



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:34 PM 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 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

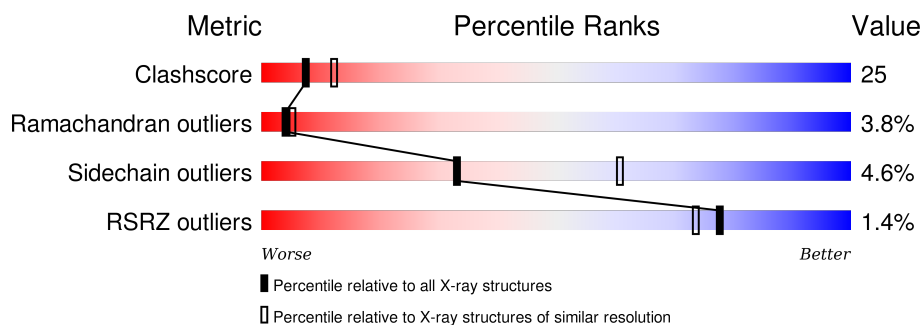
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	 55% 38% . . .
1	B	513	 49% 43% . .
1	C	513	 54% 39% . .
1	D	513	 50% 41% . . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16332 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.

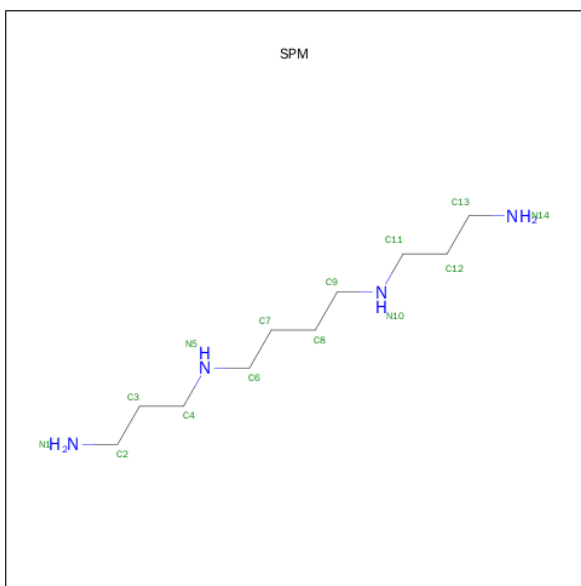
- Molecule 1 is a protein called FMS1 protein.

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		

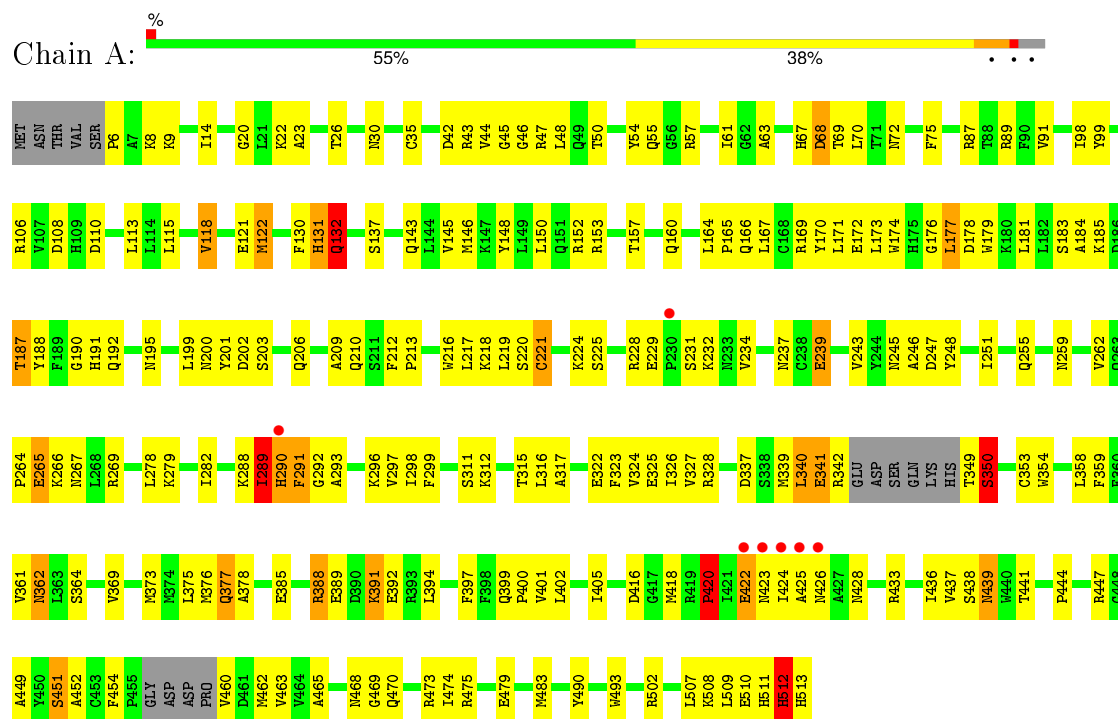
- Molecule 4 is water.

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		

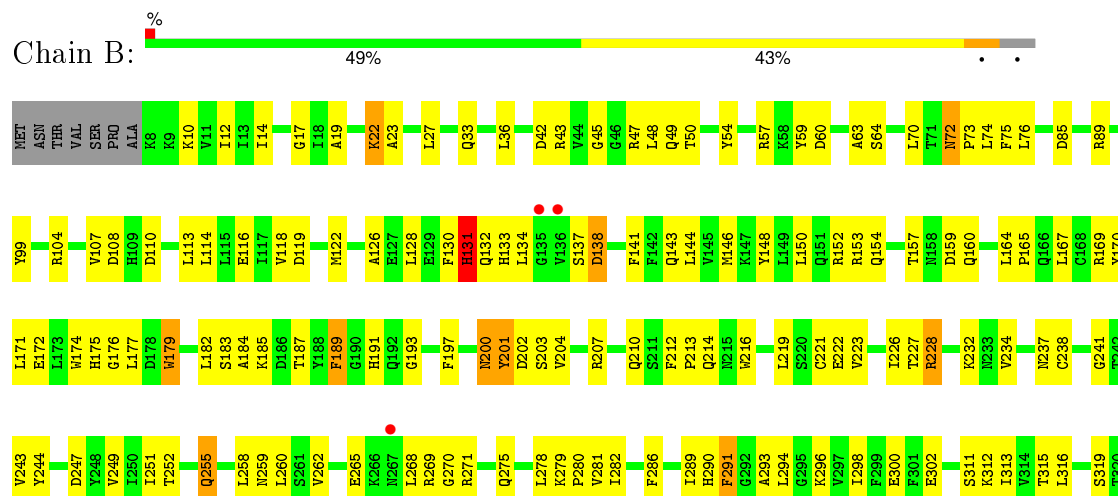
3 Residue-property plots

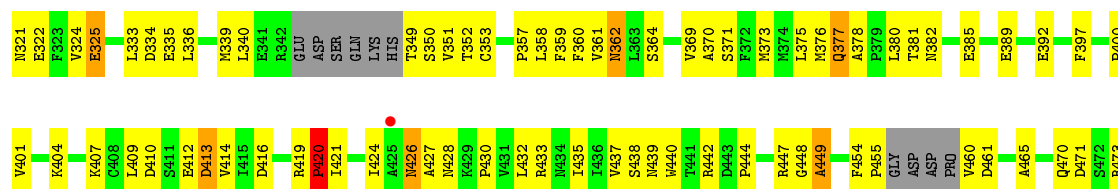
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

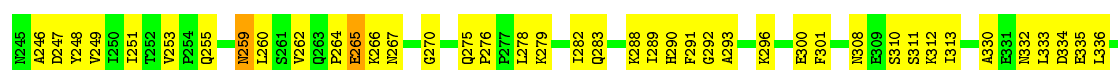
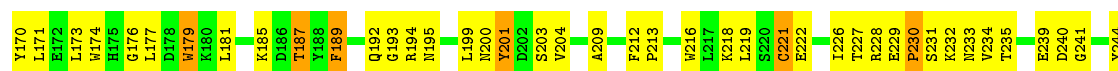
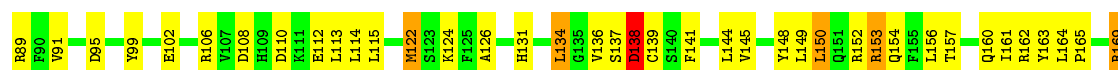
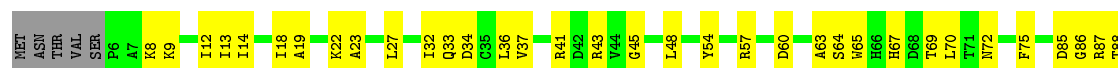


• Molecule 1: FMS1 protein

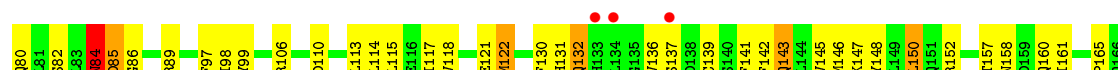


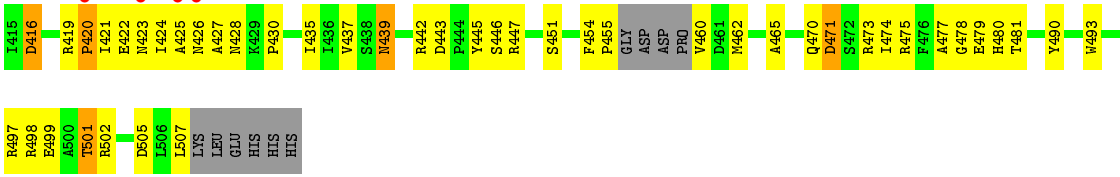


• Molecule 1: FMS1 protein



• Molecule 1: FMS1 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.309 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
2	A	14	0	26	0	0
2	B	14	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 25.

All (778) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:THR:HG22	1:D:477:ALA:HB3	1.70	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	3	4
1	B	486/513 (95%)	420 (86%)	45 (9%)	21 (4%)	3	4
1	C	489/513 (95%)	426 (87%)	49 (10%)	14 (3%)	6	9
1	D	484/513 (94%)	404 (84%)	61 (13%)	19 (4%)	4	5
All	All	1951/2052 (95%)	1668 (86%)	208 (11%)	75 (4%)	4	5

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
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

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Mol	Chain	Res	Type
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
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%)	30	56
1	B	435/454 (96%)	415 (95%)	20 (5%)	33	61
1	C	437/454 (96%)	420 (96%)	17 (4%)	39	68
1	D	433/454 (95%)	412 (95%)	21 (5%)	31	58
All	All	1744/1816 (96%)	1664 (95%)	80 (5%)	33	61

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [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](#)

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	-	48,58,58	1.40	7 (14%)	54,89,89	2.11	10 (18%)
2	SPM	A	924	-	13,13,13	0.95	1 (7%)	12,12,12	0.56	0
3	FAD	B	804	-	48,58,58	1.43	8 (16%)	54,89,89	2.54	12 (22%)
2	SPM	B	923	-	13,13,13	0.98	1 (7%)	12,12,12	0.60	0
3	FAD	C	801	-	48,58,58	1.43	9 (18%)	54,89,89	2.72	13 (24%)
2	SPM	C	921	-	13,13,13	0.98	1 (7%)	12,12,12	0.59	0
3	FAD	D	802	-	48,58,58	1.45	6 (12%)	54,89,89	2.16	11 (20%)
2	SPM	D	922	-	13,13,13	0.99	1 (7%)	12,12,12	0.61	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	-	-	0/30/50/50	0/6/6/6
2	SPM	A	924	-	-	0/11/11/11	0/0/0/0
3	FAD	B	804	-	-	0/30/50/50	0/6/6/6
2	SPM	B	923	-	-	0/11/11/11	0/0/0/0
3	FAD	C	801	-	-	0/30/50/50	0/6/6/6
2	SPM	C	921	-	-	0/11/11/11	0/0/0/0
3	FAD	D	802	-	-	0/30/50/50	0/6/6/6
2	SPM	D	922	-	-	0/11/11/11	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	FAD	C5X-N5	2.01	1.38	1.35
3	A	803	FAD	C2A-N3A	2.03	1.35	1.32
2	C	921	SPM	C9-N10	2.14	1.53	1.46
2	A	924	SPM	C9-N10	2.15	1.53	1.46
2	D	922	SPM	C9-N10	2.16	1.53	1.46
3	B	804	FAD	C1'-N10	2.16	1.50	1.48
2	B	923	SPM	C9-N10	2.18	1.54	1.46
3	D	802	FAD	C2A-N1A	2.19	1.38	1.33
3	C	801	FAD	C5'-C4'	2.19	1.55	1.51
3	A	803	FAD	C10-N1	2.19	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	FAD	C4-N3	2.36	1.37	1.33
3	D	802	FAD	C5X-N5	2.37	1.39	1.35
3	C	801	FAD	C1'-N10	2.46	1.51	1.48
3	D	802	FAD	C2A-N3A	2.48	1.36	1.32
3	A	803	FAD	C5X-N5	2.51	1.39	1.35
3	C	801	FAD	C5X-N5	2.54	1.39	1.35
3	C	801	FAD	C10-N10	2.55	1.42	1.39
3	B	804	FAD	C2A-N1A	2.56	1.38	1.33
3	A	803	FAD	C2A-N1A	2.63	1.38	1.33
3	C	801	FAD	C2A-N1A	2.63	1.38	1.33
3	B	804	FAD	C2A-N3A	2.67	1.36	1.32
3	B	804	FAD	C10-N10	2.69	1.42	1.39
3	C	801	FAD	C2A-N3A	2.76	1.37	1.32
3	A	803	FAD	C9A-N10	2.84	1.42	1.38
3	C	801	FAD	C9A-N10	3.03	1.43	1.38
3	B	804	FAD	C9A-N10	3.22	1.43	1.38
3	A	803	FAD	C4-N3	3.22	1.39	1.33
3	B	804	FAD	C4-N3	3.31	1.39	1.33
3	D	802	FAD	C4-N3	3.34	1.39	1.33
3	C	801	FAD	C4X-N5	3.59	1.39	1.33
3	B	804	FAD	C4X-N5	3.63	1.39	1.33
3	D	802	FAD	C9A-N10	3.73	1.43	1.38
3	A	803	FAD	C4X-N5	4.57	1.40	1.33
3	D	802	FAD	C4X-N5	4.95	1.41	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	804	FAD	O3P-PA-O5B	-7.39	83.34	102.94
3	C	801	FAD	O3P-PA-O5B	-6.49	85.73	102.94
3	C	801	FAD	O2A-PA-O5B	-6.39	76.25	108.46
3	C	801	FAD	O2A-PA-O1A	-5.30	83.80	112.53
3	A	803	FAD	N3A-C2A-N1A	-4.98	125.08	128.89
3	B	804	FAD	C4B-O4B-C1B	-4.97	104.25	109.72
3	B	804	FAD	C4X-C4-N3	-4.86	116.95	123.59
3	C	801	FAD	C4X-C4-N3	-4.85	116.95	123.59
3	D	802	FAD	C4X-C4-N3	-4.78	117.06	123.59
3	C	801	FAD	N3A-C2A-N1A	-4.65	125.33	128.89
3	B	804	FAD	N3A-C2A-N1A	-4.56	125.40	128.89
3	A	803	FAD	C4X-C4-N3	-4.46	117.49	123.59
3	D	802	FAD	C4B-O4B-C1B	-4.38	104.91	109.72
3	D	802	FAD	N3A-C2A-N1A	-4.32	125.59	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	804	FAD	O2A-PA-O3P	-4.00	86.96	105.09
3	A	803	FAD	C4X-C10-N10	-3.25	118.60	120.52
3	B	804	FAD	C4X-C10-N10	-3.16	118.66	120.52
3	D	802	FAD	C4-C4X-C10	-3.02	118.01	119.94
3	A	803	FAD	C4B-O4B-C1B	-2.95	106.47	109.72
3	C	801	FAD	C4B-O4B-C1B	-2.74	106.71	109.72
3	B	804	FAD	O3'-C3'-C4'	-2.65	102.06	108.75
3	A	803	FAD	C4-C4X-C10	-2.64	118.25	119.94
3	D	802	FAD	O3'-C3'-C4'	-2.37	102.77	108.75
3	C	801	FAD	O3'-C3'-C4'	-2.32	102.91	108.75
3	A	803	FAD	O3'-C3'-C4'	-2.24	103.09	108.75
3	D	802	FAD	C4X-C10-N10	-2.15	119.25	120.52
3	A	803	FAD	C9A-C5X-N5	-2.06	119.31	122.36
3	B	804	FAD	O3P-P-O5'	2.05	108.36	102.94
3	D	802	FAD	O3P-P-O5'	2.12	108.56	102.94
3	B	804	FAD	C5X-C9A-N10	2.16	119.26	117.62
3	A	803	FAD	C5X-C9A-N10	2.19	119.29	117.62
3	D	802	FAD	C4-C4X-N5	2.28	121.49	118.72
3	D	802	FAD	C1'-N10-C9A	2.30	121.44	118.86
3	C	801	FAD	C1'-N10-C9A	2.35	121.50	118.86
3	C	801	FAD	O3P-P-O5'	2.63	109.91	102.94
3	B	804	FAD	O2A-PA-O1A	3.55	131.76	112.53
3	A	803	FAD	C4X-N5-C5X	3.57	120.88	116.76
3	D	802	FAD	C4X-N5-C5X	3.60	120.91	116.76
3	C	801	FAD	C4X-N5-C5X	3.91	121.27	116.76
3	B	804	FAD	C4X-N5-C5X	3.92	121.28	116.76
3	C	801	FAD	O2A-PA-O3P	4.70	126.43	105.09
3	C	801	FAD	O5B-PA-O1A	6.20	133.67	109.62
3	C	801	FAD	C4-N3-C2	10.24	124.09	115.25
3	A	803	FAD	C4-N3-C2	10.40	124.23	115.25
3	D	802	FAD	C4-N3-C2	10.54	124.36	115.25
3	B	804	FAD	C4-N3-C2	10.75	124.54	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	FAD	3	0
3	B	804	FAD	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	FAD	1	0
3	D	802	FAD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/513 (97%)	-0.49	7 (1%) 78 74	20, 38, 63, 93	22 (4%)
1	B	492/513 (95%)	-0.46	4 (0%) 87 85	18, 37, 61, 79	37 (7%)
1	C	495/513 (96%)	-0.49	4 (0%) 87 85	19, 36, 63, 87	33 (6%)
1	D	490/513 (95%)	-0.40	12 (2%) 62 56	18, 40, 68, 92	34 (6%)
All	All	1975/2052 (96%)	-0.46	27 (1%) 78 74	18, 38, 65, 93	126 (6%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	ASN	5.3
1	D	134	LEU	4.1
1	A	425	ALA	3.9
1	B	135	GLY	3.9
1	D	232	LYS	3.8
1	D	426	ASN	3.6
1	A	424	ILE	3.6
1	B	425	ALA	3.5
1	D	230	PRO	3.0
1	D	133	HIS	2.8
1	D	137	SER	2.8
1	D	423	ASN	2.7
1	B	267	ASN	2.6
1	C	423	ASN	2.6
1	D	425	ALA	2.5
1	A	230	PRO	2.5
1	D	245	ASN	2.4
1	D	227	THR	2.3
1	D	420	PRO	2.2
1	C	415	ILE	2.2
1	C	425	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	422	GLU	2.1
1	A	426	ASN	2.1
1	D	267	ASN	2.0
1	B	136	VAL	2.0
1	A	290	HIS	2.0
1	C	419	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FAD	C	801	53/53	0.97	0.16	1.12	20,28,40,44	0
3	FAD	A	803	53/53	0.97	0.14	0.00	27,32,36,37	0
3	FAD	D	802	53/53	0.97	0.12	-0.17	28,34,39,39	0
3	FAD	B	804	53/53	0.96	0.13	-0.18	23,32,40,41	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 [i](#)

There are no such residues in this entry.