



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:55 PM GMT

PDB ID : 1MOK
Title : NADPH DEPENDENT 2-KETOPROPYL COENZYME M OXIDOREDUCTASE/CARBOXYLASE
Authors : Nocek, B.; Jang, S.B.; Jeong, M.S.; Clark, D.D.; Ensign, S.A.; Peters, J.W.
Deposited on : 2002-09-09
Resolution : 2.80 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

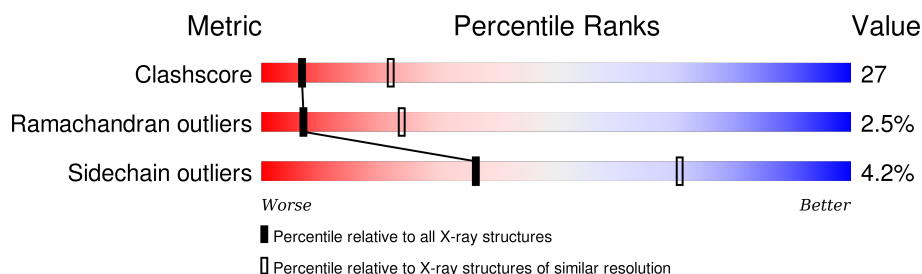
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	523	
1	B	523	
1	C	523	
1	D	523	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16304 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 orf3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	B	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	C	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	D	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			

- 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		

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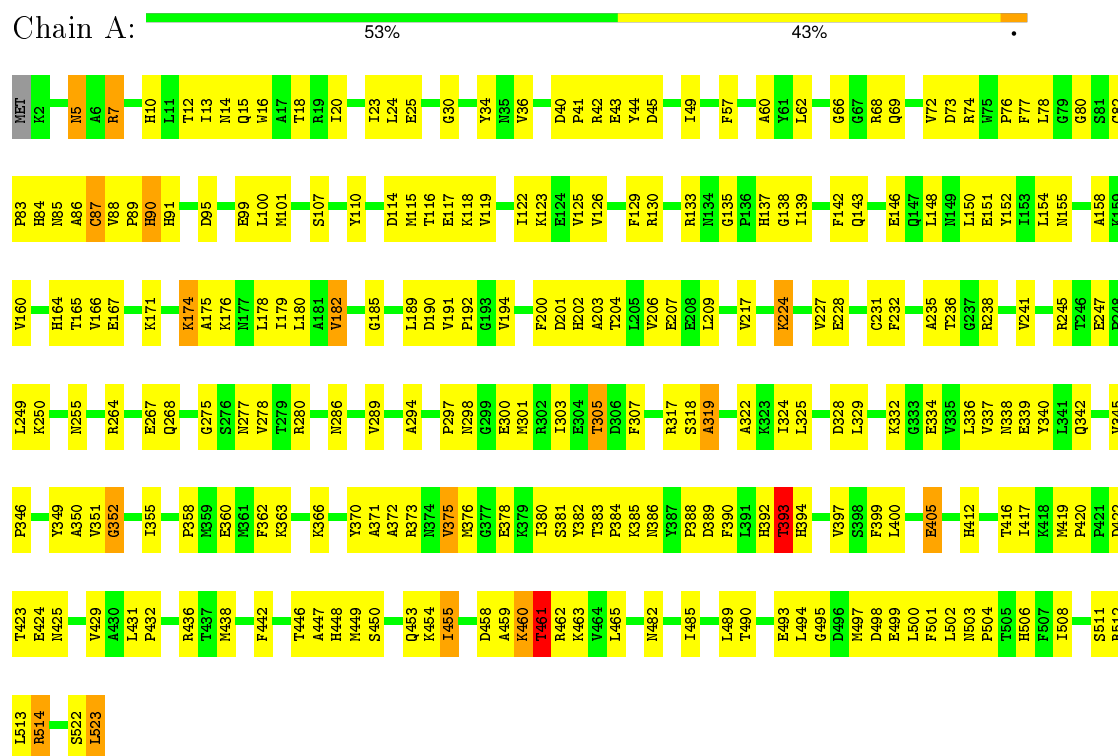
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

3 Residue-property plots

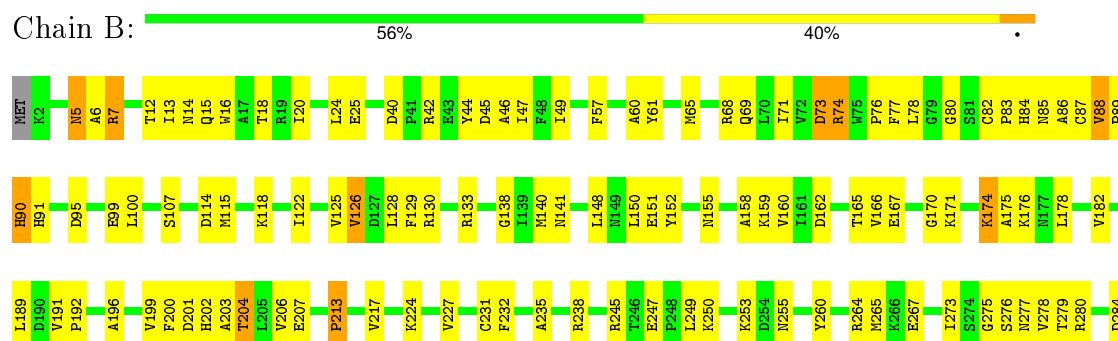
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

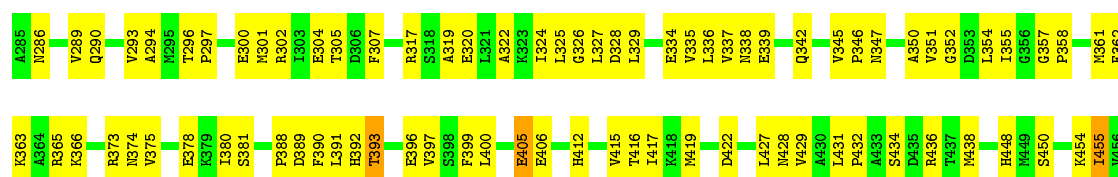
Note EDS was not executed.

• Molecule 1: orf3



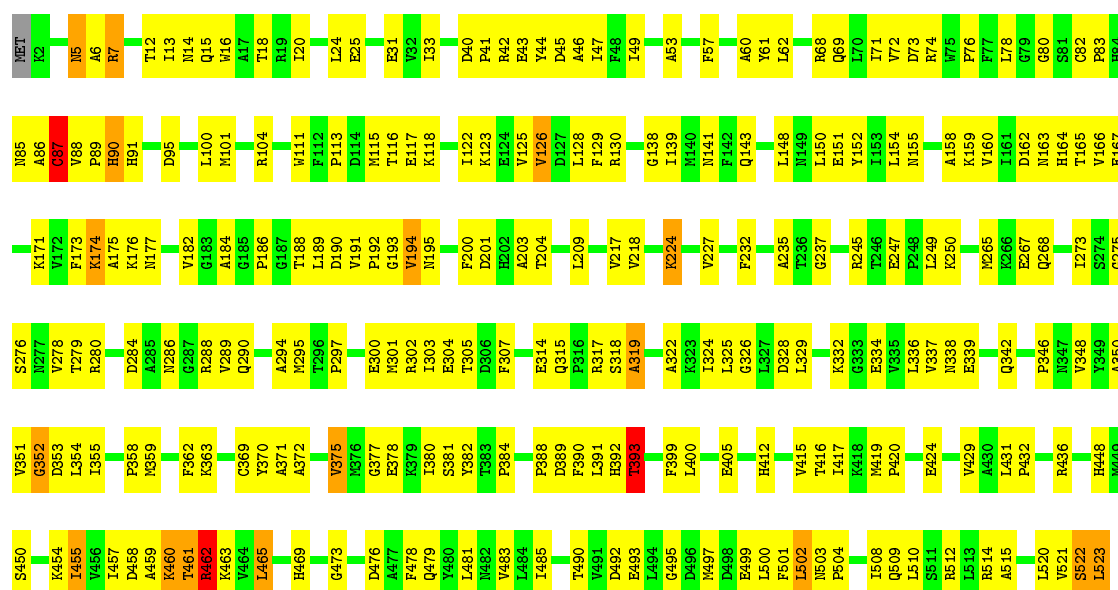
• Molecule 1: orf3





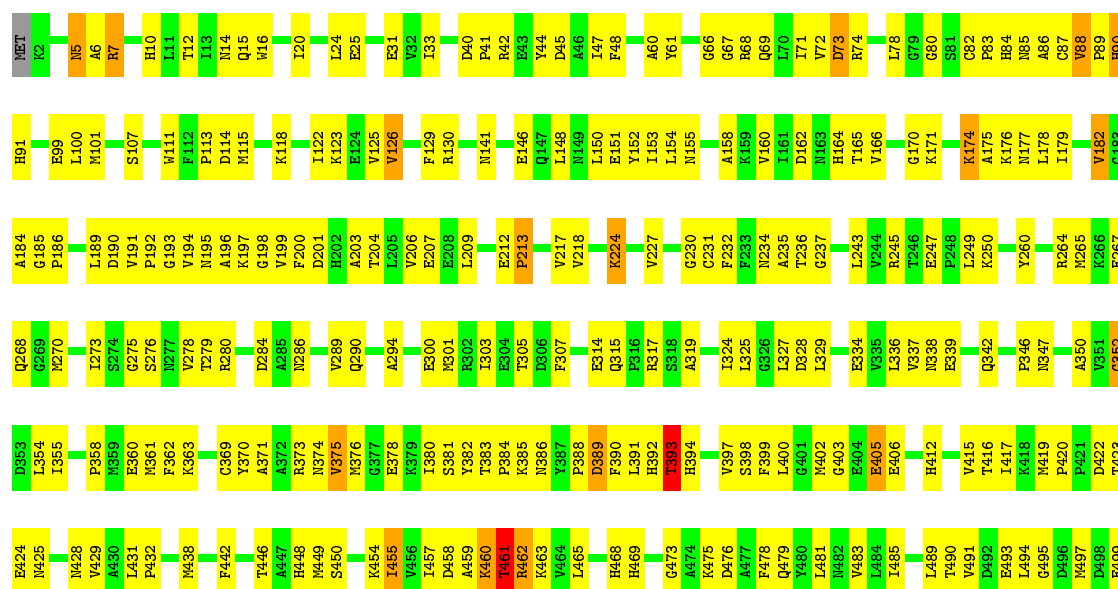
• Molecule 1: orf3

Chain C:  54% 42%



• Molecule 1: orf3

Chain D:  50% 45%



L500	F501	L502	J503	P504	T505	H506	F507	L508	Q509	L510	S511	R512	L513	R514	V521	S522	L523
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.60Å 87.50Å 100.70Å 72.00° 73.40° 69.81°	Depositor
Resolution (Å)	19.99 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (19.99-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16304	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	1/4106 (0.0%)	0.66	2/5556 (0.0%)
1	B	0.53	2/4106 (0.0%)	0.71	4/5556 (0.1%)
1	C	0.48	1/4106 (0.0%)	0.67	4/5556 (0.1%)
1	D	0.50	1/4106 (0.0%)	0.67	2/5556 (0.0%)
All	All	0.50	5/16424 (0.0%)	0.68	12/22224 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	523	LEU	C-O	-16.04	0.92	1.23
1	D	523	LEU	C-O	-15.27	0.94	1.23
1	C	523	LEU	C-O	-15.03	0.94	1.23
1	A	523	LEU	C-O	-14.81	0.95	1.23
1	B	73	ASP	C-N	-7.01	1.18	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	523	LEU	CA-C-O	12.25	145.82	120.10
1	D	523	LEU	CA-C-O	11.65	144.57	120.10
1	A	523	LEU	CA-C-O	10.93	143.06	120.10
1	C	523	LEU	CA-C-O	10.14	141.41	120.10
1	B	462	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	A	393	THR	N-CA-C	-7.20	91.57	111.00
1	C	462	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	D	393	THR	N-CA-C	-6.69	92.94	111.00
1	B	74	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	C	393	THR	N-CA-C	-6.39	93.75	111.00
1	B	393	THR	N-CA-C	-5.98	94.85	111.00
1	C	87	CYS	CA-CB-SG	5.26	123.47	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4023	0	3980	222	0
1	B	4023	0	3979	217	0
1	C	4023	0	3980	234	0
1	D	4023	0	3980	231	0
2	A	53	0	31	6	0
2	B	53	0	31	6	0
2	C	53	0	31	9	0
2	D	53	0	31	12	0
All	All	16304	0	16043	864	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 27.

All (864) 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:C:460:LYS:O	1:C:461:THR:HB	1.39	1.08
1:C:82:CYS:HA	1:C:86:ALA:HB3	1.38	1.05
1:A:82:CYS:HA	1:A:86:ALA:HB3	1.42	1.00
1:D:40:ASP:OD1	1:D:42:ARG:HG2	1.64	0.98
1:C:165:THR:HG22	1:C:174:LYS:HG3	1.46	0.97
1:C:201:ASP:H	1:C:204:THR:HG22	1.27	0.95
1:A:69:GLN:HE22	1:A:151:GLU:H	1.02	0.94
1:B:460:LYS:O	1:B:461:THR:HB	1.64	0.94
1:D:201:ASP:H	1:D:204:THR:HG22	1.34	0.93
1:A:460:LYS:O	1:A:461:THR:HB	1.69	0.93
1:B:69:GLN:HE22	1:B:151:GLU:H	0.94	0.93
1:A:201:ASP:H	1:A:204:THR:HG22	1.28	0.92
1:B:201:ASP:H	1:B:204:THR:HG22	1.34	0.92
1:D:69:GLN:HE22	1:D:151:GLU:H	0.92	0.92
1:D:82:CYS:HA	1:D:86:ALA:HB3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:VAL:HG21	1:D:249:LEU:HD21	1.53	0.90
1:D:165:THR:HG22	1:D:174:LYS:HG3	1.53	0.90
1:A:5:ASN:HD21	1:A:7:ARG:HB2	1.36	0.89
1:A:227:VAL:HG21	1:A:249:LEU:HD21	1.55	0.89
1:C:69:GLN:NE2	1:C:151:GLU:H	1.71	0.89
1:A:165:THR:HG22	1:A:174:LYS:HG3	1.55	0.88
1:B:5:ASN:HD21	1:B:7:ARG:HB2	1.38	0.88
1:D:337:VAL:HG21	1:D:355:ILE:HD13	1.55	0.88
1:C:69:GLN:HE22	1:C:151:GLU:N	1.71	0.88
1:A:350:ALA:O	1:A:355:ILE:HD11	1.74	0.88
1:A:40:ASP:OD1	1:A:42:ARG:HG2	1.73	0.88
1:B:82:CYS:HB3	1:B:83:PRO:HD3	1.55	0.87
1:D:69:GLN:HE22	1:D:151:GLU:N	1.74	0.86
1:D:460:LYS:O	1:D:461:THR:HB	1.75	0.85
1:C:69:GLN:HE22	1:C:151:GLU:H	0.87	0.83
1:D:350:ALA:O	1:D:355:ILE:HD11	1.79	0.83
1:C:227:VAL:HG21	1:C:249:LEU:HD21	1.58	0.83
1:D:69:GLN:NE2	1:D:151:GLU:H	1.75	0.81
1:A:12:THR:HB	1:A:15:GLN:HG3	1.63	0.80
1:B:227:VAL:HG21	1:B:249:LEU:HD21	1.62	0.80
1:A:126:VAL:O	1:A:130:ARG:HG3	1.82	0.80
1:B:165:THR:HG22	1:B:174:LYS:HG3	1.63	0.80
1:B:217:VAL:HG22	1:B:307:PHE:HD2	1.46	0.79
1:C:432:PRO:O	1:C:450:SER:HB2	1.82	0.79
1:C:82:CYS:CA	1:C:86:ALA:HB3	2.12	0.79
1:A:201:ASP:H	1:A:204:THR:CG2	1.96	0.78
1:B:40:ASP:OD1	1:B:42:ARG:HG2	1.82	0.78
1:C:5:ASN:HD21	1:C:7:ARG:HB2	1.48	0.78
1:A:5:ASN:ND2	1:A:7:ARG:HB2	1.99	0.78
1:D:417:ILE:HG22	1:D:455:ILE:HG22	1.66	0.78
1:A:255:ASN:HB2	1:A:405:GLU:OE1	1.83	0.78
1:A:74:ARG:O	1:A:155:ASN:HA	1.83	0.78
1:B:499:GLU:HB2	1:B:503:ASN:ND2	1.99	0.77
1:B:5:ASN:ND2	1:B:7:ARG:HB2	1.98	0.77
1:D:201:ASP:H	1:D:204:THR:CG2	1.96	0.76
1:C:40:ASP:OD1	1:C:42:ARG:HG2	1.85	0.76
1:A:82:CYS:CA	1:A:86:ALA:HB3	2.16	0.76
1:B:69:GLN:NE2	1:B:151:GLU:H	1.80	0.75
1:C:337:VAL:HG21	1:C:355:ILE:HD13	1.66	0.75
1:C:460:LYS:O	1:C:461:THR:CB	2.26	0.75
1:B:69:GLN:HE22	1:B:151:GLU:N	1.80	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:O	1:B:363:LYS:HD3	1.88	0.74
1:C:122:ILE:O	1:C:125:VAL:HG12	1.86	0.74
1:A:499:GLU:HB2	1:A:503:ASN:ND2	2.03	0.74
1:C:417:ILE:HG22	1:C:455:ILE:HG22	1.71	0.73
1:B:273:ILE:HG22	1:B:276:SER:HB2	1.70	0.73
1:D:338:ASN:HD21	1:D:342:GLN:NE2	1.87	0.72
1:C:416:THR:HG22	1:C:523:LEU:HG	1.70	0.72
1:A:160:VAL:HG11	1:A:325:LEU:HD21	1.70	0.72
1:B:337:VAL:HG21	1:B:355:ILE:HD13	1.72	0.72
1:C:355:ILE:O	1:C:355:ILE:HG22	1.89	0.72
1:A:412:HIS:HD2	1:A:458:ASP:OD2	1.72	0.72
1:D:247:GLU:HB2	1:D:250:LYS:HE2	1.71	0.72
1:B:355:ILE:HG22	1:B:355:ILE:O	1.89	0.71
1:B:74:ARG:O	1:B:155:ASN:HA	1.89	0.71
1:B:458:ASP:O	1:B:462:ARG:HA	1.91	0.71
1:D:82:CYS:CA	1:D:86:ALA:HB3	2.21	0.71
1:A:337:VAL:HG21	1:A:355:ILE:HD13	1.73	0.71
1:B:432:PRO:O	1:B:450:SER:HB2	1.90	0.71
1:D:82:CYS:HB3	1:D:83:PRO:HD3	1.70	0.71
1:A:338:ASN:HD21	1:A:342:GLN:NE2	1.88	0.71
1:B:275:GLY:O	1:B:297:PRO:HD3	1.90	0.71
1:D:328:ASP:O	1:D:329:LEU:HD23	1.91	0.70
1:C:201:ASP:H	1:C:204:THR:CG2	2.03	0.70
1:A:339:GLU:O	1:A:381:SER:HA	1.92	0.70
1:C:200:PHE:HD1	1:C:204:THR:HG23	1.55	0.70
1:B:82:CYS:HA	1:B:86:ALA:HB3	1.71	0.70
1:D:432:PRO:O	1:D:450:SER:HB2	1.91	0.70
1:A:358:PRO:O	1:A:363:LYS:HD3	1.92	0.69
1:A:490:THR:OG1	1:A:493:GLU:HG3	1.92	0.69
1:A:82:CYS:HB3	1:A:83:PRO:HD3	1.73	0.69
1:B:350:ALA:O	1:B:355:ILE:HD11	1.92	0.69
1:C:462:ARG:HB3	1:C:520:LEU:HD11	1.75	0.69
1:C:358:PRO:O	1:C:363:LYS:HD3	1.93	0.69
1:D:227:VAL:CG1	1:D:393:THR:HG22	2.22	0.68
1:B:82:CYS:HB3	1:B:83:PRO:CD	2.23	0.68
1:C:12:THR:HG22	1:C:14:ASN:H	1.58	0.68
1:A:328:ASP:HB3	1:A:336:LEU:HD12	1.76	0.68
1:B:14:ASN:O	1:B:18:THR:HG23	1.93	0.68
1:D:355:ILE:HG22	1:D:355:ILE:O	1.93	0.68
1:A:12:THR:HG22	1:A:14:ASN:H	1.58	0.68
1:C:165:THR:HG22	1:C:174:LYS:CG	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLY:HA3	2:B:524:FAD:O2P	1.92	0.68
1:D:338:ASN:HD21	1:D:342:GLN:HE21	1.39	0.68
1:D:122:ILE:O	1:D:125:VAL:HG12	1.93	0.68
1:C:5:ASN:ND2	1:C:7:ARG:HB2	2.09	0.67
1:C:476:ASP:O	1:C:479:GLN:HG3	1.93	0.67
1:D:200:PHE:HD1	1:D:204:THR:HG23	1.60	0.67
1:A:192:PRO:HG2	1:A:280:ARG:HB2	1.77	0.67
1:C:350:ALA:O	1:C:355:ILE:HD11	1.95	0.67
1:B:12:THR:HG22	1:B:14:ASN:H	1.59	0.66
1:C:352:GLY:HA3	2:C:524:FAD:O2P	1.95	0.66
1:C:87:CYS:HA	1:C:90:HIS:HD2	1.61	0.66
1:D:373:ARG:HH21	1:D:380:ILE:HG12	1.59	0.66
1:B:126:VAL:O	1:B:130:ARG:HG3	1.96	0.66
1:D:227:VAL:HG11	1:D:393:THR:HG22	1.77	0.66
1:A:338:ASN:OD1	1:A:342:GLN:HB2	1.96	0.66
1:C:49:ILE:HG22	1:C:182:VAL:HG23	1.78	0.66
1:D:378:GLU:HB3	1:D:380:ILE:HD13	1.78	0.65
1:C:497:MET:SD	1:D:483:VAL:HG21	2.37	0.65
1:D:338:ASN:OD1	1:D:342:GLN:HB2	1.97	0.65
1:B:400:LEU:HD11	1:B:485:ILE:HD12	1.79	0.65
1:C:247:GLU:HB2	1:C:250:LYS:HE2	1.79	0.65
1:D:454:LYS:HG2	1:D:455:ILE:N	2.12	0.65
1:A:417:ILE:HG22	1:A:455:ILE:HG22	1.77	0.65
1:C:337:VAL:HA	1:C:342:GLN:O	1.97	0.65
1:A:115:MET:O	1:A:118:LYS:HB3	1.97	0.65
1:A:454:LYS:HG2	1:A:455:ILE:N	2.12	0.65
1:C:113:PRO:HG3	1:D:113:PRO:HD3	1.79	0.64
1:A:494:LEU:HD23	1:A:511:SER:OG	1.97	0.64
1:C:128:LEU:HD11	1:D:442:PHE:O	1.98	0.64
1:C:160:VAL:HG11	1:C:325:LEU:HD21	1.79	0.64
1:A:378:GLU:HB3	1:A:380:ILE:HD13	1.79	0.64
1:A:62:LEU:HB2	1:A:372:ALA:HB1	1.79	0.64
1:B:227:VAL:HG11	1:B:393:THR:HG22	1.80	0.64
1:A:224:LYS:NZ	1:A:360:GLU:OE2	2.23	0.64
1:D:499:GLU:HB2	1:D:503:ASN:ND2	2.13	0.63
1:A:122:ILE:O	1:A:125:VAL:HG12	1.99	0.63
1:C:227:VAL:HG13	1:C:265:MET:HE3	1.80	0.63
1:B:227:VAL:CG1	1:B:393:THR:HG22	2.28	0.63
1:D:267:GLU:OE1	1:D:448:HIS:HE1	1.82	0.63
1:D:300:GLU:HG2	1:D:301:MET:N	2.14	0.63
1:C:45:ASP:O	1:C:177:ASN:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ARG:O	1:C:155:ASN:HA	1.99	0.62
1:C:113:PRO:HD3	1:D:113:PRO:HG3	1.79	0.62
1:B:191:VAL:CG2	1:B:192:PRO:HD2	2.29	0.62
1:C:481:LEU:O	1:C:485:ILE:HG13	1.99	0.62
1:D:44:TYR:CD1	1:D:68:ARG:HG2	2.34	0.62
1:A:87:CYS:HA	1:A:90:HIS:HD2	1.63	0.62
1:C:126:VAL:O	1:C:130:ARG:HG3	2.00	0.62
1:B:473:GLY:O	1:B:504:PRO:HG2	1.98	0.62
1:C:389:ASP:HB3	1:C:399:PHE:CE1	2.34	0.62
1:C:12:THR:HB	1:C:15:GLN:HG3	1.81	0.62
1:A:300:GLU:HG2	1:A:301:MET:N	2.14	0.62
1:D:74:ARG:HG3	2:D:524:FAD:C2A	2.29	0.62
1:C:458:ASP:O	1:C:462:ARG:HA	2.00	0.62
1:A:160:VAL:O	1:A:324:ILE:HG21	2.00	0.61
1:C:279:THR:H	1:C:294:ALA:HA	1.66	0.61
1:A:499:GLU:HB2	1:A:503:ASN:HD22	1.63	0.61
1:B:462:ARG:HB3	1:B:520:LEU:HD11	1.82	0.61
1:C:300:GLU:HG2	1:C:301:MET:N	2.15	0.61
1:A:416:THR:HG22	1:A:523:LEU:HG	1.81	0.61
1:B:300:GLU:HG2	1:B:301:MET:N	2.16	0.61
1:B:352:GLY:CA	2:B:524:FAD:O2P	2.49	0.61
1:C:499:GLU:HB2	1:C:503:ASN:ND2	2.16	0.61
1:C:476:ASP:OD1	1:D:503:ASN:HB2	2.00	0.60
1:B:182:VAL:HG12	1:B:317:ARG:HB2	1.83	0.60
1:B:24:LEU:HD13	1:B:76:PRO:HG3	1.83	0.60
1:B:191:VAL:HG22	1:B:192:PRO:HD2	1.83	0.60
1:A:495:GLY:O	1:A:512:ARG:HD3	2.01	0.60
1:D:495:GLY:O	1:D:512:ARG:HB2	2.00	0.60
1:B:86:ALA:O	1:B:90:HIS:HB3	2.02	0.60
1:C:328:ASP:O	1:C:329:LEU:HD23	2.01	0.60
1:C:502:LEU:HG	1:D:91:HIS:CD2	2.36	0.60
1:C:454:LYS:HG2	1:C:455:ILE:N	2.16	0.60
1:C:16:TRP:O	1:C:20:ILE:HG13	2.02	0.60
1:A:389:ASP:HB3	1:A:399:PHE:CE1	2.37	0.60
1:B:327:LEU:HD23	1:B:345:VAL:CG2	2.32	0.60
1:D:182:VAL:CG1	1:D:317:ARG:HB2	2.31	0.60
1:A:400:LEU:HD12	1:A:400:LEU:O	2.02	0.59
1:D:165:THR:HG22	1:D:174:LYS:CG	2.30	0.59
1:A:227:VAL:HG11	1:A:393:THR:HG22	1.83	0.59
1:C:353:ASP:OD2	2:C:524:FAD:H5'2	2.02	0.59
1:D:400:LEU:HD12	1:D:400:LEU:C	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:ASP:HB3	1:D:336:LEU:HD12	1.84	0.59
1:C:417:ILE:HG22	1:C:455:ILE:CG2	2.32	0.59
1:B:273:ILE:CG2	1:B:276:SER:HB2	2.31	0.59
1:B:338:ASN:HD21	1:B:342:GLN:HE21	1.48	0.59
1:B:378:GLU:HB3	1:B:380:ILE:HD13	1.84	0.59
1:A:60:ALA:HA	1:A:150:LEU:HD21	1.85	0.59
1:C:191:VAL:CG2	1:C:192:PRO:HD2	2.32	0.59
1:C:503:ASN:HB2	1:D:476:ASP:OD1	2.03	0.59
1:D:243:LEU:HD22	1:D:276:SER:OG	2.03	0.59
1:A:497:MET:SD	1:B:483:VAL:HG21	2.42	0.59
1:C:353:ASP:HB3	1:C:359:MET:SD	2.43	0.59
1:D:217:VAL:HG22	1:D:307:PHE:HD2	1.68	0.59
1:A:191:VAL:HG22	1:A:280:ARG:HA	1.85	0.58
1:D:12:THR:HG22	1:D:14:ASN:H	1.67	0.58
1:D:417:ILE:HG22	1:D:455:ILE:CG2	2.33	0.58
1:C:89:PRO:HB3	1:C:129:PHE:CE1	2.38	0.58
1:B:264:ARG:HG2	1:B:264:ARG:HH11	1.69	0.58
1:B:125:VAL:HG11	1:B:232:PHE:HZ	1.65	0.58
1:A:267:GLU:OE1	1:A:448:HIS:HE1	1.86	0.58
1:C:501:PHE:O	2:D:524:FAD:N3	2.34	0.58
1:B:476:ASP:O	1:B:479:GLN:HG3	2.02	0.58
1:A:180:LEU:N	1:A:349:TYR:O	2.32	0.58
1:D:191:VAL:HG22	1:D:192:PRO:HD2	1.84	0.58
1:A:95:ASP:OD2	1:B:438:MET:HG2	2.02	0.58
1:A:338:ASN:HD21	1:A:342:GLN:HE21	1.49	0.58
1:C:492:ASP:OD1	1:C:515:ALA:HB1	2.03	0.58
1:A:432:PRO:O	1:A:450:SER:HB2	2.03	0.58
1:D:160:VAL:HG11	1:D:325:LEU:HD21	1.85	0.58
1:C:463:LYS:O	1:C:465:LEU:HD13	2.03	0.58
1:A:192:PRO:HG2	1:A:280:ARG:CB	2.33	0.58
1:C:74:ARG:HG3	2:C:524:FAD:C2A	2.34	0.58
1:C:95:ASP:OD2	1:D:438:MET:HB2	2.03	0.58
1:A:355:ILE:HG22	1:A:355:ILE:O	2.04	0.58
1:B:277:ASN:O	1:B:294:ALA:HB1	2.04	0.58
1:A:90:HIS:HE1	1:A:392:HIS:HD2	1.52	0.57
1:B:412:HIS:HD2	1:B:458:ASP:OD2	1.87	0.57
1:B:328:ASP:HB3	1:B:336:LEU:HD12	1.85	0.57
1:D:89:PRO:HB3	1:D:129:PHE:CZ	2.39	0.57
1:B:389:ASP:HB3	1:B:399:PHE:CE1	2.38	0.57
1:A:489:LEU:HD21	1:A:494:LEU:HD13	1.86	0.57
1:D:300:GLU:HG2	1:D:301:MET:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:PHE:CD1	1:C:502:LEU:HA	2.38	0.57
1:C:86:ALA:O	1:C:90:HIS:HB3	2.03	0.57
1:B:115:MET:O	1:B:118:LYS:HB3	2.03	0.57
1:D:420:PRO:HB3	1:D:431:LEU:O	2.04	0.57
1:A:334:GLU:HG2	1:A:334:GLU:O	2.03	0.57
1:B:206:VAL:HG23	1:B:207:GLU:OE2	2.03	0.57
1:C:302:ARG:HH12	1:C:304:GLU:HG3	1.69	0.57
1:C:82:CYS:HB3	1:C:83:PRO:HD3	1.86	0.57
1:C:40:ASP:HB3	1:C:68:ARG:NH1	2.20	0.57
1:A:247:GLU:HB2	1:A:250:LYS:HE2	1.87	0.57
1:A:90:HIS:CE1	1:A:392:HIS:HD2	2.22	0.57
1:B:192:PRO:HG2	1:B:280:ARG:HB2	1.87	0.57
1:A:460:LYS:O	1:A:461:THR:CB	2.51	0.57
1:B:84:HIS:ND1	1:B:133:ARG:HD2	2.20	0.57
1:A:123:LYS:HA	1:A:209:LEU:HD23	1.87	0.56
1:C:461:THR:O	1:C:461:THR:HG22	2.03	0.56
1:D:126:VAL:O	1:D:130:ARG:HG3	2.05	0.56
1:C:182:VAL:HG12	1:C:317:ARG:HB2	1.87	0.56
1:B:419:MET:HB3	1:B:432:PRO:HB3	1.85	0.56
1:C:160:VAL:O	1:C:324:ILE:HG21	2.05	0.56
1:A:390:PHE:HA	1:A:397:VAL:O	2.05	0.56
1:D:403:GLY:HA2	1:D:468:HIS:NE2	2.20	0.56
1:D:459:ALA:O	1:D:460:LYS:HB2	2.04	0.56
1:B:338:ASN:HD21	1:B:342:GLN:NE2	2.02	0.56
1:A:191:VAL:CG2	1:A:192:PRO:HD2	2.35	0.56
1:A:416:THR:CG2	1:A:523:LEU:HG	2.36	0.56
1:C:245:ARG:O	1:C:275:GLY:HA2	2.05	0.56
1:C:62:LEU:HB2	1:C:372:ALA:HB1	1.88	0.56
1:B:247:GLU:HB2	1:B:250:LYS:HE2	1.88	0.56
1:A:423:THR:HB	1:B:13:ILE:HD12	1.87	0.56
1:C:192:PRO:HG2	1:C:280:ARG:HB2	1.88	0.56
1:D:370:TYR:CD1	1:D:382:TYR:HB2	2.41	0.56
1:C:378:GLU:HB3	1:C:380:ILE:HD13	1.87	0.56
1:D:358:PRO:O	1:D:363:LYS:HD3	2.05	0.56
1:C:483:VAL:HG21	1:D:497:MET:SD	2.45	0.56
1:B:49:ILE:HG22	1:B:182:VAL:HG23	1.87	0.56
1:A:191:VAL:HG22	1:A:192:PRO:HD2	1.87	0.55
1:B:454:LYS:HG2	1:B:455:ILE:N	2.21	0.55
1:C:72:VAL:CG1	1:C:158:ALA:HB2	2.35	0.55
1:D:231:CYS:SG	1:D:393:THR:HA	2.46	0.55
1:A:179:ILE:HD11	1:A:351:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:GLN:HG2	1:C:510:LEU:H	1.70	0.55
1:C:182:VAL:HG13	2:C:524:FAD:C8A	2.36	0.55
1:A:90:HIS:CD2	2:A:524:FAD:H6	2.42	0.55
1:D:191:VAL:CG2	1:D:192:PRO:HD2	2.35	0.55
1:C:400:LEU:HD12	1:C:400:LEU:C	2.27	0.55
1:C:47:ILE:HG13	1:C:175:ALA:HB2	1.88	0.55
1:D:82:CYS:HB3	1:D:83:PRO:CD	2.37	0.55
1:C:89:PRO:HB3	1:C:129:PHE:CZ	2.42	0.55
1:C:275:GLY:O	1:C:297:PRO:HD3	2.07	0.55
1:D:212:GLU:OE1	1:D:213:PRO:HD2	2.06	0.55
1:C:461:THR:O	1:C:461:THR:CG2	2.54	0.55
1:C:352:GLY:CA	2:C:524:FAD:O2P	2.55	0.55
1:D:403:GLY:HA2	1:D:468:HIS:HE2	1.72	0.55
1:B:255:ASN:HB2	1:B:405:GLU:OE1	2.07	0.55
1:B:400:LEU:C	1:B:400:LEU:HD12	2.28	0.54
1:D:89:PRO:HB3	1:D:129:PHE:CE1	2.42	0.54
1:A:227:VAL:CG1	1:A:393:THR:HG22	2.38	0.54
1:A:338:ASN:ND2	1:A:342:GLN:HE21	2.04	0.54
1:B:165:THR:HG22	1:B:174:LYS:CG	2.34	0.54
1:C:100:LEU:HB2	1:C:235:ALA:HB1	1.89	0.54
1:C:44:TYR:CD1	1:C:68:ARG:HG2	2.43	0.54
1:A:400:LEU:C	1:A:400:LEU:HD12	2.28	0.54
1:D:490:THR:OG1	1:D:493:GLU:HG3	2.07	0.54
1:A:13:ILE:HG21	1:A:139:ILE:HG12	1.89	0.54
1:A:499:GLU:OE2	1:A:512:ARG:NH2	2.39	0.54
1:A:165:THR:HG22	1:A:174:LYS:CG	2.33	0.54
1:C:217:VAL:HG22	1:C:307:PHE:HD2	1.73	0.54
1:A:400:LEU:HD11	1:A:485:ILE:CD1	2.38	0.54
1:D:171:LYS:N	1:D:171:LYS:HD2	2.23	0.54
1:C:82:CYS:N	1:C:86:ALA:HB3	2.23	0.54
1:D:73:ASP:OD1	2:D:524:FAD:H1B	2.07	0.54
1:B:481:LEU:O	1:B:485:ILE:HG13	2.07	0.54
1:D:286:ASN:HD22	1:D:286:ASN:N	2.06	0.54
1:C:339:GLU:O	1:C:381:SER:HA	2.08	0.54
1:B:90:HIS:HE1	1:B:392:HIS:HD2	1.54	0.54
1:C:20:ILE:O	1:C:24:LEU:HB2	2.08	0.54
1:C:300:GLU:HG2	1:C:301:MET:H	1.71	0.54
1:D:5:ASN:ND2	1:D:7:ARG:HB2	2.23	0.54
1:A:69:GLN:HE22	1:A:151:GLU:N	1.86	0.53
1:D:182:VAL:HG12	1:D:317:ARG:HB2	1.89	0.53
1:B:396:GLU:HB2	1:B:471:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:VAL:HG22	1:B:307:PHE:CD2	2.37	0.53
1:C:416:THR:CG2	1:C:523:LEU:HG	2.37	0.53
1:A:352:GLY:O	1:A:363:LYS:NZ	2.34	0.53
1:C:350:ALA:C	1:C:355:ILE:HD11	2.29	0.53
1:A:393:THR:OG1	1:A:394:HIS:N	2.41	0.53
1:B:90:HIS:CE1	1:B:392:HIS:HD2	2.27	0.53
1:C:191:VAL:HG22	1:C:280:ARG:HA	1.90	0.53
1:B:391:LEU:C	1:B:391:LEU:HD12	2.29	0.53
1:B:350:ALA:C	1:B:355:ILE:HD11	2.29	0.53
1:C:509:GLN:HG2	1:C:510:LEU:N	2.23	0.53
1:C:116:THR:O	1:C:117:GLU:HB2	2.09	0.53
1:D:218:VAL:HG22	1:D:303:ILE:HD13	1.91	0.53
1:B:88:VAL:HB	1:B:89:PRO:CD	2.38	0.53
1:D:74:ARG:O	1:D:155:ASN:HA	2.09	0.53
1:D:338:ASN:ND2	1:D:342:GLN:HE21	2.06	0.53
1:A:461:THR:O	1:A:463:LYS:N	2.42	0.53
1:C:189:LEU:HD21	1:C:278:VAL:HB	1.91	0.53
1:B:20:ILE:O	1:B:24:LEU:HB2	2.09	0.53
1:A:135:GLY:O	1:A:139:ILE:HG13	2.09	0.53
1:D:87:CYS:HA	2:D:524:FAD:N5	2.24	0.53
1:D:412:HIS:HD2	1:D:458:ASP:OD2	1.91	0.53
1:D:337:VAL:HA	1:D:342:GLN:O	2.09	0.52
1:C:469:HIS:ND1	1:C:469:HIS:C	2.61	0.52
1:D:264:ARG:HG2	1:D:264:ARG:NH1	2.24	0.52
1:D:42:ARG:HG3	1:D:68:ARG:HD2	1.91	0.52
1:A:417:ILE:HD13	1:A:514:ARG:HE	1.75	0.52
1:D:260:TYR:O	1:D:264:ARG:HG2	2.09	0.52
1:A:86:ALA:O	1:A:90:HIS:HB3	2.10	0.52
1:D:374:ASN:HA	1:D:378:GLU:O	2.10	0.52
1:B:400:LEU:HD11	1:B:485:ILE:CD1	2.39	0.52
1:B:461:THR:O	1:B:463:LYS:N	2.43	0.52
1:B:499:GLU:HB2	1:B:503:ASN:HD22	1.71	0.52
1:B:264:ARG:NH1	1:B:264:ARG:HG2	2.24	0.52
1:D:419:MET:HA	1:D:420:PRO:C	2.30	0.52
1:D:325:LEU:HB2	1:D:327:LEU:HD21	1.92	0.52
1:A:373:ARG:NH2	1:A:378:GLU:OE1	2.42	0.52
1:C:420:PRO:HB3	1:C:431:LEU:O	2.10	0.52
1:C:462:ARG:O	1:C:490:THR:HA	2.10	0.52
1:B:122:ILE:O	1:B:125:VAL:HG12	2.09	0.52
1:B:189:LEU:HD21	1:B:278:VAL:HB	1.92	0.51
1:D:362:PHE:CD1	1:D:363:LYS:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LYS:HA	1:C:209:LEU:HD23	1.93	0.51
1:C:267:GLU:OE1	1:C:448:HIS:HE1	1.92	0.51
1:A:89:PRO:HB3	1:A:129:PHE:CZ	2.46	0.51
1:C:391:LEU:C	1:C:391:LEU:HD12	2.31	0.51
1:B:499:GLU:HB2	1:B:503:ASN:HD21	1.76	0.51
1:D:232:PHE:O	1:D:236:THR:HG23	2.10	0.51
1:B:483:VAL:O	1:B:487:GLN:HG3	2.10	0.51
1:D:90:HIS:HD2	2:D:524:FAD:N5	2.08	0.51
1:A:247:GLU:HA	1:A:247:GLU:OE2	2.10	0.51
1:D:166:VAL:CG2	1:D:178:LEU:HD21	2.40	0.51
1:D:337:VAL:CG2	1:D:355:ILE:HD13	2.37	0.51
1:A:337:VAL:HA	1:A:342:GLN:O	2.10	0.51
1:C:490:THR:OG1	1:C:493:GLU:HG3	2.11	0.51
1:C:247:GLU:HA	1:C:247:GLU:OE2	2.10	0.51
1:B:300:GLU:HG2	1:B:301:MET:H	1.75	0.51
1:C:332:LYS:HB3	1:C:334:GLU:OE1	2.09	0.51
1:D:499:GLU:HB2	1:D:503:ASN:HD22	1.75	0.51
1:C:370:TYR:CD1	1:C:382:TYR:HB2	2.46	0.51
1:A:166:VAL:CG2	1:A:178:LEU:HD21	2.41	0.51
1:B:302:ARG:HH12	1:B:304:GLU:HG3	1.76	0.51
1:C:12:THR:HG23	1:D:424:GLU:OE2	2.10	0.51
1:A:419:MET:HB3	1:A:432:PRO:HB3	1.92	0.51
1:D:382:TYR:CE2	1:D:384:PRO:HD3	2.46	0.51
1:B:339:GLU:O	1:B:381:SER:HA	2.11	0.51
1:B:337:VAL:HA	1:B:342:GLN:O	2.11	0.51
1:B:373:ARG:NH2	1:B:378:GLU:OE1	2.44	0.51
1:B:267:GLU:OE1	1:B:448:HIS:HE1	1.93	0.51
1:C:45:ASP:HA	1:C:176:LYS:HE3	1.90	0.51
1:A:179:ILE:HD12	1:A:371:ALA:CB	2.41	0.50
1:D:264:ARG:HH11	1:D:264:ARG:HG2	1.75	0.50
1:A:88:VAL:HB	1:A:89:PRO:CD	2.41	0.50
1:D:160:VAL:O	1:D:324:ILE:HG21	2.11	0.50
1:D:415:VAL:HG23	1:D:457:ILE:HB	1.94	0.50
1:D:90:HIS:CD2	2:D:524:FAD:N5	2.79	0.50
1:C:24:LEU:HD13	1:C:76:PRO:CG	2.41	0.50
1:C:47:ILE:HG13	1:C:175:ALA:CB	2.42	0.50
1:D:339:GLU:O	1:D:381:SER:HA	2.12	0.50
1:D:334:GLU:HG2	1:D:334:GLU:O	2.11	0.50
1:B:217:VAL:CG2	1:B:307:PHE:HD2	2.20	0.50
1:D:417:ILE:HD13	1:D:514:ARG:HE	1.77	0.50
1:B:391:LEU:O	1:B:391:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:CG1	1:A:158:ALA:HB2	2.41	0.50
1:C:12:THR:HG22	1:C:14:ASN:N	2.26	0.50
1:B:159:LYS:HB2	1:B:167:GLU:HB3	1.93	0.50
1:D:280:ARG:HG2	1:D:280:ARG:HH11	1.77	0.50
1:C:400:LEU:HD23	1:C:478:PHE:CD2	2.46	0.50
1:B:416:THR:HG22	1:B:523:LEU:HG	1.92	0.50
1:D:416:THR:HG22	1:D:523:LEU:HG	1.92	0.50
1:A:91:HIS:HE1	2:A:524:FAD:O4	1.95	0.50
1:D:461:THR:HG22	1:D:463:LYS:H	1.77	0.50
1:B:182:VAL:CG1	1:B:182:VAL:O	2.60	0.50
1:D:88:VAL:HB	1:D:89:PRO:CD	2.41	0.50
1:A:352:GLY:CA	2:A:524:FAD:O2P	2.61	0.49
1:B:125:VAL:HG11	1:B:232:PHE:CZ	2.47	0.49
1:A:420:PRO:HB3	1:A:431:LEU:O	2.12	0.49
1:D:390:PHE:HA	1:D:397:VAL:O	2.11	0.49
1:C:362:PHE:CD1	1:C:363:LYS:N	2.80	0.49
1:A:419:MET:HB2	1:A:453:GLN:HG2	1.95	0.49
1:B:320:GLU:O	1:B:324:ILE:HG13	2.12	0.49
1:A:24:LEU:HD21	1:A:84:HIS:CE1	2.47	0.49
1:D:82:CYS:N	1:D:86:ALA:HB3	2.26	0.49
1:A:300:GLU:HG2	1:A:301:MET:H	1.75	0.49
1:A:43:GLU:HG2	1:A:44:TYR:N	2.26	0.49
1:C:200:PHE:CD1	1:C:204:THR:HG23	2.43	0.49
1:D:31:GLU:O	1:D:155:ASN:ND2	2.33	0.49
1:B:231:CYS:SG	1:B:393:THR:HA	2.53	0.49
1:C:191:VAL:HG22	1:C:192:PRO:HD2	1.94	0.49
1:D:509:GLN:HG2	1:D:510:LEU:H	1.77	0.49
1:B:47:ILE:HG13	1:B:175:ALA:HB2	1.94	0.49
1:C:73:ASP:OD1	2:C:524:FAD:O3B	2.26	0.49
1:C:91:HIS:CD2	1:D:502:LEU:HG	2.47	0.49
1:A:217:VAL:HG13	1:A:307:PHE:CD2	2.48	0.49
1:D:125:VAL:HG11	1:D:232:PHE:HZ	1.77	0.49
1:C:278:VAL:HA	1:C:294:ALA:HB2	1.93	0.49
1:B:327:LEU:HD23	1:B:345:VAL:HG21	1.95	0.49
1:D:206:VAL:HG23	1:D:207:GLU:OE2	2.12	0.49
1:D:115:MET:O	1:D:118:LYS:HB3	2.12	0.49
1:D:71:ILE:HB	1:D:152:TYR:HB3	1.94	0.49
1:A:337:VAL:HG11	1:A:350:ALA:HB3	1.95	0.49
1:C:192:PRO:HG2	1:C:280:ARG:CB	2.42	0.49
1:B:200:PHE:HD1	1:B:204:THR:HG23	1.78	0.49
1:D:90:HIS:CE1	1:D:392:HIS:HD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:VAL:HG11	1:C:232:PHE:HZ	1.78	0.49
1:C:278:VAL:HA	1:C:294:ALA:CB	2.42	0.49
1:B:24:LEU:HD13	1:B:76:PRO:CG	2.42	0.49
1:B:148:LEU:HB2	1:B:150:LEU:HG	1.93	0.49
1:A:82:CYS:HB3	1:A:83:PRO:CD	2.41	0.48
1:C:163:ASN:ND2	1:C:164:HIS:NE2	2.61	0.48
1:A:12:THR:HG22	1:A:14:ASN:N	2.27	0.48
1:C:16:TRP:HZ3	1:C:33:ILE:HD13	1.78	0.48
1:D:416:THR:CG2	1:D:523:LEU:HG	2.42	0.48
1:B:417:ILE:HD13	1:B:514:ARG:HE	1.78	0.48
1:B:253:LYS:HE3	1:B:406:GLU:OE1	2.13	0.48
1:B:460:LYS:O	1:B:461:THR:CB	2.49	0.48
1:B:182:VAL:HG13	2:B:524:FAD:C8A	2.44	0.48
1:B:361:MET:HG2	2:B:524:FAD:C2	2.43	0.48
1:D:101:MET:HG3	1:D:268:GLN:OE1	2.13	0.48
1:A:82:CYS:N	1:A:86:ALA:HB3	2.27	0.48
1:B:355:ILE:CG2	1:B:355:ILE:O	2.61	0.48
1:A:85:ASN:HA	1:A:89:PRO:HG3	1.95	0.48
1:C:111:TRP:CD2	1:D:100:LEU:HD21	2.49	0.48
1:D:90:HIS:CD2	2:D:524:FAD:H6	2.49	0.48
1:C:101:MET:HG3	1:C:268:GLN:OE1	2.13	0.48
1:C:502:LEU:HG	1:D:91:HIS:CG	2.49	0.48
1:A:337:VAL:CG1	1:A:350:ALA:HB3	2.43	0.48
1:C:227:VAL:CG1	1:C:393:THR:HG22	2.43	0.48
1:A:289:VAL:HG12	1:A:305:THR:O	2.14	0.48
1:D:87:CYS:HA	1:D:90:HIS:HD2	1.79	0.48
1:A:499:GLU:OE1	1:B:362:PHE:HB2	2.14	0.48
1:D:448:HIS:H	1:D:448:HIS:CD2	2.31	0.48
1:A:16:TRP:CD1	1:A:142:PHE:HB2	2.48	0.48
1:A:217:VAL:HG22	1:A:307:PHE:HD2	1.79	0.48
1:C:166:VAL:HG12	1:C:167:GLU:N	2.29	0.48
1:B:334:GLU:HG2	1:B:334:GLU:O	2.13	0.48
1:C:162:ASP:OD2	1:C:162:ASP:C	2.51	0.48
1:D:74:ARG:HG3	2:D:524:FAD:N1A	2.28	0.48
1:B:247:GLU:OE2	1:B:247:GLU:HA	2.14	0.48
1:A:148:LEU:CB	1:A:150:LEU:HG	2.44	0.48
1:B:264:ARG:O	1:B:267:GLU:HB3	2.14	0.48
1:D:462:ARG:HB3	1:D:491:VAL:HG12	1.95	0.48
1:B:495:GLY:HA2	1:B:508:ILE:O	2.14	0.48
1:B:71:ILE:HB	1:B:152:TYR:HB3	1.96	0.48
1:B:57:PHE:CD2	1:B:365:ARG:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:LEU:HD12	1:D:391:LEU:C	2.34	0.48
1:D:200:PHE:CD1	1:D:204:THR:HG23	2.46	0.48
1:D:164:HIS:O	1:D:174:LYS:HA	2.14	0.48
1:A:417:ILE:HG22	1:A:455:ILE:CG2	2.44	0.48
1:C:46:ALA:HA	1:C:177:ASN:O	2.14	0.48
1:A:513:LEU:HD11	1:B:60:ALA:HB1	1.95	0.48
1:D:245:ARG:O	1:D:275:GLY:HA2	2.14	0.48
1:C:165:THR:HA	1:C:173:PHE:O	2.14	0.47
1:B:463:LYS:O	1:B:465:LEU:HD13	2.14	0.47
1:D:73:ASP:OD2	2:D:524:FAD:O2B	2.25	0.47
1:B:192:PRO:HG2	1:B:280:ARG:CB	2.44	0.47
1:C:504:PRO:HD2	1:D:476:ASP:HB2	1.95	0.47
1:C:72:VAL:HG11	1:C:158:ALA:HB2	1.95	0.47
1:D:501:PHE:CD1	1:D:502:LEU:HA	2.49	0.47
1:D:42:ARG:NH1	1:D:66:GLY:O	2.47	0.47
1:D:499:GLU:OE2	1:D:512:ARG:NH2	2.47	0.47
1:B:148:LEU:CB	1:B:150:LEU:HG	2.44	0.47
1:A:388:PRO:HD3	1:A:482:ASN:ND2	2.28	0.47
1:A:423:THR:HB	1:B:13:ILE:CD1	2.43	0.47
1:A:286:ASN:N	1:A:286:ASN:HD22	2.11	0.47
1:A:362:PHE:CD1	1:A:363:LYS:N	2.83	0.47
1:A:420:PRO:HD3	1:A:432:PRO:HD3	1.96	0.47
1:B:495:GLY:O	1:B:512:ARG:HD3	2.15	0.47
1:C:473:GLY:HA2	1:D:473:GLY:HA2	1.97	0.47
1:C:328:ASP:HB3	1:C:336:LEU:HD12	1.96	0.47
1:A:446:THR:O	1:A:449:MET:HB2	2.15	0.47
1:D:20:ILE:O	1:D:24:LEU:HB2	2.15	0.47
1:A:100:LEU:HB2	1:A:235:ALA:HB1	1.95	0.47
1:A:185:GLY:HA2	1:A:317:ARG:NH2	2.28	0.47
1:B:490:THR:OG1	1:B:493:GLU:HG3	2.14	0.47
1:D:400:LEU:HD11	1:D:485:ILE:CD1	2.45	0.47
1:D:107:SER:OG	1:D:114:ASP:HA	2.14	0.47
1:B:78:LEU:H	1:B:141:ASN:HD21	1.63	0.47
1:D:162:ASP:OD2	1:D:165:THR:N	2.46	0.47
1:C:24:LEU:HD13	1:C:76:PRO:HG3	1.96	0.47
1:B:24:LEU:HD21	1:B:84:HIS:CE1	2.50	0.47
1:B:279:THR:H	1:B:294:ALA:HA	1.79	0.47
1:C:217:VAL:HG22	1:C:307:PHE:CD2	2.50	0.47
1:D:189:LEU:HD21	1:D:278:VAL:HB	1.96	0.47
1:D:402:MET:HA	1:D:406:GLU:OE1	2.14	0.47
1:A:101:MET:HG3	1:A:268:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:LEU:HG	1:B:91:HIS:CE1	2.49	0.47
1:C:164:HIS:O	1:C:174:LYS:HA	2.15	0.47
1:C:31:GLU:O	1:C:155:ASN:ND2	2.42	0.47
1:B:327:LEU:HD23	1:B:345:VAL:HG23	1.96	0.47
1:A:45:ASP:HA	1:A:176:LYS:HE3	1.97	0.47
1:B:160:VAL:HG11	1:B:325:LEU:HD21	1.97	0.47
1:B:346:PRO:O	1:B:347:ASN:HB2	2.15	0.47
1:A:164:HIS:O	1:A:174:LYS:HA	2.15	0.47
1:B:374:ASN:HA	1:B:378:GLU:O	2.14	0.47
1:C:391:LEU:O	1:C:391:LEU:HD12	2.14	0.47
1:A:44:TYR:CD1	1:A:68:ARG:HG2	2.49	0.47
1:A:217:VAL:HG13	1:A:307:PHE:HD2	1.79	0.47
1:B:78:LEU:HB2	1:B:140:MET:HG3	1.97	0.47
1:D:90:HIS:HE1	1:D:392:HIS:HD2	1.62	0.46
1:A:42:ARG:NH1	1:A:66:GLY:O	2.48	0.46
1:A:72:VAL:HG11	1:A:158:ALA:HB2	1.97	0.46
1:A:385:LYS:O	1:A:386:ASN:HB2	2.14	0.46
1:D:346:PRO:O	1:D:347:ASN:HB2	2.15	0.46
1:A:372:ALA:O	1:A:375:VAL:HG22	2.16	0.46
1:A:498:ASP:OD2	1:B:366:LYS:NZ	2.39	0.46
1:A:322:ALA:HB2	1:A:329:LEU:HD21	1.97	0.46
1:C:227:VAL:HG13	1:C:265:MET:CE	2.44	0.46
1:A:345:VAL:HG13	1:A:346:PRO:HD2	1.97	0.46
1:A:129:PHE:CE1	1:A:133:ARG:HD3	2.50	0.46
1:D:60:ALA:HA	1:D:150:LEU:HD21	1.97	0.46
1:A:231:CYS:SG	1:A:393:THR:HA	2.55	0.46
1:D:126:VAL:HG11	1:D:209:LEU:CD2	2.46	0.46
1:B:278:VAL:HA	1:B:294:ALA:HB2	1.97	0.46
1:B:279:THR:HB	1:B:293:VAL:HG12	1.98	0.46
1:C:372:ALA:O	1:C:375:VAL:HG22	2.14	0.46
1:D:509:GLN:HG2	1:D:510:LEU:N	2.30	0.46
1:C:501:PHE:CG	1:C:502:LEU:HA	2.50	0.46
1:C:400:LEU:HD11	1:C:485:ILE:HD12	1.97	0.46
1:D:12:THR:HB	1:D:15:GLN:HG3	1.98	0.46
1:B:171:LYS:N	1:B:171:LYS:HD2	2.29	0.46
1:A:267:GLU:OE1	1:A:448:HIS:CE1	2.67	0.46
1:D:325:LEU:CB	1:D:327:LEU:HD21	2.45	0.46
1:A:16:TRP:HB3	1:A:138:GLY:HA2	1.97	0.46
1:B:245:ARG:HG3	1:B:277:ASN:OD1	2.15	0.46
1:C:284:ASP:OD2	1:C:290:GLN:HB2	2.16	0.46
1:C:521:VAL:O	1:C:522:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:HB2	1:D:150:LEU:HG	1.98	0.46
1:D:385:LYS:O	1:D:386:ASN:HB2	2.15	0.46
1:C:461:THR:O	1:C:463:LYS:N	2.49	0.46
1:A:332:LYS:HB3	1:A:334:GLU:OE1	2.16	0.46
1:C:302:ARG:HH12	1:C:304:GLU:CG	2.28	0.46
1:C:352:GLY:C	1:C:354:LEU:H	2.19	0.46
1:B:191:VAL:HG22	1:B:280:ARG:HA	1.96	0.46
1:B:16:TRP:HB3	1:B:138:GLY:HA2	1.98	0.46
1:C:429:VAL:C	1:C:431:LEU:H	2.19	0.46
1:A:78:LEU:HD21	1:A:154:LEU:HD21	1.97	0.46
1:C:184:ALA:HB1	1:C:315:GLN:C	2.36	0.46
1:B:260:TYR:HE1	1:B:427:LEU:HD13	1.81	0.46
1:D:405:GLU:H	1:D:405:GLU:CD	2.19	0.46
1:B:390:PHE:HA	1:B:397:VAL:O	2.16	0.46
1:C:85:ASN:HB2	1:C:203:ALA:HA	1.98	0.46
1:D:80:GLY:HA3	2:D:524:FAD:O2A	2.17	0.45
1:C:355:ILE:O	1:C:355:ILE:CG2	2.59	0.45
1:D:419:MET:HB3	1:D:432:PRO:HB3	1.96	0.45
1:A:424:GLU:HG3	1:A:425:ASN:ND2	2.30	0.45
1:D:286:ASN:N	1:D:286:ASN:ND2	2.64	0.45
1:A:275:GLY:O	1:A:297:PRO:HD3	2.16	0.45
1:A:429:VAL:O	1:A:447:ALA:HB1	2.15	0.45
1:B:284:ASP:OD2	1:B:290:GLN:HB2	2.16	0.45
1:D:186:PRO:HA	1:D:314:GLU:OE1	2.16	0.45
1:D:40:ASP:HB3	1:D:68:ARG:NH1	2.32	0.45
1:A:419:MET:HA	1:A:420:PRO:C	2.36	0.45
1:C:235:ALA:C	1:C:237:GLY:H	2.19	0.45
1:A:438:MET:HB2	1:B:95:ASP:OD2	2.17	0.45
1:C:459:ALA:O	1:C:460:LYS:HB2	2.17	0.45
1:D:481:LEU:O	1:D:485:ILE:HG13	2.17	0.45
1:B:339:GLU:HB2	1:B:381:SER:HB2	1.99	0.45
1:A:14:ASN:O	1:A:18:THR:HG23	2.17	0.45
1:D:455:ILE:HG22	1:D:455:ILE:O	2.17	0.45
1:B:12:THR:HG22	1:B:14:ASN:N	2.28	0.45
1:A:77:PHE:HD1	1:A:78:LEU:O	2.00	0.45
1:A:241:VAL:HG21	1:A:303:ILE:HD12	1.99	0.45
1:D:122:ILE:O	1:D:123:LYS:C	2.55	0.45
1:C:100:LEU:HD21	1:D:111:TRP:CD2	2.52	0.45
1:D:16:TRP:O	1:D:20:ILE:HG13	2.17	0.45
1:A:167:GLU:HG3	1:A:171:LYS:O	2.16	0.45
1:D:469:HIS:ND1	1:D:469:HIS:C	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:HD1	1:A:204:THR:HG23	1.81	0.45
1:D:73:ASP:HA	2:D:524:FAD:N3A	2.32	0.45
1:A:350:ALA:C	1:A:355:ILE:HD11	2.36	0.45
1:B:476:ASP:OD1	1:B:479:GLN:NE2	2.49	0.45
1:A:388:PRO:HG2	1:B:500:LEU:HD21	1.98	0.45
1:A:116:THR:O	1:A:117:GLU:HB2	2.17	0.45
1:A:352:GLY:HA3	2:A:524:FAD:O2P	2.16	0.45
1:C:419:MET:HA	1:C:420:PRO:C	2.36	0.45
1:D:235:ALA:C	1:D:237:GLY:H	2.19	0.45
1:D:224:LYS:NZ	1:D:360:GLU:OE2	2.33	0.45
1:D:203:ALA:O	1:D:206:VAL:HG22	2.16	0.45
1:D:489:LEU:HD21	1:D:494:LEU:HD13	1.99	0.45
1:C:182:VAL:O	1:C:182:VAL:CG1	2.65	0.44
1:A:429:VAL:C	1:A:431:LEU:H	2.20	0.44
1:A:49:ILE:HG22	1:A:182:VAL:HG23	1.99	0.44
1:B:78:LEU:HB2	1:B:140:MET:CG	2.47	0.44
1:C:286:ASN:HD22	1:C:286:ASN:N	2.13	0.44
1:B:82:CYS:CA	1:B:86:ALA:HB3	2.42	0.44
1:A:318:SER:O	1:A:319:ALA:C	2.55	0.44
1:D:460:LYS:O	1:D:461:THR:CB	2.55	0.44
1:A:370:TYR:CD1	1:A:382:TYR:HB2	2.52	0.44
1:B:417:ILE:O	1:B:417:ILE:HG23	2.17	0.44
1:C:288:ARG:HG2	1:C:289:VAL:N	2.32	0.44
1:C:461:THR:O	1:C:463:LYS:HG3	2.17	0.44
1:C:502:LEU:HD23	1:C:502:LEU:N	2.31	0.44
1:D:231:CYS:SG	1:D:265:MET:HE3	2.58	0.44
1:C:43:GLU:HG2	1:C:44:TYR:N	2.32	0.44
1:C:337:VAL:CG2	1:C:355:ILE:HD13	2.42	0.44
1:B:296:THR:O	1:B:297:PRO:C	2.56	0.44
1:C:186:PRO:HA	1:C:314:GLU:OE1	2.17	0.44
1:C:13:ILE:CD1	1:D:423:THR:HB	2.47	0.44
1:B:196:ALA:O	1:B:199:VAL:HG23	2.17	0.44
1:D:284:ASP:OD2	1:D:290:GLN:HB2	2.17	0.44
1:D:393:THR:OG1	1:D:394:HIS:N	2.50	0.44
1:D:61:TYR:CD2	1:D:369:CYS:SG	3.10	0.44
1:C:6:ALA:O	1:C:7:ARG:C	2.56	0.44
1:A:16:TRP:O	1:A:20:ILE:HG13	2.18	0.44
1:A:206:VAL:HG23	1:A:207:GLU:OE2	2.17	0.44
1:A:107:SER:OG	1:A:114:ASP:HA	2.17	0.44
1:C:495:GLY:O	1:C:512:ARG:HB2	2.18	0.44
1:D:45:ASP:O	1:D:177:ASN:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:VAL:HG13	1:C:126:VAL:N	2.33	0.44
1:A:513:LEU:HD11	1:B:60:ALA:CB	2.48	0.44
1:A:57:PHE:CE1	1:B:512:ARG:HG2	2.53	0.44
1:A:119:VAL:O	1:A:119:VAL:CG2	2.65	0.44
1:A:80:GLY:O	1:A:83:PRO:HD2	2.18	0.44
1:B:459:ALA:O	1:B:460:LYS:HB2	2.18	0.44
2:D:524:FAD:H9	2:D:524:FAD:H1'1	1.87	0.44
1:C:415:VAL:HG23	1:C:457:ILE:HB	2.00	0.44
1:D:45:ASP:HA	1:D:176:LYS:HE3	2.00	0.44
1:A:119:VAL:HG23	1:A:119:VAL:O	2.18	0.44
1:C:80:GLY:O	1:C:83:PRO:HD2	2.18	0.43
1:A:228:GLU:HG2	1:A:392:HIS:HB2	2.00	0.43
1:B:84:HIS:CE1	1:B:133:ARG:CZ	3.00	0.43
1:A:148:LEU:HB3	1:A:150:LEU:HG	2.00	0.43
1:A:13:ILE:CG2	1:A:139:ILE:HG12	2.48	0.43
1:C:469:HIS:C	1:C:469:HIS:HD1	2.22	0.43
1:C:218:VAL:HG22	1:C:303:ILE:HD13	2.00	0.43
1:A:264:ARG:HA	1:A:264:ARG:NE	2.33	0.43
2:A:524:FAD:H1'1	2:A:524:FAD:H9	1.88	0.43
1:A:73:ASP:HA	2:A:524:FAD:N3A	2.34	0.43
1:A:503:ASN:O	1:A:506:HIS:CE1	2.72	0.43
1:B:352:GLY:C	1:B:354:LEU:H	2.21	0.43
1:A:372:ALA:O	1:A:376:MET:HG2	2.19	0.43
1:D:170:GLY:C	1:D:171:LYS:HD2	2.39	0.43
1:C:194:VAL:HG13	1:C:195:ASN:HD22	1.83	0.43
1:B:286:ASN:N	1:B:286:ASN:HD22	2.17	0.43
1:A:232:PHE:O	1:A:236:THR:HG23	2.18	0.43
1:B:60:ALA:HA	1:B:150:LEU:HD21	1.99	0.43
1:D:100:LEU:HB2	1:D:235:ALA:HB1	2.00	0.43
1:C:318:SER:O	1:C:319:ALA:C	2.56	0.43
1:D:162:ASP:OD2	1:D:162:ASP:C	2.57	0.43
1:B:362:PHE:C	1:B:362:PHE:CD1	2.92	0.43
1:C:362:PHE:C	1:C:362:PHE:CD1	2.91	0.43
1:C:400:LEU:HD11	1:C:485:ILE:CD1	2.48	0.43
1:B:85:ASN:HA	1:B:89:PRO:HG3	2.00	0.43
1:A:10:HIS:HA	1:A:146:GLU:OE1	2.18	0.43
1:D:184:ALA:HB1	1:D:315:GLN:C	2.38	0.43
1:B:158:ALA:H	2:B:524:FAD:C2A	2.31	0.43
1:A:20:ILE:O	1:A:24:LEU:HB2	2.17	0.43
1:A:152:TYR:CD1	1:A:154:LEU:HG	2.54	0.43
1:A:110:TYR:OH	1:B:128:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ALA:O	1:C:326:GLY:HA2	2.19	0.43
1:B:429:VAL:C	1:B:431:LEU:H	2.21	0.43
1:D:179:ILE:HD12	1:D:371:ALA:HB1	2.00	0.43
1:A:231:CYS:O	1:A:394:HIS:NE2	2.51	0.43
1:D:461:THR:O	1:D:463:LYS:N	2.51	0.43
1:A:16:TRP:HD1	1:A:142:PHE:HB2	1.84	0.43
1:A:436:ARG:NH1	1:B:99:GLU:OE1	2.52	0.43
1:D:200:PHE:HA	1:D:204:THR:HG21	2.01	0.43
1:D:424:GLU:HG3	1:D:425:ASN:ND2	2.33	0.43
1:D:458:ASP:O	1:D:462:ARG:HA	2.19	0.43
1:B:322:ALA:O	1:B:326:GLY:HA2	2.18	0.43
1:C:188:THR:OG1	1:C:189:LEU:N	2.52	0.43
1:B:89:PRO:HB3	1:B:129:PHE:CE1	2.54	0.43
1:B:170:GLY:C	1:B:171:LYS:HD2	2.39	0.43
1:B:201:ASP:OD1	1:B:201:ASP:C	2.57	0.43
1:C:476:ASP:OD2	1:D:505:THR:OG1	2.27	0.43
1:B:352:GLY:C	1:B:354:LEU:N	2.68	0.43
1:C:49:ILE:HG22	1:C:182:VAL:CG2	2.48	0.43
1:A:139:ILE:O	1:A:143:GLN:HB3	2.18	0.43
1:C:289:VAL:HG12	1:C:290:GLN:N	2.33	0.43
1:A:227:VAL:HG21	1:A:249:LEU:CD2	2.38	0.43
1:A:325:LEU:O	1:A:345:VAL:HG21	2.19	0.43
1:B:400:LEU:HD22	1:B:482:ASN:HB2	2.00	0.43
1:D:185:GLY:HA2	1:D:317:ARG:NH2	2.34	0.43
1:C:424:GLU:OE2	1:D:12:THR:HG23	2.19	0.43
1:C:159:LYS:HB2	1:C:167:GLU:HB3	2.00	0.43
1:C:273:ILE:HG22	1:C:276:SER:HB2	2.00	0.43
1:D:352:GLY:C	1:D:354:LEU:N	2.71	0.43
1:D:355:ILE:CG2	1:D:355:ILE:O	2.65	0.42
1:B:362:PHE:CD1	1:B:363:LYS:N	2.87	0.42
1:C:14:ASN:O	1:C:18:THR:HG23	2.19	0.42
2:C:524:FAD:H9	2:C:524:FAD:H1'1	1.86	0.42
1:D:279:THR:HG22	1:D:280:ARG:HG2	1.99	0.42
1:B:322:ALA:HB2	1:B:329:LEU:HD21	2.00	0.42
1:C:276:SER:HA	1:C:295:MET:O	2.18	0.42
1:A:298:ASN:CG	1:A:298:ASN:O	2.56	0.42
1:A:366:LYS:NZ	1:B:496:ASP:O	2.45	0.42
1:C:191:VAL:CG2	1:C:279:THR:O	2.67	0.42
1:C:191:VAL:CG2	1:C:280:ARG:HA	2.49	0.42
1:C:388:PRO:HG2	1:D:500:LEU:HD21	2.01	0.42
1:A:424:GLU:OE2	1:B:12:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:VAL:HA	1:D:294:ALA:HB2	2.01	0.42
1:D:371:ALA:O	1:D:375:VAL:HG13	2.19	0.42
1:B:100:LEU:HB2	1:B:235:ALA:HB1	2.01	0.42
1:C:436:ARG:NH1	1:D:99:GLU:OE1	2.52	0.42
1:C:16:TRP:HB3	1:C:138:GLY:HA2	2.02	0.42
2:C:524:FAD:HO3'	2:C:524:FAD:H5'2	1.80	0.42
1:C:53:ALA:O	1:C:57:PHE:HB2	2.19	0.42
1:C:90:HIS:CE1	1:C:392:HIS:HD2	2.37	0.42
1:B:231:CYS:SG	1:B:265:MET:HE3	2.60	0.42
1:C:499:GLU:OE2	1:C:512:ARG:NH2	2.52	0.42
1:D:476:ASP:O	1:D:479:GLN:HG3	2.18	0.42
1:A:24:LEU:HD13	1:A:76:PRO:CG	2.50	0.42
1:B:289:VAL:HG12	1:B:290:GLN:N	2.33	0.42
1:D:230:GLY:O	1:D:270:MET:HE3	2.20	0.42
1:A:201:ASP:N	1:A:204:THR:HG22	2.12	0.42
1:C:40:ASP:CB	1:C:68:ARG:NH1	2.83	0.42
1:C:338:ASN:OD1	1:C:342:GLN:HB2	2.20	0.42
1:C:191:VAL:HG23	1:C:192:PRO:HD2	2.01	0.42
1:D:501:PHE:CG	1:D:502:LEU:HA	2.54	0.42
1:A:78:LEU:CD2	1:A:154:LEU:HD21	2.50	0.42
1:D:47:ILE:HG13	1:D:175:ALA:HB2	2.02	0.42
1:D:10:HIS:HA	1:D:146:GLU:OE1	2.20	0.42
1:D:67:GLY:HA3	1:D:376:MET:CE	2.50	0.42
1:C:412:HIS:HD2	1:C:458:ASP:OD2	2.02	0.42
1:C:476:ASP:HB2	1:D:504:PRO:HD2	2.02	0.42
1:D:125:VAL:HG13	1:D:126:VAL:N	2.34	0.42
1:A:34:TYR:OH	1:A:36:VAL:HG21	2.19	0.42
1:C:346:PRO:O	1:C:348:VAL:HG23	2.20	0.42
1:A:459:ALA:O	1:A:460:LYS:HB2	2.19	0.42
1:B:200:PHE:CD1	1:B:204:THR:HG23	2.55	0.42
1:A:338:ASN:ND2	1:A:340:TYR:HD2	2.18	0.42
1:B:202:HIS:CE1	2:B:524:FAD:HM82	2.55	0.42
1:D:383:THR:HA	1:D:384:PRO:HD2	1.90	0.42
1:B:405:GLU:CD	1:B:405:GLU:H	2.22	0.42
1:C:286:ASN:ND2	1:C:286:ASN:N	2.67	0.42
1:B:521:VAL:O	1:B:522:SER:HB2	2.20	0.42
1:A:459:ALA:O	1:A:460:LYS:O	2.38	0.42
1:C:454:LYS:CG	1:C:455:ILE:N	2.82	0.42
1:A:122:ILE:HD11	1:A:238:ARG:HD2	2.02	0.42
1:B:280:ARG:HH11	1:B:280:ARG:HG2	1.85	0.42
1:C:499:GLU:O	1:C:499:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:H	1:C:141:ASN:HD21	1.68	0.42
1:C:139:ILE:O	1:C:143:GLN:HB3	2.20	0.42
1:A:383:THR:HA	1:A:384:PRO:HD2	1.89	0.42
1:B:45:ASP:O	1:B:46:ALA:HB2	2.19	0.42
1:C:60:ALA:HA	1:C:150:LEU:HD21	2.02	0.41
1:A:23:ILE:HG23	1:A:30:GLY:HA3	2.01	0.41
1:A:99:GLU:OE1	1:B:436:ARG:NH1	2.52	0.41
1:B:162:ASP:C	1:B:162:ASP:OD2	2.59	0.41
1:C:76:PRO:HB3	1:C:155:ASN:HB2	2.02	0.41
1:C:100:LEU:O	1:C:104:ARG:HG3	2.20	0.41
1:A:24:LEU:HD13	1:A:76:PRO:HG3	2.02	0.41
1:D:152:TYR:CD1	1:D:154:LEU:HG	2.55	0.41
1:D:78:LEU:H	1:D:141:ASN:HD21	1.68	0.41
1:B:415:VAL:HG23	1:B:457:ILE:HB	2.03	0.41
1:D:429:VAL:C	1:D:431:LEU:H	2.23	0.41
1:C:302:ARG:HH11	1:C:302:ARG:HG2	1.86	0.41
1:A:171:LYS:HD2	1:A:171:LYS:N	2.34	0.41
1:A:442:PHE:O	1:B:128:LEU:HD11	2.21	0.41
1:C:115:MET:O	1:C:118:LYS:HB3	2.19	0.41
1:B:61:TYR:O	1:B:65:MET:HG3	2.19	0.41
1:D:33:ILE:O	1:D:153:ILE:HA	2.20	0.41
1:D:198:GLY:H	1:D:289:VAL:HG23	1.86	0.41
1:D:86:ALA:O	1:D:90:HIS:HB3	2.19	0.41
1:A:400:LEU:HD11	1:A:485:ILE:HD13	2.01	0.41
1:D:400:LEU:HD23	1:D:478:PHE:CD2	2.55	0.41
1:A:447:ALA:C	1:A:449:MET:H	2.23	0.41
1:C:371:ALA:O	1:C:375:VAL:HG13	2.20	0.41
1:C:288:ARG:CG	1:C:289:VAL:N	2.83	0.41
1:D:521:VAL:O	1:D:522:SER:HB2	2.20	0.41
1:A:447:ALA:C	1:A:449:MET:N	2.73	0.41
1:A:179:ILE:HD12	1:A:371:ALA:HB1	2.02	0.41
1:D:71:ILE:HB	1:D:152:TYR:CB	2.50	0.41
1:D:80:GLY:O	1:D:83:PRO:HD2	2.21	0.41
1:A:495:GLY:HA2	1:A:508:ILE:O	2.20	0.41
1:B:267:GLU:OE1	1:B:448:HIS:CE1	2.74	0.41
1:A:20:ILE:HD13	1:A:137:HIS:HB3	2.02	0.41
1:D:48:PHE:CE2	1:D:179:ILE:HG21	2.56	0.41
1:C:500:LEU:HD21	1:D:388:PRO:HG2	2.01	0.41
1:D:398:SER:OG	1:D:475:LYS:HA	2.20	0.41
1:C:152:TYR:CD1	1:C:154:LEU:HG	2.55	0.41
1:D:196:ALA:O	1:D:199:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:CYS:SG	1:D:361:MET:SD	3.19	0.41
1:B:45:ASP:HA	1:B:176:LYS:HE3	2.02	0.41
1:B:6:ALA:O	1:B:7:ARG:C	2.59	0.41
1:A:503:ASN:HB2	1:B:476:ASP:OD1	2.20	0.41
1:C:122:ILE:O	1:C:125:VAL:CG1	2.63	0.41
1:B:182:VAL:CG1	1:B:317:ARG:HB2	2.49	0.41
1:B:122:ILE:O	1:B:126:VAL:CG1	2.69	0.41
1:C:88:VAL:HB	1:C:89:PRO:CD	2.51	0.41
1:B:329:LEU:HD23	1:B:335:VAL:HA	2.03	0.41
1:B:44:TYR:CD1	1:B:68:ARG:HG2	2.56	0.41
1:C:171:LYS:N	1:C:171:LYS:HD2	2.36	0.41
1:B:465:LEU:N	1:B:465:LEU:CD1	2.84	0.41
1:C:227:VAL:HG21	1:C:249:LEU:CD2	2.38	0.41
1:B:162:ASP:OD2	1:B:165:THR:N	2.53	0.41
1:B:338:ASN:ND2	1:B:342:GLN:HE21	2.15	0.41
1:C:362:PHE:HB2	1:D:499:GLU:OE1	2.20	0.41
1:D:125:VAL:HG11	1:D:232:PHE:CZ	2.56	0.41
1:D:122:ILE:O	1:D:125:VAL:CG1	2.67	0.41
1:B:122:ILE:O	1:B:126:VAL:HG13	2.21	0.41
1:B:191:VAL:HG22	1:B:192:PRO:CD	2.50	0.41
1:C:499:GLU:HB2	1:C:503:ASN:HD22	1.85	0.41
1:C:375:VAL:C	1:C:377:GLY:H	2.24	0.41
1:B:85:ASN:HB2	1:B:203:ALA:HA	2.03	0.41
1:A:89:PRO:HB3	1:A:129:PHE:CE1	2.55	0.41
1:B:523:LEU:N	1:B:523:LEU:HD12	2.36	0.41
1:A:44:TYR:HB2	1:A:175:ALA:HB2	2.02	0.41
1:C:193:GLY:O	1:C:195:ASN:N	2.54	0.41
1:C:148:LEU:CB	1:C:150:LEU:HG	2.51	0.41
1:A:500:LEU:HD21	1:B:388:PRO:HG2	2.02	0.41
1:B:107:SER:OG	1:B:114:ASP:HA	2.20	0.41
1:C:61:TYR:CD2	1:C:369:CYS:SG	3.12	0.41
1:D:72:VAL:CG1	1:D:158:ALA:HB2	2.51	0.41
1:A:189:LEU:HD21	1:A:278:VAL:HB	2.03	0.41
1:D:446:THR:O	1:D:449:MET:HB2	2.21	0.41
1:D:5:ASN:HD21	1:D:7:ARG:HB2	1.84	0.41
1:B:89:PRO:HB3	1:B:129:PHE:CZ	2.56	0.41
1:D:506:HIS:HB3	1:D:509:GLN:NE2	2.36	0.41
1:B:77:PHE:CD1	1:B:77:PHE:C	2.95	0.41
1:B:80:GLY:O	1:B:83:PRO:HD2	2.21	0.40
1:B:491:VAL:HG11	1:B:520:LEU:HD21	2.03	0.40
1:C:457:ILE:HG22	1:C:458:ASP:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LYS:CG	1:A:455:ILE:N	2.82	0.40
1:D:462:ARG:O	1:D:490:THR:HA	2.21	0.40
1:B:213:PRO:HB2	1:B:238:ARG:HE	1.86	0.40
1:D:193:GLY:O	1:D:195:ASN:N	2.54	0.40
1:C:224:LYS:HE2	1:C:390:PHE:O	2.20	0.40
1:C:201:ASP:N	1:C:204:THR:HG22	2.11	0.40
1:B:201:ASP:H	1:B:204:THR:CG2	2.18	0.40
1:B:87:CYS:HA	1:B:90:HIS:HD2	1.85	0.40
1:C:359:MET:O	2:C:524:FAD:H1'2	2.20	0.40
1:B:16:TRP:O	1:B:20:ILE:HG13	2.21	0.40
1:A:148:LEU:HB2	1:A:150:LEU:HG	2.03	0.40
1:A:182:VAL:HG12	1:A:317:ARG:HB2	2.04	0.40
1:C:71:ILE:HB	1:C:152:TYR:HB3	2.01	0.40
1:A:278:VAL:HA	1:A:294:ALA:HB2	2.03	0.40
1:A:202:HIS:CG	1:A:203:ALA:N	2.89	0.40
1:A:370:TYR:HA	1:A:373:ARG:HD3	2.03	0.40
1:D:24:LEU:HD21	1:D:84:HIS:CE1	2.57	0.40
1:A:501:PHE:CD2	1:A:502:LEU:HD23	2.56	0.40
1:D:389:ASP:HB3	1:D:399:PHE:CE1	2.57	0.40
1:B:201:ASP:N	1:B:204:THR:HG22	2.17	0.40
1:B:357:GLY:HA2	1:B:358:PRO:C	2.42	0.40
1:A:339:GLU:HB2	1:A:381:SER:HB2	2.03	0.40
1:D:503:ASN:O	1:D:504:PRO:C	2.59	0.40
1:B:12:THR:H	1:B:15:GLN:HB2	1.87	0.40
1:D:273:ILE:HG22	1:D:276:SER:HB2	2.04	0.40
1:C:370:TYR:HD1	1:C:382:TYR:CG	2.40	0.40
1:A:245:ARG:HG3	1:A:277:ASN:OD1	2.22	0.40
1:B:166:VAL:CG2	1:B:178:LEU:HD21	2.50	0.40
1:D:6:ALA:O	1:D:7:ARG:C	2.60	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	520/523 (99%)	449 (86%)	60 (12%)	11 (2%)	9	29
1	B	520/523 (99%)	447 (86%)	62 (12%)	11 (2%)	9	29
1	C	520/523 (99%)	456 (88%)	51 (10%)	13 (2%)	7	24
1	D	520/523 (99%)	450 (86%)	54 (10%)	16 (3%)	5	17
All	All	2080/2092 (99%)	1802 (87%)	227 (11%)	51 (2%)	7	24

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	A	319	ALA
1	A	462	ARG
1	B	224	LYS
1	B	462	ARG
1	C	224	LYS
1	C	462	ARG
1	C	508	ILE
1	D	224	LYS
1	D	462	ARG
1	A	461	THR
1	A	522	SER
1	B	461	THR
1	B	522	SER
1	C	352	GLY
1	C	522	SER
1	D	319	ALA
1	D	352	GLY
1	D	461	THR
1	D	522	SER
1	A	393	THR
1	A	460	LYS
1	B	213	PRO
1	B	319	ALA
1	B	434	SER
1	C	319	ALA
1	C	460	LYS
1	C	461	THR
1	A	352	GLY
1	C	393	THR
1	D	393	THR
1	A	87	CYS
1	B	428	ASN

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Mol	Chain	Res	Type
1	C	41	PRO
1	D	197	LYS
1	B	508	ILE
1	D	85	ASN
1	D	428	ASN
1	D	460	LYS
1	D	508	ILE
1	A	194	VAL
1	B	88	VAL
1	C	194	VAL
1	C	384	PRO
1	D	194	VAL
1	C	351	VAL
1	D	213	PRO
1	A	41	PRO
1	B	351	VAL
1	D	41	PRO
1	D	88	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	423/424 (100%)	407 (96%)	16 (4%)	40	74
1	B	423/424 (100%)	405 (96%)	18 (4%)	35	70
1	C	423/424 (100%)	407 (96%)	16 (4%)	40	74
1	D	423/424 (100%)	402 (95%)	21 (5%)	30	64
All	All	1692/1696 (100%)	1621 (96%)	71 (4%)	36	71

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	7	ARG
1	A	25	GLU

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Mol	Chain	Res	Type
1	A	90	HIS
1	A	174	LYS
1	A	182	VAL
1	A	190	ASP
1	A	305	THR
1	A	375	VAL
1	A	405	GLU
1	A	422	ASP
1	A	455	ILE
1	A	461	THR
1	A	465	LEU
1	A	504	PRO
1	A	514	ARG
1	B	5	ASN
1	B	7	ARG
1	B	25	GLU
1	B	73	ASP
1	B	90	HIS
1	B	126	VAL
1	B	174	LYS
1	B	204	THR
1	B	305	THR
1	B	375	VAL
1	B	405	GLU
1	B	422	ASP
1	B	455	ILE
1	B	461	THR
1	B	462	ARG
1	B	465	LEU
1	B	504	PRO
1	B	514	ARG
1	C	5	ASN
1	C	7	ARG
1	C	25	GLU
1	C	87	CYS
1	C	90	HIS
1	C	126	VAL
1	C	174	LYS
1	C	190	ASP
1	C	305	THR
1	C	375	VAL
1	C	405	GLU

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Mol	Chain	Res	Type
1	C	455	ILE
1	C	462	ARG
1	C	465	LEU
1	C	502	LEU
1	C	514	ARG
1	D	5	ASN
1	D	7	ARG
1	D	25	GLU
1	D	73	ASP
1	D	90	HIS
1	D	126	VAL
1	D	174	LYS
1	D	182	VAL
1	D	190	ASP
1	D	234	ASN
1	D	305	THR
1	D	375	VAL
1	D	389	ASP
1	D	405	GLU
1	D	422	ASP
1	D	455	ILE
1	D	461	THR
1	D	465	LEU
1	D	502	LEU
1	D	504	PRO
1	D	514	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	14	ASN
1	A	39	ASN
1	A	69	GLN
1	A	90	HIS
1	A	141	ASN
1	A	163	ASN
1	A	195	ASN
1	A	234	ASN
1	A	255	ASN
1	A	286	ASN
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	392	HIS
1	A	412	HIS
1	A	425	ASN
1	A	448	HIS
1	A	482	ASN
1	B	5	ASN
1	B	14	ASN
1	B	39	ASN
1	B	69	GLN
1	B	90	HIS
1	B	141	ASN
1	B	234	ASN
1	B	255	ASN
1	B	286	ASN
1	B	342	GLN
1	B	392	HIS
1	B	412	HIS
1	B	425	ASN
1	B	448	HIS
1	C	5	ASN
1	C	14	ASN
1	C	39	ASN
1	C	69	GLN
1	C	90	HIS
1	C	141	ASN
1	C	163	ASN
1	C	195	ASN
1	C	234	ASN
1	C	255	ASN
1	C	286	ASN
1	C	342	GLN
1	C	392	HIS
1	C	412	HIS
1	C	425	ASN
1	D	5	ASN
1	D	14	ASN
1	D	39	ASN
1	D	69	GLN
1	D	90	HIS
1	D	141	ASN
1	D	163	ASN
1	D	195	ASN

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Mol	Chain	Res	Type
1	D	234	ASN
1	D	255	ASN
1	D	286	ASN
1	D	342	GLN
1	D	392	HIS
1	D	412	HIS
1	D	425	ASN
1	D	448	HIS
1	D	482	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	524	-	48,58,58	2.75	12 (25%)	54,89,89	2.45	13 (24%)
2	FAD	B	524	-	48,58,58	2.74	15 (31%)	54,89,89	2.42	13 (24%)
2	FAD	C	524	-	48,58,58	2.70	13 (27%)	54,89,89	2.37	13 (24%)
2	FAD	D	524	-	48,58,58	2.68	15 (31%)	54,89,89	2.48	12 (22%)

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	524	-	-	0/30/50/50	0/6/6/6
2	FAD	B	524	-	-	0/30/50/50	0/6/6/6
2	FAD	C	524	-	-	0/30/50/50	0/6/6/6
2	FAD	D	524	-	-	0/30/50/50	0/6/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	524	FAD	C1'-N10	-5.33	1.42	1.48
2	B	524	FAD	C1'-N10	-4.94	1.43	1.48
2	C	524	FAD	C1'-N10	-4.21	1.44	1.48
2	B	524	FAD	C5A-C4A	-3.93	1.31	1.40
2	D	524	FAD	C1'-N10	-3.87	1.44	1.48
2	A	524	FAD	C5A-C4A	-3.82	1.31	1.40
2	D	524	FAD	C5A-C4A	-3.82	1.31	1.40
2	D	524	FAD	C5'-C4'	-3.66	1.46	1.51
2	C	524	FAD	C5A-C4A	-3.64	1.32	1.40
2	A	524	FAD	C5'-C4'	-3.50	1.46	1.51
2	C	524	FAD	C5'-C4'	-3.06	1.47	1.51
2	B	524	FAD	C5'-C4'	-3.05	1.47	1.51
2	C	524	FAD	C4-C4X	-2.64	1.36	1.41
2	B	524	FAD	C2'-C3'	-2.45	1.48	1.53
2	C	524	FAD	C2'-C3'	-2.39	1.48	1.53
2	A	524	FAD	C2B-C3B	-2.30	1.47	1.53
2	B	524	FAD	C2B-C3B	-2.28	1.47	1.53
2	D	524	FAD	C2B-C3B	-2.26	1.47	1.53
2	D	524	FAD	C2'-C3'	-2.04	1.49	1.53
2	B	524	FAD	C4-C4X	-2.01	1.37	1.41
2	B	524	FAD	C6-C7	2.03	1.43	1.37
2	D	524	FAD	C6-C7	2.05	1.43	1.37
2	D	524	FAD	O4B-C1B	2.33	1.44	1.41
2	D	524	FAD	C9A-C5X	2.41	1.47	1.42
2	A	524	FAD	C9A-C5X	2.45	1.47	1.42
2	B	524	FAD	C10-N1	2.46	1.39	1.35
2	A	524	FAD	C10-N1	2.48	1.39	1.35
2	C	524	FAD	C9A-C5X	2.63	1.48	1.42
2	D	524	FAD	C10-N1	2.75	1.40	1.35
2	C	524	FAD	C10-N1	2.87	1.40	1.35
2	B	524	FAD	C9A-C5X	3.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	524	FAD	C5X-N5	3.90	1.41	1.35
2	A	524	FAD	C5X-N5	4.16	1.42	1.35
2	B	524	FAD	C5X-N5	4.69	1.42	1.35
2	C	524	FAD	C5X-N5	4.70	1.42	1.35
2	D	524	FAD	C4-N3	4.85	1.42	1.33
2	B	524	FAD	C4-N3	5.10	1.42	1.33
2	A	524	FAD	C4-N3	5.37	1.43	1.33
2	B	524	FAD	C2A-N3A	5.47	1.41	1.32
2	C	524	FAD	C4-N3	5.60	1.43	1.33
2	B	524	FAD	C4A-N3A	5.69	1.44	1.35
2	D	524	FAD	C2A-N3A	5.78	1.42	1.32
2	A	524	FAD	C2A-N3A	6.01	1.42	1.32
2	C	524	FAD	C2A-N3A	6.01	1.42	1.32
2	A	524	FAD	C4A-N3A	6.10	1.44	1.35
2	C	524	FAD	C4A-N3A	6.39	1.45	1.35
2	C	524	FAD	C4X-N5	6.73	1.43	1.33
2	D	524	FAD	C4A-N3A	6.80	1.45	1.35
2	A	524	FAD	C4X-N5	6.83	1.44	1.33
2	D	524	FAD	C4X-N5	7.18	1.44	1.33
2	B	524	FAD	C4X-N5	7.72	1.45	1.33
2	C	524	FAD	C9A-N10	8.10	1.50	1.38
2	D	524	FAD	C9A-N10	8.30	1.50	1.38
2	B	524	FAD	C9A-N10	8.76	1.50	1.38
2	A	524	FAD	C9A-N10	9.06	1.51	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	524	FAD	C4X-C4-N3	-6.42	114.82	123.59
2	A	524	FAD	C4X-C4-N3	-6.33	114.93	123.59
2	B	524	FAD	C4X-C4-N3	-6.15	115.19	123.59
2	B	524	FAD	N3A-C2A-N1A	-6.01	124.29	128.89
2	C	524	FAD	C4X-C4-N3	-5.81	115.64	123.59
2	C	524	FAD	N3A-C2A-N1A	-5.66	124.56	128.89
2	D	524	FAD	N3A-C2A-N1A	-5.61	124.60	128.89
2	A	524	FAD	N3A-C2A-N1A	-5.38	124.78	128.89
2	D	524	FAD	C5X-C9A-N10	-3.48	114.98	117.62
2	C	524	FAD	C5X-C9A-N10	-3.30	115.11	117.62
2	A	524	FAD	C4X-C10-N10	-3.23	118.61	120.52
2	A	524	FAD	C5X-C9A-N10	-3.23	115.16	117.62
2	D	524	FAD	C4X-C10-N10	-3.23	118.62	120.52
2	B	524	FAD	C5X-C9A-N10	-3.18	115.21	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	524	FAD	C4X-C10-N10	-3.08	118.71	120.52
2	C	524	FAD	C1'-N10-C9A	-3.08	115.41	118.86
2	B	524	FAD	C1'-N10-C9A	-3.04	115.45	118.86
2	D	524	FAD	C1'-N10-C9A	-3.01	115.48	118.86
2	A	524	FAD	C1'-N10-C9A	-2.82	115.70	118.86
2	B	524	FAD	O2'-C2'-C1'	-2.73	103.25	109.94
2	C	524	FAD	O2'-C2'-C1'	-2.61	103.53	109.94
2	A	524	FAD	O2'-C2'-C1'	-2.59	103.57	109.94
2	B	524	FAD	C4X-C10-N10	-2.47	119.07	120.52
2	A	524	FAD	O3P-P-O5'	-2.45	96.44	102.94
2	C	524	FAD	O3P-P-O5'	-2.38	96.63	102.94
2	D	524	FAD	O2'-C2'-C1'	-2.35	104.17	109.94
2	C	524	FAD	C4-C4X-N5	-2.33	115.89	118.72
2	A	524	FAD	O3'-C3'-C4'	-2.31	102.94	108.75
2	D	524	FAD	O3P-P-O5'	-2.29	96.85	102.94
2	B	524	FAD	C4-C4X-N5	-2.28	115.95	118.72
2	A	524	FAD	C4-C4X-N5	-2.24	116.00	118.72
2	B	524	FAD	O3P-P-O5'	-2.18	97.16	102.94
2	B	524	FAD	O3'-C3'-C4'	-2.12	103.41	108.75
2	D	524	FAD	O3'-C3'-C4'	-2.08	103.52	108.75
2	C	524	FAD	O3'-C3'-C4'	-2.05	103.58	108.75
2	A	524	FAD	C1'-C2'-C3'	2.12	115.89	109.82
2	C	524	FAD	C1'-C2'-C3'	2.17	116.02	109.82
2	D	524	FAD	C1'-C2'-C3'	2.18	116.06	109.82
2	C	524	FAD	O3P-PA-O5B	2.38	109.25	102.94
2	B	524	FAD	C1'-C2'-C3'	2.40	116.67	109.82
2	D	524	FAD	O3P-PA-O5B	2.40	109.30	102.94
2	B	524	FAD	O2B-C2B-C3B	2.47	119.87	111.83
2	D	524	FAD	O2B-C2B-C3B	2.50	119.95	111.83
2	C	524	FAD	O2B-C2B-C3B	2.53	120.06	111.83
2	A	524	FAD	O2B-C2B-C3B	2.54	120.10	111.83
2	A	524	FAD	O3P-PA-O5B	2.66	110.00	102.94
2	B	524	FAD	O3P-PA-O5B	2.73	110.19	102.94
2	C	524	FAD	C4-N3-C2	11.68	125.34	115.25
2	B	524	FAD	C4-N3-C2	11.96	125.59	115.25
2	A	524	FAD	C4-N3-C2	12.35	125.92	115.25
2	D	524	FAD	C4-N3-C2	12.62	126.16	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	524	FAD	6	0
2	B	524	FAD	6	0
2	C	524	FAD	9	0
2	D	524	FAD	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.