



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:12 AM GMT

PDB ID : 2ZXH
Title : Structure of Aquifex aeolicus GidA in the form I crystal
Authors : Numata, T.; Osawa, T.
Deposited on : 2008-12-24
Resolution : 3.20 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

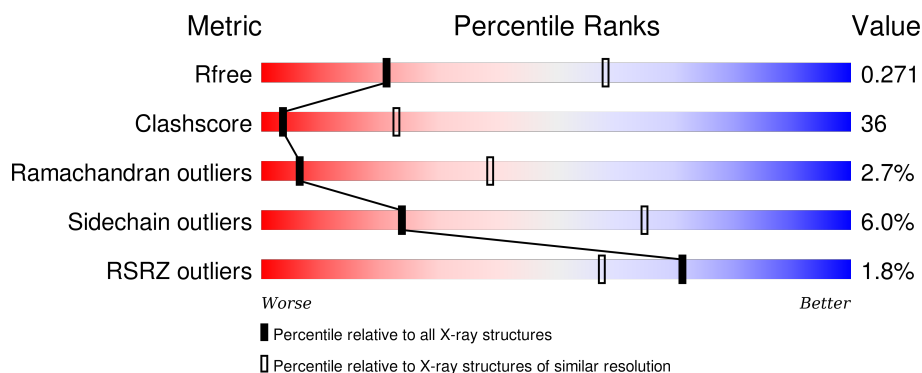
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	637	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 46%, green 44%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 46% 44% • 5% </div> </div>
1	B	637	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 49%, green 40%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 40% 49% • 6% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9714 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4804	3080	816	893	15			
1	B	601	Total	C	N	O	S	0	0	0
			4789	3070	813	891	15			

There are 40 discrepancies between the modelled and reference sequences:

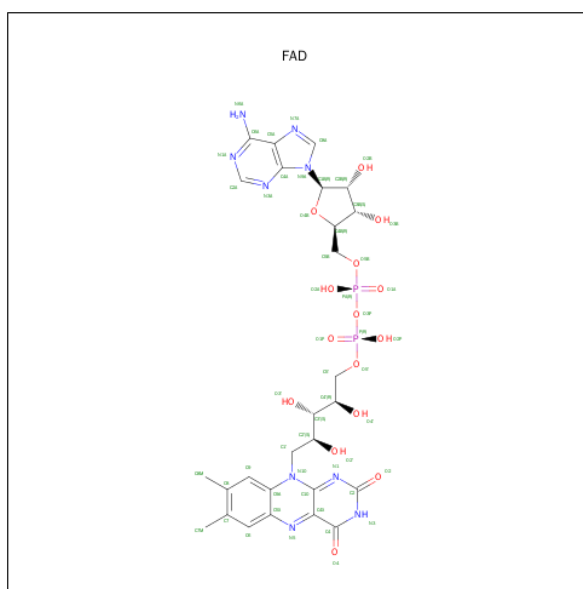
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O66962
A	-18	GLY	-	EXPRESSION TAG	UNP O66962
A	-17	SER	-	EXPRESSION TAG	UNP O66962
A	-16	SER	-	EXPRESSION TAG	UNP O66962
A	-15	HIS	-	EXPRESSION TAG	UNP O66962
A	-14	HIS	-	EXPRESSION TAG	UNP O66962
A	-13	HIS	-	EXPRESSION TAG	UNP O66962
A	-12	HIS	-	EXPRESSION TAG	UNP O66962
A	-11	HIS	-	EXPRESSION TAG	UNP O66962
A	-10	HIS	-	EXPRESSION TAG	UNP O66962
A	-9	SER	-	EXPRESSION TAG	UNP O66962
A	-8	SER	-	EXPRESSION TAG	UNP O66962
A	-7	GLY	-	EXPRESSION TAG	UNP O66962
A	-6	LEU	-	EXPRESSION TAG	UNP O66962
A	-5	VAL	-	EXPRESSION TAG	UNP O66962
A	-4	PRO	-	EXPRESSION TAG	UNP O66962
A	-3	ALA	-	EXPRESSION TAG	UNP O66962
A	-2	GLY	-	EXPRESSION TAG	UNP O66962
A	-1	SER	-	EXPRESSION TAG	UNP O66962
A	0	HIS	-	EXPRESSION TAG	UNP O66962
B	-19	MET	-	EXPRESSION TAG	UNP O66962
B	-18	GLY	-	EXPRESSION TAG	UNP O66962
B	-17	SER	-	EXPRESSION TAG	UNP O66962
B	-16	SER	-	EXPRESSION TAG	UNP O66962

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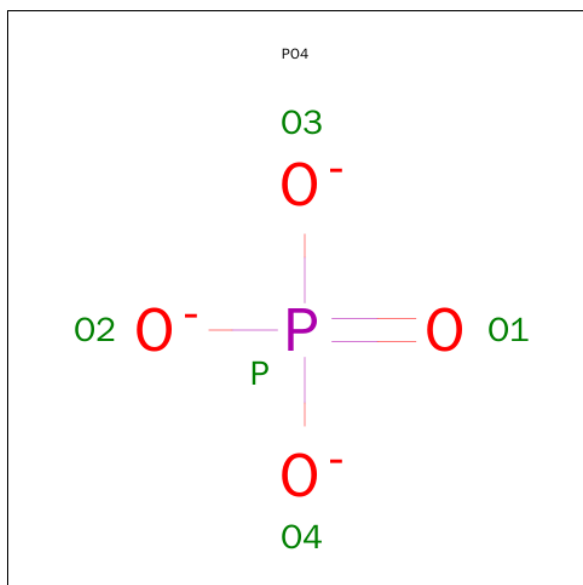
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP O66962
B	-14	HIS	-	EXPRESSION TAG	UNP O66962
B	-13	HIS	-	EXPRESSION TAG	UNP O66962
B	-12	HIS	-	EXPRESSION TAG	UNP O66962
B	-11	HIS	-	EXPRESSION TAG	UNP O66962
B	-10	HIS	-	EXPRESSION TAG	UNP O66962
B	-9	SER	-	EXPRESSION TAG	UNP O66962
B	-8	SER	-	EXPRESSION TAG	UNP O66962
B	-7	GLY	-	EXPRESSION TAG	UNP O66962
B	-6	LEU	-	EXPRESSION TAG	UNP O66962
B	-5	VAL	-	EXPRESSION TAG	UNP O66962
B	-4	PRO	-	EXPRESSION TAG	UNP O66962
B	-3	ALA	-	EXPRESSION TAG	UNP O66962
B	-2	GLY	-	EXPRESSION TAG	UNP O66962
B	-1	SER	-	EXPRESSION TAG	UNP O66962
B	0	HIS	-	EXPRESSION TAG	UNP O66962

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

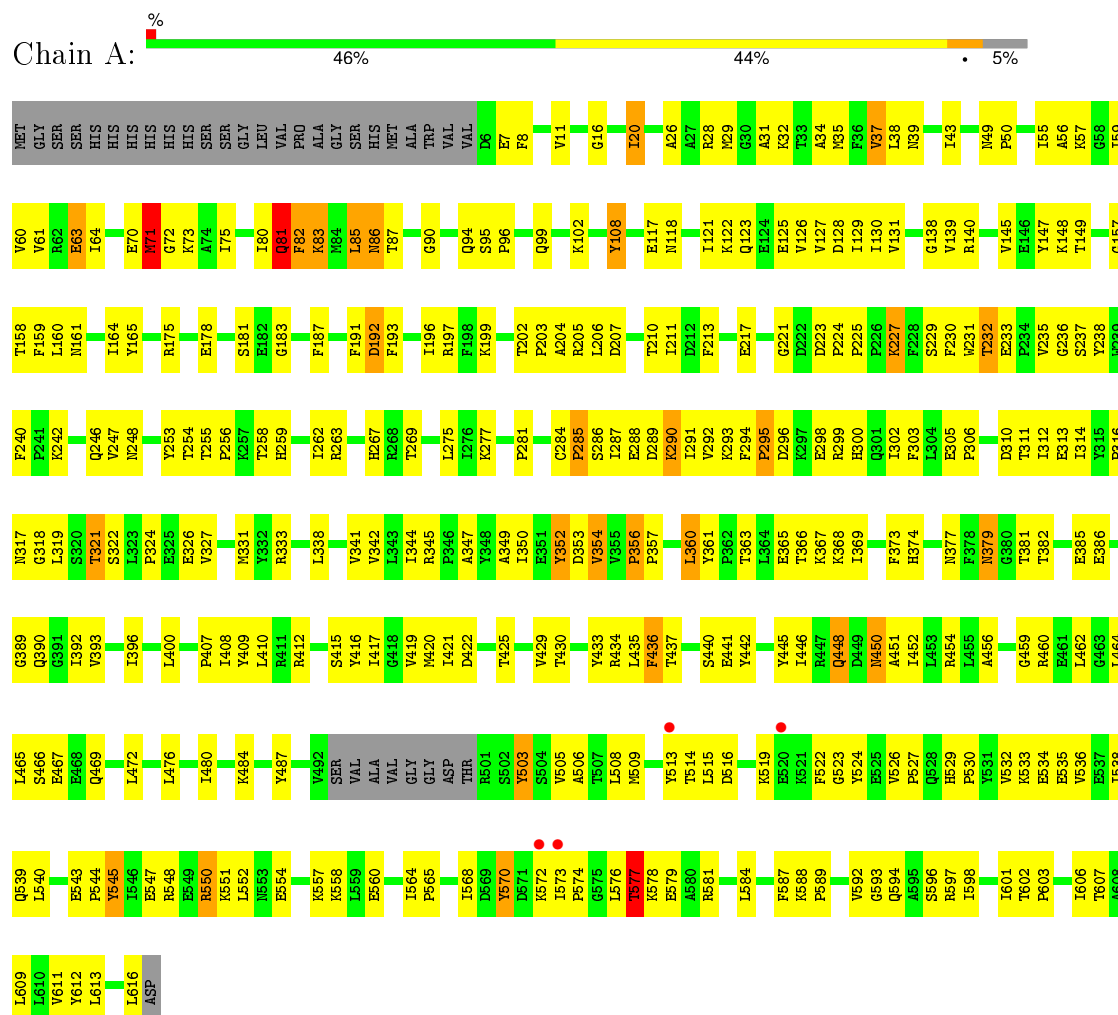


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

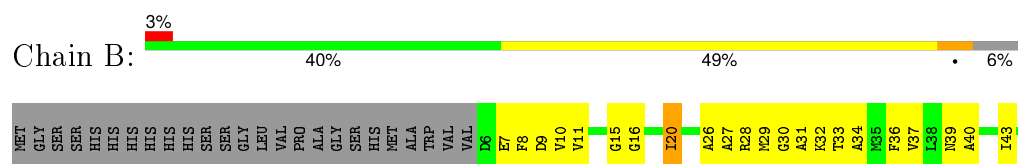
3 Residue-property plots

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: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG



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4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.64Å 213.27Å 231.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.20 40.70 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.97-3.20) 99.5 (40.70-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.18Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.242 , 0.271 0.247 , 0.271	Depositor DCC
R_{free} test set	1998 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 78473 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9714	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: PO4, 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	0.43	0/4904	0.66	0/6624
1	B	0.43	0/4889	0.65	0/6605
All	All	0.43	0/9793	0.65	0/13229

There are no bond length outliers.

There are no bond angle outliers.

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	4804	0	4871	321	0
1	B	4789	0	4854	381	1
2	A	53	0	31	4	0
2	B	53	0	31	2	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
All	All	9714	0	9787	696	1

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 36.

All (696) 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:B:20:ILE:HG21	1:B:109:MET:HE3	1.35	1.08
1:B:466:SER:HB3	1:B:469:GLN:HG3	1.32	1.06
1:B:480:ILE:HD13	1:B:535:GLU:HG2	1.44	1.00
1:A:311:THR:HG22	1:A:313:GLU:H	1.26	0.97
1:B:311:THR:HG22	1:B:313:GLU:H	1.30	0.94
1:B:7:GLU:HG2	1:B:148:LYS:HB2	1.52	0.91
1:B:87:THR:HA	1:B:94:GLN:HE21	1.36	0.90
1:B:254:THR:HG23	1:B:302:ILE:HD11	1.53	0.90
1:A:254:THR:HG23	1:A:302:ILE:HD11	1.55	0.88
1:B:211:ILE:HB	1:B:213:PHE:CE1	2.09	0.88
1:A:29:MET:HE1	1:A:396:ILE:HA	1.53	0.88
1:B:478:ARG:HH12	1:B:482:LYS:HE2	1.40	0.85
1:B:362:PRO:HG2	1:B:594:GLN:HE22	1.42	0.84
1:A:127:VAL:HG13	1:A:183:GLY:HA3	1.58	0.83
1:B:210:THR:HG21	1:B:342:VAL:HG23	1.59	0.83
1:A:225:PRO:HG2	1:A:240:PHE:HB2	1.60	0.82
1:A:87:THR:HA	1:A:94:GLN:HE21	1.45	0.81
1:B:257:LYS:O	1:B:260:GLU:HG2	1.80	0.81
1:B:508:LEU:HA	1:B:511:MET:HE3	1.64	0.80
1:A:302:ILE:HD13	1:A:319:LEU:HD11	1.65	0.79
1:B:10:VAL:HG23	1:B:33:THR:HG23	1.64	0.78
1:B:466:SER:H	1:B:469:GLN:HE21	1.31	0.78
1:B:8:PHE:CE2	1:B:34:ALA:HB2	2.19	0.78
1:B:483:TRP:HE1	1:B:528:GLN:HE21	1.32	0.77
1:B:20:ILE:HG21	1:B:109:MET:CE	2.13	0.77
1:B:412:ARG:HD2	1:B:597:ARG:NH1	2.00	0.77
1:B:29:MET:HE1	1:B:396:ILE:HG12	1.66	0.77
1:A:122:LYS:HZ3	1:A:147:TYR:HE2	1.33	0.77
1:A:357:PRO:O	1:A:360:LEU:HD12	1.86	0.76
1:A:392:ILE:O	1:A:396:ILE:HG13	1.84	0.76
1:A:287:ILE:HD12	1:A:290:LYS:HD2	1.69	0.75
1:B:362:PRO:CG	1:B:594:GLN:HE22	1.98	0.75
1:A:7:GLU:HG2	1:A:148:LYS:HB2	1.68	0.75
1:B:505:VAL:HA	1:B:508:LEU:HG	1.69	0.75
1:B:224:PRO:HD3	1:B:242:LYS:HE2	1.68	0.75
1:B:476:LEU:O	1:B:480:ILE:HG13	1.87	0.74
1:A:210:THR:HG21	1:A:342:VAL:HG23	1.68	0.74
1:A:71:MET:HE1	1:A:385:GLU:HG3	1.68	0.74
1:B:221:GLY:HA3	1:B:246:GLN:OE1	1.88	0.73
1:A:122:LYS:NZ	1:A:147:TYR:HE2	1.87	0.73
1:B:329:TRP:CD1	1:B:343:LEU:HD12	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HZ3	1:B:436:PHE:HE1	1.35	0.73
1:A:29:MET:HE1	1:A:396:ILE:HG12	1.71	0.73
1:B:565:PRO:HB2	1:B:568:ILE:HG23	1.69	0.73
1:A:161:ASN:O	1:A:197:ARG:NH2	2.21	0.73
1:B:8:PHE:CD2	1:B:34:ALA:HB2	2.23	0.73
1:A:360:LEU:HD21	1:A:374:HIS:HB2	1.71	0.73
1:A:324:PRO:HB2	1:A:327:VAL:HG23	1.71	0.72
1:B:10:VAL:HG12	1:B:151:ALA:HB3	1.71	0.72
1:B:545:TYR:H	1:B:545:TYR:HD1	1.36	0.72
1:B:573:ILE:HA	1:B:612:TYR:HD1	1.54	0.72
1:A:311:THR:HG22	1:A:313:GLU:N	2.03	0.72
1:A:476:LEU:O	1:A:480:ILE:HG13	1.90	0.72
1:A:505:VAL:HA	1:A:508:LEU:HD12	1.71	0.71
1:B:329:TRP:HD1	1:B:343:LEU:HD12	1.55	0.71
1:B:483:TRP:CZ2	1:B:527:PRO:HA	2.24	0.71
1:A:386:GLU:HG3	1:A:435:LEU:HG	1.72	0.71
1:B:594:GLN:HA	1:B:597:ARG:NH2	2.06	0.71
1:A:211:ILE:HB	1:A:213:PHE:CE1	2.25	0.71
1:B:32:LYS:HZ1	1:B:120:TYR:HE1	1.38	0.70
1:A:275:LEU:HD11	1:B:441:GLU:HG3	1.72	0.70
1:A:363:THR:HG22	1:A:408:ILE:O	1.89	0.70
1:A:160:LEU:HB3	1:A:353:ASP:HB2	1.72	0.70
1:B:37:VAL:HG12	1:B:39:ASN:H	1.57	0.70
1:A:505:VAL:O	1:A:508:LEU:HB2	1.91	0.69
1:B:55:ILE:HG22	1:B:56:ALA:N	2.07	0.69
1:B:472:LEU:O	1:B:476:LEU:HG	1.92	0.69
1:B:476:LEU:HD22	1:B:529:HIS:NE2	2.07	0.69
1:B:412:ARG:HD2	1:B:597:ARG:HH11	1.55	0.69
1:A:420:MET:HG3	1:A:433:TYR:HE1	1.57	0.69
1:A:565:PRO:HB2	1:A:568:ILE:HG23	1.75	0.69
1:A:476:LEU:HD21	1:A:529:HIS:CE1	2.27	0.68
1:A:85:LEU:HD23	1:A:86:ASN:H	1.58	0.68
1:B:70:GLU:O	1:B:72:GLY:N	2.26	0.68
1:B:207:ASP:OD1	1:B:312:ILE:HD12	1.94	0.68
1:B:466:SER:H	1:B:469:GLN:NE2	1.91	0.68
1:B:138:GLY:HA2	1:B:149:THR:HG22	1.75	0.68
1:B:478:ARG:NH1	1:B:482:LYS:HE2	2.09	0.68
1:A:313:GLU:HG2	1:A:344:ILE:HD12	1.75	0.68
1:A:589:PRO:HG3	1:A:598:ILE:HD11	1.76	0.68
1:B:521:LYS:C	1:B:522:PHE:HD2	1.96	0.67
1:A:603:PRO:O	1:A:606:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:PRO:HA	1:B:339:GLU:OE2	1.94	0.67
1:B:204:ALA:N	1:B:347:ALA:HB2	2.08	0.67
1:A:480:ILE:HD13	1:A:535:GLU:HG2	1.75	0.66
1:B:382:THR:OG1	1:B:432:PRO:HB3	1.95	0.66
1:B:480:ILE:HG23	1:B:536:VAL:HG23	1.77	0.66
1:B:450:ASN:HD22	1:B:451:ALA:N	1.93	0.66
1:B:225:PRO:HG2	1:B:240:PHE:HB2	1.77	0.66
1:A:381:THR:HG21	1:A:390:GLN:NE2	2.10	0.66
1:B:211:ILE:HB	1:B:213:PHE:HE1	1.59	0.66
1:A:545:TYR:H	1:A:545:TYR:HD1	1.43	0.66
1:A:70:GLU:O	1:A:72:GLY:N	2.28	0.65
1:A:420:MET:HG3	1:A:433:TYR:CE1	2.29	0.65
1:A:37:VAL:O	1:A:123:GLN:HA	1.96	0.65
1:B:37:VAL:HG12	1:B:39:ASN:N	2.12	0.65
1:B:60:VAL:HG21	1:B:435:LEU:CD1	2.27	0.65
1:A:247:VAL:HG12	1:A:248:ASN:N	2.12	0.65
1:A:367:LYS:NZ	1:A:587:PHE:HA	2.11	0.65
1:B:29:MET:HE1	1:B:396:ILE:HA	1.79	0.64
1:B:206:LEU:HD23	1:B:343:LEU:HD23	1.78	0.64
1:A:357:PRO:HG3	1:A:379:ASN:O	1.97	0.64
1:A:294:PHE:N	1:A:295:PRO:HD3	2.13	0.64
1:B:87:THR:HG22	1:B:94:GLN:NE2	2.13	0.64
1:A:71:MET:HE1	1:A:385:GLU:HA	1.80	0.64
1:B:362:PRO:HG2	1:B:594:GLN:NE2	2.12	0.64
1:A:568:ILE:HD11	1:A:570:TYR:CE1	2.33	0.64
1:B:573:ILE:HG12	1:B:612:TYR:CD1	2.33	0.64
1:B:452:ILE:O	1:B:456:ALA:HB2	1.98	0.64
1:B:191:PHE:O	1:B:192:ASP:HB2	1.98	0.64
1:A:204:ALA:N	1:A:347:ALA:HB2	2.12	0.64
1:B:90:GLY:O	1:B:94:GLN:HG3	1.98	0.64
1:B:328:GLN:O	1:B:332:TYR:HD2	1.81	0.63
1:A:130:ILE:HD12	1:A:130:ILE:N	2.13	0.63
1:B:59:ILE:HG12	1:B:448:GLN:HB3	1.81	0.63
1:B:67:LEU:HD21	1:B:458:LEU:HD23	1.81	0.63
1:A:448:GLN:O	1:A:448:GLN:NE2	2.31	0.63
1:A:434:ARG:HH11	1:A:434:ARG:HG2	1.63	0.63
1:B:52:ILE:HD12	1:B:71:MET:CE	2.28	0.63
1:A:60:VAL:HG21	1:A:435:LEU:CD1	2.28	0.63
1:A:8:PHE:O	1:A:149:THR:HA	1.99	0.63
1:B:360:LEU:O	1:B:367:LYS:HE3	1.99	0.63
1:B:466:SER:HB3	1:B:469:GLN:CG	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ILE:HD11	1:B:473:VAL:HG21	1.80	0.62
1:B:37:VAL:O	1:B:123:GLN:HA	1.99	0.62
1:B:311:THR:HG22	1:B:313:GLU:N	2.09	0.62
1:A:57:LYS:HB3	1:A:385:GLU:HG2	1.82	0.62
1:B:492:VAL:O	1:B:492:VAL:HG12	1.97	0.62
1:A:60:VAL:O	1:A:64:ILE:HG13	2.00	0.62
1:B:247:VAL:HG12	1:B:248:ASN:N	2.14	0.62
1:B:275:LEU:HD22	1:B:275:LEU:N	2.14	0.62
1:B:108:TYR:C	1:B:108:TYR:HD2	2.03	0.62
1:B:29:MET:HE2	1:B:464:LEU:HD21	1.82	0.62
1:A:460:ARG:CZ	1:A:467:GLU:HG2	2.29	0.62
1:B:9:ASP:OD1	1:B:150:LYS:HE3	2.00	0.62
1:B:225:PRO:HB3	1:B:246:GLN:HE22	1.64	0.62
1:B:529:HIS:CE1	1:B:531:TYR:HB3	2.34	0.61
1:B:260:GLU:O	1:B:264:LYS:HG3	2.00	0.61
1:A:366:THR:HG22	1:A:368:LYS:N	2.15	0.61
1:A:231:TRP:CZ3	1:A:469:GLN:HG2	2.35	0.61
1:B:594:GLN:N	1:B:597:ARG:HH21	1.98	0.61
1:A:284:CYS:SG	1:A:293:LYS:HD2	2.41	0.61
1:A:138:GLY:HA2	1:A:149:THR:HG22	1.82	0.61
1:A:29:MET:CE	1:A:396:ILE:HG12	2.30	0.61
1:A:129:ILE:HB	1:A:187:PHE:CE1	2.35	0.61
1:B:570:TYR:CD2	1:B:584:LEU:HB3	2.36	0.61
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.17	0.60
1:B:357:PRO:HG3	1:B:379:ASN:O	2.01	0.60
1:B:57:LYS:NZ	1:B:436:PHE:HE1	1.98	0.60
1:B:108:TYR:C	1:B:108:TYR:CD2	2.75	0.60
1:A:573:ILE:HG21	1:A:576:LEU:HD22	1.83	0.60
1:A:554:GLU:O	1:A:558:LYS:HG3	2.02	0.60
1:A:287:ILE:HD13	1:A:318:GLY:O	2.01	0.60
1:B:8:PHE:HE1	1:B:147:TYR:HD2	1.50	0.60
1:B:159:PHE:CD2	1:B:174:GLY:HA3	2.36	0.60
1:B:589:PRO:HA	1:B:594:GLN:OE1	2.00	0.60
1:B:381:THR:CG2	1:B:382:THR:N	2.65	0.60
1:B:363:THR:HG22	1:B:408:ILE:O	2.02	0.60
1:A:551:LYS:HA	1:A:554:GLU:HG3	1.83	0.59
1:A:196:ILE:HG13	1:A:354:VAL:HG12	1.83	0.59
1:B:564:ILE:HD11	1:B:592:VAL:HA	1.84	0.59
1:B:366:THR:HG22	1:B:368:LYS:N	2.17	0.59
1:B:251:ILE:N	1:B:251:ILE:HD12	2.16	0.59
1:B:11:VAL:HG23	1:B:149:THR:OG1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:TYR:CD2	1:B:612:TYR:C	2.75	0.59
1:A:450:ASN:N	1:A:450:ASN:HD22	1.99	0.59
1:A:204:ALA:O	1:A:205:ARG:HD2	2.01	0.59
1:A:574:PRO:HD3	1:A:612:TYR:HD1	1.66	0.59
1:B:227:LYS:NZ	1:B:229:SER:O	2.36	0.59
1:A:480:ILE:HG23	1:A:536:VAL:HG23	1.84	0.59
1:B:250:TRP:C	1:B:251:ILE:HD12	2.22	0.59
1:B:267:HIS:CD2	1:B:267:HIS:H	2.19	0.59
1:A:286:SER:HB2	1:A:288:GLU:OE1	2.03	0.59
1:A:82:PHE:N	1:A:82:PHE:CD1	2.70	0.59
1:B:8:PHE:O	1:B:149:THR:HA	2.03	0.59
1:A:28:ARG:HH12	1:A:70:GLU:HG2	1.68	0.59
1:B:450:ASN:O	1:B:454:ARG:HG3	2.02	0.58
1:A:196:ILE:CG1	1:A:354:VAL:HG12	2.33	0.58
1:B:29:MET:CE	1:B:464:LEU:HD21	2.32	0.58
1:B:29:MET:CE	1:B:396:ILE:HG12	2.33	0.58
1:A:247:VAL:HG12	1:A:248:ASN:H	1.68	0.58
1:A:8:PHE:CD2	1:A:34:ALA:HB2	2.38	0.58
1:B:589:PRO:HG3	1:B:598:ILE:HD11	1.86	0.58
1:A:435:LEU:C	1:A:437:THR:H	2.06	0.58
1:A:81:GLN:HB3	1:A:99:GLN:HB2	1.84	0.58
1:B:396:ILE:O	1:B:400:LEU:HG	2.04	0.58
1:B:362:PRO:CG	1:B:594:GLN:NE2	2.67	0.58
1:B:573:ILE:HA	1:B:612:TYR:CD1	2.37	0.58
1:B:62:ARG:NH1	1:B:238:TYR:CD1	2.72	0.58
1:A:8:PHE:CE2	1:A:34:ALA:HB2	2.39	0.58
1:A:514:THR:C	1:A:516:ASP:H	2.05	0.58
1:B:210:THR:HB	1:B:341:VAL:HA	1.86	0.58
1:A:160:LEU:HD23	1:A:353:ASP:CB	2.34	0.58
1:B:420:MET:HG3	1:B:433:TYR:CE1	2.38	0.58
1:B:225:PRO:HB3	1:B:246:GLN:NE2	2.19	0.57
1:A:452:ILE:O	1:A:456:ALA:HB2	2.03	0.57
1:B:442:TYR:HA	1:B:549:GLU:OE2	2.04	0.57
1:A:224:PRO:HD3	1:A:242:LYS:HE2	1.84	0.57
1:B:359:GLU:OE1	1:B:368:LYS:HE3	2.04	0.57
1:B:381:THR:HG22	1:B:382:THR:N	2.19	0.57
1:B:262:ILE:HB	1:B:291:ILE:HD13	1.84	0.57
1:A:206:LEU:HB2	1:A:314:ILE:HB	1.86	0.57
1:B:430:THR:HG23	1:B:431:GLU:HG2	1.87	0.57
1:B:191:PHE:CD2	1:B:369:ILE:HD11	2.39	0.57
1:B:514:THR:C	1:B:516:ASP:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:TRP:HD1	1:B:343:LEU:CD1	2.17	0.57
1:B:63:GLU:O	1:B:67:LEU:HD12	2.05	0.57
1:A:60:VAL:HA	1:A:63:GLU:HG3	1.85	0.57
1:A:160:LEU:HA	1:A:181:SER:OG	2.04	0.57
1:B:453:LEU:HD11	1:B:535:GLU:OE2	2.05	0.57
1:A:589:PRO:HA	1:A:594:GLN:OE1	2.04	0.57
1:A:81:GLN:HG3	1:A:247:VAL:O	2.04	0.57
1:A:365:GLU:HG3	1:A:373:PHE:CE2	2.40	0.57
1:A:584:LEU:HG	1:A:601:ILE:HD11	1.87	0.56
1:A:450:ASN:HD22	1:A:451:ALA:N	2.03	0.56
1:B:594:GLN:CA	1:B:597:ARG:NH2	2.69	0.56
1:B:81:GLN:HG3	1:B:247:VAL:O	2.05	0.56
1:B:285:PRO:HG3	1:B:434:ARG:NH2	2.21	0.56
1:B:319:LEU:HD11	1:B:335:ILE:CD1	2.36	0.56
1:A:560:GLU:OE1	1:A:597:ARG:NH2	2.38	0.56
1:B:392:ILE:O	1:B:396:ILE:HG13	2.06	0.56
1:B:82:PHE:O	1:B:83:LYS:HB3	2.06	0.56
1:B:545:TYR:CD1	1:B:545:TYR:N	2.74	0.56
1:A:389:GLY:O	1:A:392:ILE:HG22	2.05	0.56
1:A:367:LYS:HZ1	1:A:587:PHE:HA	1.71	0.56
1:A:534:GLU:O	1:A:538:ILE:HG13	2.05	0.56
1:B:450:ASN:ND2	1:B:454:ARG:HE	2.03	0.56
1:A:230:PHE:HZ	1:A:476:LEU:HD13	1.71	0.55
1:A:221:GLY:HA3	1:A:246:GLN:OE1	2.06	0.55
1:B:480:ILE:HD13	1:B:535:GLU:CG	2.28	0.55
1:A:90:GLY:O	1:A:94:GLN:HG3	2.07	0.55
1:A:275:LEU:HD23	1:A:292:VAL:HG13	1.87	0.55
1:A:210:THR:HG21	1:A:342:VAL:CG2	2.35	0.55
1:A:290:LYS:HB3	1:A:300:HIS:CE1	2.41	0.55
1:B:509:MET:CE	1:B:515:LEU:HG	2.37	0.55
1:B:483:TRP:CE3	1:B:527:PRO:HG3	2.41	0.55
1:B:275:LEU:H	1:B:275:LEU:HD22	1.72	0.55
1:B:199:LYS:HA	1:B:350:ILE:O	2.07	0.55
1:A:360:LEU:HD11	1:A:379:ASN:HD21	1.70	0.55
1:A:229:SER:HB3	1:A:232:THR:OG1	2.06	0.55
1:B:224:PRO:HB3	1:B:242:LYS:HG2	1.88	0.55
1:A:71:MET:CE	1:A:385:GLU:HA	2.37	0.55
1:A:63:GLU:OE2	1:A:454:ARG:NH2	2.38	0.55
1:A:85:LEU:HD23	1:A:86:ASN:N	2.20	0.55
1:B:247:VAL:HG12	1:B:248:ASN:H	1.69	0.55
1:A:573:ILE:HA	1:A:612:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:OE1	1:A:235:VAL:HG23	2.06	0.55
1:A:570:TYR:CE2	1:A:584:LEU:HB3	2.42	0.55
1:A:102:LYS:NZ	1:A:205:ARG:HH21	2.04	0.55
1:A:275:LEU:CD1	1:B:441:GLU:HG3	2.37	0.55
1:A:545:TYR:N	1:A:545:TYR:CD1	2.76	0.55
1:A:547:GLU:OE1	1:A:547:GLU:HA	2.07	0.55
1:B:117:GLU:HG2	1:B:118:ASN:OD1	2.07	0.54
1:B:519:LYS:HD2	1:B:526:VAL:CG2	2.37	0.54
1:B:262:ILE:HD13	1:B:287:ILE:HG23	1.89	0.54
1:B:10:VAL:HG21	1:B:26:ALA:HB1	1.90	0.54
1:B:160:LEU:HD23	1:B:353:ASP:CB	2.38	0.54
1:A:386:GLU:CG	1:A:435:LEU:HG	2.36	0.54
1:B:508:LEU:O	1:B:513:TYR:HB2	2.07	0.54
1:B:259:HIS:N	1:B:259:HIS:CD2	2.74	0.54
1:B:480:ILE:HG23	1:B:536:VAL:CG2	2.37	0.54
1:B:435:LEU:C	1:B:437:THR:H	2.10	0.54
1:A:29:MET:HE3	1:A:464:LEU:HD21	1.88	0.54
1:B:514:THR:HG22	1:B:537:GLU:OE2	2.07	0.54
1:A:199:LYS:HA	1:A:350:ILE:O	2.08	0.54
1:A:204:ALA:HB1	1:A:345:ARG:O	2.07	0.54
1:A:547:GLU:OE1	1:A:550:ARG:HD3	2.07	0.53
1:B:548:ARG:O	1:B:552:LEU:HG	2.08	0.53
1:B:32:LYS:NZ	1:B:120:TYR:HE1	2.05	0.53
1:A:108:TYR:C	1:A:108:TYR:CD2	2.81	0.53
1:A:396:ILE:O	1:A:400:LEU:HG	2.09	0.53
1:B:28:ARG:HH12	1:B:70:GLU:HG2	1.73	0.53
1:A:341:VAL:HG22	1:A:342:VAL:N	2.24	0.53
1:B:484:LYS:HE3	1:B:540:LEU:HD23	1.91	0.53
1:A:225:PRO:HG2	1:A:240:PHE:CB	2.35	0.53
1:A:366:THR:HG22	1:A:368:LYS:H	1.74	0.53
1:A:574:PRO:CD	1:A:612:TYR:HD1	2.21	0.53
1:B:366:THR:HG22	1:B:368:LYS:H	1.73	0.53
1:B:204:ALA:HB1	1:B:345:ARG:O	2.08	0.53
1:B:397:ASN:OD1	1:B:408:ILE:N	2.36	0.53
1:A:352:TYR:CD1	1:A:352:TYR:N	2.77	0.53
1:B:409:TYR:CE2	1:B:590:ILE:HD12	2.44	0.53
1:A:82:PHE:O	1:A:83:LYS:HB3	2.07	0.53
1:B:160:LEU:HD23	1:B:353:ASP:HB3	1.91	0.53
1:B:258:THR:HB	1:B:259:HIS:HD2	1.73	0.53
1:B:46:MET:SD	1:B:105:TYR:CD2	3.02	0.53
1:A:396:ILE:HD13	1:A:462:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:VAL:CA	1:B:508:LEU:HG	2.39	0.52
1:B:286:SER:HB2	1:B:288:GLU:HG2	1.91	0.52
1:B:335:ILE:HB	1:B:338:LEU:HD12	1.91	0.52
1:B:460:ARG:HD3	1:B:467:GLU:HA	1.91	0.52
1:B:510:THR:O	1:B:510:THR:HG22	2.07	0.52
1:A:128:ASP:OD1	1:A:129:ILE:N	2.42	0.52
1:A:20:ILE:HA	1:A:35:MET:HE3	1.91	0.52
1:B:492:VAL:C	1:B:502:SER:HA	2.30	0.52
1:B:507:THR:HG22	1:B:511:MET:HE2	1.91	0.52
1:B:60:VAL:HG21	1:B:435:LEU:HD13	1.91	0.52
1:B:81:GLN:HB3	1:B:99:GLN:HB2	1.91	0.52
1:B:534:GLU:O	1:B:538:ILE:HG13	2.08	0.52
1:A:526:VAL:HG11	1:A:533:LYS:HE3	1.91	0.52
1:A:259:HIS:N	1:A:259:HIS:CD2	2.78	0.52
1:A:460:ARG:NH2	1:A:467:GLU:HG2	2.25	0.52
1:A:381:THR:HG21	1:A:390:GLN:HE22	1.73	0.52
1:A:56:ALA:HB3	1:A:435:LEU:HB3	1.91	0.52
1:A:293:LYS:C	1:A:295:PRO:HD3	2.31	0.52
1:B:484:LYS:HE3	1:B:540:LEU:CD2	2.40	0.52
1:A:71:MET:CE	1:A:385:GLU:HG3	2.39	0.51
1:A:275:LEU:HD23	1:A:292:VAL:CG1	2.40	0.51
1:B:218:VAL:CG1	1:B:248:ASN:HD22	2.23	0.51
1:B:166:ILE:HD11	1:B:348:TYR:HB3	1.91	0.51
1:B:82:PHE:CD1	1:B:82:PHE:N	2.79	0.51
1:A:288:GLU:O	1:A:292:VAL:HG23	2.10	0.51
1:B:410:LEU:HD12	1:B:417:ILE:CG2	2.40	0.51
1:B:286:SER:CB	1:B:288:GLU:HG2	2.41	0.51
1:B:361:TYR:O	1:B:425:THR:HG21	2.10	0.51
1:A:108:TYR:HD2	1:A:108:TYR:C	2.14	0.51
1:B:126:VAL:HG13	1:B:139:VAL:CG1	2.41	0.51
1:B:416:TYR:O	1:B:419:VAL:HB	2.10	0.51
1:B:8:PHE:CE1	1:B:147:TYR:HD2	2.29	0.51
1:A:160:LEU:HD23	1:A:353:ASP:HB3	1.92	0.51
1:B:154:VAL:HG21	1:B:188:TYR:OH	2.11	0.51
1:A:361:TYR:OH	1:A:588:LYS:HD2	2.10	0.51
1:A:466:SER:HB3	1:A:469:GLN:HB2	1.92	0.51
1:A:393:VAL:HG21	1:A:421:ILE:HD11	1.93	0.51
1:A:60:VAL:HG21	1:A:435:LEU:HD13	1.92	0.50
1:B:440:SER:C	1:B:442:TYR:H	2.14	0.50
1:A:357:PRO:HA	1:A:360:LEU:HD12	1.94	0.50
1:A:126:VAL:HG13	1:A:139:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ARG:O	1:B:324:PRO:HD3	2.10	0.50
1:A:450:ASN:N	1:A:450:ASN:ND2	2.58	0.50
1:B:460:ARG:NH1	1:B:467:GLU:N	2.59	0.50
1:B:487:TYR:CE2	1:B:515:LEU:HD11	2.47	0.50
1:A:38:LEU:HD21	1:A:125:GLU:HG3	1.94	0.50
1:B:28:ARG:NH2	1:B:70:GLU:OE2	2.44	0.50
1:A:39:ASN:HA	1:A:123:GLN:OE1	2.12	0.50
1:B:518:VAL:O	1:B:524:TYR:HB2	2.12	0.50
1:A:255:THR:HB	1:A:256:PRO:HD2	1.93	0.50
1:A:440:SER:C	1:A:442:TYR:H	2.15	0.50
1:B:360:LEU:HD23	1:B:366:THR:HA	1.94	0.50
1:B:434:ARG:HD3	1:B:436:PHE:CE2	2.46	0.50
1:A:381:THR:CG2	1:A:390:GLN:HE22	2.24	0.50
1:A:506:ALA:HB1	1:A:540:LEU:HD22	1.92	0.50
1:B:560:GLU:HA	1:B:591:THR:HG21	1.94	0.49
1:A:202:THR:HG22	2:A:618:FAD:HM72	1.94	0.49
1:B:509:MET:CE	1:B:537:GLU:HG3	2.42	0.49
1:B:551:LYS:HA	1:B:554:GLU:HG3	1.94	0.49
1:B:480:ILE:HG21	1:B:535:GLU:HG3	1.93	0.49
1:A:290:LYS:O	1:A:300:HIS:CE1	2.66	0.49
1:B:483:TRP:CH2	1:B:527:PRO:HA	2.46	0.49
1:A:480:ILE:HD13	1:A:535:GLU:CG	2.41	0.49
1:B:324:PRO:O	1:B:328:GLN:HG3	2.12	0.49
1:A:412:ARG:HD2	1:A:597:ARG:NH1	2.26	0.49
1:B:7:GLU:O	1:B:32:LYS:HD3	2.13	0.49
1:A:94:GLN:O	1:A:448:GLN:HG2	2.11	0.49
1:A:230:PHE:CE1	1:A:236:GLY:O	2.65	0.49
1:B:16:GLY:O	1:B:20:ILE:HG13	2.11	0.49
1:A:539:GLN:O	1:A:543:GLU:HB2	2.11	0.49
1:B:363:THR:O	1:B:364:LEU:HB2	2.13	0.49
1:A:365:GLU:HG3	1:A:373:PHE:CZ	2.47	0.49
1:A:366:THR:HG22	1:A:369:ILE:H	1.78	0.49
1:A:159:PHE:CE1	1:A:175:ARG:HG3	2.48	0.49
1:A:350:ILE:HG23	1:A:350:ILE:O	2.13	0.49
1:B:203:PRO:O	1:B:205:ARG:NH1	2.46	0.49
1:A:484:LYS:NZ	1:A:539:GLN:HB3	2.27	0.49
1:B:492:VAL:O	1:B:492:VAL:CG1	2.60	0.49
1:B:209:ARG:HD3	1:B:312:ILE:HD12	1.95	0.49
1:B:570:TYR:CE2	1:B:584:LEU:HB3	2.47	0.49
1:B:26:ALA:O	1:B:31:ALA:HB3	2.13	0.48
1:B:130:ILE:HD12	1:B:130:ILE:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:CE2	1:A:452:ILE:HG12	2.47	0.48
1:A:159:PHE:HE1	1:A:175:ARG:HG3	1.78	0.48
1:A:294:PHE:C	1:A:296:ASP:H	2.15	0.48
1:B:108:TYR:HE2	1:B:112:VAL:CG2	2.26	0.48
1:B:547:GLU:OE1	1:B:550:ARG:HD3	2.13	0.48
1:B:9:ASP:OD2	1:B:32:LYS:N	2.34	0.48
1:B:412:ARG:CD	1:B:597:ARG:NH1	2.74	0.48
1:B:326:GLU:HA	1:B:329:TRP:CE3	2.49	0.48
1:B:519:LYS:O	1:B:523:GLY:HA2	2.13	0.48
1:B:286:SER:OG	1:B:288:GLU:HG2	2.13	0.48
1:B:539:GLN:O	1:B:543:GLU:HB2	2.13	0.48
1:B:544:PRO:HB2	1:B:545:TYR:HD1	1.79	0.48
1:A:213:PHE:N	1:A:213:PHE:CD1	2.81	0.48
1:A:460:ARG:NH1	1:A:467:GLU:HG2	2.28	0.48
1:A:338:LEU:O	1:A:341:VAL:HG12	2.13	0.48
1:B:52:ILE:HD12	1:B:71:MET:HE2	1.94	0.48
1:B:452:ILE:HG23	1:B:453:LEU:HD23	1.95	0.48
1:B:29:MET:HE1	1:B:396:ILE:CG1	2.39	0.48
1:A:550:ARG:HG2	1:A:550:ARG:O	2.13	0.48
1:A:363:THR:HG21	1:A:407:PRO:HB2	1.94	0.48
1:B:130:ILE:HD12	1:B:130:ILE:N	2.29	0.48
1:A:390:GLN:HG3	1:A:420:MET:HE3	1.96	0.48
1:B:519:LYS:HG3	1:B:524:TYR:O	2.13	0.48
1:A:191:PHE:O	1:A:192:ASP:HB2	2.12	0.48
1:A:564:ILE:HD11	1:A:592:VAL:HA	1.95	0.48
1:B:253:TYR:CE2	1:B:301:GLN:HG3	2.49	0.48
1:B:230:PHE:HZ	1:B:476:LEU:HD12	1.77	0.48
1:B:29:MET:HG3	1:B:464:LEU:HD21	1.96	0.48
1:B:389:GLY:O	1:B:392:ILE:HG22	2.14	0.48
1:B:545:TYR:N	1:B:545:TYR:HD1	2.07	0.48
1:A:230:PHE:CD2	1:A:452:ILE:HG12	2.48	0.48
1:B:519:LYS:HD2	1:B:526:VAL:HG23	1.96	0.48
1:A:175:ARG:NE	1:A:178:GLU:OE2	2.42	0.48
1:B:594:GLN:CA	1:B:597:ARG:HH21	2.26	0.48
1:B:507:THR:O	1:B:511:MET:HE3	2.13	0.48
1:A:460:ARG:HD3	1:A:467:GLU:HA	1.96	0.48
1:B:318:GLY:O	1:B:319:LEU:HD23	2.14	0.47
1:B:509:MET:HE3	1:B:537:GLU:HG3	1.95	0.47
1:A:80:ILE:O	1:A:81:GLN:HB2	2.13	0.47
1:B:51:ALA:HB1	1:B:98:ALA:O	2.14	0.47
1:A:140:ARG:HG2	1:A:145:VAL:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:HD22	1:B:529:HIS:CD2	2.48	0.47
1:A:480:ILE:HG23	1:A:536:VAL:CG2	2.44	0.47
1:A:514:THR:C	1:A:516:ASP:N	2.67	0.47
1:B:224:PRO:HB3	1:B:242:LYS:CG	2.45	0.47
1:A:574:PRO:HD3	1:A:612:TYR:CD1	2.46	0.47
1:B:294:PHE:N	1:B:295:PRO:HD3	2.29	0.47
1:B:186:ASP:O	1:B:190:ARG:HB2	2.14	0.47
1:A:357:PRO:HA	1:A:360:LEU:CD1	2.45	0.47
1:B:543:GLU:N	1:B:544:PRO:CD	2.78	0.47
1:A:422:ASP:OD2	1:A:597:ARG:NH1	2.48	0.47
1:A:607:THR:O	1:A:611:VAL:HG23	2.13	0.47
1:B:28:ARG:HH22	1:B:70:GLU:CG	2.28	0.47
1:B:218:VAL:HG12	1:B:220:PRO:HD3	1.95	0.47
1:A:289:ASP:O	1:A:291:ILE:N	2.48	0.47
1:B:193:PHE:CZ	1:B:366:THR:HG21	2.50	0.47
1:B:11:VAL:HG13	1:B:36:PHE:CE1	2.50	0.47
1:A:11:VAL:HG11	1:A:139:VAL:HG21	1.96	0.47
1:B:509:MET:HE1	1:B:515:LEU:N	2.29	0.47
1:B:396:ILE:HG12	1:B:464:LEU:HD11	1.97	0.47
1:A:161:ASN:HB3	1:A:197:ARG:NH2	2.30	0.47
1:B:80:ILE:O	1:B:81:GLN:HB2	2.15	0.47
1:B:210:THR:CB	1:B:341:VAL:HA	2.44	0.47
1:B:72:GLY:O	1:B:75:ILE:HG22	2.14	0.47
1:B:420:MET:HG3	1:B:433:TYR:HE1	1.79	0.47
1:B:62:ARG:NH1	1:B:238:TYR:CG	2.82	0.47
1:B:223:ASP:OD1	1:B:242:LYS:HA	2.15	0.47
1:B:165:TYR:CE1	1:B:170:MET:HG2	2.50	0.47
1:A:613:LEU:HA	1:A:616:LEU:CD1	2.45	0.47
1:A:290:LYS:O	1:A:300:HIS:HE1	1.98	0.46
1:A:509:MET:SD	1:A:515:LEU:HD23	2.55	0.46
1:B:178:GLU:HB3	1:B:179:PRO:HD2	1.97	0.46
1:A:361:TYR:O	1:A:425:THR:HG21	2.15	0.46
1:B:522:PHE:CD2	1:B:522:PHE:N	2.83	0.46
1:B:471:LYS:O	1:B:475:GLU:HB2	2.15	0.46
1:A:472:LEU:O	1:A:472:LEU:HD12	2.15	0.46
1:B:505:VAL:HA	1:B:508:LEU:CG	2.41	0.46
1:B:29:MET:CE	1:B:396:ILE:HA	2.43	0.46
1:A:356:PRO:HA	1:A:357:PRO:HD3	1.77	0.46
1:A:294:PHE:O	1:A:296:ASP:N	2.48	0.46
1:B:582:GLU:HG3	1:B:586:LYS:HE3	1.98	0.46
1:B:11:VAL:HG23	1:B:149:THR:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LYS:HG3	1:A:579:GLU:OE2	2.16	0.46
1:A:87:THR:HA	1:A:94:GLN:NE2	2.21	0.46
1:B:514:THR:C	1:B:516:ASP:N	2.69	0.46
1:A:293:LYS:HB2	1:A:294:PHE:CD2	2.51	0.46
1:A:446:ILE:O	1:A:446:ILE:HG22	2.16	0.46
1:A:437:THR:CG2	1:B:276:ILE:HG23	2.46	0.46
1:B:522:PHE:N	1:B:522:PHE:HD2	2.13	0.46
1:B:381:THR:CG2	1:B:386:GLU:HB2	2.46	0.46
1:A:247:VAL:CG1	1:A:248:ASN:N	2.78	0.46
1:B:287:ILE:CD1	1:B:290:LYS:HD2	2.45	0.46
1:A:303:PHE:HB2	1:A:317:ASN:HB3	1.97	0.46
1:B:361:TYR:OH	1:B:588:LYS:HD2	2.15	0.46
1:A:480:ILE:HG12	1:A:532:VAL:HG13	1.98	0.46
1:A:602:THR:HG21	1:B:165:TYR:CZ	2.51	0.46
1:B:40:ALA:O	1:B:43:ILE:HG13	2.15	0.46
1:A:203:PRO:HB3	1:A:316:PRO:HG2	1.98	0.46
1:B:386:GLU:O	1:B:420:MET:HE1	2.15	0.46
1:B:483:TRP:O	1:B:487:TYR:CD2	2.69	0.46
1:A:71:MET:HE1	1:A:385:GLU:CA	2.45	0.46
1:A:415:SER:HA	1:A:454:ARG:HH21	1.80	0.46
1:A:60:VAL:HG21	1:A:435:LEU:HD11	1.97	0.46
1:B:480:ILE:O	1:B:536:VAL:HG22	2.15	0.45
1:A:333:ARG:HG2	1:A:338:LEU:O	2.16	0.45
1:A:60:VAL:HG12	1:A:64:ILE:HD11	1.98	0.45
1:A:460:ARG:NH1	1:A:467:GLU:N	2.64	0.45
1:A:551:LYS:O	1:A:554:GLU:HG3	2.16	0.45
1:A:526:VAL:HG13	1:A:527:PRO:HD2	1.98	0.45
1:B:289:ASP:C	1:B:291:ILE:H	2.19	0.45
1:A:277:LYS:HG2	1:B:439:ARG:NH1	2.31	0.45
1:A:588:LYS:N	1:A:589:PRO:HD3	2.31	0.45
1:B:570:TYR:HB2	1:B:585:LYS:HE2	1.98	0.45
1:B:160:LEU:HB3	1:B:353:ASP:HB2	1.98	0.45
1:A:157:GLY:HA2	1:A:377:ASN:HB2	1.98	0.45
1:B:28:ARG:HH22	1:B:70:GLU:CD	2.18	0.45
1:B:447:ARG:NH2	1:B:450:ASN:HB3	2.32	0.45
1:A:503:TYR:CD2	1:A:503:TYR:N	2.85	0.45
1:B:366:THR:HG22	1:B:369:ILE:H	1.80	0.45
1:B:508:LEU:C	1:B:513:TYR:HB2	2.37	0.45
1:B:612:TYR:HD2	1:B:612:TYR:C	2.20	0.45
1:B:230:PHE:CE1	1:B:236:GLY:O	2.69	0.45
1:B:191:PHE:CE2	1:B:369:ILE:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ARG:HD2	1:B:502:SER:O	2.17	0.45
1:B:487:TYR:CE1	1:B:515:LEU:HD21	2.51	0.45
1:B:71:MET:O	1:B:75:ILE:HG22	2.16	0.45
1:B:324:PRO:HB2	1:B:327:VAL:HG23	1.99	0.45
1:B:287:ILE:HA	1:B:287:ILE:HD12	1.80	0.45
1:B:287:ILE:HD12	1:B:290:LYS:HD2	1.98	0.45
1:A:26:ALA:O	1:A:31:ALA:HB3	2.16	0.45
1:B:607:THR:O	1:B:611:VAL:HG23	2.17	0.45
1:B:319:LEU:HD13	1:B:331:MET:CE	2.47	0.45
1:B:573:ILE:HA	1:B:574:PRO:HD3	1.74	0.45
1:A:117:GLU:O	1:A:118:ASN:HB2	2.17	0.45
1:B:86:ASN:ND2	1:B:89:LYS:HD2	2.31	0.45
1:B:487:TYR:OH	1:B:527:PRO:HD3	2.17	0.45
1:A:505:VAL:HA	1:A:508:LEU:CD1	2.42	0.45
1:B:267:HIS:HD2	1:B:267:HIS:H	1.62	0.45
1:B:259:HIS:CD2	1:B:259:HIS:H	2.35	0.45
1:A:519:LYS:O	1:A:523:GLY:HA2	2.16	0.45
1:A:593:GLY:O	1:A:596:SER:OG	2.28	0.45
1:B:49:ASN:HA	1:B:50:PRO:HD3	1.74	0.45
1:A:29:MET:CE	1:A:464:LEU:HD21	2.47	0.44
1:B:94:GLN:O	1:B:448:GLN:HG2	2.17	0.44
1:A:386:GLU:O	1:A:420:MET:HE1	2.17	0.44
1:A:366:THR:CG2	1:A:369:ILE:H	2.30	0.44
1:A:442:TYR:OH	1:A:557:LYS:HE3	2.17	0.44
1:A:82:PHE:N	1:A:82:PHE:HD1	2.14	0.44
1:A:158:THR:HB	1:A:350:ILE:HG12	1.99	0.44
1:A:609:LEU:HD12	1:A:609:LEU:O	2.17	0.44
1:A:262:ILE:HD13	1:A:287:ILE:HG23	1.99	0.44
1:A:589:PRO:CG	1:A:598:ILE:HD11	2.45	0.44
1:A:159:PHE:HB2	2:A:618:FAD:H8A	2.00	0.44
1:A:503:TYR:HD2	1:A:503:TYR:N	2.16	0.44
1:B:452:ILE:HD11	1:B:473:VAL:CG2	2.46	0.44
1:A:400:LEU:CD1	1:A:408:ILE:HG23	2.47	0.44
1:A:547:GLU:OE1	1:A:550:ARG:CD	2.66	0.44
1:A:519:LYS:HB2	1:A:526:VAL:HG21	1.99	0.44
1:A:159:PHE:CE2	2:A:618:FAD:H2B	2.53	0.44
1:B:261:ILE:HD13	1:B:330:GLU:HG2	2.00	0.44
1:A:253:TYR:N	1:A:253:TYR:CD1	2.85	0.44
1:B:305:GLU:HA	1:B:306:PRO:HD3	1.75	0.44
1:B:87:THR:HA	1:B:94:GLN:NE2	2.18	0.44
1:A:577:THR:O	1:A:581:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:HD12	1:A:417:ILE:CG2	2.48	0.44
1:A:59:ILE:HG12	1:A:448:GLN:HB3	2.00	0.44
1:B:507:THR:HG22	1:B:507:THR:O	2.16	0.44
1:A:262:ILE:HB	1:A:291:ILE:HD13	1.99	0.44
1:B:587:PHE:O	1:B:588:LYS:C	2.55	0.44
1:A:480:ILE:O	1:A:484:LYS:HG3	2.18	0.44
1:B:70:GLU:O	1:B:71:MET:C	2.56	0.44
1:A:573:ILE:HA	1:A:574:PRO:HD3	1.75	0.44
1:B:289:ASP:C	1:B:291:ILE:N	2.71	0.44
1:B:314:ILE:HD13	1:B:314:ILE:HA	1.78	0.44
1:B:8:PHE:HE1	1:B:147:TYR:CD2	2.32	0.43
1:B:29:MET:HE2	1:B:464:LEU:HD11	2.00	0.43
1:A:568:ILE:O	1:A:568:ILE:HD12	2.18	0.43
1:B:350:ILE:HG22	2:B:618:FAD:HM73	1.98	0.43
1:A:305:GLU:HA	1:A:306:PRO:HD3	1.81	0.43
1:A:165:TYR:CZ	1:B:602:THR:HG21	2.54	0.43
1:B:511:MET:O	1:B:513:TYR:HD1	2.01	0.43
1:B:573:ILE:HD13	1:B:609:LEU:HD12	1.99	0.43
1:A:86:ASN:HD22	1:A:86:ASN:HA	1.61	0.43
1:A:460:ARG:HD2	1:A:460:ARG:HA	1.91	0.43
1:A:259:HIS:CD2	1:A:259:HIS:H	2.34	0.43
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.82	0.43
1:B:483:TRP:CE2	1:B:527:PRO:HA	2.53	0.43
1:A:275:LEU:CD2	1:A:292:VAL:HG13	2.49	0.43
1:B:422:ASP:OD2	1:B:597:ARG:NH1	2.52	0.43
1:B:56:ALA:CB	1:B:435:LEU:HB3	2.49	0.43
1:A:587:PHE:O	1:A:588:LYS:C	2.56	0.43
1:B:230:PHE:CD2	1:B:452:ILE:HG12	2.54	0.43
1:B:235:VAL:HG12	1:B:236:GLY:N	2.33	0.43
1:B:130:ILE:HD13	1:B:138:GLY:C	2.39	0.43
1:A:61:VAL:HA	1:A:64:ILE:HD12	2.01	0.43
1:A:39:ASN:OD1	1:A:39:ASN:C	2.57	0.43
1:B:197:ARG:NH1	1:B:353:ASP:OD1	2.50	0.43
1:A:164:ILE:HD12	1:A:164:ILE:N	2.32	0.43
1:B:110:LYS:HE2	1:B:114:GLU:OE2	2.19	0.43
1:B:341:VAL:HG22	1:B:342:VAL:N	2.33	0.43
1:B:568:ILE:HG13	1:B:568:ILE:O	2.19	0.43
1:B:287:ILE:O	1:B:291:ILE:HG23	2.18	0.43
1:B:519:LYS:HB2	1:B:526:VAL:HG23	2.00	0.43
1:A:548:ARG:O	1:A:552:LEU:HG	2.19	0.43
1:B:223:ASP:OD1	1:B:224:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:CD2	1:A:86:ASN:N	2.82	0.43
1:B:72:GLY:O	1:B:73:LYS:C	2.57	0.43
1:A:367:LYS:HZ3	1:A:587:PHE:HA	1.84	0.43
1:B:163:VAL:O	1:B:350:ILE:HD12	2.18	0.43
1:A:526:VAL:CG1	1:A:527:PRO:HD2	2.49	0.43
1:B:128:ASP:CG	1:B:190:ARG:HH22	2.22	0.43
1:A:572:LYS:O	1:A:612:TYR:HE1	2.01	0.43
1:B:610:LEU:HD23	1:B:610:LEU:HA	1.73	0.43
1:A:408:ILE:HG13	1:A:409:TYR:N	2.31	0.42
1:B:108:TYR:HE2	1:B:112:VAL:HG21	1.84	0.42
1:B:381:THR:HG23	1:B:386:GLU:HB2	2.00	0.42
1:A:16:GLY:O	1:A:20:ILE:HG13	2.19	0.42
1:A:258:THR:HB	1:A:259:HIS:HD2	1.84	0.42
1:B:594:GLN:HA	1:B:597:ARG:CZ	2.49	0.42
1:B:56:ALA:HB3	1:B:435:LEU:HB3	2.00	0.42
1:B:175:ARG:NE	1:B:178:GLU:OE2	2.52	0.42
1:A:459:GLY:HA3	1:A:465:LEU:HD12	2.01	0.42
1:B:588:LYS:N	1:B:589:PRO:HD3	2.35	0.42
1:B:509:MET:HE2	1:B:515:LEU:HG	2.00	0.42
1:B:108:TYR:CE2	1:B:112:VAL:CG2	3.02	0.42
1:A:193:PHE:CZ	1:A:366:THR:HG21	2.55	0.42
1:B:396:ILE:O	1:B:399:ALA:HB3	2.19	0.42
1:A:293:LYS:HB2	1:A:294:PHE:CE2	2.54	0.42
1:A:445:TYR:O	1:A:445:TYR:CG	2.73	0.42
1:A:287:ILE:HG12	1:A:319:LEU:HD23	2.01	0.42
1:A:7:GLU:O	1:A:32:LYS:HE3	2.20	0.42
1:B:450:ASN:ND2	1:B:450:ASN:N	2.67	0.42
1:A:43:ILE:HD11	1:A:121:ILE:HD13	2.00	0.42
1:A:203:PRO:CB	1:A:316:PRO:HG2	2.49	0.42
1:B:509:MET:SD	1:B:513:TYR:O	2.78	0.42
1:B:57:LYS:HD3	1:B:385:GLU:CD	2.40	0.42
1:A:532:VAL:O	1:A:536:VAL:HG23	2.19	0.42
1:B:204:ALA:H	1:B:347:ALA:HB2	1.82	0.42
1:B:275:LEU:N	1:B:275:LEU:CD2	2.83	0.42
1:B:203:PRO:HB2	1:B:316:PRO:HG2	2.02	0.42
1:B:580:ALA:HB1	1:B:601:ILE:CD1	2.49	0.42
1:B:60:VAL:O	1:B:64:ILE:HG13	2.19	0.42
1:A:159:PHE:CD2	2:A:618:FAD:H2B	2.55	0.42
1:B:491:ARG:HA	1:B:503:TYR:O	2.20	0.42
1:A:613:LEU:HA	1:A:616:LEU:HG	2.01	0.42
1:A:377:ASN:HD21	1:A:382:THR:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:PRO:O	1:B:606:ILE:HG22	2.20	0.42
1:A:299:ARG:O	1:A:299:ARG:HG3	2.18	0.42
1:B:54:GLY:O	1:B:55:ILE:C	2.59	0.41
1:B:444:LEU:HD12	1:B:549:GLU:OE1	2.20	0.41
1:A:255:THR:HB	1:A:256:PRO:CD	2.50	0.41
1:A:95:SER:HA	1:A:96:PRO:HD2	1.93	0.41
1:A:522:PHE:HB3	1:A:524:TYR:CE1	2.55	0.41
1:B:576:LEU:O	1:B:577:THR:C	2.57	0.41
1:B:319:LEU:HD11	1:B:335:ILE:HD11	2.00	0.41
1:B:490:GLU:HB2	1:B:505:VAL:HG23	2.00	0.41
1:B:504:SER:O	1:B:508:LEU:HG	2.20	0.41
1:A:70:GLU:O	1:A:71:MET:C	2.58	0.41
1:A:415:SER:HA	1:A:454:ARG:NH2	2.35	0.41
1:A:602:THR:HB	1:A:603:PRO:HD2	2.02	0.41
1:A:613:LEU:HD23	1:A:616:LEU:HD11	2.00	0.41
1:A:321:THR:OG1	1:A:322:SER:N	2.53	0.41
1:B:367:LYS:NZ	1:B:587:PHE:HA	2.36	0.41
1:B:435:LEU:C	1:B:437:THR:N	2.74	0.41
1:A:247:VAL:CG1	1:A:248:ASN:H	2.32	0.41
1:B:602:THR:HB	1:B:603:PRO:HD2	2.01	0.41
1:A:29:MET:HE1	1:A:396:ILE:CA	2.36	0.41
1:B:560:GLU:OE1	1:B:597:ARG:NH2	2.53	0.41
1:B:487:TYR:CZ	1:B:515:LEU:HD21	2.56	0.41
1:A:7:GLU:O	1:A:32:LYS:CE	2.68	0.41
1:A:71:MET:O	1:A:75:ILE:HG22	2.21	0.41
1:A:576:LEU:O	1:A:577:THR:C	2.58	0.41
1:B:410:LEU:HD12	1:B:417:ILE:HG21	2.00	0.41
1:B:202:THR:CA	1:B:320:SER:HB3	2.50	0.41
1:A:416:TYR:O	1:A:419:VAL:HB	2.21	0.41
1:B:284:CYS:HA	1:B:285:PRO:HD3	1.87	0.41
1:A:435:LEU:C	1:A:437:THR:N	2.73	0.41
1:B:291:ILE:HG13	1:B:291:ILE:O	2.18	0.41
1:B:213:PHE:CD1	1:B:213:PHE:N	2.89	0.41
1:B:82:PHE:HD1	1:B:82:PHE:N	2.18	0.41
1:A:509:MET:HA	1:A:513:TYR:O	2.21	0.41
1:A:416:TYR:HD1	1:A:416:TYR:O	2.03	0.41
1:A:487:TYR:HD1	1:A:505:VAL:HG11	1.84	0.41
1:A:434:ARG:HD3	1:A:436:PHE:CZ	2.54	0.41
1:B:355:VAL:HG23	1:B:378:PHE:CZ	2.56	0.41
1:B:492:VAL:HG11	1:B:522:PHE:HE1	1.85	0.41
1:B:62:ARG:HE	1:B:96:PRO:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:HIS:NE2	1:B:555:LYS:HD2	2.36	0.41
1:B:591:THR:HB	1:B:594:GLN:H	1.86	0.41
1:A:72:GLY:O	1:A:73:LYS:C	2.59	0.41
1:A:529:HIS:C	1:A:529:HIS:CD2	2.94	0.41
1:B:450:ASN:HD22	1:B:450:ASN:N	2.17	0.41
1:A:281:PRO:HG3	1:A:294:PHE:CD1	2.55	0.41
1:A:284:CYS:HA	1:A:285:PRO:HD3	1.80	0.41
1:B:356:PRO:HA	1:B:357:PRO:HD3	1.86	0.41
1:B:363:THR:HG21	1:B:407:PRO:HB2	2.02	0.41
1:B:289:ASP:O	1:B:291:ILE:N	2.54	0.41
1:A:527:PRO:HB2	1:A:533:LYS:HB2	2.02	0.41
1:A:312:ILE:HG13	1:A:312:ILE:O	2.19	0.41
1:A:123:GLN:O	1:A:123:GLN:HG2	2.21	0.41
1:B:11:VAL:HG13	1:B:36:PHE:HE1	1.86	0.40
1:A:57:LYS:HD3	1:A:385:GLU:OE1	2.21	0.40
1:B:82:PHE:HB2	1:B:225:PRO:HB2	2.03	0.40
1:A:508:LEU:O	1:A:513:TYR:HB2	2.21	0.40
1:A:602:THR:HB	1:A:603:PRO:CD	2.51	0.40
1:A:130:ILE:CD1	1:A:130:ILE:N	2.80	0.40
1:B:338:LEU:O	1:B:341:VAL:HG12	2.21	0.40
1:B:15:GLY:HA3	1:B:37:VAL:HG22	2.03	0.40
1:B:553:ASN:O	1:B:554:GLU:C	2.59	0.40
1:B:207:ASP:HB3	1:B:210:THR:OG1	2.21	0.40
1:B:509:MET:HA	1:B:513:TYR:O	2.22	0.40
1:A:56:ALA:CB	1:A:435:LEU:HB3	2.51	0.40
1:A:450:ASN:ND2	1:A:454:ARG:HH11	2.18	0.40
1:B:27:ALA:O	1:B:30:GLY:N	2.43	0.40
1:B:189:ARG:CG	1:B:195:LEU:HD12	2.50	0.40
1:B:529:HIS:CE1	1:B:531:TYR:CB	3.03	0.40
1:B:505:VAL:O	1:B:508:LEU:HB2	2.20	0.40
1:A:207:ASP:HB3	1:A:210:THR:OG1	2.22	0.40
1:A:235:VAL:HG12	1:A:236:GLY:N	2.36	0.40
1:A:570:TYR:CD2	1:A:584:LEU:HB3	2.55	0.40
2:B:618:FAD:H4'	2:B:618:FAD:O1A	2.21	0.40
1:A:227:LYS:HE3	1:A:229:SER:O	2.21	0.40
1:A:322:SER:HB3	1:A:349:ALA:HB2	2.04	0.40
1:B:7:GLU:HG2	1:B:148:LYS:CB	2.35	0.40
1:A:450:ASN:HD21	1:A:454:ARG:HH11	1.69	0.40
1:B:203:PRO:CB	1:B:316:PRO:HG2	2.51	0.40
1:A:237:SER:OG	1:A:238:TYR:N	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:OE1	1:B:107:GLU:OE1[8_565]	1.59	0.61

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/637 (94%)	500 (84%)	84 (14%)	15 (2%)	7	41
1	B	597/637 (94%)	497 (83%)	83 (14%)	17 (3%)	6	37
All	All	1196/1274 (94%)	997 (83%)	167 (14%)	32 (3%)	6	39

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	MET
1	A	285	PRO
1	B	55	ILE
1	B	71	MET
1	B	285	PRO
1	B	527	PRO
1	A	55	ILE
1	A	81	GLN
1	A	290	LYS
1	A	577	THR
1	B	81	GLN
1	B	577	THR
1	A	295	PRO
1	B	436	PHE
1	B	528	GLN
1	A	436	PHE
1	B	270	ALA
1	B	544	PRO

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Mol	Chain	Res	Type
1	A	83	LYS
1	A	530	PRO
1	A	544	PRO
1	A	570	TYR
1	B	83	LYS
1	B	290	LYS
1	A	217	GLU
1	B	217	GLU
1	A	20	ILE
1	B	20	ILE
1	A	356	PRO
1	B	179	PRO
1	B	356	PRO
1	B	530	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	511/540 (95%)	478 (94%)	33 (6%)	21	61
1	B	510/540 (94%)	482 (94%)	28 (6%)	27	68
All	All	1021/1080 (94%)	960 (94%)	61 (6%)	24	65

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	63	GLU
1	A	71	MET
1	A	81	GLN
1	A	82	PHE
1	A	85	LEU
1	A	86	ASN
1	A	108	TYR
1	A	131	VAL

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Mol	Chain	Res	Type
1	A	192	ASP
1	A	223	ASP
1	A	227	LYS
1	A	232	THR
1	A	263	ARG
1	A	269	THR
1	A	298	GLU
1	A	310	ASP
1	A	321	THR
1	A	326	GLU
1	A	331	MET
1	A	352	TYR
1	A	354	VAL
1	A	360	LEU
1	A	379	ASN
1	A	429	VAL
1	A	430	THR
1	A	441	GLU
1	A	448	GLN
1	A	450	ASN
1	A	503	TYR
1	A	545	TYR
1	A	550	ARG
1	A	577	THR
1	B	67	LEU
1	B	81	GLN
1	B	82	PHE
1	B	86	ASN
1	B	104	ARG
1	B	108	TYR
1	B	116	GLN
1	B	192	ASP
1	B	269	THR
1	B	288	GLU
1	B	299	ARG
1	B	309	LEU
1	B	310	ASP
1	B	314	ILE
1	B	320	SER
1	B	321	THR
1	B	331	MET
1	B	379	ASN

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Mol	Chain	Res	Type
1	B	382	THR
1	B	401	ARG
1	B	429	VAL
1	B	441	GLU
1	B	450	ASN
1	B	527	PRO
1	B	530	PRO
1	B	545	TYR
1	B	577	THR
1	B	591	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	94	GLN
1	A	115	ASN
1	A	259	HIS
1	A	265	ASN
1	A	300	HIS
1	A	340	ASN
1	A	377	ASN
1	A	379	ASN
1	A	450	ASN
1	A	529	HIS
1	B	86	ASN
1	B	94	GLN
1	B	115	ASN
1	B	161	ASN
1	B	248	ASN
1	B	259	HIS
1	B	267	HIS
1	B	340	ASN
1	B	377	ASN
1	B	390	GLN
1	B	448	GLN
1	B	450	ASN
1	B	469	GLN
1	B	528	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	618	-	48,58,58	1.89	15 (31%)	54,89,89	2.12	11 (20%)
3	PO4	A	619	-	4,4,4	1.06	0	6,6,6	0.27	0
3	PO4	A	620	-	4,4,4	1.08	0	6,6,6	0.27	0
2	FAD	B	618	-	48,58,58	2.03	18 (37%)	54,89,89	2.16	9 (16%)
3	PO4	B	619	-	4,4,4	0.80	0	6,6,6	0.27	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
2	FAD	A	618	-	-	0/30/50/50	0/6/6/6
3	PO4	A	619	-	-	0/0/0/0	0/0/0/0
3	PO4	A	620	-	-	0/0/0/0	0/0/0/0
2	FAD	B	618	-	-	0/30/50/50	0/6/6/6
3	PO4	B	619	-	-	0/0/0/0	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	618	FAD	P-O2P	-3.10	1.41	1.54
2	B	618	FAD	O4-C4	-3.03	1.17	1.24
2	A	618	FAD	P-O2P	-2.89	1.42	1.54
2	B	618	FAD	PA-O2A	-2.86	1.42	1.54
2	A	618	FAD	O4-C4	-2.79	1.18	1.24
2	B	618	FAD	O4B-C4B	-2.71	1.38	1.45
2	A	618	FAD	O4B-C4B	-2.69	1.38	1.45
2	A	618	FAD	PA-O2A	-2.61	1.43	1.54
2	A	618	FAD	PA-O1A	-2.32	1.42	1.51
2	A	618	FAD	O3'-C3'	-2.30	1.37	1.43
2	A	618	FAD	C8A-N7A	-2.26	1.30	1.34
2	B	618	FAD	PA-O1A	-2.24	1.43	1.51
2	B	618	FAD	O3'-C3'	-2.17	1.37	1.43
2	B	618	FAD	C8A-N7A	-2.14	1.30	1.34
2	A	618	FAD	P-O1P	-2.10	1.43	1.51
2	B	618	FAD	P-O1P	-2.04	1.43	1.51
2	A	618	FAD	C2'-C3'	2.00	1.57	1.53
2	B	618	FAD	C6-C5X	2.03	1.44	1.41
2	B	618	FAD	C2'-C3'	2.15	1.57	1.53
2	B	618	FAD	C4X-C10	2.25	1.45	1.41
2	A	618	FAD	C6-C7	2.39	1.44	1.37
2	B	618	FAD	C4-N3	2.46	1.37	1.33
2	B	618	FAD	C6-C7	2.82	1.45	1.37
2	A	618	FAD	C4-N3	3.13	1.38	1.33
2	A	618	FAD	C5X-N5	3.31	1.40	1.35
2	B	618	FAD	C5X-N5	3.32	1.40	1.35
2	B	618	FAD	C9A-N10	3.36	1.43	1.38
2	B	618	FAD	C1'-N10	3.54	1.52	1.48
2	A	618	FAD	C10-N10	3.55	1.43	1.39
2	A	618	FAD	C9A-N10	4.01	1.44	1.38
2	A	618	FAD	C4X-N5	4.30	1.40	1.33
2	B	618	FAD	C4X-N5	4.52	1.40	1.33
2	B	618	FAD	C10-N10	4.92	1.44	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	618	FAD	N3A-C2A-N1A	-9.56	121.58	128.89
2	B	618	FAD	N3A-C2A-N1A	-9.43	121.67	128.89
2	A	618	FAD	C1B-N9A-C4A	-4.96	119.45	126.94
2	B	618	FAD	C1B-N9A-C4A	-3.95	120.98	126.94
2	B	618	FAD	C4A-C5A-N7A	-2.93	106.78	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	618	FAD	C4A-C5A-N7A	-2.39	107.28	109.48
2	A	618	FAD	O3'-C3'-C2'	-2.06	103.56	108.75
2	A	618	FAD	C1'-N10-C9A	2.15	121.27	118.86
2	A	618	FAD	O2'-C2'-C3'	2.34	114.89	109.02
2	A	618	FAD	C4-N3-C2	3.05	117.88	115.25
2	B	618	FAD	C4-N3-C2	3.09	117.92	115.25
2	B	618	FAD	O3P-P-O5'	3.18	111.37	102.94
2	A	618	FAD	O3P-P-O5'	3.21	111.44	102.94
2	A	618	FAD	C4-C4X-N5	3.22	122.63	118.72
2	A	618	FAD	O3P-PA-O5B	3.28	111.64	102.94
2	B	618	FAD	C4B-O4B-C1B	3.56	113.63	109.72
2	B	618	FAD	C4-C4X-N5	3.63	123.13	118.72
2	B	618	FAD	O3P-PA-O5B	4.36	114.51	102.94
2	A	618	FAD	C4X-N5-C5X	5.73	123.36	116.76
2	B	618	FAD	C4X-N5-C5X	5.79	123.43	116.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	618	FAD	4	0
2	B	618	FAD	2	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	603/637 (94%)	-0.20	4 (0%) 89 83	31, 60, 99, 118	0
1	B	601/637 (94%)	-0.01	18 (2%) 54 39	32, 72, 123, 147	0
All	All	1204/1274 (94%)	-0.10	22 (1%) 71 58	31, 67, 112, 147	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	513	TYR	5.1
1	B	503	TYR	4.3
1	B	527	PRO	4.1
1	B	486	PHE	3.8
1	B	522	PHE	3.7
1	B	487	TYR	3.1
1	B	572	LYS	2.9
1	B	329	TRP	2.9
1	B	505	VAL	2.7
1	B	526	VAL	2.7
1	B	243	GLY	2.5
1	B	518	VAL	2.4
1	B	91	LYS	2.4
1	A	513	TYR	2.3
1	A	573	ILE	2.3
1	B	521	LYS	2.3
1	B	524	TYR	2.3
1	A	572	LYS	2.3
1	A	520	GLU	2.2
1	B	540	LEU	2.2
1	B	490	GLU	2.2
1	B	568	ILE	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
2	FAD	B	618	53/53	0.95	0.26	1.19	39,65,78,78	0
2	FAD	A	618	53/53	0.96	0.22	0.53	23,47,66,73	0
3	PO4	A	619	5/5	0.82	0.23	-0.38	118,119,123,127	0
3	PO4	A	620	5/5	0.87	0.21	-0.68	120,122,126,127	0
3	PO4	B	619	5/5	0.93	0.16	-2.07	123,124,128,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.