



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 02:05 pm BST

PDB ID : 2BYB / pdb_00002byb
Title : Human Monoamine Oxidase B in complex with Deprenyl
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Deposited on : 2005-07-29
Resolution : 2.20 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

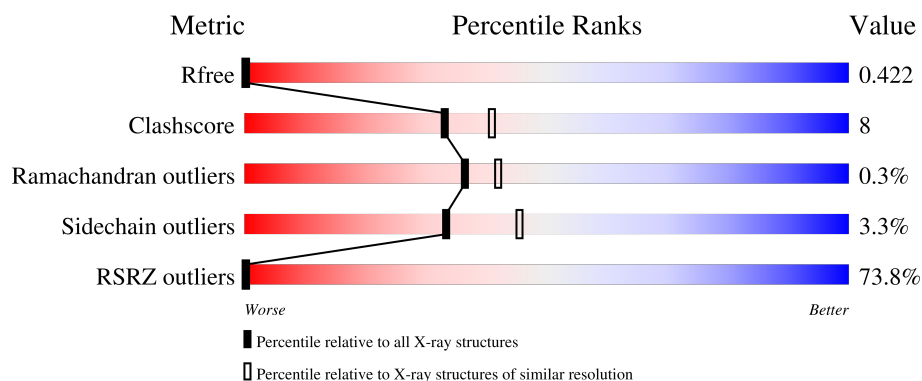
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	520	
1	B	520	

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

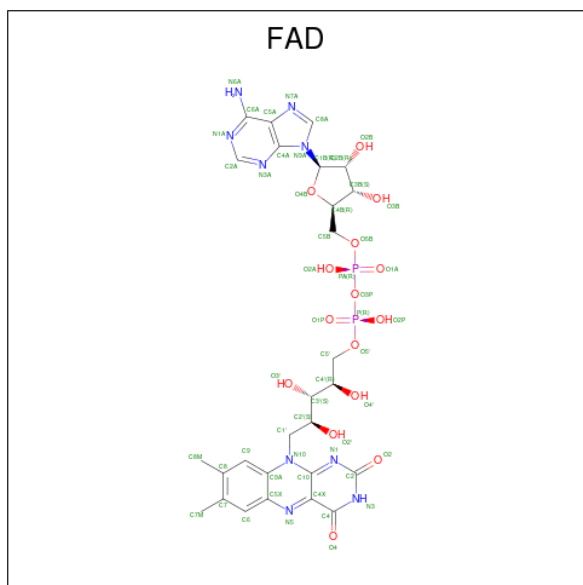
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	600	-	-	X	-

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 AMINE OXIDASE [FLAVIN-CONTAINING] B.

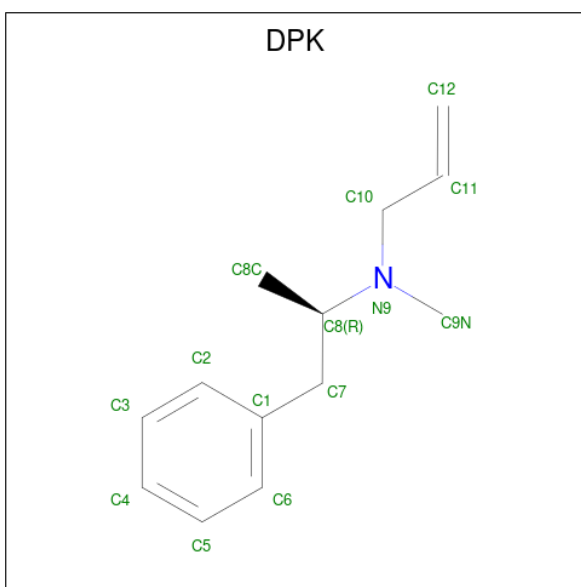
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total 3971	C 2538	N 681	O 728	S 24	0	0	0
1	B	494	Total 3940	C 2519	N 676	O 721	S 24	0	0	0

- 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 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is DEPRENYL (CCD ID: DPK) (formula: $C_{13}H_{19}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	13	1		
3	B	1	Total	C	N	0	0
			14	13	1		

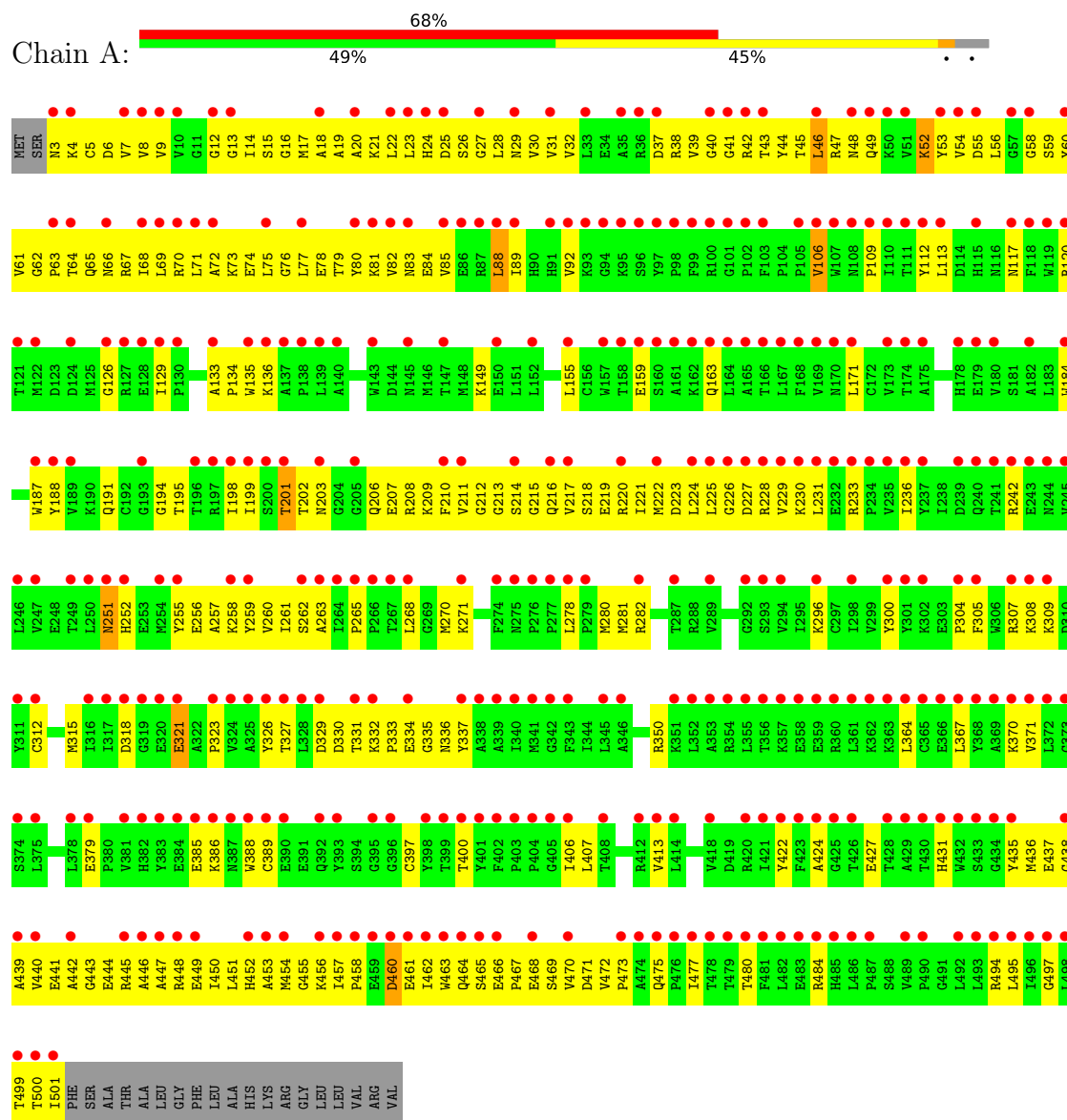
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total	O	0	0
			233	233		
4	B	256	Total	O	0	0
			256	256		

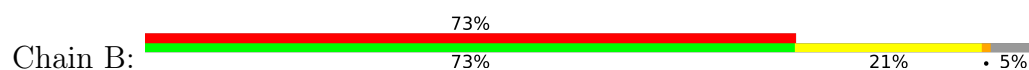
3 Residue-property plots

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

• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B



• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B



PHE	G442	P380	D318	T249	Y187	G126	Q65	MET
SER	G443	Y381	G319	L250	Y188	R127	N66	SER
ALA	E444	H382	E321	N251	V189	E128	R67	N3
THR	R445	Y383	E320	H252	K190	I129	I68	K4
ALA	A446	E384	A322	E253	Q191	P130	L69	C5
LEU	A447	E385	P323	M254	G192	S131	R70	D6
GLY	R448	K386	V324	Y255	G193	D132	L71	V7
PHE	E449	K387	A325	E256	G194	A133	A72	V8
LEU	L450	Y388	Y326	A257	T195	D133	K73	V9
ALA	L451	Q392	T327	K258	T196	A135	E74	
HIS	H452	Y393	L328	Y259	R197	K136	L75	I14
LYS	A453	Y394	D329	V260	I198	A137	G76	I15
ARG	M454	S394	D330	I261	I199	P138	L77	G16
GLY	G455	G395	T331	S262		L139	E78	M17
LEU	K456	G396	K332	A263	T202	A140	T79	
LEU	L457	C397	P333	I264	N203	E141	Y80	
VAL	P458	Y398	E334	P265	G204	E142	X81	A20
ARG	E459	T399	G335		G205	V143	Y82	K21
ARG	D460	T400	N336	L268	Q206	D144	N83	L22
VAL	E461	Y401	Y337	G269	E207	N145	E84	L23
	I462	F402	A338	M270	R208	M146	E85	H24
	V463	P403	A339	K271	K209	T147	E86	D25
	Q464	P404	I340	I272		M148	R87	S26
	S465	G405	F343	H273	G212	K149	L88	G27
	E466	I406	I344	F274	G213	E150	N29	L28
	P467	L407	L345	N275	S214	L151	T89	N29
	E468	T408	A346	P276	G215	D152	H90	V30
	S469	Q409	A347	P277	Q216	D153	H91	V31
	V470	Y410	K347	L278	V217	K154	V92	V32
	D471	G411	K348	P279	S218	L155	K93	L33
	V472	R412	A349	M280	E219	C156	G94	E34
	P473	V413	R350	R281	R220	T157	K95	A35
	A474	L414	K351	N282	I221	W157	S96	R36
	Q475	R415	L352	N283	M222	W158	P97	D37
	P476	Q416	A353		D223	S160	P98	R38
	I477	P417	R354	V289	L224	A161	F99	V39
	T478	V418	L355	I295	L225	Q162	G101	G40
	T479	D419	T356	V284	G226	Q163	P102	G41
	T480	R420	K357	I295	D227	L164	F103	R42
	F481	I421	E358	K296	R228	A165	P104	T43
	L482	Y422	E359	C297	V229	T166	P105	Y44
	E483	F423	R360	I298	K230	L167	V106	T45
	R484	A424	L361	V299	L231	F168	W107	L46
	H485	G425	K362	Y300	E232		N108	R47
	L486	T426	K363	Y301	R233	L171	N108	N48
	P487	E427	L364	K302	P234	C172	P109	Q49
	S488	T428	C365	E303	V235	V173	I110	Q49
	V489	A429	E366	P304	I236	T174	T111	K50
	P490	T430	L367	F305	Y237	A175	Y112	K52
	G491	H431	Y368	V306	I238	E176	L113	Y53
	L492	W432	A369	R307	D239	T177	D114	V54
	L493	S433	K370	K308	Q240	H178	N115	D55
	R494	G434	V371	K309	T241	E179	N116	L56
	L495	Y435		D310	R242	V180	N117	G57
	L496	M436	S374	Y311	E243	S181	F118	G58
GLY	G437	M437	L375	C312	N244	A182	W119	S59
LEU	G438	F437	E376		N245	L183	R120	Y60
THR	A439	V440	A377	M315	V245	L184	T121	V61
THR	V440		L378	I316	L246	F185	D122	G62
ILE	E441		E379	I317			D123	P63

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.84Å 225.84Å 85.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (15.00-2.20) 94.6 (15.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.237 , 0.299 0.400 , 0.422	Depositor DCC
R_{free} test set	2140 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	8534	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	2/4068 (0.0%)	1.08	2/5522 (0.0%)
1	B	1.07	9/4037 (0.2%)	1.13	7/5479 (0.1%)
All	All	1.04	11/8105 (0.1%)	1.11	9/11001 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	VAL	CA-CB	6.83	1.63	1.54
1	B	182	ALA	CA-CB	5.98	1.62	1.53
1	B	206	GLN	N-CA	5.92	1.53	1.46
1	B	82	VAL	CA-CB	5.73	1.60	1.54
1	A	477	ILE	CA-CB	5.67	1.60	1.54
1	B	175	ALA	CA-CB	-5.51	1.44	1.53
1	B	173	VAL	CA-CB	5.33	1.60	1.54
1	A	201	THR	CA-CB	5.32	1.60	1.53
1	B	207	GLU	C-O	5.31	1.30	1.24
1	B	81	LYS	C-O	5.29	1.30	1.24
1	B	196	THR	C-O	5.21	1.30	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	LEU	CA-C-N	-6.83	113.27	120.03
1	B	278	LEU	C-N-CA	-6.83	113.27	120.03
1	B	319	GLY	N-CA-C	6.30	117.93	111.95
1	A	236	ILE	CB-CA-C	-6.03	104.11	110.62
1	A	194	GLY	N-CA-C	5.97	118.13	112.04
1	B	194	GLY	N-CA-C	5.40	118.87	112.33
1	B	174	THR	N-CA-C	5.29	118.50	111.30
1	B	378	LEU	N-CA-C	-5.23	106.74	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	MET	N-CA-C	5.15	117.56	111.33

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	3971	0	3967	64	1344
1	B	3940	0	3937	64	22
2	A	53	0	29	2	60
2	B	53	0	29	2	0
3	A	14	0	17	0	0
3	B	14	0	17	1	0
4	A	233	0	0	7	132
4	B	256	0	0	16	3
All	All	8534	0	7996	125	1369

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 8.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:GLN:NE2	4:B:2244:HOH:O	1.79	1.14
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.12	0.96
1:A:92:VAL:HG22	1:A:318:ASP:OD2	1.75	0.84
1:B:414:LEU:HD12	4:B:2217:HOH:O	1.78	0.83
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.29	0.80
1:B:195:THR:O	1:B:199:ILE:HG23	1.83	0.79
1:B:28:LEU:HD11	1:B:454:MET:HE1	1.67	0.76
1:B:159:GLU:O	1:B:163:GLN:HG3	1.86	0.74
1:A:126:GLY:HA2	1:A:129:ILE:HD12	1.72	0.72
1:A:296:LYS:NZ	4:A:2139:HOH:O	2.21	0.71
1:A:195:THR:O	1:A:199:ILE:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:MET:HB3	1:B:270:MET:HB3	1.75	0.68
1:B:251:ASN:HD22	1:B:251:ASN:H	1.43	0.65
1:A:321:GLU:H	1:A:321:GLU:CD	2.04	0.65
1:A:265:PRO:HD2	1:A:268:LEU:HD12	1.79	0.65
1:B:412:ARG:HD2	4:B:2219:HOH:O	1.99	0.62
1:B:92:VAL:HG22	1:B:318:ASP:OD2	1.99	0.62
1:B:323:PRO:HD2	1:B:367:LEU:HD22	1.82	0.61
1:A:480:THR:O	1:A:484:ARG:HG3	2.00	0.61
1:A:323:PRO:HD2	1:A:367:LEU:HD22	1.83	0.60
1:A:280:MET:HE3	1:A:281:MET:HG2	1.83	0.60
1:B:84:GLU:O	1:B:84:GLU:HG2	2.01	0.60
1:A:149:LYS:HD3	4:B:2089:HOH:O	2.02	0.59
1:A:251:ASN:HD22	1:A:251:ASN:H	1.48	0.59
1:A:28:LEU:HD11	1:A:454:MET:HE1	1.85	0.58
1:B:363:LYS:HD3	4:B:2187:HOH:O	2.03	0.57
1:B:392:GLN:O	4:B:2209:HOH:O	2.17	0.57
1:B:321:GLU:H	1:B:321:GLU:CD	2.11	0.56
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.41	0.56
1:B:398:TYR:N	4:B:2102:HOH:O	2.39	0.55
1:A:270:MET:CB	1:B:270:MET:HB3	2.37	0.55
1:A:84:GLU:O	1:A:84:GLU:HG2	2.07	0.55
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.42	0.55
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.71	0.54
1:B:191:GLN:O	1:B:431:HIS:HD2	1.89	0.54
1:B:17:MET:HE3	1:B:221:ILE:HG22	1.88	0.54
1:B:116:ASN:HB3	4:B:2064:HOH:O	2.07	0.54
1:A:171:LEU:HD21	1:A:326:TYR:CG	2.43	0.54
1:A:252:HIS:NE2	1:B:248:GLU:OE2	2.33	0.54
1:B:427:GLU:O	4:B:2231:HOH:O	2.18	0.53
1:A:370:LYS:CE	4:A:2168:HOH:O	2.56	0.53
1:A:309:LYS:HE3	4:A:2144:HOH:O	2.08	0.52
1:A:270:MET:HB3	1:B:270:MET:CB	2.38	0.52
1:B:400:THR:HB	1:B:427:GLU:HG2	1.93	0.51
1:B:265:PRO:HD2	1:B:268:LEU:HD12	1.93	0.51
1:A:251:ASN:H	1:A:251:ASN:ND2	2.08	0.51
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.46	0.51
1:A:207:GLU:HG2	1:A:208:ARG:HG3	1.94	0.50
1:B:480:THR:O	1:B:484:ARG:HG3	2.11	0.50
1:B:251:ASN:H	1:B:251:ASN:ND2	2.08	0.50
1:A:88:LEU:HD12	1:A:88:LEU:N	2.27	0.49
1:A:117:ASN:HD22	1:A:120:ARG:NH2	2.02	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ALA:O	1:B:136:LYS:HB2	2.13	0.49
1:A:281:MET:HB3	1:A:413:VAL:HG21	1.95	0.49
1:B:445:ARG:HD2	1:B:463:TRP:CH2	2.47	0.49
1:B:450:ILE:O	1:B:454:MET:HG3	2.13	0.49
2:A:600:FAD:N1	2:A:600:FAD:H2'	2.28	0.48
1:A:350:ARG:HD2	1:B:410:TYR:OH	2.12	0.48
2:B:600:FAD:H2'	2:B:600:FAD:N1	2.28	0.48
1:A:389:CYS:HB3	1:B:280:MET:HG3	1.95	0.48
1:A:201:THR:O	1:A:207:GLU:HB2	2.14	0.48
1:B:174:THR:OG1	4:B:2102:HOH:O	2.20	0.48
1:B:331:THR:HG22	1:B:332:LYS:N	2.29	0.48
1:A:315:MET:HB2	1:A:327:THR:OG1	2.14	0.47
1:B:331:THR:HG22	1:B:332:LYS:H	1.80	0.47
1:B:461:GLU:O	4:B:2244:HOH:O	2.21	0.47
1:A:217:VAL:O	1:A:221:ILE:HG13	2.14	0.46
1:A:191:GLN:O	1:A:431:HIS:HD2	1.99	0.45
1:B:296:LYS:NZ	4:B:2155:HOH:O	2.47	0.45
1:A:149:LYS:CD	4:B:2089:HOH:O	2.60	0.45
1:A:400:THR:HB	1:A:427:GLU:HG2	1.97	0.45
1:B:233:ARG:HG3	1:B:251:ASN:HD21	1.80	0.45
1:A:134:PRO:HD2	1:A:135:TRP:CZ3	2.52	0.45
1:A:149:LYS:CE	4:A:2086:HOH:O	2.55	0.45
1:A:271:LYS:HG2	1:B:270:MET:O	2.16	0.45
1:B:148:MET:HE1	1:B:151:LEU:HD23	1.98	0.45
1:B:165:ALA:O	1:B:168:PHE:HB3	2.17	0.45
1:A:159:GLU:O	1:A:163:GLN:HG3	2.17	0.45
1:A:188:TYR:O	1:A:191:GLN:HG3	2.16	0.44
1:B:171:LEU:HD21	1:B:326:TYR:CG	2.52	0.44
1:B:282:ARG:O	1:B:283:ASN:C	2.59	0.44
1:B:312:CYS:O	1:B:329:ASP:HB2	2.16	0.44
1:B:117:ASN:ND2	1:B:120:ARG:HH21	1.95	0.44
1:A:117:ASN:ND2	1:A:120:ARG:HH21	2.05	0.44
1:A:406:ILE:HD11	4:B:2214:HOH:O	2.18	0.44
1:B:185:PHE:O	1:B:189:VAL:HG23	2.17	0.44
1:B:281:MET:HB3	1:B:413:VAL:HG21	1.99	0.44
1:A:370:LYS:HE3	4:A:2168:HOH:O	2.16	0.44
1:A:454:MET:HE3	1:A:456:LYS:HE3	1.99	0.44
4:A:2186:HOH:O	1:B:406:ILE:HD11	2.17	0.44
1:B:315:MET:HE3	1:B:327:THR:OG1	2.18	0.44
1:B:282:ARG:HD2	4:B:2220:HOH:O	2.16	0.43
1:B:176:GLU:OE2	1:B:346:ALA:HB1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:MET:HE3	1:B:281:MET:HG2	2.00	0.43
1:A:233:ARG:HG3	1:A:251:ASN:HD21	1.84	0.43
1:B:126:GLY:HA2	1:B:129:ILE:HD12	2.00	0.43
1:A:134:PRO:HG3	1:A:187:TRP:CD1	2.53	0.43
1:A:42:ARG:NH2	1:A:265:PRO:HG3	2.34	0.43
1:B:94:GLY:C	1:B:95:LYS:HG3	2.44	0.43
1:A:89:ILE:HG21	1:A:371:VAL:CG1	2.49	0.43
1:A:133:ALA:O	1:A:136:LYS:HB2	2.19	0.43
1:A:331:THR:HG22	1:A:332:LYS:N	2.33	0.43
1:B:237:TYR:HB3	1:B:248:GLU:HB3	2.01	0.43
3:B:601:DPK:H9N1	3:B:601:DPK:H7C2	1.85	0.42
1:A:305:PHE:HA	1:A:308:LYS:HD3	2.00	0.42
1:B:400:THR:HB	1:B:427:GLU:CG	2.49	0.42
1:A:17:MET:HE3	1:A:221:ILE:HG22	2.01	0.42
1:A:278:LEU:HD13	1:A:282:ARG:HG2	2.02	0.42
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.90	0.42
1:A:112:TYR:CD1	1:A:112:TYR:C	2.98	0.42
1:B:143:TRP:O	1:B:182:ALA:HB3	2.20	0.42
1:A:109:PRO:O	1:A:113:LEU:HG	2.20	0.42
1:A:278:LEU:N	4:A:2129:HOH:O	2.35	0.42
1:B:88:LEU:HD12	1:B:88:LEU:N	2.35	0.42
1:B:327:THR:HG21	1:B:368:TYR:CE2	2.55	0.42
1:B:343:PHE:HB2	4:B:2174:HOH:O	2.19	0.41
1:A:106:VAL:HG13	1:A:112:TYR:CD2	2.55	0.41
1:B:295:ILE:HA	1:B:386:LYS:O	2.21	0.41
1:A:60:TYR:HB3	1:A:206:GLN:HA	2.02	0.41
2:A:600:FAD:H9	2:A:600:FAD:H1'1	1.77	0.41
1:A:315:MET:HE3	1:A:327:THR:OG1	2.21	0.41
1:B:58:GLY:HA2	2:B:600:FAD:C4X	2.51	0.41
1:A:134:PRO:C	1:A:136:LYS:H	2.29	0.41
1:A:184:TRP:HB2	1:A:407:LEU:HD22	2.04	0.40
1:A:296:LYS:O	1:A:385:GLU:HA	2.22	0.40

All (1369) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NE	1:A:222:MET:CB[3_655]	0.21	1.99
1:A:76:GLY:C	2:A:600:FAD:N1[3_655]	0.29	1.91
1:A:223:ASP:O	1:A:441:GLU:OE2[3_655]	0.32	1.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:CA	1:A:441:GLU:OE1[3_655]	0.37	1.83
1:A:228:ARG:CB	1:A:462:ILE:O[3_655]	0.37	1.83
1:A:257:ALA:CB	1:A:456:LYS:CB[3_655]	0.38	1.82
1:A:53:TYR:CZ	1:A:207:GLU:C[3_655]	0.40	1.80
1:A:53:TYR:CA	1:A:207:GLU:OE2[3_655]	0.40	1.80
1:A:223:ASP:C	1:A:441:GLU:CD[3_655]	0.40	1.80
1:A:307:ARG:NH1	1:A:307:ARG:NH1[3_655]	0.40	1.80
1:A:23:LEU:CG	1:A:23:LEU:CG[3_655]	0.41	1.79
1:A:53:TYR:CD2	1:A:207:GLU:CB[3_655]	0.44	1.76
1:A:61:VAL:O	1:A:212:GLY:CA[3_655]	0.45	1.75
1:A:19:ALA:CB	1:A:22:LEU:N[3_655]	0.46	1.74
1:A:221:ILE:O	1:A:441:GLU:CA[3_655]	0.47	1.73
1:A:29:ASN:CA	1:A:449:GLU:C[3_655]	0.48	1.72
1:A:75:LEU:O	1:A:435:TYR:C[3_655]	0.48	1.72
1:A:210:PHE:CD1	1:A:210:PHE:CD1[3_655]	0.51	1.69
1:A:83:ASN:CG	1:A:335:GLY:CA[3_655]	0.52	1.68
1:A:82:VAL:O	1:A:332:LYS:CB[3_655]	0.54	1.66
1:A:29:ASN:CB	1:A:449:GLU:O[3_655]	0.56	1.64
1:A:40:GLY:CA	1:A:70:ARG:CB[3_655]	0.57	1.63
1:A:19:ALA:O	1:A:19:ALA:O[3_655]	0.59	1.61
1:A:30:VAL:CG2	1:A:448:ARG:N[3_655]	0.59	1.61
1:A:55:ASP:OD2	1:A:79:THR:CB[3_655]	0.61	1.59
1:A:67:ARG:CB	1:A:218:SER:O[3_655]	0.61	1.59
1:A:74:GLU:N	2:A:600:FAD:O4'[3_655]	0.62	1.58
1:A:74:GLU:CG	2:A:600:FAD:P[3_655]	0.63	1.57
1:A:258:LYS:O	1:A:456:LYS:NZ[3_655]	0.64	1.56
1:B:475:GLN:OE1	4:B:2058:HOH:O[3_555]	0.64	1.56
1:A:39:VAL:CA	1:A:466:GLU:OE2[3_655]	0.65	1.55
1:A:53:TYR:CE2	1:A:207:GLU:CA[3_655]	0.65	1.55
1:A:221:ILE:CA	1:A:441:GLU:N[3_655]	0.65	1.55
1:B:478:THR:O	1:B:478:THR:CB[3_555]	0.65	1.55
1:A:25:ASP:OD1	1:A:424:ALA:CB[3_655]	0.67	1.53
1:A:28:LEU:CA	1:A:450:ILE:CG1[3_655]	0.67	1.53
1:A:258:LYS:C	1:A:456:LYS:NZ[3_655]	0.68	1.52
1:A:501:ILE:C	4:A:2054:HOH:O[6_565]	0.68	1.52
1:A:84:GLU:C	1:A:336:ASN:CB[3_655]	0.69	1.51
1:A:229:VAL:CA	1:A:464:GLN:CB[3_655]	0.69	1.51
1:A:3:ASN:N	1:A:458:PRO:CB[3_655]	0.70	1.50
1:A:43:THR:OG1	1:A:69:LEU:O[3_655]	0.70	1.50
1:A:47:ARG:NE	1:A:63:PRO:CA[3_655]	0.70	1.50
1:A:54:VAL:CA	1:A:208:ARG:NH2[3_655]	0.70	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:N	1:A:219:GLU:CG[3_655]	0.71	1.49
1:A:74:GLU:CD	2:A:600:FAD:O1P[3_655]	0.71	1.49
1:A:210:PHE:N	1:A:210:PHE:N[3_655]	0.72	1.48
1:A:26:SER:CA	1:A:261:ILE:N[3_655]	0.73	1.47
1:A:42:ARG:O	1:A:73:LYS:CG[3_655]	0.73	1.47
1:A:228:ARG:N	1:A:463:TRP:CA[3_655]	0.73	1.47
1:A:26:SER:N	1:A:261:ILE:CB[3_655]	0.74	1.46
1:A:69:LEU:CB	1:A:215:GLY:CA[3_655]	0.74	1.46
1:A:32:VAL:CB	4:A:2209:HOH:O[3_655]	0.75	1.45
1:A:7:VAL:CA	1:A:451:LEU:CD2[3_655]	0.76	1.44
1:A:14:ILE:CG1	1:A:71:LEU:C[3_655]	0.76	1.44
1:A:39:VAL:CB	1:A:466:GLU:CD[3_655]	0.76	1.44
1:A:68:ILE:CB	1:A:217:VAL:N[3_655]	0.76	1.44
1:A:221:ILE:CG2	1:A:440:VAL:O[3_655]	0.76	1.44
1:A:15:SER:CB	1:A:21:LYS:CE[3_655]	0.77	1.43
1:A:46:LEU:N	1:A:472:VAL:CA[3_655]	0.77	1.43
1:A:52:LYS:CE	1:A:202:THR:N[3_655]	0.77	1.43
1:A:46:LEU:CB	1:A:473:PRO:CD[3_655]	0.78	1.42
1:A:14:ILE:CD1	1:A:72:ALA:N[3_655]	0.79	1.41
1:A:39:VAL:CG1	1:A:466:GLU:OE1[3_655]	0.79	1.41
1:A:44:TYR:CA	4:A:2216:HOH:O[3_655]	0.79	1.41
1:A:61:VAL:N	1:A:211:VAL:O[3_655]	0.79	1.41
1:A:16:GLY:N	4:A:2003:HOH:O[3_655]	0.80	1.40
1:A:83:ASN:N	1:A:332:LYS:C[3_655]	0.80	1.40
1:A:44:TYR:N	4:A:2216:HOH:O[3_655]	0.81	1.39
1:A:83:ASN:ND2	1:A:335:GLY:CA[3_655]	0.81	1.39
1:A:258:LYS:C	1:A:456:LYS:CE[3_655]	0.81	1.39
1:A:44:TYR:CE1	1:A:469:SER:C[3_655]	0.82	1.38
1:A:68:ILE:CB	1:A:217:VAL:CA[3_655]	0.82	1.38
1:A:80:TYR:CA	1:A:209:LYS:CE[3_655]	0.82	1.38
1:A:221:ILE:CG1	1:A:440:VAL:CA[3_655]	0.82	1.38
1:A:30:VAL:CG1	1:A:447:ALA:O[3_655]	0.84	1.36
1:A:44:TYR:CE2	1:A:470:VAL:CA[3_655]	0.85	1.35
1:A:53:TYR:N	1:A:207:GLU:OE1[3_655]	0.85	1.35
1:A:54:VAL:CA	1:A:208:ARG:CZ[3_655]	0.85	1.35
1:A:230:LYS:NZ	1:A:460:ASP:O[3_655]	0.85	1.35
1:A:67:ARG:CB	1:A:218:SER:C[3_655]	0.86	1.34
1:A:24:HIS:CG	1:A:446:ALA:CB[3_655]	0.87	1.33
1:A:52:LYS:CD	1:A:202:THR:N[3_655]	0.87	1.33
1:A:59:SER:OG	1:A:79:THR:N[3_655]	0.87	1.33
1:A:84:GLU:CA	1:A:336:ASN:OD1[3_655]	0.87	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:CA	1:A:462:ILE:C[3_655]	0.87	1.33
1:A:38:ARG:CB	1:A:467:PRO:C[3_655]	0.88	1.32
1:A:52:LYS:C	1:A:207:GLU:OE1[3_655]	0.88	1.32
1:A:59:SER:C	1:A:78:GLU:O[3_655]	0.88	1.32
1:A:221:ILE:C	1:A:441:GLU:CA[3_655]	0.88	1.32
1:A:229:VAL:C	1:A:464:GLN:CB[3_655]	0.88	1.32
1:A:17:MET:CB	1:A:444:GLU:OE2[3_655]	0.89	1.31
1:A:28:LEU:CB	1:A:450:ILE:CB[3_655]	0.89	1.31
1:A:7:VAL:CB	1:A:451:LEU:CD2[3_655]	0.90	1.30
1:A:46:LEU:CA	1:A:473:PRO:N[3_655]	0.90	1.30
1:A:227:ASP:CA	1:A:463:TRP:CB[3_655]	0.90	1.30
1:B:475:GLN:CD	4:B:2058:HOH:O[3_555]	0.90	1.30
1:A:29:ASN:N	1:A:450:ILE:N[3_655]	0.91	1.29
1:A:74:GLU:C	2:A:600:FAD:C4'[3_655]	0.91	1.29
1:A:220:ARG:CB	1:A:437:GLU:C[3_655]	0.91	1.29
1:A:330:ASP:CG	4:A:2046:HOH:O[3_655]	0.91	1.29
1:A:25:ASP:CA	1:A:261:ILE:CG2[3_655]	0.92	1.28
1:A:73:LYS:NZ	1:A:388:TRP:CH2[3_655]	0.92	1.28
1:A:80:TYR:N	1:A:209:LYS:CE[3_655]	0.92	1.28
1:A:227:ASP:C	1:A:463:TRP:CA[3_655]	0.92	1.28
1:A:333:PRO:CA	4:A:2154:HOH:O[3_655]	0.92	1.28
1:A:74:GLU:CB	2:A:600:FAD:O5'[3_655]	0.93	1.27
1:A:229:VAL:O	1:A:464:GLN:CA[3_655]	0.93	1.27
1:A:501:ILE:CA	4:A:2054:HOH:O[6_565]	0.93	1.27
1:A:27:GLY:O	1:A:422:TYR:CD1[3_655]	0.94	1.26
1:A:38:ARG:CA	1:A:467:PRO:N[3_655]	0.94	1.26
1:A:18:ALA:C	1:A:18:ALA:C[3_655]	0.95	1.25
1:A:30:VAL:N	1:A:448:ARG:C[3_655]	0.96	1.24
1:A:67:ARG:O	1:A:218:SER:CB[3_655]	0.96	1.24
1:A:221:ILE:CG1	1:A:440:VAL:CB[3_655]	0.96	1.24
1:A:29:ASN:N	1:A:450:ILE:CA[3_655]	0.97	1.23
1:A:30:VAL:CG1	1:A:447:ALA:C[3_655]	0.97	1.23
1:A:38:ARG:CA	1:A:467:PRO:CA[3_655]	0.98	1.22
1:A:43:THR:O	4:A:2009:HOH:O[3_655]	0.98	1.22
1:A:26:SER:C	1:A:260:VAL:O[3_655]	0.99	1.21
1:A:30:VAL:CB	1:A:448:ARG:N[3_655]	0.99	1.21
1:A:44:TYR:CE2	1:A:470:VAL:C[3_655]	0.99	1.21
1:A:77:LEU:CB	1:A:436:MET:CE[3_655]	0.99	1.21
1:A:80:TYR:CE1	1:A:80:TYR:CE1[3_655]	0.99	1.21
1:A:84:GLU:CA	1:A:336:ASN:CG[3_655]	0.99	1.21
1:A:219:GLU:C	1:A:437:GLU:OE1[3_655]	0.99	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:CA	1:A:473:PRO:O[3_655]	1.00	1.20
1:A:59:SER:CA	1:A:78:GLU:C[3_655]	1.00	1.20
1:A:66:ASN:N	1:A:219:GLU:CD[3_655]	1.00	1.20
1:A:67:ARG:NH2	1:A:222:MET:CG[3_655]	1.00	1.20
1:A:84:GLU:C	1:A:336:ASN:CG[3_655]	1.00	1.20
1:A:225:LEU:CD2	1:A:445:ARG:N[3_655]	1.00	1.20
1:A:228:ARG:N	1:A:463:TRP:N[3_655]	1.00	1.20
1:A:15:SER:CB	1:A:21:LYS:NZ[3_655]	1.01	1.19
1:A:42:ARG:C	1:A:73:LYS:CG[3_655]	1.01	1.19
1:A:85:VAL:N	1:A:336:ASN:CA[3_655]	1.01	1.19
1:A:224:LEU:O	4:A:2204:HOH:O[3_655]	1.01	1.19
1:A:330:ASP:OD2	4:A:2046:HOH:O[3_655]	1.01	1.19
1:A:68:ILE:CG2	1:A:216:GLN:C[3_655]	1.02	1.18
1:A:73:LYS:O	2:A:600:FAD:O2'[3_655]	1.02	1.18
1:A:12:GLY:O	1:A:70:ARG:NE[3_655]	1.03	1.17
1:A:43:THR:CG2	1:A:73:LYS:N[3_655]	1.03	1.17
1:A:59:SER:CA	1:A:78:GLU:CA[3_655]	1.03	1.17
1:A:260:VAL:CA	4:A:2006:HOH:O[3_655]	1.03	1.17
1:A:6:ASP:CB	1:A:450:ILE:O[3_655]	1.04	1.16
1:A:53:TYR:N	1:A:207:GLU:CD[3_655]	1.04	1.16
1:A:67:ARG:C	1:A:218:SER:CA[3_655]	1.04	1.16
1:A:329:ASP:CB	1:A:333:PRO:O[3_655]	1.04	1.16
1:A:30:VAL:CA	1:A:448:ARG:CA[3_655]	1.05	1.15
1:A:45:THR:CG2	1:A:472:VAL:CG1[3_655]	1.05	1.15
1:A:47:ARG:N	1:A:473:PRO:O[3_655]	1.05	1.15
1:A:68:ILE:CG2	1:A:217:VAL:N[3_655]	1.05	1.15
1:A:38:ARG:C	1:A:467:PRO:CD[3_655]	1.06	1.14
1:A:65:GLN:C	1:A:219:GLU:OE1[3_655]	1.06	1.14
1:A:73:LYS:NZ	1:A:388:TRP:CZ2[3_655]	1.06	1.14
1:A:5:CYS:C	1:A:451:LEU:O[3_655]	1.07	1.13
1:A:18:ALA:C	1:A:18:ALA:O[3_655]	1.07	1.13
1:A:26:SER:N	1:A:261:ILE:CA[3_655]	1.07	1.13
1:A:46:LEU:CD1	1:A:473:PRO:CG[3_655]	1.07	1.13
1:A:67:ARG:CA	1:A:218:SER:C[3_655]	1.07	1.13
1:A:78:GLU:CG	4:A:2139:HOH:O[3_655]	1.07	1.13
1:A:220:ARG:C	1:A:437:GLU:O[3_655]	1.07	1.13
1:A:27:GLY:O	1:A:422:TYR:CE1[3_655]	1.08	1.12
1:A:44:TYR:CD1	1:A:470:VAL:N[3_655]	1.08	1.12
1:A:46:LEU:N	1:A:472:VAL:N[3_655]	1.08	1.12
1:A:61:VAL:CA	1:A:216:GLN:NE2[3_655]	1.08	1.12
1:A:438:GLY:CA	4:A:2121:HOH:O[3_655]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:MET:CA	1:A:444:GLU:OE2[3_655]	1.09	1.11
1:A:18:ALA:CA	1:A:18:ALA:CA[3_655]	1.09	1.11
1:A:29:ASN:O	1:A:451:LEU:N[3_655]	1.09	1.11
1:A:38:ARG:N	1:A:467:PRO:CB[3_655]	1.09	1.11
1:A:44:TYR:CD2	1:A:471:ASP:N[3_655]	1.09	1.11
1:A:84:GLU:CB	1:A:336:ASN:OD1[3_655]	1.09	1.11
1:A:6:ASP:N	1:A:451:LEU:O[3_655]	1.10	1.10
1:A:66:ASN:CB	4:A:2119:HOH:O[3_655]	1.10	1.10
1:A:39:VAL:CB	1:A:466:GLU:OE1[3_655]	1.11	1.09
1:A:74:GLU:CD	2:A:600:FAD:P[3_655]	1.11	1.09
1:A:76:GLY:C	2:A:600:FAD:C2[3_655]	1.11	1.09
1:A:223:ASP:C	1:A:441:GLU:OE2[3_655]	1.11	1.09
1:B:479:THR:N	1:B:479:THR:N[3_555]	1.11	1.09
1:A:23:LEU:CG	1:A:23:LEU:CD1[3_655]	1.12	1.08
1:A:68:ILE:CG1	1:A:217:VAL:CG2[3_655]	1.12	1.08
1:A:224:LEU:CG	1:A:438:GLY:O[3_655]	1.12	1.08
1:A:225:LEU:CG	1:A:445:ARG:N[3_655]	1.12	1.08
1:A:15:SER:OG	1:A:21:LYS:CE[3_655]	1.13	1.07
1:A:60:TYR:CD2	1:A:211:VAL:CG2[3_655]	1.13	1.07
1:A:17:MET:SD	1:A:444:GLU:OE1[3_655]	1.14	1.06
1:A:24:HIS:CG	1:A:446:ALA:CA[3_655]	1.14	1.06
1:A:53:TYR:CZ	1:A:207:GLU:O[3_655]	1.14	1.06
1:A:53:TYR:CE2	1:A:207:GLU:C[3_655]	1.14	1.06
1:A:68:ILE:N	1:A:218:SER:N[3_655]	1.14	1.06
1:A:85:VAL:N	1:A:336:ASN:CB[3_655]	1.14	1.06
1:A:220:ARG:CB	1:A:437:GLU:CA[3_655]	1.14	1.06
1:A:257:ALA:CA	1:A:456:LYS:CA[3_655]	1.14	1.06
1:A:307:ARG:CZ	1:A:307:ARG:NH1[3_655]	1.14	1.06
1:A:336:ASN:O	4:A:2049:HOH:O[3_655]	1.14	1.06
1:A:74:GLU:CG	2:A:600:FAD:O5'[3_655]	1.15	1.05
1:A:39:VAL:CB	1:A:466:GLU:OE2[3_655]	1.16	1.04
1:A:72:ALA:O	1:A:436:MET:CG[3_655]	1.16	1.04
1:A:210:PHE:CD1	1:A:210:PHE:CE1[3_655]	1.16	1.04
1:A:220:ARG:NH1	1:A:435:TYR:CB[3_655]	1.16	1.04
1:A:221:ILE:CB	1:A:440:VAL:C[3_655]	1.16	1.04
1:A:258:LYS:CA	1:A:456:LYS:CE[3_655]	1.16	1.04
1:A:4:LYS:O	1:A:452:HIS:ND1[3_655]	1.17	1.03
1:A:17:MET:CE	1:A:444:GLU:OE1[3_655]	1.17	1.03
1:A:19:ALA:CB	1:A:21:LYS:C[3_655]	1.17	1.03
1:A:25:ASP:O	1:A:262:SER:N[3_655]	1.17	1.03
1:A:26:SER:O	1:A:260:VAL:O[3_655]	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:C	1:A:73:LYS:CD[3_655]	1.17	1.03
1:A:44:TYR:CE1	1:A:470:VAL:N[3_655]	1.17	1.03
1:A:220:ARG:CG	1:A:437:GLU:CB[3_655]	1.17	1.03
1:A:14:ILE:CG1	1:A:71:LEU:CA[3_655]	1.18	1.02
1:A:23:LEU:C	1:A:261:ILE:CD1[3_655]	1.18	1.02
1:A:46:LEU:CG	1:A:473:PRO:CG[3_655]	1.18	1.02
1:A:60:TYR:CD2	1:A:211:VAL:CB[3_655]	1.18	1.02
1:A:74:GLU:C	2:A:600:FAD:C5'[3_655]	1.18	1.02
1:A:209:LYS:N	1:A:210:PHE:O[3_655]	1.18	1.02
1:A:18:ALA:O	1:A:19:ALA:N[3_655]	1.19	1.01
1:A:32:VAL:O	1:A:464:GLN:NE2[3_655]	1.19	1.01
1:A:52:LYS:CD	1:A:202:THR:CA[3_655]	1.19	1.01
1:A:53:TYR:CA	1:A:207:GLU:CD[3_655]	1.19	1.01
1:A:59:SER:O	1:A:78:GLU:O[3_655]	1.19	1.01
1:A:73:LYS:C	2:A:600:FAD:O4'[3_655]	1.19	1.01
1:A:82:VAL:C	1:A:332:LYS:CB[3_655]	1.19	1.01
1:A:255:TYR:CE1	1:A:461:GLU:OE2[3_655]	1.19	1.01
1:A:14:ILE:CD1	1:A:71:LEU:C[3_655]	1.20	1.00
1:A:26:SER:O	1:A:260:VAL:C[3_655]	1.20	1.00
1:A:28:LEU:CB	1:A:450:ILE:CG2[3_655]	1.20	1.00
1:A:28:LEU:N	1:A:450:ILE:CG1[3_655]	1.20	1.00
1:A:45:THR:C	1:A:472:VAL:CA[3_655]	1.20	1.00
1:A:46:LEU:CA	1:A:473:PRO:CD[3_655]	1.20	1.00
1:A:47:ARG:CG	1:A:63:PRO:CB[3_655]	1.20	1.00
1:A:66:ASN:CG	4:A:2119:HOH:O[3_655]	1.20	1.00
1:A:69:LEU:CG	1:A:215:GLY:CA[3_655]	1.20	1.00
1:A:79:THR:C	1:A:209:LYS:NZ[3_655]	1.20	1.00
1:A:209:LYS:C	1:A:209:LYS:C[3_655]	1.20	1.00
1:A:209:LYS:C	1:A:210:PHE:N[3_655]	1.20	1.00
1:A:53:TYR:CD2	1:A:207:GLU:CG[3_655]	1.21	0.99
1:A:65:GLN:OE1	1:A:216:GLN:CD[3_655]	1.21	0.99
1:A:74:GLU:OE2	2:A:600:FAD:O1P[3_655]	1.21	0.99
1:A:80:TYR:N	1:A:209:LYS:NZ[3_655]	1.21	0.99
1:A:39:VAL:CG2	1:A:466:GLU:CD[3_655]	1.22	0.98
1:A:55:ASP:OD2	1:A:79:THR:OG1[3_655]	1.22	0.98
1:A:66:ASN:CA	1:A:219:GLU:CG[3_655]	1.22	0.98
1:A:67:ARG:N	1:A:219:GLU:N[3_655]	1.22	0.98
1:A:76:GLY:O	2:A:600:FAD:N1[3_655]	1.22	0.98
1:A:9:VAL:CG2	1:A:22:LEU:CD2[3_655]	1.23	0.97
1:A:26:SER:C	1:A:260:VAL:C[3_655]	1.23	0.97
1:A:29:ASN:CA	1:A:450:ILE:N[3_655]	1.23	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:CG2	1:A:457:ILE:CD1[3_655]	1.23	0.97
1:A:44:TYR:CD2	1:A:470:VAL:C[3_655]	1.23	0.97
1:A:69:LEU:CG	1:A:215:GLY:N[3_655]	1.23	0.97
1:A:74:GLU:O	2:A:600:FAD:C5'[3_655]	1.23	0.97
1:A:75:LEU:O	1:A:435:TYR:CA[3_655]	1.23	0.97
1:A:221:ILE:O	1:A:441:GLU:C[3_655]	1.23	0.97
1:A:68:ILE:CD1	1:A:217:VAL:CG2[3_655]	1.24	0.96
1:A:223:ASP:O	1:A:441:GLU:CD[3_655]	1.24	0.96
1:A:227:ASP:N	1:A:463:TRP:CB[3_655]	1.24	0.96
1:A:26:SER:CA	1:A:261:ILE:CA[3_655]	1.25	0.95
1:A:38:ARG:N	1:A:467:PRO:CG[3_655]	1.25	0.95
1:A:39:VAL:O	4:A:2215:HOH:O[3_655]	1.25	0.95
1:A:54:VAL:CB	1:A:208:ARG:NH2[3_655]	1.25	0.95
1:A:61:VAL:CB	1:A:213:GLY:O[3_655]	1.25	0.95
1:A:67:ARG:CZ	1:A:222:MET:CG[3_655]	1.25	0.95
1:A:67:ARG:CA	1:A:219:GLU:N[3_655]	1.25	0.95
1:A:6:ASP:N	1:A:451:LEU:C[3_655]	1.26	0.94
1:A:16:GLY:CA	4:A:2003:HOH:O[3_655]	1.26	0.94
1:A:25:ASP:O	1:A:261:ILE:C[3_655]	1.26	0.94
1:A:29:ASN:CA	1:A:449:GLU:O[3_655]	1.26	0.94
1:A:74:GLU:CA	2:A:600:FAD:O4'[3_655]	1.26	0.94
1:A:75:LEU:C	1:A:435:TYR:C[3_655]	1.26	0.94
1:A:81:LYS:CG	1:A:332:LYS:NZ[3_655]	1.26	0.94
1:A:84:GLU:O	1:A:336:ASN:CB[3_655]	1.26	0.94
1:A:208:ARG:O	1:A:211:VAL:CA[3_655]	1.26	0.94
1:A:228:ARG:CA	1:A:462:ILE:O[3_655]	1.26	0.94
1:A:47:ARG:NH2	1:A:62:GLY:O[3_655]	1.27	0.93
1:A:61:VAL:O	1:A:212:GLY:C[3_655]	1.27	0.93
1:A:24:HIS:ND1	1:A:446:ALA:CA[3_655]	1.28	0.92
1:A:44:TYR:CD1	1:A:469:SER:C[3_655]	1.28	0.92
1:A:65:GLN:CA	1:A:219:GLU:OE1[3_655]	1.28	0.92
1:A:221:ILE:C	1:A:441:GLU:N[3_655]	1.28	0.92
1:A:19:ALA:C	1:A:19:ALA:O[3_655]	1.29	0.91
1:A:30:VAL:C	1:A:448:ARG:CA[3_655]	1.29	0.91
1:A:32:VAL:CA	4:A:2209:HOH:O[3_655]	1.29	0.91
1:A:32:VAL:CG1	4:A:2209:HOH:O[3_655]	1.29	0.91
1:A:59:SER:CB	1:A:78:GLU:C[3_655]	1.29	0.91
1:A:69:LEU:CD2	1:A:215:GLY:N[3_655]	1.29	0.91
1:A:208:ARG:C	1:A:210:PHE:O[3_655]	1.29	0.91
1:A:220:ARG:N	1:A:437:GLU:CD[3_655]	1.29	0.91
1:A:500:THR:O	4:A:2014:HOH:O[6_565]	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:C	1:A:422:TYR:CD1[3_655]	1.30	0.90
1:A:53:TYR:CZ	1:A:208:ARG:N[3_655]	1.30	0.90
1:A:55:ASP:OD2	1:A:79:THR:CG2[3_655]	1.30	0.90
1:A:223:ASP:CA	1:A:441:GLU:CD[3_655]	1.30	0.90
1:A:5:CYS:CB	1:A:452:HIS:CA[3_655]	1.31	0.89
1:A:67:ARG:O	1:A:218:SER:CA[3_655]	1.31	0.89
1:A:3:ASN:O	1:A:458:PRO:N[3_655]	1.32	0.88
1:A:15:SER:CA	1:A:21:LYS:CE[3_655]	1.32	0.88
1:A:45:THR:N	1:A:469:SER:OG[3_655]	1.32	0.88
1:A:52:LYS:CD	1:A:201:THR:C[3_655]	1.32	0.88
1:A:75:LEU:O	1:A:436:MET:N[3_655]	1.32	0.88
1:A:500:THR:C	4:A:2014:HOH:O[6_565]	1.32	0.88
1:A:6:ASP:CG	1:A:450:ILE:O[3_655]	1.33	0.87
1:A:53:TYR:CB	1:A:207:GLU:OE2[3_655]	1.33	0.87
1:A:53:TYR:OH	1:A:207:GLU:O[3_655]	1.33	0.87
1:A:54:VAL:N	1:A:208:ARG:NH2[3_655]	1.33	0.87
1:A:65:GLN:OE1	1:A:216:GLN:OE1[3_655]	1.33	0.87
1:A:76:GLY:O	2:A:600:FAD:C2[3_655]	1.33	0.87
1:A:221:ILE:CA	1:A:440:VAL:C[3_655]	1.33	0.87
1:A:224:LEU:CD1	1:A:438:GLY:O[3_655]	1.33	0.87
1:B:478:THR:C	1:B:478:THR:C[3_555]	1.33	0.87
1:A:40:GLY:N	1:A:70:ARG:CB[3_655]	1.34	0.86
1:A:55:ASP:CG	1:A:79:THR:OG1[3_655]	1.34	0.86
1:A:59:SER:CB	1:A:79:THR:N[3_655]	1.34	0.86
1:A:75:LEU:CD2	1:A:439:ALA:N[3_655]	1.34	0.86
1:A:84:GLU:CG	1:A:336:ASN:ND2[3_655]	1.34	0.86
1:A:220:ARG:NH1	1:A:435:TYR:CG[3_655]	1.34	0.86
1:A:24:HIS:CE1	1:A:445:ARG:NH2[3_655]	1.35	0.85
1:A:28:LEU:C	1:A:450:ILE:N[3_655]	1.35	0.85
1:A:30:VAL:CB	1:A:447:ALA:C[3_655]	1.35	0.85
1:A:30:VAL:C	1:A:448:ARG:CB[3_655]	1.35	0.85
1:A:38:ARG:CB	1:A:467:PRO:O[3_655]	1.35	0.85
1:A:59:SER:N	1:A:78:GLU:CA[3_655]	1.35	0.85
1:A:60:TYR:C	1:A:211:VAL:O[3_655]	1.35	0.85
1:A:74:GLU:CA	2:A:600:FAD:C4'[3_655]	1.35	0.85
1:A:79:THR:O	1:A:209:LYS:NZ[3_655]	1.35	0.85
1:A:256:GLU:O	1:A:455:GLY:C[3_655]	1.35	0.85
1:A:14:ILE:CD1	1:A:72:ALA:CA[3_655]	1.36	0.84
1:A:58:GLY:C	1:A:77:LEU:O[3_655]	1.36	0.84
1:A:59:SER:C	1:A:78:GLU:C[3_655]	1.36	0.84
1:A:67:ARG:O	1:A:218:SER:OG[3_655]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLY:CA	2:A:600:FAD:N1[3_655]	1.36	0.84
1:A:77:LEU:N	2:A:600:FAD:C2[3_655]	1.36	0.84
1:A:77:LEU:CD2	4:A:2036:HOH:O[3_655]	1.36	0.84
1:A:82:VAL:CA	1:A:333:PRO:CD[3_655]	1.36	0.84
1:A:229:VAL:C	1:A:464:GLN:CA[3_655]	1.36	0.84
1:A:259:TYR:N	1:A:456:LYS:CE[3_655]	1.36	0.84
1:A:334:GLU:CA	4:A:2048:HOH:O[3_655]	1.36	0.84
1:A:7:VAL:O	1:A:451:LEU:CD1[3_655]	1.37	0.83
1:A:25:ASP:C	1:A:261:ILE:CA[3_655]	1.37	0.83
1:A:38:ARG:O	1:A:467:PRO:CD[3_655]	1.37	0.83
1:A:39:VAL:CG2	1:A:466:GLU:CG[3_655]	1.37	0.83
1:A:40:GLY:N	1:A:70:ARG:CG[3_655]	1.37	0.83
1:A:53:TYR:OH	1:A:207:GLU:C[3_655]	1.37	0.83
1:A:67:ARG:C	1:A:218:SER:N[3_655]	1.37	0.83
1:A:210:PHE:CG	1:A:210:PHE:CD1[3_655]	1.37	0.83
1:A:228:ARG:CB	1:A:462:ILE:C[3_655]	1.37	0.83
1:A:256:GLU:C	1:A:455:GLY:O[3_655]	1.37	0.83
1:A:5:CYS:CA	1:A:452:HIS:CA[3_655]	1.38	0.82
1:A:14:ILE:O	1:A:71:LEU:CD1[3_655]	1.38	0.82
1:A:29:ASN:CG	1:A:449:GLU:O[3_655]	1.38	0.82
1:A:44:TYR:CZ	1:A:470:VAL:CA[3_655]	1.38	0.82
1:A:75:LEU:CB	1:A:436:MET:CA[3_655]	1.38	0.82
1:A:209:LYS:O	1:A:209:LYS:CB[3_655]	1.38	0.82
1:A:255:TYR:CZ	1:A:461:GLU:OE2[3_655]	1.38	0.82
1:A:260:VAL:N	4:A:2006:HOH:O[3_655]	1.38	0.82
1:A:42:ARG:N	4:A:2044:HOH:O[3_655]	1.39	0.81
1:A:44:TYR:O	1:A:471:ASP:CB[3_655]	1.39	0.81
1:A:45:THR:CB	1:A:472:VAL:CB[3_655]	1.39	0.81
1:A:53:TYR:CG	1:A:207:GLU:CG[3_655]	1.39	0.81
1:A:74:GLU:CA	2:A:600:FAD:C5'[3_655]	1.39	0.81
1:A:82:VAL:C	1:A:332:LYS:CA[3_655]	1.39	0.81
1:A:83:ASN:CB	1:A:335:GLY:N[3_655]	1.39	0.81
1:A:422:TYR:C	4:A:2008:HOH:O[3_655]	1.39	0.81
1:A:7:VAL:N	1:A:451:LEU:CA[3_655]	1.40	0.80
1:A:8:VAL:CG2	1:A:457:ILE:CG2[3_655]	1.40	0.80
1:A:18:ALA:N	4:A:2001:HOH:O[3_655]	1.40	0.80
1:A:25:ASP:CB	1:A:261:ILE:CG2[3_655]	1.40	0.80
1:A:30:VAL:CB	1:A:448:ARG:CA[3_655]	1.40	0.80
1:A:43:THR:N	1:A:73:LYS:CB[3_655]	1.40	0.80
1:A:68:ILE:CG1	1:A:217:VAL:CB[3_655]	1.40	0.80
1:A:68:ILE:CA	1:A:217:VAL:CA[3_655]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:CD2	1:A:465:SER:O[3_655]	1.40	0.80
1:B:81:LYS:NZ	1:B:100:ARG:NH1[3_555]	1.40	0.80
1:A:47:ARG:CG	1:A:63:PRO:CG[3_655]	1.41	0.79
1:A:53:TYR:C	1:A:207:GLU:OE2[3_655]	1.41	0.79
1:A:58:GLY:CA	1:A:77:LEU:O[3_655]	1.41	0.79
1:A:257:ALA:N	1:A:456:LYS:CA[3_655]	1.41	0.79
1:A:24:HIS:CB	1:A:446:ALA:CA[3_655]	1.42	0.78
1:A:25:ASP:C	1:A:261:ILE:CB[3_655]	1.42	0.78
1:A:25:ASP:C	1:A:261:ILE:CG2[3_655]	1.42	0.78
1:A:38:ARG:CB	1:A:467:PRO:CA[3_655]	1.42	0.78
1:A:42:ARG:O	1:A:73:LYS:CD[3_655]	1.42	0.78
1:A:68:ILE:CD1	1:A:217:VAL:CB[3_655]	1.42	0.78
1:A:224:LEU:N	1:A:441:GLU:CG[3_655]	1.42	0.78
1:A:227:ASP:C	1:A:463:TRP:N[3_655]	1.42	0.78
1:A:228:ARG:CA	1:A:463:TRP:N[3_655]	1.42	0.78
1:A:332:LYS:CD	4:A:2047:HOH:O[3_655]	1.42	0.78
1:A:14:ILE:C	1:A:71:LEU:CD1[3_655]	1.43	0.77
1:A:42:ARG:CB	4:A:2010:HOH:O[3_655]	1.43	0.77
1:A:43:THR:CB	1:A:69:LEU:O[3_655]	1.43	0.77
1:A:46:LEU:CA	1:A:472:VAL:C[3_655]	1.43	0.77
1:A:68:ILE:CA	1:A:218:SER:N[3_655]	1.43	0.77
1:A:210:PHE:CE2	1:A:214:SER:CB[3_655]	1.43	0.77
1:A:219:GLU:O	1:A:437:GLU:OE1[3_655]	1.43	0.77
1:B:478:THR:O	1:B:478:THR:OG1[3_555]	1.43	0.77
1:A:23:LEU:CD1	1:A:23:LEU:CD2[3_655]	1.44	0.76
1:A:28:LEU:CB	1:A:450:ILE:CG1[3_655]	1.44	0.76
1:A:44:TYR:CG	1:A:470:VAL:N[3_655]	1.44	0.76
1:A:45:THR:CA	1:A:472:VAL:CB[3_655]	1.44	0.76
1:A:45:THR:CG2	1:A:472:VAL:CB[3_655]	1.44	0.76
1:A:47:ARG:CD	1:A:63:PRO:CB[3_655]	1.44	0.76
1:A:59:SER:CB	1:A:78:GLU:CA[3_655]	1.44	0.76
1:A:61:VAL:C	1:A:212:GLY:C[3_655]	1.44	0.76
1:A:83:ASN:N	1:A:332:LYS:O[3_655]	1.44	0.76
1:A:259:TYR:N	1:A:456:LYS:CD[3_655]	1.44	0.76
1:A:39:VAL:CA	1:A:466:GLU:CD[3_655]	1.45	0.75
1:A:47:ARG:CD	1:A:63:PRO:CA[3_655]	1.45	0.75
1:A:52:LYS:CG	1:A:202:THR:CA[3_655]	1.45	0.75
1:A:80:TYR:CA	1:A:209:LYS:NZ[3_655]	1.45	0.75
1:A:83:ASN:OD1	1:A:335:GLY:C[3_655]	1.45	0.75
1:A:28:LEU:CG	1:A:450:ILE:CG2[3_655]	1.46	0.74
1:A:43:THR:OG1	1:A:69:LEU:C[3_655]	1.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:CG	1:A:473:PRO:CD[3_655]	1.46	0.74
1:A:59:SER:OG	1:A:79:THR:CA[3_655]	1.46	0.74
1:A:60:TYR:CD2	1:A:211:VAL:CG1[3_655]	1.46	0.74
1:A:227:ASP:C	1:A:463:TRP:C[3_655]	1.46	0.74
1:A:255:TYR:CD2	1:A:458:PRO:CD[3_655]	1.46	0.74
1:A:30:VAL:O	1:A:448:ARG:CB[3_655]	1.47	0.73
1:A:38:ARG:N	1:A:467:PRO:CA[3_655]	1.47	0.73
1:A:39:VAL:C	1:A:466:GLU:OE2[3_655]	1.47	0.73
1:A:60:TYR:CG	1:A:211:VAL:CB[3_655]	1.47	0.73
1:A:65:GLN:C	1:A:219:GLU:CD[3_655]	1.47	0.73
1:A:74:GLU:OE1	2:A:600:FAD:O1P[3_655]	1.47	0.73
1:A:75:LEU:CD1	1:A:436:MET:O[3_655]	1.47	0.73
1:A:84:GLU:O	1:A:336:ASN:CG[3_655]	1.47	0.73
1:A:7:VAL:C	1:A:451:LEU:CG[3_655]	1.48	0.72
1:A:30:VAL:CA	1:A:448:ARG:C[3_655]	1.48	0.72
1:A:67:ARG:CZ	1:A:222:MET:CB[3_655]	1.48	0.72
1:A:68:ILE:CA	1:A:217:VAL:C[3_655]	1.48	0.72
1:A:81:LYS:CD	1:A:332:LYS:NZ[3_655]	1.48	0.72
1:A:83:ASN:O	1:A:334:GLU:CB[3_655]	1.48	0.72
1:A:84:GLU:N	1:A:336:ASN:OD1[3_655]	1.48	0.72
1:A:224:LEU:CB	1:A:442:ALA:N[3_655]	1.48	0.72
1:A:230:LYS:CE	1:A:461:GLU:CA[3_655]	1.48	0.72
1:A:5:CYS:O	1:A:455:GLY:N[3_655]	1.49	0.71
1:A:40:GLY:CA	1:A:70:ARG:CA[3_655]	1.49	0.71
1:A:42:ARG:N	4:A:2010:HOH:O[3_655]	1.49	0.71
1:A:59:SER:N	1:A:78:GLU:N[3_655]	1.49	0.71
1:A:61:VAL:O	1:A:212:GLY:N[3_655]	1.49	0.71
1:A:65:GLN:N	1:A:219:GLU:OE1[3_655]	1.49	0.71
1:A:83:ASN:CB	1:A:332:LYS:O[3_655]	1.49	0.71
1:A:221:ILE:CB	1:A:440:VAL:CA[3_655]	1.49	0.71
1:A:221:ILE:N	1:A:437:GLU:O[3_655]	1.49	0.71
1:A:336:ASN:C	4:A:2049:HOH:O[3_655]	1.49	0.71
1:A:19:ALA:CA	1:A:22:LEU:N[3_655]	1.50	0.70
1:A:26:SER:N	1:A:261:ILE:CG1[3_655]	1.50	0.70
1:A:28:LEU:CA	1:A:450:ILE:CB[3_655]	1.50	0.70
1:A:30:VAL:N	1:A:449:GLU:N[3_655]	1.50	0.70
1:A:31:VAL:CB	1:A:457:ILE:CD1[3_655]	1.50	0.70
1:A:60:TYR:CE2	1:A:211:VAL:CG2[3_655]	1.50	0.70
1:A:68:ILE:O	4:A:2018:HOH:O[3_655]	1.50	0.70
1:A:74:GLU:CG	2:A:600:FAD:O3P[3_655]	1.50	0.70
1:A:75:LEU:CD2	1:A:439:ALA:CA[3_655]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLY:O	2:A:600:FAD:C10[3_655]	1.50	0.70
1:A:83:ASN:CA	1:A:332:LYS:O[3_655]	1.50	0.70
1:A:223:ASP:C	1:A:441:GLU:OE1[3_655]	1.50	0.70
1:A:223:ASP:C	1:A:441:GLU:CG[3_655]	1.50	0.70
1:A:226:GLY:CA	1:A:463:TRP:CE3[3_655]	1.50	0.70
1:A:228:ARG:CG	1:A:462:ILE:CG2[3_655]	1.50	0.70
1:A:21:LYS:CA	1:A:443:GLY:C[3_655]	1.51	0.69
1:A:59:SER:N	1:A:77:LEU:O[3_655]	1.51	0.69
1:A:60:TYR:O	4:A:2045:HOH:O[3_655]	1.51	0.69
1:A:67:ARG:CD	1:A:222:MET:CB[3_655]	1.51	0.69
1:A:221:ILE:CG2	1:A:440:VAL:C[3_655]	1.51	0.69
1:A:230:LYS:CE	1:A:460:ASP:O[3_655]	1.51	0.69
1:A:321:GLU:OE2	1:A:499:THR:O[6_564]	1.51	0.69
1:A:7:VAL:O	1:A:451:LEU:CG[3_655]	1.52	0.68
1:A:7:VAL:CA	1:A:451:LEU:CG[3_655]	1.52	0.68
1:A:67:ARG:CG	1:A:218:SER:O[3_655]	1.52	0.68
1:A:70:ARG:O	4:A:2230:HOH:O[3_655]	1.52	0.68
1:A:80:TYR:CD1	1:A:80:TYR:OH[3_655]	1.52	0.68
1:A:225:LEU:CA	1:A:445:ARG:CB[3_655]	1.52	0.68
1:A:227:ASP:O	1:A:463:TRP:O[3_655]	1.52	0.68
1:A:230:LYS:N	1:A:464:GLN:CG[3_655]	1.52	0.68
1:A:3:ASN:O	1:A:457:ILE:C[3_655]	1.53	0.67
1:A:7:VAL:O	1:A:451:LEU:CB[3_655]	1.53	0.67
1:A:12:GLY:O	1:A:70:ARG:CD[3_655]	1.53	0.67
1:A:24:HIS:CB	1:A:446:ALA:CB[3_655]	1.53	0.67
1:A:28:LEU:N	1:A:450:ILE:CD1[3_655]	1.53	0.67
1:A:40:GLY:CA	1:A:70:ARG:CG[3_655]	1.53	0.67
1:A:45:THR:C	1:A:472:VAL:N[3_655]	1.53	0.67
1:A:61:VAL:C	1:A:212:GLY:CA[3_655]	1.53	0.67
1:A:75:LEU:C	1:A:436:MET:N[3_655]	1.53	0.67
1:A:75:LEU:CD2	1:A:439:ALA:CB[3_655]	1.53	0.67
1:A:17:MET:CG	1:A:444:GLU:OE2[3_655]	1.54	0.66
1:A:21:LYS:CA	1:A:443:GLY:O[3_655]	1.54	0.66
1:A:42:ARG:CA	4:A:2010:HOH:O[3_655]	1.54	0.66
1:A:43:THR:CG2	1:A:73:LYS:CA[3_655]	1.54	0.66
1:A:44:TYR:CE1	1:A:469:SER:O[3_655]	1.54	0.66
1:A:44:TYR:CZ	1:A:469:SER:O[3_655]	1.54	0.66
1:A:46:LEU:N	1:A:472:VAL:C[3_655]	1.54	0.66
1:A:67:ARG:NE	1:A:222:MET:CG[3_655]	1.54	0.66
1:A:83:ASN:OD1	1:A:335:GLY:CA[3_655]	1.54	0.66
1:A:219:GLU:C	1:A:437:GLU:CD[3_655]	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:CA	1:A:437:GLU:O[3_655]	1.54	0.66
1:A:225:LEU:CD1	1:A:444:GLU:C[3_655]	1.54	0.66
1:A:227:ASP:C	1:A:463:TRP:CB[3_655]	1.54	0.66
1:A:257:ALA:CB	1:A:456:LYS:CA[3_655]	1.54	0.66
1:A:321:GLU:CG	1:A:499:THR:O[6_564]	1.54	0.66
1:A:17:MET:CG	1:A:70:ARG:NH2[3_655]	1.55	0.65
1:A:53:TYR:CD2	1:A:207:GLU:CA[3_655]	1.55	0.65
1:A:55:ASP:N	1:A:208:ARG:NH1[3_655]	1.55	0.65
1:A:68:ILE:CA	1:A:217:VAL:N[3_655]	1.55	0.65
1:A:84:GLU:CB	1:A:336:ASN:CG[3_655]	1.55	0.65
1:A:208:ARG:O	1:A:211:VAL:C[3_655]	1.55	0.65
1:A:223:ASP:CB	1:A:441:GLU:OE1[3_655]	1.55	0.65
1:A:231:LEU:CG	1:A:465:SER:O[3_655]	1.55	0.65
1:A:256:GLU:O	1:A:455:GLY:O[3_655]	1.55	0.65
1:A:24:HIS:NE2	1:A:445:ARG:NH2[3_655]	1.56	0.64
1:A:28:LEU:C	1:A:450:ILE:CA[3_655]	1.56	0.64
1:A:32:VAL:O	1:A:464:GLN:CD[3_655]	1.56	0.64
1:A:44:TYR:CZ	1:A:470:VAL:N[3_655]	1.56	0.64
1:A:67:ARG:NE	1:A:222:MET:CA[3_655]	1.56	0.64
1:A:74:GLU:CA	2:A:600:FAD:O5'[3_655]	1.56	0.64
1:A:77:LEU:N	2:A:600:FAD:N1[3_655]	1.56	0.64
1:A:209:LYS:CA	1:A:210:PHE:C[3_655]	1.56	0.64
1:A:255:TYR:CZ	1:A:461:GLU:CD[3_655]	1.56	0.64
1:A:321:GLU:CD	1:A:499:THR:O[6_564]	1.56	0.64
1:A:330:ASP:OD2	4:A:2116:HOH:O[3_655]	1.56	0.64
1:A:422:TYR:O	4:A:2008:HOH:O[3_655]	1.56	0.64
1:A:47:ARG:NH1	4:A:2037:HOH:O[3_655]	1.57	0.63
1:A:53:TYR:CE2	1:A:207:GLU:CB[3_655]	1.57	0.63
1:A:59:SER:N	1:A:77:LEU:C[3_655]	1.57	0.63
1:A:80:TYR:CB	1:A:209:LYS:CD[3_655]	1.57	0.63
1:A:83:ASN:CG	1:A:335:GLY:N[3_655]	1.57	0.63
1:A:500:THR:O	4:A:2149:HOH:O[6_565]	1.57	0.63
1:A:14:ILE:CG1	1:A:72:ALA:N[3_655]	1.58	0.62
1:A:20:ALA:O	1:A:447:ALA:CB[3_655]	1.58	0.62
1:A:30:VAL:N	1:A:448:ARG:O[3_655]	1.58	0.62
1:A:38:ARG:CA	1:A:467:PRO:CB[3_655]	1.58	0.62
1:A:44:TYR:CD2	1:A:470:VAL:CA[3_655]	1.58	0.62
1:A:53:TYR:CD1	1:A:208:ARG:CG[3_655]	1.58	0.62
1:A:60:TYR:CE1	1:A:78:GLU:OE1[3_655]	1.58	0.62
1:A:65:GLN:CD	1:A:216:GLN:OE1[3_655]	1.58	0.62
1:A:69:LEU:CA	1:A:215:GLY:CA[3_655]	1.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLY:C	2:A:600:FAD:C10[3_655]	1.58	0.62
1:A:225:LEU:CD1	1:A:445:ARG:N[3_655]	1.58	0.62
1:A:422:TYR:N	4:A:2008:HOH:O[3_655]	1.58	0.62
1:A:19:ALA:CB	1:A:22:LEU:CA[3_655]	1.59	0.61
1:A:24:HIS:CD2	1:A:446:ALA:CB[3_655]	1.59	0.61
1:A:26:SER:CA	1:A:260:VAL:C[3_655]	1.59	0.61
1:A:38:ARG:CA	1:A:467:PRO:CD[3_655]	1.59	0.61
1:A:44:TYR:C	4:A:2216:HOH:O[3_655]	1.59	0.61
1:A:44:TYR:CD1	1:A:469:SER:CA[3_655]	1.59	0.61
1:A:46:LEU:C	1:A:473:PRO:N[3_655]	1.59	0.61
1:A:47:ARG:N	1:A:473:PRO:C[3_655]	1.59	0.61
1:A:52:LYS:CE	1:A:201:THR:C[3_655]	1.59	0.61
1:A:73:LYS:O	2:A:600:FAD:C2'[3_655]	1.59	0.61
1:A:80:TYR:CB	1:A:209:LYS:CE[3_655]	1.59	0.61
1:A:83:ASN:O	1:A:334:GLU:CA[3_655]	1.59	0.61
1:A:225:LEU:CD2	1:A:445:ARG:CA[3_655]	1.59	0.61
1:A:5:CYS:CB	1:A:452:HIS:N[3_655]	1.60	0.60
1:A:14:ILE:CG2	1:A:71:LEU:CG[3_655]	1.60	0.60
1:A:24:HIS:CB	1:A:446:ALA:C[3_655]	1.60	0.60
1:A:29:ASN:CB	1:A:449:GLU:C[3_655]	1.60	0.60
1:A:29:ASN:N	1:A:449:GLU:C[3_655]	1.60	0.60
1:A:43:THR:CA	1:A:73:LYS:CB[3_655]	1.60	0.60
1:A:53:TYR:CB	1:A:207:GLU:CD[3_655]	1.60	0.60
1:A:54:VAL:N	1:A:208:ARG:CZ[3_655]	1.60	0.60
1:A:66:ASN:N	1:A:219:GLU:CB[3_655]	1.60	0.60
1:A:83:ASN:CG	1:A:335:GLY:C[3_655]	1.60	0.60
1:A:223:ASP:OD2	1:A:431:HIS:O[3_655]	1.60	0.60
1:A:229:VAL:C	1:A:464:GLN:CG[3_655]	1.60	0.60
1:A:5:CYS:SG	1:A:457:ILE:CG1[3_655]	1.61	0.59
1:A:25:ASP:O	1:A:261:ILE:CA[3_655]	1.61	0.59
1:A:32:VAL:N	1:A:448:ARG:CD[3_655]	1.61	0.59
1:A:45:THR:O	1:A:472:VAL:O[3_655]	1.61	0.59
1:A:61:VAL:CG2	1:A:213:GLY:O[3_655]	1.61	0.59
1:A:228:ARG:O	1:A:461:GLU:O[3_655]	1.61	0.59
1:A:257:ALA:CA	1:A:456:LYS:CB[3_655]	1.61	0.59
1:A:44:TYR:C	1:A:469:SER:OG[3_655]	1.62	0.58
1:A:56:LEU:C	1:A:471:ASP:OD2[3_655]	1.62	0.58
1:A:83:ASN:ND2	1:A:335:GLY:N[3_655]	1.62	0.58
1:A:256:GLU:O	1:A:456:LYS:N[3_655]	1.62	0.58
1:A:257:ALA:CA	1:A:456:LYS:N[3_655]	1.62	0.58
1:A:20:ALA:N	1:A:22:LEU:CB[3_655]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:VAL:CG2	1:A:213:GLY:C[3_655]	1.63	0.57
1:A:65:GLN:CA	4:A:2120:HOH:O[3_655]	1.63	0.57
1:A:67:ARG:C	1:A:218:SER:CB[3_655]	1.63	0.57
1:A:84:GLU:O	1:A:336:ASN:ND2[3_655]	1.63	0.57
1:A:257:ALA:CB	1:A:456:LYS:CG[3_655]	1.63	0.57
1:A:15:SER:CA	1:A:21:LYS:NZ[3_655]	1.64	0.56
1:A:61:VAL:CB	1:A:216:GLN:NE2[3_655]	1.64	0.56
1:A:66:ASN:OD1	1:A:219:GLU:OE2[3_655]	1.64	0.56
1:A:69:LEU:C	4:A:2018:HOH:O[3_655]	1.64	0.56
1:A:224:LEU:N	1:A:441:GLU:CD[3_655]	1.64	0.56
1:A:6:ASP:O	1:A:454:MET:CE[3_655]	1.65	0.55
1:A:24:HIS:N	1:A:261:ILE:CD1[3_655]	1.65	0.55
1:A:27:GLY:N	1:A:260:VAL:O[3_655]	1.65	0.55
1:A:47:ARG:NE	1:A:63:PRO:N[3_655]	1.65	0.55
1:A:53:TYR:CE1	1:A:208:ARG:N[3_655]	1.65	0.55
1:A:54:VAL:O	1:A:471:ASP:O[3_655]	1.65	0.55
1:A:59:SER:OG	1:A:78:GLU:C[3_655]	1.65	0.55
1:A:67:ARG:O	1:A:218:SER:N[3_655]	1.65	0.55
1:A:83:ASN:N	1:A:333:PRO:N[3_655]	1.65	0.55
1:A:84:GLU:N	1:A:336:ASN:N[3_655]	1.65	0.55
1:A:206:GLN:O	4:A:2030:HOH:O[3_655]	1.65	0.55
1:A:501:ILE:N	4:A:2014:HOH:O[6_565]	1.65	0.55
1:A:13:GLY:O	1:A:70:ARG:NH1[3_655]	1.66	0.54
1:A:24:HIS:CE1	1:A:445:ARG:CZ[3_655]	1.66	0.54
1:A:25:ASP:OD1	1:A:424:ALA:CA[3_655]	1.66	0.54
1:A:25:ASP:CG	1:A:424:ALA:CB[3_655]	1.66	0.54
1:A:40:GLY:C	1:A:70:ARG:CG[3_655]	1.66	0.54
1:A:45:THR:C	1:A:472:VAL:C[3_655]	1.66	0.54
1:A:62:GLY:N	1:A:212:GLY:O[3_655]	1.66	0.54
1:A:68:ILE:CG1	1:A:217:VAL:CA[3_655]	1.66	0.54
1:A:259:TYR:N	1:A:456:LYS:NZ[3_655]	1.66	0.54
1:A:6:ASP:OD2	1:A:450:ILE:O[3_655]	1.67	0.53
1:A:23:LEU:CB	1:A:23:LEU:CD1[3_655]	1.67	0.53
1:A:23:LEU:CG	1:A:23:LEU:CD2[3_655]	1.67	0.53
1:A:44:TYR:CZ	1:A:469:SER:C[3_655]	1.67	0.53
1:A:53:TYR:CG	1:A:207:GLU:CB[3_655]	1.67	0.53
1:A:53:TYR:CE1	1:A:208:ARG:CG[3_655]	1.67	0.53
1:A:68:ILE:N	1:A:217:VAL:C[3_655]	1.67	0.53
1:A:75:LEU:N	2:A:600:FAD:C4'[3_655]	1.67	0.53
1:A:81:LYS:CG	4:A:2158:HOH:O[3_655]	1.67	0.53
1:A:220:ARG:CA	1:A:437:GLU:C[3_655]	1.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:NH2	4:A:2157:HOH:O[3_655]	1.67	0.53
1:B:475:GLN:NE2	4:B:2058:HOH:O[3_555]	1.67	0.53
1:A:7:VAL:C	1:A:451:LEU:CD1[3_655]	1.68	0.52
1:A:7:VAL:CB	1:A:451:LEU:CG[3_655]	1.68	0.52
1:A:26:SER:CB	1:A:261:ILE:N[3_655]	1.68	0.52
1:A:52:LYS:O	1:A:207:GLU:OE1[3_655]	1.68	0.52
1:A:65:GLN:OE1	1:A:216:GLN:CG[3_655]	1.68	0.52
1:A:67:ARG:C	1:A:218:SER:C[3_655]	1.68	0.52
1:A:67:ARG:CB	1:A:219:GLU:N[3_655]	1.68	0.52
1:A:67:ARG:CD	1:A:222:MET:N[3_655]	1.68	0.52
1:A:75:LEU:O	1:A:435:TYR:O[3_655]	1.68	0.52
1:A:75:LEU:CG	1:A:439:ALA:CB[3_655]	1.68	0.52
1:A:75:LEU:CA	1:A:435:TYR:O[3_655]	1.68	0.52
1:A:82:VAL:CB	1:A:333:PRO:CD[3_655]	1.68	0.52
1:A:202:THR:OG1	1:A:337:TYR:CE1[3_655]	1.68	0.52
1:A:220:ARG:CB	1:A:438:GLY:N[3_655]	1.68	0.52
1:A:221:ILE:CB	1:A:440:VAL:CB[3_655]	1.68	0.52
1:A:228:ARG:CG	1:A:462:ILE:O[3_655]	1.68	0.52
1:A:24:HIS:CG	1:A:446:ALA:N[3_655]	1.69	0.51
1:A:45:THR:CA	1:A:472:VAL:CG2[3_655]	1.69	0.51
1:A:52:LYS:NZ	1:A:202:THR:N[3_655]	1.69	0.51
1:A:54:VAL:N	1:A:208:ARG:NE[3_655]	1.69	0.51
1:A:56:LEU:CB	1:A:471:ASP:OD2[3_655]	1.69	0.51
1:A:82:VAL:CG1	1:A:333:PRO:CG[3_655]	1.69	0.51
1:A:82:VAL:C	1:A:332:LYS:C[3_655]	1.69	0.51
1:A:83:ASN:N	1:A:332:LYS:CA[3_655]	1.69	0.51
1:A:210:PHE:CE1	1:A:210:PHE:CE1[3_655]	1.69	0.51
1:A:220:ARG:CB	1:A:437:GLU:CB[3_655]	1.69	0.51
1:A:221:ILE:O	1:A:441:GLU:CB[3_655]	1.69	0.51
1:A:230:LYS:NZ	1:A:460:ASP:C[3_655]	1.69	0.51
1:B:81:LYS:CE	1:B:100:ARG:NH1[3_555]	1.69	0.51
1:B:478:THR:C	1:B:479:THR:N[3_555]	1.69	0.51
1:A:45:THR:O	1:A:472:VAL:C[3_655]	1.70	0.50
1:A:52:LYS:CB	1:A:202:THR:CA[3_655]	1.70	0.50
1:A:54:VAL:CA	1:A:208:ARG:NH1[3_655]	1.70	0.50
1:A:66:ASN:N	1:A:219:GLU:OE1[3_655]	1.70	0.50
1:A:82:VAL:O	1:A:332:LYS:CG[3_655]	1.70	0.50
1:A:208:ARG:O	1:A:211:VAL:N[3_655]	1.70	0.50
1:A:220:ARG:NH1	1:A:435:TYR:CD2[3_655]	1.70	0.50
1:A:226:GLY:O	4:A:2214:HOH:O[3_655]	1.70	0.50
1:A:15:SER:CA	1:A:21:LYS:CD[3_655]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:MET:CA	1:A:444:GLU:CD[3_655]	1.71	0.49
1:A:21:LYS:CB	1:A:443:GLY:CA[3_655]	1.71	0.49
1:A:25:ASP:N	1:A:261:ILE:CG2[3_655]	1.71	0.49
1:A:26:SER:O	1:A:260:VAL:CA[3_655]	1.71	0.49
1:A:38:ARG:O	1:A:467:PRO:CG[3_655]	1.71	0.49
1:A:43:THR:N	1:A:73:LYS:CG[3_655]	1.71	0.49
1:A:55:ASP:CB	1:A:79:THR:OG1[3_655]	1.71	0.49
1:A:62:GLY:CA	1:A:212:GLY:O[3_655]	1.71	0.49
1:A:68:ILE:CG2	1:A:216:GLN:CA[3_655]	1.71	0.49
1:A:255:TYR:CE2	1:A:461:GLU:CD[3_655]	1.71	0.49
1:A:258:LYS:N	1:A:456:LYS:CG[3_655]	1.71	0.49
1:A:5:CYS:CA	1:A:452:HIS:C[3_655]	1.72	0.48
1:A:24:HIS:CA	1:A:446:ALA:C[3_655]	1.72	0.48
1:A:30:VAL:CG2	1:A:447:ALA:C[3_655]	1.72	0.48
1:A:40:GLY:O	1:A:70:ARG:O[3_655]	1.72	0.48
1:A:42:ARG:CG	4:A:2010:HOH:O[3_655]	1.72	0.48
1:A:75:LEU:CB	1:A:436:MET:C[3_655]	1.72	0.48
1:A:76:GLY:O	2:A:600:FAD:N3[3_655]	1.72	0.48
1:A:80:TYR:CE1	1:A:80:TYR:CZ[3_655]	1.72	0.48
1:A:208:ARG:O	1:A:210:PHE:O[3_655]	1.72	0.48
1:A:227:ASP:OD2	4:A:2212:HOH:O[3_655]	1.72	0.48
1:B:478:THR:CA	1:B:478:THR:O[3_555]	1.72	0.48
1:A:7:VAL:N	1:A:451:LEU:CB[3_655]	1.73	0.47
1:A:28:LEU:C	1:A:450:ILE:CG1[3_655]	1.73	0.47
1:A:38:ARG:C	1:A:467:PRO:N[3_655]	1.73	0.47
1:A:39:VAL:CG2	1:A:466:GLU:OE1[3_655]	1.73	0.47
1:A:43:THR:N	1:A:73:LYS:CD[3_655]	1.73	0.47
1:A:48:ASN:CA	1:A:475:GLN:CG[3_655]	1.73	0.47
1:A:66:ASN:CA	1:A:219:GLU:CD[3_655]	1.73	0.47
1:A:67:ARG:N	1:A:219:GLU:CA[3_655]	1.73	0.47
1:A:224:LEU:C	4:A:2204:HOH:O[3_655]	1.73	0.47
1:A:230:LYS:N	1:A:464:GLN:NE2[3_655]	1.73	0.47
1:A:422:TYR:CA	4:A:2008:HOH:O[3_655]	1.73	0.47
1:B:478:THR:CA	1:B:478:THR:C[3_555]	1.73	0.47
1:A:44:TYR:CD2	1:A:470:VAL:N[3_655]	1.74	0.46
1:A:47:ARG:C	1:A:473:PRO:O[3_655]	1.74	0.46
1:A:53:TYR:CE1	1:A:208:ARG:CA[3_655]	1.74	0.46
1:A:53:TYR:CE1	1:A:207:GLU:C[3_655]	1.74	0.46
1:A:53:TYR:N	1:A:207:GLU:OE2[3_655]	1.74	0.46
1:A:56:LEU:CA	1:A:471:ASP:OD2[3_655]	1.74	0.46
1:A:61:VAL:N	1:A:211:VAL:C[3_655]	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:NZ	1:A:300:TYR:CE2[3_655]	1.74	0.46
1:A:258:LYS:N	1:A:456:LYS:CE[3_655]	1.74	0.46
1:B:478:THR:C	1:B:478:THR:CB[3_555]	1.74	0.46
1:A:14:ILE:CG2	1:A:71:LEU:CD1[3_655]	1.75	0.45
1:A:15:SER:O	1:A:21:LYS:CG[3_655]	1.75	0.45
1:A:17:MET:CB	1:A:444:GLU:CD[3_655]	1.75	0.45
1:A:45:THR:C	1:A:472:VAL:CB[3_655]	1.75	0.45
1:A:53:TYR:OH	1:A:208:ARG:N[3_655]	1.75	0.45
1:A:77:LEU:CA	2:A:600:FAD:N3[3_655]	1.75	0.45
1:A:221:ILE:CB	1:A:440:VAL:CG1[3_655]	1.75	0.45
1:A:227:ASP:CA	1:A:463:TRP:CA[3_655]	1.75	0.45
1:A:228:ARG:N	1:A:462:ILE:C[3_655]	1.75	0.45
1:A:231:LEU:CD1	1:A:465:SER:OG[3_655]	1.75	0.45
1:A:259:TYR:C	4:A:2006:HOH:O[3_655]	1.75	0.45
1:A:5:CYS:O	1:A:451:LEU:O[3_655]	1.76	0.44
1:A:14:ILE:CD1	1:A:71:LEU:O[3_655]	1.76	0.44
1:A:18:ALA:CA	1:A:18:ALA:C[3_655]	1.76	0.44
1:A:24:HIS:NE2	1:A:445:ARG:CZ[3_655]	1.76	0.44
1:A:32:VAL:O	1:A:464:GLN:OE1[3_655]	1.76	0.44
1:A:73:LYS:C	2:A:600:FAD:O2'[3_655]	1.76	0.44
1:A:75:LEU:C	1:A:435:TYR:O[3_655]	1.76	0.44
1:A:80:TYR:CD2	1:A:209:LYS:CD[3_655]	1.76	0.44
1:A:81:LYS:O	1:A:331:THR:O[3_655]	1.76	0.44
1:A:83:ASN:OD1	1:A:335:GLY:O[3_655]	1.76	0.44
1:A:329:ASP:O	1:A:333:PRO:CB[3_655]	1.76	0.44
1:A:14:ILE:CA	1:A:71:LEU:CD1[3_655]	1.77	0.43
1:A:14:ILE:CB	1:A:71:LEU:C[3_655]	1.77	0.43
1:A:14:ILE:CB	1:A:71:LEU:O[3_655]	1.77	0.43
1:A:52:LYS:CD	1:A:201:THR:O[3_655]	1.77	0.43
1:A:60:TYR:CG	1:A:211:VAL:CG1[3_655]	1.77	0.43
1:A:65:GLN:NE2	1:A:220:ARG:NH2[3_655]	1.77	0.43
1:A:81:LYS:CA	4:A:2158:HOH:O[3_655]	1.77	0.43
1:A:85:VAL:N	1:A:336:ASN:N[3_655]	1.77	0.43
1:A:220:ARG:CG	1:A:437:GLU:CG[3_655]	1.77	0.43
1:A:330:ASP:CB	4:A:2046:HOH:O[3_655]	1.77	0.43
1:A:28:LEU:CD2	1:A:259:TYR:CG[3_655]	1.78	0.42
1:A:30:VAL:C	1:A:448:ARG:C[3_655]	1.78	0.42
1:A:30:VAL:CB	1:A:447:ALA:O[3_655]	1.78	0.42
1:A:38:ARG:CD	1:A:468:GLU:O[3_655]	1.78	0.42
1:A:45:THR:CB	1:A:472:VAL:CG2[3_655]	1.78	0.42
1:A:46:LEU:C	1:A:472:VAL:C[3_655]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:CB	1:A:215:GLY:N[3_655]	1.78	0.42
1:A:74:GLU:OE1	2:A:600:FAD:P[3_655]	1.78	0.42
1:A:80:TYR:CG	1:A:209:LYS:CD[3_655]	1.78	0.42
1:A:224:LEU:CB	1:A:442:ALA:CA[3_655]	1.78	0.42
1:A:21:LYS:CG	1:A:443:GLY:CA[3_655]	1.79	0.41
1:A:26:SER:O	1:A:260:VAL:N[3_655]	1.79	0.41
1:A:28:LEU:O	1:A:450:ILE:N[3_655]	1.79	0.41
1:A:30:VAL:O	1:A:448:ARG:C[3_655]	1.79	0.41
1:A:60:TYR:CB	1:A:211:VAL:CB[3_655]	1.79	0.41
1:A:65:GLN:O	1:A:215:GLY:C[3_655]	1.79	0.41
1:A:68:ILE:C	4:A:2018:HOH:O[3_655]	1.79	0.41
1:A:73:LYS:O	2:A:600:FAD:C3'[3_655]	1.79	0.41
1:A:220:ARG:N	1:A:437:GLU:OE1[3_655]	1.79	0.41
1:A:223:ASP:N	1:A:441:GLU:OE1[3_655]	1.79	0.41
1:A:229:VAL:CB	1:A:464:GLN:CB[3_655]	1.79	0.41
1:A:259:TYR:O	4:A:2006:HOH:O[3_655]	1.79	0.41
1:A:14:ILE:CG1	1:A:71:LEU:CB[3_655]	1.80	0.40
1:A:44:TYR:CE2	1:A:470:VAL:N[3_655]	1.80	0.40
1:A:45:THR:CG2	1:A:472:VAL:CG2[3_655]	1.80	0.40
1:A:54:VAL:C	1:A:208:ARG:CZ[3_655]	1.80	0.40
1:A:54:VAL:C	1:A:208:ARG:NH1[3_655]	1.80	0.40
1:A:68:ILE:CB	1:A:216:GLN:C[3_655]	1.80	0.40
1:A:72:ALA:CB	1:A:436:MET:SD[3_655]	1.80	0.40
1:A:74:GLU:O	2:A:600:FAD:C4'[3_655]	1.80	0.40
1:A:214:SER:OG	4:A:2043:HOH:O[3_655]	1.80	0.40
1:A:217:VAL:O	1:A:440:VAL:CG2[3_655]	1.80	0.40
1:A:229:VAL:N	1:A:464:GLN:N[3_655]	1.80	0.40
1:A:3:ASN:CA	1:A:458:PRO:CB[3_655]	1.81	0.39
1:A:7:VAL:CG1	1:A:451:LEU:CD2[3_655]	1.81	0.39
1:A:13:GLY:CA	1:A:70:ARG:CD[3_655]	1.81	0.39
1:A:14:ILE:CG1	1:A:71:LEU:O[3_655]	1.81	0.39
1:A:21:LYS:N	1:A:443:GLY:O[3_655]	1.81	0.39
1:A:23:LEU:CB	1:A:23:LEU:CG[3_655]	1.81	0.39
1:A:28:LEU:CD2	1:A:259:TYR:CD1[3_655]	1.81	0.39
1:A:29:ASN:O	1:A:451:LEU:CA[3_655]	1.81	0.39
1:A:47:ARG:NE	1:A:63:PRO:C[3_655]	1.81	0.39
1:A:60:TYR:N	1:A:78:GLU:N[3_655]	1.81	0.39
1:A:60:TYR:N	1:A:78:GLU:O[3_655]	1.81	0.39
1:A:74:GLU:OE1	2:A:600:FAD:O2P[3_655]	1.81	0.39
1:A:85:VAL:CA	1:A:336:ASN:CA[3_655]	1.81	0.39
1:A:227:ASP:CB	1:A:463:TRP:CB[3_655]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASP:O	1:A:463:TRP:N[3_655]	1.81	0.39
1:A:230:LYS:CE	1:A:460:ASP:C[3_655]	1.81	0.39
1:A:230:LYS:N	1:A:464:GLN:CD[3_655]	1.81	0.39
1:A:230:LYS:CE	1:A:461:GLU:N[3_655]	1.81	0.39
1:A:312:CYS:CB	1:A:334:GLU:O[3_655]	1.81	0.39
1:A:334:GLU:CB	4:A:2048:HOH:O[3_655]	1.81	0.39
1:A:501:ILE:O	4:A:2054:HOH:O[6_565]	1.81	0.39
1:A:7:VAL:C	1:A:451:LEU:CD2[3_655]	1.82	0.38
1:A:20:ALA:CB	1:A:22:LEU:CD1[3_655]	1.82	0.38
1:A:24:HIS:CB	1:A:447:ALA:N[3_655]	1.82	0.38
1:A:32:VAL:CG2	4:A:2209:HOH:O[3_655]	1.82	0.38
1:A:39:VAL:CG1	1:A:466:GLU:CD[3_655]	1.82	0.38
1:A:47:ARG:CB	1:A:473:PRO:O[3_655]	1.82	0.38
1:A:53:TYR:CE1	1:A:208:ARG:CB[3_655]	1.82	0.38
1:A:55:ASP:CG	1:A:79:THR:CG2[3_655]	1.82	0.38
1:A:59:SER:CA	1:A:78:GLU:N[3_655]	1.82	0.38
1:A:67:ARG:CD	1:A:222:MET:CA[3_655]	1.82	0.38
1:A:71:LEU:N	1:A:218:SER:OG[3_655]	1.82	0.38
1:A:73:LYS:O	2:A:600:FAD:O4'[3_655]	1.82	0.38
1:A:76:GLY:N	2:A:600:FAD:C2'[3_655]	1.82	0.38
1:A:81:LYS:CB	4:A:2158:HOH:O[3_655]	1.82	0.38
1:A:83:ASN:O	1:A:334:GLU:C[3_655]	1.82	0.38
1:A:225:LEU:CG	1:A:441:GLU:O[3_655]	1.82	0.38
1:A:227:ASP:C	1:A:463:TRP:O[3_655]	1.82	0.38
1:A:227:ASP:N	1:A:463:TRP:CG[3_655]	1.82	0.38
1:A:463:TRP:O	4:A:2122:HOH:O[3_655]	1.82	0.38
1:A:23:LEU:CA	1:A:261:ILE:CD1[3_655]	1.83	0.37
1:A:24:HIS:ND1	1:A:446:ALA:N[3_655]	1.83	0.37
1:A:26:SER:C	1:A:261:ILE:N[3_655]	1.83	0.37
1:A:27:GLY:CA	1:A:422:TYR:CD1[3_655]	1.83	0.37
1:A:29:ASN:CA	1:A:449:GLU:CA[3_655]	1.83	0.37
1:A:30:VAL:CG2	1:A:448:ARG:CA[3_655]	1.83	0.37
1:A:41:GLY:C	4:A:2044:HOH:O[3_655]	1.83	0.37
1:A:55:ASP:CG	1:A:79:THR:CB[3_655]	1.83	0.37
1:A:59:SER:CB	1:A:78:GLU:CB[3_655]	1.83	0.37
1:A:66:ASN:CG	1:A:219:GLU:OE2[3_655]	1.83	0.37
1:A:67:ARG:CA	1:A:218:SER:CA[3_655]	1.83	0.37
1:A:77:LEU:CA	2:A:600:FAD:C2[3_655]	1.83	0.37
1:A:77:LEU:N	2:A:600:FAD:O2[3_655]	1.83	0.37
1:A:85:VAL:CG1	4:A:2142:HOH:O[3_655]	1.83	0.37
1:A:220:ARG:N	1:A:437:GLU:OE2[3_655]	1.83	0.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:CB	1:A:445:ARG:CB[3_655]	1.83	0.37
1:A:333:PRO:N	4:A:2154:HOH:O[3_655]	1.83	0.37
1:A:14:ILE:CB	1:A:71:LEU:CA[3_655]	1.84	0.36
1:A:23:LEU:O	1:A:261:ILE:CG1[3_655]	1.84	0.36
1:A:29:ASN:C	1:A:448:ARG:O[3_655]	1.84	0.36
1:A:38:ARG:N	1:A:467:PRO:N[3_655]	1.84	0.36
1:A:52:LYS:CD	1:A:202:THR:C[3_655]	1.84	0.36
1:A:59:SER:C	1:A:78:GLU:N[3_655]	1.84	0.36
1:A:67:ARG:NH2	1:A:222:MET:SD[3_655]	1.84	0.36
1:A:84:GLU:C	1:A:336:ASN:CA[3_655]	1.84	0.36
1:A:220:ARG:CD	1:A:437:GLU:CB[3_655]	1.84	0.36
1:A:221:ILE:CB	1:A:440:VAL:O[3_655]	1.84	0.36
1:A:224:LEU:CB	1:A:442:ALA:CB[3_655]	1.84	0.36
1:A:4:LYS:C	1:A:457:ILE:O[3_655]	1.85	0.35
1:A:28:LEU:C	1:A:450:ILE:CB[3_655]	1.85	0.35
1:A:43:THR:CG2	1:A:73:LYS:CB[3_655]	1.85	0.35
1:A:56:LEU:N	1:A:471:ASP:CB[3_655]	1.85	0.35
1:A:65:GLN:O	1:A:216:GLN:N[3_655]	1.85	0.35
1:A:74:GLU:CG	2:A:600:FAD:O1P[3_655]	1.85	0.35
1:A:210:PHE:CG	1:A:210:PHE:CE1[3_655]	1.85	0.35
1:A:219:GLU:CA	1:A:437:GLU:OE1[3_655]	1.85	0.35
1:A:221:ILE:O	1:A:441:GLU:N[3_655]	1.85	0.35
1:A:229:VAL:CA	1:A:464:GLN:CA[3_655]	1.85	0.35
1:A:257:ALA:CA	1:A:456:LYS:CG[3_655]	1.85	0.35
1:A:59:SER:CA	1:A:79:THR:N[3_655]	1.86	0.34
1:A:69:LEU:N	1:A:215:GLY:C[3_655]	1.86	0.34
1:A:208:ARG:CB	4:A:2118:HOH:O[3_655]	1.86	0.34
1:A:230:LYS:N	1:A:464:GLN:CB[3_655]	1.86	0.34
1:A:500:THR:OG1	4:A:2168:HOH:O[6_565]	1.86	0.34
1:A:7:VAL:C	1:A:451:LEU:CB[3_655]	1.87	0.33
1:A:17:MET:CG	1:A:70:ARG:NH1[3_655]	1.87	0.33
1:A:25:ASP:C	1:A:261:ILE:C[3_655]	1.87	0.33
1:A:31:VAL:N	1:A:448:ARG:CB[3_655]	1.87	0.33
1:A:53:TYR:CZ	1:A:207:GLU:CA[3_655]	1.87	0.33
1:A:65:GLN:O	1:A:215:GLY:O[3_655]	1.87	0.33
1:A:76:GLY:O	2:A:600:FAD:C4X[3_655]	1.87	0.33
1:A:78:GLU:CD	4:A:2139:HOH:O[3_655]	1.87	0.33
1:A:84:GLU:CB	1:A:336:ASN:ND2[3_655]	1.87	0.33
1:A:221:ILE:CG1	1:A:440:VAL:CG2[3_655]	1.87	0.33
1:A:228:ARG:NH1	1:A:445:ARG:CD[3_655]	1.87	0.33
1:A:229:VAL:CG2	1:A:448:ARG:NH2[3_655]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:O	1:A:464:GLN:CB[3_655]	1.87	0.33
1:A:312:CYS:O	1:A:334:GLU:O[3_655]	1.87	0.33
1:A:386:LYS:NZ	1:A:470:VAL:CG2[3_655]	1.87	0.33
1:A:3:ASN:C	1:A:458:PRO:CA[3_655]	1.88	0.32
1:A:3:ASN:N	1:A:458:PRO:CA[3_655]	1.88	0.32
1:A:29:ASN:C	1:A:449:GLU:C[3_655]	1.88	0.32
1:A:39:VAL:C	4:A:2215:HOH:O[3_655]	1.88	0.32
1:A:47:ARG:CZ	1:A:63:PRO:CA[3_655]	1.88	0.32
1:A:52:LYS:CG	1:A:202:THR:C[3_655]	1.88	0.32
1:A:68:ILE:CD1	1:A:217:VAL:CG1[3_655]	1.88	0.32
1:A:83:ASN:CB	1:A:335:GLY:CA[3_655]	1.88	0.32
1:A:256:GLU:C	1:A:455:GLY:C[3_655]	1.88	0.32
1:A:21:LYS:CA	1:A:443:GLY:CA[3_655]	1.89	0.31
1:A:22:LEU:O	1:A:261:ILE:CD1[3_655]	1.89	0.31
1:A:23:LEU:O	1:A:261:ILE:CD1[3_655]	1.89	0.31
1:A:25:ASP:OD2	1:A:263:ALA:CB[3_655]	1.89	0.31
1:A:38:ARG:CB	1:A:467:PRO:CB[3_655]	1.89	0.31
1:A:59:SER:CA	1:A:78:GLU:O[3_655]	1.89	0.31
1:A:59:SER:OG	1:A:79:THR:C[3_655]	1.89	0.31
1:A:59:SER:C	1:A:78:GLU:CA[3_655]	1.89	0.31
1:A:75:LEU:CG	1:A:436:MET:O[3_655]	1.89	0.31
1:A:83:ASN:ND2	1:A:335:GLY:C[3_655]	1.89	0.31
1:A:221:ILE:CG1	1:A:440:VAL:CG1[3_655]	1.89	0.31
1:A:221:ILE:C	1:A:441:GLU:CB[3_655]	1.89	0.31
1:A:228:ARG:CG	1:A:462:ILE:C[3_655]	1.89	0.31
1:A:258:LYS:CG	1:A:454:MET:CB[3_655]	1.89	0.31
1:A:18:ALA:O	1:A:18:ALA:O[3_655]	1.90	0.30
1:A:28:LEU:CD1	1:A:450:ILE:CG2[3_655]	1.90	0.30
1:A:30:VAL:O	1:A:448:ARG:CA[3_655]	1.90	0.30
1:A:80:TYR:C	1:A:209:LYS:CE[3_655]	1.90	0.30
1:A:81:LYS:CG	4:A:2156:HOH:O[3_655]	1.90	0.30
1:A:208:ARG:O	1:A:210:PHE:C[3_655]	1.90	0.30
1:A:208:ARG:N	1:A:212:GLY:N[3_655]	1.90	0.30
1:A:220:ARG:CB	1:A:437:GLU:O[3_655]	1.90	0.30
1:A:228:ARG:N	1:A:463:TRP:C[3_655]	1.90	0.30
1:A:257:ALA:C	1:A:456:LYS:CG[3_655]	1.90	0.30
1:B:102:PRO:N	1:B:475:GLN:NE2[3_555]	1.90	0.30
1:A:17:MET:SD	1:A:70:ARG:NH2[3_655]	1.91	0.29
1:A:29:ASN:O	1:A:450:ILE:C[3_655]	1.91	0.29
1:A:42:ARG:C	1:A:73:LYS:CB[3_655]	1.91	0.29
1:A:44:TYR:CE2	1:A:470:VAL:O[3_655]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:N	1:A:475:GLN:NE2[3_655]	1.91	0.29
1:A:74:GLU:CD	2:A:600:FAD:O3P[3_655]	1.91	0.29
1:A:81:LYS:N	4:A:2158:HOH:O[3_655]	1.91	0.29
1:A:224:LEU:N	1:A:441:GLU:CB[3_655]	1.91	0.29
1:A:332:LYS:CG	4:A:2047:HOH:O[3_655]	1.91	0.29
1:A:4:LYS:O	1:A:452:HIS:CE1[3_655]	1.92	0.28
1:A:6:ASP:CA	1:A:451:LEU:O[3_655]	1.92	0.28
1:A:6:ASP:OD1	1:A:454:MET:N[3_655]	1.92	0.28
1:A:17:MET:CG	1:A:70:ARG:CZ[3_655]	1.92	0.28
1:A:19:ALA:C	1:A:19:ALA:C[3_655]	1.92	0.28
1:A:24:HIS:ND1	1:A:446:ALA:CB[3_655]	1.92	0.28
1:A:27:GLY:CA	1:A:422:TYR:CB[3_655]	1.92	0.28
1:A:28:LEU:O	1:A:446:ALA:O[3_655]	1.92	0.28
1:A:38:ARG:N	1:A:467:PRO:CD[3_655]	1.92	0.28
1:A:44:TYR:CE2	1:A:471:ASP:N[3_655]	1.92	0.28
1:A:46:LEU:CA	1:A:472:VAL:CA[3_655]	1.92	0.28
1:A:85:VAL:CA	1:A:336:ASN:CB[3_655]	1.92	0.28
1:B:477:ILE:O	1:B:480:THR:N[3_555]	1.92	0.28
1:A:16:GLY:CA	4:A:2005:HOH:O[3_655]	1.93	0.27
1:A:30:VAL:N	1:A:448:ARG:CA[3_655]	1.93	0.27
1:A:40:GLY:O	4:A:2044:HOH:O[3_655]	1.93	0.27
1:A:47:ARG:N	1:A:473:PRO:N[3_655]	1.93	0.27
1:A:52:LYS:CE	1:A:202:THR:CA[3_655]	1.93	0.27
1:A:69:LEU:N	1:A:215:GLY:O[3_655]	1.93	0.27
1:A:84:GLU:C	1:A:336:ASN:ND2[3_655]	1.93	0.27
1:A:219:GLU:CB	1:A:437:GLU:OE2[3_655]	1.93	0.27
1:A:225:LEU:CD1	1:A:444:GLU:CB[3_655]	1.93	0.27
1:A:229:VAL:N	1:A:464:GLN:CB[3_655]	1.93	0.27
1:A:231:LEU:CD1	1:A:465:SER:C[3_655]	1.93	0.27
1:B:102:PRO:CD	1:B:475:GLN:NE2[3_555]	1.93	0.27
1:A:5:CYS:CA	1:A:452:HIS:O[3_655]	1.94	0.26
1:A:17:MET:N	4:A:2001:HOH:O[3_655]	1.94	0.26
1:A:29:ASN:C	1:A:451:LEU:N[3_655]	1.94	0.26
1:A:29:ASN:C	1:A:450:ILE:N[3_655]	1.94	0.26
1:A:38:ARG:CZ	4:A:2217:HOH:O[3_655]	1.94	0.26
1:A:53:TYR:CA	1:A:207:GLU:OE1[3_655]	1.94	0.26
1:A:60:TYR:CG	1:A:211:VAL:CG2[3_655]	1.94	0.26
1:A:69:LEU:N	4:A:2018:HOH:O[3_655]	1.94	0.26
1:A:72:ALA:C	1:A:436:MET:CG[3_655]	1.94	0.26
1:A:209:LYS:CA	1:A:209:LYS:C[3_655]	1.94	0.26
1:A:221:ILE:N	1:A:441:GLU:N[3_655]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:CB	4:A:2207:HOH:O[3_655]	1.94	0.26
1:A:255:TYR:CD2	1:A:461:GLU:OE1[3_655]	1.94	0.26
1:A:256:GLU:C	1:A:456:LYS:CA[3_655]	1.94	0.26
1:A:17:MET:N	1:A:444:GLU:OE2[3_655]	1.95	0.25
1:A:38:ARG:CA	1:A:467:PRO:C[3_655]	1.95	0.25
1:A:38:ARG:CA	1:A:467:PRO:CG[3_655]	1.95	0.25
1:A:40:GLY:C	1:A:70:ARG:CB[3_655]	1.95	0.25
1:A:41:GLY:N	1:A:70:ARG:CG[3_655]	1.95	0.25
1:A:42:ARG:O	1:A:73:LYS:CE[3_655]	1.95	0.25
1:A:52:LYS:CG	1:A:203:ASN:N[3_655]	1.95	0.25
1:A:53:TYR:CE2	1:A:207:GLU:O[3_655]	1.95	0.25
1:A:65:GLN:NE2	1:A:216:GLN:OE1[3_655]	1.95	0.25
1:A:68:ILE:N	1:A:218:SER:CA[3_655]	1.95	0.25
1:A:81:LYS:CB	1:A:332:LYS:NZ[3_655]	1.95	0.25
1:A:82:VAL:CB	4:A:2030:HOH:O[3_655]	1.95	0.25
1:A:220:ARG:CG	1:A:437:GLU:CA[3_655]	1.95	0.25
1:A:220:ARG:N	1:A:437:GLU:CG[3_655]	1.95	0.25
1:A:225:LEU:CD1	1:A:444:GLU:CA[3_655]	1.95	0.25
1:A:332:LYS:CE	4:A:2047:HOH:O[3_655]	1.95	0.25
1:A:333:PRO:CB	4:A:2154:HOH:O[3_655]	1.95	0.25
1:B:477:ILE:O	1:B:480:THR:CG2[3_555]	1.95	0.25
1:A:5:CYS:C	1:A:451:LEU:C[3_655]	1.96	0.24
1:A:15:SER:OG	1:A:21:LYS:CD[3_655]	1.96	0.24
1:A:15:SER:C	1:A:21:LYS:NZ[3_655]	1.96	0.24
1:A:30:VAL:CA	1:A:448:ARG:O[3_655]	1.96	0.24
1:A:31:VAL:CG1	1:A:461:GLU:CB[3_655]	1.96	0.24
1:A:39:VAL:N	1:A:466:GLU:OE2[3_655]	1.96	0.24
1:A:39:VAL:N	1:A:466:GLU:CD[3_655]	1.96	0.24
1:A:60:TYR:C	4:A:2045:HOH:O[3_655]	1.96	0.24
1:A:74:GLU:C	2:A:600:FAD:O5'[3_655]	1.96	0.24
1:A:76:GLY:C	2:A:600:FAD:O2[3_655]	1.96	0.24
1:A:84:GLU:C	1:A:336:ASN:OD1[3_655]	1.96	0.24
1:A:220:ARG:CA	1:A:437:GLU:CG[3_655]	1.96	0.24
1:A:221:ILE:O	1:A:441:GLU:O[3_655]	1.96	0.24
1:A:231:LEU:CG	1:A:465:SER:C[3_655]	1.96	0.24
1:A:304:PRO:CG	4:A:2052:HOH:O[3_655]	1.96	0.24
1:A:330:ASP:OD1	4:A:2046:HOH:O[3_655]	1.96	0.24
1:A:20:ALA:O	1:A:443:GLY:O[3_655]	1.97	0.23
1:A:24:HIS:CE1	1:A:445:ARG:NE[3_655]	1.97	0.23
1:A:45:THR:OG1	1:A:69:LEU:CD2[3_655]	1.97	0.23
1:A:46:LEU:CB	1:A:473:PRO:CG[3_655]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:VAL:C	1:A:212:GLY:O[3_655]	1.97	0.23
1:A:65:GLN:CB	1:A:216:GLN:CG[3_655]	1.97	0.23
1:A:67:ARG:C	1:A:219:GLU:N[3_655]	1.97	0.23
1:A:69:LEU:CA	4:A:2018:HOH:O[3_655]	1.97	0.23
1:A:74:GLU:N	2:A:600:FAD:C4'[3_655]	1.97	0.23
1:A:82:VAL:O	1:A:332:LYS:CA[3_655]	1.97	0.23
1:A:84:GLU:CA	1:A:336:ASN:ND2[3_655]	1.97	0.23
1:A:221:ILE:CA	1:A:441:GLU:CA[3_655]	1.97	0.23
1:A:221:ILE:CB	1:A:441:GLU:N[3_655]	1.97	0.23
1:A:225:LEU:N	1:A:441:GLU:O[3_655]	1.97	0.23
1:A:225:LEU:O	1:A:445:ARG:CG[3_655]	1.97	0.23
1:A:231:LEU:CG	1:A:465:SER:OG[3_655]	1.97	0.23
1:A:12:GLY:O	1:A:70:ARG:CZ[3_655]	1.98	0.22
1:A:14:ILE:CA	1:A:71:LEU:CA[3_655]	1.98	0.22
1:A:15:SER:OG	1:A:21:LYS:NZ[3_655]	1.98	0.22
1:A:17:MET:O	1:A:444:GLU:CG[3_655]	1.98	0.22
1:A:18:ALA:CA	1:A:18:ALA:CB[3_655]	1.98	0.22
1:A:24:HIS:CB	1:A:446:ALA:N[3_655]	1.98	0.22
1:A:28:LEU:CD2	1:A:259:TYR:CB[3_655]	1.98	0.22
1:A:30:VAL:C	1:A:448:ARG:O[3_655]	1.98	0.22
1:A:44:TYR:CE1	1:A:469:SER:CA[3_655]	1.98	0.22
1:A:68:ILE:CB	1:A:217:VAL:CB[3_655]	1.98	0.22
1:A:83:ASN:CA	1:A:332:LYS:C[3_655]	1.98	0.22
1:A:208:ARG:O	1:A:212:GLY:N[3_655]	1.98	0.22
1:A:209:LYS:CA	1:A:209:LYS:O[3_655]	1.98	0.22
1:A:229:VAL:CB	1:A:464:GLN:O[3_655]	1.98	0.22
1:A:15:SER:C	4:A:2003:HOH:O[3_655]	1.99	0.21
1:A:23:LEU:CB	1:A:23:LEU:CD2[3_655]	1.99	0.21
1:A:30:VAL:CG1	1:A:447:ALA:CA[3_655]	1.99	0.21
1:A:38:ARG:CG	1:A:467:PRO:CB[3_655]	1.99	0.21
1:A:74:GLU:CG	2:A:600:FAD:O2P[3_655]	1.99	0.21
1:A:202:THR:OG1	1:A:337:TYR:CZ[3_655]	1.99	0.21
1:A:223:ASP:N	1:A:441:GLU:CB[3_655]	1.99	0.21
1:A:223:ASP:OD2	1:A:431:HIS:C[3_655]	1.99	0.21
1:A:229:VAL:O	1:A:464:GLN:C[3_655]	1.99	0.21
1:A:329:ASP:CA	1:A:333:PRO:O[3_655]	1.99	0.21
1:A:337:TYR:N	4:A:2049:HOH:O[3_655]	1.99	0.21
1:A:26:SER:N	1:A:261:ILE:CG2[3_655]	2.00	0.20
1:A:32:VAL:CG2	1:A:448:ARG:NE[3_655]	2.00	0.20
1:A:37:ASP:C	1:A:467:PRO:CA[3_655]	2.00	0.20
1:A:38:ARG:CB	1:A:468:GLU:N[3_655]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:OG1	1:A:69:LEU:CD1[3_655]	2.00	0.20
1:A:61:VAL:CA	1:A:211:VAL:O[3_655]	2.00	0.20
1:A:65:GLN:C	1:A:219:GLU:CG[3_655]	2.00	0.20
1:A:66:ASN:CA	1:A:219:GLU:OE2[3_655]	2.00	0.20
1:A:74:GLU:O	2:A:600:FAD:O3'[3_655]	2.00	0.20
1:A:76:GLY:O	2:A:600:FAD:C4[3_655]	2.00	0.20
1:A:80:TYR:CD1	1:A:80:TYR:CZ[3_655]	2.00	0.20
1:A:82:VAL:CG1	1:A:334:GLU:OE1[3_655]	2.00	0.20
1:A:219:GLU:CA	1:A:437:GLU:OE2[3_655]	2.00	0.20
1:A:222:MET:C	1:A:441:GLU:CG[3_655]	2.00	0.20
1:A:227:ASP:O	1:A:463:TRP:C[3_655]	2.00	0.20
1:A:229:VAL:CA	1:A:464:GLN:CG[3_655]	2.00	0.20
1:A:260:VAL:CB	4:A:2006:HOH:O[3_655]	2.00	0.20
1:B:476:PRO:CB	1:B:483:GLU:OE2[3_555]	2.00	0.20
1:A:23:LEU:O	1:A:450:ILE:CD1[3_655]	2.01	0.19
1:A:27:GLY:C	1:A:422:TYR:CG[3_655]	2.01	0.19
1:A:43:THR:C	4:A:2216:HOH:O[3_655]	2.01	0.19
1:A:46:LEU:CD1	1:A:473:PRO:CB[3_655]	2.01	0.19
1:A:65:GLN:O	1:A:219:GLU:OE1[3_655]	2.01	0.19
1:A:67:ARG:CA	1:A:218:SER:O[3_655]	2.01	0.19
1:A:75:LEU:CB	1:A:436:MET:O[3_655]	2.01	0.19
1:A:79:THR:O	4:A:2138:HOH:O[3_655]	2.01	0.19
1:A:210:PHE:CD1	1:A:210:PHE:CZ[3_655]	2.01	0.19
1:A:228:ARG:NH1	1:A:445:ARG:CG[3_655]	2.01	0.19
1:A:255:TYR:CE2	1:A:461:GLU:CG[3_655]	2.01	0.19
1:A:258:LYS:N	1:A:456:LYS:CD[3_655]	2.01	0.19
1:A:6:ASP:CB	1:A:450:ILE:C[3_655]	2.02	0.18
1:A:7:VAL:CA	1:A:451:LEU:CB[3_655]	2.02	0.18
1:A:12:GLY:C	1:A:70:ARG:NE[3_655]	2.02	0.18
1:A:20:ALA:C	1:A:443:GLY:O[3_655]	2.02	0.18
1:A:26:SER:CA	1:A:261:ILE:CB[3_655]	2.02	0.18
1:A:29:ASN:O	1:A:452:HIS:N[3_655]	2.02	0.18
1:A:40:GLY:C	1:A:70:ARG:CA[3_655]	2.02	0.18
1:A:52:LYS:NZ	1:A:201:THR:CB[3_655]	2.02	0.18
1:A:53:TYR:CE1	1:A:207:GLU:O[3_655]	2.02	0.18
1:A:55:ASP:OD2	1:A:79:THR:CA[3_655]	2.02	0.18
1:A:66:ASN:CB	1:A:219:GLU:CG[3_655]	2.02	0.18
1:A:74:GLU:CB	2:A:600:FAD:P[3_655]	2.02	0.18
1:A:80:TYR:N	1:A:209:LYS:CD[3_655]	2.02	0.18
1:A:220:ARG:O	1:A:437:GLU:O[3_655]	2.02	0.18
1:A:225:LEU:CD2	1:A:444:GLU:C[3_655]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:O	1:A:456:LYS:CE[3_655]	2.02	0.18
1:A:329:ASP:CG	1:A:333:PRO:O[3_655]	2.02	0.18
2:A:600:FAD:O2A	4:A:2044:HOH:O[3_655]	2.02	0.18
1:A:14:ILE:CB	1:A:71:LEU:CG[3_655]	2.03	0.17
1:A:17:MET:SD	1:A:444:GLU:CD[3_655]	2.03	0.17
1:A:17:MET:C	4:A:2001:HOH:O[3_655]	2.03	0.17
1:A:18:ALA:CA	1:A:18:ALA:O[3_655]	2.03	0.17
1:A:26:SER:N	1:A:261:ILE:N[3_655]	2.03	0.17
1:A:29:ASN:N	1:A:449:GLU:O[3_655]	2.03	0.17
1:A:30:VAL:CG1	1:A:448:ARG:N[3_655]	2.03	0.17
1:A:40:GLY:O	1:A:70:ARG:CA[3_655]	2.03	0.17
1:A:43:THR:C	4:A:2009:HOH:O[3_655]	2.03	0.17
1:A:45:THR:CA	1:A:472:VAL:N[3_655]	2.03	0.17
1:A:45:THR:CA	1:A:472:VAL:CA[3_655]	2.03	0.17
1:A:47:ARG:CZ	1:A:63:PRO:C[3_655]	2.03	0.17
1:A:53:TYR:CD1	1:A:208:ARG:CD[3_655]	2.03	0.17
1:A:54:VAL:CA	1:A:208:ARG:NE[3_655]	2.03	0.17
1:A:62:GLY:N	1:A:212:GLY:C[3_655]	2.03	0.17
1:A:66:ASN:ND2	4:A:2119:HOH:O[3_655]	2.03	0.17
1:A:74:GLU:CB	4:A:2230:HOH:O[3_655]	2.03	0.17
1:A:82:VAL:CA	1:A:333:PRO:N[3_655]	2.03	0.17
1:A:221:ILE:CG1	1:A:440:VAL:N[3_655]	2.03	0.17
1:A:221:ILE:CD1	1:A:440:VAL:CB[3_655]	2.03	0.17
1:A:222:MET:O	1:A:441:GLU:CG[3_655]	2.03	0.17
1:A:229:VAL:CG1	1:A:464:GLN:CG[3_655]	2.03	0.17
1:A:258:LYS:C	1:A:456:LYS:CD[3_655]	2.03	0.17
1:A:321:GLU:CG	1:A:499:THR:C[6_564]	2.03	0.17
1:A:475:GLN:CD	4:A:2026:HOH:O[3_655]	2.03	0.17
1:A:3:ASN:O	1:A:458:PRO:CA[3_655]	2.04	0.16
1:A:6:ASP:OD1	1:A:453:ALA:C[3_655]	2.04	0.16
1:A:28:LEU:CD2	1:A:450:ILE:CG2[3_655]	2.04	0.16
1:A:29:ASN:C	1:A:448:ARG:C[3_655]	2.04	0.16
1:A:38:ARG:C	1:A:467:PRO:CG[3_655]	2.04	0.16
1:A:38:ARG:NH2	4:A:2217:HOH:O[3_655]	2.04	0.16
1:A:43:THR:CB	1:A:73:LYS:CB[3_655]	2.04	0.16
1:A:46:LEU:C	1:A:473:PRO:CD[3_655]	2.04	0.16
1:A:65:GLN:CG	4:A:2120:HOH:O[3_655]	2.04	0.16
1:A:66:ASN:OD1	4:A:2119:HOH:O[3_655]	2.04	0.16
1:A:68:ILE:CG1	1:A:217:VAL:N[3_655]	2.04	0.16
1:A:73:LYS:CE	1:A:388:TRP:CZ2[3_655]	2.04	0.16
1:A:73:LYS:CE	1:A:388:TRP:CH2[3_655]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:C	1:A:335:GLY:N[3_655]	2.04	0.16
1:A:220:ARG:C	1:A:437:GLU:C[3_655]	2.04	0.16
1:A:501:ILE:CA	4:A:2014:HOH:O[6_565]	2.04	0.16
1:A:7:VAL:CG2	1:A:451:LEU:CD2[3_655]	2.05	0.15
1:A:28:LEU:CB	1:A:450:ILE:CD1[3_655]	2.05	0.15
1:A:47:ARG:O	1:A:473:PRO:O[3_655]	2.05	0.15
1:A:53:TYR:C	1:A:208:ARG:NE[3_655]	2.05	0.15
1:A:59:SER:OG	1:A:79:THR:O[3_655]	2.05	0.15
1:A:68:ILE:O	1:A:214:SER:O[3_655]	2.05	0.15
1:A:222:MET:N	1:A:441:GLU:CA[3_655]	2.05	0.15
1:A:226:GLY:N	4:A:2214:HOH:O[3_655]	2.05	0.15
1:A:307:ARG:NE	1:A:307:ARG:NH1[3_655]	2.05	0.15
1:A:501:ILE:N	4:A:2054:HOH:O[6_565]	2.05	0.15
1:A:6:ASP:N	1:A:452:HIS:N[3_655]	2.06	0.14
1:A:24:HIS:CA	1:A:446:ALA:CB[3_655]	2.06	0.14
1:A:44:TYR:CA	1:A:469:SER:OG[3_655]	2.06	0.14
1:A:47:ARG:N	1:A:473:PRO:CA[3_655]	2.06	0.14
1:A:47:ARG:NE	1:A:63:PRO:CB[3_655]	2.06	0.14
1:A:52:LYS:CG	1:A:201:THR:O[3_655]	2.06	0.14
1:A:53:TYR:CE2	1:A:207:GLU:N[3_655]	2.06	0.14
1:A:61:VAL:CG1	1:A:213:GLY:O[3_655]	2.06	0.14
1:A:61:VAL:C	1:A:216:GLN:NE2[3_655]	2.06	0.14
1:A:68:ILE:CA	1:A:217:VAL:CB[3_655]	2.06	0.14
1:A:76:GLY:CA	2:A:600:FAD:C2'[3_655]	2.06	0.14
1:A:80:TYR:CG	1:A:80:TYR:OH[3_655]	2.06	0.14
1:A:82:VAL:CG1	1:A:333:PRO:CD[3_655]	2.06	0.14
1:A:224:LEU:N	1:A:441:GLU:OE2[3_655]	2.06	0.14
1:A:255:TYR:CZ	1:A:461:GLU:CG[3_655]	2.06	0.14
1:A:255:TYR:OH	1:A:461:GLU:CG[3_655]	2.06	0.14
1:A:386:LYS:CD	1:A:470:VAL:CG2[3_655]	2.06	0.14
4:A:2116:HOH:O	4:A:2155:HOH:O[3_655]	2.06	0.14
1:A:19:ALA:CB	1:A:21:LYS:O[3_655]	2.07	0.13
1:A:30:VAL:CA	1:A:448:ARG:N[3_655]	2.07	0.13
1:A:39:VAL:O	4:A:2038:HOH:O[3_655]	2.07	0.13
1:A:70:ARG:N	4:A:2018:HOH:O[3_655]	2.07	0.13
1:A:74:GLU:C	2:A:600:FAD:O4'[3_655]	2.07	0.13
1:A:81:LYS:O	1:A:332:LYS:CA[3_655]	2.07	0.13
1:A:83:ASN:CA	1:A:335:GLY:N[3_655]	2.07	0.13
1:A:84:GLU:CA	1:A:336:ASN:CB[3_655]	2.07	0.13
1:A:85:VAL:CG2	4:A:2142:HOH:O[3_655]	2.07	0.13
1:A:334:GLU:CG	4:A:2048:HOH:O[3_655]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:N	1:A:451:LEU:CD2[3_655]	2.08	0.12
1:A:19:ALA:CA	1:A:19:ALA:O[3_655]	2.08	0.12
1:A:20:ALA:C	1:A:447:ALA:CB[3_655]	2.08	0.12
1:A:44:TYR:OH	1:A:469:SER:O[3_655]	2.08	0.12
1:A:44:TYR:CB	1:A:471:ASP:OD1[3_655]	2.08	0.12
1:A:52:LYS:C	1:A:207:GLU:CD[3_655]	2.08	0.12
1:A:53:TYR:CG	1:A:207:GLU:CD[3_655]	2.08	0.12
1:A:55:ASP:OD1	1:A:79:THR:CG2[3_655]	2.08	0.12
1:A:74:GLU:CB	2:A:600:FAD:C5'[3_655]	2.08	0.12
1:A:74:GLU:N	4:A:2230:HOH:O[3_655]	2.08	0.12
1:A:82:VAL:C	1:A:333:PRO:N[3_655]	2.08	0.12
1:A:221:ILE:CD1	1:A:440:VAL:CG1[3_655]	2.08	0.12
1:A:228:ARG:CD	1:A:462:ILE:CG2[3_655]	2.08	0.12
1:A:3:ASN:C	1:A:458:PRO:N[3_655]	2.09	0.11
1:A:14:ILE:CB	1:A:71:LEU:CD1[3_655]	2.09	0.11
1:A:15:SER:O	1:A:21:LYS:CD[3_655]	2.09	0.11
1:A:17:MET:CA	1:A:444:GLU:CG[3_655]	2.09	0.11
1:A:21:LYS:N	1:A:443:GLY:C[3_655]	2.09	0.11
1:A:32:VAL:CB	1:A:448:ARG:NE[3_655]	2.09	0.11
1:A:40:GLY:O	1:A:70:ARG:C[3_655]	2.09	0.11
1:A:41:GLY:CA	4:A:2044:HOH:O[3_655]	2.09	0.11
1:A:43:THR:OG1	1:A:70:ARG:N[3_655]	2.09	0.11
1:A:46:LEU:N	1:A:471:ASP:C[3_655]	2.09	0.11
1:A:52:LYS:NZ	1:A:84:GLU:OE1[3_655]	2.09	0.11
1:A:52:LYS:CB	1:A:202:THR:CG2[3_655]	2.09	0.11
1:A:60:TYR:CA	1:A:211:VAL:CB[3_655]	2.09	0.11
1:A:61:VAL:O	1:A:213:GLY:N[3_655]	2.09	0.11
1:A:65:GLN:OE1	1:A:216:GLN:CB[3_655]	2.09	0.11
1:A:68:ILE:C	1:A:214:SER:O[3_655]	2.09	0.11
1:A:68:ILE:CG2	1:A:216:GLN:O[3_655]	2.09	0.11
1:A:69:LEU:CA	1:A:214:SER:O[3_655]	2.09	0.11
1:A:80:TYR:CD2	1:A:209:LYS:CG[3_655]	2.09	0.11
1:A:81:LYS:O	1:A:331:THR:C[3_655]	2.09	0.11
1:A:220:ARG:CZ	1:A:435:TYR:CB[3_655]	2.09	0.11
1:A:227:ASP:O	1:A:463:TRP:CA[3_655]	2.09	0.11
1:A:228:ARG:NE	1:A:462:ILE:CG2[3_655]	2.09	0.11
1:A:228:ARG:CD	1:A:445:ARG:O[3_655]	2.09	0.11
1:A:255:TYR:CE2	1:A:461:GLU:OE1[3_655]	2.09	0.11
1:A:256:GLU:C	1:A:456:LYS:C[3_655]	2.09	0.11
1:A:257:ALA:N	1:A:455:GLY:O[3_655]	2.09	0.11
1:A:3:ASN:O	1:A:457:ILE:O[3_655]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:N	1:A:458:PRO:CG[3_655]	2.10	0.10
1:A:12:GLY:C	1:A:70:ARG:CD[3_655]	2.10	0.10
1:A:17:MET:CG	1:A:444:GLU:CD[3_655]	2.10	0.10
1:A:27:GLY:CA	1:A:422:TYR:CG[3_655]	2.10	0.10
1:A:30:VAL:O	1:A:448:ARG:O[3_655]	2.10	0.10
1:A:37:ASP:C	1:A:467:PRO:CB[3_655]	2.10	0.10
1:A:46:LEU:CB	1:A:473:PRO:N[3_655]	2.10	0.10
1:A:60:TYR:CA	1:A:211:VAL:O[3_655]	2.10	0.10
1:A:61:VAL:CG2	1:A:213:GLY:CA[3_655]	2.10	0.10
1:A:65:GLN:C	1:A:219:GLU:CB[3_655]	2.10	0.10
1:A:79:THR:C	1:A:209:LYS:CE[3_655]	2.10	0.10
1:A:208:ARG:C	1:A:210:PHE:C[3_655]	2.10	0.10
1:A:221:ILE:CG1	1:A:440:VAL:C[3_655]	2.10	0.10
1:A:222:MET:CE	1:A:466:GLU:CB[3_655]	2.10	0.10
1:A:223:ASP:N	1:A:441:GLU:CG[3_655]	2.10	0.10
1:A:225:LEU:CG	1:A:445:ARG:CA[3_655]	2.10	0.10
1:A:229:VAL:O	1:A:464:GLN:N[3_655]	2.10	0.10
1:A:256:GLU:C	1:A:456:LYS:N[3_655]	2.10	0.10
1:A:257:ALA:N	1:A:456:LYS:N[3_655]	2.10	0.10
1:A:312:CYS:C	1:A:334:GLU:O[3_655]	2.10	0.10
1:A:7:VAL:CG2	1:A:28:LEU:CD1[3_655]	2.11	0.09
1:A:8:VAL:O	1:A:26:SER:OG[3_655]	2.11	0.09
1:A:28:LEU:CA	1:A:450:ILE:CD1[3_655]	2.11	0.09
1:A:37:ASP:O	1:A:467:PRO:CA[3_655]	2.11	0.09
1:A:39:VAL:N	1:A:467:PRO:CD[3_655]	2.11	0.09
1:A:44:TYR:CG	1:A:471:ASP:N[3_655]	2.11	0.09
1:A:46:LEU:N	1:A:473:PRO:N[3_655]	2.11	0.09
1:A:53:TYR:C	1:A:208:ARG:NH2[3_655]	2.11	0.09
1:A:60:TYR:CB	1:A:211:VAL:CG1[3_655]	2.11	0.09
1:A:61:VAL:CG2	1:A:213:GLY:N[3_655]	2.11	0.09
1:A:65:GLN:O	1:A:216:GLN:CA[3_655]	2.11	0.09
1:A:66:ASN:N	1:A:219:GLU:OE2[3_655]	2.11	0.09
1:A:67:ARG:CA	1:A:218:SER:CB[3_655]	2.11	0.09
1:A:68:ILE:CB	1:A:217:VAL:C[3_655]	2.11	0.09
1:A:76:GLY:CA	2:A:600:FAD:C1'[3_655]	2.11	0.09
1:A:210:PHE:CD1	1:A:210:PHE:CD2[3_655]	2.11	0.09
1:A:227:ASP:CA	1:A:463:TRP:C[3_655]	2.11	0.09
1:A:228:ARG:N	1:A:463:TRP:CB[3_655]	2.11	0.09
1:A:228:ARG:N	1:A:462:ILE:O[3_655]	2.11	0.09
1:A:255:TYR:CG	1:A:458:PRO:CD[3_655]	2.11	0.09
1:A:255:TYR:CD1	1:A:461:GLU:OE2[3_655]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:CD1	4:A:2113:HOH:O[3_655]	2.11	0.09
1:A:3:ASN:CB	4:A:2211:HOH:O[3_655]	2.12	0.08
1:A:6:ASP:CA	1:A:450:ILE:O[3_655]	2.12	0.08
1:A:27:GLY:O	1:A:422:TYR:CG[3_655]	2.12	0.08
1:A:32:VAL:CG1	4:A:2208:HOH:O[3_655]	2.12	0.08
1:A:60:TYR:CD1	1:A:78:GLU:OE1[3_655]	2.12	0.08
1:A:209:LYS:C	1:A:209:LYS:O[3_655]	2.12	0.08
1:A:220:ARG:CB	1:A:437:GLU:CG[3_655]	2.12	0.08
1:A:220:ARG:CZ	1:A:435:TYR:CG[3_655]	2.12	0.08
1:A:221:ILE:CA	1:A:440:VAL:CA[3_655]	2.12	0.08
1:A:221:ILE:CD1	1:A:440:VAL:CG2[3_655]	2.12	0.08
1:A:255:TYR:CE1	1:A:461:GLU:CD[3_655]	2.12	0.08
1:A:258:LYS:CA	1:A:456:LYS:NZ[3_655]	2.12	0.08
1:B:101:GLY:C	1:B:475:GLN:NE2[3_555]	2.12	0.08
1:A:14:ILE:CA	1:A:71:LEU:CB[3_655]	2.13	0.07
1:A:16:GLY:C	4:A:2003:HOH:O[3_655]	2.13	0.07
1:A:23:LEU:C	1:A:261:ILE:CG1[3_655]	2.13	0.07
1:A:24:HIS:CA	1:A:446:ALA:O[3_655]	2.13	0.07
1:A:39:VAL:N	1:A:466:GLU:CG[3_655]	2.13	0.07
1:A:39:VAL:CG2	1:A:466:GLU:OE2[3_655]	2.13	0.07
1:A:59:SER:O	1:A:78:GLU:C[3_655]	2.13	0.07
1:A:65:GLN:CB	4:A:2120:HOH:O[3_655]	2.13	0.07
1:A:65:GLN:CD	1:A:216:GLN:CD[3_655]	2.13	0.07
1:A:66:ASN:C	1:A:219:GLU:CG[3_655]	2.13	0.07
1:A:74:GLU:OE2	4:A:2126:HOH:O[3_655]	2.13	0.07
1:A:75:LEU:CA	1:A:435:TYR:C[3_655]	2.13	0.07
1:A:80:TYR:CD1	1:A:80:TYR:CE1[3_655]	2.13	0.07
1:A:83:ASN:O	1:A:334:GLU:N[3_655]	2.13	0.07
1:A:255:TYR:OH	1:A:461:GLU:OE2[3_655]	2.13	0.07
1:A:312:CYS:CA	1:A:334:GLU:O[3_655]	2.13	0.07
1:A:9:VAL:CG2	1:A:22:LEU:CG[3_655]	2.14	0.06
1:A:14:ILE:N	1:A:71:LEU:CA[3_655]	2.14	0.06
1:A:20:ALA:CA	1:A:447:ALA:CB[3_655]	2.14	0.06
1:A:23:LEU:CA	1:A:23:LEU:CD1[3_655]	2.14	0.06
1:A:44:TYR:CB	4:A:2216:HOH:O[3_655]	2.14	0.06
1:A:47:ARG:CZ	1:A:62:GLY:O[3_655]	2.14	0.06
1:A:69:LEU:N	1:A:215:GLY:CA[3_655]	2.14	0.06
1:A:74:GLU:CG	2:A:600:FAD:C5'[3_655]	2.14	0.06
1:A:81:LYS:CD	4:A:2156:HOH:O[3_655]	2.14	0.06
1:A:221:ILE:CD1	1:A:440:VAL:CA[3_655]	2.14	0.06
1:A:226:GLY:O	1:A:464:GLN:N[3_655]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:CD1	1:A:466:GLU:N[3_655]	2.14	0.06
1:A:466:GLU:CB	4:A:2017:HOH:O[3_655]	2.14	0.06
4:A:2050:HOH:O	4:A:2159:HOH:O[3_655]	2.14	0.06
1:B:478:THR:O	1:B:478:THR:CG2[3_555]	2.14	0.06
1:A:6:ASP:OD2	1:A:453:ALA:CB[3_655]	2.15	0.05
1:A:24:HIS:C	1:A:446:ALA:CB[3_655]	2.15	0.05
1:A:28:LEU:CA	1:A:450:ILE:CA[3_655]	2.15	0.05
1:A:29:ASN:OD1	1:A:449:GLU:O[3_655]	2.15	0.05
1:A:31:VAL:C	1:A:448:ARG:CD[3_655]	2.15	0.05
1:A:52:LYS:CB	1:A:202:THR:CB[3_655]	2.15	0.05
1:A:65:GLN:N	4:A:2120:HOH:O[3_655]	2.15	0.05
1:A:68:ILE:N	1:A:219:GLU:N[3_655]	2.15	0.05
1:A:69:LEU:CA	1:A:215:GLY:N[3_655]	2.15	0.05
1:A:73:LYS:O	2:A:600:FAD:C4'[3_655]	2.15	0.05
1:A:82:VAL:CA	1:A:332:LYS:CA[3_655]	2.15	0.05
1:A:219:GLU:C	1:A:437:GLU:OE2[3_655]	2.15	0.05
1:A:224:LEU:CD2	1:A:438:GLY:O[3_655]	2.15	0.05
1:A:227:ASP:N	1:A:463:TRP:CA[3_655]	2.15	0.05
1:A:228:ARG:CA	1:A:463:TRP:CA[3_655]	2.15	0.05
1:A:256:GLU:O	1:A:456:LYS:CA[3_655]	2.15	0.05
1:A:501:ILE:CB	4:A:2054:HOH:O[6_565]	2.15	0.05
1:A:5:CYS:O	1:A:454:MET:C[3_655]	2.16	0.04
1:A:6:ASP:C	1:A:451:LEU:CA[3_655]	2.16	0.04
1:A:29:ASN:N	1:A:450:ILE:C[3_655]	2.16	0.04
1:A:45:THR:CB	1:A:472:VAL:CG1[3_655]	2.16	0.04
1:A:45:THR:C	1:A:472:VAL:O[3_655]	2.16	0.04
1:A:52:LYS:CA	1:A:207:GLU:OE1[3_655]	2.16	0.04
1:A:54:VAL:C	1:A:208:ARG:NH2[3_655]	2.16	0.04
1:A:77:LEU:CG	1:A:436:MET:CE[3_655]	2.16	0.04
1:A:80:TYR:CD2	1:A:209:LYS:CB[3_655]	2.16	0.04
1:A:83:ASN:N	1:A:332:LYS:CB[3_655]	2.16	0.04
1:A:83:ASN:ND2	1:A:334:GLU:C[3_655]	2.16	0.04
1:A:84:GLU:CG	1:A:336:ASN:CG[3_655]	2.16	0.04
1:A:85:VAL:CB	4:A:2142:HOH:O[3_655]	2.16	0.04
1:A:210:PHE:CD2	4:A:2034:HOH:O[3_655]	2.16	0.04
1:A:210:PHE:N	1:A:210:PHE:CA[3_655]	2.16	0.04
1:A:225:LEU:CG	1:A:444:GLU:C[3_655]	2.16	0.04
1:A:227:ASP:OD2	1:A:463:TRP:CD1[3_655]	2.16	0.04
1:A:321:GLU:CG	1:A:499:THR:OG1[6_564]	2.16	0.04
1:A:15:SER:C	1:A:21:LYS:CD[3_655]	2.17	0.03
1:A:17:MET:CE	1:A:444:GLU:CD[3_655]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:C	1:A:261:ILE:CD1[3_655]	2.17	0.03
1:A:23:LEU:N	1:A:261:ILE:CD1[3_655]	2.17	0.03
1:A:25:ASP:CA	1:A:261:ILE:CB[3_655]	2.17	0.03
1:A:32:VAL:N	1:A:448:ARG:NE[3_655]	2.17	0.03
1:A:60:TYR:CA	4:A:2045:HOH:O[3_655]	2.17	0.03
1:A:68:ILE:CD1	1:A:217:VAL:CA[3_655]	2.17	0.03
1:A:69:LEU:N	1:A:214:SER:O[3_655]	2.17	0.03
1:A:69:LEU:CB	1:A:215:GLY:C[3_655]	2.17	0.03
1:A:69:LEU:CG	1:A:215:GLY:C[3_655]	2.17	0.03
1:A:74:GLU:C	2:A:600:FAD:C3'[3_655]	2.17	0.03
1:A:76:GLY:N	2:A:600:FAD:O3'[3_655]	2.17	0.03
1:A:80:TYR:CA	1:A:209:LYS:CD[3_655]	2.17	0.03
1:A:210:PHE:CE2	1:A:214:SER:CA[3_655]	2.17	0.03
1:A:219:GLU:CA	1:A:437:GLU:CD[3_655]	2.17	0.03
1:A:220:ARG:CD	1:A:437:GLU:N[3_655]	2.17	0.03
1:A:256:GLU:CA	1:A:455:GLY:O[3_655]	2.17	0.03
1:A:258:LYS:NZ	1:A:454:MET:CA[3_655]	2.17	0.03
1:A:466:GLU:CG	4:A:2017:HOH:O[3_655]	2.17	0.03
1:A:21:LYS:CB	1:A:443:GLY:C[3_655]	2.18	0.02
1:A:29:ASN:CA	1:A:450:ILE:CA[3_655]	2.18	0.02
1:A:40:GLY:N	1:A:466:GLU:OE2[3_655]	2.18	0.02
1:A:53:TYR:CZ	1:A:208:ARG:CA[3_655]	2.18	0.02
1:A:56:LEU:CD1	1:A:470:VAL:O[3_655]	2.18	0.02
1:A:74:GLU:CD	2:A:600:FAD:O2P[3_655]	2.18	0.02
1:A:83:ASN:O	1:A:335:GLY:N[3_655]	2.18	0.02
1:A:223:ASP:CG	1:A:431:HIS:CB[3_655]	2.18	0.02
1:A:227:ASP:CG	1:A:463:TRP:CD1[3_655]	2.18	0.02
1:A:228:ARG:NE	1:A:449:GLU:CG[3_655]	2.18	0.02
1:A:228:ARG:CA	1:A:462:ILE:CA[3_655]	2.18	0.02
1:A:386:LYS:NZ	1:A:470:VAL:CG1[3_655]	2.18	0.02
1:A:466:GLU:O	4:A:2017:HOH:O[3_655]	2.18	0.02
1:B:100:ARG:NE	1:B:208:ARG:NH2[3_555]	2.18	0.02
1:A:5:CYS:C	1:A:452:HIS:C[3_655]	2.19	0.01
1:A:6:ASP:O	1:A:456:LYS:CG[3_655]	2.19	0.01
1:A:14:ILE:CB	1:A:71:LEU:CB[3_655]	2.19	0.01
1:A:16:GLY:C	4:A:2001:HOH:O[3_655]	2.19	0.01
1:A:19:ALA:CA	1:A:21:LYS:N[3_655]	2.19	0.01
1:A:21:LYS:CD	1:A:439:ALA:O[3_655]	2.19	0.01
1:A:24:HIS:CA	1:A:447:ALA:N[3_655]	2.19	0.01
1:A:38:ARG:CA	1:A:466:GLU:C[3_655]	2.19	0.01
1:A:44:TYR:CG	1:A:469:SER:C[3_655]	2.19	0.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:TYR:CE1	1:A:470:VAL:CA[3_655]	2.19	0.01
1:A:47:ARG:CZ	1:A:64:THR:N[3_655]	2.19	0.01
1:A:47:ARG:CB	1:A:63:PRO:CB[3_655]	2.19	0.01
1:A:56:LEU:O	1:A:471:ASP:OD2[3_655]	2.19	0.01
1:A:60:TYR:N	1:A:78:GLU:CA[3_655]	2.19	0.01
1:A:62:GLY:N	1:A:216:GLN:CD[3_655]	2.19	0.01
1:A:81:LYS:NZ	1:A:300:TYR:CZ[3_655]	2.19	0.01
1:A:223:ASP:CA	1:A:441:GLU:CG[3_655]	2.19	0.01
1:A:223:ASP:O	1:A:441:GLU:OE1[3_655]	2.19	0.01
1:A:333:PRO:CB	4:A:2153:HOH:O[3_655]	2.19	0.01
1:A:370:LYS:NZ	1:A:497:GLY:O[6_564]	2.19	0.01
1:A:438:GLY:C	4:A:2121:HOH:O[3_655]	2.19	0.01
1:B:478:THR:C	1:B:478:THR:O[3_555]	2.19	0.01

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	497/520 (96%)	476 (96%)	20 (4%)	1 (0%)	43	51
1	B	492/520 (95%)	470 (96%)	20 (4%)	2 (0%)	30	34
All	All	989/1040 (95%)	946 (96%)	40 (4%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	LYS
1	A	52	LYS
1	B	460	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	427/444 (96%)	413 (97%)	14 (3%)	33	45
1	B	424/444 (96%)	410 (97%)	14 (3%)	33	45
All	All	851/888 (96%)	823 (97%)	28 (3%)	33	45

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	88	LEU
1	A	106	VAL
1	A	155	LEU
1	A	198	ILE
1	A	242	ARG
1	A	251	ASN
1	A	321	GLU
1	A	364	LEU
1	A	379	GLU
1	A	397	CYS
1	A	460	ASP
1	A	494	ARG
1	A	495	LEU
1	B	46	LEU
1	B	150	GLU
1	B	155	LEU
1	B	167	LEU
1	B	198	ILE
1	B	242	ARG
1	B	251	ASN
1	B	294	VAL
1	B	364	LEU
1	B	379	GLU
1	B	397	CYS
1	B	470	VAL
1	B	494	ARG

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Mol	Chain	Res	Type
1	B	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	116	ASN
1	A	117	ASN
1	A	251	ASN
1	A	416	GLN
1	A	431	HIS
1	A	464	GLN
1	B	116	ASN
1	B	117	ASN
1	B	251	ASN
1	B	431	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DPK	A	601	2	14,14,14	0.53	0	15,17,17	2.34	4 (26%)
3	DPK	B	601	2	14,14,14	0.60	0	15,17,17	2.28	3 (20%)
2	FAD	B	600	3,1	56,58,58	1.34	8 (14%)	81,89,89	2.01	23 (28%)
2	FAD	A	600	3,1	56,58,58	1.37	7 (12%)	81,89,89	1.84	22 (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
3	DPK	A	601	2	-	6/11/11/11	0/1/1/1
3	DPK	B	601	2	-	6/11/11/11	0/1/1/1
2	FAD	B	600	3,1	-	3/34/50/50	0/6/6/6
2	FAD	A	600	3,1	-	4/34/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C4X-N5	4.69	1.39	1.30
2	B	600	FAD	C4X-N5	4.55	1.39	1.30
2	B	600	FAD	C2A-N1A	3.19	1.39	1.33
2	A	600	FAD	C8A-N7A	3.01	1.37	1.31
2	B	600	FAD	C10-N1	2.91	1.39	1.33
2	A	600	FAD	C2A-N1A	2.88	1.39	1.33
2	A	600	FAD	C1'-N10	2.71	1.55	1.48
2	A	600	FAD	O4-C4	2.68	1.28	1.23
2	B	600	FAD	C8A-N7A	2.57	1.36	1.31
2	A	600	FAD	C10-N1	2.55	1.38	1.33
2	A	600	FAD	C2A-N3A	2.50	1.38	1.33
2	B	600	FAD	O4B-C4B	-2.41	1.39	1.45
2	B	600	FAD	C2A-N3A	2.33	1.38	1.33
2	B	600	FAD	C9-C9A	2.23	1.43	1.39
2	B	600	FAD	C5'-C4'	2.21	1.54	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	DPK	C9N-N9-C10	7.02	119.16	110.20
3	A	601	DPK	C9N-N9-C10	6.64	118.67	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	N3A-C2A-N1A	-6.00	119.22	128.60
2	B	600	FAD	C9A-C5X-N5	-5.22	116.75	122.43
2	A	600	FAD	C5A-C4A-N3A	-5.12	120.06	126.75
2	B	600	FAD	C5A-C4A-N3A	-4.97	120.26	126.75
2	A	600	FAD	N3A-C2A-N1A	-4.79	121.11	128.60
2	A	600	FAD	C5A-N7A-C8A	4.50	109.90	103.51
3	B	601	DPK	C11-C10-N9	4.30	121.66	112.62
2	B	600	FAD	C5A-N7A-C8A	4.29	109.60	103.51
3	A	601	DPK	C11-C10-N9	4.23	121.51	112.62
2	A	600	FAD	N9A-C8A-N7A	-4.05	108.38	113.91
2	B	600	FAD	N9A-C8A-N7A	-3.91	108.56	113.91
2	A	600	FAD	C4A-C5A-N7A	-3.84	105.94	110.62
2	B	600	FAD	C2A-N3A-C4A	3.83	120.81	111.75
3	A	601	DPK	C8C-C8-C7	-3.67	107.65	112.10
2	B	600	FAD	C4-N3-C2	-3.54	119.10	125.64
2	B	600	FAD	C10-C4X-N5	-3.53	117.37	124.86
2	B	600	FAD	C1'-N10-C9A	-3.48	114.71	120.51
2	A	600	FAD	C2A-N3A-C4A	3.45	119.91	111.75
2	A	600	FAD	O3'-C3'-C4'	-3.45	100.48	108.81
2	A	600	FAD	C9A-N10-C10	-3.28	115.66	120.77
2	A	600	FAD	C10-C4X-N5	-3.24	117.97	124.86
2	A	600	FAD	C9A-C5X-N5	-3.16	119.00	122.43
2	B	600	FAD	C4X-C10-N1	-3.13	117.47	124.73
2	A	600	FAD	C5A-C4A-N9A	3.04	109.32	105.78
2	B	600	FAD	C9A-N10-C10	-3.03	116.04	120.77
2	B	600	FAD	C4A-C5A-N7A	-2.92	107.06	110.62
2	B	600	FAD	N3A-C4A-N9A	2.80	131.69	127.08
2	B	600	FAD	C5X-N5-C4X	2.62	122.43	118.07
2	A	600	FAD	C2B-C1B-N9A	2.61	119.92	113.30
2	B	600	FAD	C2B-C1B-N9A	2.57	119.82	113.30
2	B	600	FAD	C4X-C10-N10	2.52	120.17	116.48
2	B	600	FAD	C4'-C3'-C2'	2.49	118.54	113.36
2	B	600	FAD	C4-C4X-C10	2.45	120.92	116.79
2	B	600	FAD	C4-C4X-N5	2.45	121.71	118.23
2	A	600	FAD	C6A-C5A-C4A	2.38	120.39	117.18
2	A	600	FAD	C4-C4X-C10	2.35	120.73	116.79
2	B	600	FAD	C10-N1-C2	2.34	121.58	116.90
2	B	600	FAD	C4X-C4-N3	2.33	119.11	113.19
2	A	600	FAD	C4'-C3'-C2'	2.32	118.18	113.36
2	A	600	FAD	C4X-C10-N10	2.29	119.82	116.48
2	A	600	FAD	C1'-N10-C9A	-2.25	116.76	120.51
2	A	600	FAD	C1B-N9A-C8A	2.24	132.18	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O2-C2-N1	-2.19	118.19	121.83
2	A	600	FAD	C4A-N9A-C1B	-2.19	121.37	126.59
2	A	600	FAD	C4-C4X-N5	2.15	121.29	118.23
2	A	600	FAD	N3A-C4A-N9A	2.14	130.61	127.08
2	A	600	FAD	O2-C2-N1	-2.14	118.28	121.83
3	A	601	DPK	C9N-N9-C8	2.13	117.27	113.67
2	B	600	FAD	P-O3P-PA	-2.11	125.57	132.83
3	B	601	DPK	C9N-N9-C8	2.08	117.19	113.67

There are no chirality outliers.

All (19) torsion outliers are listed below:

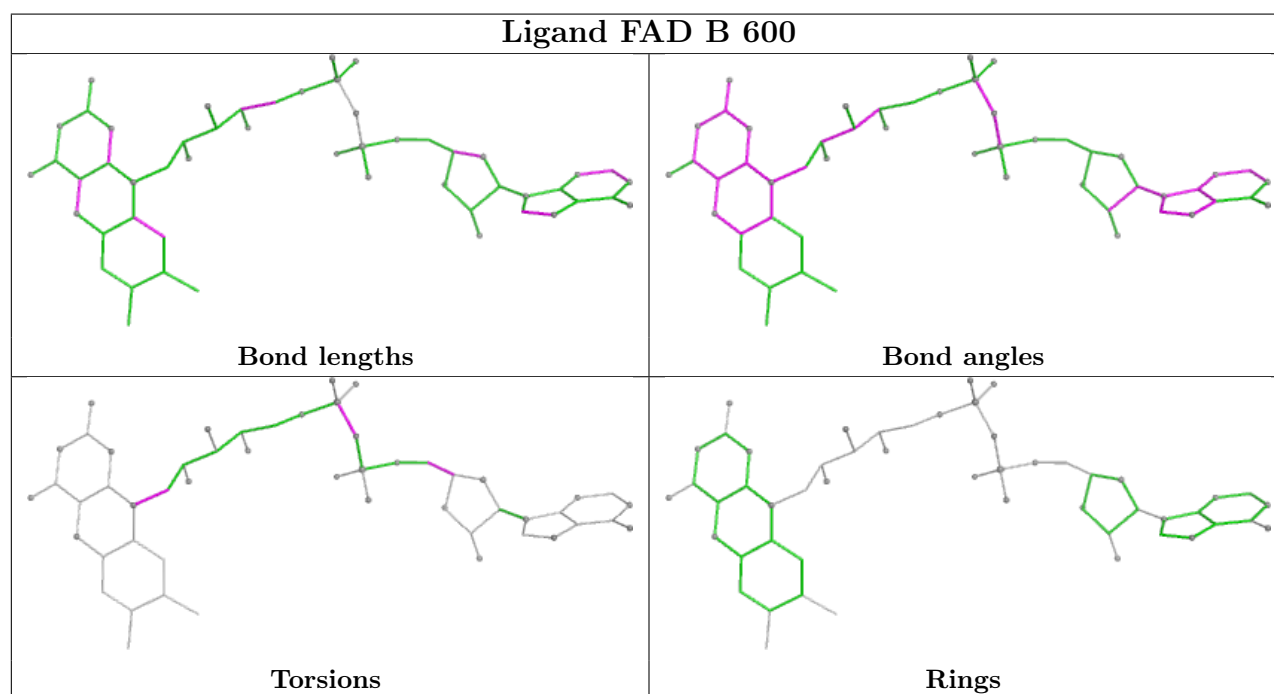
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C2'-C1'-N10-C10
2	B	600	FAD	C2'-C1'-N10-C10
2	B	600	FAD	PA-O3P-P-O5'
3	A	601	DPK	C11-C10-N9-C9N
3	A	601	DPK	C11-C10-N9-C8
3	A	601	DPK	C8C-C8-N9-C10
3	A	601	DPK	C7-C8-N9-C10
3	B	601	DPK	C11-C10-N9-C9N
3	B	601	DPK	C11-C10-N9-C8
3	B	601	DPK	C8C-C8-N9-C10
3	B	601	DPK	C7-C8-N9-C10
3	A	601	DPK	N9-C10-C11-C12
3	B	601	DPK	N9-C10-C11-C12
2	A	600	FAD	PA-O3P-P-O5'
3	A	601	DPK	C8C-C8-N9-C9N
3	B	601	DPK	C8C-C8-N9-C9N
2	A	600	FAD	C5B-O5B-PA-O2A
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B

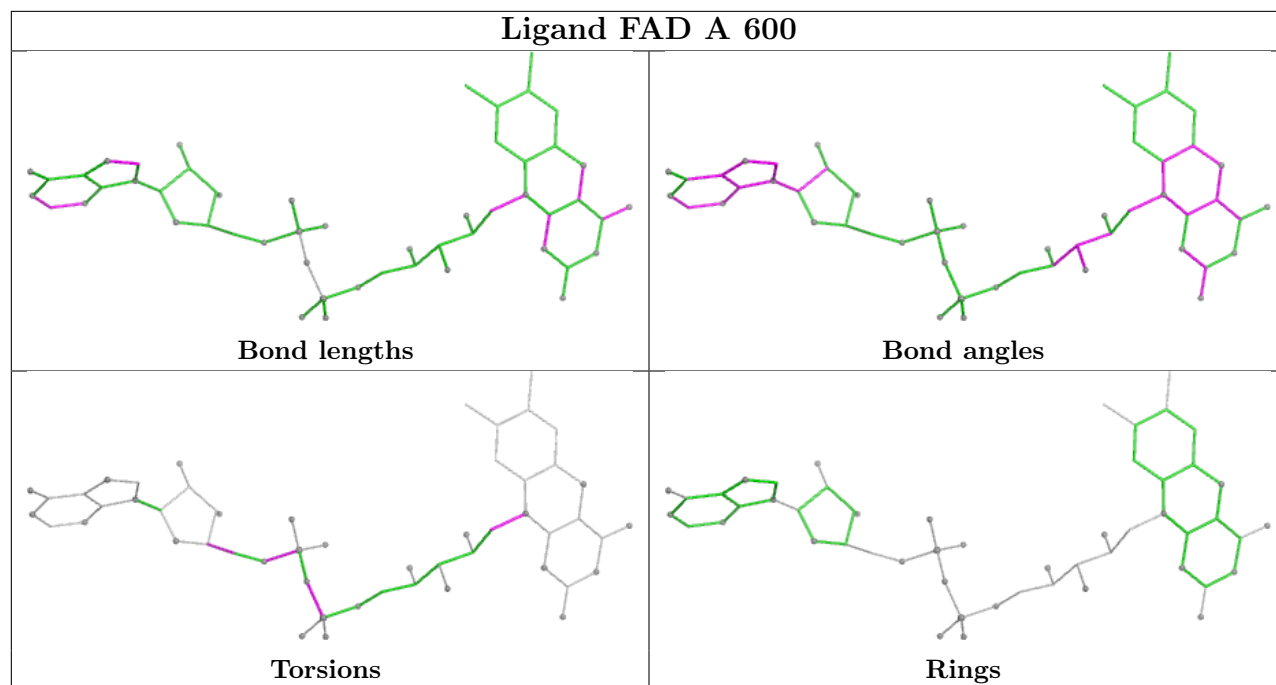
There are no ring outliers.

3 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	DPK	1	0
2	B	600	FAD	2	0
2	A	600	FAD	2	60

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	499/520 (95%)	2.76	355 (71%) 0 0	24, 31, 46, 64	0
1	B	494/520 (95%)	3.00	378 (76%) 0 0	23, 31, 42, 60	0
All	All	993/1040 (95%)	2.88	733 (73%) 0 0	23, 31, 44, 64	0

All (733) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ASN	13.6
1	B	212	GLY	11.1
1	B	495	LEU	9.2
1	B	496	ILE	8.6
1	A	496	ILE	7.3
1	B	58	GLY	7.3
1	B	460	ASP	7.2
1	A	94	GLY	7.1
1	A	481	PHE	7.1
1	A	13	GLY	6.9
1	B	43	THR	6.9
1	A	110	ILE	6.8
1	B	494	ARG	6.7
1	A	459	GLU	6.5
1	A	224	LEU	6.5
1	A	106	VAL	6.4
1	B	81	LYS	6.4
1	B	462	ILE	6.3
1	A	495	LEU	6.3
1	B	446	ALA	6.1
1	A	259	TYR	6.0
1	A	246	LEU	6.0
1	A	499	THR	5.9
1	B	92	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	226	GLY	5.8
1	A	482	LEU	5.8
1	B	455	GLY	5.8
1	A	484	ARG	5.7
1	B	224	LEU	5.7
1	B	230	LYS	5.7
1	A	498	LEU	5.6
1	B	88	LEU	5.6
1	A	475	GLN	5.6
1	A	497	GLY	5.5
1	B	395	GLY	5.5
1	A	92	VAL	5.5
1	B	451	LEU	5.5
1	B	243	GLU	5.4
1	B	265	PRO	5.4
1	B	250	LEU	5.4
1	A	433	SER	5.4
1	A	98	PRO	5.3
1	A	107	TRP	5.3
1	A	429	ALA	5.3
1	A	494	ARG	5.3
1	A	12	GLY	5.3
1	B	27	GLY	5.3
1	B	489	VAL	5.2
1	B	238	ILE	5.2
1	B	458	PRO	5.2
1	B	463	TRP	5.2
1	B	492	LEU	5.2
1	A	354	ARG	5.2
1	A	23	LEU	5.1
1	A	486	LEU	5.1
1	B	270	MET	5.1
1	B	155	LEU	5.1
1	A	245	VAL	5.1
1	B	31	VAL	5.1
1	B	461	GLU	5.1
1	B	335	GLY	5.1
1	B	336	ASN	5.0
1	A	105	PRO	5.0
1	B	215	GLY	5.0
1	A	334	GLU	5.0
1	A	133	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	442	ALA	5.0
1	B	54	VAL	5.0
1	B	107	TRP	5.0
1	B	110	ILE	5.0
1	B	246	LEU	5.0
1	B	319	GLY	5.0
1	B	221	ILE	4.9
1	A	101	GLY	4.9
1	B	453	ALA	4.9
1	B	476	PRO	4.9
1	A	492	LEU	4.9
1	A	470	VAL	4.9
1	A	501	ILE	4.9
1	B	477	ILE	4.9
1	B	156	CYS	4.8
1	B	136	LYS	4.8
1	B	252	HIS	4.8
1	A	477	ILE	4.7
1	A	229	VAL	4.7
1	A	236	ILE	4.7
1	B	481	PHE	4.7
1	A	388	TRP	4.7
1	B	16	GLY	4.7
1	B	469	SER	4.7
1	A	3	ASN	4.6
1	A	244	ASN	4.6
1	B	381	VAL	4.6
1	B	193	GLY	4.6
1	A	465	SER	4.6
1	B	465	SER	4.6
1	B	227	ASP	4.6
1	B	23	LEU	4.6
1	B	236	ILE	4.6
1	B	261	ILE	4.6
1	B	459	GLU	4.5
1	A	64	THR	4.5
1	A	163	GLN	4.5
1	B	5	CYS	4.5
1	A	302	LYS	4.5
1	A	389	CYS	4.5
1	B	103	PHE	4.5
1	B	61	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	485	HIS	4.5
1	B	66	ASN	4.5
1	A	241	THR	4.4
1	B	241	THR	4.4
1	B	345	LEU	4.4
1	B	259	TYR	4.4
1	A	37	ASP	4.4
1	A	387	ASN	4.4
1	A	243	GLU	4.4
1	A	468	GLU	4.4
1	A	462	ILE	4.4
1	B	491	GLY	4.4
1	A	487	PRO	4.4
1	B	119	TRP	4.4
1	A	363	LYS	4.3
1	B	456	LYS	4.3
1	A	205	GLY	4.3
1	B	355	LEU	4.3
1	B	482	LEU	4.3
1	B	450	ILE	4.3
1	B	429	ALA	4.3
1	A	173	VAL	4.3
1	A	189	VAL	4.3
1	A	157	TRP	4.3
1	B	394	SER	4.3
1	B	72	ALA	4.3
1	A	372	LEU	4.3
1	A	493	LEU	4.3
1	A	500	THR	4.3
1	A	41	GLY	4.3
1	A	103	PHE	4.2
1	B	361	LEU	4.2
1	A	352	LEU	4.2
1	B	189	VAL	4.2
1	B	363	LYS	4.2
1	A	476	PRO	4.2
1	B	490	PRO	4.2
1	B	159	GLU	4.2
1	A	72	ALA	4.1
1	A	461	GLU	4.1
1	B	157	TRP	4.1
1	A	318	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	258	LYS	4.1
1	B	242	ARG	4.1
1	B	255	TYR	4.1
1	B	95	LYS	4.1
1	A	252	HIS	4.0
1	B	71	LEU	4.0
1	B	113	LEU	4.0
1	A	50	LYS	4.0
1	A	383	TYR	4.0
1	A	439	ALA	4.0
1	A	373	GLY	4.0
1	A	301	TYR	4.0
1	A	203	ASN	4.0
1	A	432	TRP	4.0
1	A	138	PRO	4.0
1	B	493	LEU	4.0
1	B	53	TYR	4.0
1	B	457	ILE	4.0
1	B	106	VAL	4.0
1	A	331	THR	4.0
1	B	111	THR	4.0
1	B	303	GLU	4.0
1	B	26	SER	4.0
1	B	21	LYS	3.9
1	B	82	VAL	3.9
1	B	143	TRP	3.9
1	A	48	ASN	3.9
1	B	420	ARG	3.9
1	A	418	VAL	3.9
1	B	51	VAL	3.9
1	B	367	LEU	3.9
1	B	204	GLY	3.9
1	A	340	ILE	3.9
1	A	82	VAL	3.9
1	A	345	LEU	3.9
1	B	28	LEU	3.9
1	B	93	LYS	3.9
1	B	354	ARG	3.9
1	B	247	VAL	3.9
1	B	378	LEU	3.9
1	A	20	ALA	3.9
1	B	220	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	425	GLY	3.8
1	B	424	ALA	3.8
1	B	473	PRO	3.8
1	A	457	ILE	3.8
1	A	97	TYR	3.8
1	A	22	LEU	3.8
1	B	352	LEU	3.8
1	B	375	LEU	3.8
1	B	452	HIS	3.8
1	A	480	THR	3.8
1	B	369	ALA	3.8
1	A	463	TRP	3.8
1	B	163	GLN	3.8
1	B	187	TRP	3.8
1	B	449	GLU	3.8
1	B	105	PRO	3.8
1	B	228	ARG	3.8
1	B	410	TYR	3.7
1	B	432	TRP	3.7
1	A	33	LEU	3.7
1	B	414	LEU	3.7
1	B	260	VAL	3.7
1	B	418	VAL	3.7
1	B	320	GLU	3.7
1	B	337	TYR	3.7
1	B	239	ASP	3.7
1	B	274	PHE	3.7
1	A	119	TRP	3.7
1	A	312	CYS	3.7
1	A	71	LEU	3.7
1	B	226	GLY	3.7
1	B	464	GLN	3.7
1	B	48	ASN	3.7
1	A	255	TYR	3.7
1	A	307	ARG	3.7
1	B	100	ARG	3.7
1	B	333	PRO	3.7
1	B	59	SER	3.7
1	B	431	HIS	3.7
1	A	4	LYS	3.7
1	A	187	TRP	3.7
1	B	167	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	124	ASP	3.7
1	A	275	ASN	3.7
1	A	337	TYR	3.7
1	B	69	LEU	3.6
1	A	220	ARG	3.6
1	A	31	VAL	3.6
1	A	239	ASP	3.6
1	B	3	ASN	3.6
1	B	484	ARG	3.6
1	B	474	ALA	3.6
1	B	97	TYR	3.6
1	A	258	LYS	3.6
1	B	150	GLU	3.6
1	A	412	ARG	3.6
1	A	170	ASN	3.6
1	A	453	ALA	3.6
1	B	442	ALA	3.6
1	B	162	LYS	3.6
1	B	301	TYR	3.6
1	B	311	TYR	3.6
1	A	294	VAL	3.6
1	B	480	THR	3.6
1	B	309	LYS	3.6
1	A	225	LEU	3.6
1	A	8	VAL	3.6
1	B	448	ARG	3.5
1	A	356	THR	3.5
1	A	7	VAL	3.5
1	A	247	VAL	3.5
1	A	325	ALA	3.5
1	B	338	ALA	3.5
1	B	112	TYR	3.5
1	A	93	LYS	3.5
1	B	50	LYS	3.5
1	A	43	THR	3.5
1	B	64	THR	3.5
1	B	376	GLU	3.5
1	A	112	TYR	3.5
1	B	398	TYR	3.5
1	A	242	ARG	3.5
1	B	98	PRO	3.5
1	B	467	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	3.5
1	A	160	SER	3.5
1	A	214	SER	3.5
1	A	374	SER	3.5
1	A	24	HIS	3.5
1	A	485	HIS	3.5
1	B	435	TYR	3.5
1	A	458	PRO	3.4
1	B	175	ALA	3.4
1	B	160	SER	3.4
1	A	452	HIS	3.4
1	A	49	GLN	3.4
1	B	30	VAL	3.4
1	A	338	ALA	3.4
1	B	340	ILE	3.4
1	B	483	GLU	3.4
1	A	438	GLY	3.4
1	B	213	GLY	3.4
1	A	328	LEU	3.4
1	B	108	ASN	3.4
1	B	223	ASP	3.4
1	A	135	TRP	3.4
1	A	479	THR	3.4
1	A	178	HIS	3.4
1	B	251	ASN	3.4
1	B	318	ASP	3.4
1	A	404	PRO	3.3
1	B	358	GLU	3.3
1	B	140	ALA	3.3
1	B	279	PRO	3.3
1	B	188	TYR	3.3
1	B	422	TYR	3.3
1	A	339	ALA	3.3
1	B	257	ALA	3.3
1	B	419	ASP	3.3
1	A	155	LEU	3.3
1	A	250	LEU	3.3
1	B	192	CYS	3.3
1	B	130	PRO	3.3
1	B	359	GLU	3.3
1	B	209	LYS	3.3
1	B	237	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	182	ALA	3.3
1	B	35	ALA	3.3
1	B	85	VAL	3.3
1	B	322	ALA	3.3
1	A	319	GLY	3.3
1	B	101	GLY	3.3
1	B	344	ILE	3.3
1	A	305	PHE	3.3
1	A	300	TYR	3.3
1	B	488	SER	3.3
1	A	489	VAL	3.3
1	B	294	VAL	3.3
1	B	325	ALA	3.2
1	B	447	ALA	3.2
1	A	396	GLY	3.2
1	A	231	LEU	3.2
1	B	486	LEU	3.2
1	A	357	LYS	3.2
1	B	264	ILE	3.2
1	A	287	THR	3.2
1	B	9	VAL	3.2
1	B	275	ASN	3.2
1	B	77	LEU	3.2
1	A	266	PRO	3.2
1	B	421	ILE	3.2
1	A	426	THR	3.2
1	A	217	VAL	3.2
1	B	165	ALA	3.2
1	A	359	GLU	3.2
1	B	116	ASN	3.2
1	B	466	GLU	3.2
1	B	109	PRO	3.2
1	B	20	ALA	3.2
1	A	129	ILE	3.2
1	A	111	THR	3.2
1	A	222	MET	3.2
1	B	334	GLU	3.1
1	A	460	ASP	3.1
1	B	29	ASN	3.1
1	B	263	ALA	3.1
1	B	245	VAL	3.1
1	B	276	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	306	TRP	3.1
1	B	68	ILE	3.1
1	A	360	ARG	3.1
1	A	121	THR	3.1
1	A	309	LYS	3.1
1	A	329	ASP	3.1
1	B	283	ASN	3.1
1	B	470	VAL	3.1
1	A	188	TYR	3.1
1	A	265	PRO	3.1
1	B	134	PRO	3.1
1	A	233	ARG	3.1
1	B	79	THR	3.1
1	B	121	THR	3.1
1	A	382	HIS	3.1
1	B	347	HIS	3.1
1	A	161	ALA	3.1
1	B	413	VAL	3.1
1	B	138	PRO	3.1
1	A	100	ARG	3.1
1	B	393	TYR	3.1
1	A	293	SER	3.1
1	A	66	ASN	3.1
1	B	123	ASP	3.1
1	B	145	ASN	3.1
1	B	487	PRO	3.1
1	A	378	LEU	3.1
1	A	53	TYR	3.0
1	B	196	THR	3.0
1	B	249	THR	3.0
1	B	428	THR	3.0
1	A	117	ASN	3.0
1	A	324	VAL	3.0
1	B	362	LYS	3.0
1	B	443	GLY	3.0
1	A	254	MET	3.0
1	A	77	LEU	3.0
1	B	158	THR	3.0
1	A	127	ARG	3.0
1	A	370	LYS	3.0
1	A	96	SER	3.0
1	B	57	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	130	PRO	3.0
1	A	346	ALA	3.0
1	A	384	GLU	3.0
1	B	277	PRO	3.0
1	A	435	TYR	3.0
1	B	114	ASP	3.0
1	A	304	PRO	3.0
1	A	54	VAL	2.9
1	A	169	VAL	2.9
1	A	249	THR	2.9
1	A	430	THR	2.9
1	A	86	GLU	2.9
1	B	6	ASP	2.9
1	B	203	ASN	2.9
1	A	102	PRO	2.9
1	A	343	PHE	2.9
1	A	115	HIS	2.9
1	A	9	VAL	2.9
1	A	180	VAL	2.9
1	A	440	VAL	2.9
1	B	4	LYS	2.9
1	A	158	THR	2.9
1	A	428	THR	2.9
1	B	102	PRO	2.9
1	B	115	HIS	2.9
1	A	263	ALA	2.9
1	B	328	LEU	2.9
1	B	417	PRO	2.9
1	A	278	LEU	2.9
1	B	118	PHE	2.9
1	B	171	LEU	2.9
1	B	173	VAL	2.9
1	B	229	VAL	2.9
1	A	399	THR	2.9
1	A	421	ILE	2.9
1	B	430	THR	2.9
1	A	29	ASN	2.9
1	B	214	SER	2.8
1	A	393	TYR	2.8
1	B	70	ARG	2.8
1	B	383	TYR	2.8
1	B	39	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	388	TRP	2.8
1	B	269	GLY	2.8
1	B	122	MET	2.8
1	A	456	LYS	2.8
1	B	73	LYS	2.8
1	A	147	THR	2.8
1	A	264	ILE	2.8
1	B	445	ARG	2.8
1	A	108	ASN	2.8
1	A	425	GLY	2.8
1	B	44	TYR	2.8
1	B	60	TYR	2.8
1	B	219	GLU	2.8
1	A	274	PHE	2.8
1	B	185	PHE	2.8
1	A	355	LEU	2.8
1	A	136	LYS	2.8
1	B	349	ALA	2.8
1	B	305	PHE	2.8
1	B	8	VAL	2.8
1	B	299	VAL	2.8
1	B	24	HIS	2.7
1	B	272	ILE	2.7
1	B	471	ASP	2.7
1	A	234	PRO	2.7
1	A	379	GLU	2.7
1	B	321	GLU	2.7
1	A	364	LEU	2.7
1	B	146	MET	2.7
1	A	120	ARG	2.7
1	A	175	ALA	2.7
1	A	398	TYR	2.7
1	B	353	ALA	2.7
1	B	423	PHE	2.7
1	B	178	HIS	2.7
1	A	464	GLN	2.7
1	A	193	GLY	2.7
1	A	184	TRP	2.7
1	A	483	GLU	2.7
1	A	122	MET	2.7
1	A	70	ARG	2.7
1	B	225	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	339	ALA	2.7
1	B	346	ALA	2.7
1	B	439	ALA	2.7
1	A	431	HIS	2.7
1	B	32	VAL	2.7
1	A	198	ILE	2.7
1	B	62	GLY	2.7
1	B	76	GLY	2.7
1	A	159	GLU	2.7
1	A	390	GLU	2.7
1	A	490	PRO	2.7
1	B	190	LYS	2.7
1	A	454	MET	2.7
1	A	25	ASP	2.7
1	A	211	VAL	2.7
1	B	440	VAL	2.7
1	B	408	THR	2.7
1	A	316	ILE	2.7
1	A	317	ILE	2.7
1	A	406	ILE	2.7
1	B	94	GLY	2.7
1	B	412	ARG	2.7
1	B	22	LEU	2.7
1	A	353	ALA	2.6
1	B	49	GLN	2.6
1	A	85	VAL	2.6
1	A	235	VAL	2.6
1	A	289	VAL	2.6
1	A	478	THR	2.6
1	A	40	GLY	2.6
1	A	199	ILE	2.6
1	A	276	PRO	2.6
1	A	473	PRO	2.6
1	B	454	MET	2.6
1	A	91	HIS	2.6
1	A	171	LEU	2.6
1	A	230	LYS	2.6
1	A	35	ALA	2.6
1	B	74	GLU	2.6
1	A	311	TYR	2.6
1	A	109	PRO	2.6
1	A	88	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	361	LEU	2.6
1	B	248	GLU	2.6
1	B	330	ASP	2.6
1	A	166	THR	2.6
1	A	341	MET	2.6
1	A	413	VAL	2.6
1	B	384	GLU	2.6
1	B	135	TRP	2.6
1	B	202	THR	2.6
1	B	180	VAL	2.6
1	A	69	LEU	2.5
1	A	179	GLU	2.5
1	B	307	ARG	2.5
1	A	474	ALA	2.5
1	A	227	ASP	2.5
1	B	55	ASP	2.5
1	A	58	GLY	2.5
1	A	292	GLY	2.5
1	B	63	PRO	2.5
1	B	126	GLY	2.5
1	B	405	GLY	2.5
1	A	118	PHE	2.5
1	B	7	VAL	2.5
1	A	89	ILE	2.5
1	A	164	LEU	2.5
1	B	364	LEU	2.5
1	B	382	HIS	2.5
1	A	216	GLN	2.5
1	A	262	SER	2.5
1	B	433	SER	2.5
1	A	232	GLU	2.5
1	A	113	LEU	2.5
1	A	367	LEU	2.5
1	B	183	LEU	2.5
1	B	231	LEU	2.5
1	B	83	ASN	2.5
1	A	365	CYS	2.5
1	B	235	VAL	2.5
1	B	151	LEU	2.5
1	B	268	LEU	2.5
1	B	37	ASP	2.5
1	B	91	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	277	PRO	2.5
1	A	405	GLY	2.5
1	B	416	GLN	2.5
1	B	45	THR	2.4
1	A	368	TYR	2.4
1	A	55	ASP	2.4
1	A	424	ALA	2.4
1	B	87	ARG	2.4
1	B	133	ALA	2.4
1	B	256	GLU	2.4
1	A	267	THR	2.4
1	A	408	THR	2.4
1	B	324	VAL	2.4
1	A	386	LYS	2.4
1	A	422	TYR	2.4
1	B	153	ASP	2.4
1	A	140	ALA	2.4
1	A	403	PRO	2.4
1	A	342	GLY	2.4
1	A	434	GLY	2.4
1	A	298	ILE	2.4
1	A	371	VAL	2.4
1	B	89	ILE	2.4
1	A	36	ARG	2.4
1	A	326	TYR	2.4
1	B	300	TYR	2.4
1	A	57	GLY	2.4
1	A	271	LYS	2.4
1	A	327	THR	2.4
1	B	331	THR	2.4
1	A	423	PHE	2.4
1	B	222	MET	2.4
1	B	164	LEU	2.4
1	A	42	ARG	2.4
1	A	445	ARG	2.4
1	B	240	GLN	2.4
1	A	321	GLU	2.4
1	B	379	GLU	2.4
1	B	468	GLU	2.4
1	A	83	ASN	2.3
1	B	401	TYR	2.3
1	A	126	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	174	THR	2.3
1	B	96	SER	2.3
1	A	210	PHE	2.3
1	B	217	VAL	2.3
1	A	282	ARG	2.3
1	A	448	ARG	2.3
1	B	365	CYS	2.3
1	A	392	GLN	2.3
1	A	395	GLY	2.3
1	B	161	ALA	2.3
1	B	426	THR	2.3
1	A	385	GLU	2.3
1	B	34	GLU	2.3
1	A	332	LYS	2.3
1	A	362	LYS	2.3
1	B	117	ASN	2.3
1	A	63	PRO	2.3
1	B	438	GLY	2.3
1	B	253	GLU	2.3
1	B	198	ILE	2.3
1	A	10	VAL	2.3
1	A	75	LEU	2.3
1	A	145	ASN	2.3
1	A	401	TYR	2.3
1	A	369	ALA	2.3
1	A	420	ARG	2.3
1	B	177	THR	2.3
1	A	200	SER	2.3
1	B	15	SER	2.3
1	B	298	ILE	2.3
1	B	302	LYS	2.3
1	A	323	PRO	2.2
1	B	403	PRO	2.2
1	A	80	TYR	2.2
1	B	195	THR	2.2
1	B	385	GLU	2.2
1	A	296	LYS	2.2
1	A	375	LEU	2.2
1	B	152	LEU	2.2
1	A	128	GLU	2.2
1	A	150	GLU	2.2
1	A	18	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	154	LYS	2.2
1	B	129	ILE	2.2
1	B	317	ILE	2.2
1	A	268	LEU	2.2
1	B	99	PHE	2.2
1	A	279	PRO	2.2
1	A	240	GLN	2.2
1	A	351	LYS	2.2
1	A	196	THR	2.2
1	A	446	ALA	2.2
1	B	131	SER	2.2
1	B	327	THR	2.2
1	A	414	LEU	2.2
1	B	14	ILE	2.2
1	B	289	VAL	2.2
1	B	280	MET	2.2
1	B	402	PHE	2.2
1	A	308	LYS	2.2
1	B	308	LYS	2.2
1	B	396	GLY	2.2
1	A	201	THR	2.2
1	B	166	THR	2.2
1	A	87	ARG	2.1
1	B	120	ARG	2.1
1	A	143	TRP	2.1
1	B	407	LEU	2.1
1	B	357	LYS	2.1
1	A	27	GLY	2.1
1	A	165	ALA	2.1
1	B	374	SER	2.1
1	B	415	ARG	2.1
1	A	81	LYS	2.1
1	A	95	LYS	2.1
1	A	320	GLU	2.1
1	A	366	GLU	2.1
1	B	127	ARG	2.1
1	B	147	THR	2.1
1	B	233	ARG	2.1
1	B	356	THR	2.1
1	B	351	LYS	2.1
1	A	46	LEU	2.1
1	A	139	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	358	GLU	2.1
1	B	142	GLU	2.1
1	A	60	TYR	2.1
1	A	237	TYR	2.1
1	A	251	ASN	2.1
1	B	316	ILE	2.1
1	A	381	VAL	2.1
1	B	41	GLY	2.1
1	A	197	ARG	2.1
1	A	228	ARG	2.1
1	B	47	ARG	2.1
1	A	400	THR	2.1
1	B	312	CYS	2.1
1	A	162	LYS	2.1
1	B	315	MET	2.1
1	A	466	GLU	2.1
1	A	167	LEU	2.1
1	A	68	ILE	2.1
1	B	25	ASP	2.1
1	B	199	ILE	2.1
1	A	99	PHE	2.1
1	A	402	PHE	2.1
1	B	411	GLY	2.1
1	B	479	THR	2.0
1	A	447	ALA	2.0
1	A	449	GLU	2.0
1	B	441	GLU	2.0
1	B	56	LEU	2.0
1	B	371	VAL	2.0
1	B	194	GLY	2.0
1	A	168	PHE	2.0
1	B	148	MET	2.0
1	B	262	SER	2.0
1	B	437	GLU	2.0
1	A	137	ALA	2.0
1	A	152	LEU	2.0
1	B	149	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

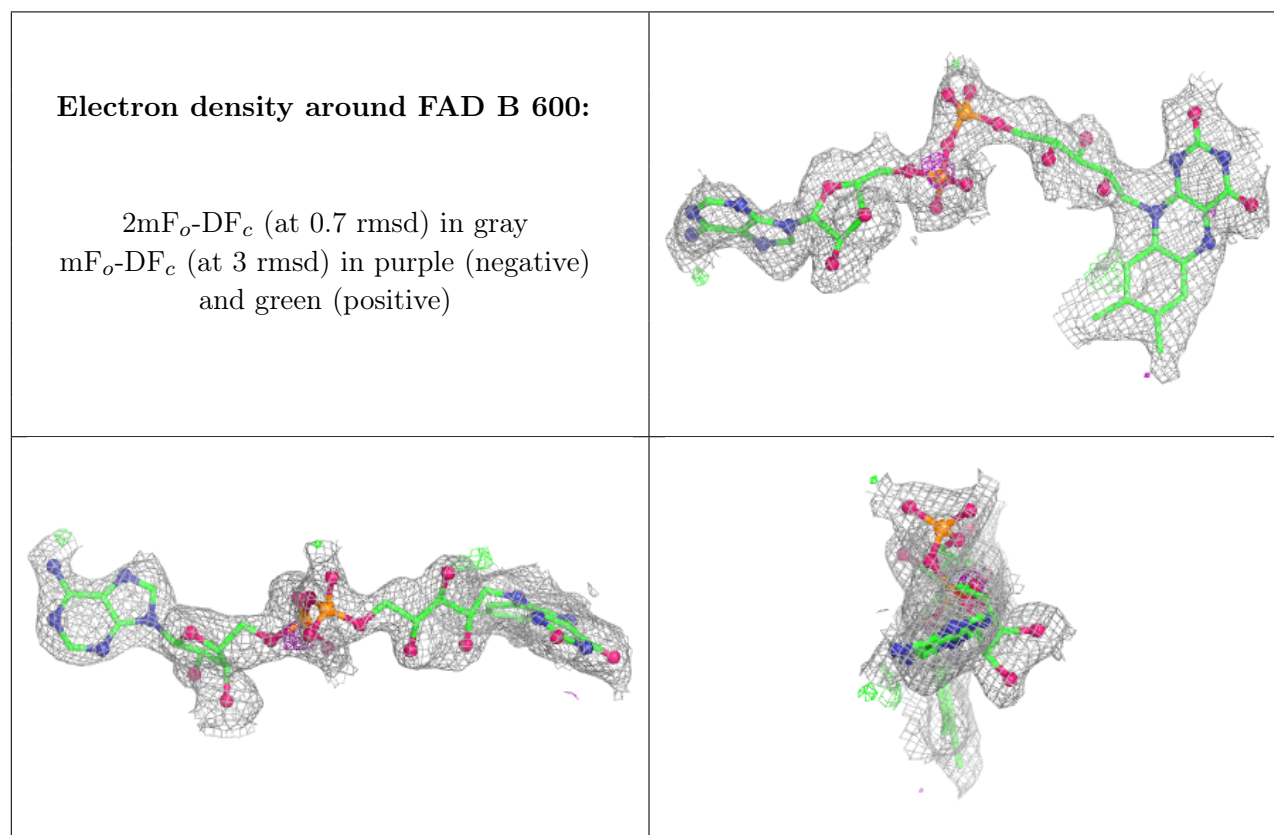
There are no oligosaccharides in this entry.

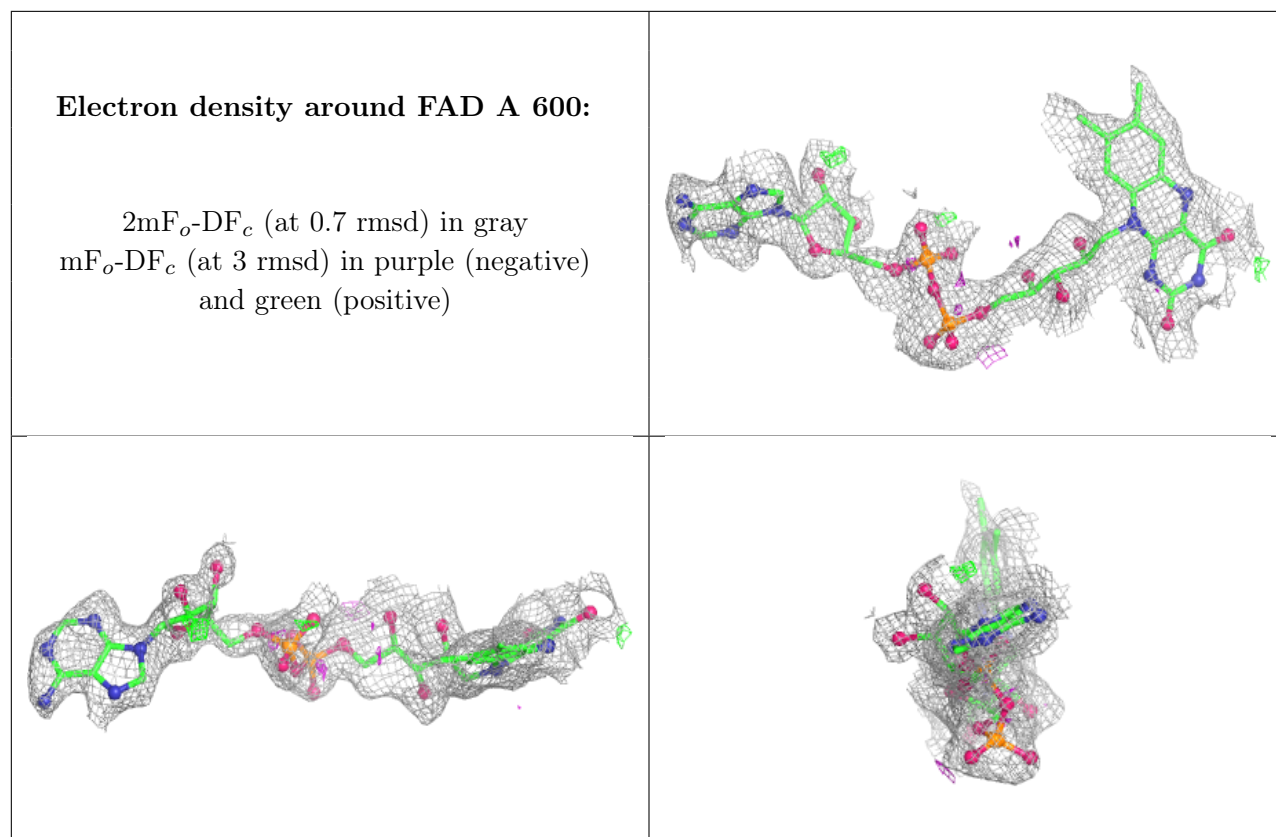
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	DPK	A	601	14/14	0.66	0.28	49,57,64,64	0
3	DPK	B	601	14/14	0.67	0.28	49,57,64,64	0
2	FAD	B	600	53/53	0.81	0.13	22,29,32,33	0
2	FAD	A	600	53/53	0.83	0.15	23,29,32,33	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.