



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 09:12 PM JST

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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

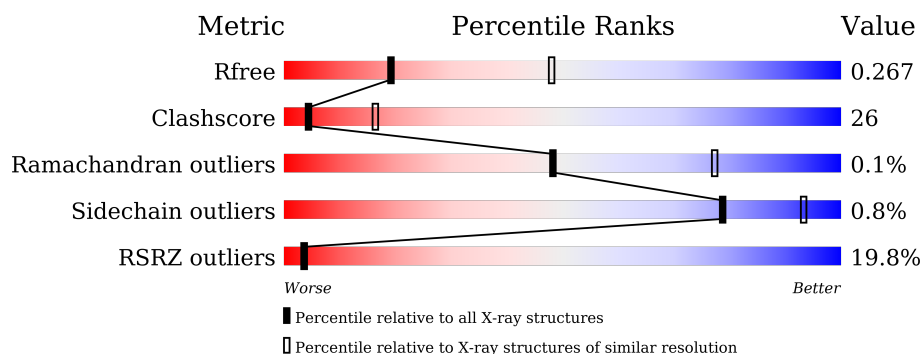
1 Overall quality at a glance

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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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	 7% 58% 32% 8%
2	F	426	 67% 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).



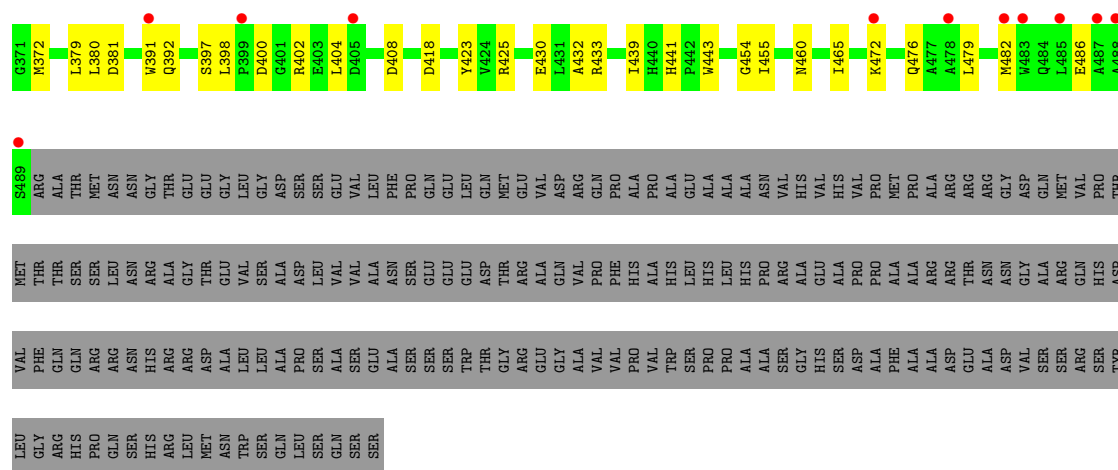
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is water.

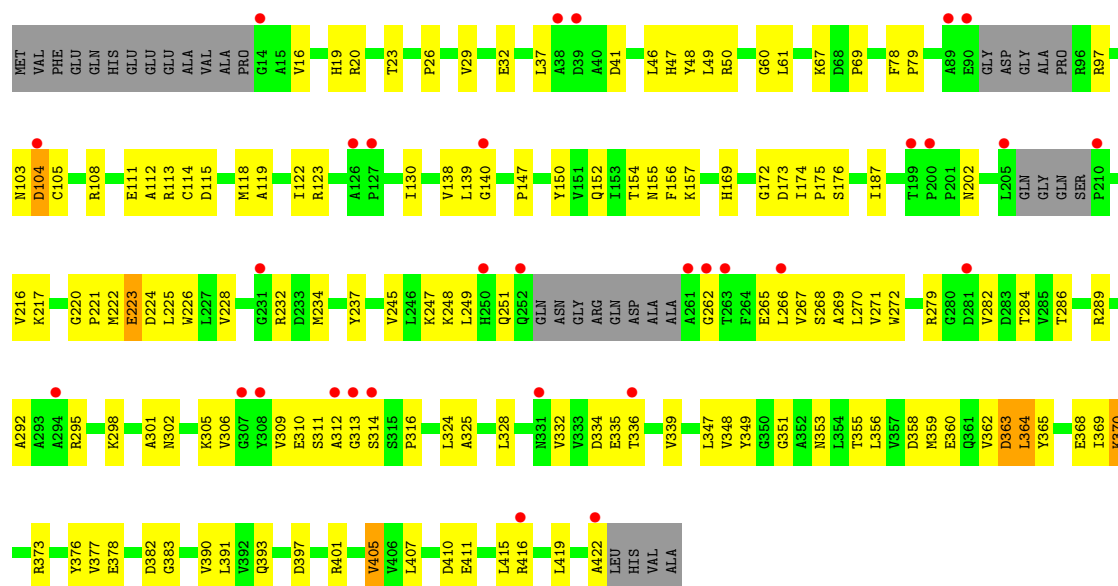
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	E	4	Total	O	0	0
			4	4		
4	B	8	Total	O	0	0
			8	8		

- Molecule 1: Cryptochrome2

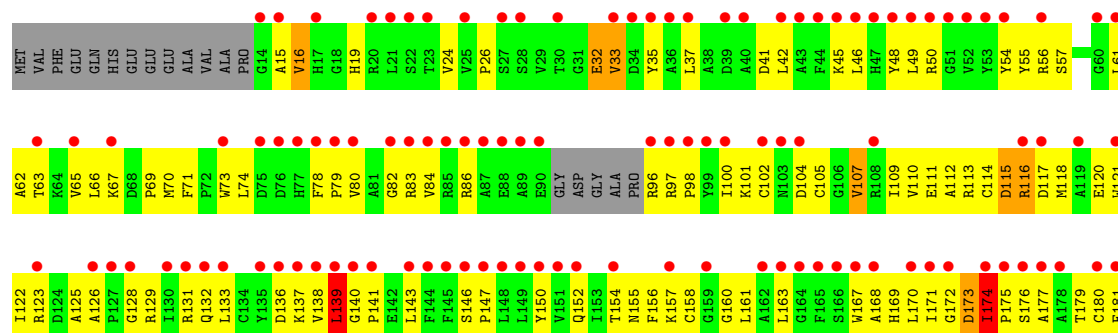




• Molecule 2: Protein ECERIFERUM 26-like



• Molecule 2: Protein ECERIFERUM 26-like





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:CG	2:E:111:GLU:HB2	2.45	0.46
2:E:20:ARG:HG2	2:E:111:GLU:HB2	1.97	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%)	44	73
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%)	37	67
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%)	86	95
1	B	414/576 (72%)	414 (100%)	0	100	100
2	E	308/332 (93%)	307 (100%)	1 (0%)	91	97
2	F	308/332 (93%)	299 (97%)	9 (3%)	37	71
All	All	1444/1816 (80%)	1432 (99%)	12 (1%)	79	93

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	A	701	-	53,58,58	0.57	1 (1%)	68,89,89	0.51	1 (1%)
3	FAD	B	701	-	53,58,58	0.47	0	68,89,89	0.49	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	701	-	-	5/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	701	-	-	7/30/50/50	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	-2.27	1.44	1.55

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	FAD	C5A-C6A-N6A	2.28	123.82	120.35
3	A	701	FAD	C5A-C6A-N6A	2.24	123.75	120.35

There are no chirality outliers.

All (12) 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	C4'-C5'-O5'-P
3	B	701	FAD	C5B-O5B-PA-O3P
3	B	701	FAD	N10-C1'-C2'-C3'
3	A	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	C5B-O5B-PA-O3P
3	B	701	FAD	P-O3P-PA-O1A
3	A	701	FAD	C5B-O5B-PA-O1A

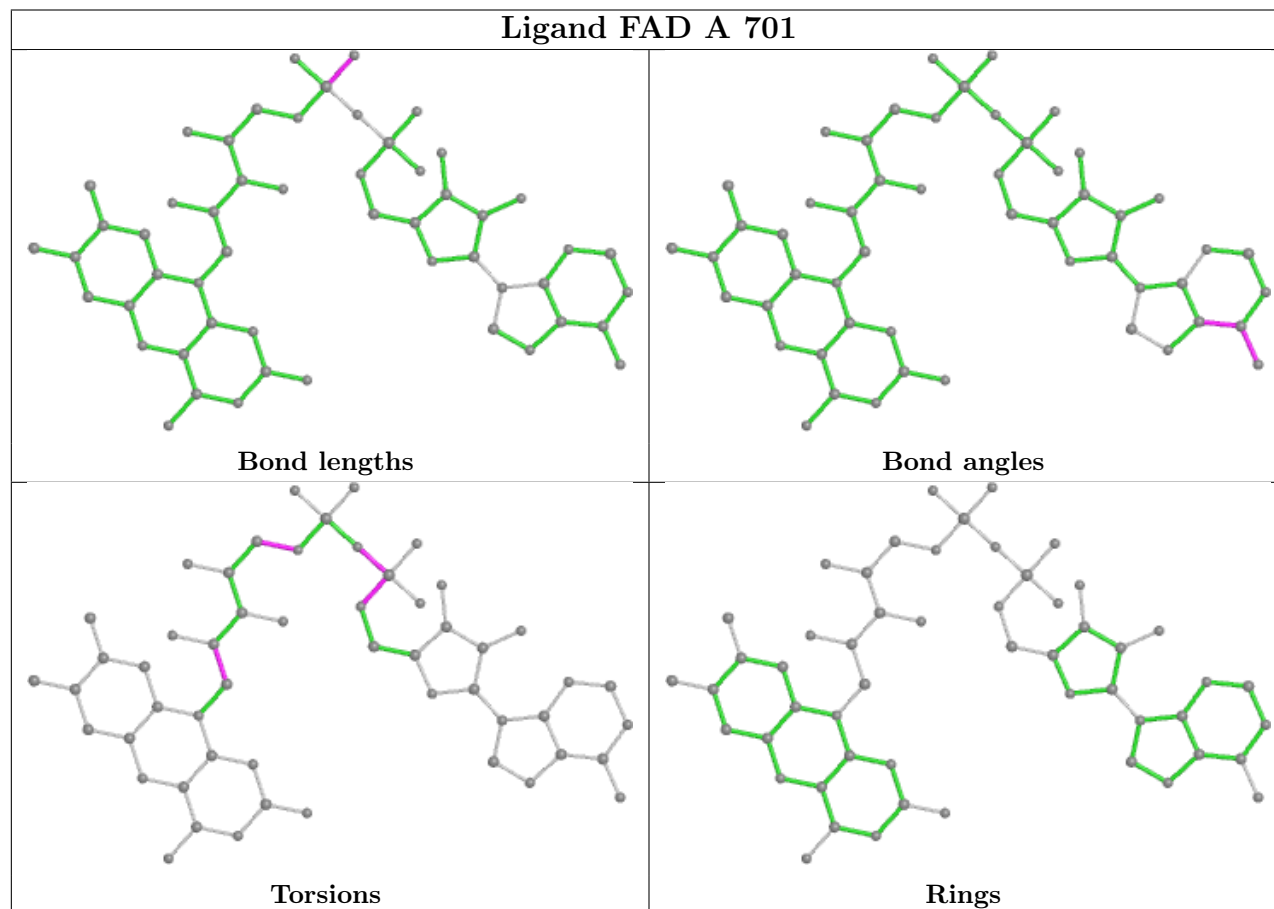
There are no ring outliers.

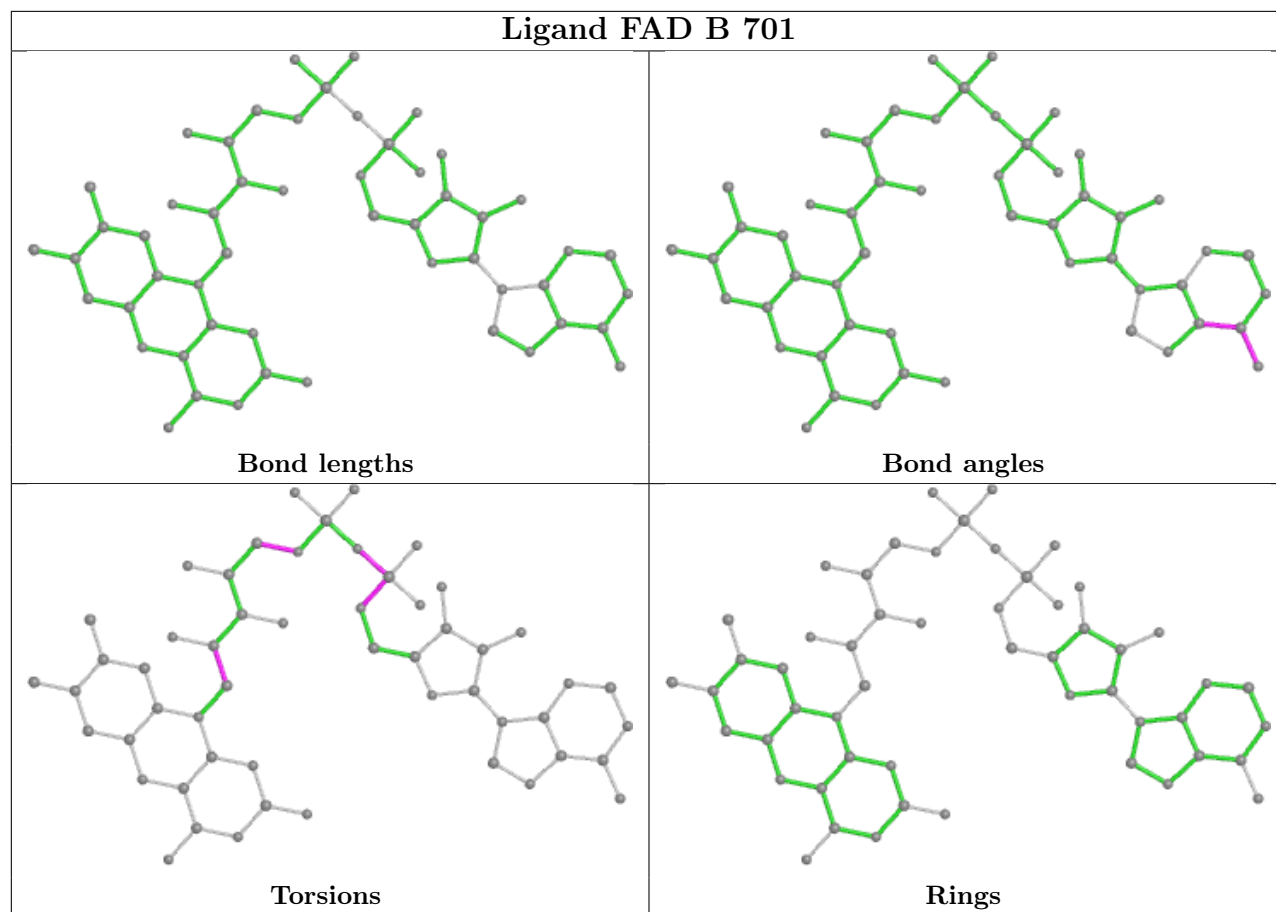
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	FAD	1	0
3	B	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%)	-0.03	14 (2%) 54 45	17, 34, 69, 106	0
1	B	488/688 (70%)	0.38	19 (3%) 44 36	23, 46, 87, 125	0
2	E	392/426 (92%)	0.59	31 (7%) 20 15	24, 59, 90, 112	0
2	F	392/426 (92%)	2.88	285 (72%) 0 0	69, 137, 173, 208	0
All	All	1760/2228 (78%)	0.87	349 (19%) 3 3	17, 54, 159, 208	0

All (349) 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	7.0
2	F	321	VAL	6.9
2	F	180	CYS	6.8
2	F	216	VAL	6.6
2	F	266	LEU	6.5
2	F	35	TYR	6.5
2	F	312	ALA	6.3
2	F	325	ALA	6.3
2	F	269	ALA	6.1
2	F	288	VAL	5.8
2	F	328	LEU	5.7
2	F	271	VAL	5.6
2	F	210	PRO	5.5
2	F	241	VAL	5.3
2	F	268	SER	5.3
2	F	261	ALA	5.2
2	F	139	LEU	5.1
2	F	36	ALA	5.1
2	F	391	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	275	VAL	5.1
2	F	299	SER	4.9
2	F	227	LEU	4.9
2	F	359	MET	4.9
2	E	199	THR	4.9
2	F	104	ASP	4.9
2	F	46	LEU	4.8
2	F	178	ALA	4.8
2	F	300	LEU	4.8
2	F	406	VAL	4.8
2	F	49	LEU	4.7
2	F	171	ILE	4.7
2	F	402	LEU	4.7
2	F	337	ALA	4.6
2	F	326	ALA	4.6
2	F	215	SER	4.6
2	F	42	LEU	4.5
2	F	212	ALA	4.5
2	F	267	VAL	4.5
2	F	98	PRO	4.5
2	F	311	SER	4.5
2	F	379	TYR	4.5
2	F	422	ALA	4.5
2	F	360	GLU	4.4
2	F	415	LEU	4.4
2	F	357	VAL	4.4
2	F	130	ILE	4.3
2	E	205	LEU	4.3
2	F	364	LEU	4.3
2	F	219	VAL	4.3
2	F	230	ALA	4.3
2	F	61	LEU	4.3
2	F	248	LYS	4.3
2	F	150	TYR	4.2
1	B	487	ALA	4.2
2	F	246	LEU	4.2
2	F	290	ALA	4.2
2	F	339	VAL	4.2
2	F	53	TYR	4.2
2	F	385	GLY	4.1
2	F	205	LEU	4.1
2	F	168	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	F	51	GLY	4.1
2	F	264	PHE	4.1
2	F	87	ALA	4.1
2	F	403	VAL	4.0
2	F	263	THR	4.0
2	F	287	VAL	4.0
1	B	488	ALA	4.0
2	F	79	PRO	4.0
2	F	99	TYR	4.0
2	F	417	ALA	4.0
2	F	165	PHE	4.0
2	F	40	ALA	3.9
2	F	195	ALA	3.9
2	F	211	ALA	3.9
2	F	308	TYR	3.9
2	F	301	ALA	3.9
2	F	100	ILE	3.9
2	F	371	GLY	3.9
2	F	77	HIS	3.9
2	F	135	TYR	3.9
2	F	181	PHE	3.9
2	F	82	GLY	3.9
2	F	226	TRP	3.8
2	E	210	PRO	3.8
2	F	349	TYR	3.8
2	F	303	GLU	3.8
2	E	416	ARG	3.8
2	F	369	ILE	3.8
2	F	60	GLY	3.8
2	F	15	ALA	3.8
2	F	394	PRO	3.8
2	F	221	PRO	3.7
2	F	239	PHE	3.7
2	F	163	LEU	3.7
2	F	408	PRO	3.7
2	F	89	ALA	3.7
2	E	307	GLY	3.7
2	F	396	ALA	3.7
2	F	240	HIS	3.7
2	F	310	GLU	3.7
2	F	354	LEU	3.6
2	F	389	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	407	LEU	3.6
2	F	67	LYS	3.6
2	F	362	VAL	3.6
2	F	297	GLY	3.6
2	F	177	ALA	3.6
2	F	45	LYS	3.6
2	E	313	GLY	3.5
2	F	14	GLY	3.5
2	F	319	THR	3.5
2	F	244	ALA	3.5
2	F	338	ALA	3.5
2	F	363	ASP	3.5
2	F	228	VAL	3.4
2	F	272	TRP	3.4
2	F	419	LEU	3.4
2	F	80	VAL	3.4
2	F	307	GLY	3.4
2	F	249	LEU	3.4
2	F	324	LEU	3.4
2	F	97	ARG	3.4
2	F	48	TYR	3.4
2	F	285	VAL	3.4
2	E	104	ASP	3.4
2	E	14	GLY	3.4
2	F	347	LEU	3.4
1	A	119	ALA	3.4
2	F	286	THR	3.4
2	F	289	ARG	3.4
1	B	489	SER	3.4
2	F	119	ALA	3.3
2	F	162	ALA	3.3
2	F	85	ARG	3.3
2	F	376	TYR	3.3
2	E	89	ALA	3.3
2	E	312	ALA	3.3
2	F	386	ASP	3.3
2	F	231	GLY	3.3
2	F	340	ALA	3.3
2	F	151	VAL	3.3
2	F	305	LYS	3.3
2	F	384	VAL	3.3
2	F	323	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	395	ASP	3.2
2	F	377	VAL	3.2
2	F	405	VAL	3.2
2	F	398	GLY	3.2
2	E	422	ALA	3.2
2	F	380	GLY	3.2
2	F	164	GLY	3.2
2	E	261	ALA	3.2
2	F	237	TYR	3.2
2	F	159	GLY	3.2
2	F	174	ILE	3.1
2	F	132	GLN	3.1
2	F	56	ARG	3.1
2	F	274	ALA	3.1
2	F	23	THR	3.1
2	F	318	LYS	3.1
2	F	44	PHE	3.1
2	F	262	GLY	3.1
1	A	311	ARG	3.1
2	F	86	ARG	3.1
2	F	242	SER	3.1
1	A	180	MET	3.1
2	F	43	ALA	3.1
2	F	52	VAL	3.0
2	F	375	VAL	3.0
2	F	78	PHE	3.0
2	F	366	GLY	3.0
2	E	126	ALA	3.0
2	E	39	ASP	3.0
2	F	170	LEU	3.0
2	F	34	ASP	3.0
2	F	250	HIS	3.0
2	F	313	GLY	3.0
2	F	126	ALA	3.0
2	F	152	GLN	3.0
2	F	317	ALA	3.0
2	F	201	PRO	2.9
2	F	329	ALA	2.9
1	A	305	PRO	2.9
2	E	263	THR	2.9
2	F	90	GLU	2.9
2	F	381	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	247	LYS	2.9
2	F	235	ALA	2.9
2	E	336	THR	2.9
2	F	54	TYR	2.9
2	F	294	ALA	2.9
2	F	332	VAL	2.9
2	F	309	VAL	2.8
2	F	148	LEU	2.8
2	F	356	LEU	2.8
2	F	102	CYS	2.8
2	F	217	LYS	2.8
2	F	149	LEU	2.8
2	F	121	TRP	2.8
2	F	128	GLY	2.8
2	E	127	PRO	2.8
2	F	146	SER	2.8
2	F	341	ALA	2.8
2	F	84	VAL	2.8
2	F	196	THR	2.8
2	F	277	LYS	2.8
2	F	252	GLN	2.8
1	A	300	SER	2.8
2	F	22	SER	2.8
2	F	176	SER	2.8
2	F	348	VAL	2.8
2	F	320	ASP	2.8
2	F	382	ASP	2.8
2	F	144	PHE	2.8
2	F	327	LEU	2.8
2	F	358	ASP	2.7
1	B	478	ALA	2.7
2	F	392	VAL	2.7
2	F	147	PRO	2.7
2	F	225	LEU	2.7
2	E	314	SER	2.7
2	F	127	PRO	2.7
2	F	141	PRO	2.7
2	F	282	VAL	2.7
2	F	21	LEU	2.7
2	F	414	SER	2.7
1	B	472	LYS	2.6
2	F	157	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	294	ALA	2.6
2	F	273	GLN	2.6
2	F	37	LEU	2.6
2	F	238	SER	2.6
2	F	281	ASP	2.6
2	F	138	VAL	2.6
2	F	352	ALA	2.6
2	F	133	LEU	2.6
2	F	361	GLN	2.6
2	F	172	GLY	2.6
2	F	188	LEU	2.6
2	F	204	PRO	2.6
2	F	189	SER	2.6
2	F	167	TRP	2.6
2	F	365	TYR	2.6
1	B	405	ASP	2.6
2	F	412	ILE	2.5
2	F	236	CYS	2.5
2	F	295	ARG	2.5
2	F	140	GLY	2.5
1	B	306	LEU	2.5
2	F	198	LEU	2.5
2	F	203	GLN	2.5
2	F	137	LYS	2.5
2	E	331	ASN	2.5
2	F	351	GLY	2.5
2	F	65	VAL	2.5
2	F	197	VAL	2.5
2	F	336	THR	2.5
2	F	292	ALA	2.5
2	F	370	LYS	2.5
1	B	309	HIS	2.5
2	F	30	THR	2.5
2	F	175	PRO	2.5
2	F	278	ILE	2.5
2	F	28	SER	2.4
2	F	123	ARG	2.4
2	F	401	ARG	2.4
1	B	399	PRO	2.4
2	E	200	PRO	2.4
2	E	90	GLU	2.4
2	F	166	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	393	GLN	2.4
1	B	485	LEU	2.4
2	F	355	THR	2.4
1	B	305	PRO	2.4
2	F	76	ASP	2.4
2	F	421	SER	2.4
1	B	180	MET	2.4
2	F	63	THR	2.4
2	E	252	GLN	2.4
2	F	200	PRO	2.4
2	F	83	ARG	2.4
1	A	85	LEU	2.3
2	F	213	PRO	2.3
2	E	281	ASP	2.3
2	F	284	THR	2.3
2	F	353	ASN	2.3
1	B	302	HIS	2.3
1	B	369	ARG	2.3
2	F	17	HIS	2.3
2	F	306	VAL	2.3
2	F	88	GLU	2.3
2	E	38	ALA	2.3
1	A	298	HIS	2.3
2	F	33	VAL	2.3
1	B	391	TRP	2.3
2	F	50	ARG	2.3
2	F	96	ARG	2.3
2	F	75	ASP	2.3
1	B	482	MET	2.3
2	F	229	PRO	2.3
2	F	103	ASN	2.2
1	A	181	CYS	2.2
2	E	140	GLY	2.2
2	F	372	GLN	2.2
1	A	208	TRP	2.2
2	F	418	ALA	2.2
2	E	266	LEU	2.2
2	F	378	GLU	2.2
2	F	224	ASP	2.2
1	A	301	SER	2.2
2	F	27	SER	2.2
1	A	91	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	400	GLY	2.2
2	F	20	ARG	2.2
2	F	116	ARG	2.2
2	F	117	ASP	2.2
2	F	136	ASP	2.2
2	F	243	ASP	2.2
2	F	154	THR	2.2
1	A	92	GLY	2.2
2	E	231	GLY	2.2
2	F	388	GLY	2.2
2	F	47	HIS	2.2
2	F	199	THR	2.1
2	E	308	TYR	2.1
2	F	143	LEU	2.1
2	F	397	ASP	2.1
2	F	145	PHE	2.1
2	F	367	LEU	2.1
1	B	483	TRP	2.1
2	E	262	GLY	2.1
2	F	193	PRO	2.1
1	B	112	ARG	2.1
2	F	131	ARG	2.1
2	F	39	ASP	2.1
2	F	25	VAL	2.1
1	A	397	SER	2.0
2	F	314	SER	2.0
2	F	184	TRP	2.0
2	F	183	LYS	2.0
2	F	280	GLY	2.0
1	B	8	ARG	2.0
2	F	108	ARG	2.0
2	F	73	TRP	2.0
1	A	176	GLY	2.0
2	E	250	HIS	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](#)

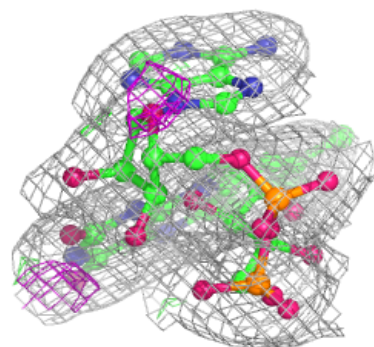
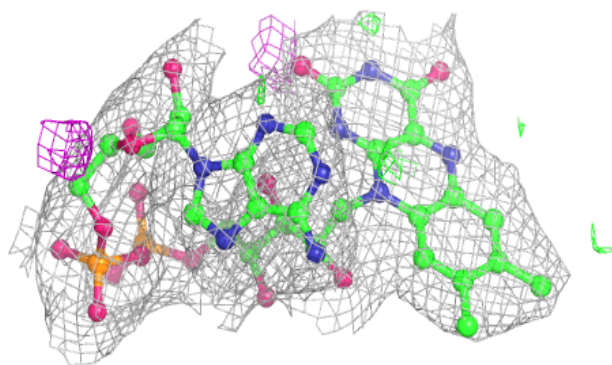
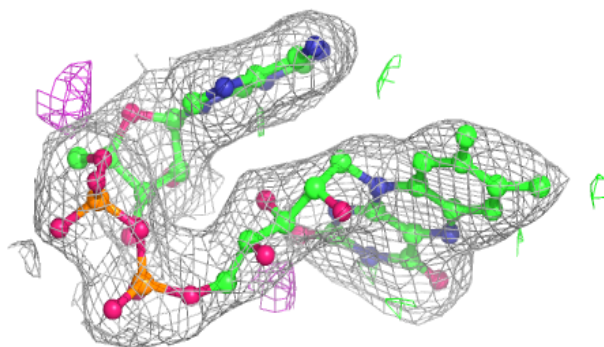
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

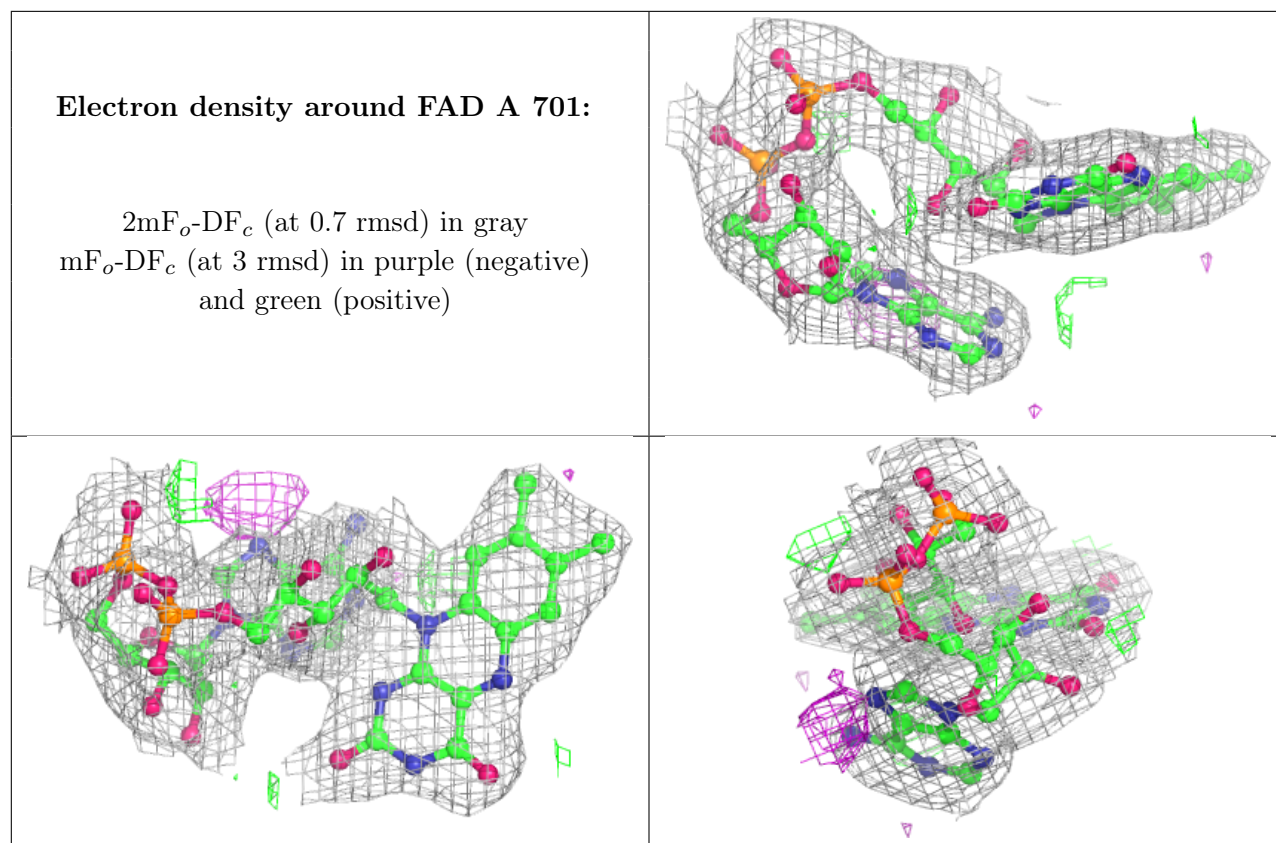
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FAD	B	701	53/53	0.94	0.10	27,38,43,48	0
3	FAD	A	701	53/53	0.96	0.07	15,27,33,37	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.