



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:35 PM GMT

PDB ID : 3ES9  
Title : NADPH-Cytochrome P450 Reductase in an Open Conformation  
Authors : Hamdane, D.; Xia, C.; Im, S.-C.; Zhang, H.; Kim, J.-J.; Waskell, L.  
Deposited on : 2008-10-05  
Resolution : 3.40 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

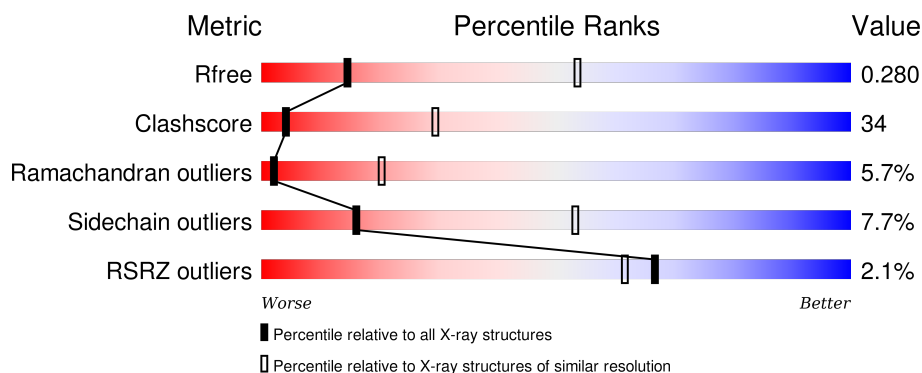
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	618	 43% 47% 7% ••
1	B	618	 4% 39% 38% 6% 17%
1	C	618	 % 32% 33% 5% • 30%

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
4	NAP	A	753	-	-	-	X
4	NAP	B	753	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12762 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.

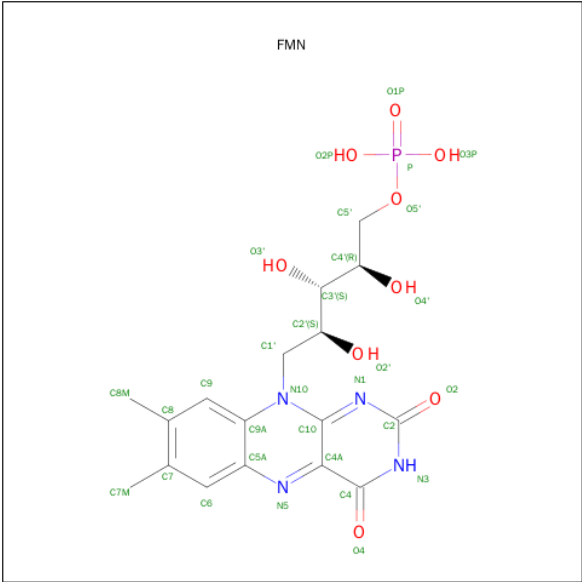
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4846	3069	834	920	23			
1	B	515	Total	C	N	O	S	0	0	0
			4138	2618	726	775	19			
1	C	435	Total	C	N	O	S	0	0	0
			3492	2212	617	647	16			

There are 12 discrepancies between the modelled and reference sequences:

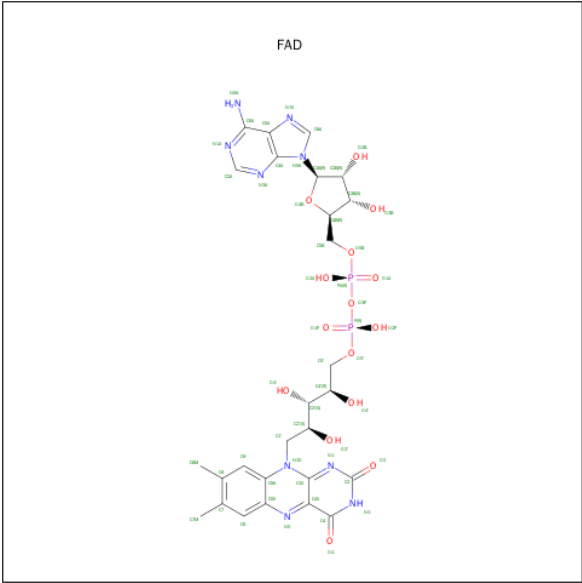
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	DELETION	UNP P00388
A	?	-	GLY	DELETION	UNP P00388
A	?	-	GLU	DELETION	UNP P00388
A	?	-	GLU	DELETION	UNP P00388
B	?	-	THR	DELETION	UNP P00388
B	?	-	GLY	DELETION	UNP P00388
B	?	-	GLU	DELETION	UNP P00388
B	?	-	GLU	DELETION	UNP P00388
C	?	-	THR	DELETION	UNP P00388
C	?	-	GLY	DELETION	UNP P00388
C	?	-	GLU	DELETION	UNP P00388
C	?	-	GLU	DELETION	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



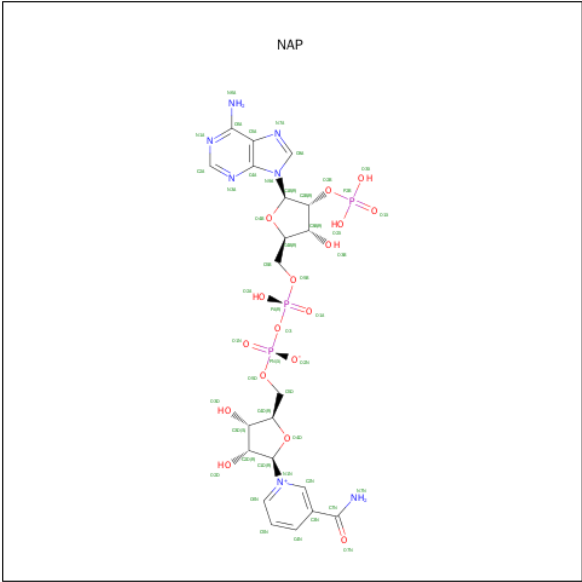
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

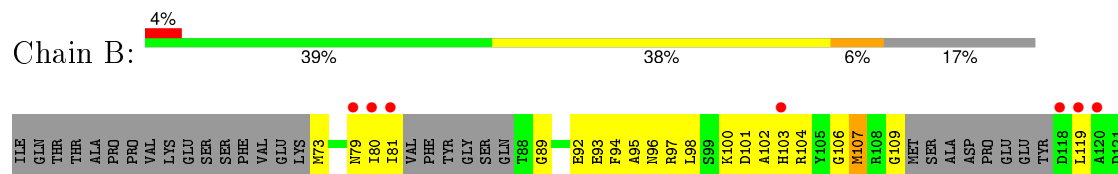
### 3 Residue-property plots

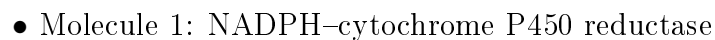
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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: NADPH-cytochrome P450 reductase

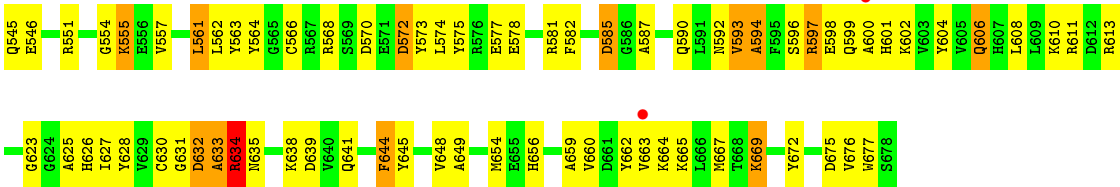


#### • Molecule 1: NADPH-cytochrome P450 reductase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.10Å 93.00Å 125.70Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	29.79 – 3.40 46.52 – 3.38	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.79-3.40) 90.3 (46.52-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.219 , 0.279 0.219 , 0.280	Depositor DCC
$R_{free}$ test set	1549 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.9	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 31581 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: FMN, NAP, 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	0.41	0/4962	0.63	0/6714
1	B	0.40	0/4233	0.66	1/5725 (0.0%)
1	C	0.36	0/3576	0.60	0/4843
All	All	0.39	0/12771	0.63	1/17282 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	PRO	N-CA-C	5.09	125.35	112.10

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	4846	0	4692	335	0
1	B	4138	0	4026	280	0
1	C	3492	0	3425	229	0
2	A	31	0	19	0	0
3	A	53	0	31	5	0
3	B	53	0	31	7	0
3	C	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	48	0	25	3	0
4	B	48	0	25	2	0
All	All	12762	0	12305	841	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 34.

All (841) 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:B:300:LEU:HD23	1:B:574:LEU:HD21	1.35	1.08
1:A:292:LEU:HD21	1:A:302:HIS:HB2	1.36	1.04
1:A:606:GLN:HE22	4:A:753:NAP:H2A	1.27	1.00
1:A:300:LEU:HD23	1:A:574:LEU:HD21	1.44	0.96
1:B:567:ARG:HD2	1:B:597:ARG:HD2	1.46	0.96
1:B:418:SER:HA	1:B:422:GLU:HB2	1.45	0.96
1:C:411:GLU:HG3	1:C:412:GLY:N	1.81	0.95
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.46	0.95
1:B:590:GLN:HE21	1:B:592:ASN:HD21	1.10	0.94
1:A:82:VAL:HG11	1:A:95:ALA:HA	1.50	0.93
1:C:606:GLN:H	1:C:606:GLN:NE2	1.67	0.92
1:B:100:LYS:HE2	1:B:354:GLU:HG3	1.49	0.92
1:B:594:ALA:HB2	1:B:608:LEU:HD11	1.50	0.91
1:C:375:LEU:O	1:C:451:LEU:HB2	1.69	0.91
1:B:568:ARG:HB2	1:B:571:GLU:HB2	1.54	0.90
1:C:288:ALA:HB3	1:C:304:GLU:HG3	1.53	0.90
1:A:454:ARG:HH22	1:A:489:VAL:HB	1.36	0.90
1:C:634:ARG:HH11	1:C:634:ARG:HB3	1.35	0.89
1:C:606:GLN:H	1:C:606:GLN:HE21	1.18	0.88
1:B:272:GLN:HA	1:B:272:GLN:HE21	1.36	0.87
1:C:257:LYS:HD3	1:C:257:LYS:O	1.74	0.86
1:B:244:GLN:HE21	1:B:350:ASN:HD21	1.23	0.86
1:C:411:GLU:HG3	1:C:412:GLY:H	1.38	0.86
1:C:371:LEU:HD23	1:C:375:LEU:HD12	1.58	0.86
1:A:464:VAL:HG12	1:A:465:HIS:H	1.40	0.85
1:A:423:ALA:HA	1:A:481:LYS:HB2	1.58	0.85
1:B:590:GLN:NE2	1:B:592:ASN:HD21	1.76	0.83
1:A:395:GLU:HG3	1:A:396:PRO:HD2	1.58	0.83
1:A:402:LEU:HD11	1:A:437:LEU:HD22	1.59	0.83
1:C:627:ILE:HG21	1:C:644:PHE:HE1	1.43	0.83
1:C:596:SER:O	1:C:597:ARG:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASP:O	1:B:344:VAL:HG23	1.79	0.83
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.59	0.82
1:C:593:VAL:HG12	1:C:594:ALA:H	1.44	0.81
1:C:484:ARG:HD2	1:C:484:ARG:H	1.45	0.81
1:C:667:MET:HA	1:C:672:TYR:HB3	1.63	0.80
1:A:327:ASP:HB3	1:A:330:LEU:HB2	1.63	0.80
1:A:326:ASN:ND2	1:A:377:ILE:HG12	1.96	0.80
1:C:291:LYS:HE2	1:C:296:THR:HG22	1.64	0.80
1:B:79:ASN:CG	1:B:80:ILE:H	1.86	0.79
1:A:184:MET:CE	1:A:188:VAL:HG23	2.12	0.79
1:B:541:MET:O	1:B:545:GLN:HG3	1.83	0.79
1:C:460:SER:HA	1:C:545:GLN:OE1	1.82	0.78
1:C:568:ARG:NH1	1:C:598:GLU:HG2	1.99	0.78
1:C:656:HIS:O	1:C:660:VAL:HG23	1.83	0.78
1:B:338:LEU:HD21	1:B:439:PRO:HD2	1.65	0.78
1:A:546:GLU:O	1:A:550:LEU:HG	1.84	0.78
1:A:452:GLN:HA	1:A:452:GLN:HE21	1.48	0.77
1:B:269:TYR:CD2	1:B:283:LEU:HD11	2.19	0.77
1:C:293:ASN:HB3	1:C:300:LEU:HD23	1.66	0.77
1:B:452:GLN:HE21	1:B:452:GLN:HA	1.50	0.77
1:B:244:GLN:HE21	1:B:350:ASN:ND2	1.82	0.76
1:A:654:MET:HB2	1:A:658:GLN:HB3	1.67	0.76
1:B:636:MET:O	1:B:640:VAL:HG23	1.86	0.76
1:B:411:GLU:HG3	1:B:412:GLY:N	2.01	0.76
1:B:402:LEU:HD11	1:B:437:LEU:HD22	1.68	0.75
1:A:371:LEU:HD23	1:A:375:LEU:HD12	1.68	0.75
1:A:488:GLY:HA2	3:A:752:FAD:O1A	1.86	0.75
1:B:378:THR:HG21	1:B:489:VAL:HG21	1.68	0.75
1:A:265:ARG:HB3	1:A:268:SER:HB3	1.69	0.75
1:A:582:PHE:HB3	1:A:587:ALA:HB3	1.69	0.75
1:B:327:ASP:HB3	1:B:330:LEU:HB2	1.69	0.75
1:C:389:LEU:HB3	1:C:437:LEU:HD11	1.67	0.75
1:C:634:ARG:HB3	1:C:634:ARG:NH1	2.02	0.74
1:C:259:TYR:HE2	1:C:266:LEU:HA	1.53	0.74
1:B:411:GLU:HG3	1:B:412:GLY:H	1.52	0.74
1:C:321:ALA:HB2	1:C:455:TYR:CE1	2.22	0.74
1:A:272:GLN:HE22	1:A:283:LEU:N	1.86	0.74
1:B:463:LYS:HG3	1:B:546:GLU:HG3	1.67	0.74
1:B:102:ALA:HB1	1:B:107:MET:O	1.88	0.73
1:C:266:LEU:HD12	1:C:266:LEU:H	1.52	0.73
1:A:455:TYR:CE1	1:A:514:ARG:HD3	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:O	1:B:227:VAL:HG23	1.88	0.73
1:C:561:LEU:H	1:C:561:LEU:HD12	1.54	0.73
1:C:259:TYR:CE2	1:C:266:LEU:HG	2.23	0.72
1:B:300:LEU:CD2	1:B:574:LEU:HD21	2.17	0.72
1:A:393:ALA:HA	1:A:436:SER:O	1.88	0.72
1:B:575:TYR:HB3	1:B:578:GLU:HB2	1.71	0.72
1:A:654:MET:HB2	1:A:658:GLN:CB	2.19	0.72
1:A:666:LEU:HD22	1:A:671:ARG:HB2	1.71	0.72
1:B:106:GLY:O	1:B:107:MET:HG3	1.89	0.72
1:C:561:LEU:N	1:C:561:LEU:HD12	2.04	0.72
1:C:649:ALA:HB2	1:C:659:ALA:HB2	1.71	0.72
1:A:96:ASN:HB3	1:A:100:LYS:HE3	1.71	0.72
1:A:348:LEU:HD12	1:A:360:PRO:HG3	1.70	0.72
1:A:113:ASP:OD1	1:A:115:GLU:HB3	1.88	0.72
1:A:434:TYR:O	1:A:437:LEU:HB3	1.91	0.71
1:A:107:MET:CE	1:A:233:VAL:HG21	2.20	0.71
1:A:634:ARG:HD2	1:A:678:SER:OG	1.89	0.71
1:C:253:MET:CE	1:C:254:ASP:H	2.01	0.71
1:A:569:SER:HB3	1:A:595:PHE:CE1	2.26	0.71
1:C:523:LYS:HB2	1:C:526:THR:OG1	1.90	0.71
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.73	0.71
1:A:654:MET:HB2	1:A:658:GLN:CG	2.21	0.70
1:B:246:GLU:HB3	1:B:351:LEU:HD21	1.73	0.70
1:A:664:LYS:HE3	1:A:664:LYS:HA	1.72	0.70
1:A:104:ARG:HD2	1:A:242:ILE:HD12	1.70	0.70
1:B:476:VAL:HG21	3:B:752:FAD:H5'2	1.71	0.70
1:A:661:ASP:HA	1:A:664:LYS:HB2	1.72	0.70
1:C:259:TYR:HB2	1:C:364:PRO:O	1.92	0.69
1:C:341:ASP:HB3	1:C:344:VAL:HG23	1.74	0.69
1:A:666:LEU:HD21	1:A:671:ARG:NH1	2.07	0.69
1:C:488:GLY:HA2	3:C:752:FAD:O1A	1.93	0.69
1:A:105:TYR:O	1:A:107:MET:N	2.25	0.69
1:B:350:ASN:HD22	1:B:351:LEU:N	1.90	0.69
1:C:265:ARG:HH11	1:C:265:ARG:HG3	1.58	0.69
1:A:254:ASP:O	1:A:257:LYS:HG2	1.92	0.69
1:A:460:SER:HB3	1:A:470:HIS:HB2	1.75	0.69
1:C:478:TYR:O	1:C:485:VAL:HG13	1.93	0.69
1:B:79:ASN:HD21	1:B:107:MET:HG2	1.58	0.69
1:A:214:GLU:HA	1:A:214:GLU:OE1	1.93	0.69
1:B:518:PHE:O	1:B:519:ARG:HD3	1.93	0.69
1:A:184:MET:HE2	1:A:188:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:MET:HB2	1:A:658:GLN:HG2	1.75	0.68
1:B:562:LEU:HD12	1:B:563:TYR:H	1.58	0.68
1:C:418:SER:HA	1:C:422:GLU:HB2	1.74	0.68
1:C:435:PRO:HA	1:C:438:ARG:NH2	2.06	0.68
1:B:479:GLU:HG2	1:B:485:VAL:HG22	1.76	0.68
1:B:254:ASP:HB3	1:B:257:LYS:HD2	1.75	0.68
1:C:645:TYR:HA	1:C:663:VAL:HG21	1.75	0.68
1:A:265:ARG:CB	1:A:268:SER:HB3	2.23	0.68
1:C:326:ASN:ND2	1:C:377:ILE:HG12	2.08	0.68
1:A:292:LEU:CD2	1:A:302:HIS:HB2	2.18	0.68
1:C:253:MET:HE2	1:C:254:ASP:H	1.58	0.68
1:A:441:ILE:HG23	1:A:442:ASP:H	1.59	0.68
1:C:324:PRO:HG2	1:C:451:LEU:HD21	1.76	0.68
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.75	0.67
1:B:409:SER:HA	1:B:413:LYS:HB2	1.75	0.67
1:A:329:ALA:O	1:A:333:GLN:HB2	1.94	0.67
1:C:302:HIS:HD2	1:C:575:TYR:OH	1.77	0.67
1:A:487:LYS:HB3	1:A:492:SER:OG	1.94	0.67
1:A:266:LEU:O	1:A:267:LYS:HB2	1.95	0.67
1:B:244:GLN:NE2	1:B:350:ASN:HD21	1.90	0.67
1:C:627:ILE:HG21	1:C:644:PHE:CE1	2.29	0.67
1:B:518:PHE:CD2	1:B:675:ASP:HB2	2.29	0.67
1:B:338:LEU:CD2	1:B:439:PRO:HD2	2.25	0.66
1:C:606:GLN:HE21	1:C:606:GLN:N	1.92	0.66
1:A:477:GLU:HG3	1:A:487:LYS:HG2	1.76	0.66
1:C:477:GLU:HG3	1:C:487:LYS:HD2	1.76	0.66
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.75	0.66
1:A:282:PHE:CE2	1:A:310:SER:HB3	2.31	0.66
1:B:395:GLU:HG2	1:B:398:GLU:HG3	1.78	0.66
1:A:484:ARG:HD2	1:A:484:ARG:H	1.60	0.66
1:A:78:ARG:NH1	1:A:110:MET:HB3	2.11	0.66
1:C:454:ARG:HG2	3:C:752:FAD:O1P	1.96	0.66
1:A:155:TRP:CZ2	1:A:161:VAL:HG11	2.31	0.66
1:A:154:ASP:O	1:A:158:GLU:HG2	1.97	0.65
1:A:566:CYS:HB2	1:A:572:ASP:OD1	1.96	0.65
1:A:452:GLN:HA	1:A:452:GLN:NE2	2.11	0.65
1:C:411:GLU:CG	1:C:412:GLY:H	2.10	0.65
1:A:272:GLN:HE22	1:A:283:LEU:H	1.43	0.65
1:B:521:PRO:O	1:B:522:PHE:HB3	1.96	0.65
1:B:100:LYS:HE2	1:B:354:GLU:CG	2.24	0.65
1:B:254:ASP:HB3	1:B:257:LYS:CD	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LYS:H	1:A:555:LYS:HD2	1.61	0.65
1:A:253:MET:HE2	1:A:257:LYS:HD3	1.77	0.64
1:A:441:ILE:HG23	1:A:442:ASP:N	2.12	0.64
1:C:240:SER:CB	1:C:387:TYR:HE1	2.10	0.64
1:B:92:GLU:O	1:B:95:ALA:HB3	1.97	0.64
1:A:184:MET:HE1	1:A:188:VAL:HG23	1.78	0.64
1:A:82:VAL:HG22	1:A:134:VAL:HB	1.79	0.64
1:B:562:LEU:HD12	1:B:563:TYR:N	2.13	0.64
1:B:664:LYS:O	1:B:668:THR:HG23	1.98	0.64
1:A:548:ALA:HB2	1:A:587:ALA:HB2	1.80	0.64
1:A:66:GLU:HG2	1:A:67:SER:N	2.13	0.64
1:C:342:LEU:H	1:C:342:LEU:HD12	1.63	0.64
1:A:86:SER:CB	1:A:91:ALA:HB3	2.25	0.63
1:B:376:ASP:OD2	1:B:378:THR:HG23	1.97	0.63
1:A:93:GLU:OE2	1:A:97:ARG:HD3	1.98	0.63
1:B:216:PHE:HE2	1:B:220:ARG:HD2	1.62	0.63
1:C:590:GLN:HE21	1:C:592:ASN:HD21	1.45	0.63
1:B:310:SER:OG	1:B:312:ILE:HG13	1.99	0.63
1:C:645:TYR:HD2	1:C:663:VAL:HG21	1.62	0.63
1:A:595:PHE:O	1:A:603:VAL:HB	1.98	0.63
1:C:568:ARG:HH12	1:C:598:GLU:HG2	1.63	0.62
1:B:79:ASN:CG	1:B:80:ILE:N	2.52	0.62
1:C:308:SER:O	1:C:309:ASP:HB2	1.98	0.62
1:C:551:ARG:CG	1:C:557:VAL:HG21	2.29	0.62
1:C:352:ASP:O	1:C:354:GLU:N	2.28	0.62
1:B:567:ARG:HB2	1:B:572:ASP:OD1	2.00	0.62
1:A:455:TYR:HE1	1:A:514:ARG:HD3	1.62	0.62
1:A:175:ASN:OD1	1:A:177:THR:HG23	2.00	0.62
1:C:599:GLN:O	1:C:601:HIS:N	2.33	0.62
1:B:627:ILE:O	1:B:628:TYR:HD2	1.82	0.61
1:A:87:GLN:HB3	1:A:140:TYR:CE1	2.35	0.61
1:A:395:GLU:HB2	1:A:436:SER:OG	2.00	0.61
1:A:632:ASP:HA	1:A:677:TRP:O	2.00	0.61
1:B:330:LEU:O	1:B:334:ILE:HG13	2.00	0.61
1:B:606:GLN:HE22	4:B:753:NAP:H2A	1.66	0.61
1:B:416:TYR:C	1:B:418:SER:H	2.04	0.61
1:B:610:LYS:O	1:B:613:ARG:HB3	2.01	0.60
1:B:79:ASN:ND2	1:B:107:MET:HG2	2.17	0.60
1:B:262:GLU:HA	1:B:269:TYR:CE1	2.35	0.60
1:A:107:MET:HE2	1:A:233:VAL:HG21	1.82	0.60
1:C:461:SER:HB2	1:C:546:GLU:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:O	1:A:242:ILE:HG22	2.01	0.60
1:C:265:ARG:HB2	1:C:268:SER:HB3	1.84	0.60
1:A:529:ILE:HD13	1:A:616:LEU:HD22	1.84	0.60
1:A:247:LEU:HD11	1:A:346:MET:HB2	1.83	0.60
1:C:633:ALA:HB2	1:C:676:VAL:HB	1.83	0.60
1:B:328:SER:O	1:B:331:VAL:HG12	2.02	0.60
1:B:259:TYR:CD2	1:B:362:PRO:HB3	2.36	0.59
1:C:544:ILE:HD11	1:C:562:LEU:HD22	1.84	0.59
1:B:302:HIS:HE1	1:B:304:GLU:HG2	1.66	0.59
1:A:145:PRO:HB3	1:A:184:MET:SD	2.42	0.59
1:A:337:ILE:HB	1:A:438:ARG:NH1	2.17	0.59
1:B:246:GLU:HB3	1:B:351:LEU:CD2	2.33	0.59
1:B:269:TYR:HD2	1:B:283:LEU:HD21	1.67	0.59
1:C:634:ARG:O	1:C:638:LYS:HG2	2.02	0.59
1:B:269:TYR:HE2	1:B:510:PRO:CG	2.16	0.59
1:C:425:ARG:HB3	1:C:430:ILE:CD1	2.33	0.59
1:A:229:GLU:OE1	1:A:387:TYR:HE2	1.86	0.59
1:B:418:SER:HA	1:B:422:GLU:CB	2.27	0.59
1:B:488:GLY:HA2	3:B:752:FAD:O1A	2.03	0.59
1:C:301:MET:CE	1:C:495:ARG:HA	2.32	0.59
1:A:118:ASP:OD2	1:A:120:ALA:HB3	2.02	0.59
1:B:528:VAL:HG23	1:B:547:ARG:NH2	2.18	0.59
1:A:324:PRO:HG2	1:A:451:LEU:HD21	1.85	0.59
1:C:575:TYR:HB3	1:C:578:GLU:HB2	1.84	0.59
1:A:378:THR:HG21	1:A:489:VAL:CG2	2.33	0.58
1:C:321:ALA:HA	1:C:454:ARG:O	2.03	0.58
1:A:454:ARG:N	1:A:454:ARG:HD2	2.17	0.58
1:C:590:GLN:HG3	1:C:592:ASN:HD21	1.68	0.58
1:C:541:MET:HA	1:C:541:MET:CE	2.33	0.58
1:C:604:TYR:HB3	1:C:606:GLN:HE22	1.67	0.58
1:A:398:GLU:OE2	1:A:434:TYR:HA	2.03	0.58
1:B:104:ARG:HB2	1:B:104:ARG:HH11	1.69	0.58
1:B:423:ALA:O	1:B:480:ALA:HB1	2.03	0.58
1:A:145:PRO:HG2	1:A:153:TYR:CG	2.38	0.58
1:C:593:VAL:O	1:C:594:ALA:HB2	2.03	0.58
1:B:262:GLU:HA	1:B:269:TYR:CD1	2.39	0.58
1:C:561:LEU:H	1:C:561:LEU:CD1	2.16	0.58
1:A:104:ARG:HD2	1:A:242:ILE:CD1	2.34	0.58
1:A:606:GLN:NE2	4:A:753:NAP:H2A	2.09	0.58
1:A:544:ILE:HD13	1:A:588:LEU:HD21	1.84	0.58
1:C:630:CYS:SG	1:C:631:GLY:N	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:HB3	1:A:92:GLU:HA	1.85	0.58
1:B:478:TYR:HE2	1:B:480:ALA:HB2	1.69	0.58
1:C:347:SER:HA	1:C:363:CYS:SG	2.44	0.58
1:B:303:LEU:HD21	1:B:494:LEU:HB3	1.84	0.58
1:A:524:SER:HB2	1:A:557:VAL:HG22	1.85	0.58
1:A:87:GLN:HB2	1:A:146:THR:HG22	1.86	0.57
1:A:272:GLN:HE22	1:A:282:PHE:HA	1.69	0.57
1:A:282:PHE:HE1	1:A:284:ALA:HA	1.69	0.57
1:A:71:GLU:O	1:A:75:LYS:HG2	2.04	0.57
1:C:667:MET:HG2	1:C:672:TYR:CD2	2.39	0.57
1:A:327:ASP:HB3	1:A:330:LEU:CB	2.33	0.57
1:C:266:LEU:HD12	1:C:266:LEU:N	2.18	0.57
1:A:158:GLU:HB2	1:B:278:ALA:CB	2.34	0.57
1:A:298:ARG:HD2	1:A:567:ARG:NH2	2.19	0.57
1:A:252:ASP:OD1	1:A:253:MET:N	2.37	0.57
1:A:233:VAL:HG12	1:A:234:GLU:N	2.18	0.57
1:C:539:PRO:HG3	1:C:630:CYS:SG	2.45	0.57
1:C:259:TYR:CE2	1:C:266:LEU:HA	2.37	0.57
1:A:283:LEU:HD23	1:A:508:LEU:CD1	2.34	0.57
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.40	0.57
1:C:383:THR:O	1:C:406:ALA:HB1	2.05	0.57
1:A:173:LEU:HD23	1:A:212:LEU:HD21	1.85	0.57
1:C:608:LEU:CD2	1:C:611:ARG:HD3	2.35	0.57
1:C:474:VAL:O	1:C:491:THR:HG21	2.05	0.57
1:B:257:LYS:HA	1:B:266:LEU:HD21	1.87	0.57
1:B:216:PHE:CE2	1:B:220:ARG:HD2	2.40	0.57
1:C:515:LYS:HD3	1:C:519:ARG:NH2	2.20	0.57
1:A:119:LEU:HG	1:A:152:PHE:CD1	2.40	0.57
1:A:103:HIS:O	1:A:105:TYR:N	2.38	0.57
1:A:189:ASP:OD2	1:A:203:LEU:HB2	2.05	0.56
1:B:222:GLN:HA	1:B:225:PRO:HD2	1.87	0.56
1:C:307:ILE:HD13	1:C:469:VAL:CG2	2.34	0.56
1:B:482:SER:O	1:B:484:ARG:HD2	2.04	0.56
1:B:376:ASP:CB	1:B:449:PRO:HG2	2.34	0.56
1:A:158:GLU:HB2	1:B:278:ALA:HB2	1.87	0.56
1:B:248:VAL:HG21	1:B:349:ASN:HD21	1.70	0.56
1:A:190:GLN:O	1:A:194:GLN:HG3	2.04	0.56
1:B:331:VAL:HG13	1:B:332:ASN:HD22	1.71	0.56
1:A:462:SER:O	1:A:466:PRO:HB3	2.06	0.56
1:B:530:MET:HB3	1:B:540:PHE:CD1	2.40	0.56
1:B:388:GLU:O	1:B:391:GLN:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:GLU:HG2	1:C:398:GLU:HG3	1.87	0.56
1:B:568:ARG:HG2	1:B:568:ARG:HH11	1.71	0.56
1:A:359:HIS:CD2	1:A:363:CYS:HB2	2.40	0.56
1:B:263:MET:H	1:B:269:TYR:HE1	1.52	0.56
1:B:567:ARG:HG3	1:B:572:ASP:OD2	2.05	0.56
1:B:298:ARG:NH1	1:B:567:ARG:NH1	2.54	0.56
1:A:283:LEU:HD23	1:A:508:LEU:HD13	1.87	0.56
1:C:592:ASN:HB3	1:C:608:LEU:HD13	1.88	0.55
1:B:303:LEU:HD22	1:B:494:LEU:HD13	1.87	0.55
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.87	0.55
1:C:551:ARG:HG2	1:C:557:VAL:HG21	1.88	0.55
1:B:125:LEU:H	1:B:126:PRO:CD	2.19	0.55
1:B:482:SER:OG	1:B:484:ARG:HG2	2.06	0.55
1:B:624:GLY:HA2	1:B:671:ARG:NH2	2.22	0.55
1:C:428:LEU:O	1:C:432:GLN:HG3	2.07	0.55
1:C:301:MET:HE1	1:C:495:ARG:HA	1.87	0.55
1:A:318:ASP:O	1:A:458:ILE:HG13	2.06	0.55
1:B:321:ALA:HB2	1:B:455:TYR:CE1	2.42	0.55
1:B:272:GLN:CA	1:B:272:GLN:HE21	2.13	0.55
1:C:358:LYS:HB3	1:C:359:HIS:CE1	2.42	0.55
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.72	0.55
1:C:551:ARG:HG3	1:C:557:VAL:HG21	1.89	0.55
1:C:602:LYS:HB3	1:C:604:TYR:HE1	1.71	0.55
1:B:392:TYR:CE1	1:B:440:PRO:HD3	2.42	0.55
1:A:569:SER:HB2	1:A:576:ARG:HH21	1.72	0.55
1:C:354:GLU:OE2	1:C:354:GLU:HA	2.06	0.55
1:B:219:TRP:C	1:B:221:GLU:H	2.10	0.55
1:B:561:LEU:CD1	1:B:561:LEU:N	2.70	0.54
1:A:241:SER:O	1:A:242:ILE:HB	2.06	0.54
1:A:70:VAL:HG21	1:A:124:SER:HB2	1.88	0.54
1:B:561:LEU:HD12	1:B:561:LEU:N	2.21	0.54
1:B:266:LEU:O	1:B:267:LYS:HB2	2.07	0.54
1:A:262:GLU:HA	1:A:269:TYR:CE1	2.42	0.54
1:B:292:LEU:CD1	1:B:302:HIS:HB2	2.37	0.54
1:B:422:GLU:O	1:B:424:ARG:HG2	2.07	0.54
1:B:594:ALA:HB2	1:B:608:LEU:CD1	2.33	0.54
1:C:590:GLN:HG3	1:C:592:ASN:ND2	2.23	0.54
1:A:152:PHE:CZ	1:A:156:LEU:HD11	2.42	0.54
1:B:426:HIS:CD2	1:B:428:LEU:HB3	2.42	0.54
1:A:540:PHE:O	1:A:544:ILE:HG13	2.08	0.54
1:B:248:VAL:HG21	1:B:349:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLN:NE2	1:A:350:ASN:HD21	2.06	0.54
1:C:334:ILE:HG12	1:C:428:LEU:HD13	1.88	0.54
1:B:627:ILE:O	1:B:628:TYR:CD2	2.61	0.54
1:B:533:PRO:HG3	1:B:636:MET:HG3	1.90	0.53
1:B:356:ASN:O	1:B:358:LYS:N	2.41	0.53
1:B:251:GLU:O	1:B:252:ASP:HB3	2.06	0.53
1:A:79:ASN:HD21	1:A:107:MET:CG	2.21	0.53
1:B:155:TRP:O	1:B:159:THR:HB	2.08	0.53
1:A:378:THR:HG21	1:A:489:VAL:HG23	1.89	0.53
1:B:292:LEU:HD11	1:B:302:HIS:HB2	1.90	0.53
1:B:217:ILE:HG22	1:B:217:ILE:O	2.08	0.53
1:A:86:SER:OG	1:A:87:GLN:N	2.40	0.53
1:A:235:ALA:O	1:A:240:SER:HB3	2.08	0.53
1:B:295:GLY:HA3	1:B:571:GLU:OE1	2.09	0.53
1:A:324:PRO:HB2	1:A:489:VAL:HG12	1.91	0.53
1:C:664:LYS:HA	1:C:667:MET:HG3	1.91	0.53
1:A:78:ARG:HH11	1:A:110:MET:HB3	1.72	0.53
1:C:389:LEU:O	1:C:392:TYR:HB2	2.09	0.53
1:A:561:LEU:HD23	1:A:563:TYR:OH	2.08	0.53
1:A:140:TYR:O	1:A:144:ASP:HB2	2.09	0.52
1:B:613:ARG:HG3	1:B:614:GLU:N	2.25	0.52
1:B:530:MET:HB3	1:B:540:PHE:CE1	2.44	0.52
1:C:307:ILE:HD13	1:C:469:VAL:HG23	1.91	0.52
1:A:308:SER:O	1:A:309:ASP:HB2	2.10	0.52
1:C:478:TYR:CE1	1:C:486:ASN:HB2	2.44	0.52
1:B:125:LEU:C	1:B:127:GLU:H	2.11	0.52
1:B:255:VAL:HA	1:B:258:VAL:CG2	2.40	0.52
1:A:635:ASN:HB3	4:A:753:NAP:N6A	2.24	0.52
1:A:272:GLN:NE2	1:A:283:LEU:H	2.07	0.52
1:B:490:ALA:N	3:B:752:FAD:O2P	2.42	0.52
1:C:245:TYR:CD2	1:C:446:GLU:HG3	2.45	0.52
1:B:403:HIS:C	1:B:405:MET:H	2.13	0.52
1:C:440:PRO:HG2	1:C:443:HIS:CB	2.40	0.52
1:A:294:GLN:O	1:A:294:GLN:HG2	2.09	0.52
1:A:356:ASN:O	1:A:358:LYS:N	2.43	0.52
1:B:161:VAL:HG13	1:B:161:VAL:O	2.10	0.52
1:C:648:VAL:HG11	1:C:662:TYR:HB3	1.91	0.52
1:B:217:ILE:O	1:B:221:GLU:HB2	2.10	0.52
1:C:371:LEU:HD23	1:C:375:LEU:CD1	2.36	0.52
1:A:105:TYR:HB3	1:A:233:VAL:HG11	1.90	0.52
1:A:133:VAL:HG12	1:A:167:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:CB	1:A:92:GLU:HA	2.40	0.51
1:A:452:GLN:CA	1:A:452:GLN:HE21	2.12	0.51
1:A:466:PRO:HG2	1:A:467:ASN:OD1	2.10	0.51
1:B:478:TYR:CE2	1:B:486:ASN:HB2	2.45	0.51
1:C:606:GLN:HG3	1:C:639:ASP:HB3	1.92	0.51
1:A:656:HIS:O	1:A:659:ALA:N	2.43	0.51
1:B:411:GLU:CG	1:B:412:GLY:H	2.21	0.51
1:A:371:LEU:CD2	1:A:375:LEU:HD12	2.40	0.51
1:A:254:ASP:HB2	1:A:257:LYS:HD2	1.91	0.51
1:A:214:GLU:O	1:A:215:ASP:C	2.47	0.51
1:A:337:ILE:HB	1:A:438:ARG:HH12	1.76	0.51
1:A:337:ILE:HD11	1:A:431:LEU:HD13	1.90	0.51
1:B:416:TYR:C	1:B:418:SER:N	2.64	0.51
1:A:525:THR:O	1:A:558:GLY:HA3	2.10	0.51
1:C:417:LEU:O	1:C:421:VAL:HB	2.10	0.51
1:B:351:LEU:O	1:B:352:ASP:HB2	2.10	0.51
1:A:464:VAL:HG12	1:A:465:HIS:N	2.17	0.51
3:B:752:FAD:O1P	3:B:752:FAD:H3'	2.11	0.51
1:B:527:PRO:HB2	1:B:625:ALA:CB	2.40	0.51
1:C:630:CYS:HA	1:C:675:ASP:O	2.10	0.51
1:A:245:TYR:HD2	1:A:446:GLU:HG3	1.74	0.51
1:A:300:LEU:CD2	1:A:574:LEU:HD21	2.29	0.51
1:A:96:ASN:O	1:A:98:LEU:N	2.43	0.51
1:C:334:ILE:HD12	1:C:377:ILE:HD12	1.91	0.51
1:C:574:LEU:O	1:C:575:TYR:C	2.49	0.51
1:C:389:LEU:HD22	1:C:439:PRO:HG3	1.93	0.51
1:B:250:HIS:CE1	1:B:347:SER:HB2	2.46	0.51
1:B:480:ALA:C	1:B:482:SER:H	2.15	0.51
1:B:474:VAL:O	1:B:491:THR:HG21	2.11	0.51
1:C:314:TYR:OH	1:C:465:HIS:O	2.24	0.51
1:A:464:VAL:O	1:A:466:PRO:HD3	2.11	0.51
1:C:515:LYS:HD3	1:C:519:ARG:HH21	1.75	0.51
1:C:318:ASP:OD1	1:C:519:ARG:NH2	2.44	0.51
1:C:521:PRO:HD3	1:C:628:TYR:OH	2.11	0.51
1:A:84:TYR:CE2	1:A:113:ASP:HB2	2.46	0.51
1:C:561:LEU:N	1:C:561:LEU:CD1	2.73	0.51
1:C:243:ARG:O	1:C:245:TYR:N	2.43	0.51
1:A:541:MET:HG3	1:A:575:TYR:CE2	2.46	0.51
1:C:506:ARG:HG3	1:C:506:ARG:HH11	1.76	0.51
1:A:394:SER:N	1:A:436:SER:O	2.44	0.50
1:B:308:SER:O	1:B:309:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HG12	1:A:83:PHE:N	2.26	0.50
1:B:269:TYR:CE2	1:B:283:LEU:HD11	2.46	0.50
1:B:606:GLN:HE22	4:B:753:NAP:C2A	2.23	0.50
1:B:331:VAL:HG13	1:B:332:ASN:N	2.26	0.50
1:C:301:MET:HG2	1:C:473:ALA:O	2.10	0.50
1:A:544:ILE:O	1:A:544:ILE:HG22	2.11	0.50
1:B:629:VAL:HG12	1:B:630:CYS:N	2.25	0.50
1:B:129:ASP:O	1:B:130:LYS:HB2	2.11	0.50
1:C:493:TRP:CH2	1:C:509:VAL:HG13	2.46	0.50
1:A:488:GLY:O	1:A:492:SER:HB2	2.12	0.50
1:B:491:THR:HG23	3:B:752:FAD:O4'	2.11	0.50
1:A:120:ALA:HA	1:A:155:TRP:CZ2	2.46	0.50
1:C:419:TRP:O	1:C:425:ARG:HD2	2.12	0.50
1:B:224:TRP:HB2	1:B:225:PRO:HD3	1.94	0.50
1:A:132:LEU:HD12	1:A:133:VAL:H	1.77	0.50
1:B:418:SER:O	1:B:422:GLU:HB3	2.11	0.50
1:B:321:ALA:HB2	1:B:455:TYR:CD1	2.47	0.50
1:B:278:ALA:HB2	1:B:512:PHE:CE2	2.47	0.50
1:B:292:LEU:HG	1:B:302:HIS:HB2	1.94	0.50
1:A:258:VAL:HG21	1:A:345:ILE:HD13	1.92	0.50
1:A:94:PHE:O	1:A:95:ALA:C	2.50	0.50
1:A:150:GLN:O	1:A:153:TYR:HB3	2.12	0.50
1:B:452:GLN:NE2	1:B:452:GLN:HA	2.23	0.50
1:A:538:ALA:HB3	1:A:539:PRO:CD	2.42	0.50
1:B:285:ALA:O	1:B:287:THR:HG23	2.12	0.50
1:B:586:GLY:C	1:B:588:LEU:H	2.13	0.50
1:A:266:LEU:O	1:A:267:LYS:CB	2.59	0.50
1:A:245:TYR:CD2	1:A:446:GLU:HG3	2.46	0.50
1:A:153:TYR:CE2	1:A:157:GLN:NE2	2.80	0.50
3:C:752:FAD:H3'	3:C:752:FAD:O1P	2.11	0.50
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.93	0.50
1:C:596:SER:O	1:C:597:ARG:CG	2.56	0.50
1:B:644:PHE:O	1:B:648:VAL:HG23	2.12	0.50
1:B:442:ASP:C	1:B:444:LEU:H	2.14	0.50
1:A:322:VAL:HG12	1:A:511:MET:HB3	1.93	0.50
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.76	0.49
1:A:518:PHE:CE2	1:A:675:ASP:HB2	2.47	0.49
1:A:80:ILE:HG23	1:A:109:GLY:CA	2.41	0.49
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.93	0.49
1:B:452:GLN:HE21	1:B:452:GLN:CA	2.17	0.49
1:B:259:TYR:CE2	1:B:362:PRO:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:VAL:HG21	1:A:497:LYS:HB3	1.94	0.49
1:A:67:SER:HB2	1:B:356:ASN:HD21	1.76	0.49
1:B:104:ARG:HB2	1:B:104:ARG:NH1	2.27	0.49
1:A:455:TYR:HE1	1:A:514:ARG:CD	2.25	0.49
1:C:409:SER:HB3	1:C:413:LYS:HD2	1.94	0.49
1:A:69:PHE:HZ	1:A:122:LEU:HD23	1.77	0.49
1:A:642:ASN:HB2	1:B:656:HIS:CD2	2.48	0.49
1:C:463:LYS:HG3	1:C:546:GLU:HG3	1.95	0.49
1:A:617:TRP:CD1	1:A:651:PHE:HB3	2.47	0.49
1:B:262:GLU:HG2	1:B:267:LYS:H	1.78	0.49
1:A:637:ALA:HB2	1:A:676:VAL:HG11	1.93	0.49
1:A:101:ASP:O	1:A:103:HIS:N	2.45	0.49
1:C:659:ALA:O	1:C:663:VAL:HG23	2.13	0.49
1:B:606:GLN:NE2	1:B:606:GLN:H	2.09	0.49
1:C:409:SER:CB	1:C:413:LYS:HD2	2.43	0.49
1:A:271:ASN:OD1	1:A:271:ASN:O	2.29	0.49
1:C:593:VAL:HG12	1:C:594:ALA:N	2.19	0.49
1:A:272:GLN:NE2	1:A:282:PHE:HA	2.27	0.49
1:C:334:ILE:CG1	1:C:428:LEU:HD13	2.42	0.49
1:C:301:MET:HE2	1:C:303:LEU:HD11	1.94	0.49
1:C:241:SER:O	1:C:242:ILE:CB	2.61	0.49
1:B:549:TRP:CE2	1:B:553:GLN:HG3	2.48	0.49
1:A:411:GLU:HA	1:A:414:GLU:HB2	1.94	0.49
1:C:581:ARG:O	1:C:585:ASP:HB2	2.13	0.49
1:C:372:THR:HG22	1:C:373:TYR:CD2	2.47	0.49
1:B:404:LYS:O	1:B:412:GLY:HA3	2.12	0.48
1:A:427:ILE:HG23	1:A:428:LEU:N	2.28	0.48
1:A:474:VAL:HG12	1:A:535:THR:HG21	1.95	0.48
1:C:665:LYS:O	1:C:669:LYS:HB2	2.12	0.48
1:A:612:ASP:O	1:A:613:ARG:C	2.51	0.48
1:A:539:PRO:HG3	1:A:630:CYS:SG	2.53	0.48
1:C:261:GLY:HA2	1:C:374:TYR:CZ	2.47	0.48
1:A:341:ASP:O	1:A:344:VAL:HG23	2.12	0.48
1:C:424:ARG:HG3	1:C:478:TYR:HE2	1.79	0.48
1:B:665:LYS:O	1:B:669:LYS:HG2	2.14	0.48
1:C:648:VAL:HG13	1:C:662:TYR:CD1	2.47	0.48
1:B:361:PHE:HB2	1:B:362:PRO:HD2	1.95	0.48
1:C:318:ASP:OD1	1:C:515:LYS:HA	2.14	0.48
1:C:402:LEU:HD21	1:C:434:TYR:CE2	2.48	0.48
1:B:331:VAL:HG23	1:B:371:LEU:HB3	1.95	0.48
1:B:599:GLN:NE2	1:B:603:VAL:HG23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:THR:O	1:B:369:THR:HG23	2.14	0.48
1:B:454:ARG:HG2	3:B:752:FAD:O1P	2.14	0.48
1:C:265:ARG:NH1	1:C:265:ARG:HG3	2.27	0.48
1:C:577:GLU:O	1:C:578:GLU:C	2.51	0.48
1:C:493:TRP:HH2	1:C:509:VAL:HG13	1.79	0.48
1:C:269:TYR:CD2	1:C:283:LEU:HD21	2.48	0.48
1:B:537:ILE:HB	1:B:564:TYR:CD1	2.48	0.48
1:B:282:PHE:HE1	1:B:307:ILE:HA	1.78	0.48
1:C:391:GLN:C	1:C:391:GLN:HE21	2.17	0.48
1:A:656:HIS:O	1:A:657:THR:C	2.50	0.48
1:C:253:MET:HG2	1:C:258:VAL:HG22	1.96	0.48
1:C:409:SER:HA	1:C:413:LYS:HB2	1.95	0.48
1:A:169:ALA:HB2	1:A:200:ILE:HG22	1.95	0.48
1:A:187:TYR:CE1	1:A:191:ARG:HD3	2.48	0.48
1:C:568:ARG:NH1	1:C:598:GLU:HA	2.29	0.48
1:A:307:ILE:HG13	1:A:467:ASN:HA	1.95	0.48
1:A:435:PRO:C	1:A:437:LEU:H	2.17	0.48
1:B:255:VAL:HA	1:B:258:VAL:HG21	1.96	0.48
1:A:253:MET:CE	1:A:253:MET:HA	2.44	0.47
1:A:262:GLU:HG2	1:A:267:LYS:H	1.78	0.47
1:C:626:HIS:HB3	1:C:628:TYR:CE1	2.48	0.47
1:C:440:PRO:HG2	1:C:443:HIS:HB2	1.95	0.47
1:A:358:LYS:HB3	1:A:359:HIS:CE1	2.49	0.47
1:A:569:SER:HA	1:A:573:TYR:HB2	1.96	0.47
1:C:370:ALA:HA	1:C:374:TYR:CD2	2.49	0.47
1:B:96:ASN:C	1:B:98:LEU:H	2.18	0.47
1:A:543:PHE:C	1:A:545:GLN:H	2.17	0.47
1:B:352:ASP:C	1:B:354:GLU:H	2.18	0.47
1:A:76:THR:OG1	1:A:78:ARG:HG2	2.15	0.47
1:A:244:GLN:HE21	1:A:350:ASN:ND2	2.13	0.47
1:A:227:VAL:HG12	1:A:227:VAL:O	2.14	0.47
1:C:456:TYR:HB3	1:C:471:ILE:HG23	1.96	0.47
1:B:352:ASP:O	1:B:354:GLU:N	2.48	0.47
1:B:533:PRO:O	1:B:534:GLY:C	2.53	0.47
1:A:627:ILE:N	1:A:671:ARG:O	2.39	0.47
1:C:253:MET:HE3	1:C:254:ASP:H	1.76	0.47
1:B:276:PHE:CD1	1:B:276:PHE:N	2.82	0.47
1:A:577:GLU:H	1:A:577:GLU:CD	2.17	0.47
1:B:406:ALA:O	1:B:407:SER:O	2.33	0.47
1:B:416:TYR:O	1:B:418:SER:N	2.47	0.47
1:A:455:TYR:CE1	1:A:514:ARG:NH1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:PHE:CE2	1:B:675:ASP:HB2	2.49	0.47
1:C:599:GLN:CG	1:C:601:HIS:CE1	2.98	0.47
1:B:442:ASP:C	1:B:444:LEU:N	2.66	0.47
1:C:327:ASP:OD1	1:C:329:ALA:HB3	2.14	0.47
1:C:294:GLN:NE2	1:C:570:ASP:HB2	2.29	0.47
1:B:351:LEU:N	1:B:351:LEU:HD23	2.30	0.47
1:C:310:SER:C	1:C:312:ILE:H	2.18	0.47
1:A:260:THR:HA	1:A:369:THR:HG21	1.97	0.47
1:C:494:LEU:HD23	1:C:494:LEU:C	2.35	0.47
1:A:332:ASN:HD22	1:A:332:ASN:C	2.13	0.47
1:B:563:TYR:CD1	1:B:592:ASN:HB2	2.50	0.47
1:A:84:TYR:HB3	1:A:95:ALA:HB2	1.97	0.47
1:A:595:PHE:HB3	1:A:598:GLU:HG2	1.97	0.47
1:A:243:ARG:NH1	1:A:442:ASP:OD2	2.41	0.47
1:B:222:GLN:CA	1:B:225:PRO:HD2	2.46	0.47
1:A:390:ALA:HB1	1:A:403:HIS:CE1	2.50	0.47
1:B:533:PRO:HD2	1:B:636:MET:CE	2.45	0.46
1:B:96:ASN:HB3	1:B:100:LYS:HE3	1.97	0.46
1:C:253:MET:HE2	1:C:254:ASP:N	2.28	0.46
1:C:307:ILE:O	1:C:307:ILE:HG13	2.15	0.46
1:C:235:ALA:HB3	1:C:391:GLN:HG2	1.97	0.46
1:A:549:TRP:HE3	1:A:550:LEU:HD23	1.80	0.46
1:A:272:GLN:HE22	1:A:282:PHE:CA	2.28	0.46
1:A:348:LEU:CD1	1:A:360:PRO:HG3	2.43	0.46
1:B:255:VAL:HG12	1:B:255:VAL:O	2.15	0.46
1:B:594:ALA:CB	1:B:608:LEU:HD11	2.32	0.46
1:C:342:LEU:N	1:C:342:LEU:HD12	2.28	0.46
1:A:119:LEU:C	1:A:121:ASP:H	2.19	0.46
1:C:568:ARG:HG2	1:C:568:ARG:HH11	1.80	0.46
1:C:648:VAL:HG21	1:C:663:VAL:HG22	1.98	0.46
1:A:101:ASP:C	1:A:103:HIS:N	2.69	0.46
1:A:458:ILE:HG22	1:A:460:SER:H	1.80	0.46
1:B:668:THR:O	1:B:669:LYS:HD3	2.16	0.46
1:A:557:VAL:HG12	1:A:558:GLY:O	2.16	0.46
1:A:116:GLU:O	1:A:117:TYR:C	2.54	0.46
1:A:187:TYR:C	1:A:189:ASP:N	2.69	0.46
1:A:211:ASN:ND2	1:A:214:GLU:HG2	2.31	0.46
1:A:155:TRP:HZ2	1:A:161:VAL:HG11	1.81	0.46
1:A:645:TYR:CE2	1:A:660:VAL:HA	2.50	0.46
1:C:321:ALA:HB2	1:C:455:TYR:CD1	2.50	0.46
1:B:288:ALA:O	1:B:303:LEU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:VAL:HG12	1:C:514:ARG:N	2.30	0.46
1:A:475:ALA:HA	1:A:491:THR:HB	1.97	0.46
1:C:390:ALA:C	1:C:392:TYR:H	2.19	0.46
1:C:418:SER:O	1:C:422:GLU:HB2	2.15	0.46
1:A:145:PRO:HG2	1:A:153:TYR:CD1	2.51	0.46
1:A:157:GLN:HG2	1:A:187:TYR:OH	2.16	0.46
1:C:310:SER:HB2	1:C:312:ILE:HG13	1.99	0.45
1:A:308:SER:O	1:A:309:ASP:CB	2.64	0.45
1:C:530:MET:O	1:C:563:TYR:N	2.46	0.45
1:B:422:GLU:O	1:B:424:ARG:N	2.49	0.45
1:A:455:TYR:CD2	1:A:455:TYR:N	2.84	0.45
1:A:262:GLU:HA	1:A:269:TYR:CD1	2.51	0.45
1:C:242:ILE:O	1:C:243:ARG:HG2	2.15	0.45
1:A:170:VAL:HG12	1:A:171:PHE:N	2.31	0.45
1:B:300:LEU:HD12	1:B:300:LEU:N	2.31	0.45
1:B:567:ARG:HD2	1:B:597:ARG:CD	2.32	0.45
1:B:254:ASP:HB3	1:B:257:LYS:HD3	1.98	0.45
1:B:302:HIS:CE1	1:B:304:GLU:HG2	2.50	0.45
1:A:567:ARG:HG3	1:A:572:ASP:OD2	2.16	0.45
1:A:337:ILE:HD12	1:A:438:ARG:HH12	1.82	0.45
1:A:244:GLN:NE2	1:A:350:ASN:ND2	2.65	0.45
1:B:244:GLN:HG3	1:B:244:GLN:O	2.17	0.45
1:C:266:LEU:CD1	1:C:266:LEU:H	2.25	0.45
1:B:627:ILE:HG21	1:B:644:PHE:CZ	2.51	0.45
1:A:358:LYS:HB3	1:A:359:HIS:ND1	2.32	0.45
1:C:245:TYR:HD2	1:C:446:GLU:HG3	1.81	0.45
1:C:283:LEU:HD23	1:C:508:LEU:HD13	1.98	0.45
1:B:573:TYR:HE1	1:B:595:PHE:HZ	1.64	0.45
1:C:299:HIS:CE1	1:C:495:ARG:HH21	2.34	0.45
1:C:405:MET:HG2	1:C:416:TYR:HB2	1.99	0.45
1:A:331:VAL:O	1:A:334:ILE:HB	2.17	0.45
1:A:446:GLU:HG2	1:A:446:GLU:O	2.15	0.45
1:A:509:VAL:O	1:A:511:MET:HG3	2.16	0.45
1:A:455:TYR:HD2	1:A:455:TYR:N	2.15	0.45
1:C:590:GLN:NE2	1:C:592:ASN:HD21	2.13	0.45
1:B:220:ARG:HG2	1:B:220:ARG:O	2.16	0.45
1:B:393:ALA:HA	1:B:436:SER:O	2.16	0.45
1:B:567:ARG:HE	1:B:597:ARG:NH1	2.15	0.45
1:A:107:MET:HE1	1:A:233:VAL:HG21	1.96	0.45
1:A:390:ALA:HB1	1:A:403:HIS:ND1	2.32	0.45
1:C:554:GLY:O	1:C:555:LYS:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:HIS:O	1:C:407:SER:HB3	2.17	0.44
1:B:459:ALA:O	1:B:460:SER:HB3	2.15	0.44
1:B:93:GLU:O	1:B:97:ARG:HG3	2.18	0.44
1:B:632:ASP:O	1:B:636:MET:HB3	2.17	0.44
1:C:316:SER:OG	1:C:461:SER:HA	2.16	0.44
1:C:358:LYS:HB3	1:C:359:HIS:ND1	2.32	0.44
1:B:156:LEU:HD23	1:B:159:THR:CG2	2.47	0.44
1:C:301:MET:HE3	1:C:495:ARG:HA	1.99	0.44
1:A:200:ILE:HA	1:A:200:ILE:HD12	1.73	0.44
1:A:385:VAL:HG13	1:A:447:LEU:HB3	1.99	0.44
1:A:272:GLN:NE2	1:A:283:LEU:N	2.60	0.44
1:C:261:GLY:HA2	1:C:374:TYR:OH	2.16	0.44
1:A:79:ASN:HD21	1:A:107:MET:HG2	1.82	0.44
1:A:175:ASN:OD1	1:A:209:ASP:HB2	2.17	0.44
1:A:643:THR:O	1:A:647:ILE:HG13	2.18	0.44
1:C:259:TYR:HE2	1:C:266:LEU:CA	2.26	0.44
1:B:159:THR:O	1:B:159:THR:HG23	2.18	0.44
1:B:403:HIS:O	1:B:405:MET:N	2.51	0.44
1:C:262:GLU:HA	1:C:269:TYR:CE1	2.51	0.44
1:B:119:LEU:N	1:B:119:LEU:HD22	2.33	0.44
1:B:81:ILE:O	1:B:81:ILE:HG23	2.18	0.44
1:C:627:ILE:HD13	1:C:644:PHE:CE1	2.52	0.44
1:A:119:LEU:C	1:A:121:ASP:N	2.70	0.44
1:A:265:ARG:HB2	1:A:268:SER:HB3	1.97	0.44
1:A:282:PHE:CD2	1:A:310:SER:HB3	2.53	0.44
1:A:664:LYS:O	1:A:667:MET:HB2	2.17	0.44
1:B:494:LEU:O	1:B:495:ARG:C	2.55	0.44
1:A:90:THR:O	1:A:93:GLU:HB3	2.18	0.44
1:A:208:ASP:O	1:A:209:ASP:C	2.56	0.44
1:A:444:LEU:C	1:A:446:GLU:H	2.21	0.44
1:A:610:LYS:O	1:A:613:ARG:HG2	2.17	0.44
1:A:313:ARG:HH11	1:A:313:ARG:HG3	1.83	0.44
1:B:591:LEU:HG	1:B:591:LEU:O	2.18	0.44
1:C:411:GLU:CG	1:C:412:GLY:N	2.59	0.44
1:B:402:LEU:HG	1:B:434:TYR:CE2	2.53	0.44
1:C:633:ALA:O	1:C:635:ASN:N	2.50	0.44
1:B:331:VAL:CG1	1:B:332:ASN:N	2.81	0.44
1:B:302:HIS:C	1:B:302:HIS:ND1	2.70	0.44
1:B:573:TYR:OH	1:B:593:VAL:HG21	2.18	0.44
1:A:199:ARG:NH1	1:A:199:ARG:HB2	2.32	0.44
1:B:480:ALA:C	1:B:482:SER:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:TYR:CE2	1:B:480:ALA:HB2	2.51	0.43
3:A:752:FAD:H3'	3:A:752:FAD:O1P	2.17	0.43
1:B:327:ASP:HB3	1:B:330:LEU:CB	2.44	0.43
1:C:649:ALA:HB1	1:C:654:MET:O	2.18	0.43
1:B:488:GLY:O	1:B:492:SER:HB3	2.18	0.43
1:A:337:ILE:HD12	1:A:431:LEU:HB3	1.99	0.43
1:B:299:HIS:CD2	1:B:495:ARG:HE	2.36	0.43
1:C:439:PRO:HB2	1:C:440:PRO:HD2	2.00	0.43
1:C:632:ASP:HA	1:C:677:TRP:O	2.17	0.43
1:C:314:TYR:HB3	1:C:513:VAL:HG21	1.99	0.43
1:B:222:GLN:C	1:B:225:PRO:HD2	2.38	0.43
1:C:413:LYS:O	1:C:417:LEU:HB2	2.17	0.43
1:A:611:ARG:HG2	1:A:612:ASP:OD2	2.17	0.43
1:A:559:GLU:OE2	1:A:619:LEU:HD21	2.18	0.43
1:A:72:LYS:HG2	1:A:72:LYS:O	2.19	0.43
1:B:73:MET:O	1:B:73:MET:HG2	2.17	0.43
1:B:617:TRP:O	1:B:617:TRP:CG	2.72	0.43
1:A:454:ARG:HG2	1:A:490:ALA:HB2	1.99	0.43
1:B:263:MET:N	1:B:269:TYR:HE1	2.16	0.43
1:B:664:LYS:HB2	1:B:664:LYS:HE3	1.81	0.43
1:B:125:LEU:N	1:B:126:PRO:CD	2.80	0.43
1:B:506:ARG:HD3	1:B:506:ARG:N	2.33	0.43
1:A:453:ALA:C	1:A:454:ARG:HD2	2.39	0.43
1:A:464:VAL:O	1:A:466:PRO:N	2.51	0.43
1:A:370:ALA:O	1:A:375:LEU:N	2.47	0.43
1:A:664:LYS:HE3	1:A:667:MET:HE3	2.00	0.43
1:A:590:GLN:NE2	1:A:592:ASN:HD21	2.17	0.43
1:A:549:TRP:CE3	1:A:550:LEU:HD23	2.53	0.43
1:B:283:LEU:CD1	1:B:283:LEU:N	2.82	0.43
1:C:390:ALA:HB1	1:C:403:HIS:CE1	2.53	0.43
1:C:262:GLU:O	1:C:374:TYR:HE1	2.02	0.43
1:C:260:THR:HG22	1:C:260:THR:O	2.18	0.43
1:C:425:ARG:HB3	1:C:430:ILE:HD11	1.99	0.43
1:A:261:GLY:HA2	1:A:373:TYR:CD2	2.53	0.43
1:C:527:PRO:HB2	1:C:625:ALA:HB2	2.00	0.43
1:B:396:PRO:O	1:B:400:GLU:HB2	2.18	0.43
1:C:484:ARG:CD	1:C:484:ARG:H	2.22	0.43
1:B:79:ASN:ND2	1:B:80:ILE:H	2.16	0.43
1:B:330:LEU:HD23	1:B:334:ILE:HD11	2.00	0.43
1:A:93:GLU:O	1:A:93:GLU:OE1	2.37	0.43
1:B:247:LEU:HD12	1:B:248:VAL:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HA	1:A:125:LEU:HD12	1.77	0.43
1:A:404:LYS:O	1:A:407:SER:N	2.47	0.43
1:C:310:SER:O	1:C:311:LYS:HB2	2.19	0.43
1:C:538:ALA:N	1:C:539:PRO:HD2	2.34	0.43
1:A:575:TYR:HA	1:A:578:GLU:OE1	2.18	0.43
1:B:425:ARG:HG3	1:B:425:ARG:HH11	1.83	0.43
1:C:638:LYS:O	1:C:641:GLN:N	2.52	0.43
1:B:160:ASP:O	1:B:162:ASP:N	2.52	0.43
1:B:551:ARG:HD3	1:B:557:VAL:HB	2.00	0.43
1:B:381:PRO:HG2	1:B:430:ILE:HD12	2.01	0.43
1:B:346:MET:SD	1:B:346:MET:C	2.97	0.43
1:A:454:ARG:HH22	1:A:489:VAL:CB	2.19	0.43
1:A:393:ALA:HA	1:A:437:LEU:HA	2.01	0.43
1:C:649:ALA:HB2	1:C:659:ALA:CB	2.46	0.43
1:A:569:SER:HB3	1:A:595:PHE:CZ	2.54	0.43
1:B:292:LEU:CG	1:B:302:HIS:HB2	2.48	0.43
1:A:271:ASN:O	1:A:271:ASN:CG	2.57	0.43
1:B:537:ILE:HG13	1:B:537:ILE:O	2.19	0.43
1:C:566:CYS:HB2	1:C:572:ASP:OD1	2.19	0.43
1:B:440:PRO:O	1:B:442:ASP:N	2.51	0.42
1:C:610:LYS:O	1:C:613:ARG:HD3	2.19	0.42
1:A:511:MET:SD	1:A:511:MET:C	2.98	0.42
1:A:383:THR:HB	1:A:406:ALA:HA	2.01	0.42
1:B:588:LEU:HD22	1:B:590:GLN:O	2.20	0.42
1:C:667:MET:CA	1:C:672:TYR:HB3	2.42	0.42
1:B:283:LEU:HD12	1:B:283:LEU:N	2.32	0.42
1:B:434:TYR:HB3	1:B:437:LEU:HB2	2.00	0.42
1:A:67:SER:HB2	1:B:356:ASN:ND2	2.35	0.42
1:A:438:ARG:NE	1:C:311:LYS:HZ3	2.16	0.42
1:C:314:TYR:CG	1:C:314:TYR:O	2.72	0.42
1:C:519:ARG:O	1:C:628:TYR:CE2	2.72	0.42
1:B:156:LEU:HA	1:B:159:THR:HG22	2.01	0.42
1:C:627:ILE:O	1:C:672:TYR:HA	2.20	0.42
1:C:368:ARG:O	1:C:372:THR:HB	2.19	0.42
1:B:333:GLN:O	1:B:337:ILE:HG22	2.20	0.42
1:B:672:TYR:CD2	1:B:672:TYR:C	2.92	0.42
1:C:452:GLN:H	1:C:452:GLN:CD	2.22	0.42
1:C:608:LEU:HD22	1:C:611:ARG:CZ	2.49	0.42
1:B:317:GLY:HA3	1:B:518:PHE:O	2.20	0.42
1:A:476:VAL:CG2	3:A:752:FAD:H5'2	2.49	0.42
1:C:593:VAL:O	1:C:608:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ARG:HD2	1:A:597:ARG:CZ	2.50	0.42
1:B:422:GLU:HB3	1:B:423:ALA:H	1.75	0.42
1:B:475:ALA:HA	1:B:491:THR:HB	2.01	0.42
1:A:168:PHE:CE1	1:A:199:ARG:HA	2.55	0.42
1:A:187:TYR:C	1:A:189:ASP:H	2.23	0.42
1:A:203:LEU:HD21	1:A:205:LEU:HD21	2.01	0.42
1:B:488:GLY:CA	3:B:752:FAD:O1A	2.68	0.42
1:A:350:ASN:C	1:A:352:ASP:H	2.22	0.42
1:B:443:HIS:O	1:B:447:LEU:HG	2.20	0.42
1:C:385:VAL:HG12	1:C:385:VAL:O	2.19	0.42
1:A:220:ARG:HB3	1:A:220:ARG:HH11	1.84	0.42
1:A:393:ALA:CA	1:A:436:SER:O	2.62	0.42
1:C:298:ARG:HH21	1:C:300:LEU:HD11	1.84	0.42
1:C:599:GLN:HG3	1:C:601:HIS:CE1	2.55	0.42
1:B:129:ASP:O	1:B:130:LYS:CB	2.67	0.42
1:B:649:ALA:HA	1:B:654:MET:HG3	2.00	0.42
1:A:464:VAL:O	1:A:465:HIS:C	2.58	0.42
1:C:252:ASP:OD1	1:C:253:MET:N	2.37	0.42
1:A:333:GLN:HB3	1:A:428:LEU:HD21	2.01	0.42
1:C:513:VAL:CG1	1:C:514:ARG:N	2.82	0.42
1:A:401:HIS:O	1:A:404:LYS:N	2.53	0.42
1:A:320:VAL:O	1:A:320:VAL:HG13	2.20	0.42
1:C:408:SER:O	1:C:409:SER:CB	2.68	0.41
1:B:539:PRO:HG3	1:B:630:CYS:SG	2.60	0.41
1:A:125:LEU:N	1:A:126:PRO:CD	2.83	0.41
1:A:335:GLY:O	1:A:339:GLY:N	2.52	0.41
1:A:392:TYR:O	1:A:437:LEU:HA	2.20	0.41
1:A:548:ALA:O	1:A:552:GLU:HG3	2.20	0.41
1:A:254:ASP:C	1:A:256:ALA:N	2.73	0.41
1:A:155:TRP:CH2	1:A:161:VAL:HG11	2.56	0.41
1:A:490:ALA:HB3	3:A:752:FAD:O1P	2.20	0.41
1:A:455:TYR:CE1	1:A:514:ARG:CD	3.00	0.41
1:A:573:TYR:CD2	1:A:573:TYR:C	2.93	0.41
1:B:276:PHE:CE1	1:B:310:SER:HB2	2.55	0.41
1:A:645:TYR:HE2	1:A:663:VAL:HB	1.85	0.41
1:B:350:ASN:HD22	1:B:351:LEU:H	1.66	0.41
1:A:454:ARG:HG2	1:A:490:ALA:CB	2.51	0.41
1:A:464:VAL:O	1:A:466:PRO:CD	2.68	0.41
1:A:664:LYS:CE	1:A:664:LYS:HA	2.44	0.41
1:C:423:ALA:O	1:C:424:ARG:HB2	2.20	0.41
1:B:626:HIS:HB3	1:B:628:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:CG2	1:B:217:ILE:O	2.68	0.41
1:B:654:MET:SD	1:B:659:ALA:HA	2.60	0.41
1:A:666:LEU:HA	1:A:666:LEU:HD23	1.94	0.41
1:A:105:TYR:C	1:A:233:VAL:HG11	2.40	0.41
1:C:551:ARG:HG2	1:C:557:VAL:CG2	2.51	0.41
1:B:569:SER:HA	1:B:595:PHE:CE1	2.55	0.41
1:A:115:GLU:HB2	1:A:148:ASN:HB2	2.02	0.41
1:C:645:TYR:O	1:C:659:ALA:HB1	2.19	0.41
1:B:564:TYR:CG	1:B:565:GLY:N	2.88	0.41
1:C:329:ALA:O	1:C:333:GLN:HG3	2.20	0.41
1:A:531:VAL:O	1:A:629:VAL:HA	2.20	0.41
1:B:563:TYR:CE1	1:B:592:ASN:ND2	2.89	0.41
1:A:567:ARG:HD2	1:A:597:ARG:NE	2.35	0.41
1:B:441:ILE:HG23	1:B:442:ASP:N	2.36	0.41
1:B:672:TYR:HD2	1:B:672:TYR:C	2.23	0.41
1:C:322:VAL:HG12	1:C:511:MET:HB3	2.02	0.41
1:B:350:ASN:ND2	1:B:351:LEU:N	2.64	0.41
1:B:464:VAL:HG12	1:B:465:HIS:CE1	2.55	0.41
1:B:94:PHE:HB3	1:B:216:PHE:CZ	2.55	0.41
1:B:528:VAL:HG12	1:B:530:MET:CG	2.51	0.41
1:C:322:VAL:O	1:C:453:ALA:HB1	2.21	0.41
1:A:82:VAL:HG11	1:A:95:ALA:CA	2.34	0.41
1:C:564:TYR:O	1:C:593:VAL:HA	2.21	0.41
1:B:80:ILE:HG23	1:B:109:GLY:HA3	2.02	0.41
1:A:569:SER:HB3	1:A:595:PHE:HE1	1.83	0.41
1:A:254:ASP:O	1:A:256:ALA:N	2.54	0.41
1:B:521:PRO:O	1:B:522:PHE:CB	2.66	0.41
1:B:104:ARG:NH1	1:B:104:ARG:CB	2.83	0.41
1:C:631:GLY:O	1:C:632:ASP:O	2.38	0.41
1:C:511:MET:O	1:C:512:PHE:HB3	2.21	0.41
1:A:321:ALA:HB3	1:A:512:PHE:CE1	2.56	0.41
1:B:520:LEU:HG	1:B:543:PHE:CE2	2.55	0.41
1:B:567:ARG:NE	1:B:597:ARG:NH1	2.69	0.41
1:C:648:VAL:CG1	1:C:662:TYR:HD1	2.34	0.41
1:A:233:VAL:CG1	1:A:234:GLU:N	2.83	0.41
1:B:321:ALA:HB3	1:B:512:PHE:CE1	2.56	0.41
1:A:175:ASN:HA	1:A:207:ASP:OD1	2.21	0.41
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.56	0.41
1:B:573:TYR:CE1	1:B:595:PHE:HZ	2.39	0.41
1:C:323:TYR:HB2	1:C:510:PRO:HB2	2.04	0.41
1:A:606:GLN:HB3	1:A:606:GLN:HE21	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:HG23	1:A:140:TYR:OH	2.21	0.40
1:A:282:PHE:CD1	1:A:283:LEU:N	2.89	0.40
1:A:573:TYR:C	1:A:573:TYR:HD2	2.24	0.40
1:C:514:ARG:O	1:C:515:LYS:C	2.59	0.40
1:A:341:ASP:OD2	1:A:341:ASP:C	2.60	0.40
1:A:330:LEU:HD12	1:A:377:ILE:HD12	2.03	0.40
1:A:187:TYR:O	1:A:189:ASP:N	2.54	0.40
1:A:156:LEU:CD1	1:A:188:VAL:HG22	2.51	0.40
1:A:96:ASN:O	1:A:100:LYS:HG3	2.21	0.40
1:B:318:ASP:OD1	1:B:519:ARG:NH2	2.50	0.40
1:A:441:ILE:CG2	1:A:442:ASP:N	2.82	0.40
1:A:247:LEU:HD12	1:A:248:VAL:H	1.86	0.40
1:A:591:LEU:O	1:A:591:LEU:HG	2.21	0.40
1:B:450:ARG:HA	1:B:450:ARG:HD2	1.84	0.40
1:B:300:LEU:CD1	1:B:300:LEU:N	2.84	0.40
1:C:596:SER:C	1:C:597:ARG:HG3	2.40	0.40
1:A:657:THR:O	1:A:658:GLN:C	2.60	0.40
1:B:411:GLU:CG	1:B:412:GLY:N	2.73	0.40
1:B:389:LEU:O	1:B:437:LEU:HD11	2.22	0.40
1:B:245:TYR:HB3	1:B:348:LEU:HD22	2.03	0.40
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.83	0.40
1:B:464:VAL:HG21	1:B:545:GLN:HB3	2.03	0.40
1:A:544:ILE:HG21	1:A:588:LEU:HG	2.04	0.40
1:A:618:LYS:HB3	1:A:618:LYS:HE2	1.93	0.40
1:C:496:ALA:O	1:C:497:LYS:C	2.60	0.40
1:A:476:VAL:HG21	3:A:752:FAD:H5'2	2.03	0.40
1:A:548:ALA:HB2	1:A:587:ALA:CB	2.50	0.40
1:A:253:MET:HA	1:A:253:MET:HE2	2.03	0.40
1:A:243:ARG:HB3	1:A:243:ARG:HE	1.75	0.40
1:C:395:GLU:HA	1:C:396:PRO:HD3	1.93	0.40
1:C:391:GLN:HG3	1:C:391:GLN:H	1.60	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	599/618 (97%)	481 (80%)	85 (14%)	33 (6%)	2	21
1	B	503/618 (81%)	374 (74%)	102 (20%)	27 (5%)	2	22
1	C	431/618 (70%)	320 (74%)	84 (20%)	27 (6%)	2	18
All	All	1533/1854 (83%)	1175 (77%)	271 (18%)	87 (6%)	2	20

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	106	GLY
1	A	240	SER
1	A	253	MET
1	A	267	LYS
1	A	357	LYS
1	A	538	ALA
1	B	161	VAL
1	B	352	ASP
1	B	353	GLU
1	B	407	SER
1	B	422	GLU
1	B	441	ILE
1	B	600	ALA
1	C	242	ILE
1	C	244	GLN
1	C	252	ASP
1	C	253	MET
1	C	353	GLU
1	C	409	SER
1	C	555	LYS
1	C	594	ALA
1	C	600	ALA
1	C	632	ASP
1	A	97	ARG
1	A	104	ARG
1	A	116	GLU
1	A	252	ASP
1	A	309	ASP
1	A	353	GLU
1	A	544	ILE

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Mol	Chain	Res	Type
1	A	555	LYS
1	A	634	ARG
1	B	404	LYS
1	B	423	ALA
1	B	534	GLY
1	C	391	GLN
1	A	102	ALA
1	A	160	ASP
1	A	209	ASP
1	B	107	MET
1	B	162	ASP
1	B	233	VAL
1	B	297	GLU
1	B	333	GLN
1	B	344	VAL
1	B	392	TYR
1	B	417	LEU
1	B	588	LEU
1	C	235	ALA
1	C	241	SER
1	C	243	ARG
1	C	515	LYS
1	C	587	ALA
1	C	633	ALA
1	C	634	ARG
1	A	146	THR
1	A	169	ALA
1	A	345	ILE
1	A	392	TYR
1	A	656	HIS
1	B	89	GLY
1	B	342	LEU
1	B	383	THR
1	B	567	ARG
1	C	362	PRO
1	C	597	ARG
1	A	156	LEU
1	A	402	LEU
1	A	445	CYS
1	C	436	SER
1	C	449	PRO
1	A	241	SER

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Mol	Chain	Res	Type
1	A	242	ILE
1	C	352	ASP
1	C	623	GLY
1	A	441	ILE
1	A	465	HIS
1	C	396	PRO
1	C	593	VAL
1	B	125	LEU
1	B	248	VAL
1	B	261	GLY
1	B	532	GLY
1	C	380	PRO
1	A	464	VAL
1	A	532	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	518/528 (98%)	477 (92%)	41 (8%)	15	52
1	B	441/528 (84%)	409 (93%)	32 (7%)	17	56
1	C	373/528 (71%)	344 (92%)	29 (8%)	16	52
All	All	1332/1584 (84%)	1230 (92%)	102 (8%)	16	53

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	81	ILE
1	A	93	GLU
1	A	98	LEU
1	A	113	ASP
1	A	117	TYR
1	A	129	ASP
1	A	146	THR

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Mol	Chain	Res	Type
1	A	182	ASN
1	A	190	GLN
1	A	198	GLN
1	A	229	GLU
1	A	252	ASP
1	A	253	MET
1	A	265	ARG
1	A	280	ASN
1	A	287	THR
1	A	303	LEU
1	A	330	LEU
1	A	332	ASN
1	A	346	MET
1	A	350	ASN
1	A	366	THR
1	A	394	SER
1	A	397	SER
1	A	403	HIS
1	A	411	GLU
1	A	414	GLU
1	A	437	LEU
1	A	454	ARG
1	A	465	HIS
1	A	484	ARG
1	A	495	ARG
1	A	522	PHE
1	A	553	GLN
1	A	555	LYS
1	A	567	ARG
1	A	573	TYR
1	A	606	GLN
1	A	664	LYS
1	A	673	SER
1	B	103	HIS
1	B	156	LEU
1	B	162	ASP
1	B	257	LYS
1	B	272	GLN
1	B	276	PHE
1	B	294	GLN
1	B	298	ARG
1	B	313	ARG

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Mol	Chain	Res	Type
1	B	346	MET
1	B	350	ASN
1	B	351	LEU
1	B	378	THR
1	B	391	GLN
1	B	403	HIS
1	B	415	LEU
1	B	452	GLN
1	B	484	ARG
1	B	506	ARG
1	B	525	THR
1	B	547	ARG
1	B	567	ARG
1	B	571	GLU
1	B	572	ASP
1	B	573	TYR
1	B	578	GLU
1	B	606	GLN
1	B	626	HIS
1	B	660	VAL
1	B	667	MET
1	B	672	TYR
1	B	673	SER
1	C	243	ARG
1	C	244	GLN
1	C	252	ASP
1	C	328	SER
1	C	330	LEU
1	C	346	MET
1	C	350	ASN
1	C	362	PRO
1	C	372	THR
1	C	391	GLN
1	C	417	LEU
1	C	422	GLU
1	C	452	GLN
1	C	472	CYS
1	C	478	TYR
1	C	484	ARG
1	C	491	THR
1	C	511	MET
1	C	535	THR

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Mol	Chain	Res	Type
1	C	541	MET
1	C	561	LEU
1	C	572	ASP
1	C	573	TYR
1	C	582	PHE
1	C	585	ASP
1	C	606	GLN
1	C	634	ARG
1	C	644	PHE
1	C	669	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	182	ASN
1	A	244	GLN
1	A	272	GLN
1	A	280	ASN
1	A	294	GLN
1	A	319	HIS
1	A	350	ASN
1	A	399	GLN
1	A	426	HIS
1	A	452	GLN
1	A	486	ASN
1	A	590	GLN
1	A	606	GLN
1	A	641	GLN
1	B	272	GLN
1	B	280	ASN
1	B	294	GLN
1	B	302	HIS
1	B	332	ASN
1	B	349	ASN
1	B	350	ASN
1	B	391	GLN
1	B	399	GLN
1	B	452	GLN
1	B	486	ASN
1	B	517	GLN
1	B	590	GLN

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Mol	Chain	Res	Type
1	B	606	GLN
1	B	626	HIS
1	B	656	HIS
1	B	658	GLN
1	C	280	ASN
1	C	302	HIS
1	C	350	ASN
1	C	359	HIS
1	C	391	GLN
1	C	403	HIS
1	C	486	ASN
1	C	583	HIS
1	C	590	GLN
1	C	606	GLN
1	C	626	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	FMN	A	751	-	32,33,33	3.16	14 (43%)	34,50,50	3.19	9 (26%)
3	FAD	A	752	-	52,58,58	3.12	25 (48%)	52,89,89	3.51	12 (23%)
4	NAP	A	753	-	45,52,52	2.35	14 (31%)	55,80,80	1.85	6 (10%)
3	FAD	B	752	-	52,58,58	3.00	24 (46%)	52,89,89	3.41	14 (26%)
4	NAP	B	753	-	45,52,52	2.42	12 (26%)	55,80,80	1.94	7 (12%)
3	FAD	C	752	-	52,58,58	2.93	24 (46%)	52,89,89	3.44	14 (26%)

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	FMN	A	751	-	-	0/18/18/18	0/3/3/3
3	FAD	A	752	-	-	0/30/50/50	0/6/6/6
4	NAP	A	753	-	-	0/27/67/67	0/5/5/5
3	FAD	B	752	-	-	0/30/50/50	0/6/6/6
4	NAP	B	753	-	-	0/27/67/67	0/5/5/5
3	FAD	C	752	-	-	0/30/50/50	0/6/6/6

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	752	FAD	PA-O5B	-2.81	1.47	1.59
3	B	752	FAD	PA-O5B	-2.77	1.47	1.59
4	B	753	NAP	PA-O5B	-2.40	1.48	1.59
3	C	752	FAD	PA-O5B	-2.39	1.49	1.59
4	A	753	NAP	PA-O5B	-2.22	1.49	1.59
2	A	751	FMN	C1'-N10	-2.20	1.46	1.48
2	A	751	FMN	P-O3P	-2.02	1.47	1.54
4	A	753	NAP	C2A-N3A	2.01	1.35	1.32
3	A	752	FAD	C2'-C3'	2.04	1.57	1.53
3	B	752	FAD	C2B-C1B	2.08	1.57	1.53
3	A	752	FAD	C6-C7	2.10	1.43	1.37
3	C	752	FAD	C6-C7	2.11	1.43	1.37
4	A	753	NAP	C2D-C1D	2.13	1.57	1.53
3	B	752	FAD	C9-C9A	2.14	1.45	1.40
4	A	753	NAP	C8A-N7A	2.15	1.38	1.34
3	C	752	FAD	C5'-C4'	2.17	1.55	1.51
3	C	752	FAD	C2B-C1B	2.18	1.57	1.53
2	A	751	FMN	C10-N1	2.18	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	752	FAD	C9-C9A	2.24	1.45	1.40
2	A	751	FMN	C9A-C5A	2.26	1.47	1.42
3	B	752	FAD	C4'-C3'	2.27	1.58	1.53
2	A	751	FMN	C4A-C10	2.32	1.45	1.40
3	B	752	FAD	C2-N3	2.36	1.43	1.38
3	C	752	FAD	C2-N3	2.36	1.43	1.38
2	A	751	FMN	C5A-N5	2.37	1.39	1.35
3	A	752	FAD	C9-C9A	2.39	1.46	1.40
3	B	752	FAD	O2'-C2'	2.41	1.48	1.43
3	C	752	FAD	C4'-C3'	2.42	1.58	1.53
4	B	753	NAP	C2D-C1D	2.42	1.57	1.53
3	A	752	FAD	C5A-C4A	2.48	1.46	1.40
3	C	752	FAD	C5X-N5	2.49	1.39	1.35
3	A	752	FAD	C8A-N7A	2.50	1.39	1.34
3	C	752	FAD	C10-N1	2.52	1.39	1.35
3	A	752	FAD	C2-N3	2.53	1.43	1.38
3	C	752	FAD	O2'-C2'	2.56	1.49	1.43
3	C	752	FAD	C4-C4X	2.68	1.46	1.41
4	A	753	NAP	C2N-N1N	2.69	1.38	1.35
3	B	752	FAD	C2A-N3A	2.70	1.36	1.32
2	A	751	FMN	C4-C4A	2.71	1.46	1.41
3	B	752	FAD	C8A-N7A	2.71	1.39	1.34
2	A	751	FMN	C8M-C8	2.72	1.56	1.51
3	A	752	FAD	C10-N10	2.74	1.42	1.39
3	C	752	FAD	C5A-C4A	2.77	1.46	1.40
3	A	752	FAD	C2A-N3A	2.79	1.37	1.32
3	A	752	FAD	C4'-C3'	2.87	1.59	1.53
3	C	752	FAD	C2A-N3A	2.90	1.37	1.32
4	A	753	NAP	O4D-C1D	2.92	1.45	1.41
3	B	752	FAD	C5A-C4A	2.93	1.47	1.40
3	A	752	FAD	C4-C4X	2.93	1.47	1.41
3	C	752	FAD	C6-C5X	2.96	1.46	1.41
4	A	753	NAP	C5A-C4A	3.03	1.47	1.40
3	C	752	FAD	C8A-N7A	3.04	1.40	1.34
4	B	753	NAP	C5A-C4A	3.04	1.47	1.40
3	A	752	FAD	C6-C5X	3.05	1.46	1.41
3	A	752	FAD	C10-N1	3.15	1.41	1.35
3	B	752	FAD	C5X-N5	3.16	1.40	1.35
4	B	753	NAP	O2D-C2D	3.16	1.50	1.43
3	A	752	FAD	C5X-N5	3.18	1.40	1.35
4	B	753	NAP	P2B-O1X	3.18	1.60	1.50
4	A	753	NAP	P2B-O1X	3.20	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	753	NAP	O2D-C2D	3.22	1.50	1.43
4	B	753	NAP	O4D-C1D	3.23	1.45	1.41
3	B	752	FAD	C6-C5X	3.26	1.46	1.41
4	B	753	NAP	C6N-N1N	3.29	1.44	1.35
3	A	752	FAD	O2'-C2'	3.31	1.50	1.43
4	A	753	NAP	C4N-C3N	3.33	1.44	1.39
4	A	753	NAP	C6N-N1N	3.34	1.44	1.35
3	B	752	FAD	C4-C4X	3.35	1.48	1.41
3	A	752	FAD	C5'-C4'	3.35	1.56	1.51
2	A	751	FMN	C9-C9A	3.35	1.48	1.40
2	A	751	FMN	C8-C7	3.39	1.50	1.41
4	B	753	NAP	C2N-N1N	3.39	1.39	1.35
3	A	752	FAD	C8-C7	3.39	1.50	1.41
3	B	752	FAD	C9A-C5X	3.51	1.50	1.42
3	B	752	FAD	C5'-C4'	3.53	1.57	1.51
3	B	752	FAD	C8-C7	3.62	1.50	1.41
3	B	752	FAD	C10-N10	3.63	1.43	1.39
4	A	753	NAP	C2A-N1A	3.71	1.41	1.33
4	B	753	NAP	C4N-C3N	3.79	1.45	1.39
3	B	752	FAD	C1'-N10	3.95	1.52	1.48
4	A	753	NAP	C7N-N7N	3.95	1.41	1.33
4	B	753	NAP	C2A-N1A	3.96	1.41	1.33
3	C	752	FAD	C1'-N10	4.03	1.52	1.48
3	C	752	FAD	C9A-C5X	4.04	1.51	1.42
3	B	752	FAD	C10-N1	4.07	1.42	1.35
3	A	752	FAD	C4X-C10	4.14	1.48	1.40
3	A	752	FAD	C9A-C5X	4.20	1.51	1.42
3	B	752	FAD	C4X-C10	4.21	1.48	1.40
4	B	753	NAP	C7N-N7N	4.22	1.41	1.33
3	C	752	FAD	C4X-C10	4.27	1.48	1.40
3	C	752	FAD	C8-C7	4.32	1.52	1.41
3	C	752	FAD	C4X-N5	4.38	1.40	1.33
3	B	752	FAD	C4X-N5	4.55	1.40	1.33
3	A	752	FAD	C4X-N5	4.80	1.40	1.33
2	A	751	FMN	C4-N3	5.07	1.42	1.33
2	A	751	FMN	C4A-N5	5.22	1.41	1.33
3	C	752	FAD	C4-N3	5.74	1.43	1.33
3	A	752	FAD	C1'-N10	5.91	1.54	1.48
3	A	752	FAD	C4-N3	5.91	1.43	1.33
3	B	752	FAD	C4-N3	6.27	1.44	1.33
3	B	752	FAD	C4A-N3A	7.04	1.45	1.35
3	C	752	FAD	C2A-N1A	7.37	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	752	FAD	C2A-N1A	7.59	1.48	1.33
3	B	752	FAD	C2A-N1A	7.71	1.48	1.33
3	A	752	FAD	C4A-N3A	7.92	1.47	1.35
2	A	751	FMN	C9A-N10	8.10	1.50	1.38
3	C	752	FAD	C4A-N3A	8.41	1.47	1.35
3	C	752	FAD	C9A-N10	8.49	1.50	1.38
3	B	752	FAD	C9A-N10	8.93	1.51	1.38
3	A	752	FAD	C9A-N10	9.55	1.52	1.38
2	A	751	FMN	C10-N10	10.49	1.51	1.39
4	A	753	NAP	C4A-N3A	10.53	1.51	1.35
4	B	753	NAP	C4A-N3A	10.59	1.51	1.35

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	752	FAD	N3A-C2A-N1A	-10.55	120.58	128.87
3	C	752	FAD	N3A-C2A-N1A	-10.49	120.63	128.87
3	B	752	FAD	N3A-C2A-N1A	-10.02	121.00	128.87
2	A	751	FMN	C4-C4A-C10	-7.50	115.14	119.94
3	C	752	FAD	C4X-C4-N3	-7.38	113.87	123.52
3	A	752	FAD	C4X-C4-N3	-7.31	113.97	123.52
3	B	752	FAD	C4X-C4-N3	-7.09	114.25	123.52
4	B	753	NAP	N3A-C2A-N1A	-6.95	123.41	128.87
3	A	752	FAD	N3-C2-N1	-6.77	116.28	127.69
3	B	752	FAD	N3-C2-N1	-6.73	116.35	127.69
4	A	753	NAP	N3A-C2A-N1A	-6.67	123.63	128.87
3	C	752	FAD	N3-C2-N1	-6.60	116.58	127.69
3	A	752	FAD	C1B-N9A-C4A	-6.43	119.63	126.81
3	B	752	FAD	O5'-P-O1P	-6.25	83.62	109.21
2	A	751	FMN	C4A-C10-N10	-6.18	116.03	120.52
3	A	752	FAD	O5'-P-O1P	-6.15	84.03	109.21
4	B	753	NAP	C2D-C1D-N1N	-5.89	102.00	113.53
3	C	752	FAD	O5'-P-O1P	-5.89	85.12	109.21
2	A	751	FMN	N3-C2-N1	-5.49	118.45	127.69
3	C	752	FAD	C1B-N9A-C4A	-5.48	120.69	126.81
3	B	752	FAD	C1B-N9A-C4A	-5.39	120.79	126.81
4	A	753	NAP	C2D-C1D-N1N	-5.36	103.02	113.53
2	A	751	FMN	C4A-C4-N3	-4.62	117.48	123.52
2	A	751	FMN	C6-C5A-N5	-3.41	114.67	118.92
2	A	751	FMN	C5A-C9A-N10	-3.35	115.07	117.58
3	C	752	FAD	O2P-P-O5'	-3.25	92.73	108.24
4	B	753	NAP	C4B-O4B-C1B	-3.17	106.29	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	752	FAD	C4-C4X-C10	-3.03	118.00	119.94
3	B	752	FAD	C4X-C10-N10	-2.98	118.35	120.52
3	C	752	FAD	C4-C4X-C10	-2.84	118.12	119.94
4	A	753	NAP	C4B-O4B-C1B	-2.80	106.68	109.64
3	A	752	FAD	C5X-C9A-N10	-2.76	115.51	117.58
3	B	752	FAD	O2P-P-O5'	-2.63	95.72	108.24
3	B	752	FAD	C5X-C9A-N10	-2.61	115.62	117.58
3	C	752	FAD	C5X-C9A-N10	-2.38	115.79	117.58
3	A	752	FAD	C6-C5X-N5	-2.30	116.05	118.92
3	B	752	FAD	C6-C5X-N5	-2.27	116.09	118.92
3	B	752	FAD	C4-C4X-C10	-2.26	118.50	119.94
3	C	752	FAD	C6-C5X-N5	-2.23	116.14	118.92
3	C	752	FAD	C4X-C10-N10	-2.23	118.90	120.52
4	A	753	NAP	O4B-C1B-C2B	-2.19	102.66	106.60
4	B	753	NAP	O3D-C3D-C4D	-2.19	104.46	111.01
2	A	751	FMN	O3P-P-O5'	-2.13	100.51	106.72
4	B	753	NAP	C1B-N9A-C4A	-2.11	124.45	126.81
2	A	751	FMN	C9A-C5A-N5	3.00	127.06	122.18
3	A	752	FAD	O2P-P-O3P	3.11	118.61	105.27
3	B	752	FAD	O2P-P-O3P	3.46	120.09	105.27
3	C	752	FAD	O2P-P-O3P	3.56	120.54	105.27
3	C	752	FAD	C1'-N10-C9A	3.95	123.41	118.83
3	A	752	FAD	C2A-N1A-C6A	4.28	126.41	118.77
3	B	752	FAD	C1'-N10-C9A	4.30	123.81	118.83
3	B	752	FAD	C2A-N1A-C6A	4.34	126.52	118.77
3	C	752	FAD	C2A-N1A-C6A	4.39	126.59	118.77
4	A	753	NAP	O4D-C1D-N1N	4.83	113.32	108.10
4	B	753	NAP	O4D-C1D-N1N	5.12	113.63	108.10
4	A	753	NAP	C2D-C3D-C4D	5.23	113.33	102.64
4	B	753	NAP	C2D-C3D-C4D	5.24	113.35	102.64
3	A	752	FAD	C1'-N10-C9A	5.72	125.46	118.83
2	A	751	FMN	C4-N3-C2	11.47	124.73	115.16
3	B	752	FAD	C4-N3-C2	14.78	127.49	115.16
3	C	752	FAD	C4-N3-C2	14.79	127.50	115.16
3	A	752	FAD	C4-N3-C2	14.87	127.56	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	752	FAD	5	0
4	A	753	NAP	3	0
3	B	752	FAD	7	0
4	B	753	NAP	2	0
3	C	752	FAD	3	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 ⓘ

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	603/618 (97%)	-0.18	1 (0%) 95 94	72, 95, 116, 136	0
1	B	515/618 (83%)	0.11	23 (4%) 37 33	65, 96, 175, 202	0
1	C	435/618 (70%)	0.03	8 (1%) 71 65	84, 116, 149, 161	0
All	All	1553/1854 (83%)	-0.02	32 (2%) 67 61	65, 101, 155, 202	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	LEU	4.6
1	B	155	TRP	4.6
1	B	164	THR	4.5
1	B	80	ILE	4.2
1	B	154	ASP	4.0
1	B	211	ASN	3.9
1	C	663	VAL	3.7
1	B	213	GLU	3.6
1	B	118	ASP	3.6
1	B	103	HIS	3.4
1	B	81	ILE	3.3
1	B	122	LEU	3.2
1	B	165	GLY	3.2
1	B	158	GLU	3.1
1	B	157	GLN	3.1
1	C	258	VAL	2.8
1	B	223	PHE	2.7
1	B	214	GLU	2.6
1	C	353	GLU	2.6
1	B	224	TRP	2.5
1	B	120	ALA	2.5
1	B	272	GLN	2.5
1	C	600	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	357	LYS	2.3
1	B	218	THR	2.3
1	B	129	ASP	2.3
1	C	358	LYS	2.3
1	C	352	ASP	2.2
1	C	365	THR	2.2
1	B	79	ASN	2.1
1	A	312	ILE	2.1
1	B	222	GLN	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
4	NAP	A	753	48/48	0.77	0.40	3.72	201,219,224,224	0
4	NAP	B	753	48/48	0.78	0.34	2.61	173,198,214,215	0
3	FAD	C	752	53/53	0.93	0.24	0.41	98,102,114,114	0
3	FAD	B	752	53/53	0.93	0.26	0.29	78,87,105,107	0
2	FMN	A	751	31/31	0.96	0.17	-0.14	102,108,109,110	0
3	FAD	A	752	53/53	0.96	0.21	-0.21	73,79,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.