



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:17 AM GMT

PDB ID : 1XPQ  
Title : Crystal structure of fms1, a polyamine oxidase from yeast  
Authors : Huang, Q.; Liu, Q.; Hao, Q.  
Deposited on : 2004-10-09  
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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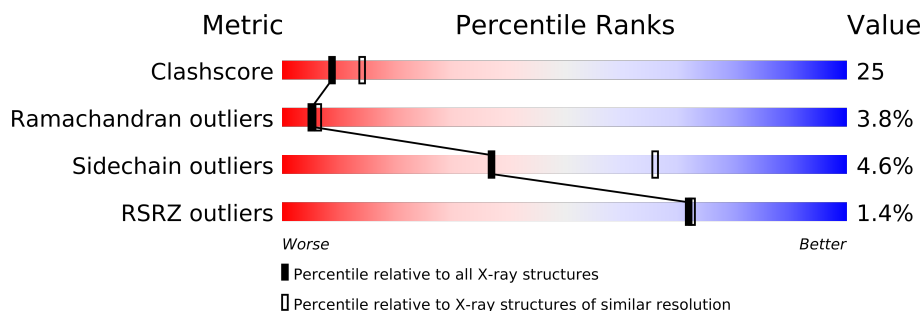
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	513	
1	B	513	
1	C	513	
1	D	513	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16332 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

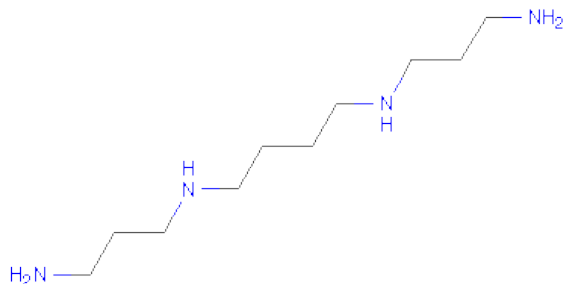
- Molecule 1 is a protein called FMS1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	86	0	0
			3997	2526	699	750	22			
1	B	492	Total	C	N	O	S	144	0	0
			3946	2496	687	741	22			
1	C	495	Total	C	N	O	S	118	0	0
			3967	2509	690	746	22			
1	D	490	Total	C	N	O	S	144	0	0
			3929	2484	684	739	22			

There are 20 discrepancies between the modelled and reference sequences:

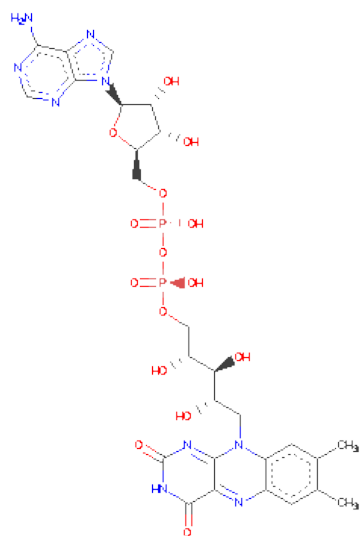
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	LEU	-	CLONING ARTIFACT	UNP P50264
A	510	GLU	-	CLONING ARTIFACT	UNP P50264
A	511	HIS	-	CLONING ARTIFACT	UNP P50264
A	512	HIS	-	CLONING ARTIFACT	UNP P50264
A	513	HIS	-	CLONING ARTIFACT	UNP P50264
B	509	LEU	-	CLONING ARTIFACT	UNP P50264
B	510	GLU	-	CLONING ARTIFACT	UNP P50264
B	511	HIS	-	CLONING ARTIFACT	UNP P50264
B	512	HIS	-	CLONING ARTIFACT	UNP P50264
B	513	HIS	-	CLONING ARTIFACT	UNP P50264
C	509	LEU	-	CLONING ARTIFACT	UNP P50264
C	510	GLU	-	CLONING ARTIFACT	UNP P50264
C	511	HIS	-	CLONING ARTIFACT	UNP P50264
C	512	HIS	-	CLONING ARTIFACT	UNP P50264
C	513	HIS	-	CLONING ARTIFACT	UNP P50264
D	509	LEU	-	CLONING ARTIFACT	UNP P50264
D	510	GLU	-	CLONING ARTIFACT	UNP P50264
D	511	HIS	-	CLONING ARTIFACT	UNP P50264
D	512	HIS	-	CLONING ARTIFACT	UNP P50264
D	513	HIS	-	CLONING ARTIFACT	UNP P50264

- Molecule 2 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	14	0
			14	10	4		
2	D	1	Total	C	N	14	0
			14	10	4		
2	B	1	Total	C	N	14	0
			14	10	4		
2	A	1	Total	C	N	14	0
			14	10	4		

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



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

- Molecule 4 is water.

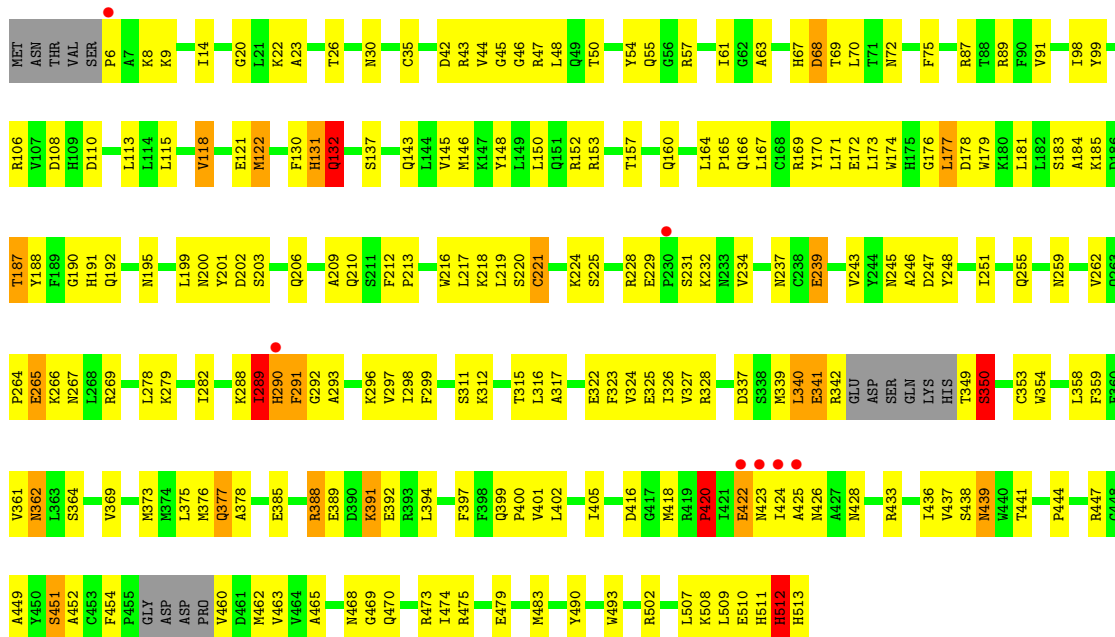
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	54	Total	O	0	0
			54	54		
4	C	66	Total	O	0	0
			66	66		
4	D	50	Total	O	0	0
			50	50		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

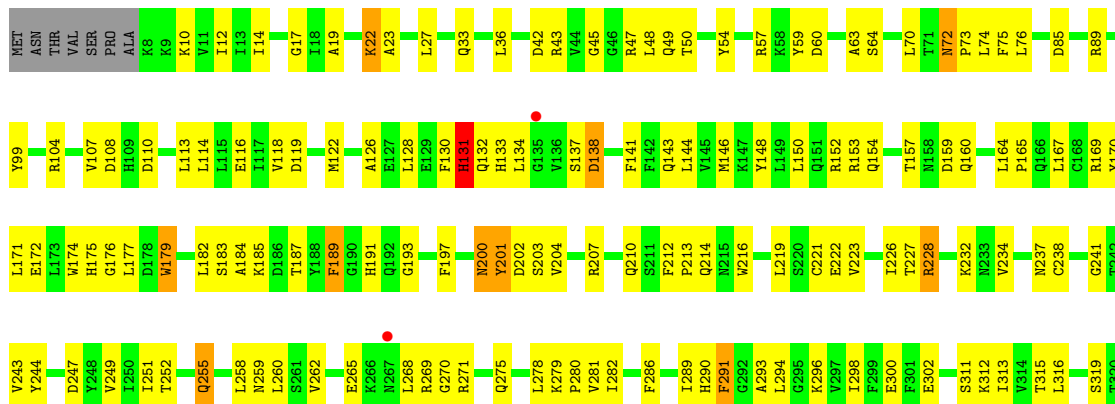
#### • Molecule 1: FMS1 protein

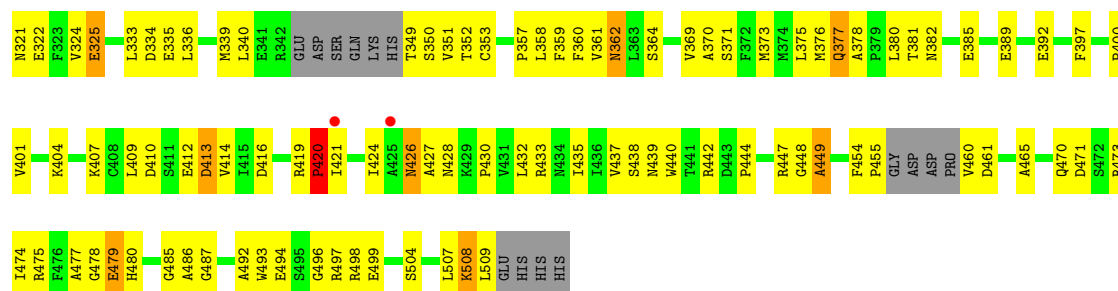
Chain A: 



#### • Molecule 1: FMS1 protein

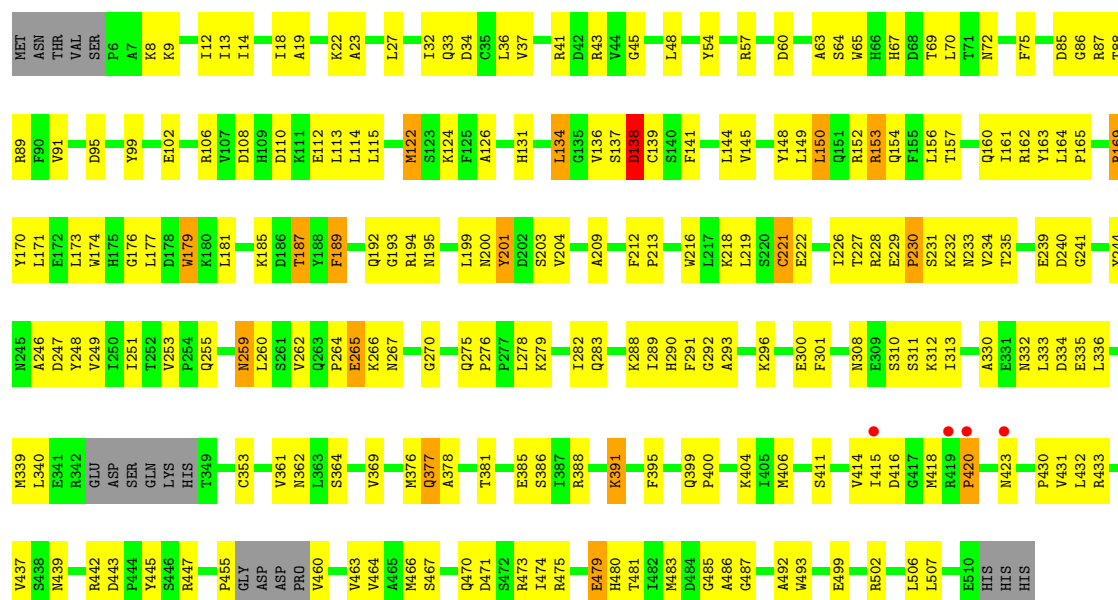
Chain B: 





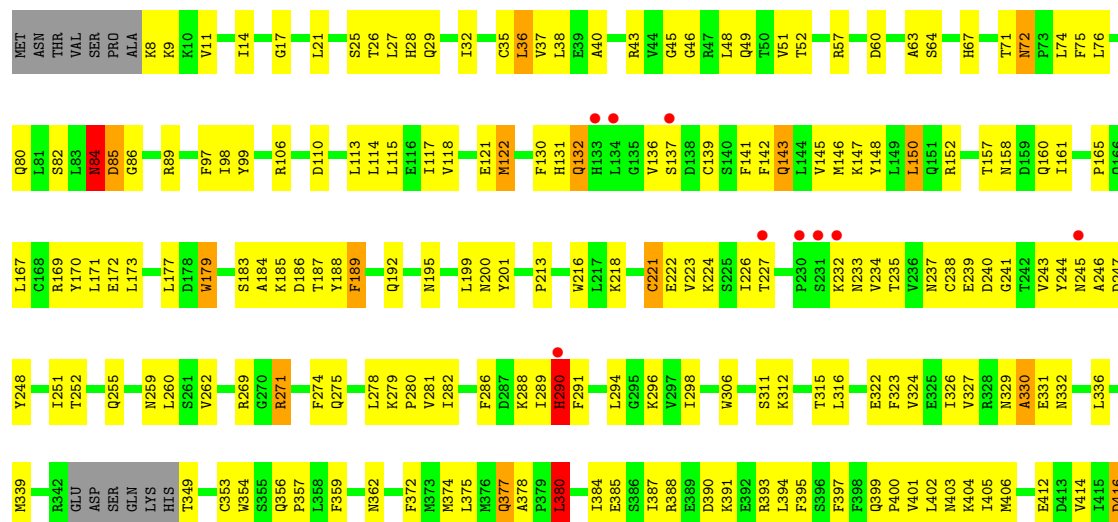
• Molecule 1: FMS1 protein

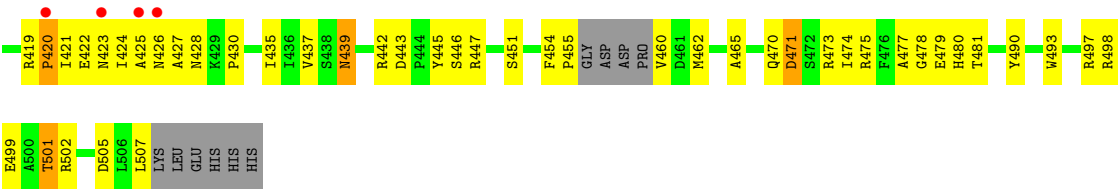
Chain C:



• Molecule 1: FMS1 protein

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.05Å 98.13Å 123.83Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	35.23 – 2.60 49.84 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.23-2.60) 73.5 (49.84-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.232 , 0.309 0.252 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 26.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 66311 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, 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	0.39	0/4080	0.64	0/5515
1	B	0.39	0/4025	0.65	0/5441
1	C	0.40	0/4047	0.64	0/5471
1	D	0.38	0/4008	0.63	1/5419 (0.0%)
All	All	0.39	0/16160	0.64	1/21846 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	380	LEU	CA-CB-CG	5.92	128.90	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3997	0	3916	202	0
1	B	3946	0	3881	217	0
1	C	3967	0	3900	159	0
1	D	3929	0	3857	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	26	0	0
2	B	14	0	26	0	0
2	C	14	0	26	0	0
2	D	14	0	26	0	0
3	A	53	0	31	3	0
3	B	53	0	31	8	0
3	C	53	0	31	1	0
3	D	53	0	31	3	0
4	A	55	0	0	1	0
4	B	54	0	0	8	0
4	C	66	0	0	2	0
4	D	50	0	0	1	0
All	All	16332	0	15782	778	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (778) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:GLY:H	1:A:451:SER:HA	1.00	1.07
1:A:289:ILE:HD11	1:A:462:MET:HG3	1.35	1.05
1:A:122:MET:HE1	1:A:145:VAL:HG22	1.39	1.05
1:D:32:ILE:HD12	1:D:507:LEU:HD12	1.40	1.02
1:D:278:LEU:HA	1:D:470:GLN:HE22	1.25	0.99
1:D:353:CYS:SG	1:D:400:PRO:HG2	2.02	0.98
1:D:278:LEU:HA	1:D:470:GLN:NE2	1.79	0.95
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.49	0.95
1:A:292:GLY:N	1:A:451:SER:HA	1.81	0.94
1:A:278:LEU:HA	1:A:470:GLN:HE22	1.32	0.94
1:A:228:ARG:HH21	1:A:232:LYS:HA	1.34	0.91
1:A:326:ILE:HD11	1:A:342:ARG:HH21	1.35	0.90
1:B:104:ARG:HD3	1:B:107:VAL:HG12	1.56	0.88
1:B:72:ASN:C	1:B:72:ASN:HD22	1.76	0.87
1:C:463:VAL:HG11	1:C:483:MET:HG2	1.54	0.87
1:C:122:MET:HE1	1:C:145:VAL:HG22	1.56	0.86
1:D:14:ILE:HD12	1:D:251:ILE:HG12	1.57	0.86
1:C:67:HIS:HA	1:C:195:ASN:HD22	1.41	0.86
1:B:353:CYS:SG	1:B:400:PRO:HB2	2.17	0.85
1:A:475:ARG:HE	1:A:502:ARG:NH1	1.75	0.84
1:A:422:GLU:HG2	1:A:423:ASN:N	1.91	0.84
1:C:150:LEU:O	1:C:153:ARG:HD2	1.78	0.84
1:D:288:LYS:C	1:D:289:ILE:HD12	1.98	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:ILE:CD1	1:A:462:MET:HG3	2.08	0.83
1:B:377:GLN:NE2	1:B:377:GLN:H	1.76	0.83
1:D:470:GLN:HB3	1:D:474:ILE:HB	1.60	0.83
1:C:193:GLY:HA2	1:D:121:GLU:HG3	1.58	0.82
1:B:14:ILE:HD12	1:B:251:ILE:HG12	1.62	0.81
1:A:326:ILE:HD11	1:A:342:ARG:NH2	1.95	0.81
1:A:172:GLU:HG2	1:A:177:LEU:O	1.80	0.81
1:A:122:MET:CE	1:A:145:VAL:HG22	2.11	0.81
1:D:359:PHE:HD2	1:D:375:LEU:HD13	1.46	0.81
1:D:173:LEU:HG	1:D:359:PHE:HB2	1.62	0.80
1:A:218:LYS:NZ	1:A:221:CYS:HB2	1.96	0.80
1:D:439:ASN:HD21	1:D:442:ARG:HD3	1.45	0.80
1:C:293:ALA:HB3	1:C:378:ALA:HB2	1.61	0.80
1:A:290:HIS:HA	1:A:451:SER:OG	1.82	0.80
1:B:322:GLU:HA	1:B:325:GLU:CG	2.11	0.80
1:C:228:ARG:HH21	1:C:232:LYS:HA	1.48	0.79
1:D:218:LYS:HD3	1:D:221:CYS:SG	2.22	0.79
1:D:288:LYS:O	1:D:289:ILE:HD12	1.83	0.79
1:D:322:GLU:O	1:D:326:ILE:HG13	1.83	0.79
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.64	0.79
1:C:288:LYS:O	1:C:289:ILE:HD13	1.84	0.77
1:B:475:ARG:HB3	1:B:499:GLU:OE1	1.85	0.77
1:B:14:ILE:CD1	1:B:226:ILE:HD11	2.15	0.77
1:C:279:LYS:HE3	1:C:470:GLN:O	1.85	0.77
1:B:222:GLU:OE2	1:B:269:ARG:HG3	1.85	0.76
1:A:278:LEU:HA	1:A:470:GLN:NE2	1.99	0.76
1:B:72:ASN:O	1:B:76:LEU:HG	1.84	0.76
1:D:227:THR:HG23	1:D:275:GLN:HB3	1.68	0.75
1:A:311:SER:HA	1:A:362:ASN:HB3	1.68	0.75
1:B:14:ILE:HD11	1:B:226:ILE:HD11	1.68	0.75
1:D:439:ASN:ND2	1:D:442:ARG:HD3	2.02	0.75
1:B:293:ALA:HB3	1:B:378:ALA:HB2	1.69	0.74
1:A:469:GLY:HA3	1:A:475:ARG:NH1	2.03	0.74
1:C:48:LEU:HD23	1:C:63:ALA:HB3	1.70	0.74
1:D:380:LEU:O	1:D:384:ILE:HG12	1.87	0.74
1:A:167:LEU:HA	1:A:316:LEU:HD21	1.69	0.74
1:C:85:ASP:O	1:C:87:ARG:N	2.21	0.73
1:A:6:PRO:HA	1:A:243:VAL:O	1.87	0.73
1:D:114:LEU:HB3	1:D:117:ILE:HD12	1.70	0.73
1:A:68:ASP:HB3	1:A:192:GLN:HB2	1.70	0.73
1:B:313:ILE:HD13	1:B:409:LEU:HD11	1.71	0.73
1:D:252:THR:HG22	1:D:477:ALA:HB3	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:48:LEU:HD23	1:D:63:ALA:HB3	1.71	0.72
1:D:171:LEU:HD13	1:D:187:THR:HG22	1.70	0.72
1:D:271:ARG:HG3	1:D:271:ARG:HH11	1.53	0.72
1:A:218:LYS:HZ2	1:A:221:CYS:HB2	1.55	0.72
1:A:166:GLN:HB3	1:A:316:LEU:HD22	1.72	0.71
1:D:247:ASP:O	1:D:473:ARG:HD2	1.90	0.71
1:B:118:VAL:HG23	1:B:164:LEU:HD13	1.73	0.71
1:A:278:LEU:CA	1:A:470:GLN:HE22	2.04	0.71
1:A:282:ILE:HG12	1:A:465:ALA:HB1	1.73	0.71
1:D:406:MET:HE1	1:D:430:PRO:HB3	1.73	0.70
1:D:224:LYS:HD2	1:D:239:GLU:HG2	1.73	0.70
1:A:228:ARG:NH2	1:A:232:LYS:HA	2.06	0.70
1:A:110:ASP:HB3	1:A:113:LEU:HB2	1.73	0.70
1:C:41:ARG:NH1	1:C:443:ASP:OD1	2.24	0.70
1:A:57:ARG:HD3	1:A:369:VAL:CG1	2.22	0.69
1:B:322:GLU:HA	1:B:325:GLU:HG2	1.73	0.69
1:A:57:ARG:HD3	1:A:369:VAL:HG13	1.74	0.69
1:C:265:GLU:OE2	1:C:267:ASN:HB3	1.93	0.69
1:D:399:GLN:HG3	1:D:403:ASN:ND2	2.07	0.69
1:D:323:PHE:O	1:D:327:VAL:HG23	1.92	0.69
1:D:148:TYR:CE1	1:D:152:ARG:HG3	2.28	0.69
1:A:192:GLN:NE2	1:B:128:LEU:HD11	2.08	0.69
1:A:224:LYS:HE2	1:A:239:GLU:HA	1.75	0.68
1:B:176:GLY:C	1:B:177:LEU:HD22	2.13	0.68
1:D:259:ASN:HA	1:D:286:PHE:HE1	1.58	0.68
1:A:167:LEU:O	1:A:170:TYR:HD2	1.75	0.68
1:C:330:ALA:HA	1:C:339:MET:HE1	1.75	0.68
1:B:460:VAL:HG12	1:B:461:ASP:H	1.59	0.68
1:B:494:GLU:OE1	1:B:497:ARG:NH2	2.24	0.68
1:A:423:ASN:HB3	1:A:426:ASN:ND2	2.08	0.68
1:B:362:ASN:HD21	1:B:364:SER:HB3	1.58	0.68
1:B:255:GLN:HG2	1:B:480:HIS:CD2	2.29	0.68
1:D:471:ASP:OD1	1:D:473:ARG:N	2.24	0.67
1:A:423:ASN:HB3	1:A:426:ASN:HD21	1.59	0.67
1:C:9:LYS:HB3	1:C:34:ASP:O	1.94	0.67
1:C:388:ARG:HB2	1:C:437:VAL:HB	1.75	0.67
1:B:72:ASN:ND2	1:B:75:PHE:H	1.92	0.67
1:A:131:HIS:O	1:A:132:GLN:HB2	1.95	0.67
1:A:157:THR:OG1	1:A:160:GLN:HG3	1.94	0.67
1:C:218:LYS:NZ	1:C:221:CYS:HB2	2.10	0.67
1:D:71:THR:OG1	1:D:192:GLN:NE2	2.27	0.67
1:C:332:ASN:OD1	1:C:335:GLU:HB2	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:349:THR:HB	4:B:965:HOH:O	1.95	0.66
1:B:64:SER:HB2	1:B:296:LYS:NZ	2.10	0.66
1:A:8:LYS:HD2	1:A:245:ASN:HD22	1.60	0.66
1:C:113:LEU:HB3	1:C:115:LEU:HG	1.77	0.66
1:B:259:ASN:O	1:B:262:VAL:HG22	1.95	0.66
1:A:67:HIS:ND1	1:A:195:ASN:ND2	2.43	0.66
1:D:72:ASN:HD22	1:D:72:ASN:C	1.99	0.66
1:C:12:ILE:HG13	1:C:246:ALA:HB2	1.78	0.66
1:A:255:GLN:HE21	1:A:290:HIS:HB2	1.60	0.66
1:A:401:VAL:O	1:A:405:ILE:HG13	1.96	0.66
1:A:165:PRO:O	1:A:169:ARG:HG3	1.95	0.65
1:D:399:GLN:N	1:D:400:PRO:HD2	2.12	0.65
1:C:218:LYS:HZ2	1:C:221:CYS:HB2	1.60	0.65
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.27	0.65
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.61	0.65
1:B:157:THR:OG1	1:B:160:GLN:HG3	1.96	0.64
1:D:48:LEU:CD2	1:D:63:ALA:HB3	2.28	0.64
1:A:247:ASP:O	1:A:473:ARG:HD2	1.96	0.64
1:C:278:LEU:HA	1:C:470:GLN:NE2	2.12	0.64
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.12	0.64
1:A:99:TYR:H	1:A:108:ASP:HB3	1.62	0.64
1:A:9:LYS:O	1:A:246:ALA:HA	1.97	0.64
1:A:248:TYR:HE1	1:A:507:LEU:HD21	1.62	0.63
1:A:399:GLN:HB3	1:A:400:PRO:HD3	1.80	0.63
1:B:439:ASN:ND2	1:B:442:ARG:HB2	2.14	0.63
1:C:213:PRO:O	1:C:216:TRP:HB2	1.98	0.63
1:A:225:SER:OG	1:A:237:ASN:HB2	1.99	0.63
1:C:278:LEU:HA	1:C:470:GLN:HE22	1.64	0.62
1:A:422:GLU:HG2	1:A:423:ASN:H	1.64	0.62
1:D:402:LEU:HB3	1:D:414:VAL:HG21	1.79	0.62
1:C:122:MET:HG2	1:C:148:TYR:CG	2.33	0.62
1:C:60:ASP:OD2	1:C:201:TYR:HB2	1.98	0.62
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.81	0.62
1:D:359:PHE:CD2	1:D:375:LEU:HD13	2.33	0.62
1:A:279:LYS:HD3	1:A:470:GLN:O	1.99	0.62
1:A:388:ARG:HD3	1:A:439:ASN:OD1	1.99	0.62
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.80	0.62
1:D:289:ILE:HG13	1:D:460:VAL:HG23	1.81	0.62
1:D:353:CYS:SG	1:D:400:PRO:CG	2.85	0.61
1:C:475:ARG:HB3	1:C:499:GLU:OE1	2.00	0.61
1:C:48:LEU:CD2	1:C:63:ALA:HB3	2.30	0.61
1:B:48:LEU:HD23	1:B:63:ALA:HB3	1.81	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:237:ASN:OD1	1:D:243:VAL:HG22	2.01	0.61
1:A:14:ILE:N	1:A:14:ILE:HD12	2.15	0.61
1:B:72:ASN:ND2	1:B:72:ASN:C	2.50	0.61
1:C:262:VAL:HG11	1:C:283:GLN:HA	1.83	0.61
1:A:323:PHE:O	1:A:327:VAL:HG23	2.01	0.61
1:A:475:ARG:HE	1:A:502:ARG:CZ	2.13	0.61
1:D:388:ARG:NH2	1:D:437:VAL:O	2.34	0.61
1:A:217:LEU:HG	1:A:219:LEU:CD2	2.30	0.61
1:B:313:ILE:CD1	1:B:409:LEU:HD11	2.31	0.61
1:A:61:ILE:O	1:A:296:LYS:HD3	2.00	0.61
1:D:282:ILE:HG12	1:D:465:ALA:HB1	1.83	0.61
1:C:110:ASP:O	1:C:114:LEU:HD23	2.00	0.61
1:C:330:ALA:HA	1:C:339:MET:CE	2.31	0.61
1:D:82:SER:O	1:D:86:GLY:HA2	2.01	0.61
1:A:251:ILE:N	1:A:251:ILE:HD12	2.15	0.61
1:B:404:LYS:HZ2	1:B:407:LYS:CE	2.14	0.60
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.36	0.60
1:A:167:LEU:HD23	1:A:167:LEU:C	2.22	0.60
1:D:475:ARG:HB3	1:D:499:GLU:OE1	2.01	0.60
1:A:279:LYS:HG3	1:A:470:GLN:OE1	2.02	0.60
1:A:259:ASN:O	1:A:262:VAL:HG22	2.02	0.60
1:C:122:MET:HG2	1:C:148:TYR:CD1	2.37	0.59
1:B:380:LEU:HD22	1:B:380:LEU:O	2.03	0.59
1:B:146:MET:CE	1:B:340:LEU:HD11	2.33	0.59
1:B:47:ARG:NE	3:B:804:FAD:O2A	2.30	0.59
1:A:98:ILE:HG12	1:A:106:ARG:NH2	2.16	0.59
1:D:259:ASN:O	1:D:262:VAL:HG22	2.02	0.59
1:C:502:ARG:O	1:C:506:LEU:HD13	2.02	0.59
1:D:443:ASP:HB3	1:D:446:SER:OG	2.02	0.59
1:A:87:ARG:HB2	1:A:89:ARG:NH1	2.18	0.59
1:D:142:PHE:O	1:D:146:MET:HG2	2.02	0.59
1:D:141:PHE:HE1	1:D:188:TYR:HH	1.50	0.59
1:C:247:ASP:O	1:C:473:ARG:HD2	2.03	0.59
1:D:130:PHE:O	1:D:132:GLN:N	2.36	0.59
1:D:269:ARG:HH11	1:D:269:ARG:HG3	1.68	0.59
1:B:460:VAL:HG12	1:B:461:ASP:N	2.17	0.59
1:A:353:CYS:SG	1:A:400:PRO:HB2	2.42	0.59
1:B:171:LEU:HD13	1:B:187:THR:HG22	1.85	0.59
1:D:9:LYS:O	1:D:246:ALA:HA	2.04	0.58
1:D:391:LYS:HA	1:D:394:LEU:HD12	1.85	0.58
1:C:260:LEU:HD11	1:C:447:ARG:NE	2.19	0.58
1:C:173:LEU:HD22	1:C:173:LEU:N	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:122:MET:HE2	1:C:145:VAL:HA	1.85	0.58
1:B:17:GLY:HA3	3:B:804:FAD:O1A	2.03	0.58
1:D:177:LEU:HD21	1:D:454:PHE:HE2	1.69	0.58
1:A:70:LEU:HD23	1:B:152:ARG:CZ	2.34	0.58
1:D:143:GLN:O	1:D:147:LYS:HG3	2.04	0.58
1:A:469:GLY:HA3	1:A:475:ARG:HH11	1.67	0.58
1:B:227:THR:HG23	1:B:275:GLN:O	2.03	0.58
1:A:297:VAL:HG22	1:A:437:VAL:HG13	1.85	0.58
1:C:176:GLY:C	1:C:177:LEU:HD22	2.23	0.58
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.67	0.58
1:D:97:PHE:CE2	1:D:359:PHE:HE1	2.22	0.58
1:D:110:ASP:HB3	1:D:113:LEU:HB2	1.86	0.58
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.86	0.58
1:C:353:CYS:SG	1:C:400:PRO:HB2	2.44	0.58
1:C:335:GLU:HG2	1:C:339:MET:HE2	1.85	0.57
1:A:218:LYS:HZ3	1:A:221:CYS:HB2	1.69	0.57
1:A:362:ASN:HD21	1:A:364:SER:HB3	1.69	0.57
1:A:265:GLU:O	1:A:267:ASN:N	2.36	0.57
1:C:67:HIS:HA	1:C:195:ASN:ND2	2.17	0.57
1:D:462:MET:HE1	1:D:480:HIS:HD2	1.70	0.57
1:D:423:ASN:O	1:D:425:ALA:N	2.38	0.57
1:B:85:ASP:OD2	1:B:89:ARG:NH2	2.33	0.57
1:D:439:ASN:HD21	1:D:442:ARG:HB2	1.68	0.57
1:C:470:GLN:HB3	1:C:474:ILE:HB	1.87	0.57
1:C:376:MET:HG3	1:C:381:THR:OG1	2.04	0.57
1:D:36:LEU:HD23	1:D:216:TRP:O	2.05	0.57
1:B:228:ARG:NH2	1:B:473:ARG:HG2	2.19	0.57
1:C:399:GLN:HB3	1:C:400:PRO:HD3	1.87	0.56
1:B:172:GLU:OE2	1:B:179:TRP:N	2.30	0.56
1:A:146:MET:CE	1:A:340:LEU:HD11	2.35	0.56
1:B:336:LEU:O	1:B:340:LEU:HG	2.05	0.56
1:C:69:THR:HB	1:C:75:PHE:CE2	2.41	0.56
1:C:157:THR:OG1	1:C:160:GLN:HG3	2.06	0.56
1:B:322:GLU:HA	1:B:325:GLU:HG3	1.87	0.56
1:B:311:SER:O	1:B:312:LYS:HD3	2.05	0.56
1:A:248:TYR:CE1	1:A:507:LEU:HD21	2.40	0.56
1:B:335:GLU:HG2	1:B:339:MET:SD	2.45	0.56
1:D:167:LEU:O	1:D:170:TYR:HD2	1.88	0.56
1:A:388:ARG:NH1	1:A:439:ASN:HB2	2.20	0.56
1:D:218:LYS:CD	1:D:221:CYS:SG	2.92	0.56
1:D:169:ARG:HD2	1:D:179:TRP:CD2	2.41	0.56
1:B:454:PHE:HB3	1:B:455:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:336:LEU:O	1:C:340:LEU:HG	2.06	0.56
1:D:72:ASN:O	1:D:76:LEU:HG	2.05	0.55
1:D:189:PHE:H	1:D:189:PHE:HD2	1.53	0.55
1:B:448:GLY:O	1:B:449:ALA:HB2	2.07	0.55
1:A:353:CYS:HB3	1:A:397:PHE:O	2.07	0.55
1:D:177:LEU:HD21	1:D:454:PHE:CE2	2.41	0.55
1:D:271:ARG:NH1	1:D:271:ARG:HG3	2.19	0.55
1:A:385:GLU:OE1	1:A:441:THR:HG23	2.07	0.55
1:D:171:LEU:HD13	1:D:187:THR:CG2	2.37	0.55
1:C:122:MET:CE	1:C:145:VAL:HG22	2.34	0.55
1:D:251:ILE:HD13	1:D:274:PHE:HZ	1.71	0.55
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.72	0.55
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.71	0.55
1:A:418:MET:O	1:A:420:PRO:HD3	2.06	0.55
1:D:222:GLU:HB3	1:D:239:GLU:HB2	1.88	0.55
1:D:372:PHE:HE2	1:D:405:ILE:HG21	1.72	0.54
1:C:240:ASP:OD1	1:C:241:GLY:N	2.41	0.54
1:C:464:VAL:HA	1:C:467:SER:HG	1.72	0.54
1:A:291:PHE:O	1:A:292:GLY:C	2.45	0.54
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.22	0.54
1:D:259:ASN:HA	1:D:286:PHE:CE1	2.40	0.54
1:B:416:ASP:OD1	1:B:416:ASP:C	2.46	0.54
1:D:150:LEU:HG	1:D:336:LEU:HD22	1.89	0.54
1:A:176:GLY:C	1:A:177:LEU:HD23	2.28	0.54
1:D:218:LYS:HE2	1:D:244:TYR:OH	2.07	0.54
1:C:41:ARG:HH12	1:C:443:ASP:CG	2.11	0.54
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.23	0.54
1:C:88:THR:HG22	1:C:199:LEU:HD12	1.88	0.54
1:D:99:TYR:O	1:D:106:ARG:HA	2.08	0.54
1:C:152:ARG:O	1:C:156:LEU:HG	2.07	0.54
1:B:189:PHE:HE1	1:B:191:HIS:NE2	2.05	0.54
1:D:387:ILE:HG13	1:D:394:LEU:HD21	1.89	0.54
1:D:40:ALA:HB1	1:D:445:TYR:CE2	2.43	0.54
1:C:64:SER:HB2	1:C:296:LYS:HZ1	1.73	0.54
1:D:11:VAL:HB	1:D:35:CYS:SG	2.48	0.54
1:B:116:GLU:O	1:B:119:ASP:HB3	2.08	0.54
1:A:424:ILE:C	1:A:426:ASN:H	2.11	0.54
1:B:479:GLU:OE2	1:B:487:GLY:HA2	2.07	0.54
1:A:209:ALA:HA	1:A:212:PHE:HE2	1.73	0.54
1:A:290:HIS:HA	1:A:451:SER:CB	2.37	0.53
1:D:45:GLY:O	1:D:48:LEU:HB2	2.08	0.53
1:C:332:ASN:ND2	1:C:335:GLU:H	2.06	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:218:LYS:CE	1:D:244:TYR:OH	2.56	0.53
1:D:478:GLY:HA2	3:D:802:FAD:O2P	2.09	0.53
1:D:139:CYS:SG	1:D:147:LYS:HE2	2.48	0.53
1:D:40:ALA:HB1	1:D:445:TYR:CZ	2.43	0.53
1:B:369:VAL:O	1:B:371:SER:N	2.40	0.53
1:B:113:LEU:CD2	1:B:159:ASP:HB3	2.38	0.53
1:D:26:THR:O	1:D:29:GLN:HB3	2.08	0.53
1:B:19:ALA:HB2	1:B:492:ALA:HB1	1.91	0.53
1:B:298:ILE:O	1:B:435:ILE:HA	2.08	0.53
1:C:54:TYR:CZ	1:C:433:ARG:HG3	2.43	0.53
1:A:292:GLY:HA3	1:A:451:SER:H	1.73	0.53
1:B:353:CYS:HB3	1:B:397:PHE:O	2.08	0.53
1:C:63:ALA:HA	3:C:801:FAD:N5	2.24	0.53
1:D:169:ARG:HD2	1:D:179:TRP:CE2	2.43	0.53
1:D:412:GLU:N	1:D:412:GLU:OE2	2.42	0.53
1:A:359:PHE:HB3	1:A:375:LEU:HB2	1.89	0.53
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.73	0.53
1:B:426:ASN:C	1:B:428:ASN:H	2.12	0.53
1:D:315:THR:O	1:D:357:PRO:HA	2.08	0.53
1:C:251:ILE:HG22	1:C:253:VAL:HG22	1.90	0.53
1:A:422:GLU:CG	1:A:423:ASN:N	2.70	0.53
1:B:293:ALA:CB	1:B:378:ALA:HB2	2.39	0.53
1:C:60:ASP:HB3	1:C:63:ALA:O	2.09	0.53
1:B:169:ARG:HB3	1:B:357:PRO:HG3	1.91	0.53
1:B:72:ASN:HD21	1:B:74:LEU:HB3	1.74	0.52
1:B:118:VAL:CG2	1:B:164:LEU:HD13	2.39	0.52
1:B:47:ARG:HA	1:B:440:TRP:CH2	2.44	0.52
1:A:217:LEU:HG	1:A:219:LEU:HD22	1.92	0.52
1:D:172:GLU:HG2	1:D:177:LEU:O	2.09	0.52
1:A:164:LEU:N	1:A:165:PRO:HD2	2.25	0.52
1:C:282:ILE:HG23	1:C:466:MET:CE	2.39	0.52
1:A:54:TYR:CD2	1:A:55:GLN:HG3	2.44	0.52
1:D:439:ASN:ND2	1:D:442:ARG:HB2	2.24	0.52
1:C:64:SER:HB2	1:C:296:LYS:NZ	2.24	0.52
1:D:67:HIS:ND1	1:D:195:ASN:ND2	2.57	0.52
1:C:218:LYS:HE3	1:C:244:TYR:OH	2.10	0.52
1:A:483:MET:CE	1:A:483:MET:HA	2.40	0.52
1:C:228:ARG:NH2	1:C:232:LYS:HA	2.23	0.52
1:C:45:GLY:O	1:C:48:LEU:HB2	2.10	0.52
1:C:416:ASP:OD1	1:C:418:MET:HG3	2.10	0.52
1:A:217:LEU:HG	1:A:219:LEU:HD21	1.92	0.52
1:C:177:LEU:HD21	1:C:292:GLY:HA2	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:189:PHE:CE1	1:B:191:HIS:NE2	2.78	0.52
1:A:349:THR:O	1:A:350:SER:OG	2.26	0.52
1:A:315:THR:OG1	1:A:358:LEU:HB2	2.10	0.52
1:C:8:LYS:O	1:C:9:LYS:HD2	2.10	0.52
1:B:47:ARG:HD3	1:B:449:ALA:O	2.09	0.52
1:B:99:TYR:HB3	1:B:316:LEU:HD11	1.91	0.52
1:A:69:THR:HB	1:A:75:PHE:CE2	2.45	0.52
1:B:10:LYS:O	1:B:247:ASP:HB2	2.10	0.51
1:B:319:SER:HA	4:B:960:HOH:O	2.09	0.51
1:A:288:LYS:O	1:A:289:ILE:HG23	2.10	0.51
1:D:353:CYS:HB3	1:D:397:PHE:O	2.10	0.51
1:C:110:ASP:HB3	1:C:113:LEU:HB2	1.90	0.51
1:A:213:PRO:O	1:A:216:TRP:HB2	2.10	0.51
1:B:138:ASP:HB2	1:B:185:LYS:HE3	1.91	0.51
1:B:414:VAL:HA	1:B:430:PRO:HG2	1.93	0.51
1:A:508:LYS:O	1:A:513:HIS:NE2	2.43	0.51
1:A:462:MET:O	1:A:463:VAL:C	2.48	0.51
1:B:361:VAL:HB	1:B:373:MET:HB3	1.91	0.51
1:A:385:GLU:O	1:A:388:ARG:HG2	2.11	0.51
1:D:462:MET:CE	1:D:480:HIS:HD2	2.23	0.51
1:A:299:PHE:CE2	1:A:402:LEU:HD11	2.46	0.51
1:D:251:ILE:HD13	1:D:274:PHE:CZ	2.45	0.51
1:B:279:LYS:HB2	1:B:280:PRO:HD2	1.92	0.51
1:B:262:VAL:HG23	1:B:262:VAL:O	2.11	0.51
1:C:377:GLN:H	1:C:377:GLN:NE2	2.08	0.51
1:A:118:VAL:HB	1:A:164:LEU:HD22	1.93	0.51
1:B:311:SER:C	1:B:312:LYS:HD3	2.30	0.51
1:B:507:LEU:O	1:B:509:LEU:N	2.43	0.51
1:D:279:LYS:HB2	1:D:280:PRO:HD2	1.93	0.51
1:C:200:ASN:O	1:C:203:SER:HB3	2.11	0.51
1:C:222:GLU:OE1	1:C:270:GLY:N	2.44	0.51
1:D:64:SER:HB2	1:D:296:LYS:NZ	2.25	0.50
1:B:377:GLN:NE2	1:B:377:GLN:N	2.53	0.50
1:B:63:ALA:HA	3:B:804:FAD:N5	2.26	0.50
1:C:290:HIS:HD2	4:C:922:HOH:O	1.93	0.50
1:D:63:ALA:HA	3:D:802:FAD:N5	2.27	0.50
1:A:63:ALA:HA	3:A:803:FAD:N5	2.26	0.50
1:A:264:PRO:O	1:A:265:GLU:HB2	2.11	0.50
1:A:349:THR:C	1:A:350:SER:OG	2.50	0.50
1:B:321:ASN:O	1:B:324:VAL:HB	2.11	0.50
1:C:138:ASP:O	1:C:139:CYS:HB3	2.11	0.50
1:A:255:GLN:OE1	1:A:289:ILE:HD12	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.52	0.50
1:A:177:LEU:HD11	1:A:452:ALA:HB3	1.94	0.50
1:A:224:LYS:CE	1:A:239:GLU:HA	2.40	0.49
1:C:95:ASP:OD2	1:C:310:SER:HA	2.12	0.49
1:C:89:ARG:O	1:C:199:LEU:HB2	2.12	0.49
1:A:143:GLN:OE1	1:A:337:ASP:OD1	2.30	0.49
1:A:172:GLU:O	1:A:176:GLY:N	2.44	0.49
1:D:380:LEU:O	1:D:380:LEU:HD22	2.12	0.49
1:B:359:PHE:CD2	1:B:375:LEU:HD22	2.47	0.49
1:D:426:ASN:O	1:D:428:ASN:N	2.45	0.49
1:C:70:LEU:HB2	1:C:192:GLN:O	2.11	0.49
1:D:145:VAL:HG11	1:D:165:PRO:HB3	1.94	0.49
1:C:149:LEU:HD22	1:C:161:ILE:HG23	1.93	0.49
1:D:167:LEU:HD23	1:D:167:LEU:C	2.32	0.49
1:A:209:ALA:HA	1:A:212:PHE:CE2	2.47	0.49
1:B:167:LEU:O	1:B:170:TYR:HD2	1.95	0.49
1:A:152:ARG:CZ	1:B:70:LEU:HD23	2.43	0.49
1:A:322:GLU:O	1:A:326:ILE:HG13	2.11	0.49
1:C:213:PRO:HB2	1:C:216:TRP:CG	2.48	0.49
1:D:227:THR:HG23	1:D:275:GLN:O	2.13	0.49
1:C:308:ASN:OD1	1:C:364:SER:HB3	2.12	0.49
1:C:57:ARG:HD3	1:C:369:VAL:CG1	2.43	0.49
1:A:70:LEU:HD23	1:B:152:ARG:NE	2.28	0.49
1:D:60:ASP:HB3	1:D:63:ALA:O	2.13	0.49
1:B:12:ILE:O	1:B:249:VAL:HA	2.12	0.49
1:D:329:ASN:O	1:D:330:ALA:C	2.51	0.49
1:B:213:PRO:HG2	1:B:216:TRP:CE2	2.47	0.49
1:B:213:PRO:HG2	1:B:216:TRP:CD2	2.47	0.49
1:D:11:VAL:HG11	1:D:27:LEU:HD11	1.94	0.48
1:B:300:GLU:O	1:B:432:LEU:HD12	2.12	0.48
1:A:470:GLN:HB3	1:A:474:ILE:HB	1.93	0.48
1:A:22:LYS:HE2	1:A:493:TRP:CZ2	2.48	0.48
1:B:148:TYR:CE1	1:B:152:ARG:HG3	2.49	0.48
1:D:184:ALA:C	1:D:186:ASP:H	2.16	0.48
1:A:219:LEU:HD22	1:A:219:LEU:N	2.27	0.48
1:D:36:LEU:HD23	1:D:37:VAL:H	1.78	0.48
1:B:241:GLY:O	1:B:243:VAL:HG23	2.13	0.48
1:C:439:ASN:ND2	1:C:442:ARG:HD3	2.27	0.48
1:D:157:THR:HG23	1:D:160:GLN:CD	2.34	0.48
1:B:392:GLU:HA	1:B:392:GLU:OE1	2.13	0.48
1:C:85:ASP:OD2	1:C:85:ASP:O	2.31	0.48
1:D:390:ASP:O	1:D:394:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:GLN:HG2	4:B:949:HOH:O	2.13	0.48
1:C:479:GLU:OE1	1:C:487:GLY:HA2	2.13	0.48
1:A:255:GLN:CD	1:A:289:ILE:HD12	2.34	0.48
1:A:234:VAL:O	1:A:245:ASN:HA	2.13	0.48
1:A:468:ASN:C	1:A:475:ARG:HH12	2.16	0.48
1:C:265:GLU:O	1:C:265:GLU:HG3	2.12	0.48
1:B:404:LYS:HZ2	1:B:407:LYS:HE2	1.78	0.48
1:D:64:SER:HB2	1:D:296:LYS:HZ1	1.78	0.48
1:C:362:ASN:HD21	1:C:364:SER:HB3	1.78	0.48
1:B:138:ASP:OD2	1:B:455:PRO:HA	2.14	0.48
1:A:153:ARG:NH2	1:A:328:ARG:O	2.46	0.48
1:C:14:ILE:CD1	1:C:226:ILE:HD11	2.44	0.48
1:B:258:LEU:HD22	4:B:954:HOH:O	2.13	0.48
1:D:353:CYS:SG	1:D:401:VAL:HG13	2.53	0.48
1:C:70:LEU:HD23	1:D:152:ARG:NH1	2.28	0.48
1:A:297:VAL:HG23	1:A:376:MET:CE	2.43	0.48
1:B:174:TRP:CZ3	1:B:191:HIS:NE2	2.82	0.48
1:D:359:PHE:HB3	1:D:375:LEU:HB2	1.95	0.48
1:C:278:LEU:CA	1:C:470:GLN:HE22	2.27	0.48
1:D:25:SER:O	1:D:29:GLN:HB2	2.13	0.48
1:D:279:LYS:HG3	1:D:281:VAL:HG12	1.95	0.48
1:B:189:PHE:HE1	1:B:191:HIS:CD2	2.31	0.48
1:C:391:LYS:H	1:C:391:LYS:HD3	1.79	0.48
1:A:289:ILE:HD11	1:A:462:MET:CG	2.25	0.47
1:B:176:GLY:HA3	1:B:294:LEU:HB2	1.95	0.47
1:C:72:ASN:HB3	1:C:75:PHE:HB3	1.96	0.47
1:D:189:PHE:N	1:D:189:PHE:HD2	2.12	0.47
1:B:99:TYR:H	1:B:108:ASP:HB3	1.79	0.47
1:D:224:LYS:CD	1:D:239:GLU:HG2	2.43	0.47
1:B:449:ALA:HA	3:B:804:FAD:HM81	1.95	0.47
1:D:28:HIS:CG	1:D:213:PRO:HD3	2.50	0.47
1:A:122:MET:HE1	1:A:145:VAL:CG2	2.29	0.47
1:D:311:SER:HA	1:D:362:ASN:HB3	1.96	0.47
1:B:419:ARG:O	1:B:420:PRO:O	2.32	0.47
1:A:171:LEU:HD11	1:A:188:TYR:CE2	2.49	0.47
1:B:290:HIS:O	1:B:291:PHE:CB	2.61	0.47
1:A:115:LEU:HB3	1:A:167:LEU:HD13	1.95	0.47
1:C:264:PRO:O	1:C:265:GLU:HB2	2.15	0.47
1:A:67:HIS:O	1:A:72:ASN:HB2	2.15	0.47
1:A:20:GLY:O	1:A:23:ALA:HB3	2.14	0.47
1:D:38:LEU:HD13	1:D:238:CYS:SG	2.54	0.47
1:D:388:ARG:NE	1:D:439:ASN:HB2	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:279:LYS:HG3	1:C:470:GLN:OE1	2.15	0.47
1:D:380:LEU:HD22	1:D:384:ILE:HG12	1.97	0.47
1:B:172:GLU:HB3	1:B:177:LEU:O	2.15	0.47
1:D:259:ASN:CA	1:D:286:PHE:HE1	2.26	0.47
1:B:64:SER:OG	1:B:197:PHE:CE1	2.67	0.47
1:B:146:MET:HE1	1:B:340:LEU:HD11	1.94	0.47
1:A:444:PRO:O	1:A:447:ARG:NE	2.47	0.47
1:A:391:LYS:HA	1:A:394:LEU:HD12	1.96	0.47
1:D:359:PHE:O	1:D:374:MET:HA	2.13	0.47
1:A:115:LEU:O	1:A:118:VAL:HG23	2.15	0.47
1:D:122:MET:HE1	1:D:148:TYR:HB2	1.96	0.47
1:D:72:ASN:ND2	1:D:75:PHE:H	2.13	0.47
1:A:87:ARG:HB2	1:A:89:ARG:HH12	1.79	0.47
1:A:206:GLN:HB3	1:A:210:GLN:NE2	2.30	0.47
1:A:26:THR:O	1:A:30:ASN:OD1	2.33	0.47
1:D:377:GLN:HG2	1:D:378:ALA:O	2.15	0.47
1:C:65:TRP:HH2	1:C:361:VAL:HG21	1.79	0.47
1:A:122:MET:HG2	1:A:148:TYR:CD2	2.50	0.47
1:C:153:ARG:HG2	1:C:154:GLN:N	2.28	0.47
1:D:375:LEU:N	1:D:375:LEU:HD12	2.30	0.47
1:D:322:GLU:OE1	1:D:322:GLU:N	2.47	0.47
1:B:237:ASN:OD1	1:B:243:VAL:HG13	2.14	0.47
1:D:72:ASN:HB3	1:D:75:PHE:HB3	1.96	0.47
1:B:213:PRO:HG2	1:B:216:TRP:CD1	2.50	0.47
1:B:54:TYR:OH	1:B:302:GLU:HG3	2.15	0.47
1:B:223:VAL:HA	1:B:238:CYS:HA	1.97	0.47
1:C:227:THR:HA	1:C:275:GLN:O	2.15	0.47
1:D:349:THR:O	1:D:349:THR:HG22	2.15	0.47
1:A:269:ARG:CZ	1:A:444:PRO:HG3	2.44	0.47
1:C:164:LEU:N	1:C:165:PRO:HD2	2.30	0.47
1:A:44:VAL:HG12	1:A:219:LEU:HD11	1.97	0.46
1:B:380:LEU:HD13	1:B:380:LEU:O	2.15	0.46
1:B:150:LEU:HG	1:B:336:LEU:HD22	1.96	0.46
1:C:248:TYR:CE2	1:C:473:ARG:HD3	2.50	0.46
1:A:171:LEU:HD13	1:A:187:THR:HG22	1.96	0.46
1:B:23:ALA:O	1:B:27:LEU:HG	2.15	0.46
1:B:270:GLY:HA2	3:B:804:FAD:H61A	1.79	0.46
1:B:213:PRO:HG2	1:B:216:TRP:CG	2.49	0.46
1:B:479:GLU:OE1	1:B:480:HIS:N	2.48	0.46
1:A:91:VAL:HG13	1:A:91:VAL:O	2.15	0.46
1:B:164:LEU:N	1:B:165:PRO:HD2	2.29	0.46
1:D:98:ILE:HG12	1:D:106:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:502:ARG:O	1:D:505:ASP:HB3	2.16	0.46
1:A:173:LEU:N	1:A:173:LEU:HD22	2.30	0.46
1:D:259:ASN:ND2	1:D:286:PHE:HD1	2.13	0.46
1:B:63:ALA:HA	3:B:804:FAD:C5X	2.46	0.46
1:D:189:PHE:N	1:D:189:PHE:CD2	2.78	0.46
1:C:229:GLU:HB3	1:C:233:ASN:O	2.16	0.46
1:A:228:ARG:HH21	1:A:232:LYS:CA	2.16	0.46
1:D:294:LEU:HD11	1:D:375:LEU:HB3	1.98	0.46
1:B:60:ASP:HB3	1:B:63:ALA:O	2.16	0.46
1:C:381:THR:O	1:C:385:GLU:HG3	2.16	0.46
1:D:183:SER:HA	1:D:455:PRO:HB3	1.97	0.46
1:C:13:ILE:HD13	1:C:23:ALA:HB3	1.98	0.46
1:B:176:GLY:O	1:B:177:LEU:HD22	2.15	0.46
1:A:449:ALA:HA	3:A:803:FAD:C8M	2.46	0.46
1:C:239:GLU:HG3	1:C:240:ASP:N	2.31	0.46
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.80	0.46
1:A:176:GLY:O	1:A:177:LEU:HD23	2.16	0.46
1:B:404:LYS:HD2	1:B:404:LYS:HA	1.72	0.46
1:D:8:LYS:N	1:D:245:ASN:ND2	2.64	0.46
1:D:157:THR:HG23	1:D:160:GLN:OE1	2.15	0.46
1:B:131:HIS:ND1	1:B:131:HIS:O	2.49	0.46
1:C:162:ARG:HD3	1:C:163:TYR:CE1	2.51	0.46
1:D:240:ASP:OD1	1:D:241:GLY:N	2.49	0.46
1:B:113:LEU:O	1:B:114:LEU:C	2.54	0.45
1:B:315:THR:O	1:B:357:PRO:HA	2.16	0.45
1:D:498:ARG:O	1:D:501:THR:HG22	2.16	0.45
1:A:121:GLU:HG3	1:B:193:GLY:HA2	1.98	0.45
1:A:470:GLN:OE1	1:A:470:GLN:HA	2.16	0.45
1:B:311:SER:HA	1:B:362:ASN:HB3	1.98	0.45
1:B:47:ARG:NH1	1:B:449:ALA:O	2.49	0.45
1:B:146:MET:HE2	1:B:340:LEU:HD11	1.97	0.45
1:C:169:ARG:HD2	1:C:179:TRP:CE2	2.50	0.45
1:C:228:ARG:HH11	1:C:228:ARG:HG2	1.82	0.45
1:B:255:GLN:HG2	1:B:480:HIS:CG	2.51	0.45
1:B:64:SER:HB2	1:B:296:LYS:HZ1	1.80	0.45
1:B:334:ASP:C	1:B:336:LEU:N	2.70	0.45
1:C:333:LEU:HD23	1:C:334:ASP:N	2.31	0.45
1:B:143:GLN:HA	1:B:143:GLN:HE21	1.80	0.45
1:A:364:SER:HA	1:A:369:VAL:O	2.15	0.45
1:D:331:GLU:O	1:D:332:ASN:HB2	2.16	0.45
1:C:36:LEU:HD12	1:C:216:TRP:O	2.16	0.45
1:A:183:SER:HB3	1:A:454:PHE:C	2.37	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:449:ALA:HA	3:A:803:FAD:HM83	1.98	0.45
1:D:395:PHE:CE2	1:D:416:ASP:HB2	2.50	0.45
1:B:381:THR:O	1:B:385:GLU:HG3	2.16	0.45
1:D:14:ILE:CD1	1:D:226:ILE:HD11	2.47	0.45
1:A:217:LEU:CD2	1:A:219:LEU:HD21	2.46	0.45
1:C:395:PHE:CE2	1:C:416:ASP:HB2	2.52	0.45
1:C:255:GLN:HB2	1:C:480:HIS:CD2	2.52	0.45
1:B:118:VAL:HG23	1:B:164:LEU:CD1	2.44	0.45
1:D:40:ALA:CB	1:D:445:TYR:CE2	3.00	0.45
1:D:17:GLY:O	1:D:21:LEU:HG	2.17	0.45
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.46	0.45
1:C:406:MET:HB3	1:C:411:SER:HB3	1.98	0.45
1:B:207:ARG:O	1:B:210:GLN:HG3	2.17	0.45
1:C:185:LYS:HG2	4:C:933:HOH:O	2.15	0.45
1:C:32:ILE:HD12	1:C:507:LEU:HD12	1.98	0.45
1:D:199:LEU:HD23	1:D:199:LEU:HA	1.82	0.45
1:A:43:ARG:HH11	1:A:43:ARG:HG3	1.82	0.45
1:A:229:GLU:C	1:A:231:SER:N	2.70	0.45
1:D:49:GLN:HE21	1:D:51:VAL:CG1	2.29	0.45
1:D:173:LEU:HG	1:D:359:PHE:CB	2.41	0.45
1:D:142:PHE:HD1	1:D:179:TRP:CH2	2.35	0.45
1:B:89:ARG:HG3	1:B:89:ARG:HH11	1.82	0.45
1:C:466:MET:HG3	1:C:481:THR:HG22	1.98	0.45
1:C:13:ILE:HB	1:C:37:VAL:HG22	1.98	0.45
1:B:213:PRO:O	1:B:216:TRP:HB2	2.17	0.44
1:B:200:ASN:HA	4:B:924:HOH:O	2.17	0.44
1:B:126:ALA:HB2	1:B:144:LEU:HD21	1.99	0.44
1:A:35:CYS:HB2	1:A:216:TRP:CZ3	2.52	0.44
1:C:311:SER:O	1:C:312:LYS:HD3	2.18	0.44
1:B:260:LEU:O	1:B:271:ARG:HD2	2.17	0.44
1:B:202:ASP:OD1	1:B:203:SER:N	2.50	0.44
1:D:419:ARG:O	1:D:421:ILE:N	2.51	0.44
1:B:201:TYR:O	1:B:204:VAL:HB	2.16	0.44
1:A:392:GLU:OE2	1:A:416:ASP:OD2	2.35	0.44
1:C:122:MET:SD	1:C:122:MET:O	2.75	0.44
1:C:22:LYS:HD3	1:C:493:TRP:NE1	2.32	0.44
1:C:102:GLU:O	1:C:404:LYS:HE2	2.18	0.44
1:D:470:GLN:O	1:D:471:ASP:HB3	2.18	0.44
1:D:399:GLN:N	1:D:400:PRO:CD	2.79	0.44
1:C:122:MET:CE	1:C:145:VAL:HG13	2.47	0.44
1:B:14:ILE:HB	1:B:251:ILE:HA	2.00	0.44
1:A:219:LEU:O	1:A:220:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:229:GLU:O	1:C:231:SER:N	2.51	0.44
1:D:89:ARG:HH11	1:D:89:ARG:HG3	1.83	0.44
1:A:72:ASN:ND2	1:A:490:TYR:CD2	2.86	0.44
1:A:437:VAL:HG12	1:A:438:SER:N	2.32	0.44
1:A:219:LEU:HD22	1:A:219:LEU:H	1.80	0.44
1:D:278:LEU:CA	1:D:470:GLN:HE22	2.13	0.44
1:A:166:GLN:CB	1:A:316:LEU:HD22	2.44	0.44
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.73	0.44
1:B:234:VAL:HG11	1:B:249:VAL:HG21	1.99	0.44
1:A:115:LEU:CB	1:A:167:LEU:HD13	2.48	0.44
1:D:406:MET:HE2	1:D:430:PRO:HG3	1.99	0.44
1:C:471:ASP:OD1	1:C:473:ARG:N	2.43	0.44
1:B:361:VAL:HG21	1:B:373:MET:HE3	1.99	0.44
1:D:377:GLN:H	1:D:377:GLN:NE2	2.16	0.44
1:C:300:GLU:O	1:C:432:LEU:HD12	2.18	0.44
1:D:8:LYS:O	1:D:9:LYS:HD3	2.18	0.43
1:B:426:ASN:HB2	1:B:427:ALA:H	1.66	0.43
1:B:99:TYR:CE2	1:B:167:LEU:HG	2.53	0.43
1:A:50:THR:OG1	1:A:202:ASP:HB3	2.17	0.43
1:B:389:GLU:HB2	4:B:950:HOH:O	2.18	0.43
1:D:255:GLN:NE2	1:D:290:HIS:O	2.52	0.43
1:D:289:ILE:O	1:D:289:ILE:CG2	2.66	0.43
1:B:496:GLY:C	1:B:498:ARG:N	2.68	0.43
1:D:142:PHE:HB2	1:D:179:TRP:CD2	2.54	0.43
1:D:169:ARG:C	1:D:171:LEU:N	2.72	0.43
1:B:175:HIS:O	1:B:177:LEU:CD2	2.66	0.43
1:A:297:VAL:CG2	1:A:376:MET:HE3	2.49	0.43
1:A:265:GLU:C	1:A:267:ASN:H	2.22	0.43
1:A:131:HIS:O	1:A:132:GLN:CB	2.65	0.43
1:B:478:GLY:HA2	3:B:804:FAD:O2P	2.18	0.43
1:A:265:GLU:C	1:A:267:ASN:N	2.72	0.43
1:B:50:THR:OG1	1:B:202:ASP:HB3	2.19	0.43
1:D:298:ILE:O	1:D:435:ILE:HA	2.18	0.43
1:A:324:VAL:O	1:A:325:GLU:C	2.57	0.43
1:D:399:GLN:HG3	1:D:403:ASN:HD21	1.81	0.43
1:D:439:ASN:HD21	1:D:442:ARG:CD	2.24	0.43
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.52	0.43
1:D:423:ASN:C	1:D:425:ALA:N	2.72	0.43
1:A:312:LYS:HD2	1:A:359:PHE:CZ	2.53	0.43
1:D:157:THR:OG1	1:D:160:GLN:HG3	2.18	0.43
1:A:178:ASP:HB3	1:A:181:LEU:HD12	2.00	0.43
1:A:289:ILE:HB	1:A:290:HIS:H	1.26	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:ILE:CD1	1:A:342:ARG:HH21	2.18	0.43
1:B:262:VAL:HG21	1:B:286:PHE:CD1	2.54	0.43
1:B:404:LYS:NZ	1:B:407:LYS:CE	2.80	0.43
1:C:12:ILE:O	1:C:249:VAL:HA	2.18	0.43
1:A:312:LYS:HD2	1:A:359:PHE:HZ	1.83	0.43
1:B:426:ASN:C	1:B:428:ASN:N	2.72	0.43
1:B:255:GLN:HA	1:B:255:GLN:NE2	2.33	0.43
1:B:334:ASP:C	1:B:336:LEU:H	2.21	0.43
1:B:122:MET:HG2	1:B:148:TYR:CD2	2.53	0.43
1:B:183:SER:O	1:B:184:ALA:C	2.57	0.43
1:C:234:VAL:HG12	1:C:235:THR:N	2.34	0.43
1:B:49:GLN:HA	4:B:963:HOH:O	2.17	0.43
1:D:289:ILE:O	1:D:290:HIS:O	2.36	0.43
1:B:302:GLU:OE2	1:B:433:ARG:NH1	2.52	0.43
1:C:414:VAL:HA	1:C:430:PRO:HG2	2.01	0.43
1:C:19:ALA:HB2	1:C:492:ALA:HB1	1.99	0.43
1:D:72:ASN:ND2	1:D:72:ASN:C	2.71	0.43
1:B:150:LEU:O	1:B:153:ARG:HG2	2.19	0.43
1:D:183:SER:N	1:D:455:PRO:HD3	2.34	0.43
1:D:497:ARG:O	1:D:501:THR:HB	2.17	0.43
1:C:43:ARG:N	1:C:219:LEU:HD13	2.34	0.43
1:D:72:ASN:HD21	1:D:490:TYR:CB	2.32	0.42
1:C:362:ASN:HD21	1:C:364:SER:CB	2.32	0.42
1:A:130:PHE:CD2	1:A:185:LYS:HE2	2.54	0.42
1:C:230:PRO:C	1:C:232:LYS:H	2.22	0.42
1:D:414:VAL:HA	1:D:430:PRO:HG2	2.01	0.42
1:A:297:VAL:HG23	1:A:376:MET:HE3	2.00	0.42
1:D:157:THR:O	1:D:161:ILE:HG13	2.20	0.42
1:C:126:ALA:HB2	1:C:144:LEU:HD21	2.01	0.42
1:B:437:VAL:HG12	1:B:438:SER:N	2.34	0.42
1:C:99:TYR:H	1:C:108:ASP:HB3	1.83	0.42
1:D:306:TRP:HB3	1:D:406:MET:HE3	2.01	0.42
1:B:169:ARG:C	1:B:171:LEU:N	2.71	0.42
1:C:333:LEU:O	1:C:336:LEU:HB3	2.18	0.42
1:C:255:GLN:HB2	1:C:480:HIS:CG	2.54	0.42
1:C:312:LYS:C	1:C:313:ILE:HG13	2.39	0.42
1:A:298:ILE:HB	1:A:436:ILE:HB	2.01	0.42
1:A:232:LYS:N	1:A:232:LYS:HD3	2.34	0.42
1:A:54:TYR:CE2	1:A:433:ARG:HG3	2.54	0.42
1:D:74:LEU:HD13	1:D:493:TRP:CD1	2.55	0.42
1:C:275:GLN:HA	1:C:276:PRO:HA	1.87	0.42
1:C:32:ILE:HG22	1:C:33:GLN:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:361:VAL:HB	1:A:373:MET:HB3	2.01	0.42
1:C:485:GLY:O	1:C:486:ALA:C	2.57	0.42
1:D:130:PHE:C	1:D:132:GLN:N	2.73	0.42
1:C:157:THR:O	1:C:161:ILE:HG13	2.20	0.42
1:B:57:ARG:HD3	1:B:369:VAL:HG13	2.00	0.42
1:C:54:TYR:CE2	1:C:433:ARG:HG3	2.55	0.42
1:A:150:LEU:O	1:A:153:ARG:HD2	2.20	0.42
1:B:43:ARG:NH1	1:B:43:ARG:HG3	2.34	0.42
1:C:169:ARG:HD2	1:C:179:TRP:CZ2	2.55	0.42
1:D:260:LEU:HD11	1:D:447:ARG:NE	2.35	0.42
1:A:512:HIS:ND1	1:A:512:HIS:C	2.73	0.42
1:D:306:TRP:HE1	1:D:362:ASN:HD21	1.67	0.42
1:C:386:SER:HA	1:C:442:ARG:CZ	2.50	0.42
1:B:154:GLN:HB2	4:B:968:HOH:O	2.20	0.42
1:B:278:LEU:CA	1:B:470:GLN:HE22	2.31	0.42
1:B:113:LEU:HD21	1:B:159:ASP:HB3	2.01	0.42
1:B:361:VAL:HG21	1:B:373:MET:CE	2.50	0.42
1:B:212:PHE:O	1:B:213:PRO:C	2.57	0.42
1:C:460:VAL:HG13	1:C:483:MET:CE	2.49	0.42
1:A:490:TYR:HA	1:A:493:TRP:HB3	2.00	0.42
1:D:354:TRP:CH2	1:D:404:LYS:HG2	2.55	0.42
1:B:444:PRO:O	1:B:447:ARG:NE	2.52	0.42
1:B:404:LYS:HZ1	1:B:407:LYS:NZ	2.18	0.42
1:B:485:GLY:O	1:B:486:ALA:C	2.58	0.42
1:B:72:ASN:HD22	1:B:73:PRO:N	2.15	0.41
1:D:385:GLU:O	1:D:388:ARG:HD2	2.20	0.41
1:D:326:ILE:HG23	1:D:339:MET:HB3	2.02	0.41
1:C:69:THR:HG23	1:C:194:ARG:O	2.19	0.41
1:C:170:TYR:CE1	1:C:171:LEU:HG	2.55	0.41
1:D:312:LYS:HD2	1:D:359:PHE:HZ	1.85	0.41
1:D:8:LYS:N	1:D:245:ASN:CG	2.74	0.41
1:D:84:ASN:HB2	1:D:85:ASP:H	1.49	0.41
1:A:122:MET:HG2	1:A:148:TYR:CG	2.55	0.41
1:B:143:GLN:HA	1:B:143:GLN:NE2	2.35	0.41
1:B:376:MET:HG3	1:B:381:THR:OG1	2.20	0.41
1:C:301:PHE:HE2	1:C:414:VAL:CG1	2.33	0.41
1:B:504:SER:O	1:B:508:LYS:HB2	2.21	0.41
1:A:317:ALA:HA	1:A:354:TRP:O	2.21	0.41
1:A:424:ILE:O	1:A:426:ASN:N	2.52	0.41
1:B:175:HIS:CD2	1:B:182:LEU:HD21	2.56	0.41
1:B:47:ARG:HA	1:B:440:TRP:CZ3	2.55	0.41
1:A:146:MET:HE1	1:A:340:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:189:PHE:O	1:D:189:PHE:CD2	2.73	0.41
1:B:57:ARG:HD2	1:B:59:TYR:OH	2.21	0.41
1:A:339:MET:O	1:A:341:GLU:N	2.48	0.41
1:B:351:VAL:HG12	1:B:352:THR:N	2.35	0.41
1:A:199:LEU:HA	1:A:199:LEU:HD23	1.86	0.41
1:D:399:GLN:HE21	1:D:403:ASN:HD21	1.68	0.41
1:D:173:LEU:HD22	1:D:173:LEU:N	2.36	0.41
1:D:46:GLY:C	1:D:48:LEU:H	2.23	0.41
1:B:432:LEU:HD12	1:B:433:ARG:H	1.85	0.41
1:D:158:ASN:HB3	1:D:324:VAL:HG11	2.01	0.41
1:B:22:LYS:NZ	1:B:493:TRP:CZ2	2.87	0.41
1:A:115:LEU:HA	1:A:118:VAL:CG2	2.50	0.41
1:D:130:PHE:C	1:D:132:GLN:H	2.24	0.41
1:B:454:PHE:N	1:B:454:PHE:CD2	2.87	0.41
1:B:130:PHE:O	1:B:131:HIS:C	2.58	0.41
1:D:89:ARG:HG3	1:D:89:ARG:NH1	2.36	0.41
1:A:184:ALA:O	1:A:185:LYS:C	2.59	0.41
1:A:377:GLN:CD	1:A:377:GLN:H	2.24	0.41
1:A:42:ASP:C	1:A:42:ASP:OD1	2.57	0.41
1:B:126:ALA:CB	1:B:144:LEU:HD21	2.50	0.41
1:A:509:LEU:O	1:A:511:HIS:N	2.53	0.41
1:D:122:MET:HG2	1:D:148:TYR:CD2	2.55	0.41
1:C:181:LEU:O	1:C:455:PRO:HD3	2.20	0.41
1:A:483:MET:HA	1:A:483:MET:HE3	2.03	0.41
1:A:462:MET:HA	1:A:462:MET:HE2	2.02	0.41
1:D:63:ALA:HA	3:D:802:FAD:C4X	2.51	0.41
1:D:113:LEU:HB3	1:D:115:LEU:HG	2.03	0.41
1:B:189:PHE:C	1:B:189:PHE:CD1	2.95	0.41
1:B:290:HIS:O	1:B:291:PHE:HB3	2.21	0.41
1:C:65:TRP:CH2	1:C:361:VAL:HG21	2.55	0.41
1:A:229:GLU:C	1:A:231:SER:H	2.24	0.41
1:A:511:HIS:O	1:A:512:HIS:HB3	2.21	0.41
1:D:52:THR:HA	1:D:57:ARG:O	2.21	0.41
1:A:174:TRP:CZ3	1:A:191:HIS:CD2	3.09	0.41
1:A:106:ARG:HB3	1:A:108:ASP:OD1	2.21	0.41
1:C:259:ASN:ND2	1:C:259:ASN:O	2.51	0.41
1:B:183:SER:HB2	1:B:454:PHE:C	2.41	0.41
1:C:464:VAL:HA	1:C:467:SER:OG	2.19	0.41
1:B:433:ARG:NH1	1:B:433:ARG:HG3	2.36	0.41
1:A:45:GLY:O	1:A:46:GLY:C	2.59	0.41
1:C:174:TRP:CE3	1:C:189:PHE:HZ	2.39	0.41
1:D:43:ARG:HA	4:D:952:HOH:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:259:ASN:O	1:C:262:VAL:HG22	2.21	0.40
1:D:390:ASP:CG	1:D:393:ARG:HB2	2.40	0.40
1:C:222:GLU:CD	1:C:445:TYR:HH	2.24	0.40
1:D:481:THR:O	1:D:498:ARG:NH1	2.52	0.40
1:B:22:LYS:HG2	1:B:493:TRP:NE1	2.36	0.40
1:C:415:ILE:HB	1:C:431:VAL:HG22	2.03	0.40
1:B:45:GLY:O	1:B:48:LEU:HB2	2.21	0.40
1:D:67:HIS:HA	1:D:195:ASN:HD22	1.87	0.40
1:C:27:LEU:CD2	1:C:32:ILE:HG13	2.51	0.40
1:A:46:GLY:C	1:A:48:LEU:H	2.24	0.40
1:A:460:VAL:N	4:A:926:HOH:O	2.54	0.40
1:B:36:LEU:HD11	1:B:244:TYR:CE2	2.56	0.40
1:D:451:SER:OG	1:D:479:GLU:OE2	2.39	0.40
1:D:248:TYR:CD2	1:D:473:ARG:HA	2.56	0.40
1:B:72:ASN:HA	1:B:73:PRO:HD2	1.99	0.40
1:B:325:GLU:H	1:B:325:GLU:HG2	1.52	0.40
1:C:18:ILE:HB	1:C:48:LEU:HD12	2.03	0.40
1:C:201:TYR:O	1:C:204:VAL:HB	2.21	0.40
1:B:259:ASN:ND2	1:B:286:PHE:CD2	2.90	0.40
1:D:36:LEU:HD23	1:D:37:VAL:N	2.36	0.40
1:D:356:GLN:HB2	1:D:357:PRO:HD2	2.03	0.40
1:D:223:VAL:HA	1:D:238:CYS:HA	2.02	0.40
1:A:43:ARG:HG3	1:A:43:ARG:NH1	2.36	0.40
1:C:99:TYR:O	1:C:106:ARG:HA	2.21	0.40
1:C:141:PHE:CD2	1:C:187:THR:HG21	2.57	0.40
1:A:463:VAL:HG21	1:A:483:MET:HE3	2.02	0.40
1:B:72:ASN:ND2	1:B:74:LEU:N	2.69	0.40
1:D:114:LEU:HD22	1:D:117:ILE:HD12	2.02	0.40
1:C:213:PRO:HD2	1:C:216:TRP:CE3	2.57	0.40
1:D:99:TYR:CE2	1:D:167:LEU:HG	2.56	0.40
1:A:418:MET:C	1:A:420:PRO:HD3	2.41	0.40
1:B:496:GLY:O	1:B:498:ARG:N	2.55	0.40
1:B:412:GLU:O	1:B:413:ASP:C	2.60	0.40
1:B:42:ASP:O	1:B:219:LEU:HD13	2.22	0.40
1:A:8:LYS:HD2	1:A:245:ASN:ND2	2.31	0.40
1:B:270:GLY:HA2	3:B:804:FAD:N6A	2.37	0.40
1:D:269:ARG:HH11	1:D:269:ARG:CG	2.34	0.40
1:A:269:ARG:O	1:A:447:ARG:NH2	2.53	0.40
1:B:358:LEU:HB3	1:B:360:PHE:CE1	2.56	0.40
1:D:234:VAL:HG12	1:D:235:THR:N	2.37	0.40
1:C:209:ALA:HA	1:C:212:PHE:CE2	2.56	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	492/513 (96%)	418 (85%)	53 (11%)	21 (4%)	4	5
1	B	486/513 (95%)	420 (86%)	45 (9%)	21 (4%)	4	5
1	C	489/513 (95%)	426 (87%)	49 (10%)	14 (3%)	7	11
1	D	484/513 (94%)	404 (84%)	61 (13%)	19 (4%)	5	6
All	All	1951/2052 (95%)	1668 (86%)	208 (11%)	75 (4%)	5	6

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ILE
1	A	290	HIS
1	A	291	PHE
1	A	420	PRO
1	B	133	HIS
1	B	137	SER
1	B	200	ASN
1	B	289	ILE
1	B	291	PHE
1	B	370	ALA
1	B	420	PRO
1	B	421	ILE
1	B	424	ILE
1	B	449	ALA
1	B	508	LYS
1	C	86	GLY
1	C	131	HIS
1	C	138	ASP
1	C	265	GLU
1	C	420	PRO
1	C	423	ASN
1	D	131	HIS
1	D	132	GLN
1	D	137	SER

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Mol	Chain	Res	Type
1	D	290	HIS
1	D	420	PRO
1	D	471	ASP
1	A	132	GLN
1	A	187	THR
1	A	200	ASN
1	A	266	LYS
1	A	422	GLU
1	A	425	ALA
1	B	131	HIS
1	B	268	LEU
1	B	426	ASN
1	C	136	VAL
1	C	169	ARG
1	D	84	ASN
1	D	200	ASN
1	D	232	LYS
1	D	416	ASP
1	D	424	ILE
1	D	427	ALA
1	A	47	ARG
1	A	350	SER
1	A	391	LYS
1	A	451	SER
1	B	134	LEU
1	B	138	ASP
1	B	232	LYS
1	C	187	THR
1	C	266	LYS
1	D	85	ASP
1	D	233	ASN
1	D	330	ALA
1	A	137	SER
1	A	265	GLU
1	A	340	LEU
1	A	439	ASN
1	A	510	GLU
1	A	512	HIS
1	B	132	GLN
1	B	265	GLU
1	B	413	ASP
1	C	134	LEU

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Mol	Chain	Res	Type
1	C	137	SER
1	D	136	VAL
1	D	185	LYS
1	B	350	SER
1	D	422	GLU
1	A	190	GLY
1	D	380	LEU
1	C	91	VAL
1	C	230	PRO

### 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	439/454 (97%)	417 (95%)	22 (5%)	34	61
1	B	435/454 (96%)	415 (95%)	20 (5%)	37	66
1	C	437/454 (96%)	420 (96%)	17 (4%)	43	74
1	D	433/454 (95%)	412 (95%)	21 (5%)	35	64
All	All	1744/1816 (96%)	1664 (95%)	80 (5%)	37	66

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	118	VAL
1	A	122	MET
1	A	131	HIS
1	A	132	GLN
1	A	177	LEU
1	A	179	TRP
1	A	201	TYR
1	A	203	SER
1	A	221	CYS
1	A	239	GLU
1	A	289	ILE
1	A	341	GLU

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Mol	Chain	Res	Type
1	A	350	SER
1	A	362	ASN
1	A	377	GLN
1	A	388	ARG
1	A	389	GLU
1	A	420	PRO
1	A	428	ASN
1	A	479	GLU
1	A	512	HIS
1	B	22	LYS
1	B	72	ASN
1	B	131	HIS
1	B	179	TRP
1	B	189	PHE
1	B	201	TYR
1	B	214	GLN
1	B	221	CYS
1	B	228	ARG
1	B	255	GLN
1	B	281	VAL
1	B	325	GLU
1	B	333	LEU
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	410	ASP
1	B	420	PRO
1	B	471	ASP
1	B	479	GLU
1	C	112	GLU
1	C	122	MET
1	C	124	LYS
1	C	134	LEU
1	C	138	ASP
1	C	150	LEU
1	C	153	ARG
1	C	179	TRP
1	C	189	PHE
1	C	201	TYR
1	C	221	CYS
1	C	259	ASN
1	C	291	PHE

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Mol	Chain	Res	Type
1	C	377	GLN
1	C	391	LYS
1	C	420	PRO
1	C	479	GLU
1	D	36	LEU
1	D	72	ASN
1	D	80	GLN
1	D	84	ASN
1	D	118	VAL
1	D	122	MET
1	D	143	GLN
1	D	150	LEU
1	D	179	TRP
1	D	189	PHE
1	D	201	TYR
1	D	221	CYS
1	D	271	ARG
1	D	290	HIS
1	D	291	PHE
1	D	316	LEU
1	D	377	GLN
1	D	380	LEU
1	D	420	PRO
1	D	439	ASN
1	D	501	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	80	GLN
1	A	143	GLN
1	A	151	GLN
1	A	192	GLN
1	A	195	ASN
1	A	210	GLN
1	A	237	ASN
1	A	245	ASN
1	A	255	GLN
1	A	318	ASN
1	A	362	ASN
1	A	426	ASN

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Mol	Chain	Res	Type
1	A	434	ASN
1	B	30	ASN
1	B	33	GLN
1	B	72	ASN
1	B	84	ASN
1	B	120	ASN
1	B	143	GLN
1	B	175	HIS
1	B	195	ASN
1	B	245	ASN
1	B	255	GLN
1	B	259	ASN
1	B	329	ASN
1	B	362	ASN
1	B	377	GLN
1	B	434	ASN
1	B	439	ASN
1	C	29	GLN
1	C	80	GLN
1	C	109	HIS
1	C	143	GLN
1	C	195	ASN
1	C	210	GLN
1	C	259	ASN
1	C	290	HIS
1	C	362	ASN
1	C	377	GLN
1	C	439	ASN
1	D	33	GLN
1	D	72	ASN
1	D	120	ASN
1	D	192	GLN
1	D	195	ASN
1	D	210	GLN
1	D	283	GLN
1	D	329	ASN
1	D	362	ASN
1	D	399	GLN
1	D	439	ASN
1	D	480	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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$
3	FAD	A	803	-	58,58,58	1.16	5 (8%)	85,89,89	1.34	8 (9%)
2	SPM	A	924	-	13,13,13	0.92	1 (7%)	12,12,12	0.56	0
3	FAD	B	804	-	58,58,58	1.27	6 (10%)	85,89,89	1.77	17 (20%)
2	SPM	B	923	-	13,13,13	0.95	1 (7%)	12,12,12	0.58	0
3	FAD	C	801	-	58,58,58	1.25	7 (12%)	85,89,89	1.95	14 (16%)
2	SPM	C	921	-	13,13,13	0.96	1 (7%)	12,12,12	0.59	0
3	FAD	D	802	-	58,58,58	1.15	6 (10%)	85,89,89	1.39	11 (12%)
2	SPM	D	922	-	13,13,13	0.96	1 (7%)	12,12,12	0.60	0

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
3	FAD	A	803	-	-	0/34/50/50	0/1/6/6
2	SPM	A	924	-	-	0/11/11/11	0/0/0/0
3	FAD	B	804	-	-	0/34/50/50	0/1/6/6
2	SPM	B	923	-	-	0/11/11/11	0/0/0/0
3	FAD	C	801	-	-	0/34/50/50	0/1/6/6
2	SPM	C	921	-	-	0/11/11/11	0/0/0/0
3	FAD	D	802	-	-	0/34/50/50	0/1/6/6
2	SPM	D	922	-	-	0/11/11/11	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	FAD	C9A-N10	3.44	1.43	1.38
3	B	804	FAD	PA-O3P	3.36	1.66	1.59
3	B	804	FAD	C9A-N10	2.97	1.43	1.38
3	C	801	FAD	C9A-N10	2.78	1.43	1.38
3	C	801	FAD	C5X-N5	2.65	1.39	1.35
3	A	803	FAD	C5X-N5	2.62	1.39	1.35
3	C	801	FAD	C1'-C2'	2.61	1.54	1.51
3	A	803	FAD	C9A-N10	2.61	1.42	1.38
3	C	801	FAD	C2A-N1A	2.53	1.38	1.33
3	A	803	FAD	C2A-N1A	2.53	1.38	1.33
3	C	801	FAD	C1'-N10	2.50	1.51	1.48
3	D	802	FAD	C5X-N5	2.48	1.39	1.35
3	C	801	FAD	C2A-N3A	2.48	1.37	1.32
3	B	804	FAD	C2A-N1A	2.46	1.38	1.33
3	B	804	FAD	C2A-N3A	2.40	1.36	1.32
3	D	802	FAD	C4X-N5	2.37	1.41	1.36
3	D	802	FAD	C2A-N3A	2.23	1.36	1.32
3	B	804	FAD	C1'-N10	2.23	1.50	1.48
2	B	923	SPM	C9-N10	2.13	1.54	1.46
3	B	804	FAD	C5X-N5	2.11	1.38	1.35
3	D	802	FAD	C2A-N1A	2.10	1.38	1.33
2	D	922	SPM	C9-N10	2.10	1.53	1.46
3	C	801	FAD	C5'-C4'	2.10	1.55	1.51
2	A	924	SPM	C9-N10	2.09	1.53	1.46
3	A	803	FAD	C4X-N5	2.09	1.40	1.36
2	C	921	SPM	C9-N10	2.08	1.53	1.46
3	D	802	FAD	C2-N3	2.07	1.41	1.37
3	A	803	FAD	C10-N1	2.02	1.39	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	FAD	O2A-PA-O5B	-6.40	76.25	108.51
3	C	801	FAD	O5B-PA-O1A	6.20	133.67	109.37
3	C	801	FAD	O3P-PA-O1A	-5.30	73.27	111.28
3	C	801	FAD	O2A-PA-O1A	-5.09	83.80	112.21
3	B	804	FAD	C4B-O4B-C1B	-5.06	104.25	109.75
3	D	802	FAD	C2-N1-C10	4.90	119.92	114.98
3	C	801	FAD	C2-N1-C10	4.70	119.71	114.98
3	C	801	FAD	O2A-PA-O3P	4.49	126.43	105.14
3	B	804	FAD	O3P-PA-O5B	-4.49	83.34	103.41
3	D	802	FAD	C4B-O4B-C1B	-4.46	104.91	109.75
3	B	804	FAD	C2-N1-C10	4.41	119.42	114.98
3	B	804	FAD	O4B-C1B-C2B	-4.38	100.05	106.77
3	B	804	FAD	O3P-PA-O1A	-4.34	80.11	111.28
3	A	803	FAD	N3A-C2A-N1A	-4.34	125.08	128.71
3	A	803	FAD	C2-N1-C10	4.24	119.26	114.98
3	B	804	FAD	C4X-N5-C5X	4.08	121.28	116.69
3	C	801	FAD	C4X-N5-C5X	4.07	121.27	116.69
3	C	801	FAD	N3A-C2A-N1A	-4.04	125.33	128.71
3	C	801	FAD	O3P-PA-O5B	-3.95	85.73	103.41
3	B	804	FAD	N3A-C2A-N1A	-3.95	125.40	128.71
3	B	804	FAD	O2A-PA-O3P	-3.83	86.96	105.14
3	A	803	FAD	C4X-C10-N10	-3.82	118.60	120.51
3	D	802	FAD	C4X-N5-C5X	3.75	120.91	116.69
3	D	802	FAD	N3A-C2A-N1A	-3.73	125.59	128.71
3	A	803	FAD	C4X-N5-C5X	3.72	120.88	116.69
3	B	804	FAD	C4X-C10-N10	-3.71	118.66	120.51
3	C	801	FAD	O4B-C1B-C2B	-3.70	101.10	106.77
3	B	804	FAD	O2A-PA-O1A	3.50	131.76	112.21
3	B	804	FAD	O4B-C1B-N9A	3.38	111.59	108.44
3	A	803	FAD	C4B-O4B-C1B	-3.02	106.47	109.75
3	A	803	FAD	O4B-C1B-C2B	-2.83	102.44	106.77
3	C	801	FAD	C4B-O4B-C1B	-2.80	106.71	109.75
3	D	802	FAD	O4B-C1B-C2B	-2.76	102.54	106.77
3	C	801	FAD	C1'-N10-C9A	2.71	121.50	118.87
3	D	802	FAD	C1'-N10-C9A	2.64	121.44	118.87
3	B	804	FAD	O3'-C3'-C4'	-2.64	102.06	108.74
3	D	802	FAD	C5'-C4'-C3'	-2.59	107.17	112.06
3	D	802	FAD	C4X-C10-N10	-2.52	119.25	120.51
3	A	803	FAD	C5X-C9A-N10	2.52	119.29	116.80
3	B	804	FAD	C5X-C9A-N10	2.50	119.26	116.80
3	D	802	FAD	O3'-C3'-C4'	-2.36	102.77	108.74
3	C	801	FAD	O3'-C3'-C4'	-2.31	102.91	108.74
3	B	804	FAD	C4'-C3'-C2'	2.25	118.34	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	FAD	O3'-C3'-C4'	-2.23	103.09	108.74
3	D	802	FAD	C5X-C9A-N10	2.23	119.00	116.80
3	B	804	FAD	C1'-N10-C9A	2.12	120.93	118.87
3	B	804	FAD	C5'-C4'-C3'	-2.08	108.14	112.06
3	B	804	FAD	P-O3P-PA	2.07	137.76	131.68
3	C	801	FAD	C5X-C9A-N10	2.07	118.84	116.80
3	D	802	FAD	N3A-C4A-N9A	2.01	129.07	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	498/513 (97%)	-0.48	7 (1%)	72 72	20, 38, 63, 93	22 (4%)
1	B	492/513 (95%)	-0.45	4 (0%)	83 85	18, 37, 61, 79	37 (7%)
1	C	495/513 (96%)	-0.47	4 (0%)	83 85	19, 36, 63, 87	33 (6%)
1	D	490/513 (95%)	-0.39	13 (2%)	52 49	18, 40, 68, 92	34 (6%)
All	All	1975/2052 (96%)	-0.45	28 (1%)	72 72	18, 38, 65, 93	126 (6%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	ASN	5.2
1	D	134	LEU	3.9
1	B	135	GLY	3.7
1	A	424	ILE	3.5
1	B	425	ALA	3.3
1	D	232	LYS	3.3
1	D	426	ASN	3.2
1	A	425	ALA	3.1
1	B	267	ASN	3.0
1	D	230	PRO	2.9
1	D	425	ALA	2.6
1	C	415	ILE	2.6
1	C	423	ASN	2.6
1	D	137	SER	2.5
1	D	245	ASN	2.5
1	D	423	ASN	2.3
1	A	230	PRO	2.3
1	D	420	PRO	2.3
1	A	290	HIS	2.2
1	A	422	GLU	2.2
1	D	133	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	227	THR	2.1
1	C	420	PRO	2.1
1	B	421	ILE	2.1
1	A	6	PRO	2.0
1	D	231	SER	2.0
1	C	419	ARG	2.0
1	D	290	HIS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FAD	C	801	53/53	0.16	0.88	20,28,40,44	0
3	FAD	A	803	53/53	0.14	0.10	27,32,36,37	0
3	FAD	B	804	53/53	0.13	-0.11	23,32,40,41	0
3	FAD	D	802	53/53	0.12	-0.23	28,34,39,39	0
2	SPM	C	921	14/14	-	-	175,178,181,181	14
2	SPM	D	922	14/14	-	-	161,165,169,169	14
2	SPM	B	923	14/14	-	-	134,138,142,142	14
2	SPM	A	924	14/14	-	-	142,144,145,145	14

## 6.5 Other polymers ⓘ

There are no such residues in this entry.