:A:133:VAL:N	2.26	0.48
1:B:168:VAL:O	1:B:168:VAL:HG23	2.14	0.48
1:B:27:ASP:O	1:B:31:ILE:HG13	2.13	0.48
1:B:553:TYR:CD1	1:B:553:TYR:N	2.82	0.48
1:A:27:ASP:O	1:A:31:ILE:HG13	2.13	0.48
1:B:267:ILE:HG22	1:B:268:TRP:O	2.14	0.48
1:A:58:HIS:O	1:A:60:PRO:HD3	2.13	0.48
1:B:230:PRO:HA	1:B:233:GLN:HG3	1.95	0.48
1:A:204:LEU:HB3	1:A:206:ASN:HD21	1.77	0.48
1:A:553:TYR:N	1:A:553:TYR:CD1	2.82	0.48
1:B:297:ARG:N	1:B:298:PRO:HD2	2.29	0.48
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.96	0.47
1:A:426:SER:O	1:A:502:GLU:HA	2.13	0.47
1:B:314:ILE:HD11	1:B:350:ARG:CA	2.40	0.47
1:A:363:ILE:CD1	1:B:363:ILE:HG23	2.45	0.47
1:A:280:LEU:HB2	1:A:395:LEU:HD22	1.96	0.47
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.70	0.47
1:A:230:PRO:HA	1:A:233:GLN:HG3	1.95	0.47
1:B:280:LEU:HB2	1:B:395:LEU:HD22	1.96	0.47
1:B:52:MET:C	1:B:53:LYS:HG3	2.35	0.47
1:B:64:MET:HE2	1:B:485:GLN:HE22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:O	1:A:164:LEU:HD23	2.13	0.47
1:A:297:ARG:N	1:A:298:PRO:HD2	2.29	0.47
1:A:386:PRO:CG	1:A:387:GLU:N	2.78	0.47
1:A:312:ARG:NH2	1:A:316:LEU:CD2	2.78	0.47
1:B:39:VAL:CG1	1:B:40:ILE:N	2.78	0.47
1:A:250:ILE:HD12	1:B:527:PHE:CE2	2.50	0.47
1:B:142:VAL:HG12	1:B:143:GLU:N	2.28	0.47
1:A:168:VAL:HG23	1:A:168:VAL:O	2.14	0.47
1:A:267:ILE:HG22	1:A:268:TRP:O	2.14	0.47
1:A:377:ALA:O	1:A:379:PRO:HD3	2.15	0.47
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.96	0.47
1:B:386:PRO:CG	1:B:387:GLU:N	2.78	0.47
1:B:97:LEU:HA	1:B:97:LEU:HD23	1.35	0.47
1:B:151:LEU:CD2	1:B:166:LEU:HD21	2.45	0.47
1:B:231:GLU:OE1	1:B:231:GLU:N	2.36	0.47
1:B:289:LEU:HD22	1:B:351:TRP:CZ2	2.49	0.47
1:A:318:ALA:O	1:A:322:GLY:N	2.42	0.46
1:A:151:LEU:CD2	1:A:166:LEU:HD21	2.45	0.46
1:A:101:SER:O	1:A:102:ILE:HD13	2.16	0.46
1:A:170:ASP:OD2	4:A:602:EPT:H112	2.15	0.46
1:A:39:VAL:CG1	1:A:40:ILE:N	2.78	0.46
1:A:472:VAL:HG23	1:A:472:VAL:O	2.13	0.46
1:B:377:ALA:O	1:B:379:PRO:HD3	2.15	0.46
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.49	0.46
1:A:487:LEU:HD12	1:A:487:LEU:O	2.16	0.46
1:A:52:MET:C	1:A:53:LYS:HG3	2.35	0.46
1:B:105:ASN:HD21	1:B:504:ARG:HH21	1.63	0.46
1:A:139:TYR:C	1:A:139:TYR:CD1	2.89	0.46
1:B:503:TYR:CZ	1:B:504:ARG:CD	2.97	0.46
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.70	0.46
1:A:315:LEU:HD22	1:A:416:TRP:CH2	2.51	0.46
1:A:237:LYS:HE3	1:B:500:TRP:NE1	2.30	0.46
1:A:559:LYS:O	1:A:560:LEU:HB2	2.16	0.46
1:B:101:SER:O	1:B:102:ILE:HD13	2.16	0.46
1:A:259:MET:CE	1:A:535:VAL:HG21	2.46	0.46
1:A:399:ASP:O	1:A:403:GLN:HG2	2.16	0.46
1:B:399:ASP:O	1:B:403:GLN:HG2	2.16	0.46
1:A:64:MET:CE	1:A:485:GLN:NE2	2.79	0.46
1:B:259:MET:CE	1:B:535:VAL:HG21	2.46	0.46
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.55	0.46
3:B:600:FAD:O3'	3:B:600:FAD:N1	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HA	1:A:102:ILE:HD13	1.52	0.45
1:B:312:ARG:NH2	1:B:316:LEU:CD2	2.78	0.45
1:A:249:TYR:O	1:B:252:GLY:HA3	2.15	0.45
1:B:351:TRP:O	1:B:352:ASN:ND2	2.49	0.45
1:B:64:MET:HE3	1:B:485:GLN:NE2	2.31	0.45
1:A:190:TYR:CD1	1:A:270:MET:HB2	2.52	0.45
1:A:195:MET:HE2	1:A:195:MET:HB2	1.76	0.45
1:B:256:GLN:HE22	1:B:504:ARG:HG2	1.81	0.45
1:B:315:LEU:HD22	1:B:416:TRP:CH2	2.51	0.45
1:A:363:ILE:HD13	1:B:363:ILE:HD13	1.99	0.45
1:A:351:TRP:O	1:A:352:ASN:ND2	2.49	0.45
3:A:600:FAD:N1	3:A:600:FAD:O3'	2.39	0.45
1:A:519:TRP:CA	1:B:218:PRO:HG3	2.45	0.45
1:A:166:LEU:HD23	1:A:269:LEU:HD22	1.98	0.45
1:A:386:PRO:CG	1:A:387:GLU:H	2.30	0.45
1:B:281:ILE:HG12	1:B:383:PHE:CD2	2.52	0.45
1:B:166:LEU:HD23	1:B:269:LEU:HD22	1.98	0.45
1:B:204:LEU:CB	1:B:206:ASN:HD21	2.30	0.45
1:B:190:TYR:CD1	1:B:270:MET:HB2	2.52	0.45
1:A:105:ASN:HD21	1:A:504:ARG:HH21	1.62	0.45
1:B:139:TYR:CD1	1:B:139:TYR:C	2.89	0.45
1:A:324:LYS:HG3	1:A:416:TRP:CZ2	2.51	0.45
1:B:64:MET:CE	1:B:485:GLN:NE2	2.79	0.45
1:A:519:TRP:CH2	1:B:211:ARG:CD	2.97	0.45
1:B:324:LYS:HG3	1:B:416:TRP:CZ2	2.51	0.45
1:B:386:PRO:CG	1:B:387:GLU:H	2.30	0.45
1:B:333:PRO:HA	1:B:453:ASP:OD1	2.17	0.45
1:A:165:TRP:N	1:A:165:TRP:CD1	2.85	0.44
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.17	0.44
1:A:256:GLN:HE22	1:A:504:ARG:HG2	1.81	0.44
1:A:469:VAL:HG12	1:A:471:ILE:HD12	1.99	0.44
1:A:503:TYR:CZ	1:A:504:ARG:CD	2.97	0.44
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.34	0.44
1:B:74:ILE:CG2	1:B:75:VAL:N	2.80	0.44
1:B:94:SER:HA	1:B:540:ILE:HD11	1.99	0.44
1:A:281:ILE:HG12	1:A:383:PHE:CD2	2.52	0.44
1:A:333:PRO:HA	1:A:453:ASP:OD1	2.17	0.44
1:A:74:ILE:CG2	1:A:75:VAL:N	2.80	0.44
1:A:8:ARG:HA	1:A:9:PRO:HD3	1.70	0.44
1:B:487:LEU:HD12	1:B:487:LEU:O	2.16	0.44
1:A:291:GLN:O	1:A:295:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:THR:HB	1:A:390:PRO:HD2	2.00	0.44
1:A:471:ILE:CD1	1:A:471:ILE:N	2.80	0.44
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.17	0.44
1:A:252:GLY:HA3	1:B:249:TYR:O	2.17	0.44
1:A:363:ILE:HG23	1:B:363:ILE:CD1	2.47	0.44
1:B:469:VAL:HG12	1:B:471:ILE:HD12	1.99	0.44
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.55	0.44
1:B:61:HIS:CD2	1:B:422:HIS:N	2.76	0.44
1:A:285:LYS:HG2	1:A:286:ASP:N	2.32	0.44
1:A:61:HIS:CD2	1:A:422:HIS:ND1	2.73	0.44
1:B:559:LYS:O	1:B:560:LEU:HB2	2.16	0.44
1:A:185:VAL:HG12	1:A:186:GLY:N	2.33	0.44
1:A:204:LEU:CB	1:A:206:ASN:HD21	2.30	0.44
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.46	0.44
1:A:267:ILE:HG23	1:A:267:ILE:HD12	1.59	0.44
1:A:318:ALA:O	1:A:321:LEU:N	2.50	0.44
1:A:28:ILE:HD13	1:A:89:LEU:CD1	2.48	0.44
1:B:291:GLN:O	1:B:295:ILE:HG13	2.17	0.44
1:A:457:THR:HG21	4:A:602:EPT:H132	1.94	0.44
1:A:398:ARG:HH21	4:A:602:EPT:H121	1.82	0.44
1:B:312:ARG:NH2	1:B:316:LEU:CG	2.81	0.44
1:B:13:PRO:HG2	1:B:95:PHE:CZ	2.53	0.43
1:B:285:LYS:HG2	1:B:286:ASP:N	2.32	0.43
1:B:349:GLY:CA	1:B:352:ASN:HD21	2.30	0.43
1:B:389:THR:HB	1:B:390:PRO:HD2	1.99	0.43
1:A:13:PRO:HG2	1:A:95:PHE:CZ	2.53	0.43
1:B:204:LEU:HB3	1:B:206:ASN:ND2	2.33	0.43
1:A:527:PHE:CE2	1:B:250:ILE:HD12	2.52	0.43
1:B:318:ALA:O	1:B:321:LEU:N	2.50	0.43
1:A:363:ILE:CD1	1:B:363:ILE:HD12	2.47	0.43
1:A:405:ILE:HA	1:A:406:PRO:HD2	1.82	0.43
1:A:439:GLN:O	1:A:442:VAL:HG12	2.19	0.43
1:B:9:PRO:CG	1:B:21:PHE:CZ	2.98	0.43
1:B:283:LEU:HD13	1:B:292:ALA:HB2	2.01	0.43
1:A:312:ARG:NH2	1:A:316:LEU:CG	2.81	0.43
1:A:94:SER:HA	1:A:540:ILE:HD11	1.99	0.43
1:A:510:MET:CE	1:A:545:LYS:HD2	2.48	0.43
1:B:39:VAL:HG12	1:B:40:ILE:N	2.32	0.43
1:A:182:GLU:O	1:A:183:ARG:HB2	2.19	0.43
1:B:165:TRP:CD1	1:B:165:TRP:N	2.85	0.43
1:B:389:THR:O	1:B:396:ARG:NH2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HB3	1:A:206:ASN:ND2	2.33	0.43
1:B:195:MET:HB2	1:B:195:MET:HE2	1.75	0.43
1:B:242:PHE:HA	1:B:243:PRO:HD3	1.55	0.43
1:B:439:GLN:O	1:B:442:VAL:HG12	2.19	0.43
1:A:280:LEU:CB	1:A:395:LEU:HD22	2.48	0.43
1:B:182:GLU:O	1:B:183:ARG:HB2	2.19	0.43
1:A:323:ASP:OD1	1:A:324:LYS:N	2.52	0.43
1:A:37:VAL:CG1	1:A:38:GLU:N	2.82	0.43
1:A:424:PHE:CD1	4:A:602:EPT:H2	2.54	0.43
1:B:253:LEU:O	1:B:257:SER:OG	2.29	0.43
1:A:349:GLY:CA	1:A:352:ASN:HD21	2.30	0.43
1:A:39:VAL:HG12	1:A:40:ILE:N	2.33	0.43
1:B:471:ILE:CD1	1:B:471:ILE:N	2.80	0.43
1:A:170:ASP:OD2	4:A:602:EPT:H101	2.18	0.42
1:A:281:ILE:CG2	1:A:381:VAL:CG2	2.97	0.42
1:B:171:LEU:HD13	1:B:411:LEU:CD2	2.45	0.42
1:B:185:VAL:HG12	1:B:186:GLY:N	2.33	0.42
1:A:289:LEU:O	1:A:293:VAL:HG23	2.20	0.42
1:A:541:ILE:HG21	1:A:541:ILE:HD13	1.85	0.42
1:B:206:ASN:N	1:B:206:ASN:HD22	2.07	0.42
1:B:323:ASP:OD1	1:B:324:LYS:N	2.52	0.42
1:A:253:LEU:O	1:A:257:SER:OG	2.29	0.42
1:A:391:GLU:HA	1:A:396:ARG:CD	2.48	0.42
1:B:391:GLU:HA	1:B:396:ARG:CD	2.48	0.42
1:B:445:LYS:HD3	1:B:449:GLU:HG3	2.01	0.42
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.75	0.42
1:A:445:LYS:HD3	1:A:449:GLU:HG3	2.02	0.42
1:A:543:PRO:HB3	1:A:550:PRO:HG2	2.02	0.42
1:A:61:HIS:CD2	1:A:422:HIS:N	2.76	0.42
1:B:102:ILE:HA	1:B:102:ILE:HD13	1.52	0.42
1:B:267:ILE:HG23	1:B:267:ILE:HD12	1.59	0.42
1:B:171:LEU:CD1	1:B:411:LEU:CD2	2.98	0.42
1:A:283:LEU:HD13	1:A:292:ALA:HB2	2.01	0.42
1:A:389:THR:O	1:A:396:ARG:NH2	2.46	0.42
1:A:90:ALA:O	1:A:94:SER:N	2.53	0.42
1:B:204:LEU:CB	1:B:206:ASN:ND2	2.83	0.42
1:B:224:GLU:H	1:B:224:GLU:CD	2.22	0.42
1:B:385:PHE:CB	1:B:386:PRO:CD	2.96	0.42
1:B:61:HIS:CD2	1:B:422:HIS:ND1	2.73	0.42
1:A:171:LEU:CD1	1:A:411:LEU:CD2	2.98	0.42
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG11	1:B:423:LEU:HD22	2.02	0.42
1:A:224:GLU:H	1:A:224:GLU:CD	2.22	0.42
1:A:204:LEU:CB	1:A:206:ASN:ND2	2.83	0.42
1:B:151:LEU:CG	1:B:166:LEU:HD21	2.50	0.42
1:B:418:PRO:HG2	1:B:474:ASN:ND2	2.31	0.42
1:B:201:GLU:OE1	1:B:211:ARG:HD2	2.20	0.41
1:B:28:ILE:HD13	1:B:89:LEU:CD1	2.48	0.41
1:B:297:ARG:HH21	1:B:432:SER:CA	2.31	0.41
1:B:427:PRO:HD2	1:B:467:HIS:O	2.20	0.41
1:B:555:HIS:HB3	1:B:559:LYS:HE3	2.02	0.41
1:A:131:LEU:O	1:A:132:GLU:HB2	2.21	0.41
1:A:363:ILE:CD1	1:B:363:ILE:CD1	2.97	0.41
1:B:37:VAL:CG1	1:B:38:GLU:N	2.82	0.41
1:B:553:TYR:HB3	1:B:558:TRP:CD1	2.56	0.41
1:A:201:GLU:OE1	1:A:211:ARG:HD2	2.20	0.41
1:A:427:PRO:HD2	1:A:467:HIS:O	2.20	0.41
1:A:527:PHE:CZ	1:A:531:LEU:HD11	2.55	0.41
1:B:289:LEU:O	1:B:293:VAL:HG23	2.20	0.41
1:B:8:ARG:HA	1:B:9:PRO:HD3	1.70	0.41
1:A:64:MET:HE3	1:A:485:GLN:NE2	2.36	0.41
1:B:405:ILE:HA	1:B:406:PRO:HD2	1.82	0.41
1:B:281:ILE:CG2	1:B:381:VAL:CG2	2.97	0.41
1:B:527:PHE:CZ	1:B:531:LEU:HD11	2.54	0.41
1:A:314:ILE:HD11	1:A:350:ARG:CB	2.51	0.41
1:A:471:ILE:O	1:A:471:ILE:HG22	2.21	0.41
1:B:105:ASN:HD21	1:B:504:ARG:NH2	2.19	0.41
1:B:543:PRO:HB3	1:B:550:PRO:HG2	2.02	0.41
1:A:427:PRO:HG2	1:A:439:GLN:OE1	2.21	0.41
3:A:600:FAD:N1	3:A:600:FAD:C3'	2.84	0.41
1:A:424:PHE:CE1	4:A:602:EPT:H2	2.55	0.41
1:B:188:THR:CB	1:B:189:PRO:CD	2.96	0.41
1:B:457:THR:HG22	1:B:458:PHE:O	2.21	0.41
3:B:600:FAD:N1	3:B:600:FAD:C3'	2.84	0.41
1:A:151:LEU:CG	1:A:166:LEU:HD21	2.50	0.41
1:A:171:LEU:HD13	1:A:411:LEU:CD2	2.45	0.41
1:A:417:LEU:HD13	1:A:472:VAL:HG23	2.02	0.41
1:A:553:TYR:HB3	1:A:558:TRP:CD1	2.56	0.41
1:B:131:LEU:O	1:B:132:GLU:HB2	2.20	0.41
1:B:209:LEU:HA	1:B:209:LEU:HD23	1.94	0.41
1:B:90:ALA:O	1:B:94:SER:N	2.53	0.41
1:A:250:ILE:HG21	1:A:250:ILE:HD13	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG11	1:A:423:LEU:HD22	2.02	0.41
1:A:457:THR:HG22	1:A:458:PHE:O	2.21	0.41
1:B:151:LEU:CD2	1:B:166:LEU:CD2	2.99	0.41
1:B:487:LEU:HD12	1:B:487:LEU:C	2.41	0.41
1:B:541:ILE:HD13	1:B:541:ILE:HG21	1.85	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.55	0.41
3:A:600:FAD:H5'2	3:A:600:FAD:H2'	1.89	0.41
1:B:418:PRO:HB2	1:B:474:ASN:HD22	1.86	0.41
1:A:128:ASN:HA	1:A:128:ASN:HD22	1.67	0.41
1:A:151:LEU:CD2	1:A:166:LEU:CD2	2.99	0.41
1:A:555:HIS:HB3	1:A:559:LYS:HE3	2.02	0.41
1:B:128:ASN:HD22	1:B:145:GLY:CA	2.31	0.41
1:B:201:GLU:C	1:B:202:VAL:HG13	2.41	0.41
1:B:284:PRO:HG2	1:B:288:ASP:OD2	2.21	0.41
1:B:417:LEU:HD13	1:B:472:VAL:HG23	2.02	0.41
1:B:427:PRO:HG2	1:B:439:GLN:OE1	2.21	0.41
1:A:418:PRO:HG2	1:A:474:ASN:ND2	2.31	0.40
1:B:348:LEU:HA	1:B:348:LEU:HD23	1.83	0.40
1:B:422:HIS:CD2	1:B:424:PHE:CZ	3.09	0.40
1:B:471:ILE:O	1:B:471:ILE:HG22	2.21	0.40
1:B:71:ALA:HB2	1:B:120:VAL:HG23	2.04	0.40
1:A:121:LEU:HD12	1:A:121:LEU:N	2.36	0.40
1:A:9:PRO:CG	1:A:21:PHE:CZ	2.98	0.40
1:A:325:ARG:O	1:A:327:TYR:N	2.54	0.40
1:A:72:SER:HB3	1:A:117:GLY:O	2.22	0.40
1:A:100:ILE:HG13	1:A:100:ILE:O	2.19	0.40
1:A:12:LEU:CB	1:A:13:PRO:CD	2.97	0.40
1:A:217:LEU:HD12	1:B:516:THR:O	2.21	0.40
1:A:284:PRO:HG2	1:A:288:ASP:OD2	2.21	0.40
1:A:468:ILE:HG21	4:A:602:EPT:C2	2.50	0.40
1:B:100:ILE:HG13	1:B:100:ILE:O	2.20	0.40
1:B:102:ILE:HG22	1:B:104:ARG:H	1.87	0.40
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.78	0.40
1:B:297:ARG:CB	1:B:298:PRO:CD	2.98	0.40
1:B:312:ARG:HG2	1:B:457:THR:CG2	2.51	0.40
1:B:325:ARG:O	1:B:327:TYR:N	2.54	0.40
1:B:72:SER:HB3	1:B:117:GLY:O	2.22	0.40
1:A:189:PRO:HD3	1:A:358:TYR:CZ	2.57	0.40
1:A:503:TYR:CD2	1:A:504:ARG:HG3	2.57	0.40
1:B:238:ILE:HD12	1:B:238:ILE:HG23	1.81	0.40
1:B:189:PRO:HD3	1:B:358:TYR:CZ	2.56	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	553/560 (99%)	503 (91%)	39 (7%)	11 (2%)	9	39
1	B	553/560 (99%)	504 (91%)	38 (7%)	11 (2%)	9	39
All	All	1106/1120 (99%)	1007 (91%)	77 (7%)	22 (2%)	9	39

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	388	ASP
1	A	418	PRO
1	A	475	LYS
1	B	46	ILE
1	B	326	SER
1	B	388	ASP
1	B	418	PRO
1	B	475	LYS
1	A	105	ASN
1	A	326	SER
1	A	391	GLU
1	A	497	ALA
1	A	559	LYS
1	B	105	ASN
1	B	391	GLU
1	B	497	ALA
1	B	559	LYS
1	A	49	GLY
1	A	170	ASP
1	B	49	GLY
1	B	170	ASP

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	475/482 (98%)	459 (97%)	16 (3%)	42	73
1	B	475/482 (98%)	459 (97%)	16 (3%)	42	73
All	All	950/964 (98%)	918 (97%)	32 (3%)	42	73

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	105	ASN
1	A	114	ARG
1	A	115	VAL
1	A	128	ASN
1	A	149	HIS
1	A	177	LEU
1	A	189	PRO
1	A	206	ASN
1	A	211	ARG
1	A	224	GLU
1	A	251	ASP
1	A	277	GLN
1	A	391	GLU
1	A	422	HIS
1	A	503	TYR
1	B	61	HIS
1	B	105	ASN
1	B	114	ARG
1	B	115	VAL
1	B	128	ASN
1	B	149	HIS
1	B	177	LEU
1	B	189	PRO
1	B	206	ASN
1	B	211	ARG
1	B	224	GLU

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Mol	Chain	Res	Type
1	B	251	ASP
1	B	277	GLN
1	B	391	GLU
1	B	422	HIS
1	B	503	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	91	ASN
1	A	105	ASN
1	A	128	ASN
1	A	197	HIS
1	A	206	ASN
1	A	240	HIS
1	A	277	GLN
1	A	306	GLN
1	A	352	ASN
1	A	485	GLN
1	A	498	ASN
1	A	520	ASN
1	B	61	HIS
1	B	91	ASN
1	B	105	ASN
1	B	128	ASN
1	B	197	HIS
1	B	206	ASN
1	B	240	HIS
1	B	277	GLN
1	B	306	GLN
1	B	352	ASN
1	B	485	GLN
1	B	498	ASN
1	B	520	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FAD	A	600	1	51,58,58	0.91	2 (3%)	54,89,89	1.44	3 (5%)
4	EPT	A	602	-	14,14,14	1.21	1 (7%)	16,16,16	1.69	5 (31%)
3	FAD	B	600	1	51,58,58	0.91	2 (3%)	54,89,89	1.44	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	600	1	-	0/28/50/50	0/6/6/6
4	EPT	A	602	-	-	0/7/7/7	0/1/1/1
3	FAD	B	600	1	-	0/28/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	EPT	C5-C4	-2.98	1.33	1.38
3	B	600	FAD	C2-N1	-2.58	1.33	1.38
3	A	600	FAD	C2-N1	-2.58	1.33	1.38
3	A	600	FAD	C4-N3	3.33	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	FAD	C4-N3	3.35	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	FAD	C4X-C4-N3	-4.94	116.45	123.48
3	A	600	FAD	C4X-C4-N3	-4.91	116.49	123.48
4	A	602	EPT	C9-C8-C7	-3.16	101.14	113.70
4	A	602	EPT	C5-C6-C1	-2.72	117.27	121.02
4	A	602	EPT	C2-C3-C4	-2.66	116.86	119.88
3	B	600	FAD	C1'-N10-C10	2.04	120.59	118.50
3	A	600	FAD	C1'-N10-C10	2.08	120.64	118.50
4	A	602	EPT	C3-C2-C1	2.34	124.25	121.02
4	A	602	EPT	C6-C5-C4	3.47	123.81	119.88
3	A	600	FAD	C4-N3-C2	7.07	121.34	115.16
3	B	600	FAD	C4-N3-C2	7.10	121.37	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	9	0
4	A	602	EPT	14	0
3	B	600	FAD	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.