



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:02 PM UTC

PDB ID : 1NIP / pdb_00001nip
Title : CRYSTALLOGRAPHIC STRUCTURE OF THE NITROGENASE IRON
PROTEIN FROM AZOTOBACTER VINELANDII
Authors : Komiya, H.; Georgiadis, M.M.; Chakrabarti, P.; Woo, D.; Kornuc, J.J.; Rees,
D.C.
Deposited on : 1992-09-29
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

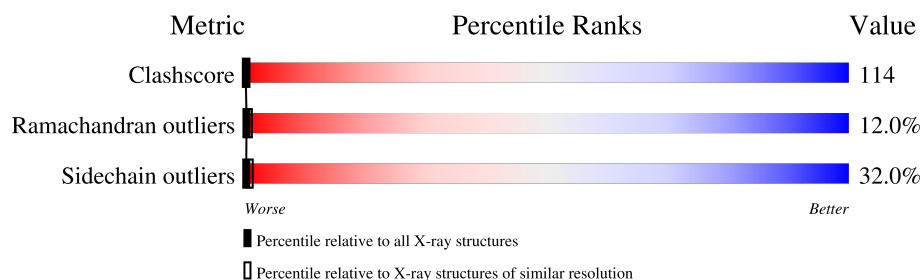
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	B	292	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4164 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.

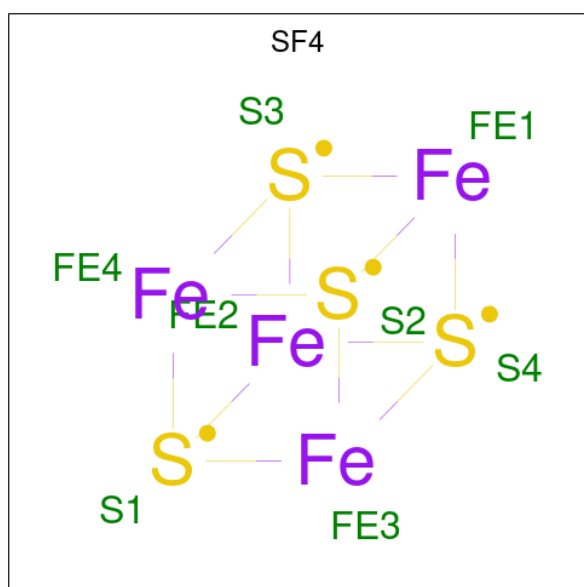
- Molecule 1 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2048	1285	342	401	20			
1	B	287	Total	C	N	O	S	0	0	0
			2062	1294	347	400	21			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

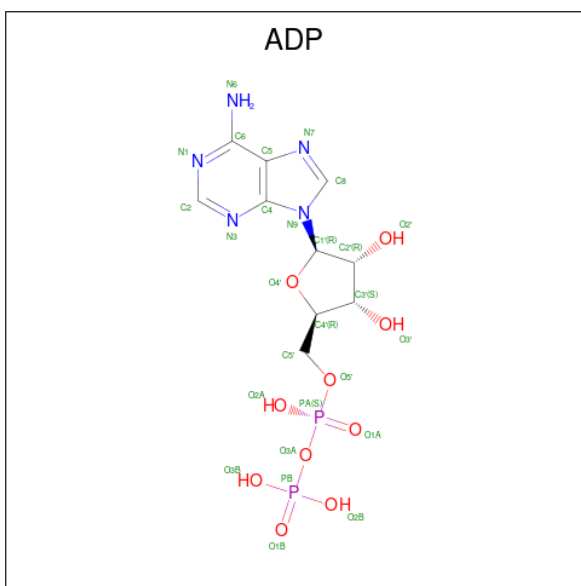
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is water.

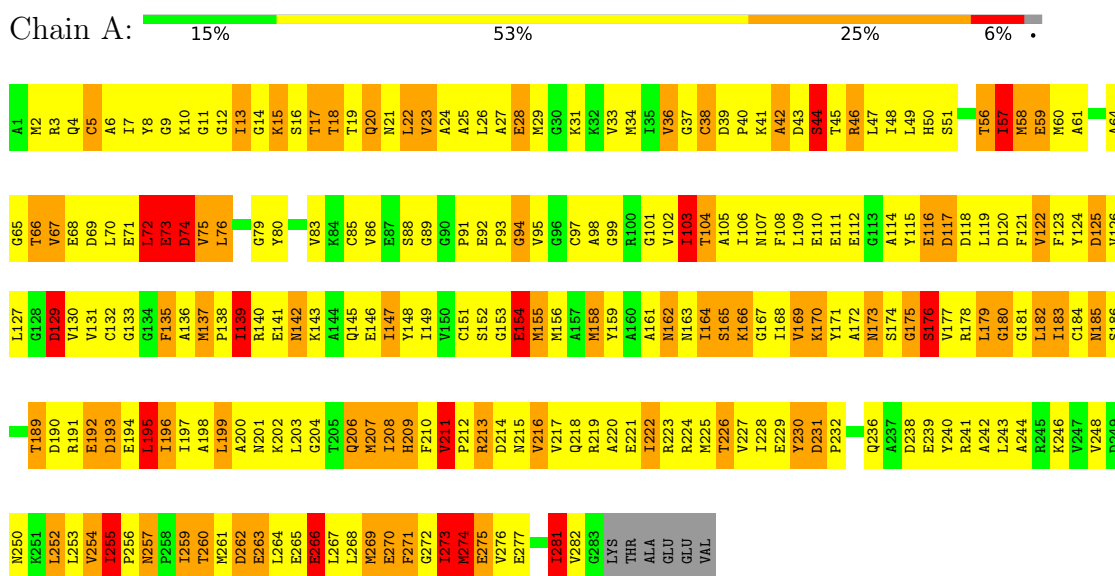
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	12	Total O 12 12	0	0

3 Residue-property plots

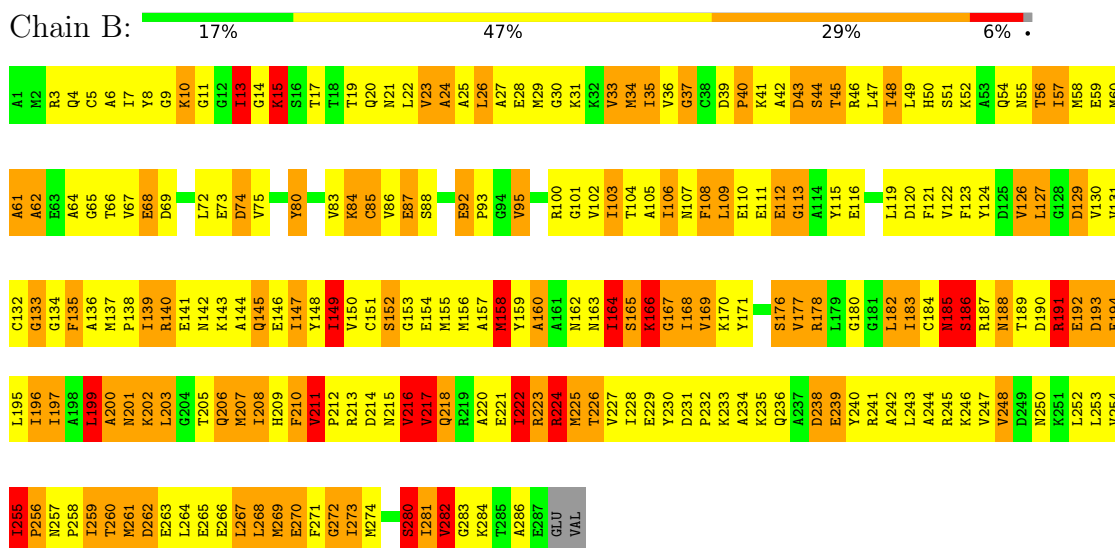
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: NITROGENASE IRON PROTEIN



• Molecule 1: NITROGENASE IRON PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.80Å 92.90Å 63.60Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ADP

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	1.19	2/2072 (0.1%)	1.66	22/2808 (0.8%)
1	B	1.14	2/2085 (0.1%)	1.70	38/2822 (1.3%)
All	All	1.16	4/4157 (0.1%)	1.68	60/5630 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	B	2	4
All	All	3	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ILE	N-CA	-6.51	1.41	1.46
1	A	112	GLU	CD-OE2	5.49	1.35	1.25
1	B	145	GLN	CD-NE2	-5.13	1.22	1.33
1	B	165	SER	CA-C	-5.08	1.47	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	VAL	N-CA-C	8.08	116.25	107.60
1	A	211	VAL	CA-C-N	8.07	127.96	120.21
1	A	211	VAL	C-N-CA	8.07	127.96	120.21
1	B	191	ARG	N-CA-C	7.78	122.21	111.55
1	B	120	ASP	CA-CB-CG	-7.24	105.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CA-CB-CG	-6.95	105.66	112.60
1	A	259	ILE	N-CA-CB	-6.84	104.28	112.07
1	B	75	VAL	CB-CA-C	-6.82	103.24	111.97
1	B	135	PHE	CA-CB-CG	-6.67	107.14	113.80
1	A	135	PHE	N-CA-C	-6.64	103.58	112.94
1	B	166	LYS	N-CA-C	-6.63	103.26	111.75
1	A	154	GLU	N-CA-C	6.45	119.78	108.75
1	B	152	SER	N-CA-C	6.33	117.75	108.14
1	A	263	GLU	N-CA-C	-6.23	104.41	111.07
1	A	189	THR	CB-CA-C	6.21	119.78	109.53
1	B	149	ILE	CB-CA-C	-6.18	105.25	111.80
1	B	186	SER	N-CA-CB	6.13	119.45	109.95
1	B	84	LYS	CB-CA-C	6.11	119.79	109.84
1	B	61	ALA	N-CA-C	-6.07	103.98	111.33
1	B	248	VAL	CB-CA-C	-5.90	104.33	111.88
1	A	274	MET	N-CA-CB	5.87	117.85	110.45
1	A	123	PHE	CA-CB-CG	-5.85	107.95	113.80
1	B	191	ARG	CB-CA-C	5.85	118.94	111.40
1	B	191	ARG	N-CA-CB	5.82	118.39	110.42
1	B	282	VAL	CA-C-N	5.81	132.80	121.41
1	B	282	VAL	C-N-CA	5.81	132.80	121.41
1	B	126	VAL	N-CA-C	5.76	117.00	108.65
1	B	160	ALA	O-C-N	5.71	128.19	122.08
1	B	255	ILE	CA-C-N	5.67	126.92	119.84
1	B	255	ILE	C-N-CA	5.67	126.92	119.84
1	B	149	ILE	N-CA-CB	-5.66	105.79	111.90
1	B	192	GLU	O-C-N	5.61	127.87	122.03
1	A	231	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	42	ALA	N-CA-C	5.61	119.05	110.36
1	B	87	GLU	N-CA-CB	5.59	119.54	110.42
1	A	154	GLU	CA-C-N	5.54	132.13	121.54
1	A	154	GLU	C-N-CA	5.54	132.13	121.54
1	B	13	ILE	CB-CA-C	-5.52	104.81	112.04
1	A	20	GLN	CA-C-N	-5.51	112.47	120.29
1	A	20	GLN	C-N-CA	-5.51	112.47	120.29
1	B	185	ASN	CA-C-N	-5.45	113.70	121.50
1	B	185	ASN	C-N-CA	-5.45	113.70	121.50
1	A	65	GLY	N-CA-C	-5.45	107.41	113.79
1	B	166	LYS	O-C-N	5.45	128.41	122.20
1	B	261	MET	O-C-N	5.44	127.91	122.03
1	A	162	ASN	N-CA-CB	-5.40	101.61	109.82
1	A	57	ILE	CB-CA-C	-5.37	105.10	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLU	N-CA-C	-5.36	105.55	111.71
1	A	257	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	86	VAL	CA-C-N	-5.29	115.73	122.77
1	B	86	VAL	C-N-CA	-5.29	115.73	122.77
1	B	167	GLY	CA-C-N	5.29	127.70	120.77
1	B	167	GLY	C-N-CA	5.29	127.70	120.77
1	B	158	MET	CB-CA-C	-5.28	102.53	110.92
1	A	183	ILE	N-CA-CB	-5.25	105.52	112.34
1	B	51	SER	N-CA-CB	5.13	118.79	110.17
1	B	40	PRO	N-CA-C	-5.12	106.54	113.40
1	B	186	SER	N-CA-C	5.10	117.88	109.76
1	B	108	PHE	CA-C-N	5.09	127.36	120.38
1	B	108	PHE	C-N-CA	5.09	127.36	120.38

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	43	ASP	CA
1	B	84	LYS	CA
1	B	191	ARG	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASP	Mainchain
1	A	139	ILE	Mainchain
1	A	269	MET	Mainchain
1	B	200	ALA	Mainchain
1	B	206	GLN	Mainchain
1	B	282	VAL	Mainchain
1	B	80	TYR	Sidechain

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	2048	0	1979	451	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2062	0	1982	483	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	8	0	0	0	0
4	B	27	0	12	29	0
5	A	5	0	0	1	0
5	B	12	0	0	4	0
All	All	4164	0	3973	922	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 114.

All (922) 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:48:ILE:HG22	1:A:79:GLY:HA3	1.25	1.11
1:A:151:CYS:HB3	1:A:196:ILE:HD11	1.34	1.07
1:A:8:TYR:CZ	1:A:126:VAL:HG11	1.97	1.00
1:A:197:ILE:HG13	1:A:207:MET:HE3	1.44	0.99
1:A:41:LYS:CD	4:B:292:ADP:H5'2	1.95	0.97
1:B:209:HIS:CD2	1:B:210:PHE:H	1.82	0.97
1:A:197:ILE:HG13	1:A:207:MET:CE	1.95	0.96
1:A:140:ARG:HG3	1:A:171:TYR:HE1	1.30	0.96
1:A:273:ILE:H	1:A:273:ILE:HD12	1.30	0.96
1:B:209:HIS:HD2	1:B:210:PHE:H	1.02	0.96
1:A:151:CYS:HB3	1:A:196:ILE:CD1	1.98	0.94
1:A:168:ILE:HD12	1:A:168:ILE:H	1.31	0.94
1:B:129:ASP:HA	4:B:292:ADP:O2'	1.67	0.93
1:A:169:VAL:HG12	1:A:170:LYS:N	1.82	0.93
1:B:10:LYS:HG2	1:B:13:ILE:CD1	2.00	0.92
1:A:6:ALA:CB	1:A:124:TYR:HB2	2.00	0.92
1:A:268:LEU:HB2	1:A:274:MET:HG2	1.52	0.92
1:A:148:TYR:HD1	1:A:181:GLY:H	1.17	0.92
1:A:209:HIS:HB2	1:A:243:LEU:HD13	1.50	0.91
1:B:8:TYR:O	1:B:15:LYS:HD2	1.71	0.90
1:A:8:TYR:HD2	1:A:164:ILE:HD11	1.34	0.90
1:B:196:ILE:HB	1:B:207:MET:HE2	1.52	0.90
1:A:161:ALA:O	1:A:164:ILE:HG22	1.72	0.90
1:B:137:MET:HE1	1:B:140:ARG:HD3	1.53	0.90
1:A:148:TYR:CE1	1:A:180:GLY:HA3	2.07	0.89
1:A:136:ALA:O	1:A:139:ILE:HB	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HD11	1:B:264:LEU:HB2	1.55	0.88
1:A:266:GLU:HG2	1:A:267:LEU:HD12	1.55	0.88
1:A:273:ILE:H	1:A:273:ILE:CD1	1.86	0.88
1:B:268:LEU:HB3	1:B:274:MET:HG2	1.55	0.88
1:A:169:VAL:O	1:A:172:ALA:N	2.07	0.88
1:A:214:ASP:O	1:A:217:VAL:HG23	1.73	0.88
1:A:236:GLN:HG3	1:A:240:TYR:CE2	2.10	0.87
1:A:142:ASN:HD21	1:A:176:SER:HB3	1.38	0.87
1:A:230:TYR:CE1	1:B:284:LYS:HA	2.10	0.87
1:B:184:CYS:HB2	1:B:196:ILE:HG13	1.55	0.87
1:B:268:LEU:HD22	1:B:273:ILE:CG2	2.04	0.87
1:B:54:GLN:HG2	1:B:55:ASN:N	1.90	0.87
1:A:33:VAL:HG22	1:A:121:PHE:HB2	1.57	0.87
1:A:8:TYR:CD2	1:A:164:ILE:HD11	2.11	0.86
1:A:141:GLU:O	1:A:143:LYS:HG2	1.76	0.85
1:B:10:LYS:HG2	1:B:13:ILE:HD13	1.58	0.85
1:A:158:MET:HE1	1:A:195:LEU:HD21	1.57	0.85
1:B:72:LEU:HD13	1:B:112:GLU:HB3	1.58	0.85
1:B:3:ARG:HB2	1:B:121:PHE:CE1	2.11	0.84
1:B:182:LEU:HD13	1:B:205:THR:HG21	1.57	0.84
1:A:151:CYS:CB	1:A:196:ILE:HD11	2.08	0.84
1:B:52:LYS:H	1:B:224:ARG:HH21	1.26	0.83
1:B:225:MET:HE1	1:B:230:TYR:HA	1.60	0.83
1:A:12:GLY:N	4:B:292:ADP:O1B	2.10	0.83
1:A:165:SER:HA	1:A:168:ILE:HD13	1.58	0.83
1:B:259:ILE:HG12	1:B:260:THR:N	1.94	0.83
1:B:6:ALA:CB	1:B:124:TYR:HB2	2.09	0.83
1:B:243:LEU:O	1:B:247:VAL:HG23	1.78	0.83
1:B:268:LEU:CB	1:B:274:MET:HG2	2.09	0.83
1:A:41:LYS:HZ2	4:B:292:ADP:C5'	1.90	0.83
1:B:160:ALA:O	1:B:164:ILE:HG13	1.77	0.82
1:A:103:ILE:HG22	1:A:104:THR:N	1.94	0.82
1:B:59:GLU:O	1:B:62:ALA:HB3	1.79	0.82
1:B:236:GLN:O	1:B:239:GLU:HB2	1.78	0.82
1:A:46:ARG:HD2	1:A:51:SER:O	1.77	0.82
1:A:140:ARG:HG3	1:A:171:TYR:CE1	2.14	0.82
1:A:209:HIS:CB	1:A:243:LEU:HD13	2.09	0.82
1:A:211:VAL:HG12	1:A:212:PRO:HD2	1.62	0.82
1:B:6:ALA:HB2	1:B:124:TYR:HB2	1.61	0.82
1:A:45:THR:HG21	1:A:49:LEU:HD12	1.60	0.81
1:B:242:ALA:O	1:B:246:LYS:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLU:OE1	1:B:239:GLU:HA	1.78	0.81
1:A:172:ALA:O	1:A:175:GLY:N	2.13	0.81
1:B:137:MET:CE	1:B:140:ARG:HD3	2.11	0.81
1:B:206:GLN:HE21	1:B:208:ILE:HD11	1.45	0.81
1:A:6:ALA:HB1	1:A:124:TYR:HB2	1.63	0.81
1:B:268:LEU:HD22	1:B:273:ILE:HG21	1.61	0.81
1:A:169:VAL:O	1:A:171:TYR:N	2.14	0.80
1:A:42:ALA:HB2	4:B:292:ADP:O2B	1.82	0.80
1:B:10:LYS:HB2	4:B:292:ADP:O2'	1.82	0.80
1:B:15:LYS:HE2	1:B:126:VAL:O	1.81	0.80
1:B:33:VAL:HG23	1:B:121:PHE:HB2	1.64	0.80
1:B:103:ILE:HG13	1:B:137:MET:HG2	1.64	0.79
1:A:45:THR:CG2	1:A:49:LEU:HD12	2.12	0.79
1:B:136:ALA:O	1:B:139:ILE:HB	1.81	0.79
1:B:214:ASP:HB3	1:B:236:GLN:NE2	1.97	0.79
1:A:57:ILE:HG13	1:A:75:VAL:CG1	2.12	0.79
1:B:206:GLN:CD	1:B:252:LEU:HD23	2.06	0.79
1:A:238:ASP:OD1	1:A:241:ARG:NH1	2.15	0.79
1:B:221:GLU:O	1:B:224:ARG:N	2.14	0.79
1:B:231:ASP:HB3	1:B:234:ALA:HB2	1.64	0.79
1:A:230:TYR:O	1:A:232:PRO:HD3	1.83	0.79
1:B:21:ASN:HD21	1:B:227:VAL:CG2	1.96	0.79
1:A:22:LEU:CD1	1:A:243:LEU:HD23	2.12	0.79
1:A:48:ILE:CG2	1:A:79:GLY:HA3	2.10	0.79
1:A:6:ALA:HB2	1:A:124:TYR:HB2	1.66	0.78
1:B:15:LYS:NZ	1:B:15:LYS:HB3	1.98	0.78
1:B:214:ASP:HB3	1:B:236:GLN:HE21	1.48	0.78
1:B:196:ILE:CB	1:B:207:MET:HE2	2.14	0.78
1:B:225:MET:HE3	1:B:230:TYR:HB2	1.66	0.78
1:B:47:LEU:O	1:B:225:MET:HA	1.83	0.78
1:B:255:ILE:N	1:B:255:ILE:HD12	1.98	0.78
1:B:282:VAL:HG13	1:B:283:GLY:N	1.99	0.78
1:B:20:GLN:OE1	1:B:47:LEU:HB2	1.82	0.78
1:B:66:THR:HG22	1:B:68:GLU:H	1.49	0.77
1:A:254:VAL:HG12	1:A:255:ILE:O	1.84	0.77
1:A:14:GLY:HA2	5:A:5011:HOH:O	1.85	0.77
1:A:57:ILE:O	1:A:60:MET:N	2.18	0.77
1:B:52:LYS:CA	1:B:224:ARG:HE	1.97	0.77
1:B:152:SER:OG	1:B:153:GLY:N	2.11	0.77
1:A:26:LEU:HD12	1:A:244:ALA:HB1	1.67	0.77
1:A:269:MET:CG	1:A:274:MET:HE2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TYR:HB3	1:A:164:ILE:HD11	1.66	0.77
1:A:268:LEU:CB	1:A:274:MET:HG2	2.15	0.77
1:A:48:ILE:HG22	1:A:79:GLY:CA	2.12	0.76
1:B:196:ILE:CG2	1:B:207:MET:HE2	2.15	0.76
1:B:156:MET:O	1:B:159:TYR:N	2.18	0.76
1:A:41:LYS:HZ2	4:B:292:ADP:H5'2	1.50	0.76
1:A:41:LYS:HD2	4:B:292:ADP:H5'2	1.67	0.76
1:A:281:ILE:HG23	1:B:223:ARG:O	1.86	0.76
1:B:58:MET:HE1	1:B:101:GLY:HA2	1.67	0.76
1:B:54:GLN:HG2	1:B:55:ASN:H	1.47	0.76
1:B:166:LYS:O	1:B:170:LYS:HG2	1.84	0.76
1:A:252:LEU:C	1:A:253:LEU:HD23	2.11	0.75
1:B:23:VAL:HG11	1:B:33:VAL:HG11	1.66	0.75
1:A:182:LEU:HD23	1:A:182:LEU:N	1.98	0.75
1:A:8:TYR:HB3	1:A:164:ILE:CD1	2.16	0.75
1:A:155:MET:HG3	1:A:156:MET:HG2	1.69	0.75
1:B:58:MET:CE	1:B:101:GLY:HA2	2.17	0.75
1:A:48:ILE:HG21	1:A:83:VAL:HB	1.69	0.74
1:B:178:ARG:HE	1:B:255:ILE:HD11	1.52	0.74
1:B:101:GLY:O	1:B:104:THR:HB	1.87	0.74
1:A:209:HIS:HE1	1:A:242:ALA:HB3	1.52	0.74
1:B:244:ALA:O	1:B:248:VAL:HG23	1.88	0.74
1:A:155:MET:CG	1:A:156:MET:HE2	2.17	0.74
1:B:56:THR:O	1:B:60:MET:HG2	1.87	0.74
1:B:64:ALA:HB1	1:B:69:ASP:CG	2.13	0.74
1:A:39:ASP:OD1	1:A:40:PRO:HD2	1.87	0.74
1:A:252:LEU:O	1:A:253:LEU:HD23	1.88	0.74
1:A:259:ILE:HG22	1:A:263:GLU:CB	2.18	0.73
1:A:266:GLU:HG2	1:A:267:LEU:N	2.01	0.73
1:B:140:ARG:HB2	1:B:171:TYR:CE2	2.24	0.73
1:A:41:LYS:NZ	4:B:292:ADP:H5'2	2.03	0.73
1:B:199:LEU:O	1:B:202:LYS:N	2.22	0.73
1:B:34:MET:HA	1:B:84:LYS:HA	1.71	0.73
1:A:57:ILE:HG13	1:A:75:VAL:HG13	1.71	0.72
1:A:274:MET:O	1:A:274:MET:HG3	1.89	0.72
1:B:182:LEU:CD1	1:B:182:LEU:N	2.52	0.72
1:B:250:ASN:OD1	1:B:252:LEU:N	2.22	0.72
1:A:137:MET:HB2	1:A:138:PRO:HD3	1.71	0.72
1:B:10:LYS:HD2	4:B:292:ADP:H1'	1.69	0.72
1:B:139:ILE:O	1:B:142:ASN:N	2.21	0.72
1:A:94:GLY:H	1:B:131:VAL:HG12	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:MET:HG2	1:A:156:MET:HE2	1.70	0.72
1:B:231:ASP:OD1	1:B:234:ALA:N	2.22	0.72
1:B:196:ILE:HD13	1:B:196:ILE:N	2.04	0.72
1:A:41:LYS:CE	4:B:292:ADP:H5'2	2.19	0.71
1:A:196:ILE:HG21	1:A:207:MET:HG3	1.70	0.71
1:B:126:VAL:HG12	1:B:127:LEU:N	2.05	0.71
1:B:21:ASN:HD21	1:B:227:VAL:HB	1.53	0.71
1:B:52:LYS:H	1:B:224:ARG:NH2	1.87	0.71
1:A:196:ILE:HG22	1:A:207:MET:CE	2.20	0.71
1:B:20:GLN:HE22	1:B:46:ARG:H	1.38	0.71
1:B:178:ARG:HH11	1:B:178:ARG:HG2	1.56	0.71
1:A:158:MET:CE	1:A:195:LEU:HD21	2.20	0.71
1:B:21:ASN:HD21	1:B:227:VAL:CB	2.04	0.71
1:B:29:MET:HE3	1:B:244:ALA:HB3	1.72	0.70
1:B:267:LEU:HD23	1:B:267:LEU:N	2.06	0.70
1:A:103:ILE:HG23	1:A:107:ASN:HD21	1.57	0.70
1:B:56:THR:CG2	1:B:59:GLU:HG3	2.21	0.70
1:B:264:LEU:O	1:B:264:LEU:HD23	1.91	0.70
1:B:3:ARG:NH2	1:B:146:GLU:OE1	2.23	0.70
1:B:282:VAL:CG1	1:B:283:GLY:N	2.53	0.70
1:A:139:ILE:O	1:A:142:ASN:N	2.24	0.70
1:B:39:ASP:OD1	1:B:41:LYS:N	2.24	0.70
1:B:72:LEU:CD1	1:B:112:GLU:HB3	2.21	0.70
1:A:186:SER:HB3	1:A:210:PHE:CE1	2.26	0.70
1:B:220:ALA:CB	1:B:227:VAL:HG22	2.21	0.70
1:A:252:LEU:O	1:A:252:LEU:HD23	1.92	0.70
1:B:3:ARG:NH1	1:B:248:VAL:HA	2.07	0.70
1:A:8:TYR:CE1	1:A:126:VAL:HG21	2.26	0.69
1:A:56:THR:OG1	1:A:59:GLU:HB2	1.92	0.69
1:A:142:ASN:HD21	1:A:176:SER:CB	2.04	0.69
1:B:196:ILE:HB	1:B:207:MET:CE	2.22	0.69
1:A:136:ALA:C	1:A:138:PRO:HD2	2.16	0.69
1:B:140:ARG:HA	1:B:171:TYR:CD2	2.26	0.69
1:A:45:THR:HG22	1:A:46:ARG:N	2.07	0.69
1:A:208:ILE:O	1:A:246:LYS:NZ	2.25	0.69
1:A:57:ILE:HG22	1:A:58:MET:N	2.05	0.69
1:A:200:ALA:O	1:A:204:GLY:N	2.25	0.69
1:A:196:ILE:HG22	1:A:207:MET:HE2	1.73	0.69
1:B:34:MET:HG3	1:B:84:LYS:HB2	1.73	0.69
1:A:165:SER:HA	1:A:168:ILE:CD1	2.22	0.69
1:A:211:VAL:CG1	1:A:212:PRO:HD2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:HG2	1:B:178:ARG:NH1	2.08	0.69
1:B:203:LEU:O	1:B:257:ASN:HB3	1.93	0.69
1:B:209:HIS:CD2	1:B:210:PHE:N	2.60	0.69
1:B:260:THR:OG1	1:B:262:ASP:HB2	1.92	0.69
1:A:60:MET:CE	1:A:74:ASP:HB3	2.23	0.69
1:B:178:ARG:HH21	1:B:255:ILE:HD11	1.58	0.69
1:A:36:VAL:HG12	1:A:38:CYS:SG	2.34	0.68
1:B:208:ILE:CG2	1:B:243:LEU:HD13	2.22	0.68
1:B:274:MET:O	1:B:274:MET:HG3	1.92	0.68
1:A:46:ARG:HE	1:A:224:ARG:HG3	1.58	0.68
1:A:238:ASP:O	1:A:241:ARG:N	2.27	0.68
1:A:26:LEU:CD1	1:A:244:ALA:HB1	2.22	0.68
1:A:218:GLN:O	1:A:221:GLU:N	2.26	0.68
1:A:41:LYS:HZ2	4:B:292:ADP:H5'1	1.58	0.68
1:B:23:VAL:CG1	1:B:33:VAL:HG11	2.23	0.68
1:B:56:THR:HG22	1:B:59:GLU:H	1.59	0.68
1:B:140:ARG:HA	1:B:171:TYR:CE2	2.28	0.68
1:A:181:GLY:C	1:A:182:LEU:HD23	2.18	0.68
1:A:194:GLU:O	1:A:197:ILE:HB	1.93	0.68
1:A:271:PHE:HB2	1:A:273:ILE:HD13	1.74	0.68
1:B:243:LEU:O	1:B:243:LEU:HD12	1.93	0.68
1:B:3:ARG:HB2	1:B:121:PHE:CD1	2.29	0.68
1:A:47:LEU:HD23	1:A:224:ARG:C	2.19	0.67
1:B:139:ILE:HG22	1:B:140:ARG:N	2.08	0.67
1:B:255:ILE:O	1:B:256:PRO:O	2.12	0.67
1:A:281:ILE:HD13	1:B:224:ARG:HB3	1.76	0.67
1:A:214:ASP:OD1	1:A:216:VAL:HB	1.94	0.67
1:B:72:LEU:HD13	1:B:112:GLU:CB	2.23	0.67
1:B:184:CYS:HB2	1:B:196:ILE:CG1	2.25	0.67
1:B:217:VAL:O	1:B:220:ALA:N	2.27	0.67
1:B:260:THR:HG1	1:B:262:ASP:HB2	1.59	0.67
1:A:26:LEU:HD23	1:A:33:VAL:HG21	1.77	0.67
1:A:26:LEU:HD23	1:A:33:VAL:CG2	2.24	0.67
1:B:22:LEU:C	1:B:22:LEU:HD23	2.20	0.67
1:B:155:MET:O	1:B:155:MET:HG2	1.93	0.67
1:A:175:GLY:O	1:A:176:SER:HB2	1.94	0.67
1:A:206:GLN:HG2	1:A:252:LEU:HD22	1.75	0.67
1:B:260:THR:HG23	1:B:263:GLU:OE1	1.95	0.67
1:A:18:THR:HG21	1:A:185:ASN:HD21	1.59	0.66
1:B:33:VAL:CG1	1:B:83:VAL:HG13	2.26	0.66
1:A:196:ILE:CG2	1:A:207:MET:HG3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:O	1:A:106:ILE:N	2.29	0.66
1:B:221:GLU:C	1:B:223:ARG:H	2.02	0.66
1:A:14:GLY:O	1:A:17:THR:N	2.29	0.66
1:A:152:SER:O	1:A:154:GLU:N	2.28	0.66
1:B:93:PRO:C	1:B:95:VAL:H	2.04	0.66
1:B:216:VAL:O	1:B:220:ALA:N	2.29	0.66
1:B:257:ASN:OD1	1:B:258:PRO:HD2	1.95	0.66
1:A:192:GLU:O	1:A:195:LEU:N	2.29	0.66
1:A:197:ILE:HG13	1:A:207:MET:HE1	1.76	0.66
1:B:126:VAL:HG12	1:B:127:LEU:H	1.59	0.66
1:B:163:ASN:C	1:B:165:SER:H	2.03	0.66
1:B:225:MET:CE	1:B:230:TYR:HA	2.26	0.65
1:A:17:THR:HG22	1:A:18:THR:N	2.11	0.65
1:A:209:HIS:HE1	1:A:242:ALA:CB	2.09	0.65
1:B:56:THR:HG22	1:B:59:GLU:HG3	1.78	0.65
1:B:154:GLU:OE2	1:B:156:MET:N	2.23	0.65
1:B:24:ALA:CB	1:B:228:ILE:HG13	2.26	0.65
1:B:188:ASN:HD21	1:B:213:ARG:HD2	1.61	0.65
1:A:186:SER:HB3	1:A:210:PHE:CZ	2.32	0.65
1:A:214:ASP:O	1:A:216:VAL:N	2.30	0.65
1:B:23:VAL:O	1:B:26:LEU:N	2.30	0.65
1:B:103:ILE:HG22	1:B:104:THR:N	2.11	0.65
1:A:147:ILE:HG22	1:A:179:LEU:HA	1.78	0.65
1:A:158:MET:HE1	1:A:195:LEU:CD2	2.27	0.65
1:B:56:THR:HB	1:B:59:GLU:CD	2.21	0.65
1:A:169:VAL:CG1	1:A:170:LYS:N	2.55	0.65
1:B:108:PHE:HD2	1:B:109:LEU:HD23	1.60	0.65
1:A:236:GLN:HG3	1:A:240:TYR:HE2	1.62	0.65
1:B:163:ASN:O	1:B:165:SER:N	2.30	0.65
1:A:196:ILE:CG2	1:A:207:MET:HE2	2.27	0.64
1:A:201:ASN:O	1:A:204:GLY:N	2.29	0.64
1:B:31:LYS:NZ	1:B:248:VAL:HG11	2.12	0.64
1:B:39:ASP:OD1	1:B:40:PRO:HD2	1.96	0.64
1:B:54:GLN:NE2	1:B:55:ASN:O	2.26	0.64
1:B:160:ALA:C	1:B:164:ILE:HG13	2.22	0.64
1:B:214:ASP:O	1:B:217:VAL:HG23	1.97	0.64
1:B:221:GLU:O	1:B:223:ARG:N	2.30	0.64
1:A:229:GLU:O	1:A:230:TYR:O	2.15	0.64
1:A:139:ILE:HG22	1:A:140:ARG:N	2.13	0.64
1:B:184:CYS:CB	1:B:196:ILE:HG13	2.26	0.64
1:B:242:ALA:C	1:B:246:LYS:HG3	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HG12	1:A:127:LEU:H	1.62	0.64
1:A:168:ILE:O	1:A:169:VAL:O	2.15	0.64
1:A:209:HIS:HB2	1:A:243:LEU:CD1	2.24	0.64
1:A:209:HIS:CE1	1:A:242:ALA:HB3	2.32	0.64
1:B:162:ASN:ND2	1:B:259:ILE:HD13	2.12	0.64
1:B:255:ILE:N	1:B:255:ILE:CD1	2.60	0.64
1:B:192:GLU:O	1:B:195:LEU:N	2.31	0.64
1:A:80:TYR:O	1:A:83:VAL:HG23	1.98	0.64
1:B:158:MET:HE2	1:B:195:LEU:HD21	1.79	0.64
1:A:21:ASN:HB2	1:A:240:TYR:CD1	2.33	0.64
1:B:162:ASN:O	1:B:166:LYS:HD3	1.97	0.64
1:B:22:LEU:CD1	1:B:243:LEU:HG	2.28	0.63
1:A:159:TYR:O	1:A:163:ASN:ND2	2.30	0.63
1:B:137:MET:HE2	1:B:141:GLU:HG2	1.81	0.63
1:B:225:MET:CE	1:B:230:TYR:HB2	2.28	0.63
1:A:273:ILE:HD12	1:A:273:ILE:N	2.07	0.63
1:B:45:THR:O	1:B:45:THR:HG22	1.96	0.63
1:B:221:GLU:C	1:B:223:ARG:N	2.56	0.63
1:B:200:ALA:HB1	1:B:205:THR:O	1.99	0.63
1:A:60:MET:HE2	1:A:74:ASP:HB3	1.79	0.63
1:B:3:ARG:HD3	1:B:121:PHE:HE1	1.64	0.63
1:A:209:HIS:CG	1:A:246:LYS:HZ2	2.16	0.63
1:B:24:ALA:HB2	1:B:226:THR:HG21	1.81	0.62
1:B:22:LEU:HD12	1:B:243:LEU:CD2	2.28	0.62
1:A:262:ASP:O	1:A:266:GLU:HB3	1.99	0.62
1:B:40:PRO:HD2	1:B:127:LEU:CD2	2.29	0.62
1:A:31:LYS:HG3	1:A:120:ASP:HB3	1.82	0.62
1:B:29:MET:HE1	1:B:245:ARG:N	2.15	0.62
1:B:25:ALA:O	1:B:28:GLU:N	2.33	0.62
1:B:197:ILE:HG12	1:B:207:MET:HE3	1.82	0.62
1:A:2:MET:HE3	1:A:119:LEU:HB2	1.81	0.62
1:A:271:PHE:CD1	1:A:271:PHE:N	2.68	0.61
1:B:58:MET:O	1:B:62:ALA:N	2.26	0.61
1:B:260:THR:HG23	1:B:263:GLU:HG3	1.82	0.61
1:B:261:MET:O	1:B:264:LEU:N	2.33	0.61
1:A:147:ILE:O	1:A:180:GLY:N	2.32	0.61
1:A:102:VAL:O	1:A:105:ALA:HB3	2.00	0.61
1:B:169:VAL:HG12	1:B:170:LYS:N	2.15	0.61
1:B:236:GLN:HG3	1:B:240:TYR:CE2	2.36	0.61
1:A:126:VAL:HG12	1:A:127:LEU:N	2.14	0.61
1:A:149:ILE:HG12	1:A:164:ILE:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:CYS:O	1:B:123:PHE:HA	2.00	0.61
1:B:33:VAL:HG22	1:B:34:MET:H	1.66	0.61
1:B:165:SER:C	1:B:167:GLY:N	2.55	0.61
1:B:236:GLN:HA	1:B:239:GLU:HB2	1.81	0.61
1:B:21:ASN:ND2	1:B:227:VAL:HB	2.15	0.60
1:A:5:CYS:HB3	1:A:146:GLU:O	2.01	0.60
1:A:33:VAL:HG12	1:A:34:MET:N	2.16	0.60
1:B:137:MET:O	1:B:141:GLU:N	2.25	0.60
1:B:254:VAL:HG12	1:B:255:ILE:N	2.16	0.60
1:B:52:LYS:HA	1:B:224:ARG:HE	1.67	0.60
1:B:31:LYS:HZ1	1:B:248:VAL:HG11	1.64	0.60
1:A:45:THR:HG21	1:A:85:CYS:HB3	1.82	0.60
1:A:73:GLU:O	1:A:75:VAL:N	2.35	0.60
1:B:13:ILE:HG22	1:B:14:GLY:N	2.16	0.60
1:B:206:GLN:NE2	1:B:208:ILE:HD11	2.13	0.60
1:B:80:TYR:OH	1:B:228:ILE:HG22	2.00	0.60
1:A:41:LYS:NZ	1:A:129:ASP:OD2	2.34	0.60
1:B:29:MET:HE3	1:B:244:ALA:CB	2.32	0.59
1:A:8:TYR:CE1	1:A:126:VAL:HG11	2.37	0.59
1:A:93:PRO:O	1:A:95:VAL:N	2.34	0.59
1:B:166:LYS:HD2	1:B:258:PRO:HB3	1.84	0.59
1:B:184:CYS:HB2	1:B:196:ILE:HG21	1.84	0.59
1:A:184:CYS:HB2	1:A:196:ILE:HD12	1.85	0.59
1:A:195:LEU:O	1:A:198:ALA:N	2.35	0.59
1:A:270:GLU:HB3	1:A:271:PHE:CD1	2.37	0.59
1:B:162:ASN:ND2	1:B:259:ILE:HG23	2.18	0.59
1:A:10:LYS:NZ	1:A:154:GLU:OE2	2.33	0.59
1:A:178:ARG:HG3	1:A:255:ILE:CD1	2.33	0.59
1:B:177:VAL:O	1:B:178:ARG:HG2	2.02	0.59
1:A:41:LYS:HD3	4:B:292:ADP:C8	2.37	0.59
1:A:92:GLU:OE2	1:A:95:VAL:O	2.20	0.59
1:A:206:GLN:HG2	1:A:252:LEU:CD2	2.33	0.59
1:A:47:LEU:HD23	1:A:225:MET:N	2.18	0.59
1:B:178:ARG:HH11	1:B:178:ARG:CG	2.16	0.59
1:B:178:ARG:NE	1:B:255:ILE:HD11	2.17	0.59
1:B:197:ILE:HG12	1:B:207:MET:CE	2.33	0.59
1:B:214:ASP:O	1:B:216:VAL:N	2.36	0.59
1:B:10:LYS:HG3	1:B:11:GLY:N	2.18	0.58
1:B:206:GLN:HE21	1:B:208:ILE:CD1	2.14	0.58
1:A:214:ASP:O	1:A:217:VAL:N	2.34	0.58
1:A:236:GLN:OE1	1:A:236:GLN:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PHE:O	1:B:138:PRO:HD2	2.04	0.58
1:B:178:ARG:NH2	1:B:255:ILE:HD11	2.19	0.58
1:B:137:MET:HE3	1:B:140:ARG:HG2	1.85	0.58
1:B:260:THR:HG23	1:B:263:GLU:CD	2.29	0.58
1:A:41:LYS:HD3	4:B:292:ADP:N7	2.19	0.58
1:A:66:THR:O	1:A:69:ASP:OD2	2.22	0.58
1:A:137:MET:N	1:A:138:PRO:HD2	2.18	0.58
1:A:106:ILE:HG22	1:A:110:GLU:OE2	2.03	0.57
1:A:248:VAL:HG12	1:A:248:VAL:O	2.04	0.57
1:A:266:GLU:O	1:A:270:GLU:N	2.33	0.57
1:B:43:ASP:HB3	1:B:46:ARG:HB2	1.85	0.57
1:A:41:LYS:HD2	4:B:292:ADP:C5'	2.34	0.57
1:A:230:TYR:C	1:B:284:LYS:CB	2.78	0.57
1:A:33:VAL:CG1	1:A:34:MET:N	2.67	0.57
1:B:182:LEU:CD1	1:B:205:THR:HG21	2.34	0.57
1:A:270:GLU:HB3	1:A:271:PHE:HD1	1.69	0.57
1:B:40:PRO:CD	1:B:41:LYS:H	2.16	0.57
1:A:259:ILE:HG22	1:A:263:GLU:HB2	1.87	0.57
1:B:162:ASN:O	1:B:165:SER:HB2	2.05	0.57
1:A:76:LEU:HD12	1:A:86:VAL:CG2	2.34	0.57
1:A:183:ILE:HD13	1:A:243:LEU:HD21	1.85	0.57
1:A:95:VAL:O	1:A:95:VAL:HG12	2.05	0.57
1:A:162:ASN:O	1:A:166:LYS:HG3	2.05	0.57
1:A:213:ARG:O	1:A:213:ARG:HG3	2.04	0.57
1:B:35:ILE:HG12	1:B:45:THR:OG1	2.04	0.57
1:B:106:ILE:O	1:B:110:GLU:HG3	2.04	0.56
1:A:259:ILE:HG22	1:A:263:GLU:HB3	1.86	0.56
1:B:24:ALA:HB1	1:B:228:ILE:HG13	1.87	0.56
1:B:225:MET:CE	1:B:230:TYR:CA	2.83	0.56
1:A:230:TYR:CD1	1:B:284:LYS:CB	2.88	0.56
1:B:22:LEU:HD12	1:B:243:LEU:HG	1.88	0.56
1:A:6:ALA:HA	1:A:124:TYR:H	1.71	0.56
1:A:110:GLU:CD	1:A:143:LYS:HZ2	2.14	0.56
1:A:197:ILE:CG1	1:A:207:MET:HE3	2.30	0.56
1:A:66:THR:HG22	1:A:68:GLU:H	1.69	0.56
1:B:208:ILE:HG22	1:B:243:LEU:HD13	1.88	0.56
1:A:271:PHE:CB	1:A:273:ILE:HD13	2.35	0.56
1:B:137:MET:CE	1:B:141:GLU:HG2	2.35	0.56
1:B:236:GLN:O	1:B:239:GLU:CB	2.53	0.56
1:B:243:LEU:HD12	1:B:247:VAL:HG23	1.88	0.56
1:A:88:SER:OG	1:A:89:GLY:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:C	1:B:62:ALA:HB3	2.31	0.55
1:B:135:PHE:C	1:B:137:MET:H	2.13	0.55
1:A:103:ILE:HG23	1:A:107:ASN:ND2	2.21	0.55
1:B:260:THR:HG23	1:B:263:GLU:CG	2.36	0.55
1:A:264:LEU:O	1:A:268:LEU:HD12	2.07	0.55
1:B:225:MET:SD	1:B:229:GLU:HG2	2.47	0.55
1:A:165:SER:O	1:A:167:GLY:N	2.39	0.55
1:A:220:ALA:HB1	1:A:225:MET:O	2.05	0.55
1:B:52:LYS:CB	1:B:224:ARG:HH21	2.20	0.55
1:A:41:LYS:NZ	4:B:292:ADP:C5'	2.64	0.55
1:A:24:ALA:O	1:A:27:ALA:HB3	2.06	0.55
1:B:105:ALA:O	1:B:108:PHE:HB3	2.07	0.55
1:B:178:ARG:HE	1:B:255:ILE:CD1	2.19	0.55
1:B:83:VAL:HG22	5:B:295:HOH:O	2.06	0.55
1:B:140:ARG:HG2	1:B:141:GLU:N	2.21	0.55
1:B:241:ARG:O	1:B:244:ALA:HB3	2.06	0.55
1:A:232:PRO:O	1:A:241:ARG:NH2	2.40	0.55
1:B:25:ALA:O	1:B:27:ALA:N	2.39	0.55
1:B:182:LEU:HD13	1:B:182:LEU:N	2.22	0.55
1:A:49:LEU:HD11	1:A:85:CYS:HB2	1.88	0.54
1:B:163:ASN:C	1:B:165:SER:N	2.61	0.54
1:B:199:LEU:O	1:B:200:ALA:C	2.50	0.54
1:A:45:THR:CG2	1:A:85:CYS:HB3	2.37	0.54
1:B:15:LYS:HB3	1:B:15:LYS:HZ2	1.69	0.54
1:A:4:GLN:O	1:A:145:GLN:N	2.24	0.54
1:A:22:LEU:HD11	1:A:243:LEU:HD23	1.88	0.54
1:B:33:VAL:HG22	1:B:34:MET:N	2.23	0.54
1:B:196:ILE:HG22	1:B:207:MET:HE2	1.90	0.54
1:A:46:ARG:HG2	1:A:47:LEU:HG	1.88	0.54
1:A:186:SER:HB2	1:A:192:GLU:OE1	2.08	0.54
1:A:137:MET:N	1:A:138:PRO:CD	2.71	0.54
1:B:10:LYS:HB2	4:B:292:ADP:HO2'	1.72	0.54
1:B:56:THR:HG23	1:B:58:MET:H	1.73	0.54
1:B:92:GLU:O	1:B:95:VAL:O	2.26	0.54
1:B:225:MET:O	1:B:225:MET:HG3	2.07	0.54
1:B:3:ARG:HD3	1:B:121:PHE:CE1	2.42	0.54
1:A:127:LEU:HG	1:A:129:ASP:H	1.73	0.54
1:B:3:ARG:O	1:B:121:PHE:HA	2.08	0.54
1:A:103:ILE:CG2	1:A:107:ASN:HD21	2.21	0.53
1:A:142:ASN:OD1	1:A:145:GLN:NE2	2.41	0.53
1:A:227:VAL:HG11	1:A:236:GLN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:MET:O	1:A:264:LEU:HB3	2.08	0.53
1:B:33:VAL:HG12	1:B:83:VAL:HG13	1.90	0.53
1:B:212:PRO:HG3	1:B:239:GLU:OE2	2.08	0.53
1:A:193:ASP:O	1:A:197:ILE:HD12	2.09	0.53
1:B:7:ILE:HG12	1:B:19:THR:OG1	2.08	0.53
1:B:21:ASN:ND2	1:B:240:TYR:CE2	2.74	0.53
1:A:41:LYS:HE3	1:A:127:LEU:HD21	1.91	0.53
1:B:210:PHE:CD1	1:B:210:PHE:C	2.85	0.53
1:B:267:LEU:HD23	1:B:267:LEU:H	1.73	0.53
1:A:259:ILE:CG2	1:A:263:GLU:HB3	2.37	0.53
1:A:218:GLN:O	1:A:220:ALA:N	2.41	0.53
1:A:263:GLU:O	1:A:267:LEU:HD13	2.09	0.53
1:B:10:LYS:HG3	4:B:292:ADP:O3'	2.09	0.53
1:B:52:LYS:N	1:B:224:ARG:HH21	2.01	0.53
1:B:255:ILE:CD1	1:B:255:ILE:H	2.22	0.53
1:A:76:LEU:HD12	1:A:86:VAL:HG21	1.91	0.52
1:A:253:LEU:HD23	1:A:253:LEU:N	2.20	0.52
1:B:106:ILE:HG21	1:B:143:LYS:HG2	1.90	0.52
1:B:109:LEU:HB3	1:B:115:TYR:CE1	2.44	0.52
1:B:150:VAL:O	1:B:150:VAL:HG12	2.06	0.52
1:A:130:VAL:O	1:A:130:VAL:HG13	2.08	0.52
1:B:10:LYS:CG	1:B:11:GLY:N	2.72	0.52
1:A:8:TYR:HE1	1:A:126:VAL:HG21	1.74	0.52
1:B:52:LYS:N	1:B:224:ARG:HE	2.07	0.52
1:B:185:ASN:O	1:B:192:GLU:OE2	2.27	0.52
1:B:187:ARG:C	1:B:189:THR:H	2.17	0.52
1:B:192:GLU:O	1:B:193:ASP:C	2.51	0.52
1:B:200:ALA:O	1:B:203:LEU:HB2	2.10	0.52
1:A:97:CYS:SG	1:A:98:ALA:N	2.82	0.52
1:B:235:LYS:O	1:B:238:ASP:OD2	2.27	0.52
1:A:169:VAL:HG12	1:A:170:LYS:H	1.68	0.52
1:A:73:GLU:C	1:A:75:VAL:H	2.16	0.52
1:B:5:CYS:HB2	1:B:123:PHE:CE1	2.45	0.52
1:B:144:ALA:O	1:B:177:VAL:HG12	2.09	0.52
1:A:13:ILE:HG22	1:A:13:ILE:O	2.09	0.52
1:B:262:ASP:O	1:B:265:GLU:HB2	2.09	0.52
1:A:165:SER:O	1:A:166:LYS:C	2.52	0.52
1:B:107:ASN:O	1:B:111:GLU:HB3	2.10	0.52
1:B:268:LEU:HB2	1:B:274:MET:HG2	1.87	0.52
1:A:2:MET:O	1:A:2:MET:HG2	2.08	0.52
1:B:4:GLN:HA	1:B:122:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:CG2	1:B:85:CYS:HB3	2.40	0.52
1:B:236:GLN:C	1:B:239:GLU:HB2	2.34	0.52
1:B:5:CYS:O	1:B:122:VAL:O	2.27	0.52
1:B:7:ILE:N	1:B:7:ILE:HD12	2.25	0.52
1:B:58:MET:HE2	1:B:101:GLY:CA	2.40	0.52
1:B:140:ARG:CA	1:B:171:TYR:CE2	2.93	0.52
1:B:163:ASN:O	1:B:166:LYS:HG2	2.10	0.52
1:A:42:ALA:O	1:A:43:ASP:OD1	2.28	0.51
1:A:271:PHE:N	1:A:271:PHE:HD1	2.07	0.51
1:B:195:LEU:HD13	1:B:271:PHE:HB2	1.92	0.51
1:B:224:ARG:O	1:B:225:MET:HB3	2.10	0.51
1:A:136:ALA:O	1:A:139:ILE:N	2.42	0.51
1:B:10:LYS:HD2	4:B:292:ADP:C1'	2.38	0.51
1:B:140:ARG:HB2	1:B:171:TYR:CZ	2.45	0.51
1:B:160:ALA:O	1:B:163:ASN:N	2.42	0.51
1:B:182:LEU:N	1:B:182:LEU:HD12	2.26	0.51
1:A:67:VAL:HG12	1:A:108:PHE:CD2	2.45	0.51
1:A:261:MET:O	1:A:264:LEU:N	2.44	0.51
1:B:22:LEU:HD11	1:B:243:LEU:HG	1.92	0.51
1:B:216:VAL:CG1	1:B:217:VAL:N	2.73	0.51
1:A:60:MET:HE3	1:A:74:ASP:HB3	1.91	0.51
1:A:230:TYR:CD1	1:B:284:LYS:HA	2.46	0.51
1:B:140:ARG:CB	1:B:171:TYR:CE2	2.94	0.51
1:B:194:GLU:O	1:B:197:ILE:HB	2.10	0.51
1:A:15:LYS:CE	1:A:125:ASP:OD1	2.58	0.51
1:B:243:LEU:HD12	1:B:243:LEU:C	2.36	0.51
1:A:208:ILE:HG22	1:A:243:LEU:CD1	2.40	0.51
1:B:124:TYR:CD2	1:B:144:ALA:HB2	2.45	0.51
1:B:3:ARG:HH12	1:B:248:VAL:HA	1.74	0.51
1:B:209:HIS:HE1	1:B:242:ALA:HB3	1.75	0.51
1:A:263:GLU:O	1:A:266:GLU:HB3	2.11	0.51
1:B:5:CYS:CB	1:B:123:PHE:CE1	2.94	0.51
1:B:109:LEU:HB3	1:B:115:TYR:HE1	1.76	0.51
1:B:20:GLN:HE21	1:B:44:SER:C	2.19	0.51
1:B:137:MET:HE1	1:B:140:ARG:CD	2.36	0.51
1:B:34:MET:HG3	1:B:84:LYS:CB	2.40	0.50
1:B:152:SER:C	1:B:154:GLU:H	2.18	0.50
1:B:225:MET:HE3	1:B:230:TYR:CB	2.37	0.50
1:B:269:MET:O	1:B:272:GLY:N	2.43	0.50
1:A:8:TYR:CD1	1:A:126:VAL:HB	2.46	0.50
1:A:179:LEU:HD23	1:A:256:PRO:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TYR:HE1	1:B:284:LYS:HA	1.72	0.50
1:B:66:THR:CG2	1:B:67:VAL:N	2.74	0.50
1:B:126:VAL:CG1	1:B:127:LEU:N	2.74	0.50
1:B:280:SER:O	1:B:281:ILE:HB	2.11	0.50
1:A:8:TYR:HB3	1:A:164:ILE:HD13	1.92	0.50
1:A:191:ARG:CB	1:A:271:PHE:HD2	2.24	0.50
1:A:266:GLU:O	1:A:269:MET:HB2	2.11	0.50
1:B:133:GLY:O	1:B:134:GLY:C	2.54	0.50
1:B:21:ASN:HD21	1:B:227:VAL:HG21	1.74	0.50
1:B:24:ALA:HB3	1:B:228:ILE:HG13	1.93	0.50
1:B:264:LEU:HD23	1:B:264:LEU:C	2.35	0.50
1:A:14:GLY:O	1:A:15:LYS:C	2.53	0.50
1:B:10:LYS:HG3	1:B:11:GLY:O	2.12	0.50
1:B:156:MET:HB3	4:B:292:ADP:O4'	2.12	0.50
1:B:156:MET:HB3	4:B:292:ADP:C1'	2.42	0.50
1:A:140:ARG:CG	1:A:171:TYR:HE1	2.14	0.50
1:A:94:GLY:N	1:B:131:VAL:HG12	2.24	0.50
1:B:209:HIS:ND1	1:B:243:LEU:HB2	2.27	0.50
1:A:265:GLU:O	1:A:268:LEU:N	2.45	0.50
1:B:135:PHE:C	1:B:137:MET:N	2.69	0.50
1:A:165:SER:C	1:A:167:GLY:N	2.68	0.49
1:B:3:ARG:HB2	1:B:121:PHE:HE1	1.71	0.49
1:B:4:GLN:NE2	1:B:143:LYS:O	2.45	0.49
1:A:46:ARG:O	1:A:50:HIS:N	2.44	0.49
1:B:178:ARG:NH2	1:B:255:ILE:HG13	2.26	0.49
1:B:137:MET:N	1:B:138:PRO:CD	2.75	0.49
1:B:140:ARG:CG	1:B:141:GLU:N	2.74	0.49
1:B:209:HIS:HD2	1:B:210:PHE:N	1.87	0.49
1:B:282:VAL:HG13	1:B:283:GLY:CA	2.43	0.49
1:A:106:ILE:HG23	1:A:115:TYR:OH	2.12	0.49
1:A:161:ALA:O	1:A:165:SER:N	2.40	0.49
1:B:34:MET:CG	1:B:84:LYS:HA	2.42	0.49
1:B:45:THR:HG21	1:B:85:CYS:HB3	1.95	0.49
1:B:156:MET:SD	4:B:292:ADP:C8	3.06	0.49
1:B:186:SER:HB2	1:B:211:VAL:O	2.12	0.49
1:B:40:PRO:HD2	1:B:127:LEU:HD22	1.92	0.49
1:B:154:GLU:OE2	1:B:156:MET:HB2	2.12	0.49
1:B:188:ASN:ND2	1:B:213:ARG:HD2	2.26	0.49
1:B:25:ALA:C	1:B:27:ALA:N	2.70	0.49
1:B:37:GLY:HA3	1:B:44:SER:HB2	1.95	0.49
1:B:236:GLN:CA	1:B:239:GLU:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:O	1:A:24:ALA:N	2.45	0.49
1:A:103:ILE:O	1:A:104:THR:C	2.55	0.49
1:A:41:LYS:HD3	4:B:292:ADP:H5'2	1.89	0.49
1:A:167:GLY:O	1:A:171:TYR:HD2	1.96	0.49
1:B:29:MET:HE2	1:B:241:ARG:HG3	1.95	0.49
1:B:56:THR:HG22	1:B:59:GLU:N	2.27	0.49
1:B:103:ILE:O	1:B:104:THR:C	2.56	0.49
1:B:188:ASN:HD21	1:B:213:ARG:CD	2.25	0.49
1:B:56:THR:HG23	1:B:58:MET:N	2.27	0.49
1:B:220:ALA:HB3	1:B:227:VAL:HG22	1.93	0.49
1:A:173:ASN:C	1:A:173:ASN:HD22	2.21	0.49
1:B:33:VAL:HG23	1:B:121:PHE:CB	2.40	0.49
1:B:52:LYS:CB	1:B:224:ARG:NH2	2.76	0.49
1:B:135:PHE:CD1	1:B:135:PHE:N	2.81	0.49
1:B:10:LYS:O	1:B:15:LYS:HD3	2.13	0.48
1:B:259:ILE:HG12	1:B:260:THR:O	2.13	0.48
1:A:238:ASP:O	1:A:242:ALA:N	2.43	0.48
1:A:156:MET:HA	1:A:159:TYR:HB3	1.95	0.48
1:B:58:MET:HE2	1:B:101:GLY:HA2	1.94	0.48
1:B:102:VAL:O	1:B:106:ILE:HG13	2.12	0.48
1:A:5:CYS:HB3	1:A:146:GLU:HB3	1.95	0.48
1:A:7:ILE:HD13	1:A:19:THR:OG1	2.11	0.48
1:A:8:TYR:OH	1:A:135:PHE:O	2.25	0.48
1:A:43:ASP:O	1:A:44:SER:C	2.55	0.48
1:A:98:ALA:O	1:A:101:GLY:N	2.46	0.48
1:A:186:SER:CB	1:A:210:PHE:CZ	2.96	0.48
1:A:236:GLN:CG	1:A:240:TYR:HE2	2.26	0.48
1:B:156:MET:O	1:B:157:ALA:C	2.55	0.48
1:B:178:ARG:NH2	1:B:255:ILE:CG1	2.76	0.48
1:A:46:ARG:CG	1:A:47:LEU:HG	2.43	0.48
1:A:171:TYR:HA	1:A:174:SER:OG	2.13	0.48
1:B:55:ASN:HB3	1:B:60:MET:SD	2.54	0.48
1:A:34:MET:HE3	1:A:36:VAL:HG23	1.96	0.48
1:A:109:LEU:HB2	1:A:115:TYR:HE1	1.78	0.48
1:B:108:PHE:O	1:B:111:GLU:HB3	2.14	0.48
1:B:183:ILE:O	1:B:183:ILE:HG22	2.13	0.48
1:B:207:MET:O	1:B:207:MET:HG2	2.12	0.48
1:A:173:ASN:C	1:A:173:ASN:ND2	2.72	0.48
1:A:272:GLY:O	1:A:275:GLU:N	2.47	0.48
1:B:72:LEU:O	1:B:74:ASP:N	2.47	0.48
1:B:102:VAL:O	1:B:103:ILE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:O	1:B:141:GLU:HB2	2.14	0.48
1:B:192:GLU:O	1:B:193:ASP:O	2.32	0.48
1:B:232:PRO:CD	1:B:233:LYS:H	2.26	0.48
1:A:5:CYS:O	1:A:122:VAL:O	2.32	0.48
1:A:15:LYS:NZ	1:A:125:ASP:OD1	2.45	0.48
1:A:186:SER:CB	1:A:210:PHE:CE1	2.95	0.48
1:A:197:ILE:O	1:A:200:ALA:HB3	2.13	0.48
1:B:22:LEU:HD23	1:B:22:LEU:O	2.13	0.48
1:B:259:ILE:CD1	1:B:260:THR:O	2.62	0.48
1:A:73:GLU:C	1:A:75:VAL:N	2.71	0.48
1:A:159:TYR:CD1	1:A:159:TYR:C	2.92	0.48
1:B:22:LEU:HD12	1:B:243:LEU:CG	2.44	0.48
1:B:34:MET:HE2	1:B:34:MET:HB3	1.70	0.48
1:B:80:TYR:O	1:B:83:VAL:HG23	2.13	0.48
1:A:108:PHE:C	1:A:108:PHE:CD1	2.92	0.47
1:A:168:ILE:H	1:A:168:ILE:CD1	2.12	0.47
1:B:56:THR:HG23	1:B:57:ILE:N	2.28	0.47
1:B:211:VAL:CG1	1:B:212:PRO:HD2	2.44	0.47
1:B:243:LEU:HA	1:B:246:LYS:HB2	1.96	0.47
1:B:254:VAL:CG1	1:B:255:ILE:N	2.77	0.47
1:A:57:ILE:CG1	1:A:75:VAL:CG1	2.86	0.47
1:A:171:TYR:HA	1:A:174:SER:CB	2.44	0.47
1:B:110:GLU:O	1:B:113:GLY:HA2	2.14	0.47
1:B:225:MET:HE3	1:B:230:TYR:CA	2.44	0.47
1:A:8:TYR:CE2	1:A:126:VAL:HG11	2.45	0.47
1:A:209:HIS:CG	1:A:246:LYS:NZ	2.82	0.47
1:A:136:ALA:O	1:A:137:MET:C	2.55	0.47
1:A:140:ARG:CG	1:A:171:TYR:CE1	2.91	0.47
1:B:3:ARG:HH12	1:B:248:VAL:CA	2.26	0.47
1:A:33:VAL:HG22	1:A:121:PHE:CB	2.36	0.47
1:A:46:ARG:HE	1:A:224:ARG:CG	2.26	0.47
1:B:208:ILE:HG21	1:B:243:LEU:CD1	2.45	0.47
1:B:232:PRO:HD2	1:B:233:LYS:H	1.80	0.47
1:B:269:MET:O	1:B:272:GLY:HA2	2.14	0.47
1:A:9:GLY:O	1:A:127:LEU:HD12	2.14	0.47
1:A:43:ASP:O	1:A:45:THR:O	2.32	0.47
1:A:192:GLU:O	1:A:193:ASP:C	2.58	0.47
1:B:186:SER:N	1:B:211:VAL:O	2.48	0.47
1:A:45:THR:O	1:A:46:ARG:HB2	2.15	0.47
1:A:109:LEU:O	1:A:114:ALA:N	2.43	0.47
1:A:116:GLU:HB2	1:A:117:ASP:H	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLN:HG2	1:B:122:VAL:HB	1.96	0.47
1:B:151:CYS:SG	1:B:152:SER:N	2.86	0.47
1:B:225:MET:CE	1:B:230:TYR:CB	2.92	0.47
1:B:239:GLU:O	1:B:242:ALA:HB3	2.15	0.47
1:A:57:ILE:C	1:A:59:GLU:N	2.71	0.47
1:A:64:ALA:HB1	1:A:69:ASP:OD2	2.15	0.47
1:B:25:ALA:HB1	1:B:241:ARG:HA	1.97	0.47
1:B:20:GLN:NE2	1:B:44:SER:O	2.38	0.47
1:B:109:LEU:CB	1:B:115:TYR:HE1	2.27	0.47
1:A:61:ALA:HB1	1:A:67:VAL:HG22	1.97	0.47
1:B:33:VAL:HG12	5:B:295:HOH:O	2.14	0.47
1:B:149:ILE:O	1:B:149:ILE:HG22	2.15	0.47
1:A:164:ILE:CG2	1:A:165:SER:N	2.77	0.46
1:A:173:ASN:HD22	1:A:174:SER:N	2.13	0.46
1:A:109:LEU:CB	1:A:115:TYR:HE1	2.28	0.46
1:A:194:GLU:CB	1:A:271:PHE:HE2	2.27	0.46
1:A:221:GLU:C	1:A:223:ARG:N	2.72	0.46
1:B:45:THR:O	1:B:45:THR:CG2	2.63	0.46
1:B:129:ASP:O	4:B:292:ADP:C2	2.68	0.46
1:A:151:CYS:SG	1:A:152:SER:N	2.88	0.46
1:A:189:THR:HB	1:A:192:GLU:HG3	1.97	0.46
1:A:238:ASP:HA	1:A:241:ARG:HB2	1.96	0.46
1:B:108:PHE:CD2	1:B:109:LEU:HD23	2.46	0.46
1:A:45:THR:HG21	1:A:49:LEU:CD1	2.39	0.46
1:A:45:THR:CG2	1:A:46:ARG:N	2.75	0.46
1:B:9:GLY:O	1:B:15:LYS:HD3	2.16	0.46
1:B:9:GLY:O	1:B:15:LYS:CD	2.63	0.46
1:B:93:PRO:O	1:B:95:VAL:N	2.45	0.46
1:B:208:ILE:CG2	1:B:243:LEU:CD1	2.91	0.46
1:B:235:LYS:HA	1:B:238:ASP:OD2	2.15	0.46
1:A:8:TYR:HD2	1:A:164:ILE:CD1	2.16	0.46
1:A:271:PHE:HB2	1:A:273:ILE:CD1	2.45	0.46
1:B:217:VAL:O	1:B:220:ALA:HB3	2.16	0.46
1:B:231:ASP:O	1:B:234:ALA:N	2.43	0.46
1:B:243:LEU:O	1:B:246:LYS:HB2	2.15	0.46
1:A:3:ARG:HD3	1:A:121:PHE:CE1	2.50	0.46
1:A:164:ILE:HG22	1:A:165:SER:N	2.30	0.46
1:B:60:MET:C	1:B:62:ALA:N	2.69	0.46
1:B:111:GLU:C	1:B:113:GLY:H	2.24	0.46
1:B:205:THR:HG23	1:B:206:GLN:N	2.30	0.46
1:A:15:LYS:O	1:A:16:SER:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HB3	1:A:253:LEU:HB3	1.98	0.46
1:B:37:GLY:CA	1:B:44:SER:HB2	2.45	0.46
1:A:3:ARG:NH1	1:A:248:VAL:HA	2.31	0.46
1:A:14:GLY:O	1:A:17:THR:HB	2.16	0.46
1:B:158:MET:HE2	1:B:195:LEU:CD2	2.46	0.46
1:B:178:ARG:HH21	1:B:255:ILE:CD1	2.24	0.46
1:B:236:GLN:O	1:B:239:GLU:N	2.48	0.46
1:A:26:LEU:CD1	1:A:244:ALA:CB	2.91	0.45
1:A:27:ALA:C	1:A:29:MET:N	2.69	0.45
1:A:151:CYS:SG	1:A:196:ILE:HD11	2.55	0.45
1:A:60:MET:HE2	1:A:74:ASP:O	2.16	0.45
1:A:66:THR:HB	1:A:69:ASP:OD2	2.16	0.45
1:A:93:PRO:C	1:A:95:VAL:H	2.22	0.45
1:A:164:ILE:O	1:A:168:ILE:HD12	2.17	0.45
1:A:266:GLU:O	1:A:269:MET:N	2.49	0.45
1:B:33:VAL:HG21	1:B:123:PHE:HD2	1.80	0.45
1:B:147:ILE:HD12	1:B:168:ILE:HD12	1.99	0.45
1:B:284:LYS:C	1:B:286:ALA:H	2.24	0.45
1:A:26:LEU:CD2	1:A:33:VAL:HG21	2.45	0.45
1:B:56:THR:CG2	1:B:58:MET:N	2.78	0.45
1:A:139:ILE:O	1:A:141:GLU:N	2.49	0.45
1:A:257:ASN:ND2	1:A:257:ASN:O	2.50	0.45
1:B:132:CYS:O	1:B:133:GLY:C	2.58	0.45
1:B:165:SER:O	1:B:166:LYS:C	2.59	0.45
1:A:36:VAL:O	1:A:38:CYS:SG	2.73	0.45
1:A:155:MET:SD	1:A:155:MET:O	2.75	0.45
1:A:212:PRO:HG2	1:A:236:GLN:HE22	1.81	0.45
1:B:26:LEU:HD21	1:B:121:PHE:CD2	2.51	0.45
1:B:49:LEU:O	1:B:50:HIS:HB2	2.17	0.45
1:B:211:VAL:HA	1:B:212:PRO:HD3	1.85	0.45
1:A:12:GLY:H	4:B:292:ADP:PB	2.33	0.45
1:B:160:ALA:HB1	1:B:164:ILE:HD11	1.99	0.45
1:B:52:LYS:CB	1:B:224:ARG:HE	2.29	0.45
1:B:126:VAL:CG1	1:B:127:LEU:H	2.26	0.45
1:B:270:GLU:C	1:B:272:GLY:H	2.24	0.45
1:A:25:ALA:O	1:A:27:ALA:N	2.50	0.45
1:A:136:ALA:O	1:A:139:ILE:CB	2.57	0.45
1:A:169:VAL:O	1:A:170:LYS:C	2.59	0.45
1:B:39:ASP:OD1	1:B:41:LYS:HB2	2.17	0.45
1:B:145:GLN:NE2	1:B:176:SER:HB2	2.32	0.45
1:A:281:ILE:HG22	1:A:281:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLU:O	1:B:269:MET:N	2.50	0.44
1:A:22:LEU:HD11	1:A:243:LEU:CD2	2.46	0.44
1:A:95:VAL:HG23	1:B:171:TYR:CE1	2.52	0.44
1:A:103:ILE:O	1:A:105:ALA:N	2.50	0.44
1:A:242:ALA:O	1:A:246:LYS:HG3	2.18	0.44
1:A:255:ILE:HD12	1:A:255:ILE:HA	1.60	0.44
1:A:266:GLU:HA	1:A:269:MET:HB2	1.99	0.44
1:B:211:VAL:HG12	1:B:212:PRO:HD2	1.99	0.44
1:B:214:ASP:O	1:B:216:VAL:HG12	2.16	0.44
1:A:137:MET:C	1:A:139:ILE:N	2.70	0.44
1:A:137:MET:CB	1:A:138:PRO:CD	2.93	0.44
1:A:214:ASP:C	1:A:216:VAL:N	2.74	0.44
1:B:108:PHE:O	1:B:111:GLU:N	2.50	0.44
1:B:158:MET:CE	1:B:195:LEU:HD21	2.46	0.44
1:A:18:THR:CG2	1:A:185:ASN:HD21	2.29	0.44
1:A:31:LYS:HG3	1:A:120:ASP:CB	2.46	0.44
1:A:3:ARG:HH12	1:A:248:VAL:HA	1.82	0.44
1:A:148:TYR:CD1	1:A:180:GLY:HA3	2.50	0.44
1:A:206:GLN:CG	1:A:252:LEU:HD22	2.43	0.44
1:A:218:GLN:O	1:A:219:ARG:C	2.60	0.44
1:A:222:ILE:HD12	1:A:222:ILE:HA	1.76	0.44
1:B:7:ILE:HG22	1:B:8:TYR:N	2.31	0.44
1:B:40:PRO:HD2	1:B:41:LYS:H	1.81	0.44
1:B:200:ALA:HB1	1:B:205:THR:C	2.42	0.44
1:A:24:ALA:HB2	1:A:226:THR:HG21	1.99	0.44
1:B:200:ALA:O	1:B:201:ASN:C	2.61	0.44
1:B:266:GLU:O	1:B:270:GLU:N	2.48	0.44
1:A:165:SER:O	1:A:168:ILE:HD12	2.18	0.44
1:A:177:VAL:O	1:A:178:ARG:HD2	2.18	0.44
1:A:11:GLY:C	4:B:292:ADP:O2A	2.61	0.44
1:A:171:TYR:HA	1:A:174:SER:HB2	2.00	0.44
1:B:102:VAL:O	1:B:105:ALA:N	2.51	0.44
1:B:241:ARG:O	1:B:244:ALA:N	2.51	0.44
1:A:8:TYR:CB	1:A:164:ILE:HD11	2.43	0.43
1:A:103:ILE:CG2	1:A:107:ASN:ND2	2.79	0.43
1:A:191:ARG:HB3	1:A:271:PHE:HD2	1.83	0.43
1:B:148:TYR:CE2	1:B:180:GLY:HA3	2.53	0.43
1:B:164:ILE:O	1:B:168:ILE:HG12	2.18	0.43
1:B:231:ASP:O	1:B:234:ALA:HB3	2.18	0.43
1:A:41:LYS:HE2	4:B:292:ADP:H2'	2.00	0.43
1:A:46:ARG:HG3	1:A:47:LEU:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG23	1:B:171:TYR:HE1	1.84	0.43
1:A:154:GLU:O	1:A:158:MET:HG2	2.18	0.43
1:A:155:MET:HG3	1:A:156:MET:CG	2.43	0.43
1:B:7:ILE:HG22	1:B:8:TYR:O	2.19	0.43
1:B:217:VAL:O	1:B:218:GLN:C	2.61	0.43
1:A:22:LEU:HD11	1:A:243:LEU:HG	1.99	0.43
1:B:35:ILE:HD13	1:B:44:SER:O	2.18	0.43
1:B:139:ILE:HD13	1:B:139:ILE:HA	1.86	0.43
1:A:72:LEU:O	1:A:76:LEU:N	2.46	0.43
1:A:204:GLY:O	1:A:254:VAL:HG11	2.18	0.43
1:A:219:ARG:NE	1:A:230:TYR:OH	2.50	0.43
1:A:246:LYS:HG3	1:A:246:LYS:H	1.61	0.43
1:B:178:ARG:HB2	1:B:253:LEU:HB3	2.00	0.43
1:B:280:SER:HB3	1:B:281:ILE:H	1.52	0.43
1:A:80:TYR:CE2	1:A:229:GLU:HG3	2.54	0.43
1:A:158:MET:HB3	1:A:158:MET:HE3	1.65	0.43
1:B:29:MET:CE	1:B:244:ALA:HB3	2.42	0.43
1:B:37:GLY:HA2	1:B:44:SER:CB	2.48	0.43
1:B:39:ASP:OD2	1:B:127:LEU:HD13	2.18	0.43
1:A:178:ARG:HG3	1:A:255:ILE:HD12	1.99	0.43
1:A:254:VAL:HG12	1:A:255:ILE:N	2.33	0.43
1:A:269:MET:O	1:A:270:GLU:C	2.61	0.43
1:B:33:VAL:N	5:B:295:HOH:O	2.28	0.43
1:B:129:ASP:OD2	4:B:292:ADP:H3'	2.18	0.43
1:B:137:MET:C	1:B:139:ILE:N	2.75	0.43
1:B:158:MET:CE	1:B:195:LEU:CD2	2.97	0.43
1:B:222:ILE:HD13	1:B:222:ILE:HA	1.85	0.43
1:A:20:GLN:HE22	1:A:46:ARG:HB3	1.82	0.43
1:A:137:MET:CB	1:A:138:PRO:HD3	2.41	0.43
1:A:189:THR:CA	1:A:192:GLU:HG3	2.48	0.43
1:B:131:VAL:HG21	1:B:163:ASN:CB	2.48	0.43
1:A:2:MET:CE	1:A:119:LEU:HB2	2.48	0.43
1:A:22:LEU:HD11	1:A:243:LEU:CG	2.48	0.43
1:A:192:GLU:O	1:A:194:GLU:N	2.51	0.43
1:A:265:GLU:O	1:A:266:GLU:C	2.60	0.43
1:B:40:PRO:CD	1:B:127:LEU:CD2	2.97	0.43
1:A:203:LEU:CD2	1:A:259:ILE:HD11	2.48	0.43
1:B:231:ASP:C	1:B:233:LYS:N	2.75	0.43
1:B:166:LYS:CD	1:B:258:PRO:HB3	2.49	0.43
1:A:103:ILE:C	1:A:105:ALA:N	2.77	0.42
1:A:264:LEU:O	1:A:265:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:CG1	1:A:277:GLU:N	2.82	0.42
1:B:48:ILE:O	1:B:50:HIS:CE1	2.72	0.42
1:A:259:ILE:HG23	1:A:263:GLU:OE1	2.19	0.42
1:B:37:GLY:HA3	1:B:87:GLU:HG2	1.99	0.42
1:B:178:ARG:NE	1:B:255:ILE:CD1	2.79	0.42
1:B:270:GLU:C	1:B:272:GLY:N	2.75	0.42
1:A:22:LEU:O	1:A:23:VAL:C	2.61	0.42
1:A:230:TYR:CG	1:A:231:ASP:N	2.86	0.42
1:B:23:VAL:O	1:B:25:ALA:N	2.52	0.42
1:A:26:LEU:C	1:A:29:MET:HB2	2.45	0.42
1:A:132:CYS:O	1:A:133:GLY:C	2.63	0.42
1:B:72:LEU:C	1:B:74:ASP:N	2.78	0.42
1:A:45:THR:O	1:A:46:ARG:CB	2.67	0.42
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.67	0.42
1:A:210:PHE:O	1:A:210:PHE:CD2	2.73	0.42
1:B:178:ARG:HH21	1:B:255:ILE:CG1	2.32	0.42
1:A:8:TYR:CE1	1:A:126:VAL:CB	3.02	0.42
1:A:8:TYR:CE1	1:A:126:VAL:CG2	2.99	0.42
1:A:12:GLY:N	4:B:292:ADP:PB	2.93	0.42
1:A:21:ASN:HB2	1:A:240:TYR:CE1	2.54	0.42
1:A:57:ILE:O	1:A:61:ALA:N	2.47	0.42
1:B:33:VAL:HG13	1:B:83:VAL:HG13	2.01	0.42
1:B:182:LEU:HD13	1:B:205:THR:CG2	2.41	0.42
1:B:186:SER:HA	1:B:192:GLU:OE2	2.19	0.42
1:A:155:MET:HG3	1:A:156:MET:HE2	1.99	0.42
1:B:93:PRO:C	1:B:95:VAL:N	2.69	0.42
1:B:132:CYS:O	1:B:135:PHE:N	2.48	0.42
1:B:236:GLN:CG	1:B:240:TYR:CE2	3.02	0.42
1:B:260:THR:CG2	1:B:263:GLU:HG3	2.47	0.42
1:B:5:CYS:HB3	1:B:123:PHE:CE1	2.55	0.42
1:B:184:CYS:SG	1:B:196:ILE:HG13	2.60	0.42
1:A:45:THR:HG23	1:A:85:CYS:SG	2.60	0.42
1:A:49:LEU:HD11	1:A:85:CYS:CB	2.50	0.42
1:A:71:GLU:O	1:A:75:VAL:HG23	2.20	0.42
1:B:35:ILE:HG23	1:B:84:LYS:O	2.20	0.42
1:B:206:GLN:NE2	1:B:208:ILE:CD1	2.79	0.42
1:A:133:GLY:O	1:A:136:ALA:HB3	2.20	0.42
1:B:58:MET:CE	1:B:101:GLY:CA	2.92	0.42
1:B:166:LYS:O	1:B:167:GLY:O	2.38	0.42
1:A:92:GLU:O	1:A:92:GLU:HG2	2.10	0.41
1:A:137:MET:O	1:A:139:ILE:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:CB	1:A:171:TYR:CE1	3.03	0.41
1:A:165:SER:O	1:A:168:ILE:N	2.53	0.41
1:A:209:HIS:CE1	1:A:242:ALA:CB	2.97	0.41
1:A:248:VAL:O	1:A:248:VAL:CG1	2.68	0.41
1:B:182:LEU:HD13	1:B:182:LEU:H	1.84	0.41
1:A:8:TYR:OH	1:A:126:VAL:HG11	2.19	0.41
1:A:110:GLU:OE1	1:A:143:LYS:NZ	2.53	0.41
1:B:127:LEU:HD12	1:B:127:LEU:HA	1.69	0.41
1:B:137:MET:HB3	1:B:138:PRO:HD3	2.02	0.41
1:A:191:ARG:HB2	1:A:271:PHE:HD2	1.84	0.41
1:A:216:VAL:HG13	1:A:216:VAL:O	2.20	0.41
1:A:228:ILE:O	1:A:229:GLU:C	2.63	0.41
1:B:178:ARG:CZ	1:B:255:ILE:HD11	2.50	0.41
1:A:21:ASN:CB	1:A:240:TYR:CD1	3.03	0.41
1:A:107:ASN:H	1:A:107:ASN:HD22	1.67	0.41
1:A:109:LEU:HB3	1:A:114:ALA:HB3	2.02	0.41
1:A:268:LEU:HB3	1:A:274:MET:HG2	2.00	0.41
1:A:98:ALA:O	1:A:102:VAL:HG23	2.19	0.41
1:A:208:ILE:CG2	1:A:243:LEU:CD1	2.98	0.41
1:B:56:THR:HG21	1:B:59:GLU:HG3	2.02	0.41
1:B:155:MET:HB2	1:B:268:LEU:HD11	2.03	0.41
1:B:177:VAL:C	1:B:178:ARG:HG2	2.45	0.41
1:A:48:ILE:HD12	1:A:48:ILE:N	2.35	0.41
1:A:260:THR:HG23	1:A:263:GLU:HG3	2.02	0.41
1:A:262:ASP:OD1	1:A:262:ASP:N	2.53	0.41
1:B:22:LEU:C	1:B:22:LEU:CD2	2.86	0.41
1:B:191:ARG:HB2	1:B:194:GLU:HG3	2.02	0.41
1:A:37:GLY:HA2	1:A:125:ASP:HB3	2.01	0.41
1:A:57:ILE:C	1:A:59:GLU:H	2.27	0.41
1:A:273:ILE:CD1	1:A:273:ILE:N	2.64	0.41
1:B:178:ARG:NH2	1:B:255:ILE:CD1	2.81	0.41
1:A:92:GLU:OE2	1:A:95:VAL:HG12	2.20	0.41
1:B:42:ALA:HB2	5:B:5025:HOH:O	2.19	0.41
1:B:142:ASN:O	1:B:143:LYS:CD	2.69	0.41
1:A:91:PRO:O	1:A:92:GLU:C	2.64	0.41
1:A:110:GLU:CD	1:A:143:LYS:NZ	2.78	0.41
1:A:169:VAL:C	1:A:171:TYR:N	2.78	0.41
1:A:189:THR:HB	1:A:192:GLU:CG	2.50	0.41
1:A:199:LEU:O	1:A:202:LYS:N	2.54	0.41
1:A:267:LEU:O	1:A:270:GLU:HB3	2.20	0.41
1:B:57:ILE:HD13	1:B:105:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:HG3	1:B:59:GLU:H	1.48	0.41
1:A:99:GLY:CA	1:A:137:MET:HG3	2.51	0.41
1:A:131:VAL:HG21	1:A:164:ILE:HG13	2.03	0.41
1:A:140:ARG:HA	1:A:171:TYR:CE1	2.55	0.41
1:A:147:ILE:HG22	1:A:147:ILE:O	2.20	0.41
1:B:34:MET:HE3	1:B:36:VAL:HG23	2.03	0.41
1:B:56:THR:O	1:B:57:ILE:C	2.62	0.41
1:B:163:ASN:HA	1:B:166:LYS:HG2	2.03	0.41
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.71	0.41
1:A:57:ILE:CG1	1:A:75:VAL:HG11	2.51	0.40
1:A:71:GLU:O	1:A:74:ASP:N	2.53	0.40
1:A:195:LEU:O	1:A:198:ALA:HB3	2.21	0.40
1:B:48:ILE:HG22	1:B:49:LEU:N	2.36	0.40
1:A:64:ALA:HB1	1:A:69:ASP:CG	2.46	0.40
1:A:102:VAL:O	1:A:103:ILE:C	2.65	0.40
1:A:213:ARG:O	1:A:213:ARG:CG	2.67	0.40
1:B:182:LEU:O	1:B:183:ILE:HG12	2.19	0.40
1:B:231:ASP:CB	1:B:234:ALA:HB2	2.41	0.40
1:B:266:GLU:O	1:B:267:LEU:C	2.64	0.40
1:A:21:ASN:HB3	1:A:240:TYR:CG	2.56	0.40
1:A:272:GLY:O	1:A:273:ILE:C	2.64	0.40
1:B:61:ALA:O	1:B:65:GLY:N	2.54	0.40
1:B:92:GLU:HA	1:B:93:PRO:HD3	1.52	0.40
1:B:245:ARG:O	1:B:248:VAL:N	2.54	0.40
1:A:236:GLN:O	1:A:239:GLU:HB2	2.21	0.40
1:A:259:ILE:CG2	1:A:263:GLU:OE1	2.68	0.40
1:A:267:LEU:HD12	1:A:267:LEU:N	2.36	0.40
1:B:103:ILE:O	1:B:106:ILE:HG13	2.20	0.40
1:B:139:ILE:O	1:B:140:ARG:C	2.63	0.40
1:B:165:SER:O	1:B:168:ILE:N	2.54	0.40
1:A:24:ALA:O	1:A:25:ALA:C	2.65	0.40
1:A:47:LEU:CD2	1:A:225:MET:N	2.83	0.40
1:A:207:MET:O	1:A:209:HIS:N	2.54	0.40
1:A:230:TYR:CD1	1:B:284:LYS:CA	3.05	0.40
1:B:50:HIS:HE1	1:B:225:MET:HB2	1.86	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	281/289 (97%)	189 (67%)	55 (20%)	37 (13%)	0	0
1	B	285/289 (99%)	173 (61%)	81 (28%)	31 (11%)	0	1
All	All	566/578 (98%)	362 (64%)	136 (24%)	68 (12%)	0	1

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	46	ARG
1	A	103	ILE
1	A	104	THR
1	A	117	ASP
1	A	155	MET
1	A	169	VAL
1	A	170	LYS
1	A	176	SER
1	A	193	ASP
1	A	208	ILE
1	A	230	TYR
1	A	273	ILE
1	A	275	GLU
1	B	26	LEU
1	B	48	ILE
1	B	62	ALA
1	B	116	GLU
1	B	119	LEU
1	B	193	ASP
1	B	215	ASN
1	B	222	ILE
1	B	256	PRO
1	B	280	SER
1	B	281	ILE

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	74	ASP
1	A	142	ASN
1	A	153	GLY
1	A	180	GLY
1	A	192	GLU
1	A	215	ASN
1	A	250	ASN
1	B	15	LYS
1	B	24	ALA
1	B	37	GLY
1	B	73	GLU
1	B	133	GLY
1	B	190	ASP
1	B	273	ILE
1	A	70	LEU
1	A	270	GLU
1	B	68	GLU
1	B	113	GLY
1	B	164	ILE
1	B	199	LEU
1	A	118	ASP
1	A	139	ILE
1	A	195	LEU
1	B	139	ILE
1	B	183	ILE
1	B	224	ARG
1	A	73	GLU
1	A	94	GLY
1	A	116	GLU
1	A	166	LYS
1	A	266	GLU
1	B	225	MET
1	A	282	VAL
1	B	30	GLY
1	B	270	GLU
1	B	272	GLY
1	A	137	MET
1	A	281	ILE
1	B	216	VAL
1	A	23	VAL
1	A	175	GLY

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Mol	Chain	Res	Type
1	B	217	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/233 (87%)	146 (72%)	57 (28%)	0	1
1	B	197/233 (84%)	126 (64%)	71 (36%)	0	0
All	All	400/466 (86%)	272 (68%)	128 (32%)	0	1

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	CYS
1	A	13	ILE
1	A	15	LYS
1	A	17	THR
1	A	18	THR
1	A	22	LEU
1	A	28	GLU
1	A	36	VAL
1	A	38	CYS
1	A	44	SER
1	A	56	THR
1	A	57	ILE
1	A	58	MET
1	A	59	GLU
1	A	66	THR
1	A	67	VAL
1	A	72	LEU
1	A	73	GLU
1	A	74	ASP
1	A	75	VAL
1	A	76	LEU
1	A	103	ILE

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Mol	Chain	Res	Type
1	A	111	GLU
1	A	122	VAL
1	A	129	ASP
1	A	147	ILE
1	A	154	GLU
1	A	158	MET
1	A	164	ILE
1	A	165	SER
1	A	173	ASN
1	A	176	SER
1	A	179	LEU
1	A	182	LEU
1	A	185	ASN
1	A	190	ASP
1	A	195	LEU
1	A	196	ILE
1	A	199	LEU
1	A	206	GLN
1	A	207	MET
1	A	209	HIS
1	A	211	VAL
1	A	213	ARG
1	A	216	VAL
1	A	222	ILE
1	A	226	THR
1	A	252	LEU
1	A	254	VAL
1	A	255	ILE
1	A	260	THR
1	A	262	ASP
1	A	266	GLU
1	A	271	PHE
1	A	273	ILE
1	A	274	MET
1	A	281	ILE
1	B	10	LYS
1	B	13	ILE
1	B	15	LYS
1	B	17	THR
1	B	23	VAL
1	B	33	VAL
1	B	34	MET

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Mol	Chain	Res	Type
1	B	35	ILE
1	B	43	ASP
1	B	44	SER
1	B	45	THR
1	B	56	THR
1	B	57	ILE
1	B	74	ASP
1	B	85	CYS
1	B	88	SER
1	B	92	GLU
1	B	95	VAL
1	B	100	ARG
1	B	103	ILE
1	B	106	ILE
1	B	109	LEU
1	B	112	GLU
1	B	127	LEU
1	B	129	ASP
1	B	130	VAL
1	B	140	ARG
1	B	147	ILE
1	B	149	ILE
1	B	158	MET
1	B	164	ILE
1	B	166	LYS
1	B	168	ILE
1	B	169	VAL
1	B	176	SER
1	B	177	VAL
1	B	178	ARG
1	B	182	LEU
1	B	185	ASN
1	B	186	SER
1	B	188	ASN
1	B	191	ARG
1	B	194	GLU
1	B	196	ILE
1	B	197	ILE
1	B	199	LEU
1	B	201	ASN
1	B	202	LYS
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	207	MET
1	B	208	ILE
1	B	210	PHE
1	B	211	VAL
1	B	216	VAL
1	B	217	VAL
1	B	218	GLN
1	B	222	ILE
1	B	223	ARG
1	B	224	ARG
1	B	226	THR
1	B	238	ASP
1	B	239	GLU
1	B	255	ILE
1	B	259	ILE
1	B	260	THR
1	B	262	ASP
1	B	267	LEU
1	B	268	LEU
1	B	269	MET
1	B	280	SER
1	B	282	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	55	ASN
1	A	107	ASN
1	A	142	ASN
1	A	145	GLN
1	A	163	ASN
1	A	173	ASN
1	A	185	ASN
1	A	201	ASN
1	A	257	ASN
1	B	145	GLN
1	B	188	ASN
1	B	209	HIS
1	B	236	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	SF4	B	290	1	0,12,12	-	-	-		
4	ADP	B	292	2	28,29,29	1.06	1 (3%)	43,45,45	2.36	3 (6%)

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	SF4	B	290	1	-	-	0/6/5/5
4	ADP	B	292	2	-	4/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	292	ADP	PA-O3A	4.57	1.64	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	292	ADP	C1'-N9-C8	-9.56	105.87	127.09
4	B	292	ADP	O2A-PA-O3A	9.38	132.62	107.27
4	B	292	ADP	O3A-PA-O1A	-6.90	89.94	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

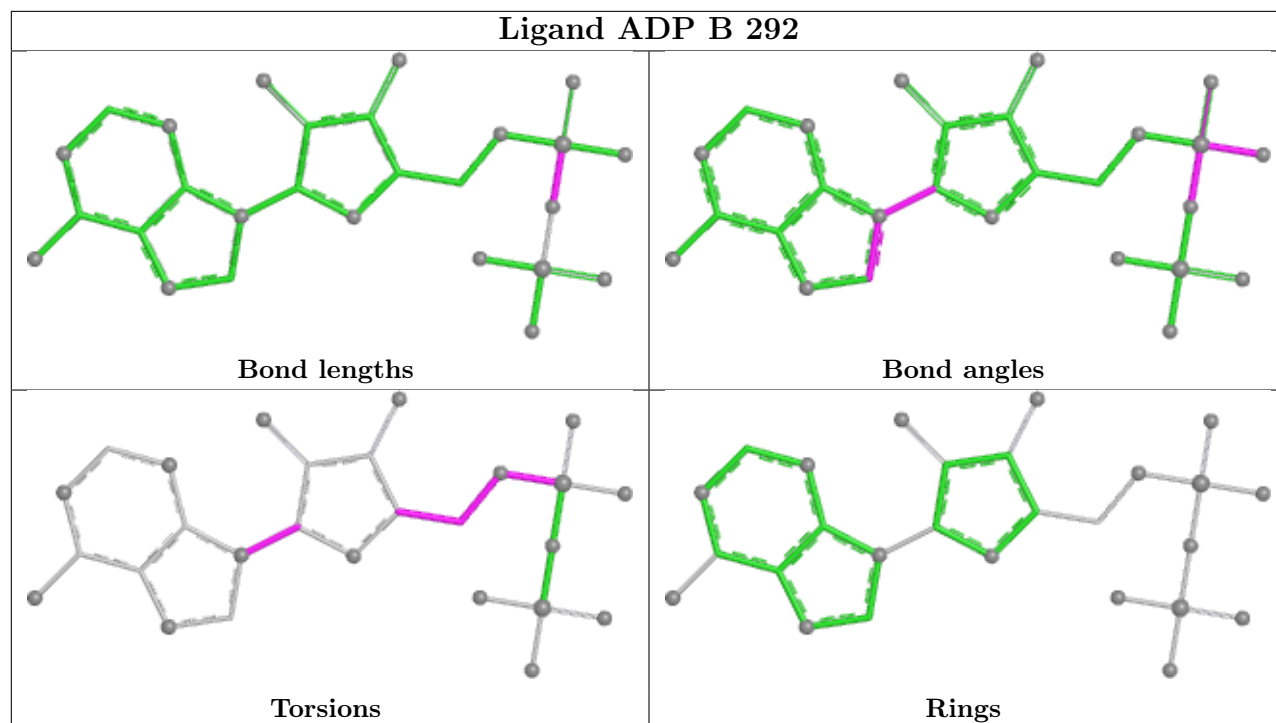
Mol	Chain	Res	Type	Atoms
4	B	292	ADP	C5'-O5'-PA-O3A
4	B	292	ADP	C2'-C1'-N9-C4
4	B	292	ADP	C3'-C4'-C5'-O5'
4	B	292	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	292	ADP	29	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.