



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:36 PM GMT

PDB ID : 1J9Z  
Title : CYPOR-W677G  
Authors : Hubbard, P.A.; Shen, A.L.; Paschke, R.; Kasper, C.B.; Kim, J.J.  
Deposited on : 2001-05-29  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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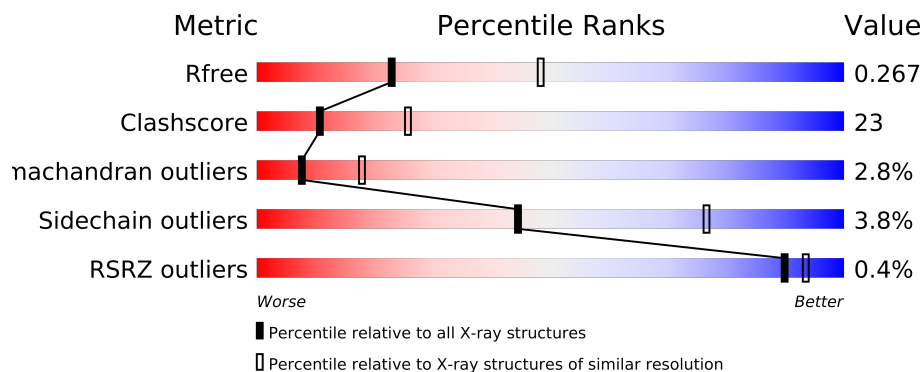
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10265 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

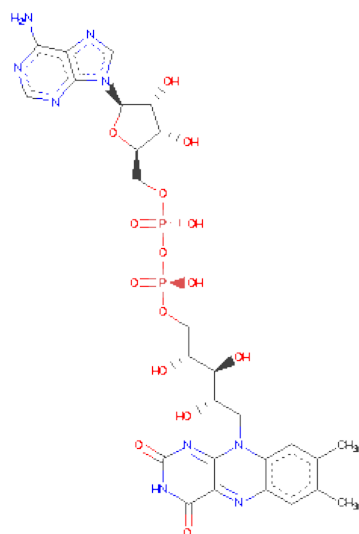
- Molecule 1 is a protein called NADPH-Cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4901	3099	844	935	23			
1	B	611	Total	C	N	O	S	0	0	0
			4890	3092	842	933	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	GLY	TRP	ENGINEERED	UNP P00388
B	677	GLY	TRP	ENGINEERED	UNP P00388

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



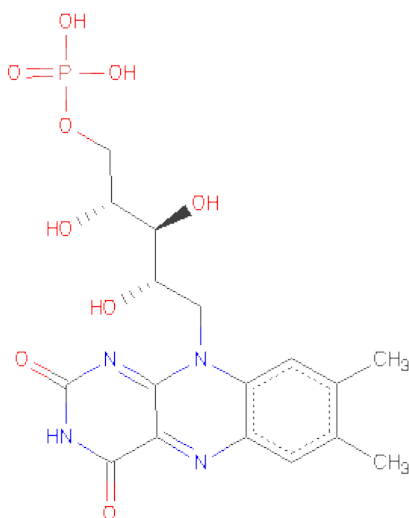
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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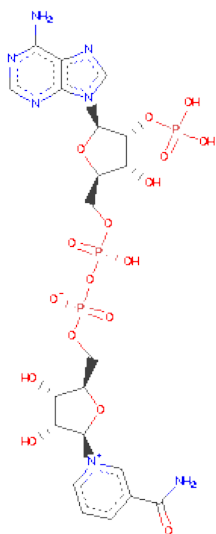
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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		

- Molecule 5 is water.

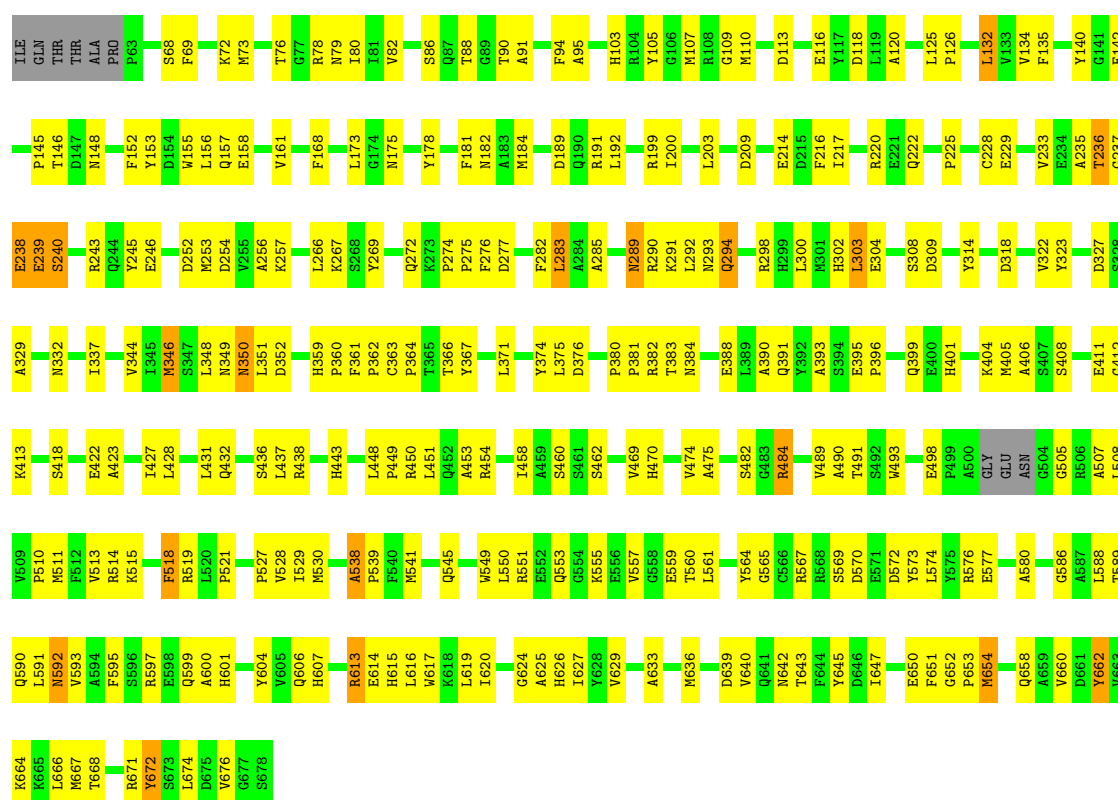
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total	O	0	0
			109	109		
5	B	101	Total	O	0	0
			101	101		

### 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.

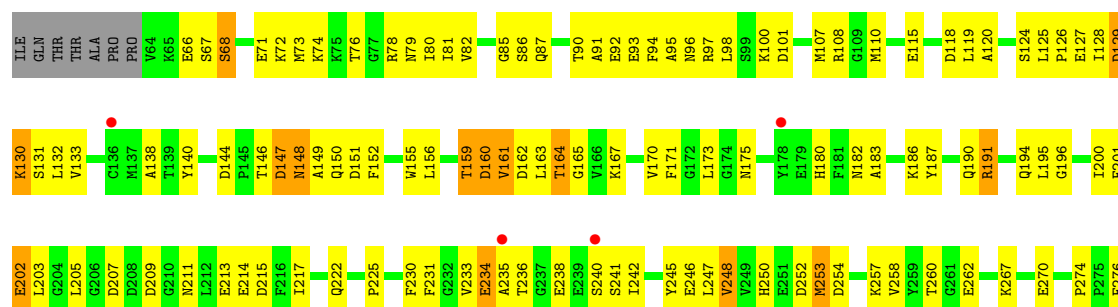
#### • Molecule 1: NADPH-Cytochrome P450 reductase

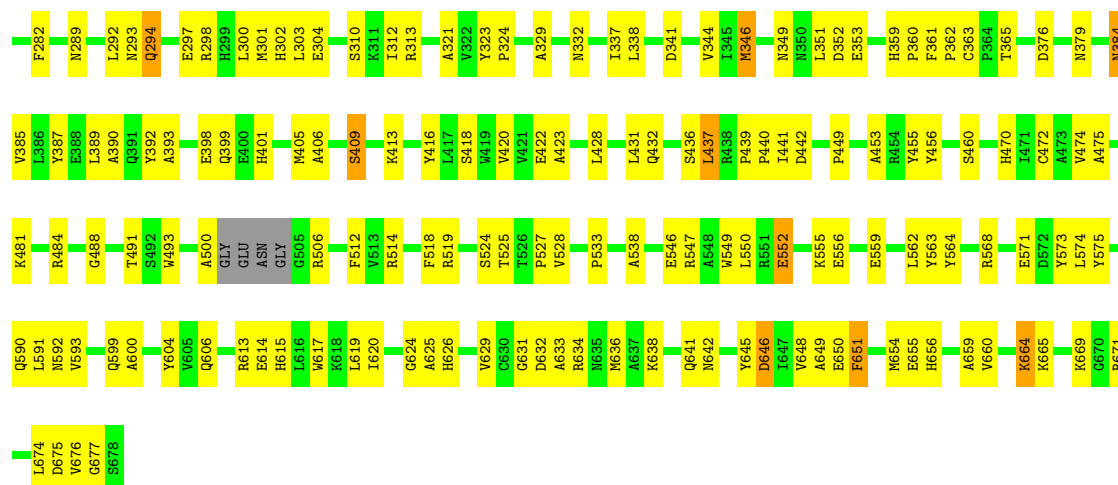
Chain A:



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

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.63Å 116.06Å 118.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.80 – 2.71	Depositor EDS
% Data completeness (in resolution range)	79.6 (30.00-2.70) 79.6 (29.80-2.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.188 , 0.270 0.187 , 0.267	Depositor DCC
$R_{free}$ test set	1535 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 7.3	EDS
Estimated twinning fraction	0.034 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 30972 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

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	0.38	0/5016	0.61	0/6784
1	B	0.37	0/5004	0.61	0/6768
All	All	0.38	0/10020	0.61	0/13552

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	456	TYR	Sidechain

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4901	0	4748	222	0
1	B	4890	0	4737	231	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	31	0	19	3	0
3	B	31	0	19	1	0
4	A	48	0	25	0	0
4	B	48	0	25	3	0
5	A	109	0	0	6	0
5	B	101	0	0	2	0
All	All	10265	0	9635	451	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (451) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.30	1.14
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.33	1.09
1:B:78:ARG:HH22	1:B:352:ASP:HB2	1.26	1.00
1:B:163:LEU:HB2	1:B:196:GLY:HA3	1.44	0.96
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.27	0.96
1:B:159:THR:HG22	1:B:161:VAL:H	1.32	0.94
1:A:86:SER:HB3	1:A:91:ALA:HB3	1.48	0.93
1:B:159:THR:HG21	1:B:161:VAL:HG13	1.54	0.90
1:B:665:LYS:HE2	1:B:669:LYS:HE3	1.53	0.90
1:B:167:LYS:HB3	1:B:200:ILE:HD11	1.53	0.88
1:B:159:THR:HG22	1:B:160:ASP:H	1.39	0.88
1:B:78:ARG:NH2	1:B:352:ASP:HB2	1.88	0.88
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.55	0.87
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.36	0.86
1:A:559:GLU:HG2	1:A:589:THR:HG21	1.58	0.86
1:A:350:ASN:HD22	1:A:351:LEU:N	1.75	0.84
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.60	0.83
1:B:294:GLN:NE2	1:B:294:GLN:H	1.75	0.83
1:A:291:LYS:NZ	1:A:293:ASN:HD21	1.77	0.81
1:A:604:TYR:H	1:A:607:HIS:CD2	1.98	0.81
1:A:590:GLN:NE2	1:A:592:ASN:HD21	1.79	0.80
1:B:68:SER:OG	1:B:71:GLU:HG2	1.82	0.78
1:B:568:ARG:HB3	1:B:568:ARG:NH2	1.98	0.78
1:A:529:ILE:HD13	1:A:616:LEU:HD22	1.67	0.76
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.67	0.76
1:B:107:MET:HE1	1:B:233:VAL:HG21	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:541:MET:O	1:A:545:GLN:HG3	1.86	0.75
1:B:409:SER:HA	1:B:413:LYS:HD3	1.67	0.75
1:A:86:SER:HA	1:A:146:THR:HG21	1.67	0.75
1:A:613:ARG:HD2	1:A:651:PHE:HE1	1.52	0.74
1:A:371:LEU:HD23	1:A:375:LEU:HD12	1.67	0.74
1:B:78:ARG:HD3	1:B:110:MET:HB2	1.68	0.73
1:A:613:ARG:NH1	1:A:613:ARG:HG2	2.02	0.73
1:B:437:LEU:HD22	1:B:439:PRO:HD3	1.69	0.73
1:A:254:ASP:O	1:A:257:LYS:HG2	1.89	0.72
1:B:159:THR:CG2	1:B:161:VAL:HG13	2.19	0.72
1:B:527:PRO:HB2	1:B:625:ALA:CB	2.14	0.72
1:A:527:PRO:HB2	1:A:625:ALA:CB	2.20	0.71
1:A:214:GLU:OE1	1:A:413:LYS:HE3	1.90	0.71
1:A:549:TRP:O	1:A:553:GLN:HG2	1.91	0.70
1:B:590:GLN:NE2	1:B:592:ASN:HD21	1.89	0.70
1:A:103:HIS:HA	1:A:107:MET:O	1.92	0.69
1:A:135:PHE:CE2	1:A:192:LEU:HD11	2.28	0.69
1:A:521:PRO:HG3	1:A:626:HIS:ND1	2.08	0.69
1:B:533:PRO:HG3	1:B:636:MET:HG3	1.76	0.68
1:A:567:ARG:HD3	1:A:597:ARG:CZ	2.24	0.68
1:B:233:VAL:O	1:B:234:GLU:HG2	1.94	0.67
1:B:323:TYR:CE2	1:B:453:ALA:HB2	2.28	0.67
1:A:86:SER:HB2	3:A:751:FMN:O3P	1.95	0.67
1:B:214:GLU:OE1	1:B:413:LYS:HE3	1.94	0.67
1:A:653:PRO:O	1:A:654:MET:HB3	1.94	0.67
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.77	0.67
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.76	0.66
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.77	0.66
1:B:360:PRO:HG2	1:B:361:PHE:CD1	2.31	0.66
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.78	0.66
1:A:350:ASN:ND2	1:A:352:ASP:H	1.94	0.65
1:A:291:LYS:NZ	1:A:293:ASN:ND2	2.42	0.65
1:B:217:ILE:HD11	1:B:406:ALA:O	1.96	0.65
1:B:568:ARG:HB3	1:B:568:ARG:HH21	1.62	0.65
1:A:590:GLN:HE21	1:A:592:ASN:HD21	1.41	0.65
1:A:246:GLU:HB3	1:A:351:LEU:CD2	2.26	0.64
1:A:217:ILE:HD11	1:A:383:THR:HG21	1.79	0.64
1:A:78:ARG:HD3	1:A:110:MET:HB3	1.80	0.64
1:B:130:LYS:HG3	1:B:231:PHE:HD1	1.61	0.64
1:A:291:LYS:HZ2	1:A:293:ASN:HD21	1.44	0.64
1:A:423:ALA:O	1:A:482:SER:HB3	1.97	0.64
1:B:302:HIS:HD2	1:B:575:TYR:OH	1.81	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.80	0.64
1:B:359:HIS:ND1	1:B:363:CYS:HB2	2.14	0.63
1:A:458:ILE:HG23	1:A:469:VAL:HG13	1.79	0.63
1:A:382:ARG:HD2	5:A:760:HOH:O	1.97	0.63
1:B:292:LEU:HD11	1:B:302:HIS:HB2	1.80	0.63
1:B:656:HIS:O	1:B:660:VAL:HG23	1.98	0.63
1:B:191:ARG:CZ	1:B:195:LEU:HD11	2.29	0.63
1:A:105:TYR:HD1	1:A:235:ALA:HA	1.63	0.62
1:A:615:HIS:O	1:A:619:LEU:HD12	1.98	0.62
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.29	0.62
1:A:344:VAL:O	1:A:366:THR:HG22	1.99	0.62
1:B:617:TRP:HZ3	1:B:648:VAL:HG22	1.64	0.62
1:A:86:SER:HB3	1:A:91:ALA:CB	2.28	0.62
1:A:314:TYR:O	1:A:462:SER:HB3	1.99	0.61
1:A:428:LEU:O	1:A:432:GLN:HG3	2.00	0.61
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.81	0.61
1:B:550:LEU:O	1:B:555:LYS:HB2	2.00	0.61
1:A:266:LEU:O	1:A:267:LYS:HB2	2.00	0.61
1:A:291:LYS:HZ1	1:A:293:ASN:HD21	1.46	0.61
1:A:395:GLU:H	1:A:436:SER:HB2	1.64	0.61
1:B:203:LEU:HG	1:B:205:LEU:HD21	1.83	0.61
1:A:418:SER:HA	1:A:422:GLU:HB3	1.81	0.61
1:B:246:GLU:HB2	1:B:351:LEU:HD21	1.82	0.60
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.66	0.60
1:B:167:LYS:HG2	1:B:230:PHE:CE2	2.36	0.60
1:A:76:THR:HB	1:A:78:ARG:NH1	2.15	0.60
1:B:214:GLU:O	1:B:217:ILE:HG22	2.01	0.60
1:A:454:ARG:HH11	1:A:489:VAL:HB	1.66	0.60
1:B:549:TRP:O	1:B:552:GLU:HG2	2.01	0.60
1:B:303:LEU:HD12	1:B:303:LEU:N	2.17	0.60
1:B:254:ASP:OD1	1:B:257:LYS:HE3	2.01	0.59
1:A:300:LEU:HD12	1:A:300:LEU:N	2.17	0.59
1:B:100:LYS:HZ3	1:B:100:LYS:HB3	1.65	0.59
1:B:129:ASP:OD1	1:B:130:LYS:HD3	2.02	0.59
1:A:239:GLU:O	1:A:240:SER:HB2	2.02	0.59
1:B:167:LYS:CB	1:B:200:ILE:HD11	2.31	0.59
1:A:401:HIS:O	1:A:405:MET:HG2	2.03	0.59
1:B:130:LYS:HG3	1:B:231:PHE:CD1	2.38	0.58
1:A:604:TYR:N	1:A:607:HIS:CD2	2.71	0.58
1:A:390:ALA:O	1:A:399:GLN:HG3	2.03	0.58
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.68	0.58
1:A:604:TYR:N	1:A:607:HIS:HD2	2.00	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:138:ALA:O	1:B:146:THR:HG23	2.03	0.58
1:B:359:HIS:HB3	1:B:360:PRO:HD2	1.86	0.58
1:A:591:LEU:O	1:A:591:LEU:HG	2.03	0.58
1:B:276:PHE:CG	1:B:282:PHE:HB2	2.38	0.58
1:A:189:ASP:HB2	1:A:203:LEU:HD13	1.85	0.58
1:A:604:TYR:H	1:A:607:HIS:HD2	1.43	0.58
1:B:528:VAL:HB	1:B:547:ARG:NH1	2.17	0.58
1:B:590:GLN:HE21	1:B:592:ASN:HD21	1.52	0.58
1:B:138:ALA:HA	1:B:173:LEU:HB2	1.85	0.58
1:A:153:TYR:CE2	1:A:157:GLN:NE2	2.72	0.58
1:A:175:ASN:OD1	1:A:209:ASP:HB2	2.04	0.58
1:B:167:LYS:HB3	1:B:200:ILE:CD1	2.30	0.58
1:A:550:LEU:O	1:A:555:LYS:HB2	2.03	0.58
1:A:664:LYS:O	1:A:668:THR:HG23	2.04	0.58
1:B:71:GLU:O	1:B:74:LYS:HB2	2.04	0.57
1:B:180:HIS:HB3	1:B:183:ALA:HB2	1.86	0.57
1:B:293:ASN:ND2	1:B:300:LEU:HD12	2.18	0.57
1:B:629:VAL:HB	1:B:674:LEU:CD2	2.34	0.57
1:B:108:ARG:HH21	1:B:108:ARG:HG2	1.69	0.57
1:A:168:PHE:O	1:A:200:ILE:HG22	2.04	0.57
1:B:159:THR:HG22	1:B:160:ASP:N	2.16	0.57
1:B:294:GLN:CD	1:B:294:GLN:H	2.08	0.57
1:A:451:LEU:HD12	5:A:759:HOH:O	2.05	0.56
1:A:662:TYR:HE1	1:A:666:LEU:HD11	1.69	0.56
1:B:125:LEU:N	1:B:126:PRO:HD2	2.21	0.56
1:B:613:ARG:HH11	1:B:613:ARG:HG2	1.70	0.56
1:B:98:LEU:O	1:B:101:ASP:HB2	2.04	0.56
1:A:626:HIS:CD2	1:A:671:ARG:HG2	2.41	0.56
1:B:393:ALA:HA	1:B:436:SER:O	2.05	0.56
1:B:182:ASN:O	1:B:186:LYS:HG3	2.06	0.56
1:B:133:VAL:O	1:B:133:VAL:HG13	2.05	0.56
1:A:437:LEU:O	1:A:438:ARG:NH1	2.37	0.56
1:A:428:LEU:HA	1:A:431:LEU:HD12	1.88	0.55
1:A:643:THR:O	1:A:647:ILE:HG13	2.05	0.55
1:B:304:GLU:HG2	1:B:470:HIS:CD2	2.40	0.55
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.88	0.55
1:A:173:LEU:C	1:A:182:ASN:HD21	2.10	0.55
1:A:614:GLU:HA	1:A:651:PHE:CE2	2.41	0.55
1:A:561:LEU:HG	1:A:590:GLN:HB2	1.88	0.55
1:A:388:GLU:O	1:A:391:GLN:HG2	2.07	0.54
1:B:186:LYS:O	1:B:190:GLN:HG2	2.06	0.54
1:B:100:LYS:NZ	1:B:100:LYS:HB3	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:VAL:HG11	1:A:95:ALA:HA	1.89	0.54
1:A:551:ARG:HH12	1:A:586:GLY:C	2.10	0.54
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.22	0.54
1:B:599:GLN:NE2	1:B:599:GLN:H	2.05	0.54
1:B:247:LEU:HD12	1:B:248:VAL:H	1.73	0.54
1:B:677:GLY:HA3	4:B:852:NAP:H71N	1.72	0.54
1:A:375:LEU:HD13	1:A:448:LEU:HD12	1.89	0.54
1:A:567:ARG:HD3	1:A:597:ARG:HD2	1.90	0.54
1:A:285:ALA:HA	1:A:508:LEU:HD23	1.90	0.53
1:A:350:ASN:HD22	1:A:351:LEU:H	1.50	0.53
1:A:660:VAL:O	1:A:664:LYS:HG3	2.08	0.53
1:B:93:GLU:O	1:B:97:ARG:HG3	2.08	0.53
1:A:82:VAL:HG22	1:A:134:VAL:HB	1.89	0.53
1:B:599:GLN:CD	1:B:599:GLN:N	2.62	0.53
1:B:514:ARG:HD2	5:B:877:HOH:O	2.08	0.53
1:B:376:ASP:OD2	1:B:379:ASN:ND2	2.42	0.53
1:B:107:MET:CE	1:B:233:VAL:HG21	2.39	0.53
1:A:294:GLN:HG3	1:A:570:ASP:HA	1.91	0.53
1:A:80:ILE:HG23	1:A:109:GLY:CA	2.38	0.53
1:A:645:TYR:CD2	1:A:660:VAL:HA	2.44	0.53
1:B:645:TYR:OH	1:B:664:LYS:HE3	2.09	0.52
1:A:591:LEU:O	1:A:593:VAL:HG23	2.09	0.52
1:B:115:GLU:HB2	1:B:148:ASN:O	2.09	0.52
1:A:236:THR:O	1:A:238:GLU:N	2.38	0.52
1:B:398:GLU:O	1:B:401:HIS:HB2	2.08	0.52
1:A:277:ASP:HB2	5:A:860:HOH:O	2.09	0.52
1:B:519:ARG:HH11	1:B:519:ARG:HG2	1.75	0.52
1:B:615:HIS:O	1:B:619:LEU:HD13	2.10	0.52
1:A:460:SER:HB3	1:A:470:HIS:CG	2.45	0.52
1:B:472:CYS:HB3	1:B:538:ALA:HB2	1.91	0.52
1:B:390:ALA:O	1:B:399:GLN:HG3	2.10	0.52
1:A:475:ALA:HA	1:A:491:THR:HB	1.91	0.52
1:B:289:ASN:OD1	1:B:303:LEU:HG	2.10	0.52
1:A:291:LYS:HE3	1:A:293:ASN:O	2.09	0.52
1:A:667:MET:HA	1:A:672:TYR:HB3	1.91	0.52
1:A:404:LYS:HG3	1:A:412:GLY:HA3	1.91	0.51
1:B:68:SER:HG	1:B:71:GLU:HG2	1.74	0.51
1:B:527:PRO:O	1:B:625:ALA:HB1	2.10	0.51
1:B:108:ARG:NH2	1:B:108:ARG:HG2	2.26	0.51
1:B:97:ARG:CZ	1:B:384:ASN:HB3	2.40	0.51
1:B:475:ALA:HA	1:B:491:THR:HB	1.91	0.51
1:A:276:PHE:CG	1:A:282:PHE:HB2	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:371:LEU:HD23	1:A:375:LEU:CD1	2.37	0.51
1:B:258:VAL:CG1	1:B:365:THR:HA	2.41	0.51
1:B:167:LYS:N	1:B:167:LYS:HD2	2.26	0.51
1:B:167:LYS:HG2	1:B:230:PHE:HE2	1.75	0.51
1:B:170:VAL:HG12	1:B:171:PHE:N	2.25	0.51
1:B:159:THR:HG22	1:B:161:VAL:N	2.14	0.51
1:A:132:LEU:HD12	1:A:132:LEU:C	2.32	0.51
1:B:626:HIS:CD2	1:B:671:ARG:HG2	2.46	0.51
1:B:428:LEU:O	1:B:432:GLN:HG3	2.11	0.50
1:A:654:MET:HB2	1:A:658:GLN:HB2	1.92	0.50
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.41	0.50
1:B:107:MET:CE	1:B:233:VAL:HG11	2.41	0.50
1:B:86:SER:HB2	1:B:91:ALA:CB	2.21	0.50
1:B:392:TYR:CD1	1:B:440:PRO:HD3	2.46	0.50
1:A:291:LYS:HZ1	1:A:293:ASN:ND2	2.05	0.50
1:A:427:ILE:HG23	1:A:428:LEU:N	2.27	0.50
1:B:546:GLU:O	1:B:549:TRP:HB3	2.12	0.50
1:A:567:ARG:HD3	1:A:597:ARG:NE	2.26	0.50
1:A:636:MET:O	1:A:640:VAL:HG23	2.12	0.50
1:B:132:LEU:H	1:B:132:LEU:HD23	1.75	0.50
1:B:376:ASP:CB	1:B:449:PRO:HG2	2.41	0.50
1:B:528:VAL:HB	1:B:547:ARG:HH11	1.77	0.50
1:B:159:THR:O	1:B:160:ASP:HB2	2.12	0.49
1:A:272:GLN:OE1	1:A:282:PHE:HA	2.12	0.49
1:A:346:MET:HG2	1:A:367:TYR:CZ	2.47	0.49
1:B:81:ILE:HG13	1:B:110:MET:O	2.12	0.49
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.94	0.49
1:A:454:ARG:NH1	1:A:489:VAL:HB	2.27	0.49
1:A:69:PHE:HD2	1:A:73:MET:HE2	1.78	0.49
1:A:222:GLN:O	1:A:225:PRO:HD2	2.12	0.49
1:A:152:PHE:CZ	1:A:156:LEU:HD11	2.47	0.49
1:A:318:ASP:OD1	1:A:515:LYS:HA	2.13	0.49
1:A:642:ASN:O	1:A:645:TYR:N	2.46	0.49
1:B:418:SER:HA	1:B:422:GLU:HB3	1.94	0.49
1:B:73:MET:HB2	1:B:78:ARG:O	2.12	0.49
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.48	0.49
1:B:353:GLU:CD	1:B:353:GLU:H	2.16	0.49
1:A:561:LEU:N	1:A:561:LEU:HD12	2.27	0.49
1:A:650:GLU:OE1	1:A:651:PHE:CE1	2.66	0.48
1:A:599:GLN:N	1:A:599:GLN:CD	2.66	0.48
1:B:78:ARG:CD	1:B:110:MET:HB2	2.42	0.48
1:A:559:GLU:OE1	1:A:619:LEU:HD21	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:TYR:HB2	5:A:825:HOH:O	2.12	0.48
1:B:162:ASP:OD1	1:B:163:LEU:N	2.47	0.48
1:A:361:PHE:HB2	1:A:362:PRO:HD2	1.94	0.48
1:B:175:ASN:HA	1:B:207:ASP:OD1	2.14	0.48
1:B:297:GLU:HG3	1:B:571:GLU:OE1	2.13	0.48
1:A:337:ILE:HB	1:B:600:ALA:HB1	1.95	0.48
1:B:617:TRP:CZ3	1:B:648:VAL:HG22	2.46	0.48
1:B:423:ALA:HA	1:B:481:LYS:HB2	1.95	0.48
1:B:293:ASN:ND2	1:B:298:ARG:O	2.46	0.48
1:B:341:ASP:HB3	1:B:344:VAL:HG23	1.96	0.48
1:B:631:GLY:N	1:B:676:VAL:HG12	2.28	0.48
1:B:79:ASN:ND2	1:B:80:ILE:HG13	2.28	0.48
1:A:560:THR:C	1:A:561:LEU:HD12	2.34	0.48
1:B:72:LYS:C	1:B:74:LYS:H	2.17	0.48
1:B:146:THR:O	1:B:147:ASP:C	2.51	0.48
1:B:231:PHE:HB2	1:B:233:VAL:HG23	1.96	0.47
1:B:360:PRO:HG2	1:B:361:PHE:CE1	2.49	0.47
1:A:427:ILE:HG23	1:A:428:LEU:H	1.79	0.47
1:A:243:ARG:NH2	1:A:443:HIS:HA	2.29	0.47
1:B:677:GLY:HA3	4:B:852:NAP:N7N	2.29	0.47
1:B:552:GLU:HG2	1:B:552:GLU:H	1.56	0.47
1:B:236:THR:CG2	1:B:238:GLU:HG2	2.43	0.47
1:A:653:PRO:O	1:A:654:MET:CB	2.61	0.47
1:B:641:GLN:NE2	1:B:645:TYR:OH	2.39	0.47
1:A:274:PRO:HA	1:A:275:PRO:C	2.34	0.47
1:B:90:THR:HG22	1:B:94:PHE:CE2	2.49	0.47
1:B:191:ARG:HD3	1:B:195:LEU:HD13	1.97	0.47
1:A:569:SER:HB3	1:A:595:PHE:CE1	2.48	0.47
1:A:625:ALA:N	1:A:671:ARG:HH21	2.12	0.47
1:A:395:GLU:OE2	1:A:396:PRO:HD2	2.15	0.47
1:B:128:ILE:HG22	1:B:131:SER:HB3	1.95	0.47
1:A:349:ASN:OD1	1:A:359:HIS:HE1	1.97	0.47
1:B:163:LEU:HG	1:B:164:THR:OG1	2.15	0.47
1:B:654:MET:SD	1:B:659:ALA:HA	2.54	0.47
1:A:474:VAL:HG13	1:A:474:VAL:O	2.14	0.47
1:B:233:VAL:O	1:B:235:ALA:N	2.48	0.47
1:B:67:SER:O	1:B:68:SER:C	2.53	0.47
1:A:408:SER:O	1:A:413:LYS:HD2	2.15	0.47
1:A:569:SER:O	1:A:576:ARG:NH1	2.46	0.47
1:B:646:ASP:HA	1:B:649:ALA:HB3	1.97	0.47
1:A:528:VAL:HG12	1:A:530:MET:HG3	1.97	0.47
1:B:338:LEU:CD2	1:B:439:PRO:HD2	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292:LEU:CD1	1:B:302:HIS:HB2	2.43	0.47
1:B:140:TYR:CD2	1:B:146:THR:HG22	2.50	0.47
1:B:247:LEU:HD11	1:B:346:MET:HB2	1.97	0.47
1:B:252:ASP:O	1:B:253:MET:HB2	2.15	0.46
1:B:201:PHE:O	1:B:202:GLU:O	2.33	0.46
1:B:159:THR:HG23	1:B:191:ARG:NH2	2.30	0.46
1:A:361:PHE:HB2	1:A:362:PRO:CD	2.46	0.46
1:B:236:THR:HG21	1:B:238:GLU:CD	2.36	0.46
1:A:292:LEU:HD11	1:A:302:HIS:HB2	1.97	0.46
1:A:236:THR:O	1:A:236:THR:HG22	2.14	0.46
1:B:209:ASP:OD1	1:B:634:ARG:NH2	2.47	0.46
1:B:124:SER:O	1:B:127:GLU:HB2	2.16	0.46
1:B:85:GLY:O	1:B:138:ALA:HB3	2.14	0.46
1:B:274:PRO:HG3	1:B:276:PHE:CE2	2.50	0.46
1:B:245:TYR:HA	1:B:349:ASN:O	2.15	0.46
1:B:233:VAL:C	1:B:235:ALA:H	2.18	0.46
1:B:147:ASP:O	1:B:149:ALA:N	2.49	0.46
1:A:308:SER:O	1:A:309:ASP:HB2	2.16	0.46
1:A:564:TYR:CG	1:A:565:GLY:N	2.84	0.46
1:B:651:PHE:H	1:B:651:PHE:HD1	1.64	0.46
1:A:86:SER:CA	1:A:146:THR:HG21	2.44	0.46
1:A:105:TYR:CD1	1:A:235:ALA:HA	2.48	0.46
1:B:301:MET:HG3	1:B:303:LEU:HD11	1.98	0.46
1:B:97:ARG:NH1	1:B:213:GLU:OE1	2.46	0.46
1:B:392:TYR:CE1	1:B:440:PRO:HD3	2.51	0.46
1:A:323:TYR:CE2	1:A:453:ALA:HB2	2.51	0.46
1:B:76:THR:OG1	1:B:78:ARG:HG3	2.16	0.46
1:B:85:GLY:O	1:B:146:THR:HG21	2.16	0.46
1:A:298:ARG:HD2	5:A:773:HOH:O	2.16	0.46
1:A:322:VAL:O	1:A:453:ALA:HA	2.16	0.46
1:A:113:ASP:HB3	1:A:116:GLU:HG3	1.98	0.46
1:A:538:ALA:HB3	1:A:539:PRO:CD	2.46	0.46
1:B:80:ILE:HG12	1:B:132:LEU:HD23	1.97	0.45
1:A:567:ARG:HD3	1:A:597:ARG:CD	2.46	0.45
1:A:577:GLU:O	1:A:580:ALA:HB3	2.15	0.45
1:B:240:SER:O	1:B:242:ILE:N	2.49	0.45
1:A:567:ARG:HD3	1:A:597:ARG:NH1	2.31	0.45
1:B:432:GLN:OE1	1:B:484:ARG:NH1	2.48	0.45
1:A:511:MET:C	1:A:511:MET:SD	2.94	0.45
1:A:588:LEU:HD13	1:A:591:LEU:HD13	1.99	0.45
1:A:289:ASN:ND2	1:A:303:LEU:HG	2.31	0.45
1:B:416:TYR:O	1:B:420:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:321:ALA:HB3	1:B:512:PHE:CE1	2.52	0.45
1:B:73:MET:HB2	1:B:78:ARG:HB2	1.98	0.45
1:A:633:ALA:HB2	1:A:676:VAL:CB	2.42	0.45
1:A:332:ASN:N	1:A:332:ASN:HD22	2.14	0.45
1:A:393:ALA:HA	1:A:436:SER:O	2.16	0.45
1:B:191:ARG:O	1:B:194:GLN:HB2	2.16	0.45
1:A:606:GLN:HE21	1:A:639:ASP:HB3	1.82	0.45
1:B:632:ASP:OD2	1:B:633:ALA:N	2.49	0.45
1:A:454:ARG:HG3	1:A:490:ALA:CB	2.46	0.45
1:A:513:VAL:HG12	1:A:514:ARG:N	2.31	0.45
1:A:484:ARG:N	1:A:484:ARG:HD2	2.31	0.45
1:B:170:VAL:HB	1:B:203:LEU:HD13	1.98	0.45
1:A:493:TRP:HH2	1:A:510:PRO:HD2	1.82	0.45
1:B:151:ASP:O	1:B:155:TRP:HB2	2.16	0.45
1:B:164:THR:HG22	1:B:165:GLY:N	2.32	0.44
1:A:88:THR:OG1	3:A:751:FMN:O1P	2.33	0.44
1:A:78:ARG:NH2	1:A:352:ASP:OD1	2.50	0.44
1:A:404:LYS:HE3	5:A:805:HOH:O	2.16	0.44
1:A:482:SER:OG	1:A:484:ARG:HD3	2.17	0.44
1:B:568:ARG:HH21	1:B:568:ARG:CB	2.27	0.44
1:A:291:LYS:HZ2	1:A:293:ASN:ND2	2.08	0.44
1:B:338:LEU:HD21	1:B:439:PRO:HD2	1.99	0.44
1:A:283:LEU:HB3	1:A:508:LEU:HD13	1.99	0.44
1:B:222:GLN:C	1:B:225:PRO:HD2	2.37	0.44
1:B:203:LEU:HG	1:B:205:LEU:CD2	2.47	0.44
1:B:203:LEU:CG	1:B:205:LEU:HD21	2.48	0.44
1:A:514:ARG:HG3	1:A:514:ARG:NH1	2.30	0.44
1:A:363:CYS:HB3	1:A:364:PRO:HA	1.98	0.44
1:B:518:PHE:CE2	1:B:675:ASP:HB2	2.52	0.44
1:A:617:TRP:CH2	1:A:652:GLY:HA2	2.53	0.44
1:A:624:GLY:HA2	1:A:671:ARG:CZ	2.48	0.44
1:B:431:LEU:HD23	1:B:437:LEU:HD13	1.99	0.44
1:B:401:HIS:O	1:B:405:MET:HG2	2.18	0.44
1:B:633:ALA:O	1:B:638:LYS:HE2	2.18	0.44
1:B:599:GLN:NE2	1:B:599:GLN:N	2.66	0.44
1:B:614:GLU:HB2	5:B:875:HOH:O	2.18	0.44
1:B:163:LEU:N	1:B:163:LEU:HD23	2.33	0.44
1:A:140:TYR:CE1	1:A:146:THR:HG22	2.53	0.44
1:A:181:PHE:O	1:A:182:ASN:HB2	2.17	0.44
1:B:488:GLY:HA3	2:B:850:FAD:O2P	2.17	0.44
1:A:624:GLY:C	1:A:671:ARG:NH2	2.72	0.43
1:B:207:ASP:OD2	1:B:209:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:519:ARG:HG2	1:B:519:ARG:NH1	2.33	0.43
1:B:441:ILE:HG23	1:B:442:ASP:N	2.33	0.43
1:B:234:GLU:O	1:B:235:ALA:HB3	2.18	0.43
1:A:645:TYR:CE2	1:A:660:VAL:HA	2.52	0.43
1:A:228:CYS:SG	1:A:233:VAL:HG23	2.58	0.43
1:B:248:VAL:HG12	1:B:250:HIS:CD2	2.53	0.43
1:A:155:TRP:CE3	1:A:156:LEU:HD23	2.52	0.43
1:A:600:ALA:HB1	1:B:337:ILE:HB	2.00	0.43
1:B:660:VAL:HG12	1:B:664:LYS:HD3	2.01	0.43
1:B:525:THR:HG22	1:B:556:GLU:O	2.19	0.43
1:B:310:SER:C	1:B:312:ILE:H	2.21	0.43
1:B:156:LEU:HB2	1:B:187:TYR:HE2	1.83	0.43
1:A:86:SER:CB	3:A:751:FMN:O3P	2.66	0.43
1:A:350:ASN:C	1:A:350:ASN:HD22	2.17	0.43
1:B:329:ALA:HA	1:B:332:ASN:HD22	1.82	0.43
1:A:175:ASN:HB3	1:A:178:TYR:HD2	1.83	0.43
1:B:624:GLY:C	1:B:671:ARG:HH21	2.22	0.43
1:B:92:GLU:HG2	1:B:96:ASN:HD21	1.82	0.43
1:A:454:ARG:HG3	1:A:490:ALA:HB3	2.00	0.43
1:A:460:SER:HB3	1:A:470:HIS:ND1	2.32	0.43
1:A:145:PRO:HA	1:A:184:MET:HG3	2.01	0.43
1:B:409:SER:HA	1:B:413:LYS:CD	2.44	0.43
1:B:606:GLN:OE1	4:B:852:NAP:H2A	2.19	0.43
1:A:348:LEU:HB2	1:A:360:PRO:CD	2.49	0.43
1:B:564:TYR:O	1:B:593:VAL:HA	2.19	0.43
1:A:374:TYR:O	1:A:450:ARG:HD2	2.18	0.43
1:B:562:LEU:HD12	1:B:563:TYR:H	1.84	0.43
1:B:82:VAL:HG11	1:B:95:ALA:HA	2.00	0.43
1:A:86:SER:H	1:A:148:ASN:HD21	1.67	0.42
1:A:72:LYS:HB2	1:A:72:LYS:HE3	1.63	0.42
1:A:662:TYR:CD1	1:A:662:TYR:C	2.92	0.42
1:A:599:GLN:HG2	1:A:601:HIS:O	2.19	0.42
1:B:385:VAL:O	1:B:389:LEU:HG	2.19	0.42
1:B:385:VAL:HG12	1:B:389:LEU:HD12	2.01	0.42
1:B:294:GLN:CD	1:B:294:GLN:N	2.71	0.42
1:A:551:ARG:NH1	1:A:586:GLY:O	2.52	0.42
1:A:245:TYR:CD1	1:A:360:PRO:HD3	2.54	0.42
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.84	0.42
1:A:235:ALA:O	1:A:238:GLU:HG3	2.20	0.42
1:B:302:HIS:CD2	1:B:575:TYR:OH	2.65	0.42
1:A:266:LEU:O	1:A:267:LYS:CB	2.66	0.42
1:B:274:PRO:HG3	1:B:276:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:ASN:HD21	1:A:107:MET:HB3	1.85	0.42
1:A:135:PHE:HE2	1:A:192:LEU:HD11	1.77	0.42
1:A:567:ARG:HH11	1:A:567:ARG:CG	2.32	0.42
1:B:651:PHE:N	1:B:651:PHE:CD1	2.88	0.42
1:B:267:LYS:HE3	1:B:270:GLU:OE1	2.20	0.42
1:A:613:ARG:HH11	1:A:613:ARG:CG	2.16	0.42
1:A:619:LEU:H	1:A:619:LEU:HD12	1.85	0.42
1:A:553:GLN:HA	1:A:553:GLN:NE2	2.35	0.42
1:A:72:LYS:O	1:A:76:THR:HG23	2.20	0.41
1:B:474:VAL:HG13	1:B:474:VAL:O	2.20	0.41
1:B:214:GLU:HA	1:B:217:ILE:HG22	2.02	0.41
1:A:238:GLU:O	1:A:239:GLU:HB2	2.20	0.41
1:A:327:ASP:OD1	1:A:329:ALA:HB3	2.20	0.41
1:B:500:ALA:O	1:B:506:ARG:HB3	2.20	0.41
1:A:125:LEU:N	1:A:126:PRO:CD	2.83	0.41
1:B:107:MET:HE2	1:B:233:VAL:HG11	2.02	0.41
1:A:78:ARG:NH1	1:A:78:ARG:HG3	2.33	0.41
1:B:140:TYR:HE2	3:B:851:FMN:O2P	2.03	0.41
1:A:189:ASP:OD2	1:A:199:ARG:HD3	2.20	0.41
1:B:604:TYR:HB3	1:B:606:GLN:OE1	2.19	0.41
1:A:380:PRO:HA	1:A:381:PRO:HD3	1.93	0.41
1:A:94:PHE:HB3	1:A:216:PHE:CE1	2.56	0.41
1:A:599:GLN:N	1:A:599:GLN:OE1	2.54	0.41
1:B:562:LEU:HD12	1:B:563:TYR:N	2.36	0.41
1:B:87:GLN:HB2	1:B:140:TYR:CZ	2.56	0.41
1:B:80:ILE:HG12	1:B:132:LEU:CD2	2.50	0.41
1:B:214:GLU:CD	1:B:413:LYS:HE3	2.40	0.41
1:B:559:GLU:OE2	1:B:619:LEU:HD21	2.20	0.41
1:B:527:PRO:O	1:B:625:ALA:CB	2.69	0.41
1:A:90:THR:HG22	1:A:173:LEU:HD21	2.02	0.41
1:A:498:GLU:O	1:A:507:ALA:HB2	2.21	0.41
1:B:323:TYR:CD2	1:B:453:ALA:HB2	2.56	0.41
1:B:460:SER:HB3	1:B:470:HIS:CG	2.56	0.41
1:B:118:ASP:C	1:B:120:ALA:H	2.24	0.41
1:A:383:THR:HB	1:A:406:ALA:HB2	2.03	0.41
1:A:300:LEU:HD22	1:A:574:LEU:HD21	2.03	0.41
1:A:118:ASP:C	1:A:120:ALA:H	2.25	0.41
1:B:138:ALA:HB2	1:B:173:LEU:HD22	2.02	0.40
1:B:564:TYR:OH	1:B:574:LEU:HG	2.20	0.40
1:A:551:ARG:NH1	1:A:586:GLY:C	2.75	0.40
1:B:324:PRO:HA	1:B:493:TRP:CD2	2.56	0.40
1:A:78:ARG:CD	1:A:110:MET:HB3	2.50	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:518:PHE:O	1:A:519:ARG:HG2	2.22	0.40
1:A:620:ILE:CD1	1:A:627:ILE:HD11	2.51	0.40
1:B:642:ASN:HA	1:B:645:TYR:CD1	2.56	0.40
1:B:321:ALA:HB2	1:B:455:TYR:CE1	2.56	0.40
1:B:150:GLN:C	1:B:152:PHE:N	2.74	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	609/622 (98%)	536 (88%)	61 (10%)	12 (2%)	11	28
1	B	607/622 (98%)	516 (85%)	69 (11%)	22 (4%)	5	11
All	All	1216/1244 (98%)	1052 (86%)	130 (11%)	34 (3%)	8	18

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	GLU
1	B	159	THR
1	B	160	ASP
1	B	202	GLU
1	B	234	GLU
1	B	241	SER
1	A	236	THR
1	A	237	GLY
1	A	654	MET
1	B	68	SER
1	B	148	ASN
1	B	164	THR
1	B	409	SER
1	B	524	SER
1	B	651	PHE

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Mol	Chain	Res	Type
1	A	253	MET
1	A	256	ALA
1	B	147	ASP
1	B	253	MET
1	A	68	SER
1	A	238	GLU
1	A	240	SER
1	A	505	GLY
1	B	119	LEU
1	B	211	ASN
1	B	620	ILE
1	B	655	GLU
1	A	538	ALA
1	A	592	ASN
1	B	161	VAL
1	B	650	GLU
1	A	161	VAL
1	B	362	PRO
1	B	248	VAL

### 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	523/530 (99%)	500 (96%)	23 (4%)	39	71
1	B	522/530 (98%)	505 (97%)	17 (3%)	50	81
All	All	1045/1060 (99%)	1005 (96%)	40 (4%)	44	76

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	142	GLU
1	A	158	GLU
1	A	220	ARG
1	A	229	GLU
1	A	239	GLU

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Mol	Chain	Res	Type
1	A	252	ASP
1	A	283	LEU
1	A	289	ASN
1	A	290	ARG
1	A	294	GLN
1	A	303	LEU
1	A	346	MET
1	A	350	ASN
1	A	384	ASN
1	A	411	GLU
1	A	484	ARG
1	A	518	PHE
1	A	572	ASP
1	A	573	TYR
1	A	613	ARG
1	A	662	TYR
1	A	672	TYR
1	B	129	ASP
1	B	130	LYS
1	B	144	ASP
1	B	191	ARG
1	B	215	ASP
1	B	260	THR
1	B	262	GLU
1	B	294	GLN
1	B	346	MET
1	B	384	ASN
1	B	387	TYR
1	B	437	LEU
1	B	552	GLU
1	B	573	TYR
1	B	591	LEU
1	B	646	ASP
1	B	664	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	150	GLN
1	A	157	GLN
1	A	182	ASN

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Mol	Chain	Res	Type
1	A	190	GLN
1	A	289	ASN
1	A	293	ASN
1	A	332	ASN
1	A	350	ASN
1	A	359	HIS
1	A	384	ASN
1	A	399	GLN
1	A	401	HIS
1	A	452	GLN
1	A	467	ASN
1	A	486	ASN
1	A	553	GLN
1	A	590	GLN
1	A	607	HIS
1	B	79	ASN
1	B	87	GLN
1	B	96	ASN
1	B	157	GLN
1	B	250	HIS
1	B	272	GLN
1	B	294	GLN
1	B	302	HIS
1	B	332	ASN
1	B	349	ASN
1	B	467	ASN
1	B	486	ASN
1	B	590	GLN
1	B	599	GLN
1	B	635	ASN
1	B	641	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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



## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	FAD	A	750	-	58,58,58	2.50	24 (41%)	85,89,89	2.16	15 (17%)
3	FMN	A	751	-	33,33,33	2.20	12 (36%)	46,50,50	2.18	10 (21%)
4	NAP	A	752	-	52,52,52	3.49	21 (40%)	80,80,80	1.86	15 (18%)
2	FAD	B	850	-	58,58,58	2.69	23 (39%)	85,89,89	2.38	19 (22%)
3	FMN	B	851	-	33,33,33	2.44	15 (45%)	46,50,50	2.31	12 (26%)
4	NAP	B	852	-	52,52,52	3.45	19 (36%)	80,80,80	1.73	14 (17%)

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	750	-	-	0/34/50/50	0/1/6/6
3	FMN	A	751	-	-	0/18/18/18	0/0/3/3
4	NAP	A	752	-	-	0/35/67/67	0/3/5/5
2	FAD	B	850	-	-	0/34/50/50	0/1/6/6
3	FMN	B	851	-	-	0/18/18/18	0/0/3/3
4	NAP	B	852	-	-	0/35/67/67	0/3/5/5

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	752	NAP	C2N-N1N	13.02	1.52	1.35
4	B	852	NAP	C2N-N1N	12.83	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	852	NAP	C4N-C3N	10.48	1.57	1.39
4	A	752	NAP	C4N-C3N	9.98	1.56	1.39
4	A	752	NAP	C4A-N3A	9.51	1.50	1.35
2	B	850	FAD	C1'-C2'	9.25	1.60	1.51
4	B	852	NAP	C4A-N3A	8.58	1.48	1.35
2	B	850	FAD	C9A-N10	7.22	1.49	1.38
3	B	851	FMN	C9A-N10	7.11	1.49	1.38
2	A	750	FAD	C9A-N10	7.00	1.49	1.38
4	A	752	NAP	C6N-C5N	6.40	1.53	1.38
3	A	751	FMN	C9A-N10	6.25	1.48	1.38
4	B	852	NAP	C6N-C5N	6.25	1.53	1.38
2	A	750	FAD	C4A-N3A	6.14	1.45	1.35
2	B	850	FAD	C10-N10	5.80	1.51	1.38
3	B	851	FMN	C10-N10	5.79	1.51	1.38
4	A	752	NAP	C7N-N7N	5.67	1.45	1.33
2	B	850	FAD	C4A-N3A	5.52	1.44	1.35
4	A	752	NAP	PA-O3	-5.50	1.49	1.59
4	B	852	NAP	PA-O3	-5.26	1.50	1.59
4	B	852	NAP	PN-O3	-5.25	1.49	1.60
4	B	852	NAP	C7N-N7N	5.24	1.44	1.33
2	A	750	FAD	C10-N10	4.95	1.49	1.38
4	A	752	NAP	PN-O3	-4.90	1.50	1.60
4	B	852	NAP	C2A-N1A	4.71	1.43	1.33
4	A	752	NAP	C2A-N1A	4.71	1.43	1.33
4	A	752	NAP	C4A-N9A	-4.65	1.31	1.37
2	A	750	FAD	C1'-C2'	4.63	1.56	1.51
3	A	751	FMN	C10-N10	4.62	1.48	1.38
2	B	850	FAD	C5'-C4'	-4.56	1.44	1.51
4	B	852	NAP	C4A-N9A	-4.43	1.31	1.37
2	B	850	FAD	C4-C4X	4.17	1.48	1.41
4	B	852	NAP	PN-O5D	-4.12	1.46	1.60
2	A	750	FAD	C5X-N5	4.06	1.41	1.35
2	A	750	FAD	C5'-C4'	-3.97	1.45	1.51
2	A	750	FAD	C9A-C5X	3.95	1.50	1.42
2	A	750	FAD	C6-C5X	3.90	1.46	1.41
2	B	850	FAD	P-O3P	-3.89	1.52	1.59
3	A	751	FMN	C1'-N10	-3.74	1.43	1.48
4	A	752	NAP	PN-O5D	-3.66	1.48	1.60
3	B	851	FMN	C9-C9A	3.61	1.47	1.40
2	B	850	FAD	C5X-N5	3.54	1.40	1.35
2	A	750	FAD	C2'-C3'	3.54	1.60	1.53
2	B	850	FAD	C2A-N3A	3.52	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	FAD	C8A-N9A	3.41	1.41	1.36
2	A	750	FAD	C8-C7	3.38	1.50	1.40
2	B	850	FAD	C6-C5X	3.38	1.45	1.41
2	B	850	FAD	C4-N3	3.29	1.42	1.37
3	B	851	FMN	C8-C7	3.19	1.50	1.40
4	B	852	NAP	P2B-O2B	-3.12	1.50	1.59
4	A	752	NAP	P2B-O2B	-3.10	1.50	1.59
3	A	751	FMN	C5A-N5	3.09	1.40	1.35
2	B	850	FAD	C8-C7	3.01	1.49	1.40
2	A	750	FAD	P-O3P	-2.97	1.54	1.59
3	B	851	FMN	C4-C4A	2.96	1.46	1.41
2	A	750	FAD	C4X-N5	2.96	1.42	1.36
3	A	751	FMN	C9-C9A	2.95	1.46	1.40
3	B	851	FMN	C1'-C2'	2.92	1.54	1.51
2	A	750	FAD	PA-O5B	-2.89	1.46	1.59
2	B	850	FAD	C9A-C5X	2.88	1.48	1.42
3	B	851	FMN	C4A-C10	2.86	1.45	1.40
2	B	850	FAD	C9-C9A	2.82	1.46	1.40
2	B	850	FAD	PA-O3P	-2.80	1.54	1.59
4	B	852	NAP	PA-O5B	-2.75	1.46	1.59
2	A	750	FAD	C6-C7	2.72	1.45	1.37
4	B	852	NAP	C8A-N9A	2.72	1.40	1.36
2	B	850	FAD	PA-O5B	-2.72	1.46	1.59
4	A	752	NAP	C8A-N7A	-2.72	1.29	1.34
3	A	751	FMN	C8-C7	2.72	1.48	1.40
2	A	750	FAD	C4-C4X	2.71	1.45	1.41
3	A	751	FMN	C4A-N5	2.70	1.41	1.36
2	A	750	FAD	C4X-C10	2.70	1.45	1.40
4	B	852	NAP	C8A-N7A	-2.69	1.29	1.34
3	B	851	FMN	C10-N1	2.67	1.40	1.35
4	A	752	NAP	C2A-N3A	2.67	1.37	1.32
2	B	850	FAD	C2'-C3'	2.64	1.59	1.53
3	A	751	FMN	C4-C4A	2.64	1.45	1.41
2	A	750	FAD	C2A-N1A	2.62	1.39	1.33
3	B	851	FMN	C4'-C3'	2.55	1.58	1.53
3	B	851	FMN	C5A-N5	2.53	1.39	1.35
4	A	752	NAP	PA-O5B	-2.51	1.47	1.59
3	B	851	FMN	C9A-C5A	2.48	1.47	1.42
4	B	852	NAP	C3N-C7N	2.46	1.54	1.50
3	A	751	FMN	C4A-C10	2.46	1.45	1.40
3	A	751	FMN	P-O3P	-2.45	1.45	1.54
4	A	752	NAP	C6A-N6A	-2.38	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	851	FMN	P-O3P	-2.35	1.46	1.54
3	B	851	FMN	C1'-N10	-2.33	1.45	1.48
2	A	750	FAD	C8A-N7A	2.33	1.39	1.34
2	B	850	FAD	C2B-C1B	2.31	1.56	1.53
2	A	750	FAD	C2A-N3A	2.30	1.36	1.32
2	A	750	FAD	C9-C9A	2.28	1.45	1.40
4	A	752	NAP	C5D-C4D	2.27	1.59	1.51
2	A	750	FAD	O4-C4	-2.27	1.20	1.24
4	A	752	NAP	C5A-C4A	-2.25	1.35	1.40
4	A	752	NAP	C3N-C7N	2.24	1.54	1.50
4	B	852	NAP	C5D-C4D	2.23	1.58	1.51
2	B	850	FAD	C4X-N5	2.23	1.40	1.36
4	B	852	NAP	C6A-N6A	-2.19	1.28	1.35
3	B	851	FMN	P-O2P	-2.18	1.46	1.54
4	B	852	NAP	P2B-O2X	-2.17	1.46	1.54
2	B	850	FAD	C6-C7	2.17	1.43	1.37
3	A	751	FMN	C6-C5A	2.16	1.44	1.41
2	A	750	FAD	PA-O3P	-2.16	1.56	1.59
4	A	752	NAP	P2B-O3X	-2.12	1.47	1.54
2	B	850	FAD	C4X-C10	2.09	1.44	1.40
4	A	752	NAP	C8A-N9A	2.08	1.39	1.36
2	B	850	FAD	C2-N3	2.08	1.41	1.37
4	B	852	NAP	C6A-C5A	2.05	1.54	1.42
3	A	751	FMN	P-O2P	-2.04	1.47	1.54
3	B	851	FMN	C8M-C8	2.03	1.55	1.51
4	A	752	NAP	C6A-C5A	2.02	1.54	1.42
2	A	750	FAD	C4A-N9A	2.02	1.40	1.37
2	B	850	FAD	O2B-C2B	2.01	1.47	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	850	FAD	C2'-C1'-N10	-13.11	95.06	112.45
2	A	750	FAD	C2'-C1'-N10	-9.87	99.36	112.45
3	A	751	FMN	C4A-C10-N10	-9.26	115.89	120.51
3	B	851	FMN	C4A-C10-N10	-8.93	116.05	120.51
2	B	850	FAD	C2-N1-C10	7.64	122.68	114.98
2	B	850	FAD	C4X-C10-N10	-7.39	116.82	120.51
2	A	750	FAD	C2-N1-C10	7.34	122.38	114.98
4	A	752	NAP	O4B-C1B-N9A	7.22	115.16	108.44
4	B	852	NAP	O4B-C1B-N9A	6.66	114.63	108.44
2	A	750	FAD	C1'-N10-C9A	6.35	125.05	118.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	752	NAP	N3A-C2A-N1A	-6.24	123.49	128.71
4	A	752	NAP	O4D-C1D-N1N	6.15	114.24	107.95
4	B	852	NAP	N3A-C2A-N1A	-6.08	123.63	128.71
2	A	750	FAD	C4X-C10-N10	-5.94	117.54	120.51
2	B	850	FAD	C1'-N10-C9A	5.79	124.50	118.87
4	A	752	NAP	O2N-PN-O1N	-4.91	103.92	118.72
3	B	851	FMN	C10-C4A-N5	4.89	126.39	120.45
3	A	751	FMN	C10-C4A-N5	4.84	126.33	120.45
3	B	851	FMN	P-O5'-C5'	4.32	130.69	118.19
3	B	851	FMN	C2-N1-C10	4.11	119.12	114.98
2	B	850	FAD	N3A-C2A-N1A	-4.11	125.27	128.71
2	A	750	FAD	C10-C4X-N5	4.02	125.34	120.45
4	B	852	NAP	O2N-PN-O1N	-3.90	106.95	118.72
3	A	751	FMN	C2-N1-C10	3.83	118.84	114.98
2	B	850	FAD	C8A-N9A-C4A	-3.80	104.00	106.90
3	B	851	FMN	C6-C5A-N5	-3.74	114.61	118.97
2	A	750	FAD	C8A-N9A-C4A	-3.74	104.04	106.90
4	B	852	NAP	O4D-C1D-N1N	3.69	111.73	107.95
4	B	852	NAP	N6A-C6A-N1A	3.69	126.61	119.36
2	B	850	FAD	C10-C4X-N5	3.59	124.81	120.45
2	A	750	FAD	N3A-C2A-N1A	-3.54	125.75	128.71
2	A	750	FAD	O4B-C1B-N9A	-3.50	105.19	108.44
4	A	752	NAP	N6A-C6A-N1A	3.49	126.22	119.36
2	A	750	FAD	C4'-C3'-C2'	3.37	120.85	113.25
3	A	751	FMN	P-O5'-C5'	3.30	127.73	118.19
3	B	851	FMN	O3P-P-O5'	-3.29	97.57	106.65
4	B	852	NAP	O7N-C7N-C3N	3.24	123.23	119.58
2	A	750	FAD	C4A-C5A-N7A	3.21	112.27	109.52
4	B	852	NAP	O7N-C7N-N7N	-3.19	117.98	122.59
2	A	750	FAD	C8A-N9A-C1B	3.12	132.53	126.38
2	A	750	FAD	C1'-N10-C10	-3.10	114.76	119.17
2	B	850	FAD	O4B-C1B-N9A	-3.10	105.56	108.44
3	B	851	FMN	C9A-C5A-N5	3.09	127.11	122.37
2	B	850	FAD	C1'-N10-C10	-3.02	114.88	119.17
4	A	752	NAP	C1B-N9A-C4A	-2.86	121.69	126.64
2	B	850	FAD	C4A-C5A-N7A	2.86	111.97	109.52
4	B	852	NAP	C4D-O4D-C1D	2.86	112.85	109.75
2	B	850	FAD	C4'-C3'-C2'	2.78	119.53	113.25
4	A	752	NAP	C4D-O4D-C1D	2.77	112.76	109.75
2	B	850	FAD	C8A-N9A-C1B	2.74	131.78	126.38
3	A	751	FMN	C9A-C5A-N5	2.70	126.51	122.37
3	A	751	FMN	C6-C5A-N5	-2.69	115.83	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	752	NAP	O7N-C7N-C3N	2.68	122.59	119.58
3	B	851	FMN	C4'-C3'-C2'	-2.65	107.25	113.25
4	A	752	NAP	C3B-C2B-C1B	-2.64	97.60	102.73
4	B	852	NAP	C2A-N1A-C6A	2.58	123.42	118.77
4	A	752	NAP	PN-O3-PA	-2.56	121.97	132.95
4	A	752	NAP	O7N-C7N-N7N	-2.55	118.90	122.59
4	B	852	NAP	C1B-N9A-C4A	-2.53	122.26	126.64
3	B	851	FMN	O4'-C4'-C3'	-2.52	102.78	109.05
4	B	852	NAP	O3X-P2B-O2B	2.51	114.32	107.09
3	A	751	FMN	O3P-P-O5'	-2.50	99.75	106.65
4	A	752	NAP	C2A-N1A-C6A	2.46	123.22	118.77
2	B	850	FAD	C5X-C9A-N10	-2.44	114.41	116.80
2	B	850	FAD	C9A-C5X-N5	2.37	126.00	122.37
2	A	750	FAD	N3-C2-N1	-2.36	116.18	121.19
2	B	850	FAD	N3-C2-N1	-2.35	116.19	121.19
3	A	751	FMN	O2P-P-O1P	2.34	118.08	110.44
4	B	852	NAP	PN-O3-PA	-2.33	122.96	132.95
2	A	750	FAD	O3'-C3'-C4'	-2.29	102.94	108.74
3	B	851	FMN	C9A-N10-C10	-2.27	119.54	121.77
3	A	751	FMN	O4'-C4'-C3'	-2.25	103.43	109.05
4	A	752	NAP	C3D-C2D-C1D	2.25	104.42	100.91
2	B	850	FAD	O2'-C2'-C1'	2.17	115.09	109.71
2	B	850	FAD	C9-C9A-N10	2.15	126.23	121.59
4	B	852	NAP	O2B-P2B-O1X	2.15	112.80	106.79
4	B	852	NAP	C2N-N1N-C1D	-2.15	114.02	119.33
2	B	850	FAD	C6-C5X-N5	-2.13	116.50	118.97
2	A	750	FAD	C9A-C5X-N5	2.12	125.62	122.37
3	A	751	FMN	C4'-C3'-C2'	-2.11	108.47	113.25
4	A	752	NAP	C8A-N9A-C1B	2.09	130.50	126.38
4	A	752	NAP	O2B-P2B-O1X	2.06	112.55	106.79
2	B	850	FAD	C2B-C1B-N9A	2.05	118.54	113.27
3	B	851	FMN	C7M-C7-C6	-2.05	115.44	120.38
3	B	851	FMN	O2P-P-O1P	2.05	117.13	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	613/622 (98%)	-0.57	0	100   100	16, 36, 57, 87	0
1	B	611/622 (98%)	-0.35	4 (0%)	84   89	16, 44, 92, 107	0
All	All	1224/1244 (98%)	-0.46	4 (0%)	90   95	16, 38, 85, 107	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ALA	3.1
1	B	178	TYR	2.6
1	B	136	CYS	2.5
1	B	240	SER	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FMN	B	851	31/31	0.28	1.33	75,91,94,94	0
4	NAP	B	852	48/48	0.13	0.81	26,34,72,74	0
3	FMN	A	751	31/31	0.16	0.53	37,55,58,58	0
2	FAD	A	750	53/53	0.14	0.19	24,30,35,35	0
4	NAP	A	752	48/48	0.13	0.15	26,40,70,74	0
2	FAD	B	850	53/53	0.12	0.10	16,21,24,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.