



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:53 pm GMT

PDB ID : 2BN4
Title : A SECOND FMN-BINDING SITE IN YEAST NADPH-CYTOCHROME
P450 REDUCTASE SUGGESTS A NOVEL MECHANISM OF ELECTRON
TRANSFER BY DIFLAVIN REDUCTASE
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Deposited on : 2005-03-18
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

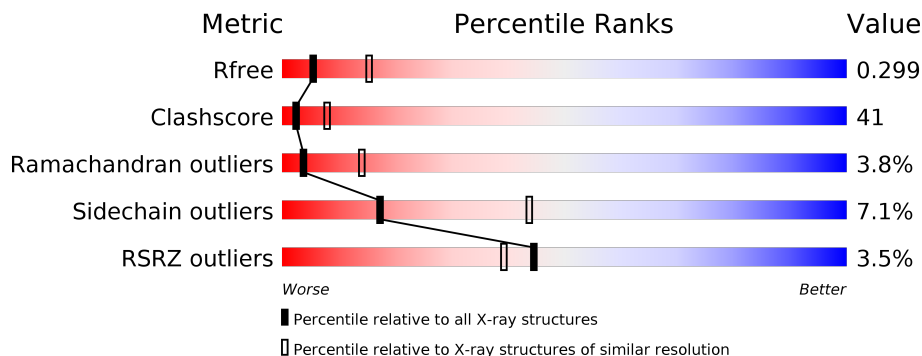
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	100719	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)

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 ≥ 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	682	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>49%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	682	<div> <div>4%</div> <div> <div></div> <div>33%</div> <div>55%</div> <div>6%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10331 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.

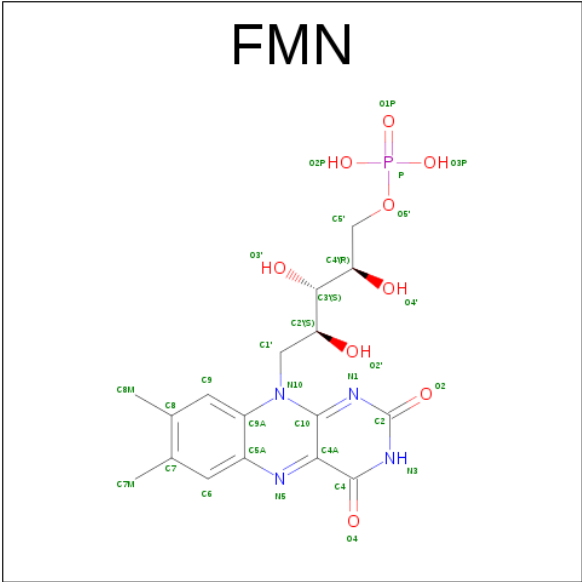
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	0	0
			5021	3202	827	977	15			
1	B	641	Total	C	N	O	S	0	0	0
			5007	3191	825	976	15			

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



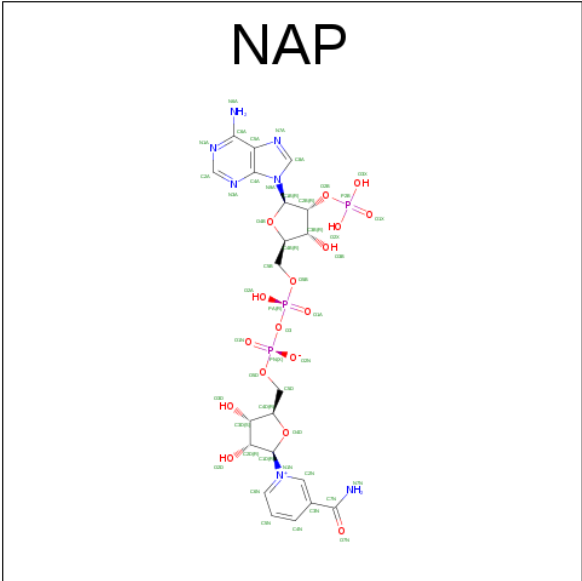
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 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-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	22	Total	O	0	0
			22	22		

E633	M634	I635	N636	G637	G638	A639	F640	I641	Y642	V643	C644	G645	D646	A647	K648	G649	M650	A651	K652	G653	V654	S655	T656	A657	L658	G659	G660	I661	L662	S663	R664	G665	K666	T669	E672	A673	T674	E675	L676	I677	L680	K681	T682	S683	G684	R685	Y686	Q687	V690	W691						
Q562	K563	N568	V569	S570	L571	G572	K573	H574	L575	L576	F577	G579	S580	R581	N582	T583	D584	D585	F586	Q589	D590	E591	E594	Y595	A596	K597	K598	L599	D600	G601	T534	P535	V536	L537	M538	L539	S540	P541	G542	T543	G544	V545	P547	F548	B549	G550	P551	L552	R553	E554	B555	V556	A557	F558	G631	F632
T494	A495	E496	T497	N498	L499	P500	V501	H502	Y503	P508	R509	K510	L511	F512	A513	N514	Y515	K516	L517	P518	V519	H520	N521	R522	R527	L528	P529	S530	T534	P535	V536	L537	M538	L539	S540	P541	G542	T543	G544	V545	P547	F548	B549	G550	P551	L552	R553	E554	B555	V556	A557	F558	G631	F632		
M426	Q427	F428	L429	T430	V431	E432	S433	V434	Q435	M436	T437	P438	R439	Y440	S441	I442	S443	S444	S445	S446	L447	S448	E449	K450	K451	Q452	T453	V454	M455	V456	I459	V460	M465	P466	E467	L468	P469	D470	A471	P472	P473	P474	V475	G476	V477	T478	T479	M480	L481	L482	R483	M484	I485	Q486	L487	N493
L360	E361	T362	G364	Q369	L370	F371	S372	S373	L374	A375	I376	Q377	Q378	A379	N380	A381	D382	V383	S384	K385	L386	L387	L390	S391	K392	D395	Q396	F397	A398	V399	I400	T402	S403	K404	Y405	F406	N407	I408	K409	D410	A411	L412	K413	Y414	L415	S416	A419	K420	W421	D422	T423	V424	P425			
D293	L294	S295	L299	Y301	D305	H306	L307	A308	V309	W310	P311	S312	N313	P314	L315	E316	F321	L322	Q323	I324	F325	R326	S327	D328	P329	E330	T331	L332	F333	L335	K336	P337	L338	D339	P340	T341	V342	K343	V344	P345	F346	P347	T348	P349	T350	T351	L352	G353	A354	K355	L356	K357	H358	Y359		
R146	Y147	M148	F150	G151	L152	G153	N154	F156	Y157	E158	F159	F160	N161	G162	A163	A164	K165	K166	K169	H170	A173	A174	G175	L179	E184	A185	G188	A189	G190	T191	T192	Y196	W199	K200	D201	I203	L207	E210	L211	L213	R215	N216	C217	T218	A219	H220	F222									
K77	S80	K81	E82	L83	W84	F87	N88	L89	N90	V91	N92	C93	N94	G95	A96	V97	N98	Y99	D100	F101	E102	S103	L104	D106	V107	P108	Y109	I110	I113	T117	Y118	G119	E120	P124	D125	N129	F130	F133	I134	C135	N136	A137	E138	A139	G140	A141	L142	S143	N144	L145						
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	LEU	ASP	ILE	MET	SER	ASP	ASP	GLY	ASP	ASP	ILE	THR	ALA	VAL	SER	SER	SER	GLY	N47	R48	D49	I50	Q52	V53	V54	K59	N60	Y61	L62	V63	A66	S67	Q68	T69	A72	E73	D74	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 77.84Å 261.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.41 – 2.91 43.41 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.1 (43.41-2.91) 91.3 (43.41-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.300 0.239 , 0.299	Depositor DCC
R_{free} test set	3256 reflections (9.89%)	DCC
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.135 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10331	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.42	0/5137	0.69	1/6978 (0.0%)
1	B	0.42	0/5120	0.68	1/6952 (0.0%)
All	All	0.42	0/10257	0.69	2/13930 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ASN	N-CA-C	-6.79	92.66	111.00
1	B	312	SER	N-CA-C	-5.11	97.21	111.00

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	5021	0	4876	362	0
1	B	5007	0	4880	463	0
2	A	53	0	31	2	0
2	B	53	0	31	4	0
3	A	31	0	19	3	0
3	B	31	0	19	2	0
4	A	40	0	19	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	40	0	19	1	0
5	A	33	0	0	3	0
5	B	22	0	0	5	0
All	All	10331	0	9894	822	0

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

All (822) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLU:HG2	1:A:436:MET:HA	1.30	1.13
1:A:528:LEU:HD23	1:A:529:PRO:HD2	1.28	1.11
1:B:59:LYS:HD3	1:B:92:MET:HB2	1.22	1.10
1:A:67:SER:HB2	1:A:72:ALA:HB3	1.39	1.05
1:B:482:LEU:HA	1:B:485:ILE:HD12	1.42	1.01
1:A:60:ASN:HD21	1:A:89:LEU:HB3	1.28	0.99
1:A:449:SER:HB3	1:A:557:ALA:HB2	1.45	0.98
1:B:327:LEU:HD11	1:B:352:ILE:HD13	1.46	0.96
1:A:379:PRO:HD2	1:A:383:VAL:HG11	1.46	0.95
1:B:225:GLN:HB3	1:B:336:LYS:HB3	1.48	0.95
1:A:322:LEU:HD13	1:A:329:PRO:HG3	1.49	0.94
1:A:60:ASN:ND2	1:A:89:LEU:HB3	1.82	0.94
1:B:467:GLU:O	1:B:469:PRO:HD3	1.68	0.93
1:B:449:SER:HB3	1:B:557:ALA:HB2	1.49	0.93
1:B:623:LYS:HE2	1:B:623:LYS:HA	1.53	0.91
1:A:612:LEU:HD23	1:A:613:PRO:HD2	1.51	0.91
1:A:647:ALA:CB	1:A:690:VAL:HG11	2.01	0.91
1:B:633:GLU:HG2	1:B:637:ASN:HD21	1.36	0.90
1:A:178:ARG:HH21	1:A:181:LYS:HA	1.34	0.90
1:A:50:ILE:HG23	1:A:51:ALA:H	1.37	0.90
1:B:278:GLU:OE2	1:B:286:ASN:HB3	1.71	0.90
1:B:105:ASN:ND2	1:B:142:LEU:HA	1.87	0.90
1:A:647:ALA:HB2	1:A:690:VAL:HG11	1.54	0.89
1:B:659:VAL:HG22	1:B:677:ILE:HG13	1.52	0.89
1:A:529:PRO:HD3	1:A:642:TYR:OH	1.72	0.89
1:B:273:ILE:HD12	1:B:485:ILE:HG21	1.55	0.88
1:B:380:ASN:ND2	1:B:382:ASP:H	1.73	0.87
1:B:67:SER:HB2	1:B:72:ALA:HB3	1.57	0.86
1:A:246:LEU:HB2	1:A:249:HIS:HD2	1.40	0.86
1:B:647:ALA:HA	1:B:650:MET:HB3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLU:OE2	1:A:436:MET:HG3	1.77	0.84
1:A:467:GLU:O	1:A:469:PRO:HD3	1.77	0.84
1:B:416:SER:HB2	1:B:419:ALA:HB3	1.60	0.84
1:B:640:PHE:HB3	1:B:642:TYR:HE1	1.42	0.84
1:B:105:ASN:HD22	1:B:142:LEU:HA	1.39	0.84
1:A:493:ASN:ND2	1:A:496:GLU:HB2	1.91	0.84
1:B:379:PRO:HD2	1:B:383:VAL:HB	1.60	0.83
1:B:87:PHE:HB2	1:B:89:LEU:HD12	1.60	0.83
1:A:648:LYS:HE3	4:A:753:NAP:N1N	1.93	0.82
1:B:185:ALA:HB1	1:B:192:THR:HG23	1.62	0.82
1:B:247:PRO:HG2	1:B:509:ARG:NH1	1.93	0.81
1:A:599:LEU:HD12	1:A:603:PHE:HB2	1.61	0.81
1:A:666:LYS:HE3	1:A:676:LEU:HD21	1.62	0.81
1:B:562:GLN:CB	1:B:568:ASN:HB3	2.11	0.80
1:A:416:SER:HB3	1:A:419:ALA:HB3	1.63	0.80
1:A:105:ASN:ND2	1:A:142:LEU:HA	1.96	0.80
1:B:327:LEU:HD11	1:B:352:ILE:CD1	2.11	0.79
1:A:247:PRO:HG2	1:A:509:ARG:NH1	1.96	0.79
1:B:540:GLY:HA3	1:B:548:PHE:HE1	1.47	0.79
1:B:238:LEU:HD12	1:B:509:ARG:HE	1.48	0.79
1:B:220:PHE:H	1:B:376:GLN:HE22	1.29	0.79
1:A:623:LYS:HA	1:A:623:LYS:HE2	1.65	0.79
1:A:130:PHE:CE1	1:A:134:ILE:HD11	2.19	0.78
1:A:54:VAL:HG13	1:A:59:LYS:HB2	1.66	0.78
1:A:130:PHE:CZ	1:A:134:ILE:HD11	2.19	0.78
1:A:318:VAL:HG13	1:A:356:ILE:HG22	1.65	0.78
1:B:68:GLN:HB2	1:B:124:PRO:HB3	1.65	0.78
1:B:640:PHE:HB3	1:B:642:TYR:CE1	2.18	0.78
1:A:49:ASP:O	1:A:53:VAL:HG23	1.84	0.78
1:B:220:PHE:H	1:B:376:GLN:NE2	1.82	0.77
1:B:508:PRO:O	1:B:511:LEU:HB2	1.87	0.75
1:A:115:ILE:HD11	1:A:163:ALA:HB1	1.67	0.75
1:A:211:LEU:HB2	1:A:213:LEU:HG	1.69	0.75
1:B:328:ASP:OD2	1:B:330:GLU:HB2	1.85	0.75
1:B:465:ASN:HB2	5:B:2016:HOH:O	1.86	0.75
1:A:260:LEU:HA	1:A:298:ASN:OD1	1.85	0.75
1:B:372:SER:HB2	1:B:391:SER:HB2	1.69	0.75
1:B:96:VAL:HG21	1:B:130:PHE:CD2	2.21	0.75
1:A:528:LEU:HD23	1:A:529:PRO:CD	2.14	0.75
1:A:226:TYR:HB2	1:A:427:GLN:HG2	1.69	0.74
1:B:322:LEU:HD13	1:B:329:PRO:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:HB3	1:A:98:ASN:ND2	2.03	0.73
1:B:327:LEU:HD12	1:B:328:ASP:N	2.03	0.73
1:B:323:SER:O	1:B:420:LYS:HE3	1.88	0.73
1:A:398:ALA:HA	1:A:402:THR:HB	1.70	0.73
1:B:59:LYS:HE2	1:B:341:THR:HG21	1.68	0.73
1:A:449:SER:HB3	1:A:557:ALA:CB	2.19	0.73
1:B:263:PHE:HD2	1:B:268:PRO:O	1.72	0.73
1:B:327:LEU:CD1	1:B:352:ILE:HD13	2.18	0.73
1:A:346:PHE:CD2	1:A:359:TYR:HB3	2.23	0.73
1:A:326:ASN:HB2	1:A:420:LYS:HD3	1.71	0.73
1:B:449:SER:O	1:B:450:GLU:HG3	1.89	0.73
1:A:230:ASN:HD22	1:A:231:GLU:HG2	1.54	0.72
1:B:535:PRO:HB2	1:B:639:ALA:HB2	1.69	0.72
1:B:437:THR:HG22	1:B:438:PRO:O	1.89	0.72
1:A:154:ASN:OD1	1:A:156:THR:HG22	1.89	0.72
1:A:426:MET:O	1:A:430:VAL:HG23	1.89	0.72
1:B:113:ILE:O	1:B:149:MET:HG3	1.89	0.72
1:A:78:LYS:HE2	1:A:367:SER:OG	1.89	0.72
1:A:59:LYS:HE2	1:A:92:MET:HB2	1.70	0.72
1:B:535:PRO:HB2	1:B:639:ALA:CB	2.19	0.72
1:A:233:THR:HG22	1:A:234:ASP:H	1.54	0.72
1:B:88:ASN:HD21	1:B:216:GLN:NE2	1.87	0.71
1:A:628:GLU:HG3	1:A:629:ASP:N	2.05	0.71
1:B:220:PHE:N	1:B:376:GLN:HE22	1.88	0.71
1:A:138:GLU:HG3	1:A:139:ALA:H	1.56	0.70
1:B:633:GLU:HG2	1:B:637:ASN:ND2	2.04	0.70
1:B:50:ILE:HG23	1:B:51:ALA:H	1.55	0.70
1:B:473:PRO:O	1:B:475:VAL:HG13	1.91	0.70
1:B:528:LEU:HD12	1:B:528:LEU:H	1.57	0.70
1:A:535:PRO:HB2	1:A:639:ALA:HB2	1.72	0.70
1:B:562:GLN:HB2	1:B:568:ASN:HB3	1.73	0.70
1:B:576:LEU:HD12	1:B:577:PHE:N	2.07	0.70
1:B:154:ASN:OD1	1:B:156:THR:HB	1.93	0.69
1:B:361:GLU:HG2	1:B:436:MET:HA	1.73	0.69
1:B:547:PRO:HG2	1:B:644:CYS:SG	2.32	0.69
1:A:233:THR:HG22	1:A:234:ASP:N	2.07	0.69
1:B:581:ARG:HD3	1:B:611:ARG:NH1	2.08	0.69
1:A:51:ALA:HB2	1:A:103:SER:O	1.93	0.68
1:A:50:ILE:HG23	1:A:51:ALA:N	2.07	0.68
1:A:565:GLY:O	1:A:567:ASN:N	2.27	0.68
1:A:144:ASN:OD1	1:B:109:VAL:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLU:HG3	1:B:401:ILE:HD12	1.75	0.68
1:A:273:ILE:HD12	1:A:485:ILE:HG21	1.76	0.68
1:B:279:LEU:HD11	1:B:289:HIS:HB2	1.76	0.68
1:A:361:GLU:HG2	1:A:436:MET:CA	2.17	0.68
1:B:528:LEU:HG	1:B:551:PHE:CD2	2.28	0.67
1:A:292:PHE:O	1:A:453:THR:HG22	1.95	0.67
1:A:97:GLU:HB2	1:A:126:GLY:O	1.94	0.67
1:B:295:SER:HA	1:B:452:GLN:NE2	2.09	0.67
1:A:236:MET:O	1:A:246:LEU:HD22	1.95	0.67
1:B:288:ILE:HD11	1:B:483:ARG:HD2	1.76	0.67
1:A:322:LEU:HD13	1:A:329:PRO:CG	2.23	0.67
1:B:380:ASN:OD1	1:B:383:VAL:HG23	1.94	0.67
1:B:445:SER:HB3	1:B:455:HIS:CG	2.29	0.67
1:A:152:LEU:H	1:A:152:LEU:HD12	1.59	0.67
1:A:370:LEU:HD13	1:A:370:LEU:O	1.95	0.67
1:B:400:GLU:C	1:B:401:ILE:HD12	2.15	0.67
1:B:514:ASN:HB2	1:B:516:LYS:HE3	1.77	0.67
1:A:100:ASP:OD1	1:A:102:GLU:HG2	1.95	0.67
1:A:476:GLY:HA3	2:A:750:FAD:O2P	1.94	0.67
1:B:481:LEU:HD13	1:B:503:TYR:CG	2.30	0.66
1:A:95:ASP:OD2	1:A:97:GLU:HB3	1.95	0.66
1:B:573:LYS:HE3	1:B:634:MET:HG2	1.77	0.66
1:A:322:LEU:CD1	1:A:329:PRO:HG3	2.26	0.66
1:A:270:ILE:HD13	1:A:511:LEU:HD22	1.77	0.66
1:B:225:GLN:NE2	1:B:336:LYS:HD3	2.09	0.66
1:A:246:LEU:HB2	1:A:249:HIS:CD2	2.28	0.66
1:B:538:MET:HE3	1:B:576:LEU:HB2	1.77	0.66
1:A:547:PRO:HG2	1:A:644:CYS:SG	2.36	0.66
1:A:625:LYS:HG3	1:A:664:ARG:HH12	1.61	0.66
1:B:130:PHE:CZ	1:B:134:ILE:HD11	2.30	0.66
1:A:646:ASP:OD1	1:A:648:LYS:HG3	1.96	0.66
1:B:352:ILE:HD11	1:B:426:MET:HG3	1.75	0.66
1:B:487:LEU:HD12	1:B:499:LEU:HD22	1.77	0.66
1:B:632:PHE:CE1	1:B:665:GLY:HA3	2.30	0.65
1:A:240:GLU:OE2	1:A:508:PRO:HB3	1.95	0.65
1:A:677:ILE:HG22	1:A:681:LYS:HE3	1.77	0.65
1:A:194:GLU:OE1	1:A:368:ARG:NH1	2.30	0.65
1:A:69:THR:HB	3:A:751:FMN:O1P	1.96	0.65
1:B:449:SER:HB3	1:B:557:ALA:CB	2.26	0.65
1:B:82:GLU:OE1	1:B:200:LYS:HD2	1.97	0.65
1:B:95:ASP:HB3	1:B:98:ASN:ND2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ALA:HB2	1:B:103:SER:O	1.97	0.65
1:B:59:LYS:HD3	1:B:92:MET:CB	2.15	0.64
1:B:152:LEU:HD12	1:B:152:LEU:H	1.62	0.64
1:B:265:LEU:HG	1:B:522:ARG:HH12	1.62	0.64
1:B:609:HIS:HB3	1:B:612:LEU:HG	1.80	0.64
1:B:327:LEU:HG	1:B:352:ILE:HG21	1.78	0.64
1:B:600:ASP:OD1	1:B:601:GLY:N	2.28	0.64
1:A:278:GLU:OE2	1:A:286:ASN:HB3	1.97	0.64
1:A:425:PRO:HB3	1:A:427:GLN:OE1	1.98	0.64
1:B:100:ASP:OD1	1:B:102:GLU:HG2	1.97	0.64
1:B:400:GLU:O	1:B:401:ILE:HD12	1.98	0.64
1:A:562:GLN:HB3	1:A:568:ASN:HA	1.79	0.63
1:B:546:ALA:HB3	1:B:547:PRO:HD3	1.80	0.63
1:A:407:ASN:H	1:A:410:ASP:HB2	1.62	0.63
1:B:327:LEU:HD12	1:B:328:ASP:H	1.62	0.63
1:A:528:LEU:HD22	1:A:555:ARG:NH2	2.14	0.63
1:A:647:ALA:HB3	1:A:690:VAL:HG11	1.79	0.63
1:B:232:ILE:HG22	1:B:232:ILE:O	1.99	0.63
1:B:233:THR:HG22	1:B:235:SER:H	1.62	0.62
1:B:327:LEU:CG	1:B:352:ILE:HG21	2.29	0.62
1:A:236:MET:HG2	1:A:349:PRO:HB2	1.81	0.62
1:B:234:ASP:HB3	1:B:247:PRO:HB2	1.79	0.62
1:B:459:ILE:HD13	4:B:753:NAP:H52N	1.81	0.62
1:A:226:TYR:HB2	1:A:427:GLN:CG	2.28	0.62
1:A:489:GLN:HA	1:A:515:TYR:CE1	2.34	0.62
1:B:268:PRO:HD3	1:B:310:TRP:CH2	2.35	0.62
1:B:322:LEU:HD21	1:B:356:ILE:HD12	1.81	0.62
1:B:439:ARG:HB2	1:B:441:TYR:HE1	1.64	0.62
1:B:513:ALA:O	1:B:514:ASN:HB2	2.00	0.62
1:A:288:ILE:N	1:A:288:ILE:HD12	2.15	0.62
1:A:95:ASP:C	1:A:97:GLU:H	2.03	0.62
1:B:421:TRP:N	1:B:421:TRP:CD1	2.68	0.62
1:B:50:ILE:HG23	1:B:51:ALA:N	2.15	0.62
1:A:363:THR:HG21	1:A:477:VAL:CG2	2.30	0.61
1:A:60:ASN:HD21	1:A:89:LEU:CB	2.07	0.61
1:B:247:PRO:CG	1:B:509:ARG:NH1	2.62	0.61
1:B:274:VAL:CG1	1:B:293:ASP:HB2	2.30	0.61
1:A:63:VAL:HG21	1:A:80:SER:OG	2.00	0.61
1:A:59:LYS:HD2	1:A:90:ASN:OD1	2.01	0.61
1:B:544:GLY:O	1:B:547:PRO:HD2	1.99	0.61
1:A:291:GLU:HG2	1:A:455:HIS:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:CD2	1:B:269:TYR:HB2	2.36	0.61
1:B:351:THR:HG23	1:B:354:ALA:H	1.66	0.61
1:A:305:ASP:OD1	1:A:523:ARG:HA	2.00	0.61
1:A:371:PHE:HE1	1:A:390:LEU:HD13	1.64	0.61
1:A:535:PRO:HB2	1:A:639:ALA:CB	2.29	0.61
1:A:152:LEU:N	1:A:152:LEU:HD12	2.15	0.61
1:B:301:TYR:CE2	1:B:454:VAL:HG22	2.36	0.61
1:B:179:LEU:HD22	1:B:210:GLU:HG3	1.80	0.61
1:B:307:LEU:HD11	1:B:519:VAL:HG11	1.83	0.61
1:A:228:VAL:O	1:A:229:LEU:HD23	2.01	0.61
1:B:361:GLU:HA	1:B:436:MET:HE3	1.82	0.61
1:B:640:PHE:CB	1:B:642:TYR:HE1	2.12	0.61
1:B:307:LEU:HD11	1:B:519:VAL:CG1	2.31	0.60
1:B:135:CYS:HA	1:B:170:HIS:CD2	2.36	0.60
1:B:331:THR:HB	1:B:352:ILE:HD12	1.82	0.60
1:B:379:PRO:HD2	1:B:383:VAL:CB	2.31	0.60
1:B:481:LEU:O	1:B:485:ILE:HG13	2.01	0.60
1:A:279:LEU:HD23	1:A:587:LEU:HD22	1.83	0.60
1:A:628:GLU:HG3	1:A:629:ASP:H	1.67	0.60
1:B:313:ASN:HD21	1:B:436:MET:HE3	1.66	0.60
1:B:273:ILE:HG12	1:B:292:PHE:CE2	2.36	0.60
1:B:573:LYS:NZ	1:B:633:GLU:OE1	2.35	0.60
1:B:152:LEU:HD12	1:B:152:LEU:N	2.17	0.60
1:B:310:TRP:HB2	1:B:518:PRO:HB2	1.83	0.60
1:B:316:GLU:OE1	1:B:502:HIS:HD2	1.84	0.60
1:B:339:ASP:OD2	1:B:341:THR:HB	2.01	0.60
1:A:318:VAL:HG13	1:A:356:ILE:CG2	2.32	0.60
1:A:335:LEU:HD11	1:A:430:VAL:HG11	1.84	0.59
1:A:94:ALA:HB1	1:A:99:TYR:CE1	2.37	0.59
1:B:247:PRO:HG2	1:B:509:ARG:HH11	1.66	0.59
1:A:96:VAL:HG21	1:A:130:PHE:CD2	2.37	0.59
1:A:105:ASN:OD1	1:A:144:ASN:HB2	2.02	0.59
1:B:185:ALA:CB	1:B:192:THR:HG23	2.31	0.59
1:A:230:ASN:ND2	1:A:231:GLU:HG2	2.16	0.59
1:B:69:THR:HG22	1:B:69:THR:O	2.03	0.59
1:B:528:LEU:HD23	1:B:555:ARG:NH1	2.18	0.59
1:A:640:PHE:HB3	1:A:642:TYR:CE1	2.38	0.59
1:B:452:GLN:HB2	5:B:2014:HOH:O	2.03	0.59
1:B:158:GLU:O	1:B:159:PHE:HB2	2.03	0.58
1:B:240:GLU:HG2	1:B:245:TYR:O	2.02	0.58
1:B:531:ASN:ND2	1:B:533:SER:HB2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:HD21	1:B:352:ILE:HD13	1.85	0.58
1:B:374:LEU:HB2	1:B:387:LEU:HD11	1.84	0.58
1:B:658:LEU:O	1:B:662:LEU:HD13	2.03	0.58
1:A:379:PRO:CD	1:A:383:VAL:HG11	2.25	0.58
1:A:232:ILE:HB	1:A:332:ILE:HD11	1.86	0.58
1:B:555:ARG:HG3	1:B:574:HIS:CE1	2.38	0.58
1:B:603:PHE:CD2	1:B:604:GLU:N	2.72	0.58
1:B:363:THR:HG21	1:B:477:VAL:CG2	2.33	0.58
1:B:582:ASN:HD21	1:B:584:ASP:HB2	1.68	0.58
1:B:346:PHE:HB2	1:B:347:PRO:HD2	1.85	0.58
1:B:277:ARG:CA	1:B:486:GLN:HE21	2.17	0.58
1:B:60:ASN:O	1:B:109:VAL:HB	2.03	0.57
1:B:276:SER:OG	1:B:486:GLN:HG2	2.03	0.57
1:B:580:SER:HB2	1:B:585:ASP:OD2	2.05	0.57
1:B:484:ASN:ND2	1:B:502:HIS:HA	2.19	0.57
1:B:95:ASP:OD2	1:B:97:GLU:HB2	2.04	0.57
1:B:380:ASN:ND2	1:B:382:ASP:N	2.49	0.57
1:A:481:LEU:HB2	1:A:503:TYR:CE2	2.40	0.57
1:B:456:VAL:HG12	1:B:456:VAL:O	2.05	0.57
1:B:646:ASP:O	1:B:647:ALA:CB	2.52	0.57
1:A:484:ASN:HD22	1:A:503:TYR:H	1.53	0.56
1:A:523:ARG:NH2	5:A:2023:HOH:O	2.37	0.56
1:A:647:ALA:HB1	1:A:651:ALA:H	1.69	0.56
1:B:263:PHE:HA	1:B:267:GLN:O	2.05	0.56
1:B:239:GLY:HA3	1:B:358:HIS:CD2	2.40	0.56
1:B:88:ASN:HD21	1:B:216:GLN:HE22	1.52	0.56
1:B:139:ALA:O	1:B:141:ALA:N	2.38	0.56
1:A:118:TYR:O	1:A:119:GLY:C	2.44	0.56
1:B:380:ASN:HD21	1:B:382:ASP:H	1.53	0.56
1:B:59:LYS:HE2	1:B:341:THR:CG2	2.35	0.56
1:B:468:LEU:O	1:B:471:ALA:HB3	2.06	0.56
1:A:138:GLU:CG	1:A:139:ALA:H	2.19	0.56
1:A:370:LEU:HD13	1:A:370:LEU:C	2.26	0.56
1:A:238:LEU:HD12	1:A:509:ARG:NE	2.20	0.55
1:A:375:ILE:HG22	1:A:384:LYS:HG3	1.88	0.55
1:A:513:ALA:O	1:A:516:LYS:HG3	2.06	0.55
1:B:352:ILE:CD1	1:B:426:MET:HG3	2.36	0.55
1:B:247:PRO:CG	1:B:509:ARG:HH11	2.19	0.55
1:B:322:LEU:CD2	1:B:356:ILE:HD12	2.36	0.55
1:B:562:GLN:HB3	1:B:568:ASN:HB3	1.88	0.55
1:B:625:LYS:HG3	1:B:664:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:VAL:HG12	2:B:750:FAD:O2B	2.06	0.55
1:B:231:GLU:C	1:B:232:ILE:HD12	2.27	0.55
1:A:537:ILE:HA	1:A:575:ILE:CG2	2.37	0.55
1:A:115:ILE:HG23	1:A:164:ALA:HB2	1.88	0.55
1:B:110:ILE:HD12	1:B:211:LEU:HD21	1.87	0.55
1:B:130:PHE:CE1	1:B:134:ILE:HD11	2.42	0.55
1:B:277:ARG:HA	1:B:486:GLN:HE21	1.72	0.55
1:B:620:VAL:O	1:B:624:LEU:HG	2.07	0.55
1:A:50:ILE:CG2	1:A:51:ALA:H	2.16	0.54
1:A:65:TYR:CZ	1:A:73:GLU:HG3	2.42	0.54
1:B:60:ASN:OD1	1:B:90:ASN:N	2.39	0.54
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.07	0.54
1:A:473:PRO:O	1:A:475:VAL:HG13	2.08	0.54
1:A:270:ILE:CD1	1:A:511:LEU:HD22	2.37	0.54
1:B:136:ASN:O	1:B:137:ALA:C	2.45	0.54
1:B:231:GLU:OE1	1:B:231:GLU:N	2.37	0.54
1:B:220:PHE:N	1:B:376:GLN:NE2	2.51	0.54
1:A:48:ARG:NH1	1:A:100:ASP:HB2	2.22	0.54
1:B:247:PRO:O	1:B:249:HIS:N	2.39	0.54
1:A:280:PHE:CD2	1:A:585:ASP:HA	2.43	0.54
1:A:322:LEU:HD21	1:A:356:ILE:HD12	1.89	0.54
1:A:85:ALA:O	1:A:218:ALA:HA	2.07	0.54
1:B:346:PHE:HB2	1:B:347:PRO:CD	2.37	0.54
1:A:211:LEU:CB	1:A:213:LEU:HG	2.36	0.54
1:A:400:GLU:C	1:A:401:ILE:HD12	2.28	0.54
1:A:445:SER:HB3	1:A:455:HIS:CG	2.43	0.54
1:A:355:ALA:HA	1:A:359:TYR:CD1	2.43	0.54
1:B:314:PRO:HB3	1:B:501:VAL:HB	1.89	0.54
1:B:199:TRP:CZ2	1:B:203:ILE:HG13	2.43	0.54
1:B:335:LEU:HD11	1:B:430:VAL:HG11	1.88	0.54
1:B:476:GLY:HA3	2:B:750:FAD:O2P	2.07	0.54
1:B:594:GLU:O	1:B:597:LYS:HB2	2.07	0.54
1:B:627:TYR:O	1:B:631:VAL:HG23	2.08	0.54
1:B:161:ASN:ND2	1:B:164:ALA:HB3	2.22	0.54
1:A:279:LEU:HB2	1:A:287:CYS:O	2.07	0.54
1:A:311:PRO:HG2	1:A:436:MET:CE	2.38	0.54
1:A:310:TRP:HB2	1:A:518:PRO:HB2	1.90	0.54
1:B:363:THR:HA	1:B:407:ASN:OD1	2.08	0.54
1:B:623:LYS:HE2	1:B:623:LYS:CA	2.32	0.54
1:B:92:MET:HG3	1:B:341:THR:OG1	2.07	0.54
1:A:346:PHE:HB2	1:A:347:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ASN:OD1	1:A:475:VAL:HG12	2.08	0.53
1:B:533:SER:O	1:B:572:GLY:HA3	2.08	0.53
1:A:460:VAL:HA	1:A:479:THR:HB	1.88	0.53
1:A:485:ILE:HG23	1:A:515:TYR:CD2	2.43	0.53
1:A:529:PRO:HG3	1:A:640:PHE:CG	2.43	0.53
1:B:555:ARG:HG3	1:B:574:HIS:HE1	1.72	0.53
1:A:105:ASN:ND2	1:A:142:LEU:CA	2.70	0.53
1:A:324:ILE:HG23	1:A:325:PHE:CD2	2.44	0.53
1:A:289:HIS:HD1	1:A:588:TYR:HE2	1.55	0.53
1:B:364:GLY:N	1:B:407:ASN:OD1	2.41	0.53
1:B:407:ASN:H	1:B:410:ASP:HB2	1.72	0.53
1:B:487:LEU:HD22	1:B:497:THR:HG21	1.89	0.53
1:A:209:ASP:O	1:A:210:GLU:C	2.46	0.53
1:A:580:SER:O	1:A:609:HIS:HA	2.09	0.53
1:B:156:THR:HG21	1:B:647:ALA:O	2.08	0.53
1:B:540:GLY:HA2	1:B:644:CYS:O	2.09	0.53
1:A:96:VAL:HG21	1:A:130:PHE:CG	2.43	0.53
1:A:501:VAL:HG23	1:A:503:TYR:CE1	2.44	0.53
1:A:647:ALA:HA	1:A:650:MET:HB3	1.89	0.53
1:B:623:LYS:HA	1:B:626:ASP:HB2	1.90	0.53
1:B:333:PHE:CD2	1:B:352:ILE:HG13	2.43	0.53
1:B:430:VAL:HG12	1:B:430:VAL:O	2.09	0.53
1:A:258:ILE:HG22	1:A:258:ILE:O	2.08	0.53
1:B:265:LEU:CD2	1:B:522:ARG:HH12	2.21	0.53
1:A:390:LEU:CD2	1:A:396:GLN:HG2	2.39	0.52
1:A:612:LEU:HD23	1:A:613:PRO:CD	2.32	0.52
1:B:232:ILE:HA	1:B:236:MET:HE1	1.91	0.52
1:B:274:VAL:HG23	1:B:275:LYS:N	2.24	0.52
1:B:98:ASN:HB2	1:B:99:TYR:CD1	2.44	0.52
1:A:599:LEU:O	1:A:600:ASP:HB2	2.10	0.52
1:B:519:VAL:HG12	1:B:520:HIS:N	2.23	0.52
1:B:330:GLU:O	1:B:332:ILE:HD12	2.09	0.52
1:A:109:VAL:HG12	1:B:144:ASN:HD21	1.74	0.52
1:A:240:GLU:HG2	1:A:245:TYR:O	2.08	0.52
1:B:104:LEU:O	1:B:107:VAL:HG23	2.10	0.52
1:B:105:ASN:OD1	1:B:144:ASN:HB2	2.08	0.52
1:A:407:ASN:HB2	1:A:410:ASP:OD2	2.10	0.52
1:A:363:THR:HG21	1:A:477:VAL:HG21	1.91	0.52
1:B:310:TRP:CD1	1:B:310:TRP:N	2.77	0.52
1:B:600:ASP:C	1:B:602:SER:H	2.13	0.52
1:B:611:ARG:HG3	1:B:611:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HD12	1:A:182:LEU:C	2.30	0.52
1:A:578:TYR:CG	1:A:579:GLY:N	2.77	0.52
1:B:49:ASP:O	1:B:53:VAL:HG23	2.09	0.52
1:B:539:ILE:HD13	1:B:624:LEU:HD11	1.92	0.52
1:B:66:ALA:HB2	1:B:96:VAL:HG11	1.92	0.52
1:A:113:ILE:O	1:A:149:MET:HG3	2.09	0.52
1:A:621:GLN:NE2	4:A:753:NAP:N1A	2.58	0.52
1:B:357:LYS:HG2	1:B:358:HIS:CE1	2.45	0.52
1:B:437:THR:HG23	1:B:438:PRO:HD2	1.91	0.52
1:B:139:ALA:C	1:B:141:ALA:H	2.13	0.52
1:B:117:THR:HA	1:B:163:ALA:HB2	1.92	0.52
1:B:223:GLN:HB2	1:B:342:VAL:HG21	1.92	0.52
1:B:73:GLU:CG	1:B:77:LYS:HE3	2.39	0.52
1:B:59:LYS:HG2	1:B:90:ASN:HD22	1.75	0.52
1:A:406:PHE:HD1	1:A:411:ALA:HA	1.76	0.51
1:B:646:ASP:O	1:B:647:ALA:HB3	2.11	0.51
1:B:59:LYS:CG	1:B:90:ASN:HD22	2.22	0.51
1:A:268:PRO:HB3	1:A:310:TRP:CE2	2.46	0.51
1:B:260:LEU:O	1:B:263:PHE:CZ	2.63	0.51
1:A:677:ILE:CG2	1:A:681:LYS:HE3	2.40	0.51
1:B:274:VAL:HG13	1:B:293:ASP:HB2	1.91	0.51
1:B:513:ALA:O	1:B:516:LYS:HE3	2.10	0.51
1:B:61:TYR:HD2	1:B:62:LEU:N	2.09	0.51
1:A:209:ASP:O	1:A:212:HIS:HD2	1.93	0.51
1:A:390:LEU:HD23	1:A:396:GLN:HG2	1.91	0.51
1:B:110:ILE:CD1	1:B:211:LEU:HD21	2.40	0.51
1:B:528:LEU:HD23	1:B:555:ARG:HH11	1.75	0.51
1:B:674:THR:O	1:B:677:ILE:HB	2.09	0.51
1:A:345:PRO:HB3	1:A:435:GLN:OE1	2.11	0.51
1:B:316:GLU:OE1	1:B:502:HIS:CD2	2.64	0.51
1:B:247:PRO:HG2	1:B:509:ARG:HH12	1.74	0.51
1:B:390:LEU:HD21	1:B:400:GLU:CG	2.41	0.51
1:A:548:PHE:O	1:A:552:ILE:HD13	2.10	0.51
1:B:519:VAL:CG1	1:B:520:HIS:N	2.74	0.51
1:A:149:MET:CE	1:A:168:GLU:HB2	2.41	0.51
1:B:265:LEU:CG	1:B:522:ARG:HH12	2.22	0.51
1:B:531:ASN:HD21	1:B:533:SER:HB2	1.76	0.51
1:A:437:THR:HG22	1:A:438:PRO:O	2.11	0.51
1:B:301:TYR:CD1	1:B:301:TYR:C	2.84	0.51
1:B:603:PHE:HD2	1:B:604:GLU:N	2.07	0.51
1:A:484:ASN:ND2	1:A:503:TYR:H	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LEU:CD1	1:A:603:PHE:HB2	2.37	0.50
1:A:621:GLN:HE21	4:A:753:NAP:C2A	2.23	0.50
1:A:95:ASP:O	1:A:97:GLU:N	2.43	0.50
1:A:324:ILE:HD11	1:A:413:LYS:HA	1.92	0.50
1:A:95:ASP:CB	1:A:98:ASN:ND2	2.74	0.50
1:B:148:ASN:ND2	1:B:207:LEU:HD21	2.25	0.50
1:B:62:LEU:HD12	1:B:92:MET:O	2.11	0.50
1:A:519:VAL:HG12	1:A:520:HIS:N	2.25	0.50
1:A:611:ARG:NE	4:A:753:NAP:O3X	2.44	0.50
1:B:577:PHE:CE2	1:B:624:LEU:HD23	2.46	0.50
1:B:666:LYS:HE3	1:B:676:LEU:HD21	1.92	0.50
1:A:647:ALA:CB	1:A:690:VAL:CG1	2.83	0.50
1:B:313:ASN:ND2	1:B:362:ILE:HG12	2.26	0.50
1:B:632:PHE:CZ	1:B:665:GLY:HA3	2.45	0.50
1:A:259:GLN:O	1:A:297:SER:HA	2.11	0.50
1:B:534:THR:HG23	1:B:638:GLY:O	2.11	0.50
1:A:233:THR:HB	1:A:236:MET:SD	2.51	0.50
1:B:400:GLU:HG3	1:B:401:ILE:CD1	2.41	0.50
1:B:460:VAL:HA	1:B:479:THR:HB	1.94	0.50
1:B:379:PRO:CD	1:B:383:VAL:HG11	2.41	0.50
1:A:107:VAL:HG12	1:A:109:VAL:H	1.77	0.50
1:A:508:PRO:HD2	1:A:511:LEU:HB3	1.94	0.50
1:A:596:ALA:HA	1:A:603:PHE:HD1	1.77	0.50
1:A:645:GLY:O	1:A:690:VAL:HG13	2.12	0.50
1:B:635:ILE:C	1:B:637:ASN:H	2.15	0.50
1:A:288:ILE:N	1:A:288:ILE:CD1	2.74	0.49
1:A:319:GLU:HA	1:A:319:GLU:OE1	2.12	0.49
1:A:316:GLU:O	1:A:320:GLN:HG3	2.12	0.49
1:B:450:GLU:OE2	1:B:553:ARG:CZ	2.60	0.49
1:B:579:GLY:O	1:B:580:SER:HB3	2.11	0.49
1:B:99:TYR:CD1	1:B:99:TYR:N	2.80	0.49
1:A:570:SER:O	1:A:571:LEU:HB2	2.12	0.49
1:B:551:PHE:CE2	1:B:642:TYR:CE2	3.00	0.49
1:B:611:ARG:HG3	1:B:611:ARG:HH11	1.78	0.49
1:A:119:GLY:HA3	1:A:122:ASP:OD1	2.12	0.49
1:A:485:ILE:HG12	1:A:505:LEU:HD22	1.95	0.49
1:B:449:SER:C	1:B:450:GLU:HG3	2.33	0.49
1:A:608:ALA:HB1	1:A:618:VAL:CG1	2.43	0.49
1:B:361:GLU:CG	1:B:436:MET:HA	2.41	0.49
1:B:551:PHE:HE2	1:B:642:TYR:CE2	2.30	0.49
1:B:646:ASP:O	1:B:691:TRP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLY:HA3	1:A:358:HIS:CD2	2.48	0.49
1:A:548:PHE:HA	1:A:551:PHE:HB2	1.93	0.49
1:B:330:GLU:O	1:B:331:THR:C	2.49	0.49
1:B:684:GLY:O	1:B:687:GLN:HG3	2.12	0.49
1:A:138:GLU:HG3	1:A:139:ALA:N	2.24	0.49
1:A:233:THR:CG2	1:A:234:ASP:N	2.76	0.49
1:B:161:ASN:HD21	1:B:164:ALA:HB3	1.76	0.49
1:B:61:TYR:HE1	1:B:207:LEU:HD13	1.77	0.49
1:B:548:PHE:HA	1:B:551:PHE:HB2	1.93	0.49
1:B:655:SER:O	1:B:659:VAL:HG23	2.12	0.49
1:A:647:ALA:HB2	1:A:650:MET:HE3	1.94	0.49
1:B:534:THR:HG21	1:B:640:PHE:CE1	2.47	0.49
1:B:263:PHE:O	1:B:264:ASP:HB3	2.12	0.49
1:B:443:ILE:HD13	1:B:454:VAL:HG13	1.94	0.48
1:A:478:THR:N	2:A:750:FAD:O1P	2.44	0.48
1:B:173:ALA:C	1:B:175:GLY:H	2.15	0.48
1:B:264:ASP:HA	1:B:520:HIS:CG	2.48	0.48
1:B:540:GLY:HA3	1:B:548:PHE:CE1	2.37	0.48
1:B:651:ALA:O	1:B:655:SER:HB2	2.13	0.48
1:A:152:LEU:HA	1:A:185:ALA:HB3	1.95	0.48
1:B:369:GLN:O	1:B:373:SER:OG	2.32	0.48
1:B:455:HIS:CD2	1:B:549:ARG:HH12	2.31	0.48
1:B:591:GLU:O	1:B:594:GLU:HB2	2.14	0.48
1:A:323:SER:O	1:A:326:ASN:N	2.44	0.48
1:B:238:LEU:HD23	1:B:351:THR:HG22	1.94	0.48
1:B:313:ASN:HD21	1:B:436:MET:CE	2.26	0.48
1:B:321:PHE:HD2	1:B:356:ILE:HD13	1.78	0.48
1:A:191:THR:O	1:A:192:THR:C	2.52	0.48
1:A:314:PRO:HB3	1:A:501:VAL:HB	1.95	0.48
1:A:532:PRO:HA	1:A:555:ARG:NH2	2.28	0.48
1:A:263:PHE:HA	1:A:267:GLN:O	2.14	0.48
1:A:475:VAL:HB	1:A:480:ASN:ND2	2.28	0.48
1:A:238:LEU:HD12	1:A:509:ARG:CD	2.43	0.48
1:A:582:ASN:HD22	1:A:582:ASN:N	2.12	0.48
1:A:609:HIS:HB2	1:A:612:LEU:HD12	1.95	0.48
1:A:272:PRO:HB3	1:A:516:LYS:HE3	1.96	0.48
1:A:325:PHE:CE1	1:A:429:LEU:HD21	2.49	0.48
1:A:355:ALA:O	1:A:360:LEU:HG	2.13	0.48
1:A:552:ILE:O	1:A:556:VAL:HG23	2.14	0.48
1:A:95:ASP:C	1:A:97:GLU:N	2.67	0.48
1:B:216:GLN:HG3	1:B:217:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ILE:CD1	1:B:624:LEU:HD11	2.44	0.48
1:A:123:PHE:N	1:A:123:PHE:CD1	2.82	0.48
1:A:211:LEU:HD12	1:A:213:LEU:HD11	1.95	0.48
1:A:379:PRO:HD2	1:A:383:VAL:CG1	2.30	0.48
1:A:440:TYR:CD1	1:A:440:TYR:N	2.82	0.48
1:A:594:GLU:OE2	1:A:594:GLU:HA	2.14	0.48
1:B:301:TYR:CD2	1:B:454:VAL:HG22	2.49	0.48
1:B:542:GLY:O	1:B:544:GLY:N	2.46	0.48
1:A:247:PRO:C	1:A:249:HIS:H	2.17	0.47
1:A:537:ILE:HA	1:A:575:ILE:HG23	1.96	0.47
1:B:529:PRO:HG3	1:B:640:PHE:CG	2.49	0.47
1:A:158:GLU:HB3	1:A:159:PHE:HD1	1.78	0.47
1:B:117:THR:O	1:B:118:TYR:CD1	2.67	0.47
1:A:274:VAL:CG1	1:A:293:ASP:HB2	2.44	0.47
1:B:578:TYR:CG	1:B:579:GLY:N	2.82	0.47
1:A:233:THR:HG22	1:A:235:SER:H	1.78	0.47
1:A:582:ASN:ND2	1:A:582:ASN:N	2.62	0.47
1:B:241:PRO:O	1:B:347:PRO:HG2	2.14	0.47
1:B:411:ALA:O	1:B:414:TYR:HB3	2.14	0.47
1:B:484:ASN:ND2	1:B:503:TYR:H	2.13	0.47
1:A:404:LYS:HB3	1:A:406:PHE:CE2	2.50	0.47
1:B:224:PHE:CZ	1:B:345:PRO:HD3	2.49	0.47
1:B:73:GLU:HG2	1:B:77:LYS:HE3	1.97	0.47
1:B:265:LEU:CD2	1:B:522:ARG:NH1	2.78	0.47
1:B:576:LEU:HD12	1:B:576:LEU:C	2.35	0.47
1:B:84:VAL:HG22	1:B:89:LEU:O	2.15	0.47
1:A:149:MET:HE1	1:A:164:ALA:O	2.15	0.47
1:A:216:GLN:HG3	1:A:217:GLU:O	2.15	0.47
1:A:374:LEU:O	1:A:375:ILE:C	2.53	0.47
1:A:325:PHE:HE2	1:A:412:LEU:HD12	1.79	0.47
1:A:528:LEU:HD22	1:A:555:ARG:CZ	2.44	0.47
1:B:294:LEU:HG	1:B:454:VAL:HG23	1.96	0.47
1:B:347:PRO:HD2	1:B:359:TYR:CZ	2.49	0.47
1:B:400:GLU:O	1:B:401:ILE:CD1	2.63	0.47
1:B:324:ILE:HD11	1:B:413:LYS:HA	1.96	0.47
1:B:501:VAL:HG23	1:B:503:TYR:CE1	2.50	0.47
1:B:272:PRO:HB3	1:B:516:LYS:HG2	1.95	0.47
1:A:240:GLU:CD	1:A:240:GLU:H	2.18	0.47
1:A:372:SER:HB2	1:A:391:SER:HB2	1.95	0.47
1:A:499:LEU:HD12	1:A:500:PRO:HD2	1.96	0.47
1:B:647:ALA:HB2	1:B:690:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG23	1:B:91:VAL:CG1	2.44	0.47
1:A:87:PHE:CD2	1:A:213:LEU:HB3	2.49	0.46
1:B:380:ASN:HD21	1:B:382:ASP:CB	2.28	0.46
1:B:493:ASN:OD1	1:B:495:ALA:HB3	2.14	0.46
1:B:483:ARG:NH2	1:B:498:ASN:OD1	2.46	0.46
1:B:568:ASN:O	1:B:569:VAL:C	2.54	0.46
1:A:422:ASP:OD1	1:A:422:ASP:O	2.31	0.46
1:A:70:GLY:O	1:A:74:ASP:N	2.46	0.46
1:B:499:LEU:HD12	1:B:500:PRO:HD2	1.97	0.46
1:A:233:THR:CG2	1:A:234:ASP:H	2.25	0.46
1:A:660:GLY:HA3	1:A:664:ARG:HH21	1.80	0.46
1:B:119:GLY:HA2	5:B:2001:HOH:O	2.15	0.46
1:B:59:LYS:HE2	1:B:341:THR:CB	2.45	0.46
1:B:619:TYR:O	1:B:622:ASP:HB2	2.15	0.46
1:B:673:ALA:O	1:B:677:ILE:HG12	2.15	0.46
1:A:69:THR:HG22	1:A:69:THR:O	2.16	0.46
1:B:156:THR:O	1:B:652:LYS:HG3	2.16	0.46
1:B:310:TRP:O	1:B:518:PRO:HD2	2.15	0.46
1:A:268:PRO:HB3	1:A:310:TRP:CZ2	2.51	0.46
1:A:541:PRO:HG3	1:A:620:VAL:HG21	1.97	0.46
1:A:552:ILE:N	1:A:552:ILE:HD12	2.31	0.46
1:A:197:MET:O	1:A:200:LYS:HB3	2.15	0.46
1:B:482:LEU:HA	1:B:485:ILE:CD1	2.31	0.46
1:A:406:PHE:CD1	1:A:411:ALA:HA	2.51	0.46
1:B:87:PHE:CB	1:B:89:LEU:HD12	2.39	0.46
1:B:50:ILE:CD1	1:B:92:MET:HE1	2.46	0.46
1:A:407:ASN:O	1:A:408:ILE:C	2.54	0.46
1:B:105:ASN:HB2	5:B:2002:HOH:O	2.16	0.46
1:B:154:ASN:ND2	1:B:188:GLY:HA2	2.31	0.46
1:B:265:LEU:HD23	1:B:522:ARG:HH22	1.81	0.46
1:B:533:SER:HA	1:B:572:GLY:H	1.81	0.46
1:B:662:LEU:HD22	1:B:677:ILE:HD11	1.96	0.46
1:A:481:LEU:HD13	1:A:503:TYR:CD2	2.51	0.46
1:A:518:PRO:C	1:A:519:VAL:HG23	2.36	0.46
1:B:66:ALA:O	1:B:124:PRO:HG2	2.16	0.46
1:B:440:TYR:CD1	1:B:440:TYR:N	2.83	0.46
1:B:48:ARG:HG2	1:B:98:ASN:O	2.16	0.46
1:A:274:VAL:O	1:A:275:LYS:HG3	2.15	0.45
1:A:565:GLY:C	1:A:567:ASN:H	2.20	0.45
1:A:541:PRO:HG3	1:A:620:VAL:CG2	2.46	0.45
1:A:82:GLU:HA	1:A:85:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:O	1:B:54:VAL:HG23	2.16	0.45
1:B:63:VAL:HG21	1:B:80:SER:HB2	1.98	0.45
1:B:91:VAL:HG12	1:B:92:MET:N	2.31	0.45
1:A:88:ASN:ND2	1:A:216:GLN:OE1	2.48	0.45
1:B:531:ASN:C	1:B:533:SER:H	2.20	0.45
1:A:291:GLU:HG2	1:A:455:HIS:ND1	2.30	0.45
1:A:493:ASN:HD22	1:A:496:GLU:HB2	1.74	0.45
1:B:404:LYS:HB3	1:B:406:PHE:CE2	2.51	0.45
1:A:311:PRO:HG2	1:A:436:MET:HE2	1.97	0.45
1:B:118:TYR:O	1:B:119:GLY:C	2.55	0.45
1:B:96:VAL:CG2	1:B:130:PHE:CG	3.00	0.45
1:B:327:LEU:CD2	1:B:352:ILE:HD13	2.47	0.45
1:B:595:TYR:C	1:B:597:LYS:H	2.20	0.45
1:A:135:CYS:HA	1:A:170:HIS:CD2	2.52	0.45
1:A:455:HIS:HD2	1:A:549:ARG:HH12	1.64	0.45
1:A:644:CYS:SG	1:A:645:GLY:N	2.89	0.45
1:B:509:ARG:O	1:B:510:LYS:C	2.55	0.45
1:B:95:ASP:OD2	1:B:97:GLU:CB	2.64	0.45
1:A:158:GLU:HB3	1:A:159:PHE:CD1	2.51	0.45
1:A:65:TYR:CE1	1:A:73:GLU:HG3	2.51	0.45
1:B:313:ASN:ND2	1:B:436:MET:CE	2.79	0.45
1:A:487:LEU:HD22	1:A:497:THR:HG21	1.98	0.45
1:B:321:PHE:CD2	1:B:356:ILE:HD13	2.51	0.45
1:B:223:GLN:HA	1:B:338:LEU:HD12	1.97	0.45
1:A:298:ASN:N	1:A:298:ASN:OD1	2.46	0.45
1:A:522:ARG:NH2	5:A:2022:HOH:O	2.33	0.45
1:A:62:LEU:HD11	1:A:64:LEU:HD21	1.99	0.45
1:B:379:PRO:HD3	1:B:383:VAL:HG11	1.99	0.45
1:B:69:THR:HB	3:B:751:FMN:O1P	2.17	0.45
1:A:263:PHE:CD2	1:A:269:TYR:HB2	2.51	0.45
1:A:316:GLU:N	1:A:316:GLU:OE2	2.42	0.45
1:A:481:LEU:O	1:A:485:ILE:HG13	2.17	0.45
1:A:647:ALA:HB2	1:A:690:VAL:CG1	2.37	0.45
1:B:150:PHE:CZ	1:B:196:TYR:HA	2.52	0.45
1:B:484:ASN:HD22	1:B:503:TYR:HD1	1.63	0.45
1:B:586:PHE:CE2	1:B:589:GLN:HA	2.52	0.45
1:A:123:PHE:N	1:A:123:PHE:HD1	2.14	0.45
1:A:274:VAL:HG11	1:A:293:ASP:HB2	1.99	0.45
1:A:343:LYS:HE3	5:A:2002:HOH:O	2.17	0.45
1:A:346:PHE:HB2	1:A:347:PRO:HD2	1.99	0.45
1:A:153:GLY:HA2	3:A:751:FMN:O2'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ALA:O	1:B:219:LYS:HG3	2.17	0.45
1:B:324:ILE:HG23	1:B:325:PHE:CD2	2.51	0.45
1:B:356:ILE:O	1:B:356:ILE:HG22	2.15	0.45
1:B:96:VAL:HG21	1:B:130:PHE:CG	2.51	0.44
1:B:425:PRO:O	1:B:428:PHE:HB3	2.17	0.44
1:B:616:LYS:O	1:B:618:VAL:HG23	2.16	0.44
1:A:115:ILE:CD1	1:A:163:ALA:HB1	2.44	0.44
1:A:421:TRP:N	1:A:421:TRP:CD1	2.85	0.44
1:B:189:ALA:O	1:B:191:THR:HG23	2.17	0.44
1:B:264:ASP:CG	1:B:265:LEU:HD12	2.38	0.44
1:B:669:THR:OG1	1:B:672:GLU:HG3	2.17	0.44
1:A:423:THR:O	1:A:425:PRO:HD3	2.17	0.44
1:B:276:SER:CB	1:B:486:GLN:HG2	2.47	0.44
1:A:333:PHE:O	1:A:349:PRO:HB3	2.17	0.44
1:A:226:TYR:CB	1:A:427:GLN:CG	2.95	0.44
1:A:690:VAL:HG12	1:A:691:TRP:N	2.32	0.44
1:A:74:ASP:OD1	1:A:434:PRO:HG3	2.17	0.44
1:B:450:GLU:OE2	1:B:553:ARG:NH1	2.49	0.44
1:B:380:ASN:HD21	1:B:382:ASP:HB3	1.82	0.44
1:B:445:SER:HB3	1:B:455:HIS:ND1	2.32	0.44
1:A:107:VAL:HA	1:A:108:PRO:HD3	1.74	0.44
1:A:232:ILE:HG13	1:A:232:ILE:O	2.18	0.44
1:A:275:LYS:HD2	1:A:291:GLU:OE1	2.17	0.44
1:A:546:ALA:HB3	1:A:547:PRO:HD3	2.00	0.44
2:B:750:FAD:HM83	3:B:751:FMN:HM82	2.00	0.44
1:A:350:THR:OG1	1:A:351:THR:N	2.51	0.44
1:B:185:ALA:HB1	1:B:192:THR:HA	2.00	0.44
1:B:333:PHE:HD2	1:B:352:ILE:HG13	1.82	0.44
1:B:289:HIS:CE1	1:B:455:HIS:CD2	3.06	0.44
1:A:518:PRO:O	1:A:519:VAL:CG2	2.66	0.44
1:A:54:VAL:O	1:A:59:LYS:HG2	2.18	0.44
1:B:129:ASN:H	1:B:129:ASN:ND2	2.16	0.44
1:B:211:LEU:HB2	1:B:213:LEU:HG	1.99	0.44
1:A:240:GLU:OE2	1:A:508:PRO:CB	2.65	0.44
1:A:322:LEU:HD22	1:A:329:PRO:HG3	1.99	0.44
1:A:542:GLY:O	1:A:543:THR:C	2.56	0.44
1:B:157:TYR:CE2	1:B:690:VAL:HG12	2.53	0.44
1:B:362:ILE:HG13	1:B:363:THR:N	2.33	0.44
1:A:87:PHE:HD2	1:A:213:LEU:HB3	1.83	0.43
1:A:96:VAL:CG2	1:A:130:PHE:CG	3.01	0.43
1:B:233:THR:HG22	1:B:234:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:TYR:CD1	1:B:405:TYR:N	2.86	0.43
1:A:224:PHE:CZ	1:A:345:PRO:HD3	2.53	0.43
1:A:61:TYR:HB3	1:A:91:VAL:HG22	2.01	0.43
1:B:371:PHE:HE1	1:B:390:LEU:HD13	1.84	0.43
1:A:411:ALA:O	1:A:414:TYR:HB3	2.17	0.43
1:A:436:MET:CE	1:A:477:VAL:HG11	2.49	0.43
1:B:117:THR:C	1:B:118:TYR:CD1	2.92	0.43
1:B:332:ILE:N	1:B:332:ILE:HD12	2.33	0.43
1:B:277:ARG:C	1:B:486:GLN:HE21	2.22	0.43
1:B:599:LEU:O	1:B:602:SER:HB2	2.18	0.43
1:A:149:MET:HE2	1:A:168:GLU:HB2	2.00	0.43
1:A:494:ILE:O	1:A:497:THR:OG1	2.30	0.43
1:A:51:ALA:O	1:A:55:THR:HG23	2.19	0.43
1:B:487:LEU:CD2	1:B:497:THR:HG21	2.48	0.43
1:B:536:VAL:HB	1:B:574:HIS:CD2	2.53	0.43
1:B:528:LEU:HB3	1:B:555:ARG:HH12	1.83	0.43
1:B:582:ASN:CG	1:B:583:THR:N	2.68	0.43
1:A:608:ALA:HB1	1:A:618:VAL:HG13	2.00	0.43
1:B:654:VAL:O	1:B:657:ALA:HB3	2.18	0.43
1:A:385:GLU:O	1:A:389:LEU:HG	2.18	0.43
1:A:404:LYS:HD3	1:A:406:PHE:CZ	2.54	0.43
1:A:581:ARG:NH1	1:A:611:ARG:HH12	2.17	0.43
1:A:588:TYR:O	1:A:589:GLN:C	2.57	0.43
1:B:329:PRO:O	1:B:351:THR:OG1	2.36	0.43
1:B:603:PHE:HD2	1:B:604:GLU:H	1.65	0.43
1:A:209:ASP:O	1:A:212:HIS:CD2	2.72	0.43
1:A:519:VAL:CG1	1:A:520:HIS:N	2.81	0.43
1:B:440:TYR:OH	1:B:522:ARG:NH2	2.51	0.43
1:B:531:ASN:C	1:B:533:SER:N	2.71	0.43
1:B:609:HIS:CB	1:B:612:LEU:HG	2.46	0.43
1:A:108:PRO:HB2	1:B:144:ASN:HD22	1.84	0.43
1:A:338:LEU:O	1:A:339:ASP:HB3	2.18	0.43
1:A:226:TYR:CB	1:A:427:GLN:HG2	2.46	0.43
1:A:558:PHE:CE2	1:A:562:GLN:HG3	2.54	0.43
1:B:138:GLU:O	1:B:141:ALA:CB	2.67	0.43
1:B:164:ALA:O	1:B:165:LYS:C	2.58	0.43
1:B:646:ASP:OD1	1:B:648:LYS:HB3	2.19	0.43
1:A:159:PHE:CD1	1:A:159:PHE:N	2.86	0.43
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.92	0.43
1:B:305:ASP:OD1	1:B:527:ARG:NH2	2.48	0.43
1:B:597:LYS:O	1:B:599:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASP:N	1:A:267:GLN:O	2.48	0.42
1:A:440:TYR:CE2	1:A:522:ARG:NH2	2.87	0.42
1:A:556:VAL:O	1:A:560:GLU:HB2	2.19	0.42
1:B:265:LEU:HG	1:B:522:ARG:NH1	2.33	0.42
1:B:378:ALA:CB	1:B:384:LYS:HB2	2.49	0.42
1:B:395:ASP:O	1:B:398:ALA:HB3	2.18	0.42
1:B:308:ALA:HA	1:B:439:ARG:O	2.19	0.42
1:B:503:TYR:N	1:B:503:TYR:CD1	2.87	0.42
1:B:582:ASN:OD1	1:B:583:THR:N	2.52	0.42
1:A:84:VAL:HG13	1:A:88:ASN:HA	2.01	0.42
1:B:333:PHE:O	1:B:349:PRO:HB3	2.18	0.42
1:B:377:PHE:HE2	1:B:428:PHE:CD1	2.36	0.42
1:B:390:LEU:HD22	1:B:397:PHE:HA	2.01	0.42
1:A:390:LEU:CD1	1:A:415:LEU:HD21	2.49	0.42
1:A:513:ALA:O	1:A:514:ASN:HB2	2.20	0.42
1:A:638:GLY:HA2	1:A:685:ARG:CZ	2.49	0.42
1:B:105:ASN:ND2	1:B:142:LEU:CA	2.72	0.42
1:B:439:ARG:HG3	1:B:478:THR:OG1	2.19	0.42
1:B:633:GLU:O	1:B:636:ASN:N	2.53	0.42
1:A:325:PHE:O	1:A:326:ASN:HB3	2.19	0.42
1:A:508:PRO:HD2	1:A:511:LEU:CB	2.49	0.42
1:B:276:SER:HA	1:B:289:HIS:O	2.19	0.42
1:B:329:PRO:HA	1:B:352:ILE:HG22	2.01	0.42
1:B:95:ASP:OD2	1:B:97:GLU:HG3	2.19	0.42
1:A:528:LEU:HD13	1:A:555:ARG:NH1	2.35	0.42
1:A:607:VAL:CG1	1:A:608:ALA:N	2.82	0.42
1:A:459:ILE:HD13	4:A:753:NAP:H52N	2.02	0.42
1:B:360:LEU:O	1:B:362:ILE:N	2.50	0.42
1:B:390:LEU:C	1:B:392:LYS:N	2.73	0.42
1:B:642:TYR:CD1	1:B:642:TYR:N	2.87	0.42
1:B:94:ALA:HB1	1:B:99:TYR:CE1	2.55	0.42
1:B:247:PRO:C	1:B:249:HIS:N	2.73	0.42
1:B:327:LEU:HD21	1:B:352:ILE:CG2	2.50	0.42
1:B:528:LEU:CD1	1:B:528:LEU:H	2.28	0.42
1:A:333:PHE:CD1	1:A:333:PHE:C	2.92	0.42
1:B:223:GLN:HG2	1:B:431:GLU:OE1	2.20	0.42
1:B:424:VAL:HG11	1:B:429:LEU:HD21	2.01	0.42
1:A:686:TYR:CD2	1:A:686:TYR:C	2.92	0.42
1:B:257:GLY:O	1:B:258:ILE:C	2.58	0.42
1:B:346:PHE:CD2	1:B:359:TYR:HB3	2.55	0.42
1:B:528:LEU:HD12	1:B:528:LEU:N	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:SER:HB3	1:B:547:PRO:HG3	2.01	0.42
1:A:286:ASN:O	1:A:460:VAL:HG23	2.20	0.42
1:A:528:LEU:HD11	1:A:555:ARG:HG2	2.02	0.42
1:A:74:ASP:OD2	1:A:78:LYS:NZ	2.53	0.42
1:A:194:GLU:CG	1:A:394:LYS:HG3	2.50	0.42
1:B:268:PRO:HB3	1:B:310:TRP:CE2	2.55	0.42
1:B:528:LEU:CD2	1:B:555:ARG:HH11	2.33	0.42
1:B:573:LYS:O	1:B:634:MET:HE3	2.19	0.42
1:B:633:GLU:O	1:B:634:MET:C	2.58	0.42
1:B:325:PHE:CE1	1:B:429:LEU:HD11	2.54	0.41
1:B:50:ILE:HD11	1:B:92:MET:HE1	2.02	0.41
1:B:534:THR:HG21	1:B:640:PHE:CD1	2.55	0.41
1:B:676:LEU:O	1:B:680:LEU:HG	2.20	0.41
1:A:563:LYS:C	1:A:565:GLY:H	2.24	0.41
1:A:618:VAL:O	1:A:618:VAL:HG12	2.20	0.41
1:B:481:LEU:HD13	1:B:503:TYR:CD2	2.56	0.41
1:B:581:ARG:HD3	1:B:611:ARG:HH12	1.83	0.41
1:A:393:ASP:O	1:A:394:LYS:C	2.57	0.41
1:B:289:HIS:CE1	1:B:455:HIS:HD2	2.39	0.41
1:B:333:PHE:C	1:B:333:PHE:CD1	2.93	0.41
1:A:138:GLU:CG	1:A:139:ALA:N	2.83	0.41
1:A:371:PHE:O	1:A:387:LEU:HD22	2.19	0.41
1:A:531:ASN:C	1:A:533:SER:H	2.22	0.41
1:B:453:THR:HG22	1:B:454:VAL:N	2.34	0.41
1:B:74:ASP:OD1	1:B:434:PRO:HG3	2.20	0.41
1:A:136:ASN:O	1:A:137:ALA:C	2.58	0.41
1:A:346:PHE:CZ	1:A:430:VAL:HG13	2.55	0.41
1:B:267:GLN:O	1:B:268:PRO:O	2.38	0.41
1:B:356:ILE:HG23	1:B:362:ILE:HG21	2.03	0.41
1:B:371:PHE:CE1	1:B:390:LEU:HD13	2.56	0.41
1:B:408:ILE:HD13	1:B:433:VAL:HG22	2.03	0.41
1:B:586:PHE:CD2	1:B:589:GLN:HB2	2.56	0.41
1:B:612:LEU:HA	1:B:613:PRO:HD3	1.89	0.41
1:B:63:VAL:HB	1:B:93:CYS:HA	2.02	0.41
1:A:393:ASP:HB3	1:A:396:GLN:HB3	2.02	0.41
1:A:485:ILE:O	1:A:486:GLN:C	2.58	0.41
1:B:423:THR:O	1:B:425:PRO:HD3	2.21	0.41
1:B:499:LEU:HA	1:B:500:PRO:HD3	1.74	0.41
1:B:536:VAL:HG12	1:B:538:MET:HG3	2.02	0.41
1:A:555:ARG:HD2	1:A:571:LEU:HD11	2.02	0.41
1:B:336:LYS:HA	1:B:337:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PHE:HB2	1:B:89:LEU:CD1	2.42	0.41
1:A:363:THR:HG21	1:A:477:VAL:HG23	2.02	0.41
1:A:57:ASN:HB3	1:A:59:LYS:HD3	2.03	0.41
1:A:581:ARG:HD3	1:A:611:ARG:HG3	2.02	0.41
1:A:666:LYS:HE3	1:A:676:LEU:CD2	2.40	0.41
1:A:82:GLU:HA	1:A:85:ALA:CB	2.50	0.41
1:B:224:PHE:HA	1:B:336:LYS:O	2.19	0.41
1:B:337:PRO:HB3	1:B:342:VAL:O	2.20	0.41
1:A:223:GLN:NE2	1:A:342:VAL:HG22	2.35	0.41
1:A:229:LEU:HB2	1:A:332:ILE:HG22	2.03	0.41
1:A:403:SER:O	1:A:467:GLU:HG3	2.20	0.41
1:A:578:TYR:CD1	1:A:579:GLY:N	2.86	0.41
1:B:374:LEU:O	1:B:375:ILE:C	2.59	0.41
1:B:374:LEU:CB	1:B:387:LEU:HD11	2.50	0.41
1:B:87:PHE:O	1:B:88:ASN:HB2	2.21	0.41
1:B:98:ASN:HB2	1:B:99:TYR:CE1	2.55	0.41
1:A:123:PHE:CD2	1:A:131:GLU:HB2	2.55	0.41
1:A:632:PHE:CE2	1:A:636:ASN:ND2	2.89	0.41
1:B:240:GLU:HB3	1:B:245:TYR:CB	2.51	0.41
1:B:344:VAL:HA	1:B:345:PRO:HD3	1.83	0.41
1:B:377:PHE:HB3	1:B:423:THR:HB	2.02	0.41
1:B:433:VAL:HA	1:B:434:PRO:HD3	1.80	0.41
1:B:539:ILE:HG23	1:B:620:VAL:HG21	2.02	0.41
1:A:146:ARG:HD3	1:B:146:ARG:NH1	2.35	0.41
1:A:240:GLU:CG	1:A:245:TYR:O	2.68	0.41
1:A:380:ASN:O	1:A:383:VAL:HB	2.21	0.41
1:A:609:HIS:CB	1:A:612:LEU:HD12	2.49	0.41
1:B:370:LEU:O	1:B:374:LEU:HG	2.20	0.41
1:B:485:ILE:HG23	1:B:515:TYR:HD2	1.85	0.41
1:B:95:ASP:HB3	1:B:98:ASN:HD21	1.83	0.41
1:A:316:GLU:OE1	1:A:501:VAL:HA	2.21	0.40
1:B:202:SER:OG	1:B:203:ILE:N	2.53	0.40
1:B:301:TYR:CE1	1:B:447:SER:HA	2.55	0.40
1:B:390:LEU:C	1:B:392:LYS:H	2.24	0.40
1:A:690:VAL:O	3:A:751:FMN:HM72	2.21	0.40
1:B:161:ASN:ND2	5:B:2003:HOH:O	2.54	0.40
1:B:166:LYS:O	1:B:169:LYS:HB3	2.21	0.40
1:B:572:GLY:O	1:B:574:HIS:CD2	2.73	0.40
1:B:621:GLN:OE1	1:B:653:GLY:HA3	2.22	0.40
1:B:157:TYR:OH	1:B:691:TRP:HA	2.22	0.40
1:A:362:ILE:HG13	1:A:363:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:VAL:HG12	1:A:608:ALA:N	2.36	0.40
1:B:269:TYR:N	1:B:519:VAL:O	2.55	0.40
1:A:553:ARG:NH1	1:A:553:ARG:HG2	2.36	0.40
1:A:677:ILE:HD13	1:A:677:ILE:HA	1.86	0.40
1:B:223:GLN:C	1:B:338:LEU:HD12	2.41	0.40
1:B:223:GLN:CA	1:B:338:LEU:HD12	2.52	0.40
1:B:620:VAL:HG23	1:B:621:GLN:N	2.37	0.40
1:B:662:LEU:HD22	1:B:677:ILE:CD1	2.50	0.40
1:B:441:TYR:HH	2:B:750:FAD:HO4'	1.66	0.40
1:A:582:ASN:HB2	1:A:583:THR:H	1.74	0.40
1:B:107:VAL:HG12	1:B:109:VAL:H	1.86	0.40
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.84	0.40
1:B:609:HIS:HB2	1:B:612:LEU:CD1	2.52	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	639/682 (94%)	513 (80%)	105 (16%)	21 (3%)	4	17
1	B	637/682 (93%)	504 (79%)	106 (17%)	27 (4%)	3	11
All	All	1276/1364 (94%)	1017 (80%)	211 (16%)	48 (4%)	4	14

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ASP
1	A	508	PRO
1	A	566	GLY
1	B	233	THR
1	B	241	PRO

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Mol	Chain	Res	Type
1	B	571	LEU
1	B	646	ASP
1	B	647	ALA
1	A	127	ALA
1	A	232	ILE
1	A	331	THR
1	A	526	PHE
1	A	571	LEU
1	B	119	GLY
1	B	140	GLY
1	B	248	SER
1	B	268	PRO
1	B	497	THR
1	B	570	SER
1	A	143	SER
1	A	241	PRO
1	A	261	GLY
1	A	529	PRO
1	B	264	ASP
1	B	331	THR
1	B	401	ILE
1	B	543	THR
1	B	594	GLU
1	A	50	ILE
1	A	96	VAL
1	A	192	THR
1	A	253	ARG
1	A	462	ASN
1	A	639	ALA
1	B	133	PHE
1	B	137	ALA
1	B	379	PRO
1	B	569	VAL
1	A	613	PRO
1	B	311	PRO
1	B	514	ASN
1	B	596	ALA
1	B	598	LYS
1	B	636	ASN
1	B	649	GLY
1	A	500	PRO
1	A	311	PRO

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Mol	Chain	Res	Type
1	B	468	LEU

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	548/592 (93%)	508 (93%)	40 (7%)	16	42
1	B	549/592 (93%)	511 (93%)	38 (7%)	18	45
All	All	1097/1184 (93%)	1019 (93%)	78 (7%)	17	44

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	62	LEU
1	A	97	GLU
1	A	104	LEU
1	A	160	PHE
1	A	161	ASN
1	A	182	LEU
1	A	194	GLU
1	A	209	ASP
1	A	236	MET
1	A	272	PRO
1	A	283	ASN
1	A	284	ASP
1	A	285	ARG
1	A	286	ASN
1	A	319	GLU
1	A	330	GLU
1	A	341	THR
1	A	346	PHE
1	A	350	THR
1	A	371	PHE
1	A	375	ILE

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Mol	Chain	Res	Type
1	A	387	LEU
1	A	423	THR
1	A	427	GLN
1	A	453	THR
1	A	455	HIS
1	A	457	THR
1	A	511	LEU
1	A	526	PHE
1	A	582	ASN
1	A	586	PHE
1	A	600	ASP
1	A	612	LEU
1	A	618	VAL
1	A	662	LEU
1	A	667	SER
1	A	670	THR
1	A	682	THR
1	A	686	TYR
1	B	48	ARG
1	B	60	ASN
1	B	61	TYR
1	B	81	LYS
1	B	104	LEU
1	B	120	GLU
1	B	125	ASP
1	B	156	THR
1	B	161	ASN
1	B	265	LEU
1	B	283	ASN
1	B	285	ARG
1	B	301	TYR
1	B	341	THR
1	B	344	VAL
1	B	346	PHE
1	B	352	ILE
1	B	361	GLU
1	B	369	GLN
1	B	373	SER
1	B	385	GLU
1	B	387	LEU
1	B	402	THR
1	B	422	ASP

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Mol	Chain	Res	Type
1	B	423	THR
1	B	446	SER
1	B	470	ASP
1	B	483	ARG
1	B	511	LEU
1	B	522	ARG
1	B	583	THR
1	B	586	PHE
1	B	590	ASP
1	B	626	ASP
1	B	648	LYS
1	B	676	LEU
1	B	682	THR
1	B	686	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	60	ASN
1	A	68	GLN
1	A	88	ASN
1	A	98	ASN
1	A	161	ASN
1	A	170	HIS
1	A	212	HIS
1	A	216	GLN
1	A	223	GLN
1	A	230	ASN
1	A	249	HIS
1	A	267	GLN
1	A	320	GLN
1	A	455	HIS
1	A	484	ASN
1	A	502	HIS
1	A	514	ASN
1	A	582	ASN
1	A	621	GLN
1	A	630	GLN
1	A	637	ASN
1	B	68	GLN
1	B	90	ASN

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Mol	Chain	Res	Type
1	B	98	ASN
1	B	129	ASN
1	B	161	ASN
1	B	170	HIS
1	B	212	HIS
1	B	216	GLN
1	B	225	GLN
1	B	259	GLN
1	B	267	GLN
1	B	313	ASN
1	B	326	ASN
1	B	358	HIS
1	B	376	GLN
1	B	380	ASN
1	B	452	GLN
1	B	455	HIS
1	B	484	ASN
1	B	502	HIS
1	B	531	ASN
1	B	567	ASN
1	B	574	HIS
1	B	589	GLN
1	B	637	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	51,58,58	1.81	9 (17%)	54,89,89	2.01	5 (9%)
3	FMN	A	751	-	31,33,33	1.66	5 (16%)	38,50,50	3.17	11 (28%)
4	NAP	A	753	-	36,43,52	1.10	2 (5%)	42,67,80	1.97	4 (9%)
2	FAD	B	750	-	51,58,58	1.99	10 (19%)	54,89,89	2.08	4 (7%)
3	FMN	B	751	-	31,33,33	1.79	6 (19%)	38,50,50	3.14	13 (34%)
4	NAP	B	753	-	36,43,52	1.06	1 (2%)	42,67,80	2.03	9 (21%)

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	-	-	0/28/50/50	0/6/6/6
3	FMN	A	751	-	-	0/16/18/18	0/3/3/3
4	NAP	A	753	-	-	0/23/59/67	0/4/4/5
2	FAD	B	750	-	-	0/28/50/50	0/6/6/6
3	FMN	B	751	-	-	0/16/18/18	0/3/3/3
4	NAP	B	753	-	-	0/23/59/67	0/4/4/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	FAD	C5A-C4A	-2.22	1.35	1.40
4	A	753	NAP	C5A-N7A	-2.18	1.32	1.39
2	A	750	FAD	C5A-C4A	-2.17	1.35	1.40
3	B	751	FMN	P-O2P	-2.15	1.46	1.54
3	A	751	FMN	P-O2P	-2.03	1.46	1.54
2	B	750	FAD	O4B-C1B	2.01	1.44	1.41
2	A	750	FAD	O4B-C1B	2.06	1.44	1.41
3	B	751	FMN	C5A-N5	2.06	1.38	1.35
2	B	750	FAD	C9A-C5X	2.09	1.46	1.42
3	A	751	FMN	C5A-N5	2.25	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	753	NAP	C4A-N3A	2.83	1.39	1.35
2	A	750	FAD	C9-C8	2.93	1.45	1.37
2	B	750	FAD	C4A-N3A	2.98	1.39	1.35
2	B	750	FAD	C9-C8	3.12	1.46	1.37
2	A	750	FAD	C5X-N5	3.12	1.40	1.35
4	B	753	NAP	C4A-N3A	3.16	1.40	1.35
3	B	751	FMN	C5'-C4'	3.28	1.56	1.51
2	B	750	FAD	C5X-N5	3.33	1.40	1.35
2	A	750	FAD	C4A-N3A	3.41	1.40	1.35
3	A	751	FMN	C9A-N10	3.53	1.43	1.38
3	B	751	FMN	C4A-N5	3.76	1.38	1.33
2	A	750	FAD	C10-N1	4.05	1.38	1.33
2	B	750	FAD	C10-N1	4.07	1.39	1.33
3	A	751	FMN	C4-N3	4.28	1.40	1.33
3	B	751	FMN	C4-N3	4.38	1.41	1.33
3	A	751	FMN	C4A-N5	4.56	1.39	1.33
3	B	751	FMN	C9A-N10	4.61	1.44	1.38
2	B	750	FAD	C4-N3	4.75	1.41	1.33
2	A	750	FAD	C4-N3	4.79	1.41	1.33
2	A	750	FAD	C4X-N5	5.15	1.40	1.33
2	A	750	FAD	C9A-N10	5.52	1.46	1.38
2	B	750	FAD	C9A-N10	6.14	1.46	1.38
2	B	750	FAD	C4X-N5	6.22	1.42	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	753	NAP	N3A-C2A-N1A	-8.90	121.11	128.86
4	B	753	NAP	N3A-C2A-N1A	-8.58	121.39	128.86
3	B	751	FMN	C4A-C4-N3	-5.80	115.23	123.48
2	A	750	FAD	C4X-C4-N3	-5.70	115.36	123.48
3	A	751	FMN	C4A-C4-N3	-5.64	115.45	123.48
2	B	750	FAD	C4X-C4-N3	-5.62	115.48	123.48
3	A	751	FMN	C4A-C10-N10	-5.20	116.91	120.52
4	A	753	NAP	C1B-N9A-C4A	-5.01	117.97	126.64
3	B	751	FMN	C4A-C10-N10	-4.66	117.28	120.52
4	B	753	NAP	C1B-N9A-C4A	-4.54	118.79	126.64
3	A	751	FMN	C4-C4A-C10	-4.42	116.39	119.96
3	B	751	FMN	C4-C4A-C10	-4.30	116.48	119.96
3	B	751	FMN	C4A-N5-C5A	-3.73	112.83	116.76
3	A	751	FMN	C4A-N5-C5A	-3.69	112.87	116.76
3	B	751	FMN	C6-C5A-N5	-2.94	115.51	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	751	FMN	C4-C4A-N5	-2.49	115.95	118.68
2	A	750	FAD	O5'-C5'-C4'	-2.33	103.14	109.36
3	A	751	FMN	C6-C5A-N5	-2.27	116.31	118.97
3	B	751	FMN	O2P-P-O5'	-2.26	100.73	106.73
4	B	753	NAP	O4B-C1B-C2B	-2.24	102.67	106.59
4	B	753	NAP	O3B-C3B-C2B	2.05	117.01	111.18
3	A	751	FMN	P-O5'-C5'	2.14	124.20	118.30
2	A	750	FAD	O2B-C2B-C3B	2.18	118.81	111.83
4	B	753	NAP	C3D-C2D-C1D	2.21	105.67	101.42
3	B	751	FMN	C1'-N10-C10	2.27	120.83	118.50
4	B	753	NAP	C2D-C3D-C4D	2.28	107.06	102.62
3	A	751	FMN	O3'-C3'-C2'	2.37	114.69	108.82
4	A	753	NAP	O3X-P2B-O2X	2.42	117.36	107.61
2	B	750	FAD	O2B-C2B-C3B	2.46	119.71	111.83
4	B	753	NAP	O3X-P2B-O2X	2.49	117.67	107.61
3	B	751	FMN	C1'-N10-C9A	2.54	120.68	118.35
4	A	753	NAP	C4A-C5A-N7A	2.65	111.97	109.41
4	B	753	NAP	C4A-C5A-N7A	2.85	112.17	109.41
3	A	751	FMN	C9A-C5A-N5	2.95	126.62	122.24
3	B	751	FMN	C9A-C5A-N5	3.01	126.72	122.24
3	B	751	FMN	P-O5'-C5'	3.30	127.38	118.30
4	B	753	NAP	O4D-C1D-C2D	3.62	109.33	104.74
3	A	751	FMN	C1'-N10-C10	4.45	123.07	118.50
2	A	750	FAD	C1'-N10-C9A	4.79	122.74	118.35
3	A	751	FMN	C10-C4A-N5	5.60	127.03	120.59
2	B	750	FAD	C1'-N10-C9A	5.88	123.74	118.35
3	B	751	FMN	C10-C4A-N5	6.07	127.57	120.59
2	A	750	FAD	C4-N3-C2	10.95	124.74	115.16
2	B	750	FAD	C4-N3-C2	11.20	124.96	115.16
3	B	751	FMN	C4-N3-C2	13.33	126.82	115.16
3	A	751	FMN	C4-N3-C2	13.68	127.13	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	FAD	2	0
3	A	751	FMN	3	0
4	A	753	NAP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	FAD	4	0
3	B	751	FMN	2	0
4	B	753	NAP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	643/682 (94%)	0.20	18 (2%)	53 49	35, 62, 89, 109	0
1	B	641/682 (93%)	0.20	27 (4%)	37 32	42, 69, 91, 118	0
All	All	1284/1364 (94%)	0.20	45 (3%)	44 39	35, 66, 90, 118	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	658	LEU	4.1
1	B	325	PHE	3.8
1	A	325	PHE	3.5
1	B	335	LEU	3.5
1	B	292	PHE	3.5
1	B	563	LYS	3.2
1	A	241	PRO	3.1
1	B	307	LEU	3.0
1	B	508	PRO	3.0
1	A	185	ALA	2.9
1	B	641	ILE	2.8
1	B	299	ILE	2.8
1	B	662	LEU	2.8
1	A	120	GLU	2.7
1	A	220	PHE	2.7
1	A	245	TYR	2.6
1	A	335	LEU	2.6
1	A	314	PRO	2.6
1	B	482	LEU	2.5
1	B	101	PHE	2.5
1	A	101	PHE	2.5
1	A	588	TYR	2.5
1	B	521	VAL	2.4
1	B	620	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	379	PRO	2.4
1	B	374	LEU	2.3
1	A	231	GLU	2.3
1	A	321	PHE	2.3
1	B	603	PHE	2.3
1	A	171	LEU	2.2
1	B	184	GLU	2.2
1	A	130	PHE	2.2
1	A	50	ILE	2.1
1	B	260	LEU	2.1
1	A	415	LEU	2.1
1	B	676	LEU	2.1
1	B	558	PHE	2.1
1	B	661	ILE	2.1
1	B	571	LEU	2.1
1	B	274	VAL	2.1
1	B	231	GLU	2.0
1	A	324	ILE	2.0
1	B	430	VAL	2.0
1	B	236	MET	2.0
1	B	360	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAP	B	753	40/48	0.91	0.20	-0.06	88,92,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAP	A	753	40/48	0.95	0.20	-0.09	52,59,79,82	0
2	FAD	B	750	53/53	0.95	0.20	-0.13	49,60,67,69	0
3	FMN	B	751	31/31	0.95	0.17	-0.15	49,60,66,66	0
2	FAD	A	750	53/53	0.97	0.18	-0.23	29,47,58,60	0
3	FMN	A	751	31/31	0.97	0.17	-0.36	39,52,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.