



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:13 PM UTC

PDB ID : 4K03 / pdb_00004k03
Title : Crystal structure of Drosophila Cryprochrome
Authors : Berndt, A.; Wolf, E.
Deposited on : 2013-04-03
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 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

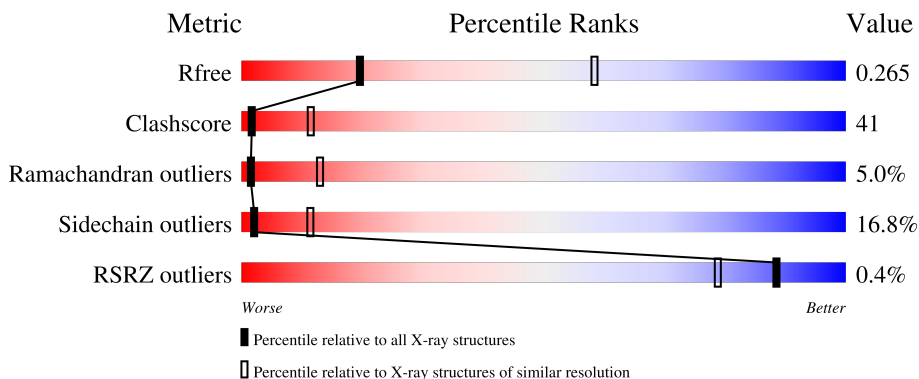
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	561	34%46%13%6%
1	B	561	34%46%15%..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8746 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 Cryptochrome-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4238	2707	749	758	24			
1	B	543	Total	C	N	O	S	0	0	0
			4350	2775	769	781	25			

There are 38 discrepancies between the modelled and reference sequences:

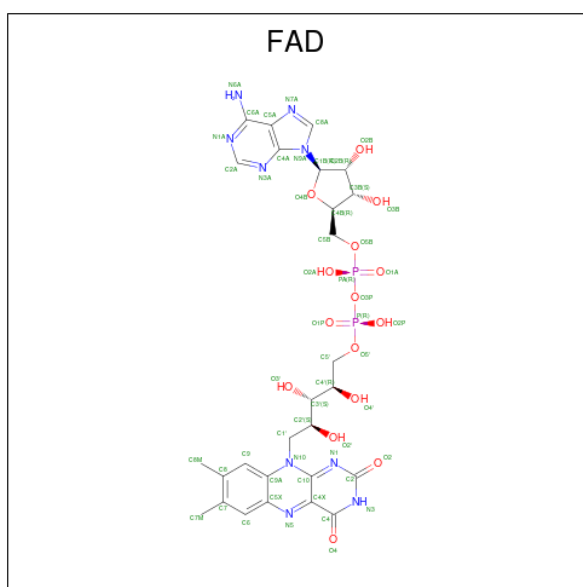
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O77059
A	-17	ALA	-	expression tag	UNP O77059
A	-16	MET	-	expression tag	UNP O77059
A	-15	GLY	-	expression tag	UNP O77059
A	-14	SER	-	expression tag	UNP O77059
A	-13	GLY	-	expression tag	UNP O77059
A	-12	ILE	-	expression tag	UNP O77059
A	-11	GLN	-	expression tag	UNP O77059
A	-10	ARG	-	expression tag	UNP O77059
A	-9	PRO	-	expression tag	UNP O77059
A	-8	THR	-	expression tag	UNP O77059
A	-7	SER	-	expression tag	UNP O77059
A	-6	THR	-	expression tag	UNP O77059
A	-5	SER	-	expression tag	UNP O77059
A	-4	SER	-	expression tag	UNP O77059
A	-3	LEU	-	expression tag	UNP O77059
A	-2	VAL	-	expression tag	UNP O77059
A	-1	ALA	-	expression tag	UNP O77059
A	0	ALA	-	expression tag	UNP O77059
B	-18	GLY	-	expression tag	UNP O77059
B	-17	ALA	-	expression tag	UNP O77059
B	-16	MET	-	expression tag	UNP O77059
B	-15	GLY	-	expression tag	UNP O77059
B	-14	SER	-	expression tag	UNP O77059
B	-13	GLY	-	expression tag	UNP O77059

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	ILE	-	expression tag	UNP O77059
B	-11	GLN	-	expression tag	UNP O77059
B	-10	ARG	-	expression tag	UNP O77059
B	-9	PRO	-	expression tag	UNP O77059
B	-8	THR	-	expression tag	UNP O77059
B	-7	SER	-	expression tag	UNP O77059
B	-6	THR	-	expression tag	UNP O77059
B	-5	SER	-	expression tag	UNP O77059
B	-4	SER	-	expression tag	UNP O77059
B	-3	LEU	-	expression tag	UNP O77059
B	-2	VAL	-	expression tag	UNP O77059
B	-1	ALA	-	expression tag	UNP O77059
B	0	ALA	-	expression tag	UNP O77059

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		

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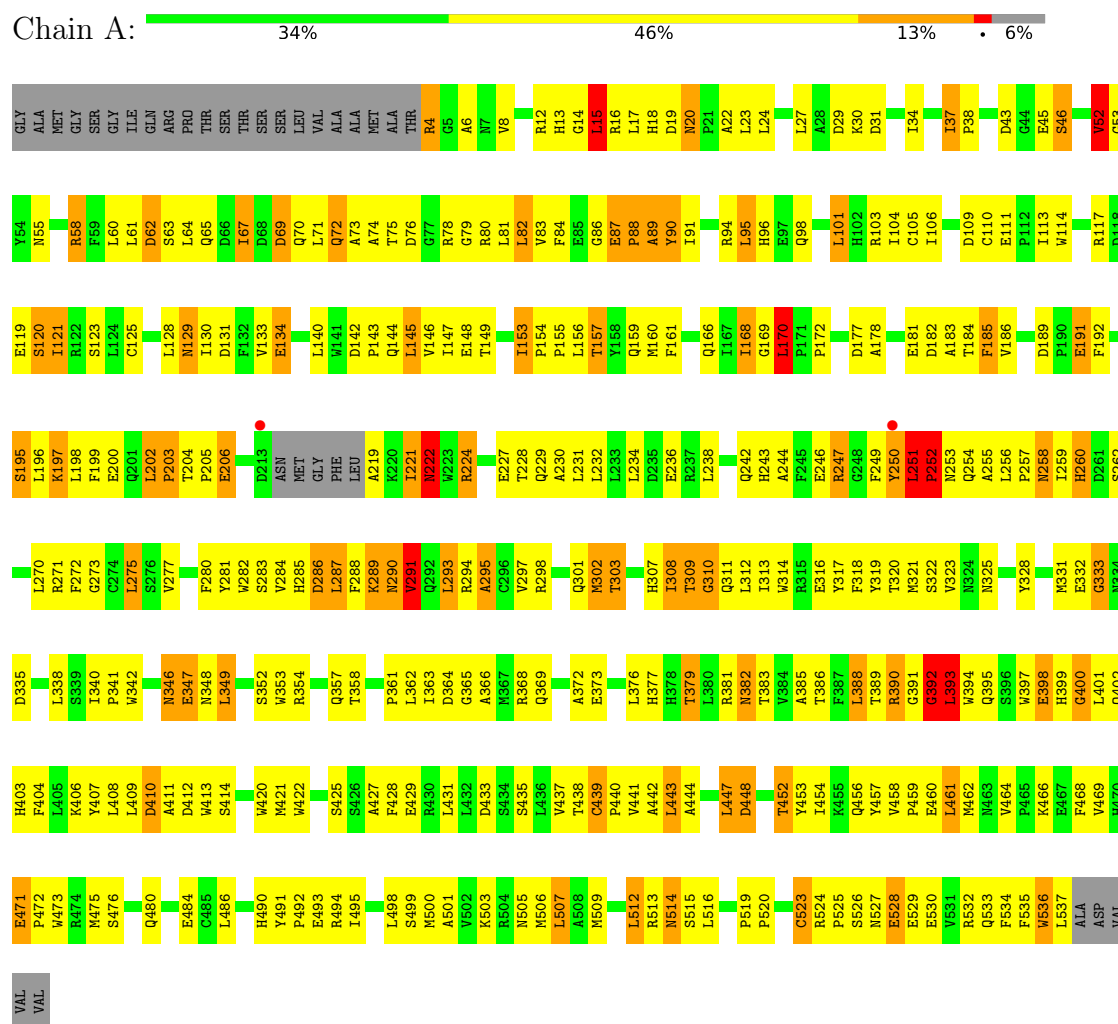
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	25	Total	O	0	0
			25	25		

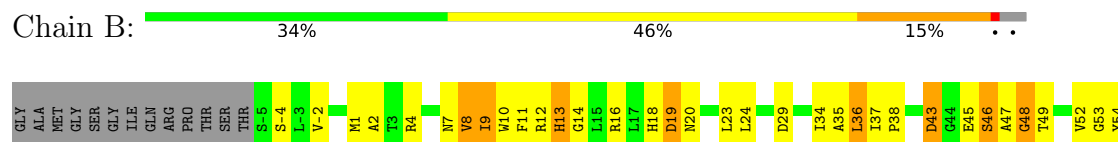
3 Residue-property plots

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

• Molecule 1: Cryptochrome-1



• Molecule 1: Cryptochrome-1



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.12Å 121.81Å 79.72Å 90.00° 114.78° 90.00°	Depositor
Resolution (Å)	40.49 – 3.20 40.49 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.49-3.20) 99.7 (40.49-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.188 , 0.269 0.186 , 0.265	Depositor DCC
R_{free} test set	1041 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.64	0/4355	1.07	30/5929 (0.5%)
1	B	0.64	0/4469	1.12	30/6082 (0.5%)
All	All	0.64	0/8824	1.09	60/12011 (0.5%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	CYS	CA-C-N	12.86	132.63	119.64
1	B	439	CYS	C-N-CA	12.86	132.63	119.64
1	A	20	ASN	CA-C-N	11.86	132.21	119.05
1	A	20	ASN	C-N-CA	11.86	132.21	119.05
1	B	20	ASN	CA-C-N	9.81	129.94	119.05
1	B	20	ASN	C-N-CA	9.81	129.94	119.05
1	B	464	VAL	CA-C-N	9.80	132.09	119.84
1	B	464	VAL	C-N-CA	9.80	132.09	119.84
1	B	219	ALA	N-CA-C	-8.87	99.09	110.53
1	A	255	ALA	N-CA-C	-8.25	101.68	112.41
1	A	170	LEU	CA-C-N	-7.58	112.57	120.38
1	A	170	LEU	C-N-CA	-7.58	112.57	120.38
1	B	535	PHE	N-CA-C	-7.18	99.23	110.36
1	A	291	VAL	N-CA-C	-6.88	95.03	109.34
1	B	62	ASP	N-CA-C	-6.80	104.24	112.54
1	A	439	CYS	CA-C-N	6.78	128.32	119.84
1	A	439	CYS	C-N-CA	6.78	128.32	119.84
1	A	202	LEU	CA-C-N	6.55	128.03	119.84
1	A	202	LEU	C-N-CA	6.55	128.03	119.84
1	B	137	SER	N-CA-C	-6.55	99.70	108.74
1	B	251	LEU	N-CA-C	-6.51	99.78	109.42
1	B	299	GLY	N-CA-C	-6.40	104.66	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ILE	CB-CA-C	-6.37	102.75	112.05
1	A	37	ILE	CA-C-N	6.33	127.75	119.84
1	A	37	ILE	C-N-CA	6.33	127.75	119.84
1	B	471	GLU	CA-C-N	6.29	127.43	120.45
1	B	471	GLU	C-N-CA	6.29	127.43	120.45
1	A	392	GLY	CA-C-N	6.28	133.01	121.70
1	A	392	GLY	C-N-CA	6.28	133.01	121.70
1	B	211	TYR	N-CA-C	6.16	118.44	108.41
1	B	217	PHE	N-CA-C	6.15	117.87	108.52
1	B	13	HIS	N-CA-C	-6.14	102.86	108.75
1	B	-2	VAL	N-CA-C	-5.98	104.87	113.07
1	A	52	VAL	N-CA-C	5.98	116.48	108.11
1	B	333	GLY	N-CA-C	-5.95	107.05	115.43
1	A	393	LEU	N-CA-C	5.94	127.62	111.00
1	A	222	ASN	N-CA-C	5.84	117.13	107.73
1	A	242	GLN	N-CA-C	-5.83	104.55	111.03
1	A	200	GLU	N-CA-C	-5.83	105.83	113.12
1	B	284	VAL	CB-CA-C	-5.82	104.25	111.70
1	B	222	ASN	N-CA-C	5.80	118.93	110.17
1	A	323	VAL	N-CA-C	5.80	115.98	110.42
1	B	67	ILE	CB-CA-C	-5.69	103.75	112.05
1	B	412	ASP	N-CA-C	-5.68	102.99	110.43
1	A	62	ASP	N-CA-C	-5.57	105.11	111.07
1	A	400	GLY	N-CA-C	-5.53	108.08	115.32
1	B	392	GLY	N-CA-C	-5.53	104.77	112.18
1	B	19	ASP	N-CA-C	-5.50	103.80	111.39
1	B	220	LYS	N-CA-C	5.49	122.50	110.80
1	B	515	SER	N-CA-C	-5.45	102.55	110.24
1	A	166	GLN	N-CA-C	-5.42	107.03	113.97
1	A	251	LEU	CA-CB-CG	5.42	135.26	116.30
1	A	333	GLY	N-CA-C	-5.39	108.67	115.08
1	A	439	CYS	N-CA-C	5.38	117.35	109.71
1	B	113	ILE	CB-CA-C	-5.30	102.60	111.29
1	A	448	ASP	CA-C-N	5.15	124.47	118.85
1	A	448	ASP	C-N-CA	5.15	124.47	118.85
1	B	488	GLY	N-CA-C	-5.13	105.19	111.35
1	A	185	PHE	N-CA-C	5.07	116.57	107.80
1	B	312	LEU	N-CA-C	-5.02	107.01	113.23

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	4238	0	4076	355	0
1	B	4350	0	4190	362	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
3	A	27	0	0	1	0
3	B	25	0	0	1	0
All	All	8746	0	8328	703	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG13	1:A:298:ARG:H	0.97	1.09
1:A:192:PHE:CZ	1:A:196:LEU:HD22	2.04	0.93
1:A:297:VAL:CG1	1:A:298:ARG:H	1.81	0.92
1:A:17:LEU:HD12	1:A:70:GLN:OE1	1.70	0.91
1:A:297:VAL:HG13	1:A:298:ARG:N	1.79	0.91
1:A:257:PRO:HD3	1:A:536:TRP:CD1	2.10	0.87
1:A:250:TYR:OH	1:B:528:GLU:HB3	1.75	0.87
1:B:298:ARG:CB	1:B:300:VAL:HG23	2.04	0.87
1:B:297:VAL:HB	1:B:298:ARG:CB	2.06	0.86
1:A:146:VAL:HG11	1:A:161:PHE:CE1	2.10	0.86
1:B:408:LEU:HB2	1:B:411:ALA:HB2	1.58	0.86
1:B:58:ARG:HH11	1:B:58:ARG:CG	1.87	0.85
1:A:461:LEU:HD22	1:A:469:VAL:HG23	1.59	0.84
1:B:321:MET:HE3	1:B:336:ILE:HD13	1.59	0.84
1:A:58:ARG:HB3	1:A:58:ARG:NH1	1.91	0.84
1:B:46:SER:HA	1:B:114:TRP:CZ3	2.12	0.83
1:A:408:LEU:HB2	1:A:411:ALA:HB2	1.58	0.83
1:A:247:ARG:HG2	1:A:247:ARG:HH11	1.40	0.83
1:A:303:THR:HG21	1:B:301:GLN:HE22	1.44	0.82
1:A:392:GLY:HA2	1:A:394:TRP:N	1.94	0.81
1:A:29:ASP:O	1:A:34:ILE:HB	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ALA:HA	1:B:247:ARG:NH1	1.96	0.81
1:A:287:LEU:HD23	1:A:288:PHE:CE1	2.15	0.81
1:B:473:TRP:CG	1:B:494:ARG:HH21	1.99	0.81
1:B:224:ARG:HG3	1:B:229:GLN:HG2	1.64	0.80
1:B:290:ASN:O	1:B:291:VAL:HG23	1.80	0.80
1:A:247:ARG:HG2	1:A:247:ARG:NH1	1.95	0.80
1:A:369:GLN:HG3	1:A:457:TYR:CZ	2.17	0.80
1:A:303:THR:HG21	1:B:301:GLN:NE2	1.97	0.79
1:B:96:HIS:HD2	1:B:128:LEU:HD13	1.46	0.79
1:A:84:PHE:CE1	1:A:198:LEU:HB2	2.18	0.79
1:B:13:HIS:NE2	1:B:271:ARG:NH1	2.31	0.79
1:B:204:THR:HB	1:B:206:GLU:OE1	1.82	0.78
1:A:501:ALA:O	1:A:505:ASN:ND2	2.16	0.78
1:A:13:HIS:NE2	1:A:271:ARG:NH1	2.32	0.77
1:A:58:ARG:CG	1:A:58:ARG:HH11	1.96	0.77
1:A:157:THR:HG22	1:A:160:MET:HB2	1.65	0.77
1:B:497:ASP:OD1	1:B:500:MET:HG3	1.85	0.77
1:A:435:SER:HA	1:A:438:THR:HB	1.66	0.77
1:A:459:PRO:C	1:A:461:LEU:H	1.93	0.77
1:B:11:PHE:C	1:B:12:ARG:HG3	2.08	0.76
1:A:58:ARG:HH11	1:A:58:ARG:CB	1.98	0.76
1:B:448:ASP:OD2	1:B:453:TYR:HB3	1.85	0.76
1:B:58:ARG:HH11	1:B:58:ARG:HG3	1.49	0.76
1:A:277:VAL:HG23	1:A:312:LEU:HD13	1.68	0.76
1:B:162:LEU:O	1:B:166:GLN:HG3	1.87	0.75
1:A:290:ASN:C	1:A:290:ASN:HD22	1.95	0.75
1:A:427:ALA:O	1:A:513:ARG:NH1	2.20	0.75
1:A:394:TRP:O	1:A:394:TRP:CD1	2.39	0.74
1:B:229:GLN:OE1	1:B:229:GLN:HA	1.87	0.74
1:B:321:MET:HE2	1:B:328:TYR:OH	1.87	0.74
1:A:471:GLU:HB3	1:A:473:TRP:CZ2	2.22	0.74
1:A:103:ARG:HG2	1:A:131:ASP:HB3	1.67	0.74
1:B:125:CYS:HB3	1:B:130:ILE:O	1.87	0.73
1:A:362:LEU:HD22	1:A:444:ALA:HB2	1.68	0.73
1:A:125:CYS:HB3	1:A:130:ILE:O	1.88	0.73
1:A:247:ARG:HH21	1:A:252:PRO:HD2	1.53	0.73
1:A:389:THR:HG22	1:A:395:GLN:O	1.89	0.72
1:A:58:ARG:HB3	1:A:58:ARG:HH11	1.50	0.72
1:B:280:PHE:HE1	1:B:308:ILE:HD11	1.55	0.72
1:A:429:GLU:HG3	1:A:525:PRO:HG2	1.72	0.72
1:B:149:THR:C	1:B:151:GLY:H	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:O	1:A:91:ILE:HG13	1.90	0.71
1:A:287:LEU:HD23	1:A:288:PHE:HE1	1.52	0.71
1:A:398:GLU:O	1:A:402:GLN:HG2	1.90	0.71
1:B:343:ALA:H	1:B:394:TRP:HD1	1.36	0.71
1:A:155:PRO:HB3	1:A:160:MET:HB3	1.72	0.71
1:A:96:HIS:HD2	1:A:128:LEU:HD13	1.55	0.70
1:B:467:GLU:HG2	1:B:468:PHE:CE2	2.26	0.70
1:B:380:LEU:O	1:B:384:VAL:HG22	1.92	0.70
1:B:393:LEU:H	1:B:496:ILE:CD1	2.05	0.70
1:A:331:MET:HE1	1:A:342:TRP:HD1	1.58	0.69
1:B:327:ASN:OD1	1:B:330:ARG:HD2	1.92	0.69
1:A:58:ARG:HH11	1:A:58:ARG:HG3	1.57	0.69
1:B:529:GLU:OE2	1:B:532:ARG:NH2	2.26	0.69
1:A:15:LEU:HA	1:A:67:ILE:HD11	1.74	0.69
1:B:159:GLN:HG2	1:B:526:SER:CB	2.22	0.69
1:B:179:ARG:NH1	1:B:181:GLU:HG3	2.07	0.69
1:B:358:THR:HG22	1:B:495:ILE:CD1	2.22	0.69
1:B:113:ILE:HD11	1:B:413:TRP:CD2	2.28	0.69
1:A:516:LEU:HD13	1:A:520:PRO:HD3	1.74	0.68
1:B:467:GLU:HG2	1:B:468:PHE:CD2	2.28	0.68
1:A:143:PRO:O	1:A:147:ILE:HG13	1.93	0.68
1:A:534:PHE:CD2	1:A:534:PHE:O	2.46	0.68
1:B:165:VAL:O	1:B:165:VAL:HG23	1.92	0.68
1:B:257:PRO:HD3	1:B:536:TRP:CE3	2.28	0.68
1:A:8:VAL:HG12	1:A:104:ILE:HA	1.76	0.68
1:A:290:ASN:HD22	1:A:291:VAL:N	1.91	0.67
1:B:321:MET:HE1	1:B:523:CYS:SG	2.34	0.67
1:A:224:ARG:HG2	1:A:229:GLN:HB2	1.75	0.67
1:A:290:ASN:C	1:A:290:ASN:ND2	2.53	0.67
1:A:364:ASP:O	1:A:368:ARG:HG3	1.94	0.67
1:A:89:ALA:HB2	1:A:120:SER:OG	1.95	0.66
1:A:301:GLN:HG3	1:A:303:THR:HG23	1.75	0.66
1:A:346:ASN:HB3	1:A:349:LEU:HB2	1.76	0.66
1:B:516:LEU:HD21	1:B:520:PRO:HG3	1.77	0.66
1:B:412:ASP:HB2	1:B:415:VAL:HB	1.78	0.66
1:A:146:VAL:HG11	1:A:161:PHE:HE1	1.60	0.66
1:B:159:GLN:HG2	1:B:526:SER:HB3	1.77	0.66
1:B:248:GLY:O	1:B:250:TYR:CE2	2.49	0.66
1:B:72:GLN:HG2	1:B:80:ARG:HD3	1.77	0.66
1:A:238:LEU:HD11	1:A:283:SER:HB2	1.77	0.65
1:A:512:LEU:HG	1:A:513:ARG:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLY:HA3	1:B:185:PHE:CE1	2.30	0.65
1:B:346:ASN:HB3	1:B:349:LEU:HD13	1.78	0.65
1:B:389:THR:HG22	1:B:395:GLN:O	1.97	0.65
1:A:75:THR:O	1:A:78:ARG:HB2	1.96	0.65
1:A:491:TYR:CD1	1:A:492:PRO:HD2	2.31	0.65
1:A:221:ILE:O	1:A:222:ASN:HB3	1.97	0.64
1:B:247:ARG:NH1	1:B:252:PRO:HD3	2.13	0.64
1:A:4:ARG:NH1	1:A:4:ARG:HA	2.11	0.64
1:A:331:MET:HE1	1:A:342:TRP:CD1	2.31	0.64
1:B:46:SER:OG	1:B:117:ARG:NH1	2.31	0.64
1:B:192:PHE:CE1	1:B:196:LEU:HD13	2.33	0.64
1:B:392:GLY:C	1:B:393:LEU:O	2.38	0.64
1:B:464:VAL:CG1	1:B:465:PRO:HD2	2.27	0.64
1:B:8:VAL:HG12	1:B:104:ILE:HA	1.78	0.63
1:A:104:ILE:HD12	1:A:125:CYS:SG	2.38	0.63
1:B:162:LEU:HD12	1:B:162:LEU:H	1.62	0.63
1:B:258:ASN:OD1	1:B:258:ASN:C	2.41	0.63
1:B:260:HIS:H	1:B:260:HIS:CD2	2.17	0.63
1:B:461:LEU:HD22	1:B:464:VAL:CG2	2.29	0.63
1:B:486:LEU:O	1:B:489:VAL:O	2.17	0.63
1:A:191:GLU:O	1:A:195:SER:HB3	1.98	0.63
1:B:491:TYR:CD1	1:B:492:PRO:HD2	2.34	0.63
1:A:249:PHE:O	1:A:250:TYR:HB2	1.99	0.63
1:B:438:THR:HG22	1:B:439:CYS:N	2.13	0.63
1:B:113:ILE:O	3:B:704:HOH:O	2.16	0.63
1:B:388:LEU:HA	1:B:393:LEU:HD12	1.79	0.63
1:B:514:ASN:CG	1:B:515:SER:H	2.06	0.63
1:B:72:GLN:CG	1:B:80:ARG:HD3	2.29	0.62
1:B:427:ALA:O	1:B:513:ARG:HD3	1.99	0.62
1:A:363:ILE:CD1	1:A:383:THR:HG22	2.28	0.62
1:A:392:GLY:HA3	1:A:505:ASN:HD21	1.64	0.62
1:B:248:GLY:O	1:B:249:PHE:O	2.18	0.62
1:B:301:GLN:HG3	1:B:303:THR:HG23	1.81	0.62
1:B:331:MET:HE1	1:B:342:TRP:HD1	1.65	0.62
1:A:206:GLU:H	1:A:206:GLU:CD	2.07	0.62
1:A:90:TYR:C	1:A:90:TYR:CD2	2.77	0.62
1:B:230:ALA:HB1	1:B:275:LEU:HB2	1.82	0.62
1:B:297:VAL:CB	1:B:298:ARG:CB	2.78	0.62
1:A:125:CYS:O	1:A:129:ASN:N	2.33	0.61
1:B:358:THR:HG22	1:B:495:ILE:HD13	1.81	0.61
1:A:366:ALA:O	1:A:376:LEU:HD11	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLU:HG3	1:A:525:PRO:HB2	1.81	0.61
1:B:343:ALA:H	1:B:394:TRP:CD1	2.18	0.61
1:A:250:TYR:HE1	1:B:532:ARG:NH1	1.98	0.61
1:B:515:SER:O	1:B:516:LEU:HB3	2.00	0.61
1:B:46:SER:O	1:B:47:ALA:HB3	2.01	0.61
1:A:23:LEU:HD12	1:A:23:LEU:O	2.01	0.61
1:B:71:LEU:O	1:B:75:THR:HG23	2.01	0.61
1:B:72:GLN:OE1	1:B:80:ARG:HD3	2.00	0.61
1:B:321:MET:HG2	1:B:321:MET:O	2.00	0.61
1:B:87:GLU:O	1:B:91:ILE:HG13	1.99	0.61
1:B:137:SER:O	1:B:138:HIS:HB3	2.00	0.61
1:B:213:ASP:OD1	1:B:216:GLY:HA2	2.01	0.61
1:A:234:LEU:HD22	1:A:275:LEU:HD11	1.83	0.60
1:A:22:ALA:HB1	1:A:105:CYS:HB3	1.83	0.60
1:A:394:TRP:HB2	1:A:505:ASN:OD1	2.01	0.60
1:B:247:ARG:HG2	1:B:248:GLY:O	2.01	0.60
1:A:156:LEU:HA	1:A:321:MET:HE2	1.83	0.60
1:B:464:VAL:HG13	1:B:465:PRO:HD2	1.82	0.60
1:A:390:ARG:HH21	1:A:433:ASP:CG	2.09	0.60
1:B:43:ASP:HB3	1:B:45:GLU:H	1.66	0.60
1:A:358:THR:HG22	1:A:495:ILE:HD13	1.84	0.60
1:A:250:TYR:CD1	1:B:529:GLU:HB2	2.35	0.60
1:A:358:THR:O	1:A:495:ILE:HG23	2.01	0.60
1:A:535:PHE:O	1:A:536:TRP:HB2	2.01	0.60
1:A:428:PHE:CE2	1:A:519:PRO:HB3	2.37	0.60
1:B:351:GLN:O	1:B:355:LEU:HG	2.02	0.60
1:A:392:GLY:HA3	1:A:505:ASN:ND2	2.17	0.59
1:B:387:PHE:O	1:B:392:GLY:O	2.20	0.59
1:B:522:HIS:CD2	1:B:524:ARG:HB3	2.38	0.59
1:A:459:PRO:HD3	3:A:709:HOH:O	2.02	0.59
1:B:474:ARG:HG3	1:B:474:ARG:HH11	1.67	0.59
1:B:516:LEU:O	1:B:516:LEU:HD22	2.02	0.59
1:B:159:GLN:O	1:B:162:LEU:HD12	2.02	0.59
1:B:249:PHE:O	1:B:250:TYR:O	2.19	0.59
1:A:472:PRO:HD2	1:A:473:TRP:CZ3	2.38	0.59
1:A:498:LEU:O	1:A:499:SER:C	2.46	0.59
1:A:258:ASN:C	1:A:258:ASN:OD1	2.45	0.59
1:A:293:LEU:HD23	1:A:303:THR:HA	1.85	0.59
1:A:392:GLY:HA2	1:A:394:TRP:H	1.64	0.59
1:A:358:THR:HA	1:A:495:ILE:CG2	2.32	0.59
1:B:1:MET:HA	1:B:4:ARG:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:HG2	1:A:90:TYR:HB3	1.84	0.58
1:A:441:VAL:C	1:A:443:LEU:H	2.10	0.58
1:A:250:TYR:HE1	1:B:532:ARG:HH12	1.50	0.58
1:A:293:LEU:O	1:A:303:THR:HG22	2.03	0.58
1:A:346:ASN:O	1:A:348:ASN:N	2.37	0.58
1:B:280:PHE:CE1	1:B:308:ILE:HD11	2.38	0.58
1:A:346:ASN:O	1:A:349:LEU:N	2.36	0.58
1:A:459:PRO:C	1:A:461:LEU:N	2.55	0.58
1:A:106:ILE:HD11	1:A:134:GLU:OE2	2.03	0.58
1:A:294:ARG:O	1:A:295:ALA:HB2	2.03	0.58
1:B:293:LEU:N	1:B:293:LEU:HD22	2.19	0.58
1:A:386:THR:O	1:A:391:GLY:HA3	2.03	0.58
1:A:119:GLU:OE1	1:A:119:GLU:HA	2.02	0.58
1:B:288:PHE:O	1:B:289:LYS:C	2.46	0.58
1:A:410:ASP:O	1:A:411:ALA:C	2.46	0.58
1:B:354:ARG:O	1:B:371:LEU:HD11	2.05	0.57
1:A:96:HIS:CD2	1:A:128:LEU:HD13	2.38	0.57
1:A:250:TYR:HE1	1:B:532:ARG:NH2	2.02	0.57
1:B:156:LEU:HD11	1:B:336:ILE:HG22	1.87	0.57
1:A:429:GLU:HG3	1:A:525:PRO:CG	2.34	0.57
1:A:75:THR:HB	1:A:78:ARG:NH1	2.19	0.57
1:A:229:GLN:HA	1:A:229:GLN:OE1	2.03	0.57
1:A:252:PRO:HB3	1:A:253:ASN:CB	2.34	0.57
1:A:27:LEU:O	1:A:30:LYS:HG3	2.05	0.57
1:A:486:LEU:HD13	1:A:490:HIS:HE1	1.69	0.57
1:B:237:ARG:HG3	1:B:238:LEU:N	2.20	0.57
1:B:377:HIS:O	1:B:380:LEU:HB2	2.05	0.57
1:B:37:ILE:HG12	1:B:186:VAL:HG11	1.85	0.57
1:B:127:GLU:HG2	1:B:128:LEU:HD23	1.87	0.57
1:A:20:ASN:HB3	1:A:23:LEU:HB3	1.86	0.57
1:A:429:GLU:HG3	1:A:525:PRO:CB	2.35	0.57
1:B:435:SER:HA	1:B:438:THR:HB	1.86	0.57
1:A:52:VAL:HG22	1:A:53:GLY:O	2.04	0.56
1:A:87:GLU:CG	1:A:90:TYR:HB3	2.35	0.56
1:A:46:SER:OG	1:A:117:ARG:NH1	2.38	0.56
1:B:104:ILE:HD12	1:B:130:ILE:HG21	1.87	0.56
1:A:286:ASP:O	1:A:288:PHE:N	2.38	0.56
1:A:514:ASN:C	1:A:516:LEU:N	2.64	0.56
1:B:11:PHE:O	1:B:12:ARG:HG3	2.04	0.56
1:B:96:HIS:HD2	1:B:128:LEU:CD1	2.17	0.56
1:A:43:ASP:HA	1:A:86:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HD11	1:A:448:ASP:HB2	1.87	0.56
1:A:516:LEU:CD1	1:A:520:PRO:HD3	2.35	0.56
1:B:343:ALA:N	1:B:394:TRP:HD1	2.01	0.56
1:A:111:GLU:OE2	1:A:413:TRP:HB3	2.05	0.56
1:A:472:PRO:HD2	1:A:473:TRP:CE3	2.40	0.56
1:A:391:GLY:O	1:A:392:GLY:O	2.24	0.56
1:A:257:PRO:HD3	1:A:536:TRP:NE1	2.20	0.55
1:B:242:GLN:HA	1:B:245:PHE:HB3	1.88	0.55
1:A:219:ALA:N	1:A:372:ALA:HB1	2.21	0.55
1:B:329:ASP:OD2	1:B:413:TRP:HZ2	1.89	0.55
1:B:527:ASN:O	1:B:531:VAL:HG23	2.05	0.55
1:B:293:LEU:N	1:B:293:LEU:CD2	2.68	0.55
1:A:530:GLU:HA	1:A:533:GLN:NE2	2.21	0.55
1:B:358:THR:O	1:B:494:ARG:HA	2.07	0.55
1:A:111:GLU:HB2	1:A:114:TRP:CD1	2.42	0.55
1:A:297:VAL:CG1	1:A:307:HIS:HB2	2.37	0.55
1:A:280:PHE:HE1	1:A:308:ILE:HD11	1.71	0.55
1:A:381:ARG:HD3	2:A:601:FAD:C9A	2.37	0.55
1:B:96:HIS:CD2	1:B:128:LEU:HD13	2.36	0.55
1:B:98:GLN:HG2	1:B:192:PHE:CE1	2.41	0.55
1:B:361:PRO:O	1:B:365:GLY:N	2.34	0.55
1:B:461:LEU:HD22	1:B:464:VAL:HG21	1.89	0.55
1:A:147:ILE:HG23	1:A:154:PRO:N	2.22	0.55
1:A:295:ALA:HA	1:B:299:GLY:O	2.07	0.55
1:A:369:GLN:HG3	1:A:457:TYR:CE1	2.42	0.55
1:A:388:LEU:O	1:A:388:LEU:HG	2.07	0.55
1:A:95:LEU:HD12	1:A:192:PHE:HE2	1.71	0.55
1:A:388:LEU:HD23	1:A:389:THR:HG23	1.88	0.55
1:B:58:ARG:CG	1:B:58:ARG:NH1	2.59	0.55
1:B:401:LEU:HG	1:B:405:LEU:CD1	2.37	0.55
1:B:418:GLY:HA2	1:B:421:MET:CE	2.37	0.55
1:B:360:PHE:CE2	1:B:494:ARG:HB3	2.41	0.54
1:B:516:LEU:O	1:B:517:ILE:C	2.50	0.54
1:B:321:MET:HE1	1:B:523:CYS:HB2	1.89	0.54
1:A:63:SER:O	1:A:67:ILE:HG13	2.07	0.54
1:B:58:ARG:HG3	1:B:58:ARG:NH1	2.21	0.54
1:A:20:ASN:O	1:A:24:LEU:HG	2.08	0.54
1:A:196:LEU:O	1:A:197:LYS:HB2	2.07	0.54
1:B:486:LEU:O	1:B:487:ILE:C	2.51	0.54
1:A:182:ASP:CG	1:A:182:ASP:O	2.51	0.54
1:A:363:ILE:HD11	1:A:440:PRO:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLN:HA	1:B:162:LEU:HD11	1.90	0.54
1:A:24:LEU:HD21	1:A:178:ALA:HB2	1.89	0.54
1:A:168:ILE:HG22	1:A:169:GLY:N	2.23	0.54
1:A:247:ARG:O	1:A:247:ARG:HG3	2.06	0.54
1:A:8:VAL:CG1	1:A:104:ILE:HG23	2.38	0.54
1:A:95:LEU:HD12	1:A:192:PHE:CE2	2.43	0.54
1:A:459:PRO:O	1:A:461:LEU:N	2.41	0.54
1:A:476:SER:O	1:A:480:GLN:HG3	2.08	0.54
1:A:509:MET:HA	1:A:512:LEU:HD23	1.90	0.54
1:B:52:VAL:HG22	1:B:53:GLY:N	2.23	0.53
1:B:247:ARG:O	1:B:248:GLY:C	2.51	0.53
1:B:324:ASN:O	1:B:326:PRO:HD3	2.08	0.53
1:B:394:TRP:CZ3	1:B:505:ASN:HB3	2.43	0.53
1:A:38:PRO:HB2	1:A:81:LEU:HA	1.90	0.53
1:B:345:PRO:HA	1:B:395:GLN:OE1	2.08	0.53
1:B:7:ASN:ND2	1:B:34:ILE:HG21	2.24	0.53
1:A:90:TYR:C	1:A:90:TYR:HD2	2.17	0.53
1:A:72:GLN:HG3	1:A:80:ARG:HG2	1.89	0.53
1:A:503:LYS:O	1:A:507:LEU:HD22	2.08	0.53
1:B:90:TYR:C	1:B:90:TYR:CD2	2.86	0.53
1:B:361:PRO:O	1:B:364:ASP:N	2.41	0.53
1:A:69:ASP:O	1:A:70:GLN:C	2.51	0.53
1:A:109:ASP:OD2	1:A:117:ARG:NH2	2.37	0.53
1:A:368:ARG:NH1	1:A:458:VAL:HG13	2.24	0.53
1:B:16:ARG:HD2	1:B:18:HIS:CE1	2.43	0.53
1:B:248:GLY:O	1:B:250:TYR:CD2	2.62	0.53
1:A:205:PRO:HB2	1:A:206:GLU:OE2	2.09	0.53
1:A:302:MET:O	1:A:302:MET:HG3	2.07	0.53
1:B:159:GLN:HA	1:B:162:LEU:CD1	2.39	0.53
1:A:60:LEU:O	1:A:64:LEU:HG	2.09	0.53
1:A:428:PHE:CZ	1:A:519:PRO:HB3	2.43	0.53
1:A:461:LEU:HD23	1:A:464:VAL:CG2	2.39	0.53
1:B:412:ASP:O	1:B:416:CYS:HB2	2.09	0.53
1:A:340:ILE:CD1	1:A:425:SER:HA	2.39	0.53
1:A:363:ILE:HD11	1:A:440:PRO:CB	2.39	0.53
1:B:46:SER:CA	1:B:114:TRP:CZ3	2.88	0.53
1:B:46:SER:CA	1:B:114:TRP:HZ3	2.22	0.53
1:B:79:GLY:HA3	1:B:185:PHE:CZ	2.44	0.53
1:B:353:TRP:O	1:B:367:MET:HG3	2.09	0.53
1:A:62:ASP:O	1:A:65:GLN:HB3	2.10	0.52
1:B:149:THR:O	1:B:151:GLY:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:VAL:O	1:B:490:HIS:HB2	2.07	0.52
1:B:10:TRP:CE2	1:B:12:ARG:HD3	2.44	0.52
1:B:217:PHE:O	1:B:218:LEU:HB2	2.09	0.52
1:B:459:PRO:C	1:B:461:LEU:H	2.17	0.52
1:A:394:TRP:CE3	1:A:505:ASN:HB3	2.44	0.52
1:A:422:TRP:CZ2	1:A:525:PRO:HA	2.44	0.52
1:A:535:PHE:O	1:A:536:TRP:CB	2.56	0.52
1:B:137:SER:O	1:B:138:HIS:CB	2.58	0.52
1:B:216:GLY:O	1:B:217:PHE:CG	2.63	0.52
1:B:433:ASP:HB3	1:B:506:MET:HG2	1.92	0.52
1:A:87:GLU:HG2	1:A:90:TYR:CB	2.39	0.52
1:B:149:THR:C	1:B:151:GLY:N	2.64	0.52
1:A:358:THR:HA	1:A:495:ILE:HG21	1.91	0.52
1:A:406:LYS:HD3	1:A:407:TYR:CE2	2.45	0.52
1:B:112:PRO:HD2	1:B:413:TRP:HZ3	1.74	0.52
1:B:46:SER:HA	1:B:114:TRP:HZ3	1.67	0.52
1:B:454:ILE:O	1:B:458:VAL:HB	2.10	0.52
1:A:16:ARG:O	1:A:20:ASN:ND2	2.41	0.51
1:B:321:MET:O	1:B:321:MET:CG	2.57	0.51
1:A:288:PHE:O	1:A:289:LYS:C	2.53	0.51
1:A:362:LEU:HB2	1:A:444:ALA:HB2	1.91	0.51
1:B:16:ARG:HD3	1:B:273:GLY:O	2.10	0.51
1:B:58:ARG:HH11	1:B:58:ARG:HG2	1.69	0.51
1:A:96:HIS:HD2	1:A:128:LEU:CD1	2.20	0.51
1:A:250:TYR:CE1	1:B:532:ARG:NH1	2.76	0.51
1:B:358:THR:HG22	1:B:495:ILE:HD11	1.92	0.51
1:A:251:LEU:O	1:A:252:PRO:C	2.54	0.51
1:A:6:ALA:HB1	1:A:37:ILE:HD11	1.92	0.51
1:A:8:VAL:HG23	1:A:37:ILE:O	2.10	0.51
1:A:250:TYR:HE1	1:B:532:ARG:CZ	2.23	0.51
1:A:516:LEU:O	1:A:516:LEU:HD12	2.11	0.51
1:B:514:ASN:CG	1:B:515:SER:N	2.67	0.51
1:B:112:PRO:HD2	1:B:413:TRP:CZ3	2.46	0.51
1:A:369:GLN:OE1	1:A:376:LEU:HD23	2.10	0.51
1:A:397:TRP:C	1:A:399:HIS:H	2.19	0.51
1:A:260:HIS:ND1	1:A:260:HIS:N	2.47	0.51
1:B:36:LEU:HD23	1:B:38:PRO:HD3	1.92	0.51
1:B:52:VAL:CG2	1:B:53:GLY:N	2.73	0.51
1:A:110:CYS:O	1:A:111:GLU:C	2.53	0.51
1:B:12:ARG:HH22	1:B:106:ILE:HD12	1.76	0.51
1:A:14:GLY:O	1:A:16:ARG:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLU:OE2	1:B:413:TRP:HB3	2.10	0.50
1:B:158:TYR:CE2	1:B:162:LEU:HD21	2.45	0.50
1:B:515:SER:O	1:B:516:LEU:CB	2.57	0.50
1:B:535:PHE:N	1:B:535:PHE:CD2	2.79	0.50
1:A:247:ARG:HH11	1:A:247:ARG:CG	2.14	0.50
1:A:448:ASP:CG	1:A:448:ASP:O	2.52	0.50
1:B:72:GLN:CD	1:B:80:ARG:HD3	2.35	0.50
1:A:94:ARG:O	1:A:98:GLN:HG2	2.11	0.50
1:B:18:HIS:O	1:B:19:ASP:C	2.54	0.50
1:B:71:LEU:HD23	1:B:180:LEU:HD13	1.92	0.50
1:B:111:GLU:HB2	1:B:114:TRP:CD1	2.47	0.50
1:B:239:LYS:O	1:B:240:VAL:C	2.53	0.50
1:B:383:THR:OG1	1:B:443:LEU:HD23	2.10	0.50
1:A:349:LEU:O	1:A:352:SER:HB2	2.11	0.50
1:A:17:LEU:HD23	1:A:23:LEU:HD22	1.92	0.50
1:B:79:GLY:O	1:B:80:ARG:HG2	2.10	0.50
1:B:392:GLY:O	1:B:393:LEU:HB2	2.10	0.50
1:A:325:ASN:O	1:A:328:TYR:HB2	2.11	0.50
1:A:346:ASN:OD1	1:A:349:LEU:HD22	2.11	0.50
1:A:524:ARG:HG2	1:A:525:PRO:HD2	1.93	0.50
1:B:46:SER:N	1:B:114:TRP:HZ3	2.09	0.50
1:B:301:GLN:O	1:B:307:HIS:HB3	2.11	0.50
1:B:386:THR:O	1:B:391:GLY:HA3	2.12	0.50
1:A:431:LEU:HB2	1:A:528:GLU:OE2	2.12	0.49
1:B:19:ASP:OD1	1:B:175:THR:HG23	2.11	0.49
1:B:488:GLY:O	1:B:489:VAL:C	2.55	0.49
1:B:508:ALA:HA	1:B:511:SER:HB2	1.94	0.49
1:A:86:GLY:HA3	1:A:91:ILE:HD11	1.93	0.49
1:B:93:ARG:HH22	1:B:127:GLU:CD	2.20	0.49
1:A:514:ASN:O	1:A:516:LEU:N	2.45	0.49
1:B:13:HIS:CD2	1:B:271:ARG:NH1	2.79	0.49
1:B:244:ALA:CA	1:B:247:ARG:NH1	2.73	0.49
1:A:101:LEU:HB3	1:A:130:ILE:HD13	1.95	0.49
1:B:107:GLU:OE2	1:B:138:HIS:HB2	2.12	0.49
1:A:58:ARG:NH1	1:A:58:ARG:CB	2.62	0.49
1:A:441:VAL:O	1:A:443:LEU:N	2.46	0.49
1:B:342:TRP:CG	1:B:396:SER:HA	2.48	0.49
1:B:389:THR:O	1:B:390:ARG:CB	2.60	0.49
1:A:394:TRP:O	1:A:394:TRP:CG	2.66	0.49
1:B:282:TRP:O	1:B:286:ASP:HB2	2.13	0.49
1:A:106:ILE:HD11	1:A:134:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ASN:O	1:A:291:VAL:HG23	2.12	0.49
1:B:67:ILE:HA	1:B:70:GLN:HB2	1.95	0.49
1:B:113:ILE:HD11	1:B:413:TRP:CG	2.48	0.49
1:A:145:LEU:O	1:A:149:THR:N	2.40	0.49
1:B:136:VAL:O	1:B:136:VAL:HG12	2.10	0.49
1:B:293:LEU:HD21	1:B:303:THR:HA	1.94	0.49
1:A:536:TRP:O	1:A:537:LEU:HD23	2.12	0.49
1:A:78:ARG:NH2	1:A:183:ALA:O	2.46	0.49
1:A:79:GLY:HA3	1:A:185:PHE:CG	2.48	0.49
1:B:364:ASP:O	1:B:368:ARG:HG3	2.13	0.49
1:B:401:LEU:HG	1:B:405:LEU:HD11	1.93	0.49
1:B:458:VAL:HG12	1:B:458:VAL:O	2.11	0.49
1:B:238:LEU:HD11	1:B:283:SER:HB2	1.94	0.48
1:A:260:HIS:HD2	1:A:452:THR:HG22	1.77	0.48
1:B:511:SER:O	1:B:514:ASN:OD1	2.31	0.48
1:A:103:ARG:HG2	1:A:131:ASP:CB	2.41	0.48
1:B:75:THR:O	1:B:78:ARG:HB2	2.14	0.48
1:A:55:ASN:HB3	1:A:409:LEU:HD21	1.95	0.48
1:B:248:GLY:O	1:B:249:PHE:C	2.56	0.48
1:A:15:LEU:HB2	1:A:272:PHE:O	2.14	0.48
1:A:159:GLN:HG2	1:A:526:SER:HB3	1.95	0.48
1:B:69:ASP:O	1:B:70:GLN:C	2.56	0.48
1:B:376:LEU:HD22	1:B:380:LEU:HD12	1.94	0.48
1:A:250:TYR:HE1	1:B:532:ARG:HH22	1.55	0.48
1:B:393:LEU:H	1:B:496:ILE:HD13	1.76	0.48
1:A:282:TRP:HZ3	1:A:285:HIS:CE1	2.32	0.48
1:A:293:LEU:H	1:A:303:THR:HB	1.78	0.48
1:A:309:THR:HG23	1:A:313:ILE:HD11	1.95	0.48
1:A:468:PHE:CD2	1:A:475:MET:HG2	2.49	0.48
1:B:229:GLN:OE1	1:B:229:GLN:CA	2.61	0.48
1:B:346:ASN:CB	1:B:349:LEU:HD22	2.44	0.48
1:A:16:ARG:HD3	1:A:273:GLY:O	2.13	0.48
1:B:113:ILE:O	1:B:113:ILE:HG22	2.13	0.48
1:B:279:ARG:O	1:B:283:SER:OG	2.27	0.48
1:B:379:THR:HG23	1:B:536:TRP:CD1	2.49	0.48
1:A:281:TYR:C	1:A:281:TYR:CD2	2.91	0.48
1:B:271:ARG:CG	1:B:412:ASP:OD2	2.62	0.48
1:A:453:TYR:O	1:A:454:ILE:C	2.57	0.48
1:B:465:PRO:O	1:B:466:LYS:HB2	2.14	0.48
1:A:466:LYS:HA	1:A:469:VAL:HG12	1.96	0.47
1:B:401:LEU:HD13	1:B:417:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:O	1:B:238:LEU:HB2	2.14	0.47
1:A:310:GLY:HA2	1:A:313:ILE:HG12	1.95	0.47
1:A:428:PHE:CE1	1:A:519:PRO:HD3	2.49	0.47
1:B:297:VAL:CA	1:B:298:ARG:CB	2.92	0.47
1:B:325:ASN:O	1:B:328:TYR:HB2	2.15	0.47
1:A:314:TRP:O	1:A:317:TYR:HB3	2.15	0.47
1:A:528:GLU:HG2	1:A:532:ARG:NH1	2.29	0.47
1:A:244:ALA:HA	1:A:247:ARG:NH1	2.30	0.47
1:A:256:LEU:HB2	1:A:257:PRO:HD2	1.96	0.47
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.76	0.47
1:A:529:GLU:HB2	1:B:250:TYR:CD2	2.49	0.47
1:B:309:THR:O	1:B:313:ILE:HG12	2.14	0.47
1:A:37:ILE:HG23	1:A:186:VAL:HG21	1.96	0.47
1:A:471:GLU:HA	1:A:473:TRP:CZ3	2.49	0.47
1:B:93:ARG:HH12	1:B:128:LEU:HD21	1.80	0.47
1:B:514:ASN:O	1:B:515:SER:C	2.57	0.47
1:A:140:LEU:H	1:A:316:GLU:CD	2.23	0.47
1:A:144:GLN:O	1:A:148:GLU:HB2	2.15	0.47
1:A:159:GLN:HG2	1:A:526:SER:CB	2.45	0.47
1:A:484:GLU:HG3	1:A:484:GLU:O	2.15	0.47
1:B:172:PRO:O	1:B:278:ARG:HG2	2.15	0.47
1:B:328:TYR:HA	1:B:334:ASN:HD21	1.80	0.47
1:B:450:ASP:OD2	1:B:466:LYS:HE3	2.14	0.47
1:B:527:ASN:OD1	1:B:530:GLU:N	2.38	0.47
1:A:297:VAL:HG12	1:A:307:HIS:HB2	1.96	0.47
1:B:69:ASP:O	1:B:71:LEU:N	2.48	0.47
1:B:356:GLY:C	1:B:364:ASP:OD1	2.58	0.47
1:B:443:LEU:HD13	1:B:446:ARG:NH2	2.30	0.47
1:A:206:GLU:CD	1:A:206:GLU:N	2.73	0.47
1:A:250:TYR:CE1	1:B:529:GLU:HB2	2.50	0.47
1:B:9:ILE:C	1:B:9:ILE:HD13	2.39	0.47
1:A:160:MET:O	1:A:161:PHE:C	2.58	0.46
1:A:286:ASP:O	1:A:287:LEU:C	2.57	0.46
1:A:18:HIS:O	1:A:19:ASP:C	2.58	0.46
1:B:280:PHE:CG	1:B:312:LEU:HD11	2.50	0.46
1:A:43:ASP:OD1	1:A:46:SER:HB2	2.16	0.46
1:A:88:PRO:C	1:A:90:TYR:H	2.23	0.46
1:A:459:PRO:O	1:A:462:MET:HG3	2.15	0.46
1:A:500:MET:HE2	1:A:500:MET:HA	1.97	0.46
1:A:8:VAL:CG1	1:A:104:ILE:HA	2.43	0.46
1:A:14:GLY:O	1:A:16:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:C	1:A:230:ALA:N	2.73	0.46
1:B:262:SER:HB3	1:B:263:PRO:CD	2.46	0.46
1:B:498:LEU:O	1:B:499:SER:C	2.58	0.46
1:A:8:VAL:HG13	1:A:8:VAL:O	2.16	0.46
1:B:23:LEU:O	1:B:23:LEU:HD12	2.15	0.46
1:B:224:ARG:CG	1:B:229:GLN:HE21	2.29	0.46
1:A:79:GLY:HA3	1:A:185:PHE:CD2	2.51	0.46
1:B:52:VAL:HG22	1:B:53:GLY:O	2.15	0.46
1:B:321:MET:HE1	1:B:523:CYS:CB	2.46	0.46
1:B:474:ARG:HG3	1:B:474:ARG:NH1	2.30	0.46
1:A:88:PRO:C	1:A:90:TYR:N	2.71	0.46
1:A:461:LEU:HD23	1:A:464:VAL:HG21	1.98	0.46
1:B:121:ILE:O	1:B:122:ARG:C	2.59	0.46
1:B:158:TYR:HE2	1:B:162:LEU:HD21	1.81	0.46
1:B:410:ASP:O	1:B:411:ALA:C	2.57	0.46
1:B:473:TRP:CD1	1:B:494:ARG:HH21	2.33	0.46
2:B:601:FAD:H3B	2:B:601:FAD:H5'2	1.98	0.46
1:B:34:ILE:HD13	1:B:34:ILE:N	2.31	0.46
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.72	0.46
1:A:340:ILE:HA	1:A:341:PRO:HD3	1.83	0.46
1:B:337:CYS:O	1:B:338:LEU:C	2.58	0.46
1:B:368:ARG:HH22	1:B:460:GLU:CD	2.23	0.46
1:B:388:LEU:HG	1:B:389:THR:HG23	1.98	0.46
1:A:358:THR:HA	1:A:495:ILE:HG23	1.97	0.45
1:B:346:ASN:HB3	1:B:349:LEU:HD22	1.97	0.45
1:A:15:LEU:HD23	1:A:15:LEU:H	1.81	0.45
1:A:280:PHE:O	1:A:284:VAL:HG23	2.16	0.45
1:A:309:THR:HG22	1:A:310:GLY:N	2.30	0.45
1:B:9:ILE:C	1:B:9:ILE:CD1	2.89	0.45
1:B:217:PHE:CZ	1:B:368:ARG:HD3	2.52	0.45
1:B:287:LEU:HD23	1:B:288:PHE:CE1	2.51	0.45
1:A:311:GLN:HB3	2:A:601:FAD:O4B	2.16	0.45
1:B:10:TRP:CZ3	1:B:121:ILE:HD12	2.51	0.45
1:B:211:TYR:O	1:B:213:ASP:N	2.49	0.45
1:B:519:PRO:HA	1:B:520:PRO:HD3	1.83	0.45
1:A:362:LEU:HD22	1:A:444:ALA:CB	2.40	0.45
1:A:385:ALA:HB1	1:A:420:TRP:CZ3	2.52	0.45
1:B:119:GLU:OE2	1:B:126:ARG:NH2	2.50	0.45
1:B:409:LEU:HA	1:B:409:LEU:HD23	1.69	0.45
1:A:147:ILE:HG23	1:A:153:ILE:C	2.42	0.45
1:A:527:ASN:HB2	1:B:250:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:OE1	1:B:137:SER:HB3	2.16	0.45
1:B:378:HIS:NE2	1:B:534:PHE:O	2.47	0.45
1:A:83:VAL:O	1:A:199:PHE:HD2	2.00	0.45
1:A:94:ARG:HB3	1:A:192:PHE:HE1	1.82	0.45
1:A:288:PHE:O	1:A:290:ASN:O	2.35	0.45
1:B:431:LEU:O	1:B:431:LEU:HD12	2.15	0.45
1:B:47:ALA:O	1:B:48:GLY:C	2.60	0.45
1:B:202:LEU:HD12	1:B:203:PRO:HD2	1.98	0.45
1:A:106:ILE:O	1:A:106:ILE:HG13	2.17	0.45
1:A:232:LEU:HD23	1:A:232:LEU:C	2.42	0.45
1:B:377:HIS:ND1	1:B:379:THR:OG1	2.50	0.45
1:A:247:ARG:O	1:A:247:ARG:CG	2.62	0.44
1:B:38:PRO:HG2	1:B:81:LEU:HA	1.99	0.44
1:B:7:ASN:OD1	1:B:103:ARG:HB2	2.17	0.44
1:B:290:ASN:O	1:B:291:VAL:CG2	2.60	0.44
1:B:441:VAL:O	1:B:445:LYS:HG3	2.18	0.44
1:B:480:GLN:HB3	1:B:485:CYS:O	2.18	0.44
1:A:161:PHE:HE1	1:A:320:THR:HG21	1.83	0.44
1:A:353:TRP:CH2	1:A:400:GLY:HA2	2.53	0.44
1:A:392:GLY:HA2	1:A:393:LEU:C	2.42	0.44
1:B:238:LEU:HA	1:B:238:LEU:HD23	1.47	0.44
1:B:23:LEU:HD12	1:B:23:LEU:C	2.43	0.44
1:B:256:LEU:HB2	1:B:257:PRO:HD2	1.99	0.44
1:B:346:ASN:O	1:B:349:LEU:HB2	2.17	0.44
1:B:418:GLY:HA2	1:B:421:MET:HE3	1.99	0.44
1:B:536:TRP:O	1:B:537:LEU:C	2.60	0.44
1:A:69:ASP:O	1:A:72:GLN:N	2.49	0.44
1:A:192:PHE:CE1	1:A:196:LEU:HD22	2.49	0.44
1:A:270:LEU:CD2	1:A:275:LEU:HD23	2.47	0.44
1:B:297:VAL:HG21	1:B:307:HIS:CD2	2.52	0.44
1:A:297:VAL:HG11	1:A:307:HIS:HB2	2.00	0.44
1:B:271:ARG:HG3	1:B:412:ASP:OD2	2.16	0.44
1:A:222:ASN:C	1:A:222:ASN:HD22	2.25	0.44
1:A:294:ARG:O	1:A:295:ALA:CB	2.65	0.44
1:A:361:PRO:O	1:A:365:GLY:N	2.39	0.44
1:B:184:THR:C	1:B:185:PHE:CD2	2.95	0.44
1:B:273:GLY:C	1:B:275:LEU:N	2.75	0.44
1:A:142:ASP:O	1:A:144:GLN:N	2.50	0.44
1:A:534:PHE:CD2	1:A:534:PHE:C	2.96	0.44
1:A:202:LEU:HG	1:A:203:PRO:HD2	1.99	0.44
1:A:38:PRO:HG2	1:A:71:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LYS:O	1:A:466:LYS:HG2	2.18	0.43
1:A:534:PHE:O	1:A:534:PHE:CG	2.71	0.43
1:B:35:ALA:HB2	1:B:184:THR:HB	2.00	0.43
1:B:154:PRO:O	1:B:156:LEU:HD23	2.18	0.43
1:B:162:LEU:O	1:B:163:HIS:C	2.56	0.43
1:B:385:ALA:HB1	1:B:420:TRP:CZ3	2.53	0.43
1:B:54:TYR:CG	1:B:212:GLY:HA2	2.53	0.43
1:A:154:PRO:HB2	1:A:321:MET:HA	1.99	0.43
1:B:270:LEU:HD21	1:B:280:PHE:HD2	1.83	0.43
1:A:29:ASP:OD2	1:A:103:ARG:NH1	2.52	0.43
1:B:211:TYR:C	1:B:213:ASP:H	2.26	0.43
1:A:17:LEU:HD23	1:A:23:LEU:CD2	2.49	0.43
1:A:192:PHE:O	1:A:196:LEU:HB2	2.18	0.43
1:A:280:PHE:CG	1:A:312:LEU:HD11	2.54	0.43
1:A:354:ARG:HB3	1:A:403:HIS:CE1	2.54	0.43
1:B:242:GLN:HB2	1:B:287:LEU:HD11	2.00	0.43
1:B:528:GLU:O	1:B:532:ARG:HG3	2.19	0.43
1:A:381:ARG:HB3	2:A:601:FAD:C8	2.49	0.43
1:A:401:LEU:HD13	1:A:420:TRP:CD1	2.53	0.43
1:B:29:ASP:HB3	1:B:34:ILE:HG12	1.99	0.43
1:B:478:GLU:H	1:B:478:GLU:HG2	1.50	0.43
1:A:74:ALA:O	1:A:181:GLU:HA	2.19	0.43
1:A:221:ILE:CB	1:A:373:GLU:OE2	2.66	0.43
1:A:353:TRP:CZ3	1:A:400:GLY:HA2	2.54	0.43
1:B:242:GLN:O	1:B:245:PHE:HB3	2.19	0.43
1:A:318:PHE:O	1:A:319:TYR:C	2.62	0.42
1:B:46:SER:H	1:B:114:TRP:HZ3	1.66	0.42
1:B:293:LEU:HD23	1:B:303:THR:HB	2.00	0.42
1:A:104:ILE:HG13	1:A:130:ILE:HG21	2.01	0.42
1:A:361:PRO:HB2	1:A:454:ILE:HD13	2.01	0.42
1:A:486:LEU:HD13	1:A:490:HIS:CE1	2.52	0.42
1:B:369:GLN:O	1:B:370:LEU:C	2.62	0.42
1:B:421:MET:HE3	1:B:421:MET:HB2	1.91	0.42
1:A:297:VAL:CG1	1:A:298:ARG:N	2.52	0.42
1:B:292:GLN:O	1:B:293:LEU:C	2.62	0.42
1:A:338:LEU:HD12	1:A:425:SER:O	2.19	0.42
1:A:379:THR:O	1:A:382:ASN:HB2	2.18	0.42
1:B:452:THR:HG22	1:B:453:TYR:N	2.33	0.42
1:B:471:GLU:CB	1:B:473:TRP:CZ2	3.02	0.42
1:B:361:PRO:O	1:B:364:ASP:HB2	2.19	0.42
1:B:410:ASP:OD1	1:B:411:ALA:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:O	1:A:82:LEU:HG	2.20	0.42
1:A:438:THR:HG22	1:A:439:CYS:N	2.34	0.42
1:B:60:LEU:O	1:B:64:LEU:HG	2.20	0.42
1:B:85:GLU:HB2	1:B:199:PHE:CE2	2.55	0.42
1:B:108:GLN:HG3	1:B:109:ASP:N	2.35	0.42
1:B:319:TYR:HA	1:B:414:SER:CB	2.49	0.42
1:B:382:ASN:O	1:B:383:THR:C	2.61	0.42
1:B:56:ARG:HD3	1:B:408:LEU:O	2.19	0.42
1:B:272:PHE:C	1:B:274:CYS:H	2.27	0.42
1:B:443:LEU:CD1	1:B:446:ARG:NH2	2.83	0.42
1:A:282:TRP:CZ3	1:A:285:HIS:ND1	2.88	0.42
1:A:286:ASP:O	1:A:289:LYS:N	2.52	0.42
1:A:309:THR:O	1:A:311:GLN:N	2.53	0.42
1:A:421:MET:HE3	1:A:421:MET:HB2	1.87	0.42
1:B:8:VAL:CG1	1:B:104:ILE:HG23	2.49	0.42
1:B:9:ILE:CG1	1:B:23:LEU:HA	2.49	0.42
1:B:68:ASP:C	1:B:68:ASP:OD1	2.62	0.42
1:B:342:TRP:HA	1:B:394:TRP:CD1	2.55	0.42
1:B:365:GLY:HA2	1:B:458:VAL:HG23	2.01	0.42
1:B:459:PRO:C	1:B:461:LEU:N	2.78	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD12	1.70	0.42
1:A:244:ALA:HA	1:A:247:ARG:HG2	2.02	0.42
1:A:439:CYS:HA	1:A:440:PRO:HD3	1.66	0.42
1:B:343:ALA:O	1:B:344:LYS:C	2.61	0.42
1:B:16:ARG:NH2	1:B:137:SER:OG	2.53	0.42
1:B:497:ASP:OD1	1:B:500:MET:CG	2.61	0.42
1:A:383:THR:HG23	1:A:440:PRO:HG3	2.01	0.41
1:B:244:ALA:HB1	1:B:251:LEU:HD12	2.02	0.41
1:B:246:GLU:O	1:B:247:ARG:C	2.61	0.41
1:A:105:CYS:HA	1:A:133:VAL:HB	2.01	0.41
1:A:357:GLN:HB3	1:A:492:PRO:HG3	2.01	0.41
1:B:101:LEU:HB2	1:B:130:ILE:CD1	2.51	0.41
1:B:488:GLY:C	1:B:489:VAL:O	2.61	0.41
1:A:88:PRO:O	1:A:90:TYR:N	2.52	0.41
1:A:400:GLY:HA3	1:A:420:TRP:CZ2	2.56	0.41
1:A:447:LEU:HD12	1:A:447:LEU:HA	1.68	0.41
1:B:93:ARG:NH1	1:B:128:LEU:HD21	2.35	0.41
1:B:309:THR:HG22	1:B:310:GLY:N	2.34	0.41
1:B:327:ASN:O	1:B:330:ARG:HG3	2.21	0.41
1:B:522:HIS:O	1:B:524:ARG:NH1	2.53	0.41
1:A:321:MET:SD	1:A:523:CYS:HB2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:CD1	1:A:383:THR:CG2	2.98	0.41
1:B:94:ARG:HD3	1:B:94:ARG:HA	1.76	0.41
1:B:108:GLN:HG3	1:B:109:ASP:H	1.85	0.41
1:B:296:CYS:SG	1:B:299:GLY:C	3.04	0.41
1:A:244:ALA:HB1	1:A:251:LEU:HD22	2.02	0.41
1:B:394:TRP:HZ3	1:B:505:ASN:HB3	1.86	0.41
1:B:398:GLU:O	1:B:402:GLN:HG2	2.20	0.41
1:A:103:ARG:HG2	1:A:131:ASP:OD2	2.21	0.41
1:A:252:PRO:CB	1:A:253:ASN:C	2.93	0.41
1:A:288:PHE:O	1:A:290:ASN:N	2.54	0.41
1:B:43:ASP:HB2	1:B:45:GLU:O	2.21	0.41
1:B:363:ILE:CD1	1:B:440:PRO:HB3	2.51	0.41
1:A:13:HIS:O	1:A:272:PHE:O	2.38	0.41
1:A:18:HIS:CE1	1:A:231:LEU:HD21	2.55	0.41
1:A:303:THR:CG2	1:B:301:GLN:NE2	2.78	0.41
1:A:332:GLU:HG2	1:A:333:GLY:H	1.86	0.41
1:B:37:ILE:CG1	1:B:186:VAL:HG11	2.51	0.41
1:B:72:GLN:OE1	1:B:80:ARG:CD	2.69	0.41
1:B:85:GLU:HB2	1:B:199:PHE:CZ	2.55	0.41
1:B:156:LEU:HD11	1:B:336:ILE:CG2	2.49	0.41
1:B:192:PHE:CZ	1:B:196:LEU:HD13	2.55	0.41
1:B:389:THR:O	1:B:390:ARG:HG2	2.20	0.41
1:B:23:LEU:O	1:B:24:LEU:C	2.63	0.41
1:B:342:TRP:CD1	1:B:396:SER:HA	2.55	0.41
1:B:343:ALA:N	1:B:394:TRP:CD1	2.84	0.41
1:B:439:CYS:HA	1:B:440:PRO:HD3	1.54	0.41
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.86	0.41
1:B:491:TYR:HA	1:B:492:PRO:HD3	1.92	0.41
1:A:404:PHE:CD2	1:A:420:TRP:NE1	2.89	0.41
1:B:2:ALA:O	1:B:99:VAL:HG23	2.20	0.41
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.92	0.41
1:A:20:ASN:O	1:A:23:LEU:HB3	2.21	0.40
1:A:121:ILE:H	1:A:121:ILE:HG12	1.36	0.40
1:A:202:LEU:HA	1:A:203:PRO:HD2	1.91	0.40
1:A:311:GLN:O	1:A:314:TRP:HB2	2.21	0.40
1:B:12:ARG:NH2	1:B:106:ILE:HD12	2.36	0.40
1:B:219:ALA:O	1:B:220:LYS:CB	2.65	0.40
1:B:349:LEU:HD23	1:B:393:LEU:HD22	2.03	0.40
1:B:429:GLU:HB3	1:B:432:LEU:HD12	2.03	0.40
1:A:119:GLU:O	1:A:120:SER:C	2.64	0.40
1:A:377:HIS:HE1	1:A:536:TRP:CZ3	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:CD1	1:A:70:GLN:OE1	2.57	0.40
1:A:168:ILE:CG2	1:A:169:GLY:N	2.83	0.40
1:A:310:GLY:CA	1:A:313:ILE:HG12	2.51	0.40
1:A:397:TRP:C	1:A:399:HIS:N	2.77	0.40
1:A:453:TYR:O	1:A:456:GLN:N	2.54	0.40
1:A:493:GLU:O	1:A:494:ARG:C	2.63	0.40
1:B:238:LEU:O	1:B:239:LYS:C	2.63	0.40
1:B:387:PHE:O	1:B:393:LEU:HB2	2.21	0.40
1:A:12:ARG:HD3	1:A:12:ARG:N	2.36	0.40
1:A:61:LEU:HB3	1:A:202:LEU:HD21	2.04	0.40
1:A:243:HIS:O	1:A:247:ARG:HG2	2.21	0.40
1:A:433:ASP:O	1:A:506:MET:HE3	2.20	0.40
1:B:179:ARG:NH1	1:B:181:GLU:CG	2.81	0.40
1:B:181:GLU:H	1:B:181:GLU:HG2	1.67	0.40
1:B:383:THR:OG1	1:B:443:LEU:CD2	2.70	0.40
1:B:476:SER:O	1:B:480:GLN:HG3	2.21	0.40
1:A:15:LEU:HD23	1:A:15:LEU:N	2.37	0.40
1:A:17:LEU:HD12	1:A:70:GLN:CD	2.43	0.40
1:A:79:GLY:HA3	1:A:185:PHE:CD1	2.56	0.40
1:A:189:ASP:O	1:A:192:PHE:N	2.49	0.40
1:A:427:ALA:CB	1:A:512:LEU:HD21	2.51	0.40
1:B:158:TYR:O	1:B:162:LEU:HD12	2.20	0.40
1:B:223:TRP:CD1	1:B:223:TRP:N	2.90	0.40
1:B:235:ASP:HA	1:B:238:LEU:HB2	2.03	0.40
1:B:406:LYS:HB3	1:B:407:TYR:CD2	2.57	0.40
1:B:461:LEU:HD22	1:B:464:VAL:HG23	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	525/561 (94%)	409 (78%)	90 (17%)	26 (5%)	1	13
1	B	541/561 (96%)	444 (82%)	70 (13%)	27 (5%)	1	13
All	All	1066/1122 (95%)	853 (80%)	160 (15%)	53 (5%)	1	13

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	221	ILE
1	A	252	PRO
1	A	254	GLN
1	A	291	VAL
1	A	347	GLU
1	A	392	GLY
1	A	393	LEU
1	B	221	ILE
1	B	249	PHE
1	B	250	TYR
1	B	517	ILE
1	A	76	ASP
1	A	227	GLU
1	A	250	TYR
1	A	287	LEU
1	A	289	LYS
1	A	295	ALA
1	B	70	GLN
1	B	150	ASN
1	B	216	GLY
1	B	290	ASN
1	B	466	LYS
1	B	489	VAL
1	A	88	PRO
1	A	310	GLY
1	A	382	ASN
1	A	442	ALA
1	A	460	GLU
1	A	515	SER
1	B	110	CYS
1	B	218	LEU
1	B	239	LYS
1	B	293	LEU
1	B	390	ARG

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Mol	Chain	Res	Type
1	B	393	LEU
1	A	69	ASP
1	A	73	ALA
1	A	172	PRO
1	A	203	PRO
1	A	286	ASP
1	B	-4	SER
1	B	14	GLY
1	B	66	ASP
1	B	88	PRO
1	B	262	SER
1	B	274	CYS
1	A	89	ALA
1	B	252	PRO
1	B	487	ILE
1	B	48	GLY
1	B	240	VAL
1	B	212	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/488 (92%)	375 (84%)	72 (16%)	2	13
1	B	458/488 (94%)	378 (82%)	80 (18%)	2	10
All	All	905/976 (93%)	753 (83%)	152 (17%)	2	11

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	15	LEU
1	A	31	ASP
1	A	45	GLU
1	A	46	SER

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Mol	Chain	Res	Type
1	A	52	VAL
1	A	58	ARG
1	A	72	GLN
1	A	82	LEU
1	A	87	GLU
1	A	90	TYR
1	A	95	LEU
1	A	101	LEU
1	A	113	ILE
1	A	120	SER
1	A	121	ILE
1	A	123	SER
1	A	129	ASN
1	A	134	GLU
1	A	145	LEU
1	A	153	ILE
1	A	157	THR
1	A	168	ILE
1	A	170	LEU
1	A	177	ASP
1	A	184	THR
1	A	191	GLU
1	A	195	SER
1	A	197	LYS
1	A	204	THR
1	A	206	GLU
1	A	222	ASN
1	A	224	ARG
1	A	236	GLU
1	A	246	GLU
1	A	247	ARG
1	A	251	LEU
1	A	252	PRO
1	A	258	ASN
1	A	260	HIS
1	A	262	SER
1	A	275	LEU
1	A	290	ASN
1	A	293	LEU
1	A	302	MET
1	A	303	THR
1	A	308	ILE

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Mol	Chain	Res	Type
1	A	309	THR
1	A	322	SER
1	A	335	ASP
1	A	346	ASN
1	A	347	GLU
1	A	349	LEU
1	A	379	THR
1	A	388	LEU
1	A	390	ARG
1	A	398	GLU
1	A	410	ASP
1	A	412	ASP
1	A	414	SER
1	A	437	VAL
1	A	443	LEU
1	A	447	LEU
1	A	452	THR
1	A	461	LEU
1	A	471	GLU
1	A	507	LEU
1	A	512	LEU
1	A	514	ASN
1	A	523	CYS
1	A	528	GLU
1	A	536	TRP
1	B	8	VAL
1	B	9	ILE
1	B	36	LEU
1	B	43	ASP
1	B	46	SER
1	B	49	THR
1	B	58	ARG
1	B	62	ASP
1	B	75	THR
1	B	80	ARG
1	B	81	LEU
1	B	83	VAL
1	B	87	GLU
1	B	94	ARG
1	B	99	VAL
1	B	116	GLU
1	B	120	SER

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Mol	Chain	Res	Type
1	B	121	ILE
1	B	123	SER
1	B	134	GLU
1	B	136	VAL
1	B	153	ILE
1	B	156	LEU
1	B	157	THR
1	B	162	LEU
1	B	164	THR
1	B	165	VAL
1	B	170	LEU
1	B	175	THR
1	B	177	ASP
1	B	184	THR
1	B	191	GLU
1	B	196	LEU
1	B	204	THR
1	B	218	LEU
1	B	228	THR
1	B	237	ARG
1	B	242	GLN
1	B	256	LEU
1	B	258	ASN
1	B	260	HIS
1	B	274	CYS
1	B	276	SER
1	B	283	SER
1	B	290	ASN
1	B	293	LEU
1	B	296	CYS
1	B	300	VAL
1	B	301	GLN
1	B	303	THR
1	B	308	ILE
1	B	309	THR
1	B	322	SER
1	B	330	ARG
1	B	335	ASP
1	B	346	ASN
1	B	352	SER
1	B	369	GLN
1	B	379	THR

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Mol	Chain	Res	Type
1	B	380	LEU
1	B	383	THR
1	B	386	THR
1	B	406	LYS
1	B	414	SER
1	B	437	VAL
1	B	438	THR
1	B	447	LEU
1	B	456	GLN
1	B	460	GLU
1	B	467	GLU
1	B	478	GLU
1	B	487	ILE
1	B	498	LEU
1	B	500	MET
1	B	503	LYS
1	B	507	LEU
1	B	511	SER
1	B	516	LEU
1	B	517	ILE
1	B	524	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	108	GLN
1	A	222	ASN
1	A	290	ASN
1	A	402	GLN
1	A	403	HIS
1	A	463	ASN
1	A	505	ASN
1	A	533	GLN
1	B	32	GLN
1	B	55	ASN
1	B	96	HIS
1	B	108	GLN
1	B	242	GLN
1	B	301	GLN
1	B	307	HIS
1	B	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
2	FAD	A	601	-	58,58,58	0.49	0	85,89,89	1.14	6 (7%)
2	FAD	B	601	-	58,58,58	0.72	1 (1%)	85,89,89	1.08	5 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	3/34/50/50	0/6/6/6
2	FAD	B	601	-	-	3/34/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	PA-O3P	4.40	1.64	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O3P-PA-O1A	-6.87	90.04	110.70
2	A	601	FAD	O3P-PA-O1A	-5.62	93.78	110.70
2	A	601	FAD	O3P-P-O1P	-3.50	100.18	110.70
2	B	601	FAD	O3P-P-O1P	-3.41	100.43	110.70
2	A	601	FAD	C2'-C1'-N10	3.35	126.03	110.20
2	A	601	FAD	O2P-P-O3P	3.03	115.46	107.27
2	A	601	FAD	C1'-C2'-C3'	2.85	117.39	109.66
2	A	601	FAD	O2A-PA-O3P	-2.54	100.41	107.27
2	B	601	FAD	C2'-C1'-N10	2.29	121.02	110.20
2	B	601	FAD	O2P-P-O1P	2.04	121.91	112.44
2	B	601	FAD	C1'-C2'-C3'	2.03	115.17	109.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	C4'-C5'-O5'-P
2	A	601	FAD	P-O3P-PA-O1A
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	P-O3P-PA-O1A

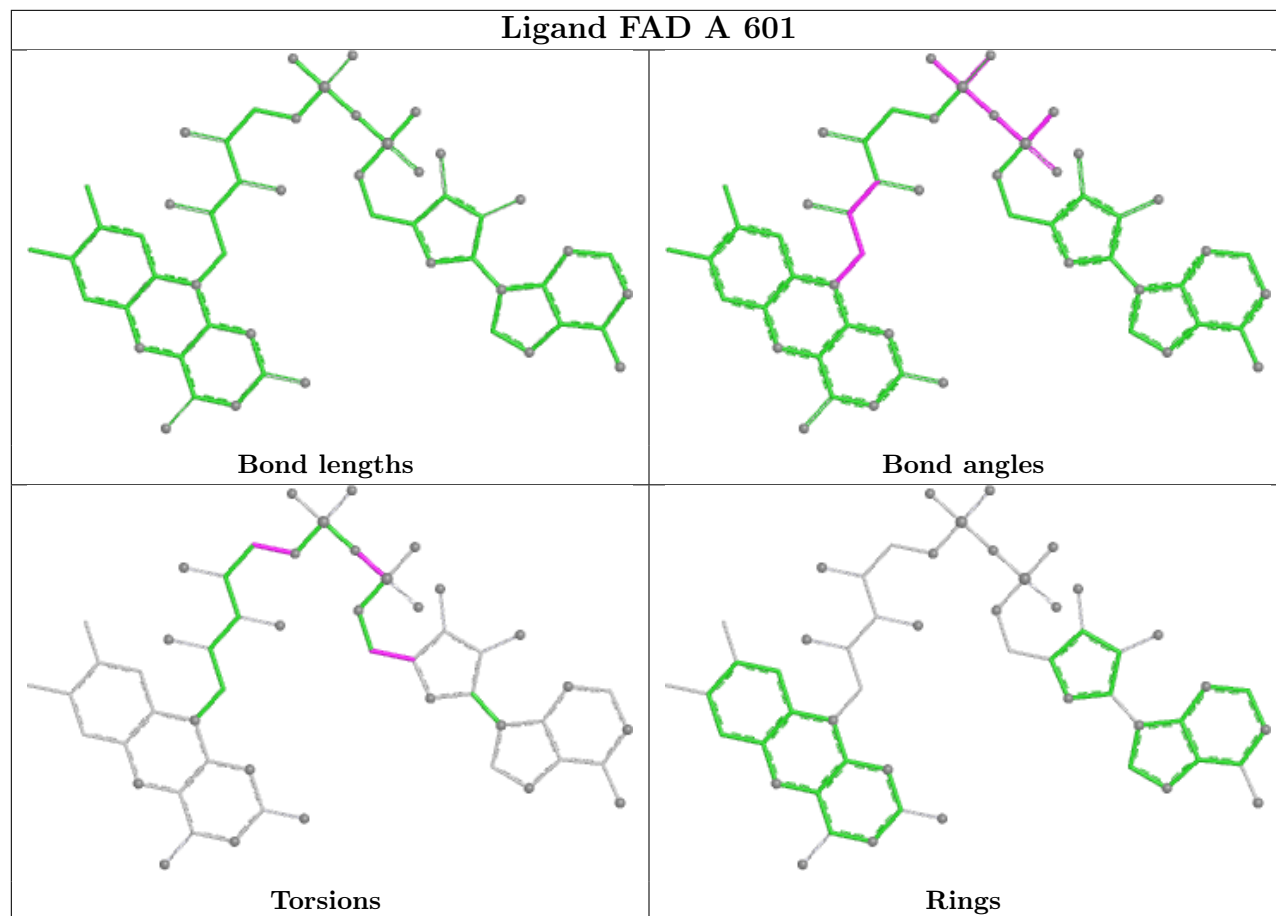
There are no ring outliers.

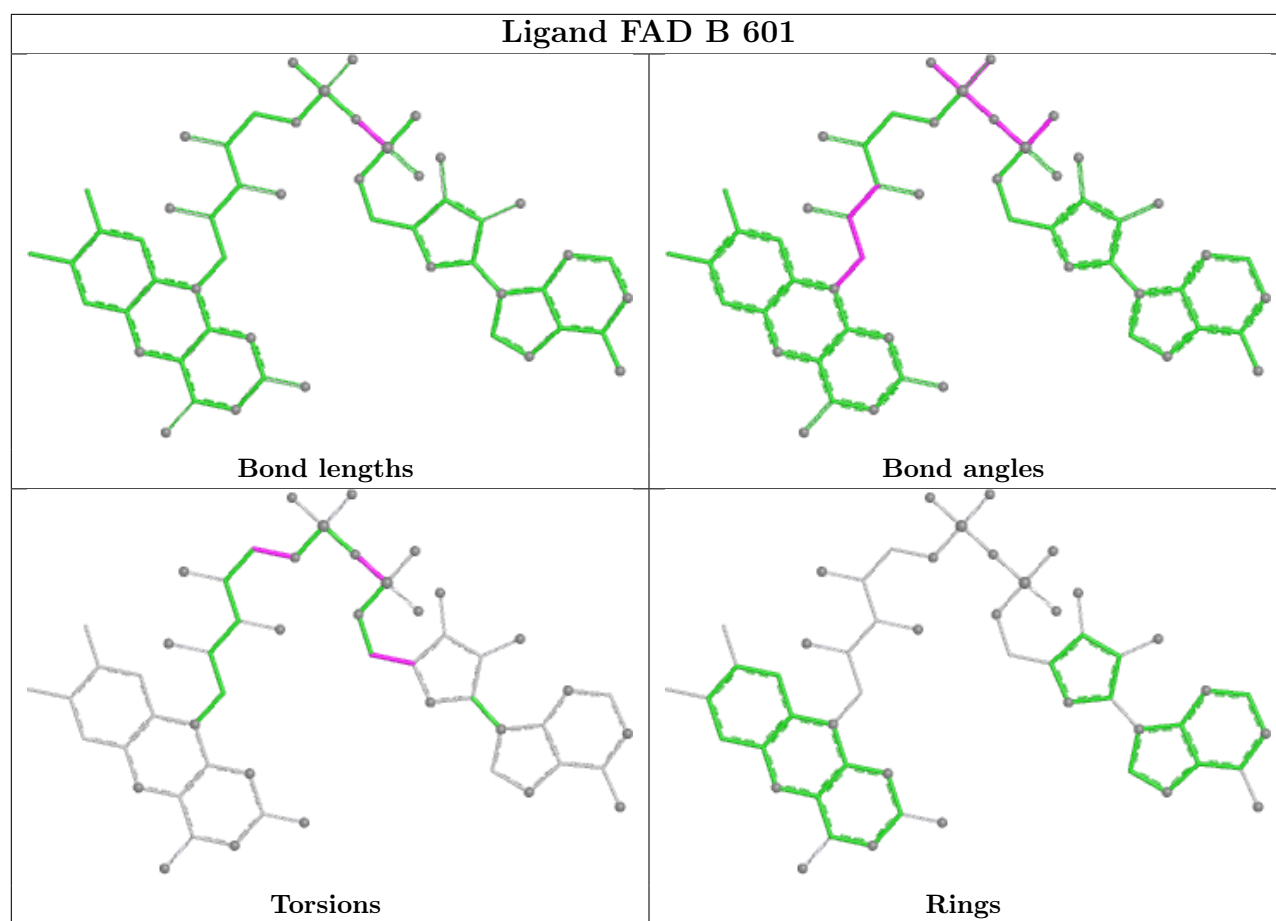
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	3	0
2	B	601	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	529/561 (94%)	-0.44	2 (0%) 88 79	23, 52, 87, 135	0
1	B	543/561 (96%)	-0.39	2 (0%) 88 79	17, 54, 92, 161	0
All	All	1072/1122 (95%)	-0.42	4 (0%) 88 79	17, 54, 90, 161	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	TYR	3.4
1	A	213	ASP	2.7
1	B	218	LEU	2.5
1	B	219	ALA	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

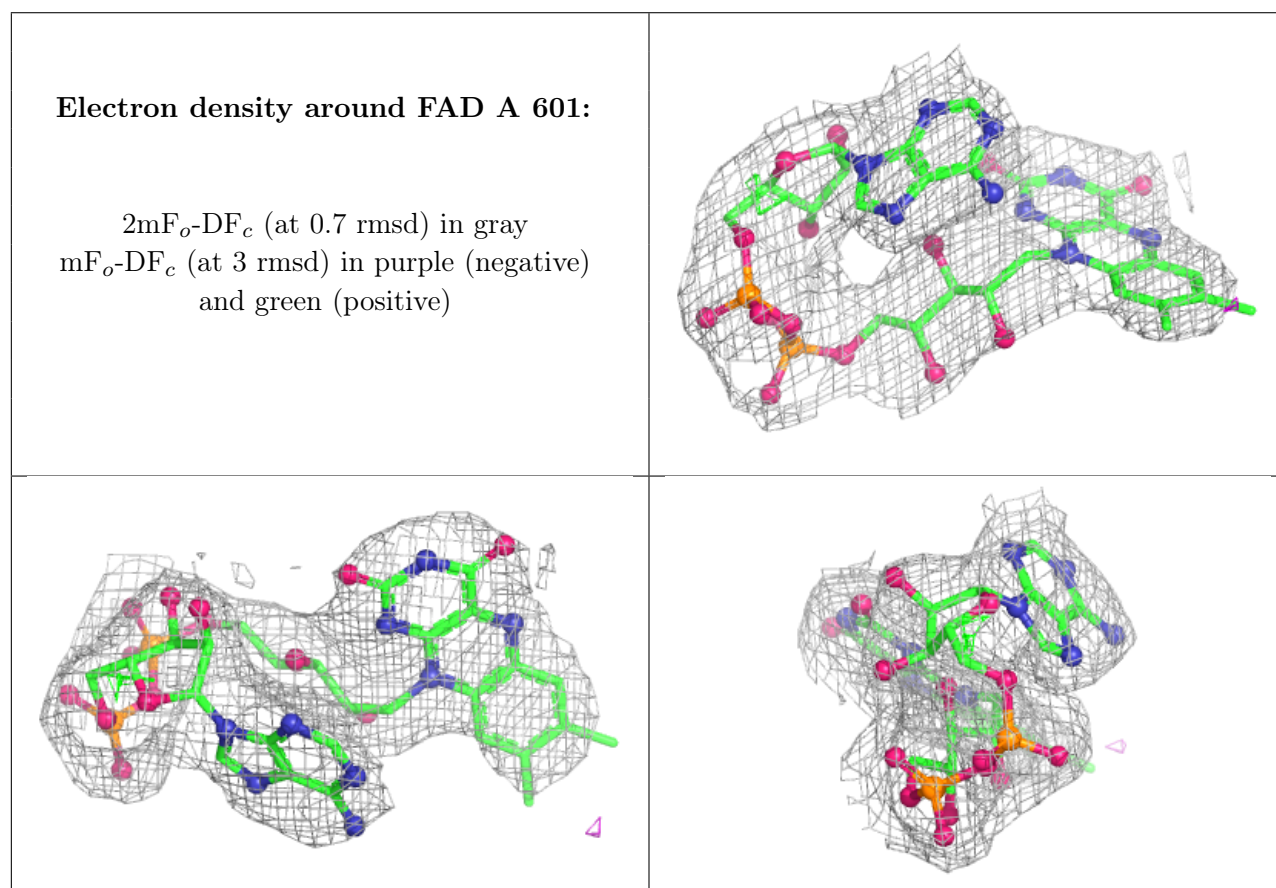
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	601	53/53	0.97	0.08	37,37,60,60	0

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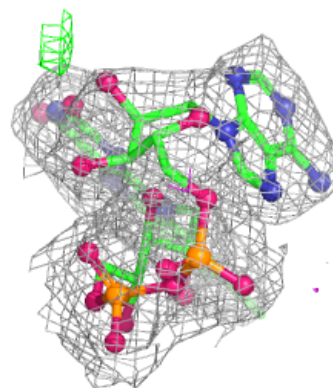
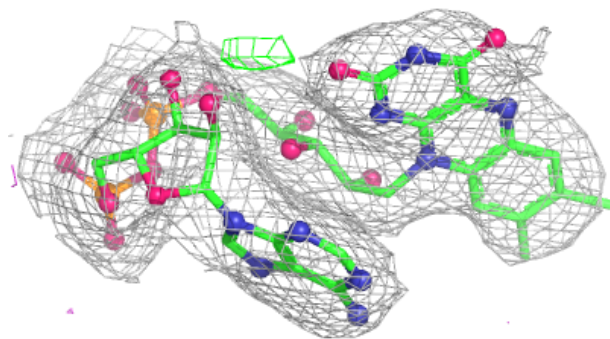
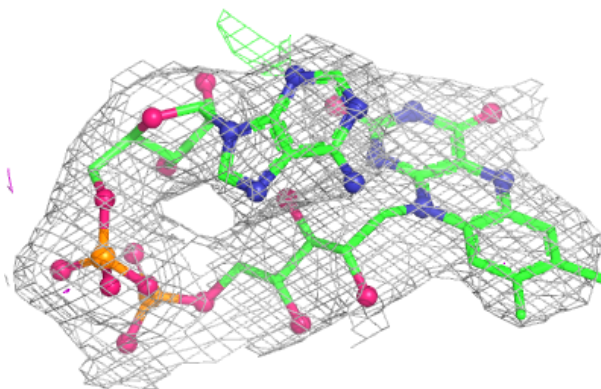
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	601	53/53	0.97	0.08	39,39,63,63	0

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 601:

$2mF_o-DF_c$ (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.