



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:40 am GMT

PDB ID : 1BHY  
Title : LOW TEMPERATURE MIDDLE RESOLUTION STRUCTURE OF P64K  
FROM MASC DATA  
Authors : Ramin, M.; Shepard, W.; Fourme, R.; Kahn, R.  
Deposited on : 1998-06-10  
Resolution : 4.18 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

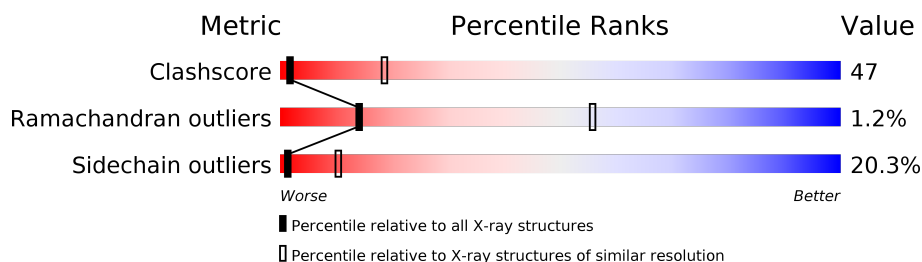
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.18 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))
Clashscore	112137	1024 (4.70-3.66)
Ramachandran outliers	110173	1022 (4.72-3.62)
Sidechain outliers	110143	1007 (4.72-3.62)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	482	

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

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

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3616 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 P64K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	3563	2249	616	679	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ALA	GLY	CONFLICT	UNP Q51225
A	553	TYR	CYS	CONFLICT	UNP Q51225

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



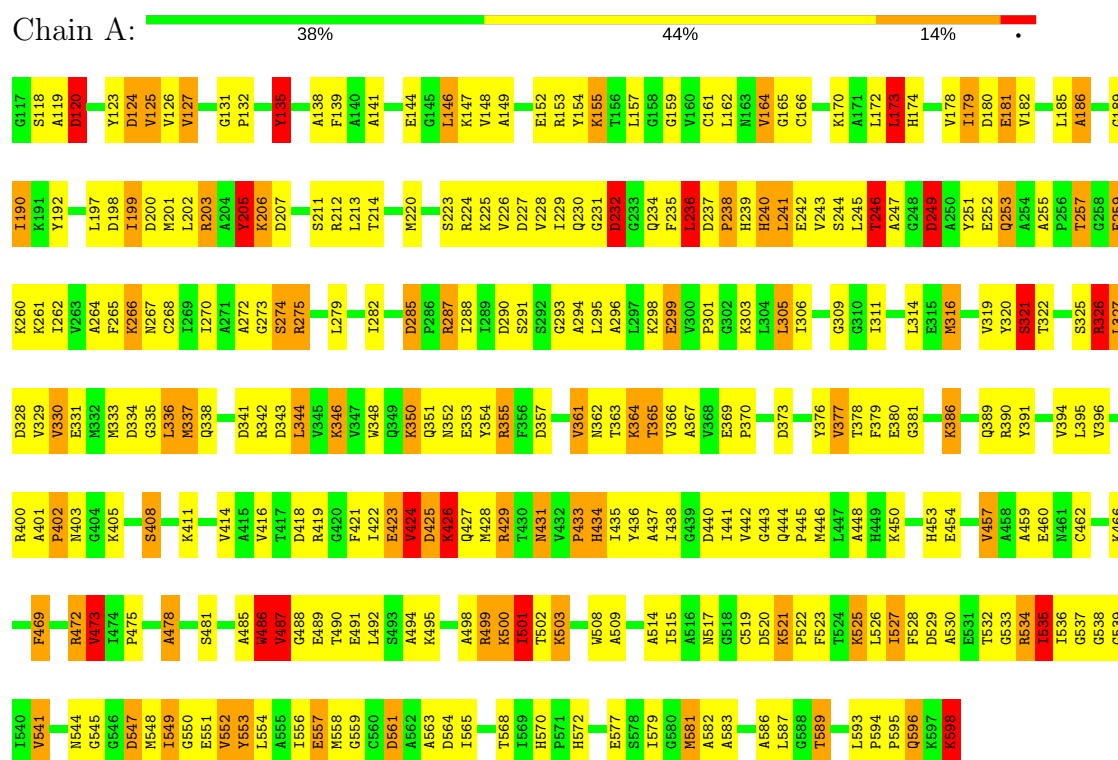
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

### 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 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.

Note EDS was not executed.

#### • Molecule 1: P64K



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.62Å 140.62Å 77.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.18	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-4.18)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.338 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 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	1.35	5/3629 (0.1%)	2.06	102/4917 (2.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	598	LYS	C-OXT	7.30	1.37	1.23
1	A	321	SER	CB-OG	6.91	1.51	1.42
1	A	274	SER	CB-OG	6.47	1.50	1.42
1	A	402	PRO	C-N	6.02	1.48	1.34
1	A	598	LYS	C-O	5.45	1.33	1.23

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	TYR	CB-CG-CD1	-19.69	109.19	121.00
1	A	355	ARG	NE-CZ-NH2	-19.16	110.72	120.30
1	A	275	ARG	NE-CZ-NH2	-15.56	112.52	120.30
1	A	534	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	A	553	TYR	CB-CG-CD2	13.92	129.35	121.00
1	A	287	ARG	NE-CZ-NH1	-13.55	113.52	120.30
1	A	425	ASP	CB-CG-OD2	-11.92	107.58	118.30
1	A	135	TYR	CB-CG-CD1	-11.78	113.93	121.00
1	A	198	ASP	CB-CG-OD1	11.26	128.43	118.30
1	A	287	ARG	CD-NE-CZ	-10.71	108.61	123.60
1	A	203	ARG	NE-CZ-NH1	-10.50	115.05	120.30
1	A	400	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	A	487	VAL	CB-CA-C	-9.62	93.12	111.40
1	A	203	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	A	253	GLN	N-CA-CB	9.20	127.15	110.60
1	A	541	VAL	CB-CA-C	-9.10	94.11	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	NH1-CZ-NH2	8.98	129.28	119.40
1	A	534	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	A	581	MET	CA-CB-CG	-8.42	98.99	113.30
1	A	290	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	124	ASP	CB-CG-OD2	8.02	125.52	118.30
1	A	423	GLU	OE1-CD-OE2	7.95	132.84	123.30
1	A	135	TYR	CB-CG-CD2	7.86	125.71	121.00
1	A	227	ASP	CB-CG-OD1	7.74	125.27	118.30
1	A	473	VAL	N-CA-CB	-7.55	94.88	111.50
1	A	400	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	A	232	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	A	249	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	365	THR	N-CA-CB	7.12	123.82	110.30
1	A	203	ARG	CG-CD-NE	7.11	126.73	111.80
1	A	553	TYR	CA-CB-CG	-7.04	100.02	113.40
1	A	355	ARG	NH1-CZ-NH2	7.03	127.13	119.40
1	A	205	TYR	CB-CG-CD1	7.03	125.22	121.00
1	A	192	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	A	501	ILE	N-CA-CB	-6.95	94.81	110.80
1	A	535	ILE	CB-CA-C	-6.94	97.72	111.60
1	A	205	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	A	424	VAL	N-CA-CB	-6.79	96.57	111.50
1	A	173	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	275	ARG	NH1-CZ-NH2	6.63	126.69	119.40
1	A	472	ARG	CD-NE-CZ	6.62	132.87	123.60
1	A	423	GLU	N-CA-CB	6.60	122.48	110.60
1	A	425	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	190	ILE	N-CA-CB	6.42	125.56	110.80
1	A	326	ARG	N-CA-C	-6.26	94.10	111.00
1	A	561	ASP	N-CA-CB	6.26	121.86	110.60
1	A	253	GLN	CB-CG-CD	6.25	127.84	111.60
1	A	535	ILE	N-CA-CB	6.11	124.86	110.80
1	A	487	VAL	N-CA-CB	6.11	124.93	111.50
1	A	490	THR	N-CA-CB	6.09	121.88	110.30
1	A	469	PHE	N-CA-C	-6.05	94.66	111.00
1	A	460	GLU	OE1-CD-OE2	6.03	130.53	123.30
1	A	240	HIS	CA-CB-CG	-6.01	103.39	113.60
1	A	253	GLN	O-C-N	6.00	132.29	122.70
1	A	181	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	A	173	LEU	CB-CG-CD1	5.98	121.16	111.00
1	A	598	LYS	CA-C-O	-5.94	107.62	120.10
1	A	541	VAL	CA-CB-CG1	-5.90	102.05	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	N-CA-CB	5.86	121.15	110.60
1	A	326	ARG	N-CA-CB	5.84	121.12	110.60
1	A	589	THR	N-CA-CB	-5.78	99.32	110.30
1	A	548	MET	CA-C-O	-5.74	108.05	120.10
1	A	246	THR	N-CA-CB	-5.69	99.49	110.30
1	A	547	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	A	236	LEU	CA-C-O	5.62	131.89	120.10
1	A	135	TYR	CB-CA-C	5.61	121.62	110.40
1	A	499	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	473	VAL	CB-CA-C	5.59	122.01	111.40
1	A	273	GLY	O-C-N	-5.58	113.78	122.70
1	A	120	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	448	ALA	N-CA-CB	-5.51	102.39	110.10
1	A	486	TRP	N-CA-CB	5.47	120.45	110.60
1	A	596	GLN	CB-CG-CD	5.42	125.69	111.60
1	A	192	TYR	N-CA-CB	5.36	120.25	110.60
1	A	226	VAL	CA-C-N	5.36	128.98	117.20
1	A	424	VAL	CB-CA-C	5.35	121.56	111.40
1	A	124	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	A	557	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	A	242	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	257	THR	N-CA-CB	-5.28	100.26	110.30
1	A	201	MET	CG-SD-CE	5.28	108.65	100.20
1	A	326	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	186	ALA	CA-C-N	-5.25	105.64	117.20
1	A	539	GLY	N-CA-C	-5.25	99.98	113.10
1	A	299	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	A	267	ASN	CB-CG-OD1	-5.24	111.12	121.60
1	A	501	ILE	CB-CA-C	5.23	122.07	111.60
1	A	541	VAL	N-CA-CB	5.22	122.99	111.50
1	A	434	HIS	O-C-N	5.22	131.05	122.70
1	A	557	GLU	CA-C-N	5.21	128.67	117.20
1	A	197	LEU	CB-CA-C	-5.18	100.36	110.20
1	A	478	ALA	N-CA-C	-5.18	97.02	111.00
1	A	224	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	353	GLU	CA-CB-CG	5.13	124.69	113.40
1	A	423	GLU	CB-CA-C	-5.11	100.19	110.40
1	A	224	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	285	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	548	MET	CA-C-N	5.09	128.40	117.20
1	A	275	ARG	CG-CD-NE	-5.06	101.17	111.80
1	A	547	ASP	OD1-CG-OD2	5.05	132.89	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	547	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	3563	0	3580	340	0
2	A	53	0	31	9	0
All	All	3616	0	3611	340	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 47.

All (340) 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:475:PRO:CA	1:A:553:TYR:OH	1.83	1.25
1:A:426:LYS:HE2	1:A:426:LYS:H	1.02	1.13
1:A:275:ARG:NH1	1:A:403:ASN:HD22	1.46	1.13
1:A:386:LYS:H	1:A:386:LYS:HD2	1.10	1.10
1:A:521:LYS:N	1:A:522:PRO:HD3	1.59	1.10
1:A:199:ILE:HD13	1:A:200:ASP:N	1.68	1.07
1:A:275:ARG:HH11	1:A:403:ASN:ND2	1.52	1.07
1:A:487:VAL:HG11	1:A:553:TYR:CE1	1.91	1.06
1:A:144:GLU:HA	1:A:144:GLU:OE1	1.54	1.03
1:A:534:ARG:HH11	1:A:559:GLY:HA2	1.22	1.02
1:A:475:PRO:N	1:A:553:TYR:OH	1.93	1.01
1:A:475:PRO:HA	1:A:553:TYR:OH	1.56	1.01
1:A:295:LEU:HG	1:A:316:MET:HE3	1.40	1.01
1:A:230:GLN:CG	1:A:246:THR:HG22	1.89	1.01
1:A:230:GLN:HG2	1:A:246:THR:HG22	1.04	1.00
1:A:534:ARG:NH1	1:A:559:GLY:HA2	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:PRO:HB3	1:A:553:TYR:CE2	1.99	0.98
1:A:295:LEU:HG	1:A:316:MET:CE	1.93	0.97
1:A:521:LYS:N	1:A:522:PRO:CD	2.29	0.96
1:A:538:GLY:HA3	1:A:552:VAL:HG21	1.48	0.95
1:A:303:LYS:HG2	1:A:326:ARG:HG2	1.49	0.94
1:A:487:VAL:HG13	1:A:553:TYR:OH	1.70	0.92
1:A:487:VAL:CG1	1:A:553:TYR:CE1	2.52	0.92
1:A:426:LYS:HE2	1:A:426:LYS:N	1.84	0.91
1:A:550:GLY:O	1:A:553:TYR:HB2	1.70	0.91
1:A:230:GLN:HG2	1:A:246:THR:CG2	1.98	0.91
1:A:275:ARG:HH11	1:A:403:ASN:HD22	0.91	0.91
1:A:501:ILE:HD11	1:A:536:ILE:HD11	1.50	0.90
1:A:321:SER:HB3	1:A:355:ARG:NH1	1.87	0.90
1:A:453:HIS:HB3	1:A:469:PHE:HE1	1.36	0.89
1:A:386:LYS:HD2	1:A:386:LYS:N	1.88	0.88
1:A:475:PRO:HA	1:A:553:TYR:HH	1.34	0.88
1:A:521:LYS:H	1:A:522:PRO:HD3	1.34	0.88
1:A:426:LYS:CE	1:A:426:LYS:H	1.87	0.86
1:A:331:GLU:OE2	1:A:333:MET:HG2	1.77	0.84
1:A:144:GLU:CA	1:A:144:GLU:OE1	2.25	0.84
1:A:331:GLU:HG2	1:A:335:GLY:O	1.77	0.83
1:A:199:ILE:HD13	1:A:200:ASP:H	1.42	0.82
1:A:257:THR:HG22	1:A:259:GLU:H	1.44	0.82
1:A:321:SER:HB3	1:A:355:ARG:HH11	1.43	0.82
1:A:288:ILE:HG23	1:A:394:VAL:CG2	2.09	0.82
1:A:386:LYS:H	1:A:386:LYS:CD	1.91	0.82
1:A:428:MET:HG2	1:A:457:VAL:HG22	1.61	0.82
1:A:509:ALA:HA	1:A:520:ASP:HB2	1.59	0.82
1:A:508:TRP:HB2	1:A:522:PRO:O	1.80	0.82
1:A:475:PRO:HB3	1:A:553:TYR:HE2	1.43	0.81
1:A:521:LYS:HE2	1:A:522:PRO:HG3	1.61	0.81
1:A:475:PRO:CB	1:A:553:TYR:OH	2.28	0.81
1:A:247:ALA:N	1:A:255:ALA:O	2.13	0.80
1:A:120:ASP:HA	1:A:262:ILE:O	1.81	0.80
1:A:288:ILE:HG23	1:A:394:VAL:HG22	1.62	0.80
1:A:236:LEU:CD2	1:A:262:ILE:HD12	2.12	0.79
1:A:595:PRO:HB2	1:A:598:LYS:HD3	1.65	0.79
1:A:501:ILE:HD11	1:A:536:ILE:CD1	2.11	0.79
1:A:132:PRO:HD2	2:A:600:FAD:O5'	1.82	0.79
1:A:500:LYS:CG	1:A:530:ALA:HB3	2.12	0.78
1:A:416:VAL:HG22	1:A:422:ILE:HG12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:HG2	1:A:501:ILE:HD12	1.67	0.76
1:A:501:ILE:HG12	1:A:527:ILE:HD12	1.68	0.74
1:A:352:ASN:HB3	1:A:355:ARG:HD2	1.67	0.74
1:A:376:TYR:CE1	1:A:390:ARG:HG3	2.23	0.74
1:A:234:GLN:HG3	1:A:408:SER:OG	1.87	0.74
1:A:561:ASP:O	1:A:564:ASP:HB2	1.88	0.74
1:A:508:TRP:CD1	1:A:523:PHE:HA	2.22	0.73
1:A:373:ASP:O	1:A:390:ARG:HD2	1.88	0.73
1:A:500:LYS:HG2	1:A:530:ALA:HB3	1.69	0.73
1:A:487:VAL:HG13	1:A:553:TYR:CZ	2.24	0.73
1:A:535:ILE:N	1:A:535:ILE:HD12	2.03	0.73
1:A:155:LYS:HD2	1:A:249:ASP:HA	1.68	0.72
1:A:489:GLU:HB3	1:A:527:ILE:HD11	1.71	0.72
1:A:235:PHE:HB2	1:A:408:SER:O	1.89	0.72
1:A:123:TYR:O	1:A:265:PHE:HA	1.89	0.72
1:A:475:PRO:CB	1:A:553:TYR:CZ	2.73	0.72
1:A:305:LEU:HD22	1:A:306:ILE:H	1.54	0.71
1:A:444:GLN:OE1	1:A:445:PRO:HA	1.90	0.71
1:A:231:GLY:HA2	1:A:246:THR:HB	1.70	0.71
1:A:487:VAL:HG12	1:A:488:GLY:H	1.54	0.71
1:A:501:ILE:CD1	1:A:536:ILE:HD11	2.20	0.71
1:A:529:ASP:HB3	1:A:532:THR:OG1	1.90	0.71
1:A:444:GLN:OE1	1:A:446:MET:N	2.24	0.70
1:A:298:LYS:HE2	1:A:299:GLU:HG2	1.74	0.70
1:A:589:THR:O	1:A:589:THR:HG22	1.92	0.70
1:A:428:MET:HG2	1:A:457:VAL:CG2	2.22	0.69
1:A:521:LYS:CE	1:A:522:PRO:HG3	2.21	0.69
1:A:535:ILE:H	1:A:535:ILE:HD12	1.56	0.69
1:A:487:VAL:HG13	1:A:553:TYR:HH	1.57	0.69
1:A:127:VAL:HG11	1:A:138:ALA:HB2	1.75	0.68
1:A:257:THR:HG22	1:A:259:GLU:HB2	1.75	0.68
1:A:475:PRO:CG	1:A:553:TYR:CZ	2.77	0.67
1:A:473:VAL:HG22	1:A:487:VAL:HG12	1.76	0.67
1:A:475:PRO:CB	1:A:553:TYR:CE2	2.74	0.67
1:A:475:PRO:HB3	1:A:553:TYR:CZ	2.30	0.67
1:A:444:GLN:HA	1:A:444:GLN:OE1	1.95	0.67
1:A:162:LEU:HD12	1:A:162:LEU:O	1.95	0.67
1:A:305:LEU:CD2	1:A:306:ILE:H	2.08	0.66
1:A:489:GLU:HG2	1:A:501:ILE:CD1	2.25	0.66
1:A:179:ILE:O	1:A:182:VAL:HG22	1.96	0.66
1:A:500:LYS:HG3	1:A:530:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:HE2	1:A:220:MET:HE3	1.60	0.65
1:A:499:ARG:HG2	1:A:501:ILE:CD1	2.26	0.65
1:A:165:GLY:HA2	2:A:600:FAD:HM72	1.78	0.65
1:A:414:VAL:HA	1:A:431:ASN:HD21	1.60	0.65
1:A:206:LYS:HG2	1:A:207:ASP:N	2.11	0.64
1:A:351:GLN:OE1	1:A:521:LYS:HD3	1.96	0.64
1:A:550:GLY:C	1:A:553:TYR:HB2	2.18	0.64
1:A:487:VAL:CG1	1:A:553:TYR:CZ	2.80	0.64
1:A:124:ASP:HB2	1:A:147:LYS:O	1.95	0.64
1:A:487:VAL:HG11	1:A:553:TYR:HE1	1.55	0.64
1:A:303:LYS:HG2	1:A:326:ARG:CG	2.27	0.64
1:A:186:ALA:O	1:A:189:GLY:N	2.27	0.64
1:A:236:LEU:HD22	1:A:262:ILE:HD12	1.80	0.64
1:A:153:ARG:O	1:A:246:THR:HG21	1.97	0.63
1:A:305:LEU:HD22	1:A:306:ILE:N	2.13	0.63
1:A:154:TYR:CZ	1:A:252:GLU:HA	2.33	0.63
1:A:386:LYS:CD	1:A:386:LYS:N	2.58	0.63
1:A:350:LYS:HE3	1:A:350:LYS:HA	1.79	0.63
1:A:344:LEU:HD23	1:A:541:VAL:HG22	1.80	0.62
1:A:500:LYS:HG3	1:A:530:ALA:CB	2.29	0.62
1:A:487:VAL:HG13	1:A:553:TYR:CE1	2.34	0.62
1:A:494:ALA:O	1:A:498:ALA:N	2.32	0.62
1:A:173:LEU:HD13	1:A:319:VAL:CG1	2.30	0.62
1:A:529:ASP:O	1:A:533:GLY:N	2.31	0.61
1:A:475:PRO:HG3	1:A:553:TYR:CE2	2.35	0.61
1:A:549:ILE:HD12	1:A:550:GLY:N	2.15	0.61
1:A:491:GLU:OE2	1:A:525:LYS:NZ	2.31	0.61
1:A:351:GLN:OE1	1:A:521:LYS:HE3	2.00	0.61
1:A:499:ARG:CG	1:A:501:ILE:HD12	2.31	0.60
1:A:431:ASN:O	1:A:433:PRO:HD3	2.01	0.60
1:A:527:ILE:HG13	1:A:527:ILE:O	1.94	0.60
1:A:519:CYS:O	1:A:522:PRO:CD	2.50	0.60
1:A:589:THR:O	1:A:589:THR:CG2	2.50	0.60
1:A:199:ILE:C	1:A:199:ILE:HD13	2.21	0.60
1:A:489:GLU:HG2	1:A:501:ILE:HD13	1.84	0.60
1:A:186:ALA:HA	1:A:190:ILE:O	2.02	0.59
1:A:336:LEU:O	1:A:337:MET:C	2.39	0.59
1:A:363:THR:HG22	1:A:381:GLY:HA3	1.84	0.59
1:A:453:HIS:HB3	1:A:469:PHE:CE1	2.27	0.59
1:A:491:GLU:OE2	1:A:525:LYS:CE	2.51	0.59
1:A:544:ASN:O	1:A:547:ASP:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD21	1:A:330:VAL:HG22	1.85	0.59
1:A:436:TYR:CE2	1:A:462:CYS:SG	2.95	0.59
1:A:427:GLN:O	1:A:428:MET:HB2	2.03	0.58
1:A:164:VAL:HG11	1:A:252:GLU:OE1	2.03	0.58
1:A:475:PRO:CD	1:A:553:TYR:OH	2.52	0.58
1:A:125:VAL:O	1:A:148:VAL:HA	2.04	0.58
1:A:429:ARG:HG2	1:A:436:TYR:CE1	2.39	0.57
1:A:436:TYR:HE2	1:A:462:CYS:HG	1.48	0.57
1:A:161:CYS:HB2	2:A:600:FAD:O2'	2.04	0.57
1:A:436:TYR:HE2	1:A:462:CYS:SG	2.27	0.57
1:A:475:PRO:CD	1:A:553:TYR:CZ	2.88	0.56
1:A:305:LEU:HD11	1:A:379:PHE:CE1	2.40	0.56
1:A:239:HIS:CE1	1:A:434:HIS:CD2	2.93	0.56
1:A:240:HIS:CD2	1:A:264:ALA:HB2	2.40	0.56
1:A:336:LEU:HD23	1:A:348:TRP:HZ3	1.70	0.56
1:A:572:HIS:HB2	1:A:577:GLU:OE1	2.06	0.56
1:A:321:SER:CB	1:A:355:ARG:HH11	2.15	0.56
1:A:487:VAL:HG12	1:A:488:GLY:N	2.21	0.56
1:A:367:ALA:HB3	1:A:378:THR:HB	1.88	0.55
1:A:275:ARG:NH1	1:A:403:ASN:ND2	2.25	0.55
1:A:501:ILE:CG1	1:A:536:ILE:HD11	2.36	0.55
1:A:343:ASP:OD1	1:A:525:LYS:NZ	2.39	0.55
1:A:341:ASP:HB3	1:A:343:ASP:OD1	2.07	0.55
1:A:509:ALA:O	1:A:515:ILE:HD11	2.06	0.55
1:A:295:LEU:CG	1:A:316:MET:CE	2.79	0.55
1:A:494:ALA:HB2	1:A:501:ILE:HD13	1.88	0.55
1:A:173:LEU:HD13	1:A:319:VAL:HG12	1.89	0.54
1:A:551:GLU:HG2	1:A:579:ILE:HD13	1.89	0.54
1:A:330:VAL:HG21	1:A:379:PHE:CE1	2.43	0.54
1:A:146:LEU:N	1:A:146:LEU:HD13	2.23	0.54
1:A:475:PRO:CG	1:A:553:TYR:CE2	2.91	0.54
1:A:257:THR:CG2	1:A:259:GLU:HB2	2.37	0.54
1:A:274:SER:HB2	1:A:401:ALA:O	2.07	0.54
1:A:526:LEU:HD22	1:A:582:ALA:HB3	1.91	0.53
1:A:305:LEU:HD11	1:A:379:PHE:CZ	2.44	0.53
1:A:500:LYS:CG	1:A:530:ALA:CB	2.83	0.53
1:A:335:GLY:HA2	1:A:361:VAL:HG21	1.90	0.52
1:A:364:LYS:HB2	1:A:380:GLU:HB3	1.91	0.52
1:A:508:TRP:HB2	1:A:522:PRO:HD2	1.91	0.52
1:A:521:LYS:HG3	1:A:522:PRO:HD3	1.91	0.52
1:A:472:ARG:HG3	1:A:557:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLU:HG2	1:A:501:ILE:HD11	1.91	0.52
1:A:486:TRP:CE3	1:A:486:TRP:N	2.78	0.52
1:A:521:LYS:NZ	1:A:522:PRO:HG3	2.24	0.51
1:A:275:ARG:N	1:A:401:ALA:O	2.43	0.51
1:A:367:ALA:HB3	1:A:378:THR:CB	2.41	0.51
1:A:520:ASP:C	1:A:522:PRO:CD	2.78	0.51
1:A:162:LEU:HD12	1:A:162:LEU:C	2.31	0.51
1:A:291:SER:O	1:A:295:LEU:HD12	2.11	0.51
1:A:491:GLU:OE1	1:A:503:LYS:HE2	2.11	0.51
1:A:440:ASP:OD1	2:A:600:FAD:H5'1	2.11	0.51
1:A:440:ASP:OD2	1:A:446:MET:HB3	2.11	0.51
1:A:232:ASP:C	1:A:232:ASP:OD1	2.48	0.51
1:A:550:GLY:HA2	1:A:553:TYR:CD2	2.46	0.51
1:A:141:ALA:O	1:A:144:GLU:HB2	2.10	0.51
1:A:377:VAL:HG13	1:A:391:TYR:CE2	2.46	0.50
1:A:361:VAL:HG13	1:A:362:ASN:N	2.27	0.50
1:A:414:VAL:HG21	1:A:435:ILE:HG21	1.94	0.50
1:A:425:ASP:O	1:A:427:GLN:N	2.45	0.50
1:A:321:SER:HB2	1:A:327:LEU:HD11	1.92	0.49
1:A:550:GLY:HA2	1:A:553:TYR:HB2	1.94	0.49
1:A:165:GLY:HA2	2:A:600:FAD:C7M	2.43	0.49
1:A:472:ARG:HE	1:A:556:ILE:CG2	2.24	0.49
1:A:563:ALA:HA	1:A:587:LEU:HD11	1.95	0.49
1:A:508:TRP:CE3	1:A:522:PRO:HG2	2.48	0.49
1:A:351:GLN:OE1	1:A:521:LYS:CE	2.60	0.49
1:A:424:VAL:HG13	1:A:428:MET:HA	1.93	0.49
1:A:438:ILE:O	1:A:441:ILE:HG22	2.12	0.49
1:A:442:VAL:HG12	1:A:443:GLY:N	2.26	0.49
1:A:459:ALA:O	1:A:462:CYS:HB2	2.12	0.49
1:A:550:GLY:CA	1:A:553:TYR:HB2	2.43	0.49
1:A:561:ASP:H	1:A:564:ASP:HB2	1.77	0.48
1:A:395:LEU:HD12	1:A:396:VAL:N	2.28	0.48
1:A:405:LYS:HG3	1:A:416:VAL:HG11	1.94	0.48
1:A:241:LEU:HA	1:A:241:LEU:HD12	1.68	0.48
1:A:421:PHE:CD2	1:A:443:GLY:HA2	2.49	0.48
1:A:453:HIS:CB	1:A:469:PHE:HE1	2.16	0.48
1:A:473:VAL:HG13	1:A:553:TYR:CE1	2.48	0.48
1:A:517:ASN:HD22	1:A:517:ASN:N	2.11	0.48
1:A:293:GLY:O	1:A:294:ALA:C	2.52	0.48
1:A:237:ASP:O	1:A:239:HIS:N	2.46	0.48
1:A:364:LYS:O	1:A:380:GLU:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HB3	1:A:403:ASN:HD21	1.79	0.48
1:A:236:LEU:HB3	1:A:240:HIS:HB2	1.96	0.48
1:A:350:LYS:HA	1:A:350:LYS:CE	2.42	0.48
1:A:508:TRP:CB	1:A:522:PRO:O	2.58	0.48
1:A:489:GLU:O	1:A:537:GLY:HA3	2.13	0.48
1:A:268:CYS:HB3	1:A:435:ILE:HG12	1.96	0.47
1:A:293:GLY:O	1:A:296:ALA:N	2.35	0.47
1:A:475:PRO:HG3	1:A:553:TYR:CZ	2.48	0.47
1:A:425:ASP:OD1	1:A:427:GLN:HB2	2.14	0.47
1:A:251:TYR:O	1:A:252:GLU:HB2	2.14	0.47
1:A:593:LEU:HB3	1:A:594:PRO:HD2	1.95	0.47
1:A:155:LYS:HD2	1:A:249:ASP:CG	2.35	0.47
1:A:127:VAL:CG1	1:A:138:ALA:HB2	2.44	0.47
1:A:229:ILE:CG2	1:A:243:VAL:HG11	2.44	0.47
1:A:174:HIS:O	1:A:178:VAL:HG23	2.14	0.47
1:A:431:ASN:N	1:A:431:ASN:HD22	2.12	0.47
1:A:131:GLY:O	1:A:135:TYR:HD2	1.97	0.47
1:A:472:ARG:NE	1:A:556:ILE:CG2	2.78	0.47
1:A:328:ASP:OD1	1:A:357:ASP:HB2	2.14	0.46
1:A:550:GLY:HA2	1:A:553:TYR:HD2	1.80	0.46
1:A:551:GLU:OE2	1:A:570:HIS:NE2	2.40	0.46
1:A:473:VAL:HG13	1:A:553:TYR:HE1	1.79	0.46
1:A:230:GLN:CG	1:A:246:THR:CG2	2.73	0.46
1:A:429:ARG:HG2	1:A:436:TYR:HE1	1.78	0.46
1:A:487:VAL:CG1	1:A:553:TYR:HE1	2.16	0.46
1:A:243:VAL:HG12	1:A:245:LEU:HD23	1.97	0.46
1:A:311:ILE:HG23	1:A:478:ALA:HA	1.98	0.46
1:A:520:ASP:C	1:A:522:PRO:HD3	2.30	0.46
1:A:211:SER:HA	1:A:214:THR:OG1	2.16	0.46
1:A:237:ASP:HA	1:A:411:LYS:O	2.15	0.46
1:A:377:VAL:HG13	1:A:391:TYR:HE2	1.80	0.46
1:A:499:ARG:HG3	1:A:500:LYS:N	2.30	0.46
1:A:502:THR:HB	1:A:528:PHE:HB2	1.96	0.46
1:A:251:TYR:CD1	1:A:252:GLU:HG3	2.50	0.46
1:A:595:PRO:HB2	1:A:598:LYS:CD	2.42	0.46
1:A:376:TYR:HA	1:A:389:GLN:O	2.16	0.45
1:A:351:GLN:OE1	1:A:521:LYS:CD	2.63	0.45
1:A:279:LEU:HB2	1:A:282:ILE:HD12	1.97	0.45
1:A:244:SER:HA	1:A:260:LYS:HG2	1.99	0.45
1:A:247:ALA:O	1:A:255:ALA:N	2.32	0.45
1:A:485:ALA:HB1	1:A:549:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:CA	1:A:262:ILE:O	2.59	0.45
1:A:305:LEU:CD2	1:A:306:ILE:N	2.76	0.45
1:A:274:SER:CB	1:A:401:ALA:O	2.64	0.45
1:A:336:LEU:N	1:A:336:LEU:CD1	2.80	0.44
1:A:489:GLU:CB	1:A:527:ILE:HD11	2.45	0.44
1:A:554:LEU:O	1:A:558:MET:HG2	2.17	0.44
1:A:166:CYS:HA	2:A:600:FAD:N5	2.32	0.44
1:A:440:ASP:CG	1:A:446:MET:HB3	2.37	0.44
1:A:301:PRO:HD2	1:A:320:TYR:CD1	2.52	0.44
1:A:365:THR:HG23	1:A:377:VAL:HG23	2.00	0.44
1:A:595:PRO:HG3	1:A:598:LYS:NZ	2.32	0.44
1:A:131:GLY:HA2	1:A:159:GLY:HA3	1.98	0.44
1:A:425:ASP:O	1:A:428:MET:N	2.39	0.44
1:A:124:ASP:O	1:A:266:LYS:HB2	2.18	0.44
1:A:126:VAL:HG22	1:A:149:ALA:HB3	2.00	0.44
1:A:166:CYS:SG	2:A:600:FAD:C4X	3.06	0.44
1:A:199:ILE:HG12	1:A:203:ARG:NH2	2.33	0.44
1:A:272:ALA:HB3	1:A:441:ILE:HD13	2.00	0.44
1:A:270:ILE:O	1:A:437:ALA:HA	2.17	0.43
1:A:165:GLY:HA2	2:A:600:FAD:C7	2.48	0.43
1:A:199:ILE:O	1:A:203:ARG:HB2	2.18	0.43
1:A:565:ILE:O	1:A:568:THR:HB	2.18	0.43
1:A:526:LEU:HD12	1:A:526:LEU:HA	1.78	0.43
1:A:298:LYS:HE2	1:A:299:GLU:CG	2.47	0.43
1:A:501:ILE:HA	1:A:528:PHE:O	2.18	0.43
1:A:237:ASP:HB2	1:A:238:PRO:HD2	2.01	0.43
1:A:529:ASP:OD2	1:A:532:THR:OG1	2.35	0.43
1:A:330:VAL:HG12	1:A:363:THR:OG1	2.19	0.42
1:A:519:CYS:C	1:A:522:PRO:HD3	2.39	0.42
1:A:583:ALA:O	1:A:586:ALA:HB3	2.19	0.42
1:A:287:ARG:HD3	1:A:287:ARG:HH11	1.36	0.42
1:A:424:VAL:HG21	1:A:437:ALA:HB3	2.01	0.42
1:A:544:ASN:O	1:A:545:GLY:C	2.58	0.42
1:A:535:ILE:HG12	1:A:565:ILE:HD11	2.01	0.42
1:A:123:TYR:CE2	1:A:149:ALA:HB2	2.54	0.42
1:A:157:LEU:HD11	1:A:228:VAL:HG21	2.01	0.42
1:A:251:TYR:CE1	1:A:252:GLU:HG3	2.55	0.42
1:A:275:ARG:NH1	1:A:275:ARG:HG2	2.35	0.42
1:A:522:PRO:HB2	1:A:541:VAL:O	2.19	0.42
1:A:282:ILE:HG21	1:A:288:ILE:HG21	2.01	0.42
1:A:131:GLY:O	1:A:135:TYR:CD2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PRO:HG3	1:A:161:CYS:HB3	2.02	0.42
1:A:180:ASP:OD1	1:A:322:THR:HG23	2.19	0.42
1:A:354:TYR:CD2	1:A:354:TYR:C	2.91	0.42
1:A:274:SER:CA	1:A:401:ALA:O	2.67	0.42
1:A:583:ALA:O	1:A:586:ALA:N	2.53	0.42
1:A:240:HIS:NE2	1:A:264:ALA:HB2	2.35	0.41
1:A:514:ALA:HB1	1:A:519:CYS:O	2.19	0.41
1:A:152:GLU:O	1:A:230:GLN:HA	2.20	0.41
1:A:119:ALA:CB	1:A:261:LYS:HA	2.51	0.41
1:A:450:LYS:HE3	1:A:454:GLU:OE1	2.19	0.41
1:A:535:ILE:H	1:A:535:ILE:CD1	2.21	0.41
1:A:486:TRP:N	1:A:486:TRP:HE3	2.18	0.41
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.41	0.41
1:A:309:GLY:O	1:A:314:LEU:HD11	2.20	0.41
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.86	0.41
1:A:274:SER:HA	1:A:402:PRO:HA	2.03	0.41
1:A:405:LYS:HE3	1:A:418:ASP:HA	2.03	0.41
1:A:414:VAL:CG2	1:A:435:ILE:HG21	2.50	0.41
1:A:152:GLU:OE1	2:A:600:FAD:H1B	2.21	0.41
1:A:346:LYS:HE2	1:A:346:LYS:HB2	1.94	0.41
1:A:394:VAL:O	1:A:394:VAL:CG2	2.68	0.41
1:A:425:ASP:C	1:A:427:GLN:N	2.73	0.41
1:A:202:LEU:O	1:A:205:TYR:N	2.54	0.40
1:A:424:VAL:HG22	1:A:429:ARG:C	2.40	0.40
1:A:515:ILE:HD13	1:A:515:ILE:HG21	1.91	0.40
1:A:549:ILE:HD12	1:A:550:GLY:H	1.83	0.40
1:A:155:LYS:HE2	1:A:155:LYS:HB2	1.45	0.40
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.79	0.40
1:A:457:VAL:HG11	1:A:469:PHE:HA	2.02	0.40
1:A:519:CYS:O	1:A:522:PRO:CG	2.69	0.40
1:A:522:PRO:CB	1:A:541:VAL:O	2.70	0.40
1:A:549:ILE:HD12	1:A:549:ILE:C	2.41	0.40
1:A:155:LYS:HD2	1:A:249:ASP:CA	2.45	0.40
1:A:336:LEU:HD23	1:A:348:TRP:CZ3	2.55	0.40
1:A:119:ALA:HB1	1:A:261:LYS:HA	2.03	0.40
1:A:369:GLU:HA	1:A:370:PRO:HD3	1.77	0.40
1:A:572:HIS:HA	1:A:577:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	480/482 (100%)	445 (93%)	29 (6%)	6 (1%)	14	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	SER
1	A	185	LEU
1	A	238	PRO
1	A	426	LYS
1	A	285	ASP
1	A	337	MET

### 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	364/364 (100%)	290 (80%)	74 (20%)	1	10

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASP
1	A	125	VAL
1	A	127	VAL
1	A	135	TYR
1	A	146	LEU

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Mol	Chain	Res	Type
1	A	155	LYS
1	A	164	VAL
1	A	170	LYS
1	A	172	LEU
1	A	173	LEU
1	A	179	ILE
1	A	181	GLU
1	A	199	ILE
1	A	205	TYR
1	A	206	LYS
1	A	212	ARG
1	A	223	SER
1	A	225	LYS
1	A	232	ASP
1	A	236	LEU
1	A	241	LEU
1	A	246	THR
1	A	249	ASP
1	A	253	GLN
1	A	259	GLU
1	A	266	LYS
1	A	305	LEU
1	A	316	MET
1	A	321	SER
1	A	325	SER
1	A	326	ARG
1	A	327	LEU
1	A	329	VAL
1	A	330	VAL
1	A	334	ASP
1	A	336	LEU
1	A	338	GLN
1	A	342	ARG
1	A	344	LEU
1	A	346	LYS
1	A	350	LYS
1	A	361	VAL
1	A	364	LYS
1	A	366	VAL
1	A	377	VAL
1	A	386	LYS
1	A	408	SER

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Mol	Chain	Res	Type
1	A	419	ARG
1	A	423	GLU
1	A	424	VAL
1	A	426	LYS
1	A	429	ARG
1	A	431	ASN
1	A	433	PRO
1	A	457	VAL
1	A	466	LYS
1	A	473	VAL
1	A	481	SER
1	A	486	TRP
1	A	487	VAL
1	A	492	LEU
1	A	495	LYS
1	A	500	LYS
1	A	501	ILE
1	A	503	LYS
1	A	521	LYS
1	A	525	LYS
1	A	527	ILE
1	A	535	ILE
1	A	549	ILE
1	A	552	VAL
1	A	581	MET
1	A	596	GLN
1	A	598	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	230	GLN
1	A	403	ASN
1	A	431	ASN
1	A	517	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	600	1	51,58,58	2.38	19 (37%)	54,89,89	2.82	20 (37%)

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	600	1	3/3/9/9	0/28/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C1'-N10	-9.97	1.38	1.48
2	A	600	FAD	O4B-C4B	-3.71	1.36	1.45
2	A	600	FAD	C5'-C4'	-3.15	1.47	1.51
2	A	600	FAD	PA-O2A	-2.82	1.41	1.55
2	A	600	FAD	C9A-C5X	-2.69	1.37	1.42
2	A	600	FAD	P-O1P	-2.10	1.43	1.50
2	A	600	FAD	O3B-C3B	2.24	1.48	1.43
2	A	600	FAD	C9A-N10	2.29	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C2'-C3'	2.36	1.58	1.53
2	A	600	FAD	O4B-C1B	2.39	1.44	1.41
2	A	600	FAD	C9-C9A	2.40	1.45	1.40
2	A	600	FAD	C4-N3	2.43	1.37	1.33
2	A	600	FAD	C5B-C4B	2.45	1.59	1.51
2	A	600	FAD	C4A-N3A	2.47	1.39	1.35
2	A	600	FAD	O2B-C2B	2.68	1.49	1.43
2	A	600	FAD	C6-C5X	2.75	1.45	1.41
2	A	600	FAD	C2A-N3A	3.90	1.38	1.32
2	A	600	FAD	C10-N1	4.25	1.39	1.33
2	A	600	FAD	C4X-N5	4.61	1.40	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C4-C4X-C10	-6.71	114.53	119.96
2	A	600	FAD	O5'-P-O1P	-5.11	88.65	109.25
2	A	600	FAD	O2P-P-O1P	-4.50	88.99	112.28
2	A	600	FAD	O2A-PA-O1A	-4.41	89.45	112.28
2	A	600	FAD	C4B-O4B-C1B	-4.38	105.11	109.77
2	A	600	FAD	C1B-N9A-C4A	-4.16	119.44	126.64
2	A	600	FAD	O3B-C3B-C4B	-3.82	99.93	111.09
2	A	600	FAD	O5B-C5B-C4B	-2.91	98.67	109.00
2	A	600	FAD	C7M-C7-C6	-2.87	113.15	120.34
2	A	600	FAD	C9-C9A-C5X	-2.20	115.78	119.58
2	A	600	FAD	C6-C5X-N5	-2.16	116.43	118.97
2	A	600	FAD	O2'-C2'-C3'	-2.01	104.10	109.09
2	A	600	FAD	C6-C5X-C9A	2.17	121.82	119.00
2	A	600	FAD	N3A-C2A-N1A	2.24	130.81	128.86
2	A	600	FAD	C7M-C7-C8	2.84	126.67	120.72
2	A	600	FAD	O2P-P-O5'	3.12	122.88	108.14
2	A	600	FAD	O4B-C4B-C3B	3.75	112.63	105.17
2	A	600	FAD	C4-C4X-N5	5.46	124.67	118.68
2	A	600	FAD	C5X-C9A-N10	5.84	121.99	117.66
2	A	600	FAD	C1'-N10-C9A	9.42	126.98	118.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	600	FAD	C4'
2	A	600	FAD	C2'
2	A	600	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	9	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.