



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:56 AM UTC

PDB ID : 9LPG / pdb_00009lpg
Title : Crystal structure of maize CRY-GL2 photoreceptor complex
Authors : Liu, Y.; Zhang, P.
Deposited on : 2025-01-24
Resolution : 2.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

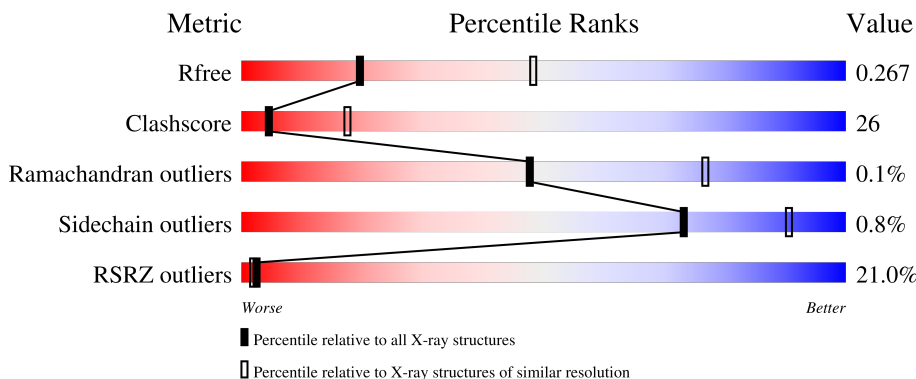
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	688	2% 54% 16% 29%
1	B	688	3% 51% 19% 29%
2	E	426	9% 58% 32% 8%
2	F	426	69% 32% 55% 5% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13981 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cryptochrome2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3947	2534	694	708	11			
1	B	488	Total	C	N	O	S	0	0	0
			3947	2534	694	708	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	TRP	engineered mutation	UNP B8A2L5
B	368	ALA	TRP	engineered mutation	UNP B8A2L5

- Molecule 2 is a protein called Protein ECERIFERUM 26-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	392	Total	C	N	O	S	0	0	0
			2974	1888	518	554	14			
2	F	392	Total	C	N	O	S	0	0	0
			2974	1888	518	554	14			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	E	4	Total	O	0	0
			4	4		
4	B	8	Total	O	0	0
			8	8		

- Molecule 1: Cryptochrome2







4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.35Å 217.06Å 228.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.17 – 2.80 42.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	77.4 (42.17-2.80) 91.4 (42.17-2.80)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.14_3260: 000)	Depositor
R, R_{free}	0.232 , 0.267 0.232 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13981	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	3/4070 (0.1%)	0.60	5/5550 (0.1%)
1	B	0.20	0/4070	0.44	1/5550 (0.0%)
2	E	0.29	1/3035 (0.0%)	0.69	11/4123 (0.3%)
2	F	0.51	1/3035 (0.0%)	1.12	26/4123 (0.6%)
All	All	0.35	5/14210 (0.0%)	0.72	43/19346 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	PRO	C-O	-6.76	1.15	1.24
1	A	206	PRO	C-O	-6.21	1.16	1.23
2	E	103	ASN	C-O	-5.46	1.17	1.24
1	A	205	THR	C-O	-5.30	1.19	1.24
2	F	407	LEU	N-CA	5.19	1.50	1.45

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	364	LEU	N-CA-C	-11.67	99.57	114.04
2	F	371	GLY	N-CA-C	10.59	126.32	114.67
2	E	139	LEU	N-CA-C	-9.80	95.03	109.15
2	E	363	ASP	N-CA-C	-8.61	97.13	109.96
2	F	408	PRO	N-CA-C	-8.51	97.13	110.50
1	B	137	GLU	N-CA-C	-7.82	105.71	114.62
2	F	33	VAL	N-CA-CB	7.25	123.19	111.23
2	F	316	PRO	N-CA-C	-7.21	103.17	113.47
2	E	223	GLU	N-CA-C	7.20	122.19	111.04
2	E	32	GLU	N-CA-C	-7.19	98.80	109.15
2	E	363	ASP	CB-CA-C	7.08	120.35	110.16
2	F	32	GLU	N-CA-C	-7.05	99.46	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	223	GLU	N-CA-C	6.85	121.66	111.04
2	F	413	ASP	N-CA-C	-6.79	103.80	111.07
1	A	181	CYS	CB-CA-C	-6.71	99.24	109.50
2	E	105	CYS	N-CA-C	-6.55	104.94	113.12
2	F	116	ARG	CA-C-N	-6.41	113.88	122.72
2	F	116	ARG	C-N-CA	-6.41	113.88	122.72
2	F	354	LEU	CB-CA-C	-6.36	99.16	109.72
2	F	372	GLN	CA-C-N	-6.03	109.69	123.15
2	F	372	GLN	C-N-CA	-6.03	109.69	123.15
2	F	409	GLY	N-CA-C	5.93	120.07	112.83
1	A	301	SER	N-CA-C	-5.85	98.34	110.80
2	F	246	LEU	CA-C-N	-5.81	112.59	122.11
2	F	246	LEU	C-N-CA	-5.81	112.59	122.11
2	F	370	LYS	N-CA-C	-5.80	98.43	110.80
2	F	116	ARG	N-CA-C	-5.79	100.25	109.23
2	F	251	GLN	CA-C-O	-5.57	115.68	122.64
2	F	173	ASP	CB-CA-C	-5.56	99.32	111.71
2	F	405	VAL	CA-C-N	-5.54	115.45	122.37
2	F	405	VAL	C-N-CA	-5.54	115.45	122.37
2	F	174	ILE	N-CA-C	5.53	120.82	108.88
2	E	370	LYS	N-CA-C	-5.53	99.91	108.31
2	E	104	ASP	CB-CA-C	5.51	121.38	110.42
2	F	139	LEU	N-CA-C	-5.50	101.76	109.96
1	A	206	PRO	CB-CA-C	-5.47	104.40	111.46
1	A	90	ASP	N-CA-C	-5.22	104.66	111.02
2	E	312	ALA	N-CA-C	-5.16	106.58	112.92
1	A	311	ARG	CB-CG-CD	-5.12	99.52	111.30
2	F	174	ILE	N-CA-CB	-5.12	104.04	111.21
2	E	313	GLY	CA-C-O	-5.09	111.72	120.57
2	F	115	ASP	CA-C-N	5.03	130.59	122.29
2	F	115	ASP	C-N-CA	5.03	130.59	122.29

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	3947	0	3828	87	1
1	B	3947	0	3828	111	1
2	E	2974	0	2964	113	0
2	F	2974	0	2961	421	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
4	A	21	0	0	0	1
4	B	8	0	0	0	1
4	E	4	0	0	0	0
All	All	13981	0	13643	722	2

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 26.

All (722) 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)
2:F:174:ILE:CG2	2:F:359:MET:HE1	1.28	1.56
2:F:308:TYR:CE1	2:F:333:VAL:HG11	1.48	1.44
2:F:308:TYR:CG	2:F:333:VAL:HG21	1.53	1.42
1:B:472:LYS:NZ	1:B:476:GLN:HE21	1.18	1.39
2:F:174:ILE:CG2	2:F:359:MET:CE	2.00	1.37
2:F:391:LEU:HD21	2:F:393:GLN:OE1	1.20	1.34
1:B:472:LYS:HZ2	1:B:476:GLN:NE2	1.25	1.31
2:F:174:ILE:HG21	2:F:359:MET:CE	1.55	1.31
2:F:360:GLU:OE2	2:F:392:VAL:CG1	1.79	1.30
2:F:15:ALA:HA	2:F:116:ARG:NH2	1.45	1.29
2:F:285:VAL:CG2	2:F:354:LEU:O	1.80	1.29
2:F:139:LEU:HD11	2:F:143:LEU:CD1	1.64	1.25
2:F:125:ALA:HB1	2:F:416:ARG:NH2	1.55	1.21
2:F:63:THR:CG2	2:F:67:LYS:HE3	1.72	1.19
1:A:177:ASP:OD1	1:A:179:SER:OG	1.63	1.17
2:F:174:ILE:HB	2:F:359:MET:HE3	1.24	1.17
2:F:245:VAL:O	2:F:249:LEU:HD13	1.41	1.16
2:F:407:LEU:HD22	2:F:412:ILE:CG1	1.77	1.15
2:F:114:CYS:SG	2:F:116:ARG:NE	2.22	1.13
2:F:405:VAL:HG13	2:F:407:LEU:HD13	1.21	1.12
2:F:15:ALA:CA	2:F:116:ARG:HH21	1.61	1.12
2:F:357:VAL:HB	2:F:391:LEU:HA	1.15	1.12
2:F:285:VAL:HG22	2:F:354:LEU:O	1.47	1.11
2:F:33:VAL:O	2:F:102:CYS:HB2	1.49	1.11
2:F:268:SER:HB3	2:F:356:LEU:HD23	1.22	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:308:TYR:CD2	2:F:333:VAL:HG21	1.86	1.10
2:F:285:VAL:HG23	2:F:354:LEU:O	1.49	1.10
2:F:308:TYR:O	2:F:333:VAL:HG22	1.53	1.08
2:F:407:LEU:HD22	2:F:412:ILE:HG12	1.32	1.08
2:F:360:GLU:OE2	2:F:392:VAL:HG12	1.45	1.07
2:F:139:LEU:CD1	2:F:143:LEU:HD12	1.84	1.07
2:F:114:CYS:SG	2:F:116:ARG:CD	2.43	1.06
2:F:360:GLU:OE2	2:F:392:VAL:HG11	1.53	1.06
2:F:308:TYR:CZ	2:F:333:VAL:HG11	1.90	1.04
2:F:289:ARG:HA	2:F:358:ASP:HB3	1.40	1.04
2:F:174:ILE:CB	2:F:359:MET:HE3	1.90	1.01
2:F:359:MET:O	2:F:362:VAL:CG1	2.08	1.01
2:F:356:LEU:HA	2:F:390:VAL:HG23	1.40	1.00
2:F:246:LEU:HA	2:F:249:LEU:HD22	1.42	1.00
2:F:174:ILE:CB	2:F:359:MET:CE	2.40	1.00
2:F:391:LEU:CD2	2:F:393:GLN:OE1	2.10	1.00
2:F:308:TYR:CE1	2:F:333:VAL:CG1	2.44	0.99
2:E:113:ARG:HE	2:E:157:LYS:HZ3	1.00	0.98
2:F:24:VAL:HG22	2:F:109:ILE:HD11	1.47	0.96
2:F:405:VAL:HG22	2:F:407:LEU:HD11	1.43	0.96
2:F:83:ARG:CZ	2:F:105:CYS:HB3	1.98	0.94
2:F:125:ALA:HB1	2:F:416:ARG:HH22	1.32	0.94
1:B:136:TRP:O	1:B:136:TRP:CD1	2.20	0.94
2:E:113:ARG:NE	2:E:157:LYS:NZ	2.15	0.93
2:F:308:TYR:CG	2:F:333:VAL:CG2	2.50	0.93
2:F:391:LEU:HD21	2:F:393:GLN:CD	1.93	0.93
1:A:308:ALA:O	1:A:311:ARG:HG3	1.67	0.93
2:F:139:LEU:CD1	2:F:143:LEU:CD1	2.42	0.93
1:A:91:THR:OG1	1:A:181:CYS:SG	2.27	0.93
2:F:405:VAL:CG2	2:F:407:LEU:HD11	1.99	0.92
2:F:308:TYR:H	2:F:333:VAL:HG23	1.33	0.92
2:F:390:VAL:HG12	2:F:405:VAL:HG23	1.50	0.92
2:F:174:ILE:HB	2:F:359:MET:CE	1.97	0.92
2:F:362:VAL:O	2:F:364:LEU:HD12	1.68	0.92
2:F:114:CYS:SG	2:F:116:ARG:HD2	2.10	0.92
2:F:273:GLN:HG3	2:F:316:PRO:O	1.70	0.91
2:E:113:ARG:NE	2:E:157:LYS:HZ3	1.68	0.91
1:A:85:LEU:HA	1:A:88:VAL:HG12	1.49	0.91
2:F:139:LEU:HD11	2:F:143:LEU:HD12	0.91	0.90
2:F:189:SER:HB3	2:F:370:LYS:HA	1.52	0.90
1:A:88:VAL:HG21	1:A:122:ILE:HD12	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ARG:HH22	1:B:98:PHE:HD1	1.18	0.90
2:F:264:PHE:HB3	2:F:360:GLU:OE1	1.71	0.89
2:F:56:ARG:HG3	2:F:375:VAL:CG2	2.02	0.89
2:F:359:MET:O	2:F:362:VAL:HG12	1.72	0.89
2:F:308:TYR:N	2:F:333:VAL:CG2	2.35	0.89
2:E:113:ARG:HG2	2:E:155:ASN:HB2	1.55	0.89
2:F:357:VAL:CB	2:F:391:LEU:HA	2.02	0.88
2:F:405:VAL:HG13	2:F:407:LEU:CD1	2.02	0.88
2:F:308:TYR:CZ	2:F:333:VAL:CG1	2.57	0.88
2:F:407:LEU:HD22	2:F:412:ILE:HG13	1.52	0.88
2:F:391:LEU:CD2	2:F:393:GLN:CD	2.46	0.88
2:F:308:TYR:CD2	2:F:333:VAL:CG2	2.56	0.87
2:F:238:SER:OG	2:F:404:THR:HG22	1.73	0.86
1:A:69:ALA:HB2	1:A:173:ILE:HD11	1.56	0.86
1:A:89:ARG:NH1	1:A:120:GLU:OE1	2.08	0.86
2:F:308:TYR:N	2:F:333:VAL:HG23	1.90	0.86
2:F:308:TYR:CD1	2:F:333:VAL:HG21	2.11	0.85
2:F:405:VAL:CG1	2:F:407:LEU:HD13	2.06	0.85
2:F:45:LYS:HG3	2:F:46:LEU:HD12	1.56	0.85
2:F:63:THR:HG23	2:F:67:LYS:HE3	1.56	0.84
2:F:83:ARG:HD3	2:F:105:CYS:SG	2.17	0.84
2:F:359:MET:O	2:F:362:VAL:HG13	1.75	0.84
2:F:174:ILE:CG2	2:F:359:MET:HE3	2.04	0.84
2:F:237:TYR:HB3	2:F:412:ILE:HD13	1.59	0.84
2:F:174:ILE:HG22	2:F:359:MET:CE	2.07	0.84
1:A:177:ASP:CG	1:A:179:SER:OG	2.21	0.84
1:B:6:TRP:CZ3	1:B:8:ARG:NH1	2.45	0.84
2:F:360:GLU:CD	2:F:392:VAL:HG12	2.02	0.84
2:F:97:ARG:HH12	2:F:204:PRO:HB2	1.44	0.83
2:F:184:TRP:HA	2:F:187:ILE:HD12	1.60	0.83
2:F:46:LEU:HD22	2:F:347:LEU:HD11	1.61	0.82
2:E:37:LEU:O	2:E:97:ARG:NH2	2.11	0.82
2:F:174:ILE:HD12	2:F:359:MET:SD	2.19	0.82
2:F:405:VAL:HG22	2:F:407:LEU:CD1	2.08	0.82
2:F:37:LEU:HD11	2:F:42:LEU:HG	1.61	0.82
1:B:8:ARG:NH2	1:B:99:ASN:O	2.13	0.81
2:F:32:GLU:O	2:F:33:VAL:HG23	1.80	0.81
2:F:37:LEU:HD22	2:F:170:LEU:HD11	1.60	0.81
2:F:234:MET:HE3	2:F:386:ASP:HA	1.61	0.81
2:E:113:ARG:HE	2:E:157:LYS:NZ	1.72	0.81
2:E:305:LYS:HD2	2:E:336:THR:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:285:VAL:HG23	2:F:354:LEU:HB3	1.63	0.81
2:F:272:TRP:HZ3	2:F:328:LEU:HD11	1.46	0.80
2:F:360:GLU:HA	2:F:393:GLN:HA	1.64	0.80
2:E:368:GLU:HG3	2:E:373:ARG:HG2	1.62	0.80
2:F:125:ALA:HB1	2:F:416:ARG:HH21	1.46	0.80
2:F:308:TYR:H	2:F:333:VAL:CG2	1.93	0.80
2:E:279:ARG:HD3	2:E:411:GLU:OE2	1.82	0.79
2:F:315:SER:O	2:F:319:THR:OG1	1.99	0.79
1:B:306:LEU:HD12	1:B:307:LEU:H	1.48	0.79
2:F:308:TYR:CE2	2:F:333:VAL:HB	2.18	0.79
2:F:308:TYR:CD1	2:F:333:VAL:HG11	2.15	0.78
2:E:237:TYR:HD1	2:E:416:ARG:HH21	1.31	0.78
2:F:63:THR:CG2	2:F:67:LYS:CE	2.57	0.78
2:F:114:CYS:SG	2:F:116:ARG:CZ	2.71	0.78
2:E:16:VAL:HG12	2:E:114:CYS:HB2	1.66	0.77
2:E:292:ALA:HA	2:E:295:ARG:HG3	1.66	0.77
2:F:272:TRP:CZ3	2:F:328:LEU:HD11	2.19	0.77
2:F:264:PHE:O	2:F:268:SER:OG	2.00	0.77
1:B:312:PHE:O	1:B:482:MET:HG3	1.83	0.76
2:F:97:ARG:NH1	2:F:204:PRO:CB	2.48	0.76
1:B:85:LEU:HD11	1:B:120:GLU:HG3	1.68	0.76
2:F:356:LEU:HA	2:F:390:VAL:CG2	2.15	0.75
1:B:312:PHE:O	1:B:482:MET:CG	2.34	0.75
2:F:189:SER:HA	2:F:370:LYS:HG2	1.68	0.75
2:F:15:ALA:CA	2:F:116:ARG:NH2	2.32	0.75
1:B:472:LYS:NZ	1:B:476:GLN:NE2	2.00	0.74
2:F:360:GLU:CG	2:F:392:VAL:HG12	2.16	0.74
2:F:139:LEU:HD23	2:F:226:TRP:CE3	2.21	0.74
2:F:16:VAL:HG23	2:F:113:ARG:O	1.88	0.74
2:F:97:ARG:NH1	2:F:204:PRO:HB2	2.02	0.74
2:F:237:TYR:HB3	2:F:412:ILE:CD1	2.18	0.74
2:F:276:ALA:HA	2:F:282:VAL:HG21	1.70	0.74
2:E:334:ASP:OD1	2:E:336:THR:HG22	1.87	0.73
2:F:139:LEU:HD21	2:F:143:LEU:HD11	1.69	0.73
2:F:168:ALA:O	2:F:171:ILE:HG22	1.88	0.73
1:A:63:SER:O	1:A:67:LEU:HD12	1.88	0.73
2:F:37:LEU:CD2	2:F:170:LEU:HD11	2.18	0.73
1:B:472:LYS:HZ3	1:B:476:GLN:HE21	1.36	0.73
2:F:117:ASP:O	2:F:120:GLU:HB3	1.89	0.72
2:F:62:ALA:O	2:F:65:VAL:HG22	1.89	0.72
1:B:306:LEU:HD12	1:B:307:LEU:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:269:ALA:HB1	2:F:324:LEU:HG	1.70	0.72
1:B:136:TRP:O	1:B:136:TRP:HD1	1.73	0.72
2:E:113:ARG:NH2	2:E:157:LYS:HZ2	1.87	0.72
1:B:6:TRP:CE3	1:B:8:ARG:NH1	2.58	0.72
2:F:272:TRP:NE1	2:F:282:VAL:HG12	2.04	0.72
1:A:169:PRO:HG3	1:B:264:LEU:HD22	1.71	0.72
2:F:136:ASP:O	2:F:137:LYS:HG3	1.90	0.72
2:E:113:ARG:CZ	2:E:157:LYS:NZ	2.52	0.71
2:E:237:TYR:CE1	2:E:416:ARG:NE	2.58	0.71
2:F:215:SER:OG	2:F:335:GLU:OE2	2.09	0.71
2:F:308:TYR:O	2:F:333:VAL:CG2	2.36	0.71
1:B:69:ALA:HB2	1:B:173:ILE:HD11	1.73	0.71
2:F:408:PRO:HB2	2:F:411:GLU:HG3	1.72	0.71
2:F:37:LEU:CD1	2:F:42:LEU:HG	2.20	0.71
1:B:425:ARG:HG2	1:B:432:ALA:HA	1.74	0.70
2:F:350:GLY:H	2:F:355:THR:CG2	2.04	0.70
2:F:125:ALA:CB	2:F:416:ARG:HH22	2.04	0.70
2:E:237:TYR:CD1	2:E:416:ARG:NH2	2.59	0.70
2:F:197:VAL:HG12	2:F:298:LYS:HG2	1.74	0.70
2:F:37:LEU:HD22	2:F:170:LEU:CD1	2.21	0.70
2:F:86:ARG:HH11	2:F:96:ARG:HD2	1.57	0.70
2:F:237:TYR:CE1	2:F:416:ARG:NH2	2.58	0.70
2:F:83:ARG:CZ	2:F:105:CYS:CB	2.69	0.69
2:F:139:LEU:CG	2:F:143:LEU:CD1	2.70	0.69
2:E:115:ASP:HA	2:E:157:LYS:HG2	1.75	0.69
2:F:83:ARG:NH1	2:F:105:CYS:HB3	2.06	0.69
2:F:350:GLY:H	2:F:355:THR:HG23	1.57	0.69
2:F:48:TYR:CZ	2:F:138:VAL:HB	2.28	0.69
2:F:41:ASP:HA	2:F:302:ASN:HD22	1.58	0.69
2:F:54:TYR:CE2	2:F:122:ILE:HD11	2.27	0.69
2:E:289:ARG:HG2	2:E:358:ASP:HB3	1.74	0.68
2:F:272:TRP:HE1	2:F:282:VAL:HG12	1.57	0.68
1:B:88:VAL:HB	1:B:93:ALA:HB3	1.75	0.68
2:F:268:SER:CB	2:F:356:LEU:HD23	2.12	0.68
2:F:63:THR:HG22	2:F:67:LYS:HE3	1.71	0.68
2:F:83:ARG:CD	2:F:105:CYS:HB2	2.24	0.68
2:F:360:GLU:CD	2:F:401:ARG:HD2	2.18	0.67
2:F:392:VAL:HA	2:F:403:VAL:HG22	1.76	0.67
1:B:306:LEU:HD11	1:B:392:GLN:HG2	1.76	0.67
2:F:169:HIS:CE1	2:F:173:ASP:HA	2.30	0.67
2:F:264:PHE:HB3	2:F:360:GLU:CD	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:SER:H	2:F:372:GLN:HE22	1.41	0.67
2:F:289:ARG:HA	2:F:358:ASP:CB	2.20	0.67
1:A:171:LYS:O	1:A:172:ARG:HG3	1.94	0.67
2:E:113:ARG:CZ	2:E:157:LYS:HZ2	2.07	0.67
2:E:266:LEU:HD23	2:E:325:ALA:CB	2.25	0.67
2:F:61:LEU:HA	2:F:65:VAL:HG21	1.75	0.66
2:F:126:ALA:HB3	2:F:129:ARG:HG2	1.76	0.66
2:F:285:VAL:CG2	2:F:354:LEU:HB3	2.25	0.66
1:B:402:ARG:NH1	1:B:408:ASP:OD2	2.26	0.66
1:B:310:LEU:HD22	1:B:482:MET:HE1	1.76	0.66
2:F:239:PHE:CE2	2:F:419:LEU:HD13	2.31	0.66
2:E:61:LEU:HD13	2:E:369:ILE:HD12	1.78	0.66
2:E:282:VAL:O	2:E:316:PRO:HG2	1.95	0.66
2:F:415:LEU:HD23	2:F:419:LEU:HD23	1.77	0.66
2:F:139:LEU:HD13	2:F:146:SER:OG	1.96	0.65
1:B:454:GLY:O	1:B:460:ASN:ND2	2.29	0.65
2:E:216:VAL:HG11	2:E:348:VAL:HG22	1.78	0.65
2:E:358:ASP:OD1	2:E:360:GLU:HG2	1.96	0.65
2:E:140:GLY:HA2	2:E:225:LEU:HD13	1.78	0.65
1:A:309:HIS:CE1	1:A:397:SER:OG	2.50	0.65
2:F:15:ALA:HA	2:F:116:ARG:HH21	0.66	0.64
2:F:73:TRP:HB2	2:F:187:ILE:HD13	1.79	0.64
2:F:125:ALA:CB	2:F:416:ARG:NH2	2.47	0.64
2:F:405:VAL:CG1	2:F:407:LEU:CD1	2.71	0.64
2:F:287:VAL:HG22	2:F:356:LEU:HB2	1.79	0.64
2:F:57:SER:H	2:F:372:GLN:NE2	1.95	0.64
2:F:240:HIS:HE1	2:F:242:SER:HA	1.63	0.64
1:A:30:VAL:HG21	1:A:91:THR:HG21	1.80	0.64
2:F:55:TYR:O	2:F:118:MET:HE1	1.98	0.63
2:F:271:VAL:O	2:F:275:VAL:HG23	1.98	0.63
2:F:55:TYR:CD2	2:F:369:ILE:HD12	2.33	0.63
2:F:390:VAL:CG1	2:F:405:VAL:HG23	2.26	0.63
2:F:117:ASP:CG	2:F:158:CYS:HB3	2.23	0.63
2:E:61:LEU:HD13	2:E:369:ILE:CD1	2.29	0.63
1:B:301:SER:O	1:B:305:PRO:HB3	1.99	0.63
2:E:232:ARG:NH1	2:E:410:ASP:OD2	2.32	0.63
2:F:139:LEU:CD1	2:F:143:LEU:HD13	2.27	0.62
1:A:365:GLN:OE1	1:A:474:ARG:NH2	2.28	0.62
2:F:324:LEU:O	2:F:328:LEU:HD13	2.00	0.62
2:F:359:MET:HB3	2:F:362:VAL:HG11	1.81	0.62
1:A:130:ASP:O	1:A:288:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HG12	1:B:95:HIS:HB2	1.80	0.62
2:F:69:PRO:HB3	2:F:187:ILE:HG22	1.81	0.62
2:F:200:PRO:HD2	2:F:298:LYS:HD3	1.81	0.62
2:F:183:LYS:HE2	2:F:186:GLN:HE22	1.64	0.62
1:B:6:TRP:CZ2	1:B:8:ARG:HD3	2.35	0.61
2:F:83:ARG:NE	2:F:105:CYS:HB2	2.16	0.61
2:E:266:LEU:HD23	2:E:325:ALA:HB3	1.82	0.61
2:E:311:SER:OG	2:E:314:SER:O	2.17	0.61
2:F:225:LEU:HD23	2:F:227:LEU:H	1.64	0.61
2:E:46:LEU:HD23	2:E:226:TRP:C	2.26	0.61
2:F:174:ILE:CD1	2:F:359:MET:SD	2.88	0.61
2:F:56:ARG:HG3	2:F:375:VAL:HG21	1.82	0.61
2:F:63:THR:HG22	2:F:67:LYS:CE	2.30	0.61
2:F:197:VAL:O	2:F:198:LEU:HD23	2.01	0.61
2:F:389:ALA:H	2:F:406:VAL:HG12	1.66	0.61
1:A:468:LEU:HD22	2:E:29:VAL:HG21	1.83	0.60
2:E:360:GLU:OE1	2:E:401:ARG:NE	2.32	0.60
2:F:308:TYR:CE2	2:F:333:VAL:CB	2.83	0.60
2:F:45:LYS:HB3	2:F:170:LEU:HD23	1.83	0.60
2:F:139:LEU:HD21	2:F:143:LEU:CD1	2.30	0.60
2:F:274:ALA:O	2:F:278:ILE:HG12	2.01	0.60
1:B:306:LEU:HD11	1:B:392:GLN:CG	2.30	0.60
2:F:173:ASP:N	2:F:176:SER:OG	2.35	0.60
2:F:63:THR:HG21	2:F:67:LYS:HE3	1.73	0.60
2:F:182:ASN:O	2:F:186:GLN:HG3	2.02	0.60
2:F:333:VAL:HG23	2:F:333:VAL:O	2.01	0.60
2:E:113:ARG:HG2	2:E:155:ASN:CB	2.31	0.60
1:B:6:TRP:CH2	1:B:8:ARG:HD3	2.37	0.60
2:F:156:PHE:HB2	2:F:158:CYS:SG	2.42	0.59
2:F:376:TYR:OH	2:F:378:GLU:OE1	2.20	0.59
2:F:391:LEU:CG	2:F:393:GLN:CD	2.75	0.59
1:A:66:ARG:NH1	1:B:268:ASN:OD1	2.35	0.59
2:F:83:ARG:CD	2:F:105:CYS:CB	2.81	0.59
2:F:97:ARG:HH11	2:F:204:PRO:HB3	1.67	0.59
2:F:114:CYS:SG	2:F:116:ARG:CG	2.91	0.59
2:F:360:GLU:HG3	2:F:392:VAL:O	2.02	0.59
2:F:389:ALA:H	2:F:406:VAL:CG1	2.15	0.59
1:B:312:PHE:O	1:B:482:MET:SD	2.60	0.59
2:F:379:TYR:HB2	2:F:393:GLN:HE22	1.67	0.59
2:F:379:TYR:O	2:F:404:THR:HG21	2.03	0.59
1:A:91:THR:O	1:A:91:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:SER:HA	1:B:253:ARG:HH22	1.68	0.59
2:F:183:LYS:HD3	2:F:193:PRO:HB2	1.84	0.59
1:B:472:LYS:O	1:B:472:LYS:HD3	2.02	0.59
2:F:391:LEU:HG	2:F:393:GLN:CD	2.28	0.59
1:A:268:ASN:OD1	1:B:66:ARG:NH1	2.36	0.59
2:F:73:TRP:NE1	2:F:180:CYS:SG	2.75	0.59
1:A:392:GLN:HB3	1:A:398:LEU:HD13	1.85	0.59
2:E:172:GLY:HA2	2:E:301:ALA:O	2.04	0.58
2:F:97:ARG:NH1	2:F:204:PRO:HB3	2.18	0.58
2:F:189:SER:CB	2:F:370:LYS:HA	2.28	0.58
1:A:65:ARG:HH21	1:A:71:LYS:HB3	1.69	0.58
1:B:8:ARG:NH2	1:B:98:PHE:CD1	2.67	0.58
2:F:348:VAL:HG13	2:F:349:TYR:CD1	2.38	0.58
1:B:312:PHE:HB3	1:B:482:MET:HG3	1.86	0.58
2:F:382:ASP:OD1	2:F:383:GLY:N	2.33	0.58
2:F:388:GLY:HA2	2:F:406:VAL:HG13	1.85	0.58
2:E:173:ASP:OD1	2:E:176:SER:OG	2.22	0.58
2:E:359:MET:HE3	2:E:391:LEU:HB3	1.86	0.58
2:F:83:ARG:NE	2:F:105:CYS:CB	2.67	0.58
2:F:83:ARG:NH2	2:F:147:PRO:HG3	2.18	0.57
2:F:359:MET:HB2	2:F:391:LEU:HD11	1.86	0.57
2:E:306:VAL:H	2:E:336:THR:HB	1.69	0.57
2:F:49:LEU:HD11	2:F:174:ILE:HG12	1.85	0.57
2:F:308:TYR:CA	2:F:333:VAL:CG2	2.82	0.57
2:F:342:PHE:CE1	2:F:346:VAL:HG13	2.39	0.57
2:E:26:PRO:HD2	2:E:104:ASP:HB3	1.85	0.57
2:E:60:GLY:O	2:E:370:LYS:NZ	2.37	0.57
2:E:220:GLY:O	2:E:221:PRO:C	2.46	0.57
1:A:85:LEU:O	1:A:89:ARG:HG3	2.03	0.57
2:E:113:ARG:NH2	2:E:157:LYS:NZ	2.50	0.57
2:F:172:GLY:HA2	2:F:301:ALA:O	2.05	0.57
2:F:291:ASP:OD2	2:F:293:ALA:HB3	2.04	0.57
2:E:289:ARG:HG2	2:E:358:ASP:CB	2.34	0.57
2:F:56:ARG:CG	2:F:375:VAL:HG21	2.34	0.57
1:B:85:LEU:HD12	1:B:116:MET:HE1	1.86	0.57
1:B:138:VAL:HG13	1:B:155:ARG:HG3	1.85	0.57
2:F:131:ARG:HH22	2:F:382:ASP:HB2	1.69	0.57
2:E:232:ARG:NH2	2:E:410:ASP:OD2	2.36	0.57
2:F:48:TYR:O	2:F:381:MET:HG3	2.05	0.57
2:F:183:LYS:HD3	2:F:193:PRO:CB	2.34	0.57
1:A:348:LEU:O	1:A:353:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:286:THR:O	2:F:355:THR:HA	2.05	0.57
1:A:59:HIS:CE1	1:A:209:GLN:HB2	2.40	0.56
2:E:49:LEU:HD11	2:E:174:ILE:HG12	1.87	0.56
2:F:61:LEU:CD1	2:F:161:LEU:HD22	2.35	0.56
2:F:37:LEU:HD13	2:F:41:ASP:HB2	1.87	0.56
2:F:174:ILE:HG21	2:F:359:MET:HE1	0.59	0.56
2:F:350:GLY:HA2	2:F:387:GLU:HB2	1.86	0.56
1:B:136:TRP:O	1:B:136:TRP:CG	2.57	0.56
2:F:285:VAL:HG23	2:F:354:LEU:C	2.27	0.56
1:A:312:PHE:HB3	1:A:485:LEU:HD13	1.88	0.56
1:B:102:TYR:OH	1:B:134:GLU:OE2	2.23	0.56
2:F:158:CYS:SG	2:F:160:GLY:N	2.79	0.56
2:F:237:TYR:CB	2:F:412:ILE:HD13	2.34	0.56
2:F:350:GLY:C	2:F:387:GLU:HB2	2.30	0.56
1:A:85:LEU:CA	1:A:88:VAL:HG12	2.29	0.56
2:E:112:ALA:O	2:E:154:THR:HA	2.06	0.56
2:F:32:GLU:O	2:F:33:VAL:CG2	2.53	0.56
2:F:185:ALA:HB2	2:F:367:LEU:HD12	1.87	0.56
2:F:407:LEU:CD2	2:F:412:ILE:HG13	2.30	0.56
2:E:415:LEU:HG	2:E:419:LEU:HD23	1.86	0.56
1:A:24:ARG:O	1:A:24:ARG:HG2	2.05	0.56
2:E:284:THR:HG22	2:E:310:GLU:HB2	1.88	0.56
2:E:328:LEU:HD21	2:E:356:LEU:HD13	1.87	0.56
2:F:86:ARG:NH1	2:F:96:ARG:HD2	2.20	0.56
2:F:315:SER:O	2:F:319:THR:N	2.39	0.56
2:F:321:VAL:HA	2:F:324:LEU:HD21	1.88	0.56
2:F:56:ARG:HG3	2:F:375:VAL:HG22	1.84	0.55
1:A:208:TRP:CE3	1:A:209:GLN:HG3	2.42	0.55
2:F:289:ARG:HE	2:F:358:ASP:CG	2.14	0.55
2:F:391:LEU:O	2:F:403:VAL:HA	2.07	0.55
2:E:156:PHE:C	2:E:157:LYS:HE2	2.32	0.55
2:F:49:LEU:CD1	2:F:174:ILE:HG12	2.36	0.55
2:F:406:VAL:C	2:F:407:LEU:HD12	2.31	0.55
1:A:434:LEU:HD12	1:A:435:PRO:HD2	1.87	0.55
1:B:425:ARG:HG3	1:B:439:ILE:HD11	1.87	0.55
2:F:115:ASP:HA	2:F:157:LYS:HG3	1.87	0.55
2:F:143:LEU:HD22	2:F:224:ASP:HA	1.87	0.55
1:B:94:THR:OG1	1:B:95:HIS:ND1	2.31	0.55
1:B:348:LEU:O	1:B:353:ARG:NH1	2.40	0.55
1:A:313:PHE:CE2	1:A:315:TRP:CE3	2.95	0.54
2:F:33:VAL:C	2:F:102:CYS:HB2	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:ARG:HB3	2:F:96:ARG:HG2	1.88	0.54
2:F:114:CYS:SG	2:F:116:ARG:HG3	2.47	0.54
1:B:312:PHE:CB	1:B:482:MET:HG3	2.37	0.54
2:F:296:SER:OG	2:F:303:GLU:OE1	2.05	0.54
2:E:130:ILE:HD11	2:E:378:GLU:HG3	1.89	0.54
1:B:11:LEU:HD12	1:B:247:PHE:HB3	1.88	0.54
1:B:392:GLN:HB3	1:B:398:LEU:HD23	1.88	0.54
1:B:47:ARG:HH21	1:B:193:GLU:HB3	1.72	0.54
2:E:309:VAL:HG22	2:E:332:VAL:HA	1.90	0.54
2:F:266:LEU:HD23	2:F:266:LEU:O	2.08	0.54
2:F:56:ARG:CG	2:F:375:VAL:CG2	2.82	0.53
1:B:398:LEU:HD12	1:B:400:ASP:H	1.73	0.53
2:F:73:TRP:HB2	2:F:187:ILE:CD1	2.39	0.53
2:F:141:PRO:HD3	2:F:225:LEU:HD12	1.90	0.53
2:F:415:LEU:HA	2:F:418:ALA:HB3	1.89	0.53
2:F:139:LEU:HG	2:F:143:LEU:HD13	1.90	0.53
2:F:86:ARG:HD2	2:F:96:ARG:CD	2.39	0.53
1:A:12:ARG:HB2	1:A:208:TRP:HD1	1.74	0.53
2:F:61:LEU:HA	2:F:65:VAL:CG2	2.39	0.53
2:F:308:TYR:CZ	2:F:333:VAL:CB	2.91	0.53
1:B:321:TYR:CD1	1:B:465:ILE:HD11	2.42	0.53
2:F:83:ARG:HD3	2:F:105:CYS:CB	2.37	0.53
2:F:362:VAL:O	2:F:364:LEU:CD1	2.49	0.53
2:E:272:TRP:HE1	2:E:282:VAL:HG12	1.73	0.53
1:B:52:TRP:HE3	1:B:380:LEU:HD22	1.72	0.53
2:F:362:VAL:HG22	2:F:364:LEU:HG	1.91	0.53
2:F:397:ASP:OD1	2:F:399:ARG:HB2	2.09	0.53
2:F:389:ALA:N	2:F:406:VAL:CG1	2.72	0.53
2:F:389:ALA:N	2:F:406:VAL:HG12	2.24	0.53
2:F:243:ASP:HA	2:F:246:LEU:HB3	1.90	0.52
2:F:139:LEU:CG	2:F:143:LEU:HD13	2.40	0.52
1:A:175:SER:HB2	1:A:178:LEU:HD11	1.90	0.52
2:E:237:TYR:CE1	2:E:416:ARG:CZ	2.93	0.52
2:F:139:LEU:HD12	2:F:140:GLY:H	1.73	0.52
2:E:270:LEU:HD11	2:E:422:ALA:HB1	1.91	0.52
1:B:39:GLU:OE1	1:B:109:ARG:NH1	2.36	0.52
2:F:42:LEU:HD21	2:F:98:PRO:HD2	1.91	0.52
2:F:114:CYS:HB3	2:F:156:PHE:CD1	2.45	0.52
2:F:243:ASP:O	2:F:246:LEU:HB3	2.10	0.52
2:F:272:TRP:CD1	2:F:282:VAL:HG12	2.45	0.52
1:B:17:PRO:HD2	1:B:99:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:NH2	1:B:182:PRO:HD2	2.24	0.52
2:F:228:VAL:HG11	2:F:347:LEU:HG	1.91	0.52
1:B:109:ARG:HD2	1:B:113:LEU:HD13	1.91	0.52
2:F:86:ARG:NH1	2:F:86:ARG:HB2	2.25	0.52
2:F:327:LEU:HD12	2:F:331:ASN:CG	2.35	0.52
2:F:360:GLU:CG	2:F:401:ARG:HD2	2.40	0.52
1:A:138:VAL:HG23	1:A:155:ARG:HG3	1.90	0.51
2:F:121:TRP:CZ2	2:F:129:ARG:HB3	2.45	0.51
2:F:272:TRP:CH2	2:F:285:VAL:HG12	2.45	0.51
1:A:98:PHE:O	1:A:126:SER:HA	2.09	0.51
1:A:454:GLY:O	1:A:460:ASN:ND2	2.43	0.51
2:F:277:LYS:NZ	2:F:418:ALA:HB1	2.25	0.51
2:F:346:VAL:O	2:F:347:LEU:HD13	2.11	0.51
2:E:115:ASP:HA	2:E:157:LYS:CG	2.40	0.51
2:F:123:ARG:HB2	2:F:123:ARG:NH1	2.26	0.51
2:F:273:GLN:NE2	2:F:317:ALA:O	2.43	0.51
2:F:321:VAL:HA	2:F:324:LEU:CD2	2.41	0.51
2:F:359:MET:HB2	2:F:393:GLN:HG2	1.91	0.51
1:B:52:TRP:CH2	1:B:243:PRO:HB2	2.46	0.51
2:F:84:VAL:HG11	2:F:139:LEU:HD21	1.92	0.51
2:F:364:LEU:HB3	2:F:377:VAL:HG11	1.91	0.51
2:E:169:HIS:CE1	2:E:173:ASP:HA	2.46	0.51
2:F:273:GLN:HG3	2:F:316:PRO:C	2.35	0.51
2:E:118:MET:O	2:E:122:ILE:HG12	2.10	0.51
2:F:35:TYR:HB3	2:F:100:ILE:HB	1.91	0.51
2:F:246:LEU:HD22	2:F:246:LEU:O	2.11	0.51
1:B:17:PRO:HD2	1:B:99:ASN:HD21	1.76	0.51
2:F:41:ASP:HA	2:F:302:ASN:ND2	2.23	0.51
2:F:115:ASP:CB	2:F:157:LYS:HG3	2.41	0.51
2:F:349:TYR:HD2	2:F:381:MET:SD	2.33	0.51
2:E:289:ARG:HA	2:E:358:ASP:HB3	1.92	0.50
2:E:41:ASP:OD1	2:E:302:ASN:HB2	2.11	0.50
2:F:350:GLY:CA	2:F:387:GLU:HB2	2.42	0.50
2:F:405:VAL:CG2	2:F:407:LEU:CD1	2.75	0.50
1:A:12:ARG:HD3	1:A:248:GLY:O	2.12	0.50
1:A:208:TRP:CZ3	1:A:209:GLN:HG3	2.46	0.50
1:B:104:PRO:HD3	1:B:295:SER:OG	2.12	0.50
2:F:78:PHE:CG	2:F:79:PRO:HD3	2.46	0.50
2:F:243:ASP:OD2	2:F:399:ARG:HD2	2.11	0.50
2:F:359:MET:HB3	2:F:362:VAL:CG1	2.41	0.50
1:A:30:VAL:HG21	1:A:91:THR:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PHE:CD1	1:B:222:PRO:HG2	2.47	0.50
1:B:372:MET:HG2	1:B:391:TRP:CD1	2.46	0.50
2:F:305:LYS:HA	2:F:336:THR:HG21	1.92	0.50
2:F:393:GLN:HB3	2:F:394:PRO:HD2	1.92	0.50
1:B:87:LEU:O	1:B:91:THR:HG23	2.11	0.50
1:B:218:PHE:HD1	1:B:222:PRO:HG2	1.76	0.50
2:F:173:ASP:CG	2:F:302:ASN:HA	2.37	0.50
2:E:328:LEU:HD21	2:E:356:LEU:CD1	2.41	0.50
2:F:97:ARG:HH11	2:F:204:PRO:CB	2.20	0.50
2:F:112:ALA:O	2:F:154:THR:HA	2.12	0.50
2:F:131:ARG:NH2	2:F:382:ASP:HB2	2.27	0.50
2:E:305:LYS:CD	2:E:336:THR:HG21	2.36	0.50
2:F:139:LEU:HD12	2:F:140:GLY:N	2.26	0.50
2:E:113:ARG:HB3	2:E:157:LYS:HZ1	1.77	0.49
2:E:202:ASN:OD1	2:E:298:LYS:NZ	2.42	0.49
2:F:74:LEU:HD11	2:F:107:VAL:HG13	1.94	0.49
2:F:147:PRO:HD2	2:F:150:TYR:OH	2.12	0.49
2:E:382:ASP:OD1	2:E:383:GLY:N	2.44	0.49
2:F:197:VAL:HB	2:F:298:LYS:HA	1.95	0.49
2:F:305:LYS:HA	2:F:336:THR:CG2	2.43	0.49
1:A:425:ARG:NH1	1:A:439:ILE:HD12	2.26	0.49
1:B:74:THR:N	1:B:183:SER:OG	2.34	0.49
2:F:198:LEU:HD21	2:F:300:LEU:HB2	1.95	0.49
2:F:273:GLN:O	2:F:273:GLN:HG2	2.11	0.49
2:E:173:ASP:OD2	2:E:175:PRO:HD2	2.11	0.49
2:F:86:ARG:HD2	2:F:96:ARG:HD2	1.95	0.49
2:F:121:TRP:CZ3	2:F:133:LEU:HD21	2.48	0.49
1:A:6:TRP:NE1	1:A:34:VAL:HG12	2.28	0.49
1:A:177:ASP:OD2	1:A:179:SER:OG	2.31	0.49
2:F:213:PRO:HD3	2:F:342:PHE:HD2	1.77	0.49
1:A:13:VAL:HG22	1:A:208:TRP:CE2	2.48	0.49
1:A:420:HIS:O	1:A:425:ARG:NH2	2.44	0.49
2:F:243:ASP:HA	2:F:246:LEU:CB	2.43	0.49
2:F:308:TYR:CB	2:F:333:VAL:HG21	2.32	0.49
2:F:408:PRO:HG2	2:F:411:GLU:OE1	2.12	0.49
2:F:86:ARG:HH11	2:F:86:ARG:HB2	1.78	0.49
1:B:482:MET:O	1:B:486:GLU:N	2.46	0.49
2:F:161:LEU:HD21	2:F:163:LEU:HD21	1.95	0.49
2:F:283:ASP:OD2	2:F:316:PRO:HD3	2.13	0.48
1:B:288:ARG:O	1:B:291:SER:OG	2.25	0.48
1:B:353:ARG:HH21	1:B:379:LEU:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:HD2	3:B:701:FAD:O2'	2.13	0.48
2:F:349:TYR:HB2	2:F:384:VAL:HG12	1.94	0.48
2:F:391:LEU:HG	2:F:393:GLN:HG3	1.95	0.48
2:E:118:MET:HG3	2:E:156:PHE:CE2	2.49	0.48
2:F:139:LEU:CD2	2:F:143:LEU:CD1	2.92	0.48
2:F:266:LEU:HG	2:F:325:ALA:HB2	1.95	0.48
1:A:37:PRO:HB2	1:A:44:TYR:CE2	2.49	0.48
1:A:415:TYR:CZ	2:E:67:LYS:HE2	2.49	0.48
2:F:198:LEU:CD2	2:F:300:LEU:HB2	2.44	0.48
2:F:288:VAL:HG21	2:F:349:TYR:CE1	2.48	0.48
1:A:406:ARG:NH1	1:A:408:ASP:OD1	2.34	0.48
2:F:169:HIS:HE1	2:F:173:ASP:HA	1.75	0.48
2:F:192:LYS:HD3	2:F:193:PRO:O	2.14	0.48
1:A:91:THR:O	1:A:91:THR:CG2	2.62	0.48
1:A:6:TRP:HE1	1:A:34:VAL:HG12	1.79	0.48
1:A:81:ALA:HB2	1:A:113:LEU:CD1	2.44	0.48
1:B:29:VAL:O	1:B:175:SER:HB3	2.14	0.48
1:A:156:CYS:HA	1:A:159:MET:HG2	1.96	0.47
2:F:183:LYS:HE2	2:F:186:GLN:NE2	2.27	0.47
2:F:335:GLU:O	2:F:339:VAL:HG23	2.14	0.47
2:E:69:PRO:HB3	2:E:187:ILE:HG22	1.96	0.47
2:F:70:MET:O	2:F:74:LEU:HG	2.15	0.47
2:E:247:LYS:O	2:E:251:GLN:HG2	2.14	0.47
2:F:292:ALA:HA	2:F:295:ARG:CD	2.44	0.47
2:F:308:TYR:CA	2:F:333:VAL:HG21	2.43	0.47
2:F:55:TYR:CE2	2:F:369:ILE:HD12	2.48	0.47
2:F:66:LEU:HD23	2:F:188:LEU:HD11	1.97	0.47
1:B:351:ARG:O	1:B:354:VAL:HG22	2.14	0.47
2:F:215:SER:HB2	2:F:286:THR:HG21	1.95	0.47
2:F:232:ARG:HA	2:F:232:ARG:HD3	1.64	0.47
2:E:286:THR:O	2:E:355:THR:HA	2.14	0.47
1:B:74:THR:H	1:B:183:SER:HG	1.55	0.47
2:F:19:HIS:HA	2:F:111:GLU:O	2.15	0.47
2:F:109:ILE:N	2:F:109:ILE:HD12	2.29	0.47
2:F:216:VAL:HG11	2:F:339:VAL:HG13	1.97	0.47
2:F:327:LEU:O	2:F:331:ASN:HB2	2.15	0.47
2:F:413:ASP:OD1	2:F:413:ASP:C	2.56	0.47
1:A:437:GLU:OE1	2:E:23:THR:OG1	2.33	0.47
2:E:152:GLN:OE1	2:E:154:THR:OG1	2.32	0.47
1:B:215:LEU:HD22	1:B:250:LEU:HD21	1.96	0.47
2:F:181:PHE:O	2:F:184:TRP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:308:TYR:CZ	2:F:333:VAL:HB	2.50	0.47
2:E:364:LEU:HB3	2:E:377:VAL:HG11	1.96	0.47
1:B:212:ASP:OD1	1:B:254:LYS:NZ	2.43	0.47
2:E:237:TYR:CE1	2:E:416:ARG:NH2	2.82	0.47
2:E:41:ASP:HA	2:E:302:ASN:HD22	1.80	0.46
2:F:80:VAL:HG22	2:F:171:ILE:HD11	1.98	0.46
2:F:115:ASP:HB3	2:F:157:LYS:HG3	1.97	0.46
2:F:128:GLY:O	2:F:132:GLN:HG3	2.15	0.46
2:E:19:HIS:HA	2:E:111:GLU:O	2.15	0.46
2:F:175:PRO:CG	2:F:295:ARG:NH2	2.78	0.46
1:A:77:SER:OG	1:A:78:ALA:N	2.49	0.46
1:A:171:LYS:HE2	1:B:157:LEU:O	2.15	0.46
1:B:309:HIS:CE1	1:B:310:LEU:HG	2.49	0.46
1:B:309:HIS:CE1	1:B:397:SER:HB2	2.51	0.46
2:F:349:TYR:HB2	2:F:384:VAL:CG1	2.45	0.46
2:F:220:GLY:O	2:F:221:PRO:C	2.58	0.46
2:E:119:ALA:O	2:E:123:ARG:HG2	2.15	0.46
2:F:79:PRO:HB2	2:F:300:LEU:HD21	1.97	0.46
2:F:407:LEU:HB2	2:F:412:ILE:HG13	1.98	0.46
2:E:20:ARG:HG2	2:E:111:GLU:HB2	1.97	0.46
2:E:20:ARG:CG	2:E:111:GLU:HB2	2.45	0.46
2:F:26:PRO:HD2	2:F:104:ASP:HB3	1.96	0.46
2:F:202:ASN:N	2:F:202:ASN:HD22	2.14	0.46
2:F:223:GLU:O	2:F:224:ASP:OD1	2.33	0.46
2:F:305:LYS:HD3	2:F:336:THR:CB	2.45	0.46
2:F:175:PRO:HG3	2:F:295:ARG:NH2	2.31	0.46
2:E:78:PHE:CG	2:E:79:PRO:HD3	2.51	0.46
2:E:262:GLY:N	2:E:265:GLU:OE2	2.47	0.46
2:E:324:LEU:HD23	2:E:324:LEU:HA	1.74	0.46
1:B:3:ILE:HG21	1:B:22:ALA:CB	2.46	0.46
1:B:10:ASP:OD1	1:B:10:ASP:N	2.49	0.46
1:B:130:ASP:OD1	1:B:288:ARG:NH2	2.48	0.46
2:F:167:TRP:CE2	2:F:177:ALA:HB2	2.50	0.46
2:F:288:VAL:O	2:F:358:ASP:CB	2.64	0.46
2:E:47:HIS:CE1	2:E:349:TYR:H	2.33	0.46
1:A:77:SER:OG	1:A:79:ASP:N	2.47	0.45
2:F:82:GLY:C	2:F:83:ARG:HD2	2.42	0.45
1:B:300:SER:HB3	1:B:305:PRO:HA	1.98	0.45
2:F:167:TRP:CZ2	2:F:171:ILE:HG23	2.51	0.45
1:A:383:ASP:HB3	1:A:386:SER:HB2	1.98	0.45
1:A:425:ARG:HG2	1:A:432:ALA:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:TYR:CG	2:F:238:SER:N	2.84	0.45
1:B:8:ARG:NH2	1:B:98:PHE:HD1	1.98	0.45
1:B:353:ARG:NH2	1:B:381:ASP:OD2	2.49	0.45
2:F:61:LEU:HD11	2:F:161:LEU:HD22	1.96	0.45
2:F:234:MET:HE1	2:F:408:PRO:HG3	1.98	0.45
2:F:284:THR:HG22	2:F:310:GLU:OE2	2.17	0.45
1:A:212:ASP:OD2	1:A:254:LYS:NZ	2.46	0.45
1:A:372:MET:HG2	1:A:391:TRP:CD1	2.51	0.45
2:F:210:PRO:HB2	2:F:211:ALA:H	1.62	0.45
2:E:220:GLY:O	2:E:222:MET:HG2	2.17	0.45
1:A:138:VAL:HG13	1:A:293:TYR:CE2	2.52	0.45
1:A:200:LEU:HD13	1:A:380:LEU:HD21	1.99	0.45
2:F:117:ASP:OD2	2:F:158:CYS:HB3	2.17	0.45
2:F:360:GLU:HG2	2:F:392:VAL:HG12	1.98	0.45
2:F:311:SER:CB	2:F:316:PRO:HG3	2.47	0.45
2:F:315:SER:C	2:F:319:THR:HG1	2.11	0.45
2:F:357:VAL:HB	2:F:390:VAL:O	2.16	0.45
1:B:372:MET:HG2	1:B:391:TRP:NE1	2.32	0.44
2:F:48:TYR:HB3	2:F:50:ARG:NH1	2.32	0.44
2:F:246:LEU:O	2:F:249:LEU:HB2	2.18	0.44
2:F:350:GLY:O	2:F:387:GLU:HB2	2.16	0.44
2:F:131:ARG:NH2	2:F:382:ASP:OD2	2.50	0.44
1:A:245:LEU:HD23	1:A:250:LEU:HB3	1.99	0.44
1:B:52:TRP:CE2	1:B:206:PRO:HB3	2.52	0.44
2:F:306:VAL:HG11	2:F:339:VAL:HG21	1.99	0.44
1:A:461:TYR:CD1	1:A:462:PRO:HD2	2.53	0.44
2:F:80:VAL:HA	2:F:171:ILE:HD11	1.99	0.44
2:F:285:VAL:HA	2:F:353:ASN:CB	2.47	0.44
2:F:362:VAL:O	2:F:364:LEU:N	2.51	0.44
2:F:392:VAL:C	2:F:393:GLN:HG3	2.42	0.44
1:B:311:ARG:NH1	1:B:486:GLU:OE2	2.50	0.44
1:A:208:TRP:CZ2	1:B:264:LEU:HD21	2.53	0.44
1:A:425:ARG:NH1	1:A:434:LEU:O	2.51	0.44
1:B:133:TYR:CE1	1:B:159:MET:HG2	2.53	0.44
1:B:404:LEU:HG	1:B:479:LEU:HD11	1.99	0.44
1:B:367:PRO:HD2	1:B:370:TRP:CE3	2.52	0.44
2:F:376:TYR:HH	2:F:378:GLU:CD	2.24	0.44
1:A:4:VAL:HB	1:A:96:VAL:HG22	1.99	0.44
1:A:208:TRP:HZ2	1:B:264:LEU:HD21	1.83	0.44
1:B:37:PRO:HD2	1:B:76:ARG:HH12	1.83	0.44
1:A:373:LYS:HA	1:A:373:LYS:HD2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:349:TYR:HA	2:F:355:THR:HG21	1.99	0.43
2:E:122:ILE:HG23	2:E:376:TYR:CD2	2.53	0.43
1:B:418:ASP:OD2	1:B:423:TYR:HB3	2.18	0.43
2:F:61:LEU:HD13	2:F:369:ILE:HD13	2.00	0.43
2:F:348:VAL:O	2:F:355:THR:HG21	2.18	0.43
2:F:391:LEU:CD2	2:F:393:GLN:NE2	2.82	0.43
2:E:268:SER:HB2	2:E:356:LEU:HD22	1.99	0.43
2:F:41:ASP:OD1	2:F:302:ASN:HB2	2.18	0.43
2:F:55:TYR:HB3	2:F:372:GLN:NE2	2.33	0.43
1:A:219:LEU:HD23	1:A:223:LEU:HD22	2.00	0.43
2:F:139:LEU:HD23	2:F:226:TRP:CZ3	2.52	0.43
1:A:133:TYR:OH	1:A:161:TYR:O	2.37	0.43
1:A:313:PHE:HE2	1:A:315:TRP:CE3	2.36	0.43
1:A:351:ARG:HD2	1:A:351:ARG:HA	1.73	0.43
2:E:269:ALA:O	2:E:272:TRP:HB3	2.18	0.43
1:B:441:HIS:HA	1:B:443:TRP:CZ3	2.53	0.43
2:F:55:TYR:HB3	2:F:372:GLN:HE22	1.84	0.43
2:F:397:ASP:CG	2:F:399:ARG:HB2	2.43	0.43
1:A:85:LEU:HA	1:A:88:VAL:CG1	2.36	0.43
1:B:77:SER:HB3	1:B:83:ALA:HB2	2.00	0.43
2:F:173:ASP:OD2	2:F:302:ASN:HA	2.18	0.43
2:E:147:PRO:HD2	2:E:150:TYR:OH	2.19	0.43
1:B:37:PRO:HD2	1:B:76:ARG:NH1	2.33	0.43
1:B:107:LEU:HD11	1:B:296:PHE:HD1	1.84	0.43
1:B:351:ARG:O	1:B:355:VAL:HG23	2.19	0.43
2:F:175:PRO:O	2:F:179:THR:HG23	2.18	0.43
2:F:283:ASP:O	2:F:310:GLU:HA	2.19	0.43
2:F:308:TYR:C	2:F:333:VAL:CG2	2.91	0.43
2:F:306:VAL:HG23	2:F:336:THR:HG23	2.00	0.43
2:F:308:TYR:C	2:F:333:VAL:HG22	2.35	0.43
1:B:242:SER:HB3	1:B:243:PRO:HD3	2.01	0.43
1:A:104:PRO:HD2	1:A:384:LEU:HD22	2.00	0.42
1:A:242:SER:HB3	3:A:701:FAD:H5'2	2.00	0.42
1:A:314:PRO:HG2	1:A:314:PRO:O	2.19	0.42
1:A:333:PRO:HG2	1:A:439:ILE:O	2.19	0.42
2:F:309:VAL:HG11	2:F:328:LEU:CD1	2.49	0.42
2:F:360:GLU:CD	2:F:401:ARG:CD	2.90	0.42
2:E:113:ARG:CG	2:E:155:ASN:HB2	2.38	0.42
2:E:113:ARG:HH21	2:E:157:LYS:NZ	2.15	0.42
2:E:223:GLU:O	2:E:224:ASP:OD1	2.36	0.42
1:B:302:HIS:O	1:B:305:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:365:TYR:O	2:E:373:ARG:HD3	2.19	0.42
1:B:8:ARG:NH1	1:B:98:PHE:CD1	2.84	0.42
2:F:55:TYR:OH	2:F:367:LEU:HG	2.19	0.42
2:F:369:ILE:O	2:F:370:LYS:C	2.63	0.42
1:B:15:ASP:HA	1:B:167:LEU:HB2	2.00	0.42
2:F:49:LEU:HD13	2:F:174:ILE:HG23	2.02	0.42
2:F:240:HIS:CE1	2:F:242:SER:HA	2.49	0.42
1:B:35:TRP:HB2	1:B:186:LEU:HD13	2.01	0.42
1:B:159:MET:HG3	1:B:160:PRO:HD2	2.01	0.42
2:E:234:MET:HE2	2:E:407:LEU:C	2.44	0.42
2:E:272:TRP:NE1	2:E:282:VAL:HG12	2.34	0.42
2:E:108:ARG:HG2	2:E:147:PRO:HG2	2.02	0.42
2:E:247:LYS:HD2	2:E:247:LYS:HA	1.94	0.42
2:E:335:GLU:O	2:E:339:VAL:HG23	2.20	0.42
2:F:183:LYS:NZ	2:F:194:GLU:H	2.17	0.42
2:E:356:LEU:HD23	2:E:390:VAL:CG1	2.49	0.42
2:F:63:THR:O	2:F:67:LYS:HG3	2.20	0.42
1:A:138:VAL:HG13	1:A:293:TYR:HE2	1.85	0.42
2:F:63:THR:HG22	2:F:67:LYS:CD	2.50	0.42
2:F:74:LEU:CD1	2:F:107:VAL:HG13	2.50	0.42
2:F:280:GLY:C	2:F:282:VAL:HG23	2.45	0.42
1:A:75:ARG:HA	1:A:75:ARG:HD3	1.59	0.41
1:A:102:TYR:OH	1:A:134:GLU:OE2	2.34	0.41
1:B:191:GLU:HA	1:B:194:ARG:HG3	2.02	0.41
2:F:110:VAL:HB	2:F:152:GLN:HG3	2.01	0.41
2:F:114:CYS:N	2:F:155:ASN:O	2.52	0.41
2:F:246:LEU:HD21	2:F:263:THR:OG1	2.19	0.41
1:A:104:PRO:HD2	1:A:384:LEU:CD2	2.50	0.41
1:B:35:TRP:CH2	1:B:45:PRO:HG2	2.55	0.41
1:B:267:SER:HB2	1:B:275:GLU:CD	2.45	0.41
1:B:350:ASP:O	1:B:353:ARG:HB2	2.19	0.41
1:B:367:PRO:O	1:B:370:TRP:HB2	2.21	0.41
1:A:406:ARG:HH12	1:A:408:ASP:CG	2.24	0.41
2:E:228:VAL:HG11	2:E:347:LEU:CD2	2.51	0.41
2:E:248:LYS:HG2	2:E:249:LEU:HD13	2.02	0.41
2:E:362:VAL:O	2:E:363:ASP:C	2.63	0.41
1:B:304:ARG:HG2	1:B:308:ALA:HB3	2.02	0.41
2:F:189:SER:OG	2:F:370:LYS:N	2.48	0.41
2:F:205:LEU:CD1	2:F:341:ALA:HA	2.50	0.41
2:F:391:LEU:HG	2:F:393:GLN:CG	2.50	0.41
2:E:245:VAL:O	2:E:249:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:ILE:HG13	2:F:376:TYR:CD2	2.55	0.41
2:F:331:ASN:OD1	2:F:331:ASN:N	2.51	0.41
2:F:381:MET:HE3	2:F:384:VAL:HG11	2.03	0.41
1:A:257:HIS:CE1	1:B:168:LEU:HG	2.55	0.41
1:A:99:ASN:HB3	1:A:129:SER:HB3	2.03	0.41
2:E:267:VAL:O	2:E:271:VAL:HG23	2.20	0.41
1:B:335:VAL:O	1:B:339:MET:HG2	2.20	0.41
2:F:69:PRO:HB3	2:F:187:ILE:CG2	2.48	0.41
2:F:285:VAL:CG2	2:F:354:LEU:C	2.79	0.41
2:F:285:VAL:HA	2:F:353:ASN:HB3	2.02	0.41
2:F:360:GLU:O	2:F:394:PRO:HD3	2.20	0.41
2:E:217:LYS:HD3	2:E:351:GLY:O	2.21	0.41
2:F:97:ARG:HA	2:F:98:PRO:HD3	1.81	0.41
2:F:114:CYS:HB3	2:F:156:PHE:HD1	1.83	0.41
2:F:277:LYS:HZ3	2:F:418:ALA:HB1	1.86	0.41
1:A:425:ARG:HD3	1:A:432:ALA:O	2.21	0.41
2:E:48:TYR:HB3	2:E:50:ARG:NH1	2.34	0.41
2:E:284:THR:O	2:E:353:ASN:HB3	2.21	0.41
2:E:397:ASP:OD1	2:E:397:ASP:N	2.53	0.41
2:E:405:VAL:HG13	2:E:407:LEU:HG	2.02	0.41
2:F:24:VAL:HG12	2:F:71:PHE:CZ	2.56	0.41
2:F:46:LEU:HD21	2:F:222:MET:HE3	2.03	0.41
2:F:233:ASP:OD1	2:F:233:ASP:N	2.53	0.41
1:A:138:VAL:HG23	1:A:155:ARG:CG	2.51	0.41
2:E:391:LEU:HB2	2:E:393:GLN:HE21	1.86	0.41
1:B:430:GLU:O	1:B:455:ILE:HD11	2.21	0.41
2:F:272:TRP:CZ2	2:F:285:VAL:HB	2.56	0.41
2:E:305:LYS:HD3	2:E:305:LYS:HA	1.84	0.40
2:F:243:ASP:OD2	2:F:399:ARG:NH1	2.53	0.40
2:E:232:ARG:CZ	2:E:410:ASP:OD2	2.69	0.40
1:B:259:VAL:CG1	1:B:278:CYS:HB3	2.52	0.40
2:F:200:PRO:HA	2:F:201:PRO:HD3	1.96	0.40
1:B:357:ALA:HB1	1:B:391:TRP:CZ3	2.57	0.40
2:F:359:MET:SD	2:F:391:LEU:HD11	2.61	0.40
1:A:215:LEU:HD13	1:A:255:VAL:HG22	2.02	0.40
2:E:48:TYR:CZ	2:E:138:VAL:HB	2.57	0.40
2:F:74:LEU:HD11	2:F:107:VAL:CG1	2.51	0.40
2:F:307:GLY:HA3	2:F:333:VAL:O	2.21	0.40
2:F:384:VAL:HG21	2:F:406:VAL:HG11	2.02	0.40
1:A:116:MET:HE3	1:A:116:MET:HB2	1.68	0.40
2:F:275:VAL:HG11	2:F:354:LEU:HD11	2.03	0.40

All (2) 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:196:SER:OG	1:B:433:ARG:O[3_654]	2.15	0.05
4:A:820:HOH:O	4:B:808:HOH:O[3_654]	2.15	0.05

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	486/688 (71%)	458 (94%)	27 (6%)	1 (0%)	43	72
1	B	486/688 (71%)	463 (95%)	23 (5%)	0	100	100
2	E	384/426 (90%)	358 (93%)	26 (7%)	0	100	100
2	F	384/426 (90%)	359 (94%)	24 (6%)	1 (0%)	36	66
All	All	1740/2228 (78%)	1638 (94%)	100 (6%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	363	ASP
1	A	305	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	414/576 (72%)	412 (100%)	2 (0%)	81	93
1	B	414/576 (72%)	414 (100%)	0	100	100
2	E	308/332 (93%)	307 (100%)	1 (0%)	86	95
2	F	308/332 (93%)	299 (97%)	9 (3%)	37	73
All	All	1444/1816 (80%)	1432 (99%)	12 (1%)	73	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	SER
1	A	181	CYS
2	E	405	VAL
2	F	16	VAL
2	F	101	LYS
2	F	107	VAL
2	F	139	LEU
2	F	174	ILE
2	F	303	GLU
2	F	355	THR
2	F	362	VAL
2	F	412	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	298	HIS
1	A	309	HIS
1	A	392	GLN
1	A	411	GLN
2	E	169	HIS
2	E	182	ASN
2	E	251	GLN
1	B	99	ASN
1	B	210	ASN
1	B	271	ASN
1	B	309	HIS
1	B	451	GLN
1	B	476	GLN
2	F	19	HIS

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Mol	Chain	Res	Type
2	F	202	ASN
2	F	372	GLN
2	F	393	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	FAD	B	701	-	58,58,58	0.34	0	85,89,89	0.32	0
3	FAD	A	701	-	58,58,58	0.45	1 (1%)	85,89,89	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	701	-	-	7/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	701	-	-	4/34/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	FAD	P-O2P	-2.31	1.44	1.55

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FAD	N10-C1'-C2'-C3'
3	B	701	FAD	C5B-O5B-PA-O1A
3	B	701	FAD	C5B-O5B-PA-O2A
3	B	701	FAD	C5B-O5B-PA-O3P
3	B	701	FAD	N10-C1'-C2'-C3'
3	B	701	FAD	C4'-C5'-O5'-P
3	A	701	FAD	P-O3P-PA-O2A
3	B	701	FAD	P-O3P-PA-O2A
3	A	701	FAD	C4'-C5'-O5'-P
3	B	701	FAD	P-O3P-PA-O1A
3	A	701	FAD	P-O3P-PA-O1A

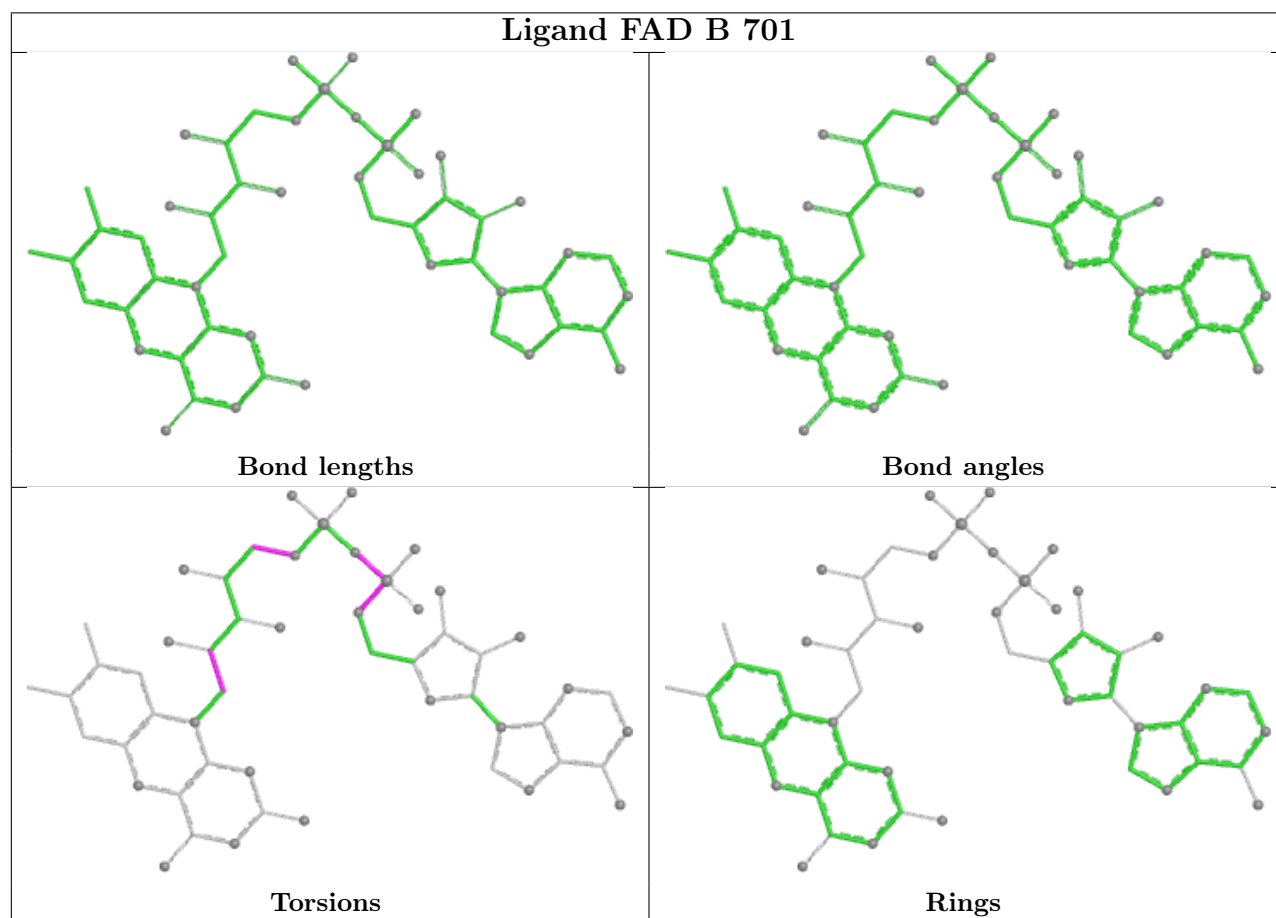
There are no ring outliers.

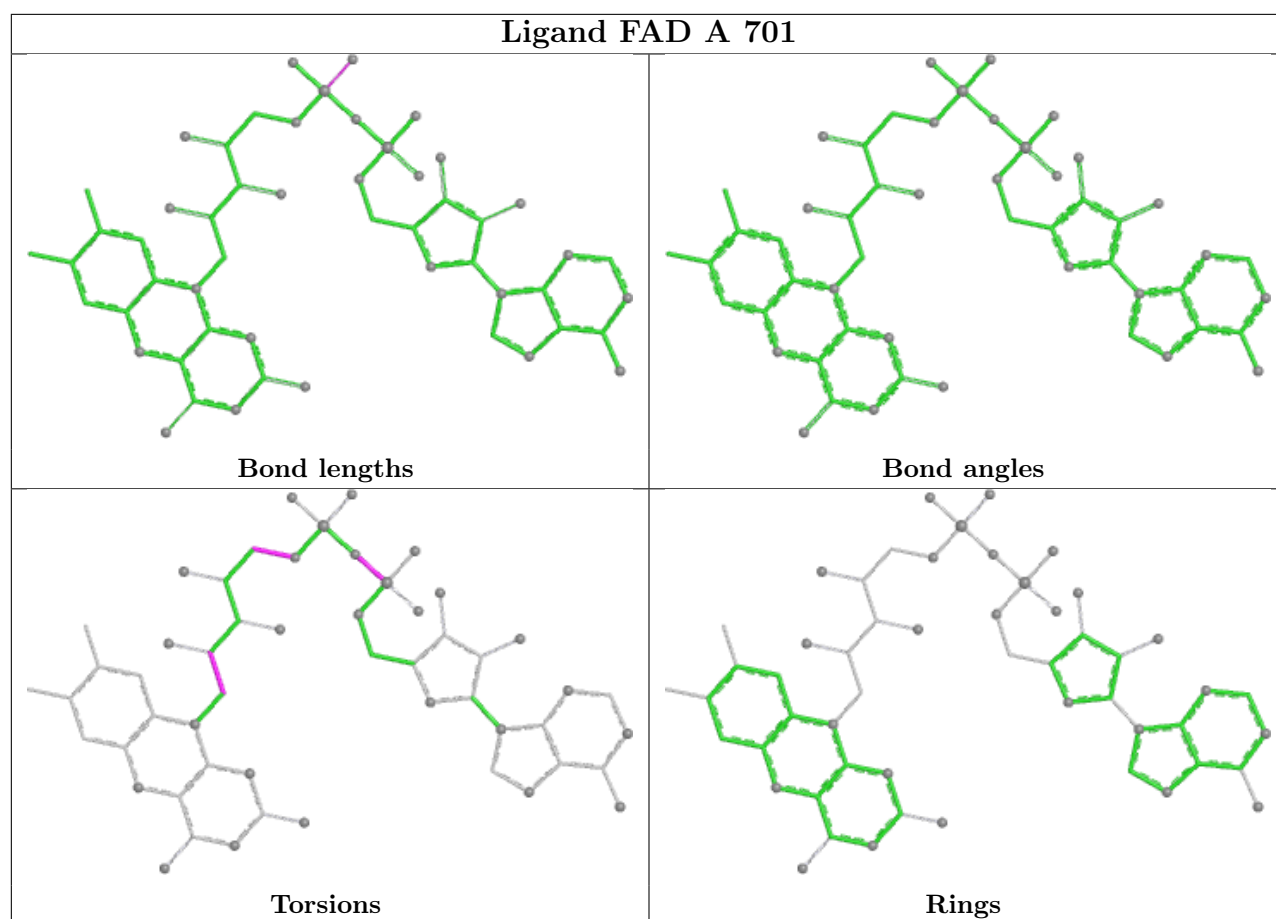
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	FAD	1	0
3	A	701	FAD	1	0

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

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	488/688 (70%)	0.12	14 (2%) 53 43	17, 34, 69, 106	0
1	B	488/688 (70%)	0.52	23 (4%) 36 29	23, 46, 87, 125	0
2	E	392/426 (92%)	0.73	37 (9%) 14 10	24, 59, 90, 112	0
2	F	392/426 (92%)	2.98	296 (75%) 0 0	69, 137, 173, 208	0
All	All	1760/2228 (78%)	1.00	370 (21%) 2 2	17, 54, 159, 208	0

All (370) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	245	VAL	8.8
2	F	322	ALA	7.2
2	F	270	LEU	7.1
2	F	180	CYS	7.0
2	F	321	VAL	7.0
2	F	216	VAL	6.7
2	F	266	LEU	6.6
2	F	35	TYR	6.6
2	F	312	ALA	6.3
2	F	325	ALA	6.3
2	F	269	ALA	6.2
2	F	288	VAL	5.9
2	F	328	LEU	5.8
2	F	271	VAL	5.7
2	F	210	PRO	5.6
2	F	241	VAL	5.4
2	F	268	SER	5.4
2	F	261	ALA	5.2
2	F	139	LEU	5.2
2	F	391	LEU	5.2
2	F	36	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	275	VAL	5.1
2	F	227	LEU	5.0
2	F	359	MET	5.0
2	F	299	SER	5.0
2	F	46	LEU	5.0
2	E	199	THR	4.9
2	F	300	LEU	4.9
2	F	104	ASP	4.9
2	F	178	ALA	4.9
2	F	406	VAL	4.9
2	F	49	LEU	4.8
2	F	402	LEU	4.8
2	F	171	ILE	4.8
2	F	337	ALA	4.7
2	F	42	LEU	4.7
2	F	98	PRO	4.6
2	F	326	ALA	4.6
2	F	212	ALA	4.6
2	F	215	SER	4.6
2	F	267	VAL	4.6
2	F	379	TYR	4.6
2	F	311	SER	4.6
2	F	415	LEU	4.5
2	F	422	ALA	4.5
2	F	357	VAL	4.4
2	F	360	GLU	4.4
2	E	205	LEU	4.4
2	F	364	LEU	4.4
2	F	130	ILE	4.4
2	F	219	VAL	4.4
2	F	61	LEU	4.4
2	F	230	ALA	4.3
2	F	150	TYR	4.3
2	F	246	LEU	4.3
2	F	53	TYR	4.3
1	B	487	ALA	4.3
2	F	248	LYS	4.3
2	F	264	PHE	4.3
2	F	290	ALA	4.3
2	F	339	VAL	4.3
2	F	205	LEU	4.3
2	F	385	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	51	GLY	4.2
2	F	168	ALA	4.2
2	F	87	ALA	4.2
2	F	79	PRO	4.1
2	F	403	VAL	4.1
2	F	165	PHE	4.1
2	F	263	THR	4.1
2	F	287	VAL	4.1
1	B	488	ALA	4.1
2	F	99	TYR	4.1
2	F	308	TYR	4.1
2	F	417	ALA	4.0
2	F	40	ALA	4.0
2	F	195	ALA	4.0
2	F	211	ALA	4.0
2	F	371	GLY	4.0
2	F	135	TYR	4.0
2	F	181	PHE	4.0
2	F	301	ALA	4.0
2	F	100	ILE	4.0
2	F	226	TRP	4.0
2	F	77	HIS	4.0
2	F	82	GLY	4.0
2	E	210	PRO	4.0
2	F	349	TYR	3.9
2	F	60	GLY	3.9
2	F	239	PHE	3.9
2	F	369	ILE	3.9
2	F	394	PRO	3.9
2	F	221	PRO	3.9
2	F	15	ALA	3.9
2	F	163	LEU	3.8
2	F	408	PRO	3.8
2	F	303	GLU	3.8
2	E	416	ARG	3.8
2	E	307	GLY	3.8
2	F	89	ALA	3.8
2	F	240	HIS	3.8
2	F	396	ALA	3.8
2	F	354	LEU	3.8
2	F	407	LEU	3.7
2	F	389	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	297	GLY	3.7
2	F	310	GLU	3.7
2	F	362	VAL	3.7
2	F	177	ALA	3.7
2	E	313	GLY	3.7
2	F	14	GLY	3.7
2	F	67	LYS	3.7
2	F	319	THR	3.6
2	F	244	ALA	3.6
2	F	338	ALA	3.6
2	F	45	LYS	3.6
2	F	272	TRP	3.6
2	F	363	ASP	3.6
2	F	419	LEU	3.6
2	F	307	GLY	3.5
2	F	228	VAL	3.5
2	F	249	LEU	3.5
2	F	324	LEU	3.5
2	F	48	TYR	3.5
2	F	80	VAL	3.5
2	E	14	GLY	3.5
2	F	285	VAL	3.5
2	F	347	LEU	3.5
2	E	104	ASP	3.5
2	F	286	THR	3.5
2	F	376	TYR	3.5
1	A	119	ALA	3.5
2	F	97	ARG	3.4
1	B	489	SER	3.4
2	F	119	ALA	3.4
2	F	162	ALA	3.4
2	F	231	GLY	3.4
2	E	89	ALA	3.4
2	E	312	ALA	3.4
2	F	386	ASP	3.4
2	F	289	ARG	3.4
2	F	340	ALA	3.4
2	F	151	VAL	3.4
2	F	85	ARG	3.4
2	F	384	VAL	3.3
2	F	398	GLY	3.3
2	F	377	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	395	ASP	3.3
2	F	405	VAL	3.3
2	F	380	GLY	3.3
2	F	305	LYS	3.3
2	E	422	ALA	3.3
2	F	164	GLY	3.3
2	F	237	TYR	3.3
2	F	323	GLU	3.3
2	F	159	GLY	3.3
2	E	261	ALA	3.3
2	F	44	PHE	3.3
2	F	174	ILE	3.2
2	F	274	ALA	3.2
2	F	132	GLN	3.2
2	F	23	THR	3.2
2	F	262	GLY	3.2
1	A	180	MET	3.2
2	F	78	PHE	3.2
2	F	242	SER	3.2
2	F	43	ALA	3.2
2	F	56	ARG	3.2
2	F	318	LYS	3.2
2	F	366	GLY	3.2
2	F	52	VAL	3.1
2	F	375	VAL	3.1
1	A	311	ARG	3.1
2	F	86	ARG	3.1
2	F	170	LEU	3.1
2	E	126	ALA	3.1
2	E	39	ASP	3.1
2	F	313	GLY	3.1
2	F	250	HIS	3.1
2	F	34	ASP	3.1
2	F	126	ALA	3.1
2	F	201	PRO	3.1
2	F	317	ALA	3.0
2	F	152	GLN	3.0
1	A	305	PRO	3.0
2	F	329	ALA	3.0
2	F	381	MET	3.0
2	E	263	THR	3.0
2	F	54	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	336	THR	3.0
2	F	235	ALA	3.0
2	F	90	GLU	3.0
2	F	102	CYS	3.0
2	F	294	ALA	3.0
2	F	332	VAL	3.0
2	F	247	LYS	2.9
2	F	121	TRP	2.9
2	F	148	LEU	2.9
2	F	356	LEU	2.9
2	F	309	VAL	2.9
2	F	149	LEU	2.9
2	F	128	GLY	2.9
2	E	127	PRO	2.9
2	F	144	PHE	2.9
2	F	146	SER	2.9
2	F	84	VAL	2.9
2	F	341	ALA	2.9
2	F	196	THR	2.9
2	F	327	LEU	2.9
2	F	217	LYS	2.9
2	F	320	ASP	2.9
2	F	348	VAL	2.9
2	F	382	ASP	2.9
1	A	300	SER	2.9
2	F	22	SER	2.9
2	F	176	SER	2.9
2	F	252	GLN	2.8
2	F	277	LYS	2.8
2	F	358	ASP	2.8
2	F	147	PRO	2.8
1	B	478	ALA	2.8
2	F	392	VAL	2.8
2	F	225	LEU	2.8
2	F	127	PRO	2.8
2	F	141	PRO	2.8
2	F	21	LEU	2.8
2	E	314	SER	2.8
2	F	282	VAL	2.8
2	F	37	LEU	2.8
2	F	414	SER	2.8
2	E	294	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	133	LEU	2.7
2	F	281	ASP	2.7
2	F	172	GLY	2.7
2	F	238	SER	2.7
2	F	273	GLN	2.7
2	F	138	VAL	2.7
2	F	188	LEU	2.7
2	F	352	ALA	2.7
2	F	167	TRP	2.7
1	B	472	LYS	2.7
2	F	157	LYS	2.7
2	F	204	PRO	2.7
2	F	361	GLN	2.7
2	F	236	CYS	2.7
2	F	365	TYR	2.7
2	F	189	SER	2.7
2	F	140	GLY	2.7
1	B	405	ASP	2.7
1	B	306	LEU	2.7
2	F	198	LEU	2.7
2	F	412	ILE	2.6
2	F	351	GLY	2.6
2	F	336	THR	2.6
2	E	331	ASN	2.6
2	F	65	VAL	2.6
2	F	197	VAL	2.6
2	F	203	GLN	2.6
2	F	292	ALA	2.6
1	B	309	HIS	2.6
2	F	295	ARG	2.6
2	F	175	PRO	2.6
2	F	137	LYS	2.6
2	F	30	THR	2.6
1	B	399	PRO	2.6
2	E	200	PRO	2.6
2	F	370	LYS	2.6
2	F	278	ILE	2.6
2	F	28	SER	2.5
1	B	485	LEU	2.5
2	F	166	SER	2.5
1	B	305	PRO	2.5
1	B	180	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	90	GLU	2.5
2	F	355	THR	2.5
2	F	393	GLN	2.5
2	F	123	ARG	2.5
2	F	401	ARG	2.5
2	F	76	ASP	2.5
2	F	421	SER	2.5
2	F	200	PRO	2.5
2	F	63	THR	2.5
1	A	85	LEU	2.5
2	F	213	PRO	2.5
2	E	252	GLN	2.5
2	E	281	ASP	2.4
2	F	284	THR	2.4
1	B	302	HIS	2.4
2	F	17	HIS	2.4
2	F	353	ASN	2.4
2	F	83	ARG	2.4
1	B	391	TRP	2.4
1	A	181	CYS	2.4
2	F	306	VAL	2.4
1	A	208	TRP	2.4
2	E	38	ALA	2.4
1	A	298	HIS	2.4
1	B	482	MET	2.4
2	F	229	PRO	2.4
2	E	140	GLY	2.4
2	F	33	VAL	2.4
1	B	369	ARG	2.4
2	F	75	ASP	2.4
2	F	88	GLU	2.4
2	E	266	LEU	2.4
2	F	103	ASN	2.3
2	F	418	ALA	2.3
2	F	372	GLN	2.3
2	F	50	ARG	2.3
2	F	96	ARG	2.3
2	F	400	GLY	2.3
2	F	224	ASP	2.3
1	A	301	SER	2.3
2	F	27	SER	2.3
1	A	91	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLY	2.3
2	E	231	GLY	2.3
2	F	388	GLY	2.3
2	F	378	GLU	2.3
2	F	117	ASP	2.3
2	F	136	ASP	2.3
2	F	243	ASP	2.3
2	F	47	HIS	2.3
2	F	154	THR	2.3
2	E	308	TYR	2.3
2	F	145	PHE	2.3
2	F	143	LEU	2.3
1	B	483	TRP	2.3
2	F	20	ARG	2.3
2	F	116	ARG	2.3
2	F	199	THR	2.3
2	F	367	LEU	2.2
2	F	397	ASP	2.2
2	E	262	GLY	2.2
2	F	193	PRO	2.2
2	F	39	ASP	2.2
2	F	184	TRP	2.2
2	F	25	VAL	2.2
2	F	73	TRP	2.2
2	F	280	GLY	2.2
1	A	397	SER	2.2
2	F	314	SER	2.2
1	B	112	ARG	2.1
2	F	131	ARG	2.1
1	A	176	GLY	2.1
2	E	250	HIS	2.1
2	F	183	LYS	2.1
2	F	31	GLY	2.1
1	B	397	SER	2.1
1	B	8	ARG	2.1
2	F	108	ARG	2.1
1	B	471	ALA	2.1
2	F	298	LYS	2.1
2	F	161	LEU	2.1
2	E	117	ASP	2.1
2	E	289	ARG	2.1
2	E	323	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	134	CYS	2.0
2	E	375	VAL	2.0
2	F	18	GLY	2.0
2	F	291	ASP	2.0
2	F	293	ALA	2.0
2	F	118	MET	2.0
1	B	314	PRO	2.0
2	F	113	ARG	2.0
2	E	286	THR	2.0
2	E	329	ALA	2.0
2	F	32	GLU	2.0
2	F	55	TYR	2.0
1	B	139	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

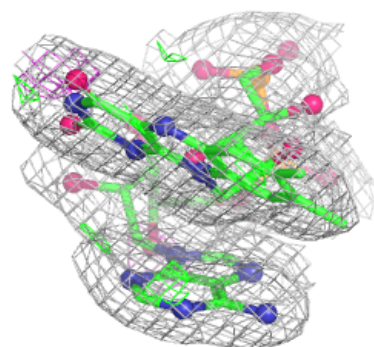
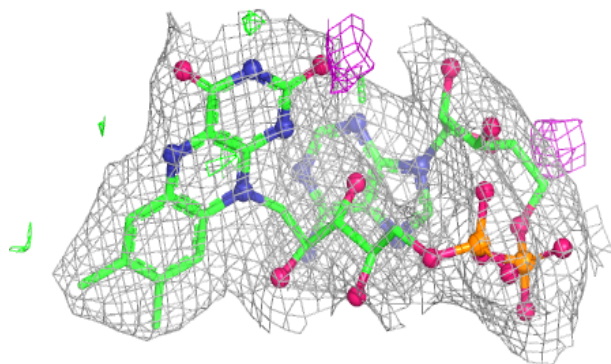
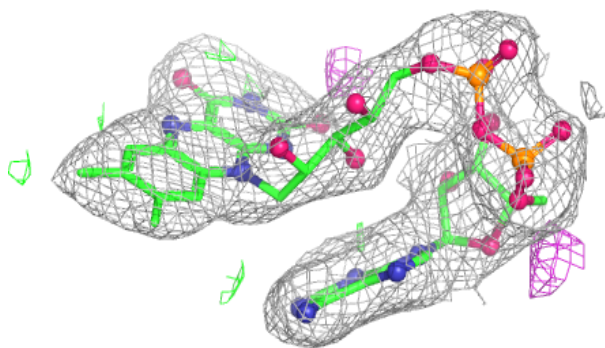
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	B	701	53/53	0.94	0.10	27,38,43,48	0
3	FAD	A	701	53/53	0.96	0.07	15,27,33,37	0

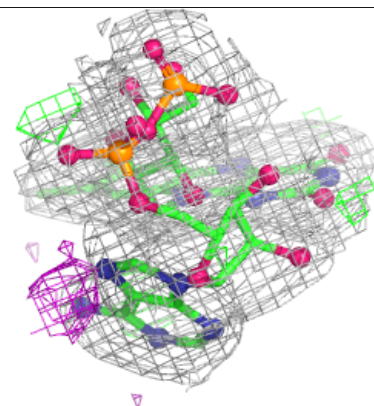
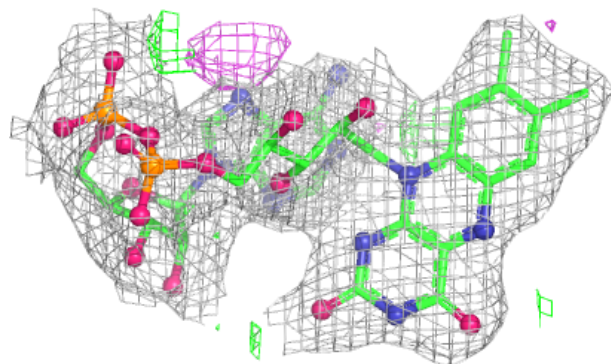
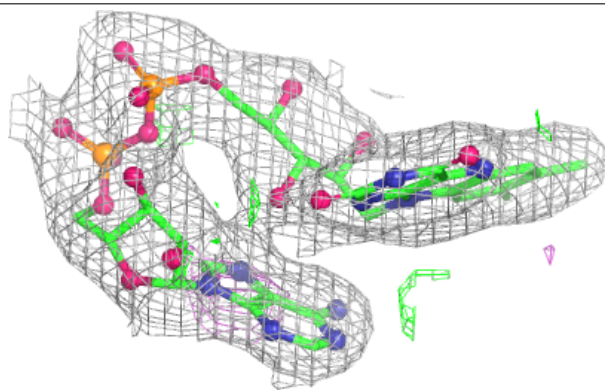
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD B 701:

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

**Electron density around FAD A 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.