



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:56 PM GMT

PDB ID : 4K03  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

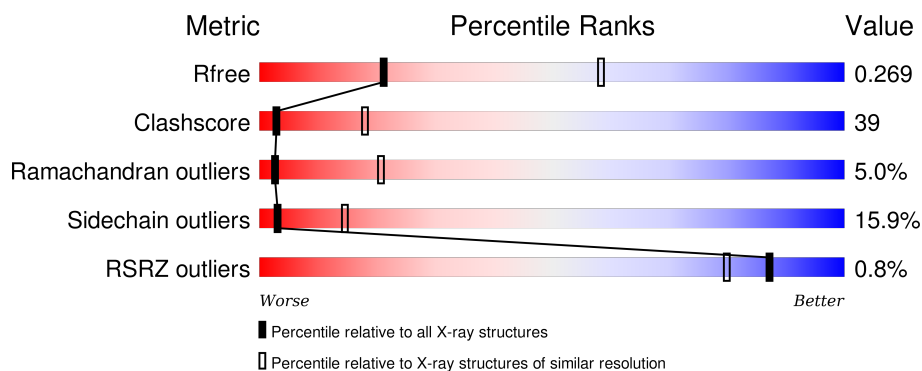
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	561	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 36%, yellow 46%, orange 12%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>36%</span> <span>46%</span> <span>12%</span> <span>• 6%</span> </div> </div>
1	B	561	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 37%, yellow 48%, orange 11%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>37%</span> <span>48%</span> <span>11%</span> <span>• •</span> </div> </div>

## 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:

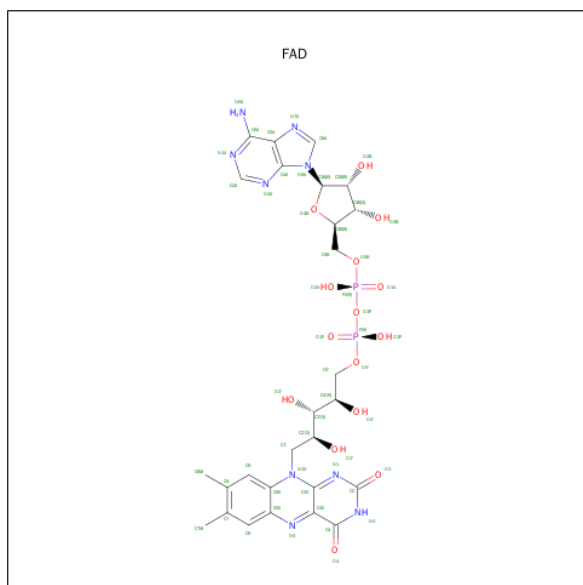
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	EXPRESSION TAG	UNP O77059
A	-17	ALA	-	EXPRESSION TAG	UNP O77059
A	-16	MET	-	EXPRESSION TAG	UNP O77059
A	-15	GLY	-	EXPRESSION TAG	UNP O77059
A	-14	SER	-	EXPRESSION TAG	UNP O77059
A	-13	GLY	-	EXPRESSION TAG	UNP O77059
A	-12	ILE	-	EXPRESSION TAG	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 (three-letter code: 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		

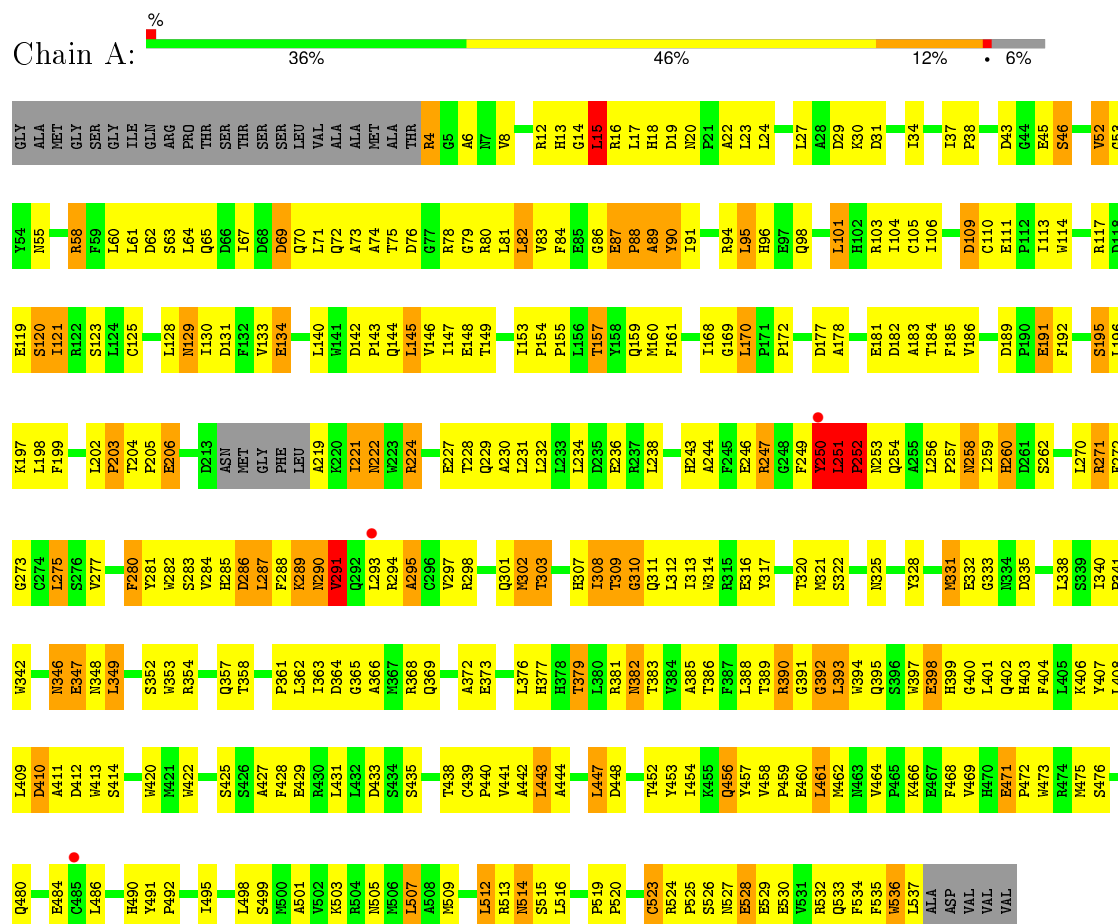
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	B	25	Total 25	O 25	0	0

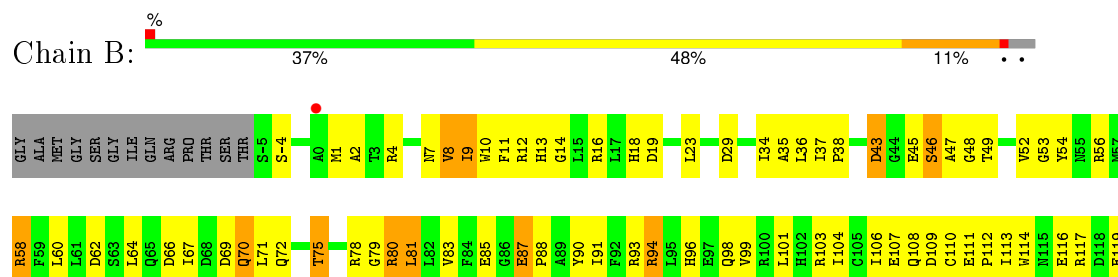
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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



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C485	C416	V415	L349	S276	P203	S120
L486	A417	C416	L350	V277	T204	I121
I487	G418	A417	Q351	R278	P205	R122
G488	G419	G418	S352	R279	E206	S123
V489	V420	V419	W353	F280	Y211	L124
H490	H421	H420	R354	V281	G212	C125
Y491	Y421	Y420	L355	V282	D213	R126
P492	A427	A427	G356	S283	Y212	E127
E493	F428	F428	Q357	D286	G216	L128
R494	E429	E429	T358	L287	F217	I130
I495	R430	R430	G359	L288	L218	E134
I496	L431	L431	F360	F288	A219	K135
D497	L432	L432	P361	K289	K220	V136
L498	D433	D433	L362	V290	I221	S137
S499	S434	S434	I363	V291	N222	H138
M500	S435	S435	L364	Q292	W223	
	L436	L436	G365	L293	R224	
K503	V437	V437	A366	C296	T228	T149
H504	T438	T438	M367	V297	T228	M150
M505	C439	C439	R368	R298	Q229	G151
M506	P440	P440	L371	G299	A230	G152
L507	V441	V441		V300	L231	I153
A508	A442	A442	L376	Q301	L232	P154
	L443	L443	R377	K302	L233	P155
	A444	A444	H378	T303	L234	L156
S511	R445	R445	T379	H307	D235	L157
L512	R446	R446	L380	I308	R237	Q159
M513	L447	L447		T309	L238	
M514	D448	D448	T383	G310	K239	L162
S515	P449	P449	A384	Q311	V240	H163
L516	D450	D450	A385	L312	E241	T164
T517	G451	G451	T386	I313	Q242	V165
T518	T452	T452	F387	F319	H243	Q166
P519	Y453	Y453	L388	T319	A244	
P620	P454	P454	I454	T320	F245	L170
P621	K455	K455	T389	K321	E246	P171
M622	Q456	Q456	R390	S322	R247	P172
C523	T457	T457	G391	V323	G248	
R524	V458	V458	L392	I324	F249	T175
P525	P459	P459	W393	N325	Y250	A176
S526	E460	E460	Q394	P326	L251	D177
M527	L461	L461	Q395	N327	P252	A178
M528			S396	V328	A179	
E529			W397	I328	L180	
E530	V464	V464	E398	K330	E181	
V531	P465	P465	L401	K331	N258	
M532	K466	K466	Q402	L334	I259	T184
G533	E467	E467		D335	H260	F185
F534	F468	F468	L405	I336	D261	V186
F535			K406	C337	P263	
M536	E471	E471	W407	L338	L270	F192
L537	P472	P472	L408		R271	L196
ALA	W473	W473	D410	K342	F272	
ASP	R474	R474	A411	A343	G273	F199
VAL	W475	W475	W412	P345	C274	
VAL	S476	S476	Q479		L275	
VAL	A477	A477				
VAL	E478	E478				
	Q479	Q479				
	Q480	Q480				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.12Å 121.81Å 79.72Å 90.00° 114.78° 90.00°	Depositor
Resolution (Å)	40.49 – 3.20 46.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.49-3.20) 99.7 (46.60-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.188 , 0.269 0.188 , 0.269	Depositor DCC
$R_{free}$ test set	1041 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 85.4	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 20371 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/4355	0.71	3/5929 (0.1%)
1	B	0.50	0/4469	0.72	1/6082 (0.0%)
All	All	0.51	0/8824	0.72	4/12011 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LEU	CA-CB-CG	8.68	135.26	115.30
1	A	393	LEU	N-CA-C	6.16	127.62	111.00
1	A	291	VAL	N-CA-C	-5.91	95.03	111.00
1	B	232	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	343	0
1	B	4350	0	4190	342	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
3	A	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	1	0
All	All	8746	0	8328	670	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 39.

All (670) 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:297:VAL:HG13	1:A:298:ARG:N	1.79	0.98
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: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:CG	1:B:58:ARG:HH11	1.87	0.85
1:A:461:LEU:HD22	1:A:469:VAL:HG23	1.59	0.84
1:A:58:ARG:NH1	1:A:58:ARG:HB3	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:HH11	1:A:247:ARG:HG2	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HH11	1:A:58:ARG:CG	1.96	0.77
1:A:13:HIS:NE2	1:A:271:ARG:NH1	2.32	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: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:HG3	1:B:58:ARG:HH11	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:427:ALA:O	1:A:513:ARG:NH1	2.20	0.75
1:A:394:TRP:CD1	1:A:394:TRP:O	2.39	0.74
1:B:229:GLN:OE1	1:B:229:GLN:HA	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:HH11	1:A:58:ARG:HB3	1.50	0.72
1:B:11:PHE:C	1:B:12:ARG:HG3	2.08	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:A:459:PRO:C	1:A:461:LEU:H	1.93	0.71
1:A:287:LEU:HD23	1:A:288:PHE:HE1	1.52	0.71
1:A:87:GLU:O	1:A:91:ILE:HG13	1.90	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:A:290:ASN:C	1:A:290:ASN:HD22	1.95	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:B:321:MET:HE3	1:B:523:CYS:HB2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:467:GLU:HG2	1:B:468:PHE:CD2	2.28	0.68
1:A:516:LEU:HD13	1:A:520:PRO:HD3	1.74	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:A:224:ARG:HG2	1:A:229:GLN:HB2	1.75	0.67
1:B:149:THR:C	1:B:151:GLY:H	1.98	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:248:GLY:O	1:B:250:TYR:CE2	2.49	0.66
1:B:159:GLN:HG2	1:B:526:SER:HB3	1.77	0.66
1:B:72:GLN:HG2	1:B:80:ARG:HD3	1.77	0.66
1:A:512:LEU:HG	1:A:513:ARG:N	2.10	0.65
1:A:238:LEU:HD11	1:A:283:SER:HB2	1.77	0.65
1:B:346:ASN:HB3	1:B:349:LEU:HD13	1.78	0.65
1:B:79:GLY:HA3	1:B:185:PHE:CE1	2.30	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:B:247:ARG:NH1	1:B:252:PRO:HD3	2.13	0.64
1:A:221:ILE:O	1:A:222:ASN:HB3	1.97	0.64
1:A:4:ARG:HA	1:A:4:ARG:NH1	2.11	0.64
1:B:321:MET:HE2	1:B:328:TYR:HE1	1.62	0.64
1:B:46:SER:OG	1:B:117:ARG:NH1	2.31	0.64
1:B:464:VAL:CG1	1:B:465:PRO:HD2	2.27	0.64
1:B:192:PHE:CE1	1:B:196:LEU:HD13	2.33	0.64
1:B:8:VAL:HG12	1:B:104:ILE:HA	1.78	0.63
1:B:162:LEU:HD12	1:B:162:LEU:H	1.62	0.63
1:A:104:ILE:HD12	1:A:125:CYS:SG	2.38	0.63
1:B:461:LEU:HD22	1:B:464:VAL:CG2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:LEU:O	1:B:489:VAL:O	2.17	0.63
1:B:260:HIS:CD2	1:B:260:HIS:H	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:A:290:ASN:C	1:A:290:ASN:ND2	2.53	0.62
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:B:301:GLN:HG3	1:B:303:THR:HG23	1.81	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:A:363:ILE:CD1	1:A:383:THR:HG22	2.28	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
1:A:429:GLU:HG3	1:A:525:PRO:HB2	1.81	0.61
1:A:250:TYR:HE1	1:B:532:ARG:NH1	1.98	0.61
1:B:321:MET:HE3	1:B:336:ILE:HD13	1.81	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:321:MET:O	1:B:321:MET:HG2	2.00	0.61
1:B:72:GLN:OE1	1:B:80:ARG:HD3	2.00	0.61
1:B:71:LEU:O	1:B:75:THR:HG23	2.01	0.61
1:B:137:SER:O	1:B:138:HIS:HB3	2.00	0.61
1:B:87:GLU:O	1:B:91:ILE:HG13	1.99	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: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:22:ALA:HB1	1:A:105:CYS:HB3	1.83	0.60
1:B:464:VAL:HG13	1:B:465:PRO:HD2	1.82	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:535:PHE:O	1:A:536:TRP:HB2	2.01	0.60
1:A:250:TYR:CD1	1:B:529:GLU:HB2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:O	1:A:495:ILE:HG23	2.01	0.60
1:B:351:GLN:O	1:B:355:LEU:HG	2.02	0.60
1:A:428:PHE:CE2	1:A:519:PRO:HB3	2.37	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:516:LEU:O	1:B:516:LEU:HD22	2.02	0.59
1:B:474:ARG:HH11	1:B:474:ARG:HG3	1.67	0.59
1:B:249:PHE:O	1:B:250:TYR:O	2.19	0.59
1:B:159:GLN:O	1:B:162:LEU:HD12	2.02	0.59
1:A:119:GLU:HA	1:A:119:GLU:OE1	2.02	0.59
1:A:472:PRO:HD2	1:A:473:TRP:CZ3	2.38	0.59
1:B:392:GLY:C	1:B:393:LEU:O	2.38	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
1:A:87:GLU:HG2	1:A:90:TYR:HB3	1.84	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:B:258:ASN:OD1	1:B:258:ASN:C	2.41	0.58
1:B:280:PHE:CE1	1:B:308:ILE:HD11	2.38	0.58
1:A:346:ASN:O	1:A:348:ASN:N	2.37	0.58
1:A:346:ASN:O	1:A:349:LEU:N	2.36	0.58
1:B:514:ASN:CG	1:B:515:SER:H	2.06	0.58
1:B:293:LEU:N	1:B:293:LEU:HD22	2.19	0.58
1:A:294:ARG:O	1:A:295:ALA:HB2	2.03	0.58
1:A:106:ILE:HD11	1:A:134:GLU:OE2	2.03	0.58
1:A:386:THR:O	1:A:391:GLY:HA3	2.03	0.58
1:B:321:MET:HE2	1:B:328:TYR:CE1	2.38	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:206:GLU:H	1:A:206:GLU:CD	2.07	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:90:TYR:CD2	1:A:90:TYR:C	2.77	0.57
1:A:252:PRO:HB3	1:A:253:ASN:CB	2.34	0.57
1:A:229:GLN:OE1	1:A:229:GLN:HA	2.03	0.57
1:A:75:THR:HB	1:A:78:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:HIS:O	1:B:380:LEU:HB2	2.05	0.57
1:A:27:LEU:O	1:A:30:LYS:HG3	2.05	0.57
1:B:237:ARG:HG3	1:B:238:LEU:N	2.20	0.57
1:A:486:LEU:HD13	1:A:490:HIS:HE1	1.69	0.57
1:B:127:GLU:HG2	1:B:128:LEU:HD23	1.87	0.57
1:B:37:ILE:HG12	1:B:186:VAL:HG11	1.85	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:87:GLU:CG	1:A:90:TYR:HB3	2.35	0.56
1:A:52:VAL:HG22	1:A:53:GLY:O	2.04	0.56
1:B:104:ILE:HD12	1:B:130:ILE:HG21	1.87	0.56
1:A:46:SER:OG	1:A:117:ARG:NH1	2.38	0.56
1:A:286:ASP:O	1:A:288:PHE:N	2.38	0.56
1:B:96:HIS:HD2	1:B:128:LEU:CD1	2.17	0.56
1:B:11:PHE:O	1:B:12:ARG:HG3	2.04	0.56
1:A:43:ASP:HA	1:A:86:GLY:O	2.05	0.56
1:A:259:ILE:HD11	1:A:448:ASP:HB2	1.87	0.56
1:B:343:ALA:N	1:B:394:TRP:HD1	2.01	0.56
1:A:516:LEU:CD1	1:A:520:PRO:HD3	2.35	0.56
1:A:472:PRO:HD2	1:A:473:TRP:CE3	2.40	0.56
1:A:111:GLU:OE2	1:A:413:TRP:HB3	2.05	0.56
1:A:250:TYR:HH	1:B:528:GLU:HB3	1.71	0.56
1:A:391:GLY:O	1:A:392:GLY:O	2.24	0.56
1:A:390:ARG:HH21	1:A:433:ASP:CG	2.09	0.55
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:B:329:ASP:OD2	1:B:413:TRP:HZ2	1.89	0.55
1:A:219:ALA:N	1:A:372:ALA:HB1	2.21	0.55
1:B:527:ASN:O	1:B:531:VAL:HG23	2.05	0.55
1:B:293:LEU:CD2	1:B:293:LEU:N	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:297:VAL:CG1	1:A:307:HIS:HB2	2.37	0.55
1:A:111:GLU:HB2	1:A:114:TRP:CD1	2.42	0.55
1:B:96:HIS:CD2	1:B:128:LEU:HD13	2.36	0.55
1:A:280:PHE:HE1	1:A:308:ILE:HD11	1.71	0.55
1:B:461:LEU:HD22	1:B:464:VAL:HG21	1.89	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:A:381:ARG:HD3	2:A:601:FAD:C9A	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:HG3	1:A:457:TYR:CE1	2.42	0.55
1:A:388:LEU:HG	1:A:388:LEU:O	2.07	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:95:LEU:HD12	1:A:192:PHE:HE2	1.71	0.55
1:B:58:ARG:CG	1:B:58:ARG:NH1	2.59	0.55
1:A:459:PRO:C	1:A:461:LEU:N	2.55	0.55
1:A:388:LEU:HD23	1:A:389:THR:HG23	1.88	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:A:498:LEU:O	1:A:499:SER:C	2.46	0.54
1:A:258:ASN:OD1	1:A:258:ASN:C	2.45	0.54
1:B:58:ARG:NH1	1:B:58:ARG:HG3	2.21	0.54
1:A:63:SER:O	1:A:67:ILE:HG13	2.07	0.54
1:A:196:LEU:O	1:A:197:LYS:HB2	2.07	0.54
1:A:20:ASN:O	1:A:24:LEU:HG	2.08	0.54
1:A:363:ILE:HD11	1:A:440:PRO:CG	2.37	0.54
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:247:ARG:HG3	1:A:247:ARG:O	2.06	0.54
1:A:168:ILE:HG22	1:A:169:GLY:N	2.23	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:509:MET:HA	1:A:512:LEU:HD23	1.90	0.54
1:A:8:VAL:CG1	1:A:104:ILE:HG23	2.38	0.54
1:A:476:SER:O	1:A:480:GLN:HG3	2.08	0.54
1:B:394:TRP:CZ3	1:B:505:ASN:HB3	2.43	0.53
1:B:52:VAL:HG22	1:B:53:GLY:N	2.23	0.53
1:B:324:ASN:O	1:B:326:PRO:HD3	2.08	0.53
1:B:345:PRO:HA	1:B:395:GLN:OE1	2.08	0.53
1:A:38:PRO:HB2	1:A:81:LEU:HA	1.90	0.53
1:B:7:ASN:ND2	1:B:34:ILE:HG21	2.24	0.53
1:A:441:VAL:C	1:A:443:LEU:H	2.10	0.53
1:A:72:GLN:HG3	1:A:80:ARG:HG2	1.89	0.53
1:B:288:PHE:O	1:B:289:LYS:C	2.46	0.53
1:A:503:LYS:O	1:A:507:LEU:HD22	2.08	0.53
1:A:410:ASP:O	1:A:411:ALA:C	2.46	0.53
1:B:361:PRO:O	1:B:364:ASP:N	2.41	0.53
1:B:248:GLY:O	1:B:250:TYR:CD2	2.62	0.53
1:A:109:ASP:OD2	1:A:117:ARG:NH2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:159:GLN:HA	1:B:162:LEU:CD1	2.39	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: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:428:PHE:CZ	1:A:519:PRO:HB3	2.43	0.53
1:A:60:LEU:O	1:A:64:LEU:HG	2.09	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:A:363:ILE:HD11	1:A:440:PRO:CB	2.39	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:340:ILE:CD1	1:A:425:SER:HA	2.39	0.53
1:B:149:THR:O	1:B:151:GLY:N	2.41	0.52
1:B:489:VAL:O	1:B:490:HIS:HB2	2.07	0.52
1:A:62:ASP:O	1:A:65:GLN:HB3	2.10	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:A:535:PHE:O	1:A:536:TRP:CB	2.56	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: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: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:B:58:ARG:HG2	1:B:58:ARG:HH11	1.69	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:A:250:TYR:CE1	1:B:532:ARG:NH1	2.76	0.51
1:A:96:HIS:HD2	1:A:128:LEU:CD1	2.20	0.51
1:B:358:THR:HG22	1:B:495:ILE:HD11	1.92	0.51
1:A:331:MET:HE1	1:A:342:TRP:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ASN:C	1:A:516:LEU:N	2.64	0.51
1:B:418:GLY:HA2	1:B:421:MET:HE2	1.91	0.51
1:A:250:TYR:HE1	1:B:532:ARG:CZ	2.23	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:516:LEU:HD12	1:A:516:LEU:O	2.11	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:B:52:VAL:CG2	1:B:53:GLY:N	2.73	0.51
1:B:36:LEU:HD23	1:B:38:PRO:HD3	1.92	0.51
1:A:260:HIS:N	1:A:260:HIS:ND1	2.47	0.51
1:B:12:ARG:HH22	1:B:106:ILE:HD12	1.76	0.51
1:B:149:THR:C	1:B:151:GLY:N	2.64	0.51
1:A:14:GLY:O	1:A:16:ARG:N	2.44	0.50
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:CD2	1:B:535:PHE:N	2.79	0.50
1:A:247:ARG:HH11	1:A:247:ARG:CG	2.14	0.50
1:A:94:ARG:O	1:A:98:GLN:HG2	2.11	0.50
1:B:111:GLU:HB2	1:B:114:TRP:CD1	2.47	0.50
1:B:71:LEU:HD23	1:B:180:LEU:HD13	1.92	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:392:GLY:O	1:B:393:LEU:HB2	2.10	0.50
1:B:79:GLY:O	1:B:80:ARG:HG2	2.10	0.50
1:A:346:ASN:OD1	1:A:349:LEU:HD22	2.11	0.50
1:A:325:ASN:O	1:A:328:TYR:HB2	2.11	0.50
1:B:301:GLN:O	1:B:307:HIS:HB3	2.11	0.50
1:B:46:SER:N	1:B:114:TRP:HZ3	2.09	0.50
1:A:524:ARG:HG2	1:A:525:PRO:HD2	1.93	0.50
1:B:386:THR:O	1:B:391:GLY:HA3	2.12	0.50
1:B:508:ALA:HA	1:B:511:SER:HB2	1.94	0.49
1:B:516:LEU:O	1:B:517:ILE:C	2.50	0.49
1:B:19:ASP:OD1	1:B:175:THR:HG23	2.11	0.49
1:B:136:VAL:O	1:B:136:VAL:HG12	2.10	0.49
1:A:431:LEU:HB2	1:A:528:GLU:OE2	2.12	0.49
1:A:86:GLY:HA3	1:A:91:ILE:HD11	1.93	0.49
1:B:244:ALA:CA	1:B:247:ARG:NH1	2.73	0.49
1:B:13:HIS:CD2	1:B:271:ARG:NH1	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ASN:O	1:A:516:LEU:N	2.45	0.49
1:A:101:LEU:HB3	1:A:130:ILE:HD13	1.95	0.49
1:B:486:LEU:O	1:B:487:ILE:C	2.51	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: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:441:VAL:O	1:A:443:LEU:N	2.46	0.49
1:A:182:ASP:O	1:A:182:ASP:CG	2.51	0.49
1:A:394:TRP:CG	1:A:394:TRP:O	2.66	0.49
1:B:282:TRP:O	1:B:286:ASP:HB2	2.13	0.49
1:B:113:ILE:HD11	1:B:413:TRP:CG	2.48	0.49
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:A:106:ILE:HD11	1:A:134:GLU:HB2	1.94	0.49
1:B:293:LEU:HD21	1:B:303:THR:HA	1.94	0.49
1:A:145:LEU:O	1:A:149:THR:N	2.40	0.49
1:A:536:TRP:O	1:A:537:LEU:HD23	2.12	0.49
1:B:247:ARG:O	1:B:248:GLY:C	2.51	0.49
1:A:78:ARG:NH2	1:A:183:ALA:O	2.46	0.49
1:B:364:ASP:O	1:B:368:ARG:HG3	2.13	0.49
1:B:458:VAL:O	1:B:458:VAL:HG12	2.11	0.49
1:B:401:LEU:HG	1:B:405:LEU:HD11	1.93	0.49
1:A:79:GLY:HA3	1:A:185:PHE:CG	2.48	0.49
1:B:238:LEU:HD11	1:B:283:SER:HB2	1.94	0.48
1:A:90:TYR:HD2	1:A:90:TYR:C	2.17	0.48
1:B:511:SER:O	1:B:514:ASN:OD1	2.31	0.48
1:A:260:HIS:HD2	1:A:452:THR:HG22	1.77	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:B:90:TYR:CD2	1:B:90:TYR:C	2.86	0.48
1:A:55:ASN:HB3	1:A:409:LEU:HD21	1.95	0.48
1:A:15:LEU:HB2	1:A:272:PHE:O	2.14	0.48
1:B:376:LEU:HD22	1:B:380:LEU:HD12	1.94	0.48
1:A:159:GLN:HG2	1:A:526:SER:HB3	1.95	0.48
1:A:69:ASP:O	1:A:70:GLN:C	2.51	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:293:LEU:H	1:A:303:THR:HB	1.78	0.48
1:B:229:GLN:CA	1:B:229:GLN:OE1	2.61	0.48
1:B:346:ASN:CB	1:B:349:LEU:HD22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:HG23	1:A:313:ILE:HD11	1.95	0.48
1:A:282:TRP:HZ3	1:A:285:HIS:CE1	2.32	0.48
1:A:468:PHE:CD2	1:A:475:MET:HG2	2.49	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:379:THR:HG23	1:B:536:TRP:CD1	2.49	0.48
1:B:279:ARG:O	1:B:283:SER:OG	2.27	0.48
1:B:271:ARG:CG	1:B:412:ASP:OD2	2.62	0.48
1:B:321:MET:CE	1:B:336:ILE:HD13	2.44	0.48
1:B:459:PRO:C	1:B:461:LEU:H	2.17	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
1:B:234:LEU:O	1:B:238:LEU:HB2	2.14	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:428:PHE:CE1	1:A:519:PRO:HD3	2.49	0.47
1:A:448:ASP:CG	1:A:448:ASP:O	2.52	0.47
1:A:310:GLY:HA2	1:A:313:ILE:HG12	1.95	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:256:LEU:HB2	1:A:257:PRO:HD2	1.96	0.47
1:A:244:ALA:HA	1:A:247:ARG:NH1	2.30	0.47
1:A:529:GLU:HB2	1:B:250:TYR:CD2	2.49	0.47
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.76	0.47
1:B:309:THR:O	1:B:313:ILE:HG12	2.14	0.47
1:B:93:ARG:HH12	1:B:128:LEU:HD21	1.80	0.47
1:A:471:GLU:HA	1:A:473:TRP:CZ3	2.49	0.47
1:A:37:ILE:HG23	1:A:186:VAL:HG21	1.96	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:159:GLN:HG2	1:A:526:SER:CB	2.45	0.47
1:B:172:PRO:O	1:B:278:ARG:HG2	2.15	0.47
1:A:484:GLU:HG3	1:A:484:GLU:O	2.15	0.47
1:A:144:GLN:O	1:A:148:GLU:HB2	2.15	0.47
1:A:297:VAL:HG12	1:A:307:HIS:HB2	1.96	0.47
1:A:288:PHE:O	1:A:289:LYS:C	2.53	0.47
1:B:69:ASP:O	1:B:71:LEU:N	2.48	0.47
1:B:443:LEU:HD13	1:B:446:ARG:NH2	2.30	0.47
1:A:250:TYR:CE1	1:B:529:GLU:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:O	1:A:252:PRO:C	2.54	0.46
1:B:280:PHE:CG	1:B:312:LEU:HD11	2.50	0.46
1:B:514:ASN:CG	1:B:515:SER:N	2.67	0.46
1:A:459:PRO:O	1:A:462:MET:HG3	2.15	0.46
1:A:43:ASP:OD1	1:A:46:SER:HB2	2.16	0.46
1:A:14:GLY:O	1:A:16:ARG:HG2	2.16	0.46
1:A:8:VAL:CG1	1:A:104:ILE:HA	2.43	0.46
1:B:262:SER:HB3	1:B:263:PRO:CD	2.46	0.46
1:B:224:ARG:CG	1:B:229:GLN:HE21	2.29	0.46
1:A:8:VAL:O	1:A:8:VAL:HG13	2.16	0.46
1:A:397:TRP:C	1:A:399:HIS:H	2.19	0.46
1:B:23:LEU:HD12	1:B:23:LEU:O	2.15	0.46
1:B:474:ARG:NH1	1:B:474:ARG:HG3	2.30	0.46
1:B:52:VAL:HG22	1:B:53:GLY:O	2.15	0.46
1:A:79:GLY:HA3	1:A:185:PHE:CD2	2.51	0.46
1:A:461:LEU:HD23	1:A:464:VAL:HG21	1.98	0.46
1:B:158:TYR:HE2	1:B:162:LEU:HD21	1.81	0.46
1:A:110:CYS:O	1:A:111:GLU:C	2.53	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:B:388:LEU:HG	1:B:389:THR:HG23	1.98	0.46
1:A:340:ILE:HA	1:A:341:PRO:HD3	1.83	0.46
1:B:346:ASN:HB3	1:B:349:LEU:HD22	1.97	0.45
1:B:72:GLN:CD	1:B:80:ARG:HD3	2.35	0.45
1:B:18:HIS:O	1:B:19:ASP:C	2.54	0.45
1:A:358:THR:HA	1:A:495:ILE:HG23	1.97	0.45
1:B:239:LYS:O	1:B:240:VAL:C	2.53	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: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:309:THR:HG22	1:A:310:GLY:N	2.30	0.45
1:B:10:TRP:CZ3	1:B:121:ILE:HD12	2.51	0.45
1:B:519:PRO:HA	1:B:520:PRO:HD3	1.83	0.45
1:B:211:TYR:O	1:B:213:ASP:N	2.49	0.45
1:A:311:GLN:HB3	2:A:601:FAD:O4B	2.16	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:HD23	1:B:409:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASN:HB2	1:B:250:TYR:OH	2.17	0.45
1:B:488:GLY:O	1:B:489:VAL:C	2.55	0.45
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: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:A:83:VAL:O	1:A:199:PHE:HD2	2.00	0.45
1:B:431:LEU:HD12	1:B:431:LEU:O	2.15	0.45
1:B:93:ARG:HH22	1:B:127:GLU:CD	2.20	0.45
1:B:202:LEU:HD12	1:B:203:PRO:HD2	1.98	0.45
1:B:377:HIS:ND1	1:B:379:THR:OG1	2.50	0.45
1:A:106:ILE:HG13	1:A:106:ILE:O	2.17	0.45
1:A:247:ARG:CG	1:A:247:ARG:O	2.62	0.44
1:B:38:PRO:HG2	1:B:81:LEU:HA	1.99	0.44
1:B:290:ASN:O	1:B:291:VAL:CG2	2.60	0.44
1:B:7:ASN:OD1	1:B:103:ARG:HB2	2.17	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:B:238:LEU:HD23	1:B:238:LEU:HA	1.47	0.44
1:A:353:TRP:CH2	1:A:400:GLY:HA2	2.53	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:A:192:PHE:CE1	1:A:196:LEU:HD22	2.49	0.44
1:A:69:ASP:O	1:A:72:GLN:N	2.49	0.44
1:B:297:VAL:HG21	1:B:307:HIS:CD2	2.52	0.44
1:A:270:LEU:CD2	1:A:275:LEU:HD23	2.47	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: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:A:142:ASP:O	1:A:144:GLN:N	2.50	0.44
1:A:202:LEU:HG	1:A:203:PRO:HD2	1.99	0.44
1:A:466:LYS:HG2	1:A:466:LYS:O	2.18	0.43
1:B:248:GLY:O	1:B:249:PHE:C	2.56	0.43
1:B:154:PRO:O	1:B:156:LEU:HD23	2.18	0.43
1:A:534:PHE:CG	1:A:534:PHE:O	2.71	0.43
1:A:38:PRO:HG2	1:A:71:LEU:HD13	1.99	0.43
1:B:35:ALA:HB2	1:B:184:THR:HB	2.00	0.43
1:B:385:ALA:HB1	1:B:420:TRP:CZ3	2.53	0.43
1:A:88:PRO:C	1:A:90:TYR:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:O	1:B:70:GLN:C	2.56	0.43
1:B:54:TYR:CG	1:B:212:GLY:HA2	2.53	0.43
1:B:270:LEU:HD21	1:B:280:PHE:HD2	1.83	0.43
1:A:154:PRO:HB2	1:A:321:MET:HA	1.99	0.43
1:A:29:ASP:OD2	1:A:103:ARG:NH1	2.52	0.43
1:A:192:PHE:O	1:A:196:LEU:HB2	2.18	0.43
1:A:17:LEU:HD23	1:A:23:LEU:CD2	2.49	0.43
1:A:280:PHE:CG	1:A:312:LEU:HD11	2.54	0.43
1:B:528:GLU:O	1:B:532:ARG:HG3	2.19	0.43
1:B:242:GLN:HB2	1:B:287:LEU:HD11	2.00	0.43
1:A:281:TYR:C	1:A:281:TYR:CD2	2.91	0.43
1:A:354:ARG:HB3	1:A:403:HIS:CE1	2.54	0.43
1:A:381:ARG:HB3	2:A:601:FAD:C8	2.49	0.43
1:B:29:ASP:HB3	1:B:34:ILE:HG12	1.99	0.43
1:A:441:VAL:C	1:A:443:LEU:N	2.72	0.43
1:A:401:LEU:HD13	1:A:420:TRP:CD1	2.53	0.43
1:A:453:TYR:O	1:A:454:ILE:C	2.57	0.43
1:B:478:GLU:HG2	1:B:478:GLU:H	1.50	0.43
1:A:221:ILE:CB	1:A:373:GLU:OE2	2.66	0.43
1:A:74:ALA:O	1:A:181:GLU:HA	2.19	0.43
1:B:242:GLN:O	1:B:245:PHE:HB3	2.19	0.43
1:A:353:TRP:CZ3	1:A:400:GLY:HA2	2.54	0.43
1:B:293:LEU:HD23	1:B:303:THR:HB	2.00	0.42
1:B:46:SER:H	1:B:114:TRP:HZ3	1.66	0.42
1:A:104:ILE:HG13	1:A:130:ILE:HG21	2.01	0.42
1:A:486:LEU:HD13	1:A:490:HIS:CE1	2.52	0.42
1:A:361:PRO:HB2	1:A:454:ILE:HD13	2.01	0.42
1:A:297:VAL:CG1	1:A:298:ARG:N	2.52	0.42
1:B:452:THR:HG22	1:B:453:TYR:N	2.33	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:471:GLU:CB	1:B:473:TRP:CZ2	3.02	0.42
1:B:410:ASP:OD1	1:B:411:ALA:N	2.47	0.42
1:B:514:ASN:O	1:B:515:SER:C	2.57	0.42
1:B:361:PRO:O	1:B:364:ASP:HB2	2.19	0.42
1:A:438:THR:HG22	1:A:439:CYS:N	2.34	0.42
1:A:38:PRO:O	1:A:82:LEU:HG	2.20	0.42
1:B:60:LEU:O	1:B:64:LEU:HG	2.20	0.42
1:A:140:LEU:H	1:A:316:GLU:CD	2.23	0.42
1:B:85:GLU:HB2	1:B:199:PHE:CE2	2.55	0.42
1:B:219:ALA:O	1:B:220:LYS:CB	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:ARG:HD3	1:B:408:LEU:O	2.19	0.42
1:B:443:LEU:CD1	1:B:446:ARG:NH2	2.83	0.42
1:B:309:THR:HG22	1:B:310:GLY:N	2.34	0.42
1:A:286:ASP:O	1:A:289:LYS:N	2.52	0.42
1:B:8:VAL:CG1	1:B:104:ILE:HG23	2.49	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:A:309:THR:O	1:A:311:GLN:N	2.53	0.42
1:A:282:TRP:CZ3	1:A:285:HIS:ND1	2.88	0.42
1:B:9:ILE:CG1	1:B:23:LEU:HA	2.49	0.42
1:A:160:MET:O	1:A:161:PHE:C	2.58	0.42
1:A:244:ALA:HA	1:A:247:ARG:HG2	2.02	0.42
1:A:286:ASP:O	1:A:287:LEU:C	2.57	0.42
1:A:439:CYS:HA	1:A:440:PRO:HD3	1.66	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD12	1.70	0.42
1:B:497:ASP:OD1	1:B:500:MET:CG	2.61	0.42
1:A:88:PRO:C	1:A:90:TYR:H	2.23	0.42
1:B:331:MET:HE1	1:B:342:TRP:HD1	1.84	0.42
1:B:16:ARG:NH2	1:B:137:SER:OG	2.53	0.42
1:B:356:GLY:C	1:B:364:ASP:OD1	2.58	0.42
1:B:368:ARG:HH22	1:B:460:GLU:CD	2.23	0.42
1:A:206:GLU:CD	1:A:206:GLU:N	2.73	0.42
1:B:9:ILE:HD13	1:B:9:ILE:C	2.39	0.42
1:B:244:ALA:HB1	1:B:251:LEU:HD12	2.02	0.41
1:A:383:THR:HG23	1:A:440:PRO:HG3	2.01	0.41
1:A:18:HIS:O	1:A:19:ASP:C	2.58	0.41
1:B:101:LEU:HB2	1:B:130:ILE:CD1	2.51	0.41
1:A:357:GLN:HB3	1:A:492:PRO:HG3	2.01	0.41
1:A:105:CYS:HA	1:A:133:VAL:HB	2.01	0.41
1:B:498:LEU:O	1:B:499:SER:C	2.58	0.41
1:A:228:THR:C	1:A:230:ALA:N	2.73	0.41
1:B:93:ARG:NH1	1:B:128:LEU:HD21	2.35	0.41
1:A:88:PRO:O	1:A:90:TYR:N	2.52	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: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:410:ASP:O	1:B:411:ALA:C	2.57	0.41
1:A:363:ILE:CD1	1:A:383:THR:CG2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:MET:SD	1:A:523:CYS:HB2	2.60	0.41
1:B:9:ILE:CD1	1:B:9:ILE:C	2.89	0.41
1:B:108:GLN:HG3	1:B:109:ASP:H	1.85	0.41
1:B:94:ARG:HD3	1:B:94:ARG:HA	1.76	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:288:PHE:O	1:A:290:ASN:N	2.54	0.41
1:B:162:LEU:O	1:B:163:HIS:C	2.56	0.41
1:B:121:ILE:O	1:B:122:ARG:C	2.59	0.41
1:B:363:ILE:CD1	1:B:440:PRO:HB3	2.51	0.41
1:B:43:ASP:HB2	1:B:45:GLU:O	2.21	0.41
1:A:13:HIS:O	1:A:272:PHE:O	2.38	0.41
1:A:303:THR:CG2	1:B:301:GLN:NE2	2.78	0.41
1:B:389:THR:O	1:B:390:ARG:HG2	2.20	0.41
1:B:156:LEU:HD11	1:B:336:ILE:CG2	2.49	0.41
1:B:72:GLN:OE1	1:B:80:ARG:CD	2.69	0.41
1:B:192:PHE:CZ	1:B:196:LEU:HD13	2.55	0.41
1:B:37:ILE:CG1	1:B:186:VAL:HG11	2.51	0.41
1:B:85:GLU:HB2	1:B:199:PHE:CZ	2.55	0.41
1:A:18:HIS:CE1	1:A:231:LEU:HD21	2.55	0.41
1:A:332:GLU:HG2	1:A:333:GLY:H	1.86	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:461:LEU:HA	1:B:461:LEU:HD23	1.86	0.41
1:B:491:TYR:HA	1:B:492:PRO:HD3	1.92	0.41
1:B:439:CYS:HA	1:B:440:PRO:HD3	1.54	0.41
1:B:337:CYS:O	1:B:338:LEU:C	2.58	0.41
1:B:376:LEU:HA	1:B:376:LEU:HD23	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:A:20:ASN:O	1:A:23:LEU:HB3	2.21	0.40
1:B:12:ARG:NH2	1:B:106:ILE:HD12	2.36	0.40
1:B:349:LEU:HD23	1:B:393:LEU:HD22	2.03	0.40
1:A:311:GLN:O	1:A:314:TRP:HB2	2.21	0.40
1:A:202:LEU:HA	1:A:203:PRO:HD2	1.91	0.40
1:A:121:ILE:HG12	1:A:121:ILE:H	1.36	0.40
1:B:429:GLU:HB3	1:B:432:LEU:HD12	2.03	0.40
1:A:377:HIS:HE1	1:A:536:TRP:CZ3	2.39	0.40
1:A:17:LEU:CD1	1:A:70:GLN:OE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:O	1:B:393:LEU:HB2	2.21	0.40
1:A:310:GLY:CA	1:A:313:ILE:HG12	2.51	0.40
1:A:168:ILE:CG2	1:A:169:GLY:N	2.83	0.40
1:A:453:TYR:O	1:A:456:GLN:N	2.54	0.40
1:A:243:HIS:O	1:A:247:ARG:HG2	2.21	0.40
1:B:179:ARG:NH1	1:B:181:GLU:CG	2.81	0.40
1:B:181:GLU:HG2	1:B:181:GLU:H	1.67	0.40
1:A:147:ILE:HG23	1:A:153:ILE:C	2.42	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:61:LEU:HB3	1:A:202:LEU:HD21	2.04	0.40
1:A:12:ARG:N	1:A:12:ARG:HD3	2.36	0.40
1:A:189:ASP:O	1:A:192:PHE:N	2.49	0.40
1:A:15:LEU:HD23	1:A:15:LEU:N	2.37	0.40
1:B:158:TYR:O	1:B:162:LEU:HD12	2.20	0.40
1:A:427:ALA:CB	1:A:512:LEU:HD21	2.51	0.40
1:B:461:LEU:HD22	1:B:464:VAL:HG23	2.01	0.40
1:B:273:GLY:C	1:B:275:LEU:N	2.75	0.40
1:B:235:ASP:HA	1:B:238:LEU:HB2	2.03	0.40
1:A:79:GLY:HA3	1:A:185:PHE:CD1	2.56	0.40
1:A:232:LEU:HD23	1:A:232:LEU:C	2.42	0.40
1:B:223:TRP:CD1	1:B:223:TRP:N	2.90	0.40
1:B:406:LYS:HB3	1:B:407:TYR:CD2	2.57	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%)	3	21
1	B	541/561 (96%)	444 (82%)	70 (13%)	27 (5%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1066/1122 (95%)	853 (80%)	160 (15%)	53 (5%)	<b>3</b> <b>21</b>

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
1	B	393	LEU
1	A	69	ASP

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Mol	Chain	Res	Type
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%)	377 (84%)	70 (16%)	3	15
1	B	458/488 (94%)	384 (84%)	74 (16%)	3	14
All	All	905/976 (93%)	761 (84%)	144 (16%)	3	14

All (144) 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
1	A	52	VAL
1	A	58	ARG

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	87	GLU
1	A	90	TYR
1	A	95	LEU
1	A	101	LEU
1	A	109	ASP
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	157	THR
1	A	170	LEU
1	A	177	ASP
1	A	184	THR
1	A	191	GLU
1	A	195	SER
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	250	TYR
1	A	251	LEU
1	A	252	PRO
1	A	258	ASN
1	A	260	HIS
1	A	262	SER
1	A	271	ARG
1	A	275	LEU
1	A	280	PHE
1	A	290	ASN
1	A	302	MET
1	A	303	THR
1	A	308	ILE
1	A	309	THR
1	A	322	SER
1	A	331	MET

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Mol	Chain	Res	Type
1	A	335	ASP
1	A	346	ASN
1	A	347	GLU
1	A	349	LEU
1	A	379	THR
1	A	390	ARG
1	A	398	GLU
1	A	410	ASP
1	A	412	ASP
1	A	414	SER
1	A	443	LEU
1	A	447	LEU
1	A	456	GLN
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	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	116	GLU
1	B	120	SER
1	B	121	ILE
1	B	123	SER
1	B	134	GLU
1	B	153	ILE
1	B	162	LEU
1	B	164	THR

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Mol	Chain	Res	Type
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	228	THR
1	B	237	ARG
1	B	242	GLN
1	B	258	ASN
1	B	260	HIS
1	B	261	ASP
1	B	271	ARG
1	B	274	CYS
1	B	276	SER
1	B	280	PHE
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	379	THR
1	B	383	THR
1	B	386	THR
1	B	390	ARG
1	B	412	ASP
1	B	414	SER
1	B	437	VAL
1	B	438	THR
1	B	447	LEU
1	B	456	GLN

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Mol	Chain	Res	Type
1	B	460	GLU
1	B	467	GLU
1	B	478	GLU
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	524	ARG
1	B	535	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	222	ASN
1	A	290	ASN
1	A	402	GLN
1	A	403	HIS
1	A	505	ASN
1	A	533	GLN
1	B	55	ASN
1	B	96	HIS
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 carbohydrates 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	-	48,58,58	1.08	5 (10%)	54,89,89	2.63	10 (18%)
2	FAD	B	601	-	48,58,58	1.06	5 (10%)	54,89,89	2.62	7 (12%)

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	-	-	0/30/50/50	0/6/6/6
2	FAD	B	601	-	-	0/30/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-N5	-2.42	1.29	1.33
2	A	601	FAD	C10-N10	-2.24	1.36	1.39
2	A	601	FAD	C10-N1	-2.17	1.32	1.35
2	B	601	FAD	C10-N10	-2.11	1.36	1.39
2	B	601	FAD	C10-N1	-2.02	1.32	1.35
2	B	601	FAD	C9A-N10	2.01	1.41	1.38
2	B	601	FAD	C4X-C10	2.55	1.45	1.41
2	A	601	FAD	C4X-C10	2.63	1.45	1.41
2	A	601	FAD	C4-N3	2.87	1.38	1.33
2	B	601	FAD	C4-N3	3.12	1.38	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4X-C4-N3	-6.85	114.22	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4X-C4-N3	-6.57	114.60	123.59
2	B	601	FAD	C4X-C10-N10	-6.36	116.77	120.52
2	A	601	FAD	C4X-C10-N10	-6.25	116.84	120.52
2	B	601	FAD	C4-C4X-C10	-3.88	117.46	119.94
2	A	601	FAD	C4-C4X-C10	-3.82	117.50	119.94
2	B	601	FAD	P-O3P-PA	-3.41	123.16	132.73
2	A	601	FAD	C2B-C1B-N9A	-2.62	110.28	114.29
2	A	601	FAD	P-O3P-PA	-2.60	125.44	132.73
2	A	601	FAD	O2P-P-O3P	2.29	115.46	105.09
2	A	601	FAD	C1'-C2'-C3'	2.65	117.39	109.82
2	A	601	FAD	O3P-P-O5'	4.34	114.44	102.94
2	B	601	FAD	O3P-P-O5'	5.10	116.46	102.94
2	B	601	FAD	O3P-PA-O5B	6.70	120.70	102.94
2	A	601	FAD	O3P-PA-O5B	7.48	122.79	102.94
2	A	601	FAD	C4-N3-C2	12.23	125.81	115.25
2	B	601	FAD	C4-N3-C2	12.32	125.90	115.25

There are no chirality outliers.

There are no torsion outliers.

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	529/561 (94%)	-0.29	3 (0%)	90 84	23, 52, 87, 135	0
1	B	543/561 (96%)	-0.19	6 (1%)	82 72	17, 54, 92, 161	0
All	All	1072/1122 (95%)	-0.24	9 (0%)	87 80	17, 54, 90, 161	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	CYS	3.0
1	B	0	ALA	2.9
1	B	490	HIS	2.7
1	B	461	LEU	2.7
1	B	473	TRP	2.3
1	A	293	LEU	2.2
1	A	485	CYS	2.2
1	B	472	PRO	2.1
1	A	250	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FAD	A	601	53/53	0.96	0.19	0.09	37,37,60,60	0
2	FAD	B	601	53/53	0.96	0.17	-0.28	39,39,63,63	0

## 6.5 Other polymers

There are no such residues in this entry.